MITOCW | 0. Introduction to Part II: Quantum mechanical methods

JEFFREY GROSSMAN: So we're very excited about this class. And, excuse me, this is the only time I get you until after spring break. So I'm not going to-- well I'll see you, maybe, but in terms of this class, I come on after spring break and then I get you for the rest of the semester. And so what I want to do in the next 20 minutes is just give you a little preview of what's coming.

Now, did you, Professor Wheeler, did you talk about laptops and stuff? So let me talk about that for a minute. Any of you who had me in 3012 know that, for me, what I would prefer is that when I'm lecturing, that you don't have your laptops open and you're not pulling your sort of under the table texting, unless-- now there is an exception. Who knows the exception? Can anybody remember?

Nobody actually took me up on this last fall, but if you really feel so inspired by what I'm talking about or what we're talking about that you need to send a tweet and summarize it, or you need to broadcast this information that you're getting in the class out to more people to bring them in, then that's OK. Otherwise, I'd really prefer it because if you open your laptop, what you're doing is you're creating a field of view for all the people behind you to get distracted. Same with the phone under the table trick, right? A lot of people see that. It's a little distracting.

The point of the class is discussion, right? So we're going to have slides, we're going to talk about slides, but if you don't ask questions, it's a lot less useful. You won't learn as much. So I really like getting interrupted. Just, like, yell out something. I don't know.

In 3012, the key word was "entropy." You could yell out "entropy" any time, and I'd turn around and we'd talk. Here, it could be, like, "quantum" would be a good one, right?

But I really want you to ask the question when you have it, because if we have a discussion on the spot about your question, that's a learning moment, right? That's a chance to learn more for everyone. So I mean, the studies are in. I'm not just being kind of touchy feely about learning here. There's a lot of rigorous studies about how people learn best. And it's in those discussions where you learn the most. So please, interact. Ask questions.

Now I'm going to motivate quantum mechanics. And how many of you have seen quantum mechanics before? How many of you have never seen quantum mechanics? It's OK.

See, the thing is, what's going to be really-- so here's the thing. You don't have to have seen quantum mechanics to feel your complete oneness and total enjoyment of the quantum mechanical simulations we're going to do. This is going to be really exciting whether you've seen quantum or not because we're going to kind of start slowly and then we're going to learn how to simulate the behavior of quantum mechanics. So what I want to do today is just tell you sort of why this is exciting and why this is important. OK?

OK, so that's what-- and I'll give you a more detailed outline when I come on for my part after spring break, but those are sort of the highlights of what we're going to touch on. Now I thought that-- OK, so I think Professor Wheeler may have shown this, right? So did you show the computers?

Does anybody know where the fastest computer on the planet is? We've gotten a lot faster, right? So some of these were actually here. The Whirlwind was here. So you can see the number of operations per second has increased dramatically, right?

Where's the fastest computer in the world today? Good guess. Yeah. Anybody know who has it? It's Google, right? It's Google. And I keep emailing them, and they don't respond to my emails, because I want to get some cycles on that machine. But they actually need to build power plants for those computers.

And Professor Wheeler showed that there's like one little rack where your simulations are going to go. Well Google has like thousands of those. Now I thought I'd share my own personal history here. Has anybody seen either of these in a museum? This is the good old days. We used to call it the Trash-80. It was a couple of years ago.

But that's how I grew up, just working on machines like this. And then there was this one which had a cartridge you could put in. You could save your data to a tape. OK? Do you remember that? No, you're too young. Yeah.

So now, when you save data to a tape, you literally are-- like, you guys think about megabytes, gigabytes. You would save like a 10k file and it would take you 10 minutes, OK? And it would have these beeps. Anyway, someday you can check it out in the museum.

But my favorite is the startup screen, right? So this one would just come on and it would say "ready." I like that. Right? So those are the old days.

OK, so Professor Wheeler talked about this. He talked about how I'm not even on here. I'm all the way down here. Hey. You know? But last but not least, right? Bottom but really important, because we're talking about bottom-up materials understanding and design, and this level-- understanding and being able to compute this level is going to be important for all the rest of the levels, right?

Now, what we're going to talk about when I come on in the second half is not just those potentials, right? So quantum mechanics gets you those potentials between atoms that you can then feed into there to there to there to there, but it also gets you real materials behaviors directly that you cannot get in any other way. Somebody tell me a quantum mechanical object that's just like really quantumy.

What makes you think quantum? Electrons, yes. I love that. That's another word. If you want to say electrons any time, in the middle of a sentence, say electrons. Scream it out. That's it, right? Electrons are quantum mechanical objects, right? You really need quantum mechanics to know what an electron is doing.

