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PROFESSOR: So today we begin our study of solids and in particular of conductivity in solids and periodic potentials, and that diagram will mean something in a few weeks. So before I get started, questions on everything previous? Yeah.

AUDIENCE: So when you're talking about fermions and bosons [INAUDIBLE]. Statistics. So we said That you had to write the statement particular way for fermions with a minus sign particular.

PROFESSOR: Yes.

AUDIENCE: Well, we were assuming that you had to write the statement a product statement of the two. Will it be that you can't do that sometimes because they can't be separated.

PROFESSOR: Absolutely. That's a wonderful question. We'll come to that in the second next to the last lecture where we'll talk about something called entanglement, which is really what you're talking about. But here's the crucial thing, for fermions, so what I wrote last time, I said suppose we have two particles that are identical one is in the state we know one is in the state χ of x and the other is in the state described by ϕ of x . I'm going to call the position of the first vertical x and the position of the second particle y . And I can write the two states without property, well, three. I could fill many, but two in particular of the following form, χ of x ϕ of y plus or minus χ of y ϕ of x .

And the point of this linear combination is that when they exchange positions, the x and y So here this is the amplitude for the first particle will be an x , and the second particle to be a y . If I switch the sign or the positions to ψ plus minus of yx or if the first particle is at y , the second particle is at x , this is equal to just swap these two terms, plus or minus ψ plus minus of x,y .

So this wave function has been contracted to ensure that under the exchange of the position of the two particles, the wave function stays the same up to a sign. This plus sign is associated with systems we call bosons, and the minus sign is associated with systems we call fermions. Now as I've discussed previously, this is a persistent property of a system. If a system is bosonic, at some moment in time, it will always be bosonic. If it's fermionic in some moment in time, it will always be fermionic, and that is a consequence of the fact that the exchange operator that swaps the two particles commutes with the energy eigenfunction if they're identical particles.

And so if it commutes with the energy operator, then its value is preserved under time evolution with that energy operator. So now the question that was asked is, if this is our definition of bosons and fermions, is it true that you can always write the wave function in this form of differences of products of two states?

Well, the answer is both yes and no. The answer is yes for sufficiently-simple systems. The answer is no when you have many, many particles, and we can't always write it as a simple product of two states. We can't always write as the sum of two terms.

What you will discover if you studied multi-particle systems in 805 and 806 is that there's a nice way of organizing this anti symmetrization property, and it doesn't necessarily have two terms, but it may have many, many terms. With that said, this is not the defining property. This is really the defining property, whether your a boson or a fermion. OK? Cool. Yeah.

AUDIENCE: So I had a question about fermions. [INAUDIBLE] the explanation being makes perfect sense about why two things can't be in the same state.

PROFESSOR: Yeah.

AUDIENCE: But Used in 804-4, during recitation one of the instructors said, well actually, this takes like really hard quantum field theory to actually prove this. What does that actually mean?

PROFESSOR: OK. Good. So the question is, look, there's this legendary statement that this fact that the Pauli exclusion principle is incredibly hard and requires the magical details of quantum field theory to explain, and that some surprising. So your recitation lecturer said this to you.

AUDIENCE: Yes.

PROFESSOR: I'm sure I love this person dearly, but I disagree with him in an important way. So there are two things are confusing. Two things that require explanation I should say. One, we can explain at the level of 804, and the other does require machinery, but it's not crazy complicated machinery. So let me tell you what we can explain with 804, and then let me sketch for you how the more sophisticated argument goes.

So this fact, the basic fact that wave functions can be symmetric or anti-symmetric, and when you have identical particles, they must be either symmetric or anti-symmetric. This follows from the statement that we have identical particles. If you have identical particles, it must be true that under the exchange, they are either even or odd. They're either symmetric or anti-symmetric under exchange.

So if we have an exchange of identical particles, we need to have identical symmetric or identical anti-symmetric. And now it's just an empirical question. What particles in the world are identical bosons and what particles are identical fermions.

Identical fermions? Well, how could you tell the difference? You can tell that identical fermions do not want to be the same state, and identical bosons do as we saw last time, as an extra factor of two for two particles that are actually n for n particles.

So bosons want to be in the same state. Fermions want to not be in the same state, so if we just look at the world and say, which particles are well modeled by assuming we have bosons, which particles are well modeled by assuming we have fermions. And answer turns out to be the following, any particle that has intrinsic angular momentum, which is a half integer, any particle which spin like the electron,

which has a limit to $1/2$ and we'll study that in more detail later, any particle that has half-integer intrinsic angular momentum empirically turns out to be a fermion.

Take two electrons, take their wave function, and swap the positions of the two electrons, the wave function picks up the minus sign. Take two neutrons, also spin $1/2$. Swap them and you pick up a minus sign. It's a fermion. Take two particles of light, two photons, swap them and you get a plus sign, and these guys have integer spin. Angular momentum of light is 1, and similarly, if we could, for the Higgs boson, if you take two Higgs bosons and swap them, you'll discover that they're bosons and as a consequence there's a plus sign under exchange.

So that is not surprising, it's just an observable property of the world. The thing that's shocking is why that's true, right? Why is it that things that have half-integer angular momentum, which sounds like an independent property from whether they're bosonic or whether identical bosons are identified, why is it that all things with half-integer angular momentum or spin are fermions, and all things with integer angular momentum like light or the Higgs boson or me we're for bosonic, we're identical with an even sign, and that requires quantum field theory.

But it's not insanely difficult. It requires the barest minima of quantum field theory. So anyone who wants to understand, come to my office hours and I happily explain that. It takes about 15 minutes just to give you the basics of quantum field theory, just the bare basics. It's pretty straightforward. But it's a beautiful thing about relativistic quantum mechanics, so I'm going to turn this all around.

So let's look at the history. The history of this was people looked at atomic spectra and said, this is bizarre. It almost fits what we get from central potential except it does buy this factor of two integer indices. Ah-ha. There must be an extra quantum number and on top of that, so the spin, the two possible states of the electron. And secondly, it must be that electrons can't be in the same state. So it sounds like that's two hypotheses.

Now, if you take those two hypotheses, everything else follows. Fine. What Dirac discovered when he studied the relativistic version of the Schrodinger equation,

which really is quantum field theory, but when he studied the relativistic version of electrons, quantum mechanical relativistic version, he discovered that these two things are linked. It is cool. I grant you.

So you he discovered that these two things are linked, and he identified what's referred to as the spin statistics theorem. If you know the spin, you determine the statistics. So exactly how that works, that does require a little bit of effort-- that's the 15 minutes-- but you can dispense with that entirely and not be at all shocked by anything if you just accept two principles instead of one, first, that electrons are anti-fermionic, so they don't want to be the same state, and secondly, they have half-integer spin.

AUDIENCE: Given that the only thing that's really measurable is [ψ^2 the square ψ^2] or non-square of the wave function and the way the function itself is never completely actually, measurable. Is there a mathematical reason why exchange can't transform a wave function just by arbitrary phase? It has to be plus or minus 1?

PROFESSOR: Well, the reason it has to be plus or minus 1 for two particles, so you said a couple of things. Let me answer the first part. So what I will call the first part of your question is, why did it have to be plus or minus 1. Why couldn't it have been an arbitrary phase? And the reason is that if you do this exchange operation twice for two particles, you get back the same thing. And that's what I mean by saying I have identical particles.

