ELEMENTS OF MODERN PHYSICS

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Lec 7: Solution of Schroedinger Equation for 1D potentials

Good morning, all of you. Let me just go back and complete something that were unfinished on the last occasion. So we will talk about different representations in quantum mechanics. They are called a Schrodinger representation, Heisenberg representation and interaction representation. And then we'll talk about solution of Schrodinger equation in simple 1D potential. They would involve particle in a box, step barrier or a barrier or rather a well, potential well, so to say, and then a bound state problem. So these are the plans for today. And let me start with this Schrodinger representation. And what we mean by that is that the one is that the wave function is time dependent. And the operators are time independent. So all the operators are time independent and we obtain the time dependence of the wave functions by solving this equation, which is the Schrodinger equation, which is what we have seen. And, of course, they also, the wave functions also depend on the position coordinate. Right now, we are just talking about the time dependence. And this gives you the solution that psi of t is equal to exponential minus i E t over h cross psi of 0.

And so this is that factor that we have talked about or there's a time evolution operator. Now, if you write it as an operator, then you have to write it as exponential minus IHT over H cross. But since we are, you know, talking about so E is the eigenvalue of H. So that's how this E appears. And these are called stationary states because the mod psi square is independent of time. And in the other representation, that is the Heisenberg representation, we have just the reverse. We have the wave functions that they do not depend upon time. and the operators are time dependent, okay. And the time dependence of the operators, they are written in this particular fashion.

It is i H t over h cross O at 0. O is any operator, any arbitrary operator. It's exponential minus i H t by h cross and so on. Now, this H is, of course, at this moment is really the H0. So, you can write it as H0 as well, which means that there is a non-interacting Hamiltonian. There is no interaction involved here, which we are going to take into account just now, in the next slide, where we talk about the interaction representation. So, these operators they obey an equation of motion which is given by d O d t, that is the commutation of O and H, this is a function of t of course. So, the time evolution of the operator or the equation of motion for the operator is the commutation of O with H. So, this is called a EOM or the equation of motion. Now, in case an operator is not, it does not depend upon time or say for example, some operator that commutes with Hamiltonian for all t. And then, of course, O is the constant of motion. So, let us talk about the interaction representation, which is more involved.

Schrödinger representations.

1) wave function is time dependent.
2) operators are time independent.

$$e^{-iHt/\hbar}$$

$$i\hbar \frac{d\psi(t)}{dt} = H\psi(t). \Rightarrow \psi(t) = e^{-iEt/\hbar}\psi(0).$$

Heisenberg representations

1) wave function time independent.
2) operators are time dependent.

$$O(t) = e^{iHt/\hbar} O(0) e^{-iHt/\hbar} = e^{iH_0t/\hbar} O(0) e^{-iH_0t/\hbar}$$

$$i\hbar \frac{dO(t)}{dt} = [O(t), H] \rightarrow \text{EOM}$$

And this is really for the interacting system. And in this case, both the wave function is time dependent and operators are time dependent as well. OK, so both are time dependent and the time dependency are given as, you know, the psi of t is equal to exponential I H naught t by h cross, exponential minus i H t by h cross psi of 0. And of course, it is true that the h 0 and h, they do not commute, which means that this h is actually comprising of a non-interacting part, which is what we have taken in the earlier case. Say this case, we can write it as H0, okay? And these E corresponds to the E0, those are non-interacting energies. And then we have done this, the same thing for, you know, for this Heisenberg representation. But in this particular case, where both psi and O are time dependent, the wave function is the transforms as or rather it is, it can be written as exponential i H naught t by h cross exponential minus i H t by h cross and operating or on psi 0 multiplied by psi 0.

Remember, you can't combine these two exponentials because when you try to combine the exponentials, it automatically means that the two operators that are in the exponent, they commute. And in this case, they do not commute. So, you have to leave it like this. And because if it does, if you know H0 and H, they commute, then of course, there is no problem. I mean, then interacting systems will have no special, you know, status or rather they do not have to be dealt with anything different than the non-interacting systems, but we know that it happens. Just to give you a clue, exponential A into exponential B is not equal to exponential A plus B and is equal to exponential A plus B when A and B commute. So, that is what it is. So, what we can do is that we can look for the time or rather this expectation values of operators and let us take an expectation values of an operator O.