And it turns out that knowing what an electron is doing is really important for a lot of properties, OK? So I'm going to give you a sense of that in this little preview today. OK, so we're all the way down there. Now there are a lot of quantum mechanists and some of you may recognize some of these people. So these are the people.

And you can tell, in contrast to thermodynamicists, they don't have mutton chops, right? And I don't know that we could say there's a trend here. I mean they look nice here. A little less. Well anyway, they look-- these were some really smart people. These are revolutionizing sort of the way we understand and view the world. And we'll talk about what their contributions were as we sort of start the quantum part. OK?

And we'll talk about the problems. You see, because they had this thing for a long time. Right? They had classical physics which described the world really well.

Did we need quantum mechanics to send people to the moon? Turns out, no, right? So we can do a lot without quantum mechanics, but there started to become these problems that classical mechanics couldn't describe.

OK, and so we'll talk about those as well. I'm not going to talk about them now. But those problems became so great, that it just sort pushed these great thinkers of the time, of 100 years ago into developing a completely new theory for the world, for the way we view the world.

Here's one of the funny things about quantum mechanics. This is a quantum mechanical ball. And I just threw it into a wall. Right, and look at what happened.

Now, we'll talk about this later. A quantum mechanical ball is not a ball. It's a spread out thing, right? It has a probability associated with it. But look at what happens there, right? Look at this. What's going on? Somebody tell me what's happening.

What is it? Tunneling. Now, is tunneling something that happens in like real systems and materials? Yeah, you bet it does. Electrons do it all the time. And if you can't predict this kind of tunneling behavior correctly then you can't design optoelectronic materials, right, at least if you want to know what the electrons are going to do, which is pretty important.

OK, now, it turns out that, OK, so that's a quantum mechanical ball thrown into a wall. Uh-oh, OK. And then there is this very simple reaction that shows the behavior of the electrons. We already saw that, so I'm going to skip that.

But so this can be complex, right? Things are going like through walls. That's weird. Isn't that kind of weird? I mean, that's weird. If I throw a ball into a wall, you don't usually expect part of it to keep going, right? You expect it to bounce back.

But if I throw an electron into that wall, some of it will keep going, right? And this is even weirder. If I start mixing materials together and reacting them, those electrons can behave really, really weirdly. That's quantum mechanics.

And we'll come to feel our enjoyment and oneness with that weirdness. It's really fun actually. It's really fun to think about how weird it is.

The nice sort of thing, and also the really hard thing about quantum mechanics is that there's really only one equation that we're going to care about. This is it. Right, that's the Schrodinger equation. And you can see that it's just a partial differential equation. It shouldn't be so bad, right?

Well, so it turns out that this equation tells us everything that we need to know for quantum mechanics. It tells us about this thing. That's the wave function. OK, and the wave function is the word we use to describe that ball, that quantum mechanical ball. OK, it's that weird shape, right?

And it turns out that if we can solve that equation, then I can get the shape of PSI. And then I know a lot about the quantum mechanics of the system. Now, here's what happens when you try to solve that equation.

Here's this equation written in very simple form, H PSI equals E PSI. Don't worry about that. We'll get to that when we talk about quantum mechanics in the second half of the class.

Again, we're not going to do sort of like quantum 101. We're going to really talk about the key essence of quantum mechanics. OK? We're not going to go into great detail of mathematics of it. OK, but it's basically a simple equation that you need to solve.

So here is that quantum mechanical ball. This is just representing that wave. Right? This is a plane wave. And I'm throwing it into a wall.

And I just happen to put another wall behind it, spaced like that, right? Now, how would you solve that equation? What's the first thing you might try? Don't say ask Siri.

Actually, you could ask Siri. Wolfram Alpha Pro is coming out. So could you put this in a Mathematica? Right? Yeah.

You could, right? It's an equation. It's got boundaries. It's got initial conditions. And here's what you get, OK. So that's a quantum mechanical ball. It's the simplest one you could get. It's just a little shape that you throw into two walls. And these are the equations you have to solve.

Now, the fun part about this, which the students in this class two years ago did not think was that fun when I gave this on a homework assignment was that Wolfram Alpha cannot handle it. Wolfram, Mathematica, Matlab, you name it, chokes, right? You cannot solve these eight equations and eight unknowns unless you do some tricks, and [INAUDIBLE] tricks first.

I won't give another problem like this, I promise. But the point of this was not meant to drive the students crazy. That really wasn't the point. The point was just to illustrate how hard this equation actually turns out to be to solve, OK?