Because I could quibble with this. You could say, well look, you could define some different notion of exchange, or under exchange, I pick up an extra phase. I swap them and then I swap them and I swap them again, I get a phase. But here's the problem with that. The problem with that is, and this can be dealt with, but an interesting question is if it can only be dealt with in two dimensions or it can be dealt with in general number of dimensions. This is a story called anyons, which Frank Wilczek here has really pounded hard on.

But here's the basic question. So does the wave function have a single value? I'd like to think it does. The wave function really should have a single value. If it has

multiple values, then it's ambiguous what the value of the wave function is there. That's not good. That mean you have to specify more than just the wave function, you have to specify which of the values the wave function takes in a particular point in the value of the wave function.

So if under double exchange we've returned to the original configuration, you pick up a phase, something is screwed. You must be able to tell whether or not you've exchanged twice, and here's why you can tell. Because while it's true that you can't tell the overall phase, imagine if I take my system and I put in a splitter and I have a beam splitter I could think of it as a two-split experiment, one component of that wave function I will double swap and the other component I will not. And then I will interfere them. I will combine them back together, do an interference experiment.

So you measure that relative phase. So that relative phase definitely matters. Do you just see that point? So it's true that they overall phase they can't measure, but by doing a superposition and only exchanging one of the superposition pairs, by physically separating those, then you can see that in interference experiments again.

So you can still deal with this, but it requires being able to know whether or not you can exchange, so there has to be some way of telling that you sort of entwined these guys, and that's something you could do in two dimensions. It turns out to be difficult to do in general number of dimensions. Well, it's an act of research topic. If you want to a more detailed answer, ask me later.

OK. One more question. Yeah.

AUDIENCE: [INAUDIBLE].

PROFESSOR: Yeah. it has precisely one observable property, which is this sign, this it's eigenvalue, value, and you can tell because the wave function either vanishes when you take the two points together or it doesn't. So that's it.

AUDIENCE: So it's not like the momentum [INAUDIBLE]. So it's only basically just [INAUDIBLE].

PROFESSOR: Yeah. It's less interesting than position or momentum. It has two eigenvalues rather than many. But it's no less interesting than, for example, spin. It contains information that you can learn about system. OK. One more.

AUDIENCE: I was wondering why you can write this fermion as two electrons I guess when it seems to me [INAUDIBLE].

PROFESSOR: That's a fantastic question. OK. Good. I was going to gloss over this. That's a fantastic question. So here's the question. Look, I have in my box here, I have a hydrogen atom, and I've quantized the cooling potential, and I know what the energy eigenvalues are for the cooling potential, and I put the electron in one of those states. And I say the wave function describing my system as sign is equal to ψ for some particular ψ That's what we've been doing.

But there are a lot of electrons in the world. In fact, there are electrons in the walls. There are electrons in your nose. There are electrons everywhere, and they are fermion. So the wave function describing the entire system must be invariant up to a sign under the exchange of any two electrons. If I take this electron and I swap it with an electron in Matt's ear-- Hi, Matt-- then the wave function had better pick up a minus sign.

So what business do I ever have writing a single wave function for a single electron. Is that your question?

AUDIENCE: Yes.

PROFESSOR: That's an excellent question. So let me answer that.

So suppose I have two electrons, and I have the wave function for two electrons x and y . I mean, I write this as if it's in one dimension. This is some position, some position, but this generally is just an arbitrary number of dimensions, and one is in the state ψ of x , and the other is in the state ψ of y . But I know that I can't have this be the state because it must be invariant under swapping x and y of two minus signs. So I need minus ψ at y ψ at x , and let's normalize this, so $1/\sqrt{2}$. So that's our electron.

Now, at this point, you might really worry, because say χ is the electron is the wave function bound to my atom, and ϕ is the wave function for the electron bound to an atom in Matt's ear. So we've just in writing this. Why can we do that? Well, let's think about this. What does the combination of terms give us?

What do they tell us is that they're interference term. If I ask them what's the probability to find an electron at x and an electron at y , this is equal to, well, it's this whole quantity norm squared sine norm squared, which is equal to $1/2$, and then there's a term where this gets term squared, this term squared, and then two cross terms.

So the first term gives us the χ at x norm squared ϕ at y norm squared. The second term gives us plus χ at y norm squared ϕ at x norm squared plus twice the real part of I'm going to write this subscript χ sub x ϕ y , complex conjugate, complex conjugate χ y ϕ x .

Everybody agree? That's just the norm squared of everything.

AUDIENCE: Shouldn't that be minus?

PROFESSOR: Oh, shoot. Sorry. Thank you. Minus. Yes, minus. Importantly minus. Now, let's be a little more explicit about this. Saying that χ is the state localized at the hydrogen, then that's as if the hydrogen is here. If the proton is here, then the wave function for χ has a norm squared that looks like this.

And if I say that ϕ is the state corresponding to being localized, at Matt's ear, then here is the ear, and here is the wave function for it, so that's ϕ . So let's then ask, what's the probability that I find the first electron here and the second electron here? Well, if this is x , and this is y , what's the probability that I find a particle there and a particle there?

Well, what's this term? Well, it's χ of x , which is not so small-- that's just some number-- times ϕ of y , some value norm squared, so this is some number. What about this one? What's χ of y ? Well, χ of y , this is all sharply-localized wave

function over here χ , and it's 0 out here.

The probability that an electron bound to the hydrogen is found far away is exponentially small as we've seen from the wave functions of hydrogen. It's bound. So this is the negligibility small as is ψ of x . ψ of x is negligibility do small. The wave function is localized around the ear, but x is way over there by the hydrogen. It's exponentially small. This term is also exponentially small.

Now in here, what about this? χ of x ψ of y , that's good. Those are both fine, but χ of y ψ of x ψ of x , these are both negligibility small, so these terms go away. So this is just equal to χ of x norm squared ψ of y norm squared. And this is what you would get approximately, and that approximately is fantastically good as they get far apart. This χ of x is just the probability that the particle that x given that it was in the wave function bound to the hydrogen, and ditto given that it was bound to the ear. Cool?

So the important thing is when fermions are separated and the wave functions are localized, you can treat them independently. When the fermions are not separated or when their wave functions are not localized, you can't treat them independently and you have to include all the terms. That cool? OK. Yeah.

AUDIENCE: That's times $1/2$, right?

PROFESSOR: Yeah, that is times $1/2$. What did I do? I'm screwing something up with the normalization. Ask me that after lecture. It's a good question. I'm screwing something up. I'm not going to get the factor of 2 straightened out right now. OK. Does that answer your question? OK. Good. This is a really deep-- it's important that this is true. I'm going to stop questions because I need to pick up with what we need to do.

So this is a really important question because if it weren't true that you could independently deal with these electron, then everything we did up until now in quantum mechanics would have been totally useless for any identical particles. And since as far as we can tell, all fundamental particles are identical, this would have

been very bad.

So with that, let's move on to the study of solids. So I want to pick up where your problem set left off. The last part of your problem set, which I hope everyone did, the left part of your problem set involved looking at this simulation from the PhET people of a particle in a series of n wells. And I want to look at the result, at least the results that I got for that simulation.