And in the Schrodinger representation, so let me write it as SCH representation. And this is equal to say we are because we are trying to calculate this expectation value. So this is O at 0 and psi 2 at t. Now, if you look at the transformation of these wave functions, they are exponential. So, let me write it as exponential minus i H naught t by h cross psi of 0. That gives a form that it is been operated upon by an operator. So, this is equal to psi 1 0 exponential i H naught t by h cross O of 0 exponential minus i H naught t by h cross and then you have a psi 2 of 0 and this is nothing but O of t. And you would write the expectation value of an operator O of t between the eigenstates or between the wave functions as this, which is the same as the Heisenberg representation. Okay, so the expectation values which are really related to the observables, they have to, you know, preserve their form. And let us show that as well for the interaction representation. And so we now have a psi 1 t, O of t, psi 2 t.

Interaction representation

1) ψ is time dependent.
2) O is " "

$$\psi(t) = \underbrace{e^{iH_0 t/\hbar}\, e^{-iHt/\hbar}}\, \psi(0).$$

$H = H_0$

$[H_0, H] \neq 0$

$e^{A} e^{B} \neq e^{A+B}$

$= e^{A+B}$ when $[A,B]=0$

Expectation values.

Sch rep. $\langle \psi_1(t) | O(0) | \psi_2(t) \rangle$

Heisenberg rep. $\langle \psi_1(0) | \underbrace{e^{iH_0 t/\hbar}\, O(0)\, e^{-iH_0 t/\hbar}}_{O(t)} | \psi_2(0) \rangle$

So, remember that O(t) is an arbitrary operator which could be anything, say for example, Hamiltonian, angular momentum, linear momentum, etc. So, we have a psi 1 0. Then we have an exponential of i H t by h cross. Remember, when you take the conjugate or this bra, then you need to change the ordering of the operators. And so that is what we did here. And exponential minus i H naught t by h cross. You can drop the h cross because it has to be, you know, carried around, you can put h cross equal to 1. And then, so this is, this part is nothing but the psi of psi 1 of t, okay? And then we'll write down this exponential i H naught t by h cross, then O of, okay, let's, this means O of 0, then exponential minus i H naught t by h cross. So, then now this is nothing but O of t. So, and now we are going to write exponential H0 t by h cross exponential minus i H t by h cross and finally, we have a psi 1 at 0. So, this not psi 1, sorry, psi 2. So, this is psi 2 of t. So, that is the expectation value in the interaction representation. So, these two, let me use a color here, These two are going to give me one and these two will together will give me one. And that will tell you that this has a form which is psi one of zero.

And then you have an exponential i H t over h cross. and O and then exponential minus IHT over h cross and then you have a psi 2 of 0. So, this is the, so it preserves the form of the expectation value and if you, you know, you can now sort of write down the equation for or rather the equation of motion or the Schrodinger equation. In this particular case, with this definition or rather in the interaction representation, which is exponential i H t H naught t by h cross exponential minus i H t by h cross. So remember that not only you can combine the exponentials, you can't change the order as well. Because this exponential is nothing but a series of, you know, power series of this H naught and H, that is full H, where H equal to H naught plus H prime. Sorry, I forgot to write this. So, H equal to H naught plus H prime. And that is what you should, you know, sort of, you cannot change the order of this. So, you have a d dt of psi of t and it is e exponential i H naught t by h cross with the H naught minus H. There are two terms because you have two terms, two exponential terms and you have a minus i H t by h cross and psi of 0.

So, what you can do is that this H 0 minus H is nothing but because H is equal to H 0 plus H prime. So H0 minus H is minus H prime and that's equal to minus exponential i H naught t by h cross H prime exponential minus i H naught t by h cross psi of 0. And what you can do is that you can introduce this the outer product or this identity operator here. which is minus i exponential i H naught t by h cross H prime exponential minus i H naught t by h cross. Now, I'm going to use this exponential i minus i H naught t by h cross. exponential i H naught t by h cross and then exponential minus i H t. Sorry, I wrote it twice. This is not required. So minus and then there is a plus and then there is a minus I H naught t by h cross and so on. And then, of course, the psi of zero. So what I did is that I have not here rather I have introduced the identity here, which is through this. OK, so this is equal to one. So I've just introduced a one there. And so this tells you that the equation of motion for the wave function in the interaction representation is minus i H prime t psi of t. So, it is interesting to note that the time evolution of the operator is not given by either H naught, which is the non-interacting Hamiltonian.