It looks simple. It's deceivingly simple. We can't solve it even today without making approximations. And the only reason we can solve it today for real materials is because we've figured out how to make really important algorithmic approximations, OK? The only Nobel Prize given in computation was given for that. I think that might be on my next slide. And computers have gotten really fast.

OK, so I'm skipping ahead of myself. This is a quote. So before that, before we figured out how to solve that equation for real materials, people like Dirac, really smart people were feeling a little bit hopeless. Right, 1929, "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known."

What's he talking about? What's completely known? Yeah, how? How come? Right? They had kind of nailed it. Right, like in the late 1800s, they were like looking at the world and saying, why? This doesn't compute.

And then they sort of spent 30 years developing the theory of quantum mechanics. And that's why he's saying it's kind of completely known. And the difficulty is only that the exact application of these laws leads to equations, much too complicated to be soluble. Right? That was 1929.

He did say later if there's no complete agreement between the results of one's work and the experiment, one should not allow oneself to be too discouraged. I like that quote.

It turns out that happens in simulation quite a bit, right? And that has to do with the fact that you can't solve the equations exactly. You have to make approximations. And knowing where you are in accuracy phase space is something that's very important in this class. And we'll be talking about that a lot. OK? But don't be discouraged.

Nice words of encouragement from Dirac. OK, so that Nobel Prize I was talking about, that was actually shared. But one of the people who won it was Walter Cohn. And he won it because of an approximation, which I'll talk about a little bit when we go into quantum mechanics.

And it turns out that you still can't solve the equations of quantum mechanics without making approximations. Even with the fastest comp-- how many transistors are on the fastest-- how many transistors can we put on a chip today? Does anybody know?

10 billion? That's a good guess. I think 3 is where we're at. And how many neurons in your brain? 100 billion, right? So we're getting close. We're getting real close. They're catching up, man.

It costs as much money to make a transistor on a chip with 3 billion transistors on it as it does to print a single letter in a newspaper. OK, so we are very good at printing lots of transistors. That has dramatically accelerated how much CPU power we have. And it's still worthless, worthless for the equations of quantum mechanics, unless you make simplifications. So we're going to have to talk about those simplifications. Because they're still not solvable unless you make these simplifications.

And that's why the Nobel Prize was given for it. That's how important it is. OK?

Once you do that, once you know the model, once you develop that model that Professor Wheeler talked about for quantum mechanics, then you can go ahead and do simulations. And you can get some really interesting properties out. Like in this case, this is lead titanate. And there's some really interesting magnetic properties that have to do with where those electrons are.

So I'm going to just give you a couple of sort of motivational slides for why understanding these electrons is so important. OK, and then I'll stop. How many know what this is? Yeah.

Quantum dots? Yeah. What's happening here? Why are they different colors?

AUDIENCE: Different energy bands.

JEFFREY GROSSMAN: OK, and somebody said, what's the reason for that? Different sizes. Different sizes. Isn't that weird? Why is that?

AUDIENCE: [INAUDIBLE]

JEFFREY GROSSMAN: That's a good try. Not quite right. Good guess. Any other ideas?

Well, there's always the go to answer, quantum. It's quantum mechanics. Right? It's quantum mechanics. This is red and that's blue. Aqua? Purple? I don't know. Because of quantum mechanics, right?

Let's break that down. It has to do with-- this isn't really breaking that down, but it's related because it's nanotechnology. OK? So I'm going to explain that in just a minute.

Nanotechnology. Well, you all know about nanotechnology. The scientist in*Spider-Man* was a nanotechnologist. Did you know that? And *The Incredible Hulk,* because of nanotechnology, right? So that's how Hollywood views nanotechnology.

But why am I telling you about nano? Well, because the effects I'm about to describe is because of nanotechnology. You hear a lot about nanotechnology, and there's a lot of hype around it. There's also a lot of there there, OK?

And I love this, in case you haven't seen the size scales. I know you've probably all seen too much nano. But I love this one where you're sitting on top of some random dude, and then you go out. Have you guys seen this? 10 times, 100 times, 1,000, right? And you keep going out, OK, and that's how far you are when you go out by 10 to the 9th.

And then you start again and you go in by the same amount, right? And so that's sort of just trying to give you a sense of the scales, right? So that's nano is going in by the same amount you'd be going out to get to here, right? It's kind of cool.

It's small stuff. Why is that interesting? Oh, the press seems to know. It's because super cows and nanotechnology will make ice cream healthy.