So let's see, here are the data points that I got-- shall I make that larger? Is that impossible to see? Those are the data points that I pulled off of PhET just the same way you did. You look, you point, you move the cursor, and you pull off the data points. So those are approximately then. And this is for 1, 2, 3, 4, 5, 6, 7, 8, 10 wells, and here's the plot of them as a function of the index which state they are.

So as a function, this is the first state. This is the second state, third, fourth, et cetera. Here are the energies vertically. And hopefully, you all got to plot some more of this and they seem to become bunched together, and the energy of the ground state without the potential was this. So I'm not going to add in a parabola corresponding to a free particle with the associated wavelengths. Remember I asked you to say take that state that looks most like a momentum. eigenstate with a definite wavelength and calculate the energy of a free particle with the corresponding wavelength.

So this parabola-- I should make this smaller-- is a parabola describing a free particle which agrees with those free particle energies at the three points where you're supposed to compute them. So there's the parabola. And so what I've done here is I've grouped them together into the bands of states. So vertically we have energy. On the horizontal side, we have n but remember that n is also corresponding kind to a momentum because each state wiggles and especially the states at the top of each band have a reasonably well-defined momenta, and so they look a lot like momentum eigenstates.

So I'm going to interpret this horizontal direction, it's something like a momentum. And at the top of the states, it certainly makes sense, but then what it actually is is

just the number the level, and what we see is that the energy is a function of the level is close-- near the top anyway-- to the energy of a free particle, but the actual allowed energies are bound. So which energies correspond to allowed states, and which energies have no allowed states associated with them is encoded in this diagram. Are we cool with that?

In this shaded region, there are states with an energy in that region, at least approximately, and in this unshaded region, there aren't any. And in each band, there are n energy eigenstates, and each band corresponds to one of the bound states of the potential. OK. Everyone cool with that?

So does this look more or less like what y'all got?

AUDIENCE: Yes.

PROFESSOR: Good. OK. Questions about this before I move on? It's an important one. And let me just remind you of a couple of facts about this PhET simulation so here's what we see if we have the single well. We have three states 1, 0, two nodes, two zeroes, and they satisfy the node theorem.

If we have many states, then if we look at the bottom state in each well. So there's the bottom state and the bottom band. It has no zeroes. It satisfies the node theorem, and the top one by comparison looks extremely similar. It looks extremely similar to the ground state, which is the orange one, the lowest energy state.

It is a little higher energy. You can see that because the curvature is greater. If you look at the top and bottom of each wave function, you see that the curvature is greater for the yellow guy, which is the guy at the top of the band, and the yellow guy, meanwhile, looks like a wave with a definite wavelength. But a general state in here doesn't have any simple symmetry properties. It's not periodic. It's not approximately periodic. Well, that one's kind of approximately periodic.

But the top guy and the bottom guy look approximately periodic. They have some nice symmetry properties. But in general, they're just not translationally invariant. They're not symmetric. They don't have any simple, nice structure. They are just

some horrible, ugly things. The bottom though and the top guy always have some nice symmetry property. Anyway to keep that in mind.

And the last thing I want you to note from all of this is that as we make the potential barriers stronger, two things happen. First off, bands become very narrow, the gaps between them become very large, and secondly, the wave functions take now an even more sort of complicated and messy, which is more obvious that the wave functions are not periodic.

This thing it looks almost periodic, but is periodic with some funny period, and it's not a single period by any stretch of the imagination. OK. So any questions about the wave functions in here? Yeah.

AUDIENCE: In this one, there is an overall [INAUDIBLE] period. [INAUDIBLE]

PROFESSOR: Excellent. OK. So let me give you a little bit of intuition for that. So suppose I have a big box. What's the ground state? What does the ground state look like? Yeah. Good. Everyone's doing this. That's good. So the ground state looks like this, and the first excited state is going to do something like this, and so on. Cool.

And what's the third excited state going to look like? I guess I shouldn't do that. The third excited state is going to do something like this. Cool?

Now, meanwhile, imagine I take my periodic well and I add to it a bunch of delta function scatterers with some strength. When the strength is zero, I just recover my original well. When the strength is non-zero though, we know that what a delta function is going to do is, it's going to make a little kink. It's going to induce a little condition on the first derivative at the delta function. So what's going to this ground state when we turn a little tiny bit of that delta function?

Yeah. What we're going to get is, we're going to get something that kinks at each of the delta functions. But it still has to have those boundary conditions. Everybody cool with that?

And as we make the delta function stronger and stronger, the effect of this is going

to eventually be to give us something that looks like-- yeah? Now that should look a lot like that. Everyone cool with that? Meanwhile, what's going to happen to the second guy?

Well the second guy, same thing. The effect on the second state is going to be-- cool? I'm not sure of I need the sound effects. So let's magnify and let's look at the second state here. Ooh, it's going to be hard to deal with that tiny energy splitting.

Come on finger, you can do this. There we go. There is two. Ah-ha. That looks a lot like this. Yes, that second state looks an awful lot like this. And let's go back to that funny state that we were looking at before. Let' see if I can get it. Should be the third guy here.

So there's a second guy in the third band. Again, you see an envelope and then the fluctuation from being in the third state and in the second state in this band as well. So on the other hand, what's the scale of the energy splitting due to a well of it this width compared to the energy splitting between states due to a well of this width?

A wide well means that its states are close together. An ENDOR well means the states are far apart. So what state do we have? We have the state that was the ground state of the whole box with a correction due to the delta function versus states which are, for example, excited states in the box. The splitting between this state and this state is going to be much larger than the splitting between this state and this state, just because this is a tiny little well and so the link scale is much shorter, the energy is much greater. That's the intuition you should have from these guys. So when you see that there's some approximate structure, let's see let's make this nice and separated again. And Oh, yeah. these are kind of difficult to control when they're so close together.

The trouble with touch pads. There we go. OK. There we go. That was the guy we were looking at before. And so you see that there is an overall envelope which has three maxima, and then there's the n inside each well. It's got two zeroes inside each well. And it's that envelope which is coming from the fact that you're in a box and the two zeroes inside each well, which is coming from this.

All the states here in this band are of the form two zeroes inside the well. All the states here are the form two zeroes is inside each well in this band except they're being modulated by an overall sine wave due to the fact that they're in a box. And so they're very closely split states with a different overall modulation but with each state inside each band corresponding to either the ground state for the individual well or the first excited state in the individual well or the second excited state.

So each band corresponds to which excited state you are inside the well, and which state you are within the band is your modulation of the overall wave from being inside a box. That make sense?

AUDIENCE: I guess so, but why does the overall modulation have a smaller effect than the--

PROFESSOR: Great. If I have a well that's this wide, what are the ground state energies? And let's say the width is L . What are the energies in this square well, an infinite well with L ? Yeah, but what are the eigenvalues?

AUDIENCE: [INAUDIBLE].

PROFESSOR: $E_{\text{sub } n}$.

AUDIENCE: [INAUDIBLE].