$$\langle \psi_1(t) | O(t) | \psi_2(t) \rangle = \langle \psi_1(0) | \underbrace{e^{iHt/\hbar} e^{-iH_0t/\hbar}}_{\psi_1(t)} \underbrace{\left(e^{iH_0t/\hbar} \, O \, e^{-iH_0t/\hbar} \right)}_{O(t)} \underbrace{e^{iH_0t/\hbar} e^{-iHt/\hbar} | \psi_2(0) \rangle}_{\psi_2(t)}$$

$$= \langle \psi_1(0) | \, e^{iHt/\hbar} \, O \, e^{-iHt/\hbar} | \psi_2(0) \rangle .$$

Sch. Eqn.

$$\frac{d}{dt} \psi(t) = i e^{iH_0t/\hbar} (H_0 - H) e^{-iHt/\hbar} \psi(0). \qquad H = H_0 + H'$$

$$= -i e^{iH_0t/\hbar} H' e^{-iHt/\hbar} \psi(0).$$

$$= -i e^{iH_0t/\hbar} H' \underbrace{e^{-iH_0t/\hbar} e^{+iH_0t/\hbar}}_{\mathbb{1}} e^{-iHt/\hbar} \psi(0)$$

$$\boxed{\frac{d}{dt} \psi(t) = -i H'(t) \psi(t)}$$

or H, which is a full Hamiltonian. In fact, it is given by this interaction term, and that justifies the name interaction representation. Okay, so what we have learned is that there are different representations, and these representations are important. They sort of tell you that if you really resort to the calculation of the expectation values, then the expectation values will be independent of the representation because they would simply be related to the experimental observables. All right, let us go on to the general solution of the Schrödinger equation. So, this is the Schrödinger equation that you see: minus h square by 2m. Now, why is it written as u? It is for a reason that we have this psi of x t, and which can be written as, say, u of x and some f of t. So, right now, we are dealing with the time-independent Schrödinger equation, and that is why the space part is written as u. But nevertheless, if you see in some texts that they have written it as psi of x, it really does not matter. I mean, they mean the same thing. It is u is a function of x, and it has either the form of a wave or a decaying solution, which is what we are going to see, okay.

So, this is the form for this wave function and rather the Schrödinger equation, where V0 is the potential energy, which is a constant potential energy. That is, the potential energy is not dependent on the distance, and it has a certain value. The wave function is going to be continuous across that potential discontinuity. And it's always going to be continuous, even if the discontinuity is infinite. That is, even if you have a delta function discontinuity, you still have the wave function to be continuous. But what is not going to be continuous is the derivative of the wave function for an infinite discontinuity. So, if you have a delta function, then the du dx is not going to be continuous, but nevertheless, it is going to be discontinuous by a known amount. So, which is fine, which is something that we are going to see later. And so, this is the equation for a constant potential V0, and E is the total energy. You can write this system or rather this equation as a second-order linear differential equation where the double derivative with respect to space is equal to some minus of some constant, which we call as k square.

General Solution of Schrodinger Equation

$\psi(x,t) = u(x) f(t)$, $u(x) \to \psi(x)$

$$\frac{-\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V_0 u(x) = Eu(x) \quad \Rightarrow \quad \frac{d^2u(x)}{dx^2} = -\underbrace{\frac{2m(E-V_0)}{\hbar^2}}_{k^2} u(x)$$

For $E > V_0$, $u(x) = Ae^{+ikx} + Be^{-ikx}$ $\quad k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ (Wavevector) $\quad k$ is positive and real

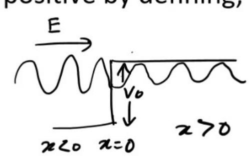
An alternative solution can be written as,

$$u(x) = A\sin(kx) + B\cos(kx)$$

$\frac{d^2y}{dx^2} = -\omega^2 x$

For $E < V_0$, k becomes imaginary, however we still use it as real and positive by defining,

$$\kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \quad \Rightarrow \quad u(x) = Ae^{+\kappa x} + Be^{-\kappa