That's actually still my favorite article about nanotechnology. It's about healthy ice cream.

Actually, my favorite part of this is the definition. I love this definition. It is also experimenting with nanotechnology or the science of invisibly tiny things. Right? We just saw them. They're red and blue. They're not invisible.

OK, right, I highlighted it. OK, back to that example, right? So why am I connecting nano here? Well, because quantum feels nano a lot. Quantum and nano very often go hand in hand.

Now, it depends how nano you mean. Some people say they're working on nano, and they're really at like 0.8 microns. That's sort of cheating, right?

But not really. Hey, this is like some millions of nanometers. I guess that's working on nano.

If I take a bulk semiconductor, what's a semiconductor? It's this picture. Somebody give me an example of a semiconductor material.

AUDIENCE: Silicon?

JEFFREY GROSSMAN: Silicon. Right? What are the properties of a semiconductor. Somebody tell me one property of a semiconductor. Yeah.

AUDIENCE: [INAUDIBLE].

JEFFREY GROSSMAN: Yeah, yeah. It's got a gap. Not too big, not too small, just right. OK? We'll be coming back to that a lot, because that gap is something you can predict using quantum mechanics. You have to have quantum mechanics to predict it.

Now, it turns out that if I look at this piece of silicon, it's optically not that exciting, right? That will go along with those different colors. Right, it just sort of looks like charcoal actually, unless you process it. Might be a little shiny, but it's kind of boring.

If I take out my little nano ice cream scooper-- I'm a theorist, right? So this is how I view experiments. And you now scoop out a little piece of it. We have a name for that. That's called the quantum dot, right? That's a quantum dot. But it's nothing more than a little tiny piece. It's a nano piece, right?

What happens? What happens is if you do that, that's when you get this. Right? Why? Back to our-- you know what the answer is. Quantum mechanics, OK?

Here's the reason. Something called quantum confinement, OK? It turns out that if I create an optical excitation in this bulk semiconductor-- let's say I shine a laser on it. That's about the worst PowerPoint graphic I've ever seen.

Anyway, but it's a laser. And you shine a light on it. Well, happens is, you see these little objects that I said were very quantum mechanical, the electron. Right? What happens is the energy from the light kicks an electron out of what's called its ground state.

Well, we're going to talk about that. I'm getting really excited myself. And when it gets kicked out of its ground state it leaves behind a hole, or a positive charge, OK?

So now you've got a negative charge and a positive charge that have been made in this material. They've been made by light. Why might I be excited about that? No pun intended [INAUDIBLE].

[LAUGHTER]

Thank you, one person. If you've suffered through me last fall then, you know it. So why might I be excited about that?

AUDIENCE: Solar power?

JEFFREY GROSSMAN: Thank you. Solar power! We just made electricity from sunlight. Now, it turns out that electron, that positive and negative charge like to be a certain distance apart. Right, and bulk silicon, 5 nanometers. Right, it's called the exciton radius.

When you create an electron hole pair, they kind of like each other. Well, they're very weakly bound in silicon. But they have a distance that they like to hang out, in this case 5 nanometers. And what that means is that when I run out of real estate in the material, and I do the same thing, well, they don't have anywhere to be.

They want to be out here, but they can't be, because there's no material out there. Right, so if I'm less than that exciton radius, then my excitation is squeezed. We have a name for that. It's actually called quantum confinement.

Why? Because these are very quantum mechanical objects. You need quantum mechanics to describe them. And what you've done is you've squeezed them. You've increased their kinetic energy. And that is the reason the color changes. That's the reason the band gap changes.

And so you can see that the physical confinement of this excited state leads to this very unique quantum effect, which is that the light emitted depends on size, right? One example of many, of sort of the beauty that comes from understanding the quantum mechanics, and we're going to be able to simulate this in the second part of this class. OK?

Now, that is a really useful piece of technology. Quantum dots are being used-- does anybody know about the uses of quantum dots? I mean, they're already in companies, right? Yeah.

AUDIENCE: Solar cells.

JEFFREY GROSSMAN: Solar cells, right? LED TVs, biomarkers. It's big in the biotech.

Oh, sorry. I just stole your answer. And I didn't want to do that. Any other ideas? They're really useful, right? And they're getting more and more useful. Very interesting, all quantum mechanics.

That gets me really excited, because I work on energy. And I'm not going to do an energy talk, don't worry. But I work a lot on energy. And the fact of the matter is that this is a map of the US. And it shows where there's good to excellent resources in some renewable technologies, like PV, red and orange. Biomass, green and light green. Wind. Number one most utilized renewable resource in the world today is wind, right?