PROFESSOR: Yeah. Exactly. So they go like, I'm just going to write proportional to, n^2 over L^2 , because it's a sine wave with period $n\pi$ upon L . So the k is n upon L with constants, and that means that the energy again, constant $h^2 k^2$ upon $2m$ is k^2 , which is n^2 over L^2 . But the important thing is that the splitting between subsequent energy levels is controlled by the width. It goes like 1 over L^2 .

So if you have a very wide well, the splittings are very small, the ground state. On the other hand, if you have a thin, narrow well, then the splittings also go like L^2 , but L is very small here so the splittings are gigantic.

When we have a superposition of a big box inside of which we have a bunch of

barriers, then the splitting due to being excited in the individual wells goes like 1 over the little distance squared. Let's call this a squared. So these go like 1 over a squared, ΔE , goes like 1 over a squared, and from here it goes like if this is L , ΔE goes like 1 over L squared.

So the combined effect is that you get splittings due to both. These splittings are tiny, and these splittings are really large because this is a much smaller distance, and this is a much larger distance. Cool?

So the only question is how big in amplitude are these-- how effective are these barriers. If they were strict delta functions, then this is all we would get. And if there were no delta functions, we would just get precisely these. And when we have some barrier, we get a combination of the two, and that's what we're seeing here with the splitting.

So what I'm doing when I'm tuning the separation here I'm controlling effectively how strong is that barrier. And so as we make the barriers stronger-- there we go-- then the splittings are controlled by the individual wells, and as we make the barrier very inefficient, then the splittings are controlled by the overall box. Cool? Excellent. Other questions about the simulation? Yeah.

AUDIENCE: How close are the actual [? wavelength ?] potentials or the combinations of the original wavelength?

PROFESSOR: Excellent question. So you can answer that immediately from this. So the question is this, look, if we had arbitrarily separated wells, if we had something that looked like-- so they're very, very far separated. Then the ground state would be effectively degenerate, because the wave function or the ground state would be the completely symmetric combination of these guys-- you guys actually studied this in our problem set-- then there's also a combination where you have this, this, this. You could also take this constant this. There are many things you could do. I'm sorry, this, many combinations.

The point is since each wave function for each well effectively drops off to zero

inside, we can just linear combinations of these, and there's no penalty for using the true ground states in here because the potential is so high, that the true solution has an exponential tail, but that exponential tail is ridiculously small if the barrier is big. So in the limit that the barriers are gigantic, the true energy eigenstates are just arbitrary linear combinations of these guys, of the individual eigenstates of each individual well. Agreed?

However, when the barriers are large but finite, then the true energetic states have little tiny exponential tails, and the curvature of that little tiny exponential tail will determine exactly what the energy is. So a state that curves a little bit versus a state that curves more will have slightly different energies. So when the barriers are very, very large, the linear combinations of the individual well eigenstates should be very good approximations, but not exact. And as the barriers become less and less effective, they should become less and less exact, and we can see that right here.

So let's take the ground state. The bottom of the band is the completely symmetric combination of the ground state of each well. Everyone see that? It's just well, well, well, well. It's a completely symmetric combination.

At the top of the band is the completely anti symmetric combination, and let's put them for comparison. The top of the band is the orange one, and the bottom of the band is the yellow one. So the bottom of the band is the completely symmetric, and the top of the band is alternating combination of the ground state in each well. And all the other states inside here-- well, which are extremely difficult to-- Let's see.

There we go.

These states are also linear combinations of the ground state in each well with different coefficients in front of them. There are the different coefficients, and they are almost degenerate. But if we go to higher energy states where the barrier is less effective-- because they have high energy and the ratio between the barrier height and their energy is small-- then you see that these states are not particularly well approximated by linear combinations. And the energies correspondingly are not degenerating.

AUDIENCE: So you said linear combinations of the [INAUDIBLE].

PROFESSOR: That gives you a better approximation, but for the same reason. It's a good approximation, but it's not exact. But it becomes excellent as the barriers become infinite, even when they also go over to the infinities very well. Very good question. Yeah.

AUDIENCE: [INAUDIBLE].

PROFESSOR: Very good question. We'll come to that in little bit. We'll come to that shortly. So I'm done at the moment with the PhET simulations. I'm motivated by all this, and effectively by that question, I'm going to ask the following thing.

Look, real materials like metal in my laptop, the real material is actually a periodic potential. It's built out of a crystal of metal atoms that are bound together, and each atom is some positively-charged beast, to which some positively-charged nucleus, to which is bound an electron.

And if I want to understand properties of solids, like the fact that metals conduct electricity, a basic fact I'd like to explain, if I want to explain the fact that metals conduct electricity, but plastic doesn't, which we will be able to explain, and diamond doesn't, which is cool, if we want to explain that property, we probably ought to study the physics of electrons in periodic systems where the potential is, atom, I don't want to be stuck to you. Atom, I don't want to be stuck to you. Atom I don't want to be stuck to you. So it's a periodic well a potential.

So in order to study the physics of solids, I need to understand first the physics of electrons in periodic potentials. And these PhET simulations were a first start at that. We did it n 's wells. I want to now think about what happens if I take not n , but an infinite number of wells. What if I really strictly periodic lattice on the line? What do we expect to happen?

Well, looking at the results of these PhET simulations, as you did this for different numbers, n , what you found was the same sort of band structure. You just find for more and more wells, you find more and more states inside each band. In fact, you

find n states within each band. Both the top and bottom of the band quickly asymptote to fixed values. As we take n large, what do you expect to happen?

Well, this was a problem on your problem set. What did you predict? What should happen when you take n large?

AUDIENCE: [? It ?] depends on the experiment.

PROFESSOR: Yeah. How many states should there be in each band?

AUDIENCE: N .

PROFESSOR: N . So there are arbitrarily many. Exactly. So there should be arbitrarily many states in each band, but they all have to fit within this energy band, the width, which is asymptoting to a constant. So there has to be a continuum of states, and they're not going to be free particle states because the system has a potential. What is the shape going to be? Well, a reasonable guess is that the shape is going to be something that fills out this curve. It's going to be a little bit different from the free particle state.

So let's find out. Let's just solve the problem of an electron in a periodic potential, and look, the periodic potential is extremely similar to things we've already solved. So I want to walk you through just a basic argument. So periodic potentials. Instead of n wells, consider a system of an infinite number of wells, each one identical and just for symmetry purposes. And let the width here be L , so the period of the lattice is L .

And what I mean by that is saying, so this is V of x seeing that it's periodic is the statement as that V of x plus L is equal to V of x . Potential doesn't change if I shift it by a lattice vector,

Now there's a nice way to say this which is that, if I take the potential, v of x , and I translate it by L , I get the same potential back V of x . And more to the point, if I take the translation if I think of these as operators expressions, if I take TL and act on Vx and then the potential of Vx of x , then this is equal to V of x TL of x .

So if I think of these as operators instead of just little functions operator, operator, then if I take the translator operator and I translate V of x f of x , I'm going to get V of x plus L f of x plus L . And if I do the right-hand side I get translator of L that's f of x plus L but just times V of x . But if V of x is equal to V of x plus L -- this is V of x plus L .

So if I translate by L says take this thing and translate it, plus L f of x plus L . And on the right-hand side, we have V of x , not V of x plus L translate by L f of x , f of x plus L . And these are equal because V of x plus L is equal to V of x . Yeah.

So what that tells you is as operators translate by L and V of x commute. Equals 0. Everyone happy with that?

So you should just be able to immediately see this, the potential is periodic with period L if by translated by L , nothing should happen. So the potential respects T of L it commutes with it. So this tells you a neat thing. Remember that translate by L is equal to E to the i PL upon \hbar , so in particular, TL commutes with P because this is just a polynomial in P dL P , and in particular with P squared is equal to 0, and that just follows from the definition.

So what that tells us is that if we take the system with our periodic potential, periodic V of x plus L is equal to V of x , then the energy, which is P squared upon $2m$ of V of x commutes with TL . So in this system, with a periodic potential, is momentum conserved? What must be true for momentum to be conserved?

So momentum conservation come from a symmetry principle.

AUDIENCE: Translation invariance.

PROFESSOR: Translation invariance. In order for momentum be conserved, the system must be translationally invariant. Is the system translationally invariant? No. If I shift it by a little bit, it's not invariant. It is, however, invariant under a certain subset of translations, which is finite shifts by L .

Yeah. So it's invariant under shifts by L , which is a subset of translations, and the

legacy of that is the fact that the energy commutes with translations by L . The energy does not commute with P , because P acting on V of x , it takes the derivative and gives you the prime of x . It is not the same thing.

But we have a subset of translations under which the system is invariant, and that's good. That's less powerful than being a free particle, but it's more powerful than not knowing anything. In particular, it tells us that we can find energy eigenfunctions, which are simultaneously eigenfunctions of the energy, and, I'll call it Q for a moment, they have an eigenvalue under TL .

So we can find eigenfunctions which are simultaneously eigenfunctions the energy operator you might E of ψ E is equal to $E \psi$ E and which are eigenfunctions under translate by L on ψ E is equal to something times ψ E . So we're going to find simultaneous eigenfunctions. Everyone cool with that? Yeah.

AUDIENCE: Do you know if the momentum operator is still the momentum operator?

PROFESSOR: Sorry. Say it again.

AUDIENCE: The momentum operator is still in remission, right?

PROFESSOR: Yeah. The momentum operator is still the momentum operator. [INAUDIBLE].

AUDIENCE: Do you know if [INAUDIBLE]?

PROFESSOR: Excellent. Excellent. Good Yes. OK. So if T of L is unitary, note, T of L is unitary. And you actually showed this on a problem set before, and let me remind you a couple of facts about it. The first is that T of L is unitary, and that says that TL dagger is equal to the identity, right? But what is TL dagger?

AUDIENCE: [INAUDIBLE].

PROFESSOR: Yeah. TL dagger, well, P is remission, so we just pick up a minus sign, so TL dagger is equal to e to the minus i PL over \hbar , and we can do think of this two ways. First thing you can notice that it's clearly the inverse of that guy, by definition of the exponential, but the other is, TL is the thing that translates you by L , and this

operator, e^{-iPL} , well, I could put my H with the and that's just translation by $-L$.

So this is translated by L and then translated by $-L$. And of course, if you translate by L and then you untranslate by L , you haven't done anything with the identity. What are the eigenvalues? What are the form of the eigenvalues of a unitary operator?

AUDIENCE: [INAUDIBLE].

PROFESSOR: Well, that's true. The eigenfunctions are orthonormal, but the eigenvalues, are they real numbers?

AUDIENCE: [INAUDIBLE].

PROFESSOR: Yeah. So the eigenvalues of a unitary operator are of the form, well, imagine we're in a momentum eigenstate, for a momentum eigenstate, then P is a real number. And then the eigenvalue of T_L is $e^{iP/\hbar}$, that's a real number. So is $e^{iP/\hbar}$ a real number? That's a pure phase. It's $e^{iP/\hbar}$ a real number.

So the eigenvalues are pure phases, and this let's just do a nice thing. We can note that here the translate by L of the ψ , if these are common eigenfunctions of E and of T_L , well, T_L is unitary, its eigenvalue must be a pure phase, $e^{iP/\hbar}$ a real number. So let's call that real number α , $e^{i\alpha}$. So maybe just label this by α for the moment, and you'll see why I want to change this to q later, but for the moment let's just call it α . Everyone cool with that?

So you actually show the following thing on a problem set, but I'm going to re-drive it for you now. We can say something more about the form of an eigenfunction of the translation operator. This is quite nice.

So suppose we have a function ψ_α such that $T_L \psi_\alpha = e^{i\alpha} \psi_\alpha$. I want to know what is the form. What can I say about the function $\psi_\alpha(x)$? What can I say about the form of this function? We can actually say something really useful for this. This is going to turn out to be necessary for us.

The first thing I'm going to do is, I'm going to just make the following observation. Define the function u of x , which is equal to e^{-iqx} times ϕ . So if ϕ is an eigenfunction of T_L with an eigenvalue $e^{-i\alpha}$, and I'm just defining this function u to be e^{-iqx} times ϕ . Cool? It's just a definition. I'm going to construct some stupid u .

Note the following thing. T_L on u , if we translate u of x , this is u of $x + L$. Translating this, I get $e^{-iq(x+L)}$ goes to e^{-iqx} times e^{-iqL} times ϕ of $x + L$. But this is equal to from here e^{-iqL} times e^{-iqx} times ϕ of $x + L$.

And from ϕ of $x + L$, I know that if I translate by L to get ϕ of $x + L$, I just pick up a phase, $e^{-i\alpha}$, so $e^{-i\alpha}$ times ϕ of x . But this is equal to $e^{-i\alpha}$ times ϕ of x , putting these two terms together, and this is nothing but u of x . Yeah. So another following cool thing.

So here I define some function u with some stupid value q , which I just pulled out of thin air, and I'm just defining this function. What I've observed is that if I translate this function by L , it picks up an overall phase times its original value where the phase depends on α and on q . So then I'm going to do the following thing. This becomes really simple if I pick a particular value of q , for a special value of q , q is equal to α divided by L , then this is equal to $e^{-i\alpha}$ times ϕ of $x + L$. That's going to be equal to $e^{-i\alpha}$ times ϕ of x , which is just 1, so I have the phase, so this u of x .

So that means if I translate by L on u and I pick q is equal to α over L , I get back u , so u is periodic. Everyone see that? Question?

So as a result, I can always write my wave function ϕ and we'll now call this q or q is related to α as q is equal to α over L , every energy eigenstate can find a basis of energy eigenstates with a definite eigenvalue under the energy, a definite eigenvalue under T_L , and I can write them in the form, since u is equal to e^{-iqx} times ϕ , then ϕ is equal to e^{iqx} times u of x where q , where the eigenvalue, $e^{-i\alpha}$, is equal to e^{-iqL} and u of

x is periodic. Everyone cool with that?

It's not totally obvious how much this is helping us here, but what we've done is, we've extracted, we've observe that there is some lingering symmetry in the system, and I've used that symmetry to deduce the form of the energy eigenfunctions as best as possible. So I haven't completely determined the energy eigenfunctions, I've just determined that the energy eigenfunctions are of the form, a phase, e to the i qx , so it varies as we change x , times a periodic function.