So if you look at this, there's only a few pockets where you're sort of-- sorry, man, it's gas or oil. Now, but we don't use hardly any of these resources, right? And the reason, as we all know, is cost and efficiency.

But in so many of these technologies, not wind, in this case, but PV, biomass, and in a number of other technologies, solar fuels, the key is pushing electrons around. That's the key. It's pushing electrons up a hill, and letting the electrons fall down a hill, right?

I mean, one of the oldest ways to store energy is what? Who knows? It goes way back. Still really used around the world, including the US. Yeah.

AUDIENCE: Steam.

JEFFREY GROSSMAN: Steam is a way. That's true. Think older. Pumping water. Who said that? In the back.

Pumping water. You pump water up a hill. You hold it in a big lake. And you let it come down when you need energy, right? You pump it up when you have the energy, and let it come down when you need it is a terribly inefficient way to store energy, but it works.

And basically, what we need to do for so many of these energy technologies is figure out how to more efficiently pump electrons up a hill. That's basically what we're doing, right? And that's quantum mechanics.

Because by definition, electrons need quantum mechanics to describe. Right? So we're going to pump electrons up hills and around in the second part of this class. And you can tell your friends that. And it will impress them, I promise you.

I always like to help you make conversation when you're at the bar. Because here's a solar cell. Do I have any time left?

Yeah, I got a couple minutes. I'm almost done. I'm really almost done. Cause we're going to work on solar cells. First, we're going to spend sort of the first half of the quantum part learning about quantum, and how to simulate that equation, right? We're going to do simulations.

And then we're going to apply those simulation tools to real problems. So we're going to study solar cells, for one. And look at this. Here is how a solar cells works.

Well, that's what you see if you take like a core six class, and if you think about it from the device scale. But here's what's happening inside that solar cell.

Sunlight comes in. Squiggly lines are always sunlight, right? Squiggly line comes in. And there is that electron. You can tell. Actually, you can't. But there it is.

And it gets promoted up, cause that light has energy with it that knocks this electron up an energy. And look at what it left behind. A hole, just like I showed you in silicon, right? In those quantum dots.

But in a solar cell, you don't want them to recombine and emit light. You don't want them to shine different colors. In a solar cell, you want to get those charges out. You want to get that electron out of one side, and get that hole out of the other side, right?

Every single step here, converting the photon into an electron, electron and hole thermalize. They couple to the solar cell, and they waste all that energy coming back up to the valence and conduction band. They wasted all this heat, right?

The electron hole pair diffuses. Hello there. Welcome to 302-1. This thing can move around. This pair can move around. And

Then you've got to get them apart, right? And you got to get them out, right?

Every single step that's critical is a quantum mechanical step. Right, you cannot describe these processes unless you can solve Schrodinger's equation, OK? So we'll be talking about that and how to make solar cells better.

For example, in silicon, people put charts like this up. More than 80% of the solar cells you buy today are this. They're multi crystalline silicon, right?

Now, the solar cells in your calculators are amorphous silicon. And the reason is, they're cheap. They're very cheap. But they're very inefficient.

And so you see things-- but they could be thin and flexible. That's kind of nice. But they're just not that efficient.

And so you start seeing things like, well, here, let's compare these two crystals. Here's a crystalline. Here's amorphous. There's a gap. Difference in energy between those states that the electron gets excited to, very different.

There's absorption coefficients. Very different. There's mobilities. And this is actually what kills it. Those holes are so slow. Right?

Well, how can you compute those things? Let me hear it.

AUDIENCE: Quantum.

JEFFREY GROSSMAN: Thank you, quantum mechanics. We can calculate, and we will calculate these things for these kinds of materials. And maybe you'll find a way to make amorphous silicon have faster holes. And if you do that, please come talk to me.

[LAUGHTER]

I'd be really interested, because I've been working on that problem for many years. But these are the kinds of things we're going to do, OK, in this class.

And I'll tell you one quick story. I was at a conference on solar energy. And they gave out calculators as kind of solar powered calculators, solar energy calculators. Solar energy conference, solar powered calculators.

And we opened one up. And it turned out it was battery powered.

[LAUGHTER]

And there was a little piece of amorphous silicon solar cell in there, but it wasn't wired up. And the reason is, these are so poor in their efficiencies, right? We've all seen it. You need to be in direct sun. And you can't see it anymore. Right? Why?

If we could figure out how to boost that whole mobility, we could get their efficiencies up. They'd cost a lot less. We'd make a game changing difference. So these are the kinds of problems that we're going to work on in the second half.