So the wave function is periodic up to an overall phase, not a constant phase, a position-dependent phase. Does everybody agree with that? Questions about that?

So a couple things to note about this q , the first is, the eigenvalue under TL e to the i α , this is the eigenvalue under L also equal to e to the i qL , but if I take q to q plus 2π over L , then nothing changes to the eigenvalue, because the 2π over L times L is just 2π , e to the 2π is 1 , so we don't change the eigenvalue.

So different ways of q only correspond to different eigenvalues of translate by L of a translation by one lattice vector, one lattice basing. They only correspond to the different eigenvalues of TL if they don't differ by 2π over L . If different values of q differ by 2π over L , then they really mean the same thing because we're just talking about translate by one period. So q is equivalent to q plus 2π over L . So that's just the first thing to know.

So what have we done so far? What we've done so far is nothing whatsoever except extract, take advantage of the translational symmetry that's left, the remaining lingering little bit of translational symmetry to constrain the form of the energetic functions. What I want to do now is observe some consequences that follows immediately from this. So there are some very nice things to follow just from this. We can learn something great about the system without knowing anything else, without knowing anything about the detailed structure of the potential.

At this point, I've made no assumptions about the potential other than the fact that it's periodic. So the thing I'm about to tell you were to be true for any periodic

potential. They follow only from the structure. So let's see what they are.

So the first one is that the wave function sine of x itself with a definite value of e and a definite value of q is not periodic by L . Because under a shift by L , u is periodic, but this part picks up a phase e to the $i qL$. That's what it is to say that an eigenfunction, the translation operator. It's not periodic by L unless q is equal to 0.

So for q equals 0, there is precisely one wave function which is periodic by L .

Because if q is equal to 0, then this phase is 0. So only if q is equal to 0 is the wave function periodic. Cool?

So this should look familiar because back in the band structure, these guys are not periodic. So these states in the middle of the band, they're horrible. They're not periodic. They're some horrible things, but that top guy in the band is periodic, and it turns out that if we had made the system infinitely large, it would become exactly periodic. The fact that it has an envelope on it like this is just the fact that we have a finite number of wells, we're in a box.

If we got rid of that box and we made many, many wells, we would find it perfectly periodic. Yeah.

AUDIENCE: Could q not be something like $2\pi/L$?

PROFESSOR: Yeah, but $2\pi/L$ would be equal to, it's equivalent to q equals 0, because it corresponds to the same eigenvalue. So q 's that differ by $2\pi/L$, I'm going to call the same thing.

AUDIENCE: OK. Got it.

PROFESSOR: Good. Other questions? So the wave function is not periodic except for one special case, and we already have a guess as to which special case. It looks like it's the state on the top of the energy band, which is approximately periodic. Two, while the wave function is not periodic, the probability that you find the particle at $x + L$ is equal to the probability that you find the particle at x , and this immediately falls in this form, because when you take the norm squared, the i 's cancel out at every

point and we're left with the periodic u of x .

So the probability is equal to norm squared of u of x , which is equal to norm squared of u of x plus L because u is periodic. So probability distribution is periodic. On the one hand, this is reassuring, because if you look at the potential, the potential is perfectly periodic, and it would be really weird if you could tell by some probability, by some measure, like how likely you would find an electron here as supposed to over here, potential is the same, the probability should be the same find the electron in each spot. The problem with that logic though, is that these are wells and usually we think that when we have wells, we have bound states, and those bound states are localized. But the probability has to be invariant under translations, so it cannot be that the electron wave functions are delocalized.

The electrons wave functions must have equal overall amplitude to be in any given well. It must be invariant under translations by a lattice spacing. So that's really weird. We have a whole bunch of quantum wells, and yet there are no localized states. All the states are extended just like free particle states are extended.

It had to be this way by periodicity, but it should surprise you a little bit. Anyway it surprises me. I shouldn't tell you what to be surprised by. Yeah.

AUDIENCE: To normalize probability, what do you do?

PROFESSOR: Yeah. Excellent. OK. So this is for the same reasons that free particle wave functions aren't normalizable, these aren't going to be normalized either. So what are we going to have to do?

AUDIENCE: Build wave packets.

PROFESSOR: Yeah. We've going to have to build wave packets. In order to really meaningfully talk about that stuff, we're going to have to built wave packets. We need wave packets to make normalizable states. But the localized wave packets are necessarily not going to be energy eigenstates just like for a free particle. And so there's going to be dispersion, and the whole story that you saw three particles we're going to see again for the particles in the periodic potential. Cool?

So next thing. Therefore, all ψ sub E_q extended. This is going to have some really cool consequences, and understanding this fact in detail is going to explain to us the difference between connectivity in the middle and not conductivity in plastic.

Although there's a surprising hook in there. Naively, it would have gone the other way around.

So the last thing to say three, is that ψ sub E_q , so this is the state with definite energy and definite eigenvalue under translation E to the $i qL$. Yeah. And you showed on a problem set that if you take a wave function, you multiply it by E to the $i qx$, what have you done to the expectation value of the momentum?

AUDIENCE: You've increased it by q .

PROFESSOR: You've increased it by q , right? This is the boost it by q operation. So q incidentally has units of a wave number, so times \hbar has units of a momentum. q is like a momentum. Is q a momentum? Well, we can answer that question by asking, is this an eigenfunction of P ? Is it an eigenfunction a momentum operator?

And the answer is definitely not. That's an eigenfunction of a momentum operator. I take a derivative, I get q times i and I multiply by \hbar , I get $\hbar q$, momentum, but when I have this extra periodic function, this thing together is no longer an eigenfunction of q , because u is some periodic function, which is necessarily not a momentum eigenfunction.

So this guy is not a momentum eigenfunction. You can see that by just taking the derivative. I get one term that picks up a q from this, but I get another term that gets a derivative with respect to u , and that's not proportional with the constant to $u e$ to the $i qx$ unless u is in the form e to the $i kx$. But if u is in the form e to the $i kx$, this is just a free particle wave function, which it can't be if we have a periodic potential.

So finally q is not a momentum eigenstate. And correspondingly, q and more important $\hbar q$ is not a momentum, I'll say the momentum in the sense that it's not the eigenvalue of the momentum operator. However, it has-- semi colon-- it has units of momentum. And not only does it have units of momentum, it's the thing that

tells you how the state transforms under translations. It translates by an e to the $i qL$ under translations by L . And there is usually what momentum is. it's the constant that tells you how the state transfers under momentum.

So it's kind of like a momentum, but it's not the eigenvalue of the momentum operator. We have a name for it. We call it the crystal momentum, and we'll understand what it does for us. Part of the goal for the next two lectures is going to be to understand exactly what this crystal moment is. So for the moment, I'm just giving it a name sort of like the beginning we give super position a name, and we'll exploit its properties basically now.

So these are the things that follow just from periodicity. I didn't know anything about the potential. I just used periodicity. So before we move on to talking about a specific potential, you all have questions about the general structure of periodic systems like this. Yeah.

AUDIENCE: What's the difference between the ψ and the [INAUDIBLE]?

PROFESSOR: Oh, excellent. I shouldn't have used ψ , I should have used ϕ . Thanks. I'll use ψ only when we talk about general super positions and wave packets. Other questions? All right.

So with all that, let's talk about a specific potential. So far we've extracted about as much as of the physics out of the system that we can just from periodicity. In order to make more progress, in order to talk about, for example, what are the allowed energy eigenvalues and for that matter, how does that allowed energy eigenvalue depend on q , the crystal momentum, in order to answer that, we have to talk about a specific system.

So let's go ahead and talk about a specific system. I'm going to pick my favorite. Now the problem set, you're going to do something really cool about it, which I'll explain in a moment. So you'll do a general case in the problem set, but for the moment, let's work with a simple example. And the simplest example is going to be a periodic potential with the simplest possible barriers in the potential. What's the

simplest barrier? Delta function. Yes. So the potential is going to be for this example V of x is equal to sum from n is equal to minus infinity of $\hbar^2 g$ naught delta of x minus nL .

So what is this? So this is just some overall constant out front. Normally we call this V naught, but I've made g naught dimensionless by pulling out an \hbar^2 over $2nL$. L is the spacing between delta barriers. So the potential looks like this. Here is 0.

We have a delta function barrier. We have a delta function barrier L . We have a delta function barrier at $2L$, dot, dot, dot, minus L , dot, dot, dot. So there's our potential.

And I want to know what are the energy eigenfunctions for a single particle in this potential. And again, g naught is the dimensionless strength of the potential. So how do we solve this problem? Well, we've done this so many times. What we see is that in between each barrier, the particle is just free, so we know the form of the wave function between each barrier, it's just e^{ikx} plus e^{-ikx} , where k is defined from the energy $\hbar^2 k^2$ upon $2m$ is e .

At the barrier, we have to satisfy appropriate matching conditions. So I could put a and b here and c and d and e and f . And under each one of these imposed boundary conditions, and this is going to be an infinite number of coefficients with an infinite number of boundary conditions. And that sounds like it's going to take some time. But we can use something really nice. We already know that the wave function is periodic.

So suppose between 0 and L , let's say less than x , less than L the wave function ψ takes the form, and we know that ψ of eq takes the form e^{ikx} , and now some periodic function, which would write as $a e^{ikx}$ -- actually, I'm not going to write that. So in between 0 and L , it's a free particle, and it's equal to $A e^{ikx}$ plus $B e^{-ikx}$, where k is defined purely from the energy $\hbar^2 k^2$ upon $2m$ is the energy. So this is what we mean by k .

And in between $2L$ it will take the similar form, but what we can do is, we can define, so this is sine of x , between L less than x less than $2L$ ψ is equal to-- well, I could define it with new constants, but I know what it has to be because whatever the value is here it's the same as the value here up to a shift by L the translation to phase e to the $i qL$. So this is equal between L and $2L$, it's equal to e to the $i qL$ and periodicity condition, the same thing, A plus B , with the same coefficients. Everyone cool with that?

So I can now translate, so let's think about what the boundary conditions are going to have to be. At each of the delta functions, the delta function boundary condition is going to say that the slope here minus the slope here is something proportional to the amplitude here. And the slope here is going to be minus something proportional to the amplitude. But the slope here is the same as the slope here up to an overall phase from the translation. And the slope here is the same as the slope here up to a phase coming from the translation.

So we can now turn this into instead of this, the condition between the slopes here and here, I can turn that into a condition between the slopes here and here. Wow. This is horrible. Here are my two delta functions. The slope here and here, the boundary condition I put at 0 , I can translate this into the slope here up to an overall phase e to the $i qL$.

So I can turn the boundary condition here into a boundary condition between these two guys inside one domain. And so I can turn this into a problem that just involved A and B and that's it. Everyone see that? So let's do it. So questions on the basic strategy at that point?

So let's do it. So what we need is we got the general form of the wave function, and I'm going to erase this because we don't need it. Got the general form of the wave function, and then we need to impose the boundary conditions of the delta function. And in particular, let's just impose them at 0 because imposing them at 0 is going to be equivalent to imposing them everywhere else by periodicity if I use the periodicity of the wave function.

So the boundary conditions at the delta functions. So the first is that $\psi(0^+) = \psi(0^-)$, so this is a statement that the wave function is continuous. But $\psi(0^-)$ is equal to-- well, that's this point. But this point is the same as this point except the wave function picks up a phase $e^{i q L}$. This is equal to $\psi(L^-)$, right here, times $e^{i q L}$.

And we have to be careful because the statement is at the wave function here, is the wave function here times $e^{i q L}$. So the wave function here times the wave function here times $e^{i q L}$ minus. And this leads to $\psi(0^+) = \psi(0^-) e^{i q L}$. And this leads to $\psi(0^+) = \psi(0^-) e^{i q L}$. So the value right here-- is $A + B$ because it's just this wave function evaluated at $x = 0$, and this guy at L is going to be this evaluated at $x = L$ times $e^{-i q L}$. So this is equal to $A e^{i k L} + B e^{-i k L}$. So there's my first condition.

Second boundary condition is the derivative condition, and the derivative condition is that $\psi'(0^+) - \psi'(0^-) = g \psi(0)$. And this gives me that $i k A - B = g(A + B)$. So that's this guy, and now the derivative of the second guy picked up our extra phase minus $i k A e^{i k L} - B e^{-i k L} = g(A + B)$ -- this is all in the notes so I'm not going to worry too much about it-- is equal to, on the right-hand side is $g(A + B)$.

So now note the following properties of these equations. These equations determine an equation, so from the first, I'll call this 1, and I'll call this 2. So 1 implies that $A = B \times \text{something}$. It's just a linear equation. So if we pull the side over, put this over here, $A = B \times \text{something}$. Everybody agree with that? Some horrible expression of k and q times.

And 2 also gives an expression form $A = B \times \text{horrible expression}$ in terms of k and q but a different one. Call this expression 1, I'll call this expression 2. So as usual, so this is two different expressions for A given B and this only makes sense it's only a solution if these two horrible expressions are equal to each other.

And so this is what we've done many times before, and if you've set these two

expressions equal to each other and do a little bit of trigonometry, you get the following relation. Cosine of qL is equal to cosine of kL plus g naught upon $2kL$ sine kL . Where what k means is nothing other than the square root of $2ne$ upon \hbar . k is defined from that relation, and what q means is q is the eigenfunction or e to the i qL anyway, is the eigenfunction of the wave function under translation by L .

So k is really playing the role of the energy. Everyone cool with that? I just skipped the algebra, but if you do the horrible algebra from setting these two expressions equal to each other, then you get this. Yeah.

AUDIENCE: Is q some like undetermined thing as of right now, or do we know--

PROFESSOR: Excellent. What values of q are allowed by this expression? Is exactly the right question to ask here. What values of q 's are allowed for our wave function? Is there any condition on what the value q is so far? No. It could have been absolutely any number. For any number q , we can find a eigenfunction to translate by L , e to the i qL as the eigenvalue, any value of q . However, q is equivalent to q plus 2π upon L . If you skipped by 2π over L , then it's not really a different eigenvalue. It's the same eigenvalue.

So q is defined. It's any continuous number between let's say minus π over L and π over L for simplicity, make it nice and small. i could have said 0 and 2π . It doesn't make any difference, minus π and π over L . So q is a free parameter. So there exists a state. Another way to say this is that there exist states and in particular eigenstates for any value of q , for any q , and any e , so for any value of q and e which satisfy this equation corresponds to a state. There exists states for any q E satisfying this equation. Cool?

This is just like the finite well. In the case of the finite well, we go through exactly the same analysis the only difference is that we don't have the qL . What happens in the finite well case we impose a boundary condition off in infinity. So the thing has normalized, and we put another boundary condition in infinity, and what we ended up getting is something of the form roughly 1 is equal to something like this. It's actually not exactly that, but here we have kL , and if you combine these two

together, you get something kL plus a phase shift over kL and then a 1. If you multiply, you get kL is equal to cosine of kL plus a phase shift, which is exactly the form for the delta potential.

Good. So this is similar. However, here we have an extra parameter q , which is free to vary. q could be anything between minus π/L and π/L . So what does cosine of qL turn into? Well, it's anything qL can take q is $2\pi/L$ or π/L to minus π/L . So qL can go between π and minus π , so cosine of qL varies between cosine of π , which is 1 and cosine of minus π , which is minus 1.

So any value of cosine of qL between 1 minus 1 is a valid value of qL . On the other hand, if this is equal to 7, is there a q such that this is equal to 7? No. So what we need to do now is, we need to solve this equation, but it's obviously a god awful transcendental equation. So how do we solve horrible transcendental equations?

AUDIENCE: Graphically.

PROFESSOR: Graphically. So let's solve it graphically.

So to solve it graphically, that lets plot the left-hand side and the right-hand side as a function of qL . So in this direction, I'm going to plot cosine of qL . That's the left side. And cosine of qL we know is going to vary between plus 1 and minus 1. Because q between q is equal to π/L , and q is equal to minus π/L .

And in the horizontal direction, I'm going to plot kL . And when kL is 0, remember that the definition of kL is that E , the energy eigenvalue is equal to $\hbar^2 k^2$ upon $2m$. And what we're looking for are points, are any common solution to this equation where there's a value of q and a value of E of k such that these two expressions are equal to each other. Yeah.

AUDIENCE: [INAUDIBLE].

PROFESSOR: Sorry?

AUDIENCE: [INAUDIBLE].

PROFESSOR: Oh, sorry. Thank you. This is qL is equal to 0 and qL is equal to π . Thank you. Yes. Are there types of other questions? So kL equals 0 is going to be equal to 0, k equals 0, and this is going to be a function of kL . I'm going to plot it as a function of kL because that's what shows up. But remember that k is nothing but code for E .

And so what we're looking for a common solutions of that equation. Now let's first just plot. So if this is 0, let's just plot cosine of kL , the right-hand side cosine of kL plus g naught over $2kL$ sine kL . And let's do this first for the free particle.

Oh, I wish I had colored chalk. For the free particle, free is going to be g naught equals 0. There is a potential and the potential is 0 times the delta function, which is not so much delta function. So for free particle when g is equal to 0, that second term vanishes, and we have cosine of qL is equal to cosine of kL . Kale, if you fry it, it's crispy.

So what is that going to be? Well, this has an obvious solution which is that q is equal to k , but the problem is, q is only defined up to 2π over L , so mod 2π over L . Well, let's see what this looks like in here. So for the free particle what does this tell us? So for the free particle, let me just write this as therefore, q is equal to L or q is equal to k , and therefore E is equal to $\hbar^2 q^2$.

So any q or E are allowed such that q^2 is equal E times 2 upon \hbar^2 squared. So that's just the usual condition. It's the free particle has energy $\hbar^2 k^2$ upon $2m$, and we just chose to call it k equals q . So what we're doing is instead of organizing things as momentum eigenstates of the free particle or organizing the free particle energy eigenstates in terms of transient by L eigenstates. Perfectly valid. It commutes with the energy operator.

What does this look like? Well, cosine of kL is cosine of qL , when k is equal to 0, q is equal to 0. So we get this. And the points, when the points where qL is equal to π or minus 1, these are the points where we get the qL is equal to $n\pi$ or equivalently plus or minus kL is equal to $n\pi$ plus or minus $n\pi$.

So this is n is 1, n is 2, n is 3. Everyone cool with that? And these guys are 2π

times n or $2n$ plus 1 $2n$ π . And I really want this to be odd, so n odd. And this is n π kL so n π for n even. Everyone cool with that? So that's what it would look like for a free particle.

What happens if we don't have a free particle? What happens if we have the interacting potential? So now let's have g naught equal to 1 or 0 . And again, here is plus 1 . Here is minus 1 . And we're plotting as a function of kL . And now it changes, so let g naught be a small, positive number. If g naught is a small, positive number, then near k goes to 0 . Sine goes like it's argument, and so that means kL over kL we get cosine of 0 , which is 1 , plus g naught over 2 .

So at 0 , the value of the right-hand side is greater than 1 . Is there an energy eigenvalue with energy equal to 0 ? No. We have to wait until cosine gets sufficiently small and sine is increasing, so what does this curve do? It looks like this. It's again periodic with the appropriate period, but the amplitude of the deviation from the free particle is falling off as we go to higher and higher values.

So we've taken this point and pushed it out. So what does this tell us? Well, remember that there is an energy eigenfunction with a given q and remember this is cosine of qL , there is an energy eigenvalue. There exists an energy eigenstate with an e and TL eigenstate for any E and q such that there exists a solution.

And so what does that mean? Well, is there an energy eigenvalue with this value of E or this value of k ? No. Right? Because here's the right-hand side and the left-hand side is any value in here. There's a q for which any left-hand side is any value between 1 and minus 1 . So there's no value of q you can pick so the left-hand side is equal to the right-hand side for the value of k .

And similarly here, here, here, here, here, specifically for this value of k or this value of the energy, E minimum, there's one value of q . This one. q is equal to 0 where there is an energy eigenstate. So there's a minimum energy in the system. What about for this value of energy? Yeah. There's exactly one solution there, and actually if you're careful, it's 2 because it's the cosine of qL . q could have been positive or negative.

So we have a solution here with this value of energy and with this value of cosine qL . Any q that gives us this value of cosine qL is going to work, and that's one of two values. And similarly for each of these guys, there's a state for every value of energy in this region until we get here, and when we get here, this is E maximum. If we go to any higher energy, any higher k , then there's no solution for any value of q and any value of E .

So what we get are these bands, continuous bands for any energy separated by gaps and then again continuous bands for any energy and bands for any energy. So all of these shaded in regions, any energy in this region corresponds to a state and similarly here.

So here's the upshot of all this. We're going to study the details of this in detail next time. When we have a periodic potential, every energy eigenfunction is extended through the entire material. Every energy eigenfunction is extended across the entire lattice. None of them are localized. And that's like a free particle.

However, not every energy is an allowed energy. Only some energies are allowed. Some energies do not correspond to allowed energy eigenfunctions eigenvalues, and some energies do. And they come in continuous bands of allowed energies and continuous gaps of disallowed energies. And it's going to turn out to be exactly this structure of bands and gaps, or band gaps, that is going to give us the structure of conductivity in metals and explain to us why we don't have conductivity in plastic. We'll pick up on that next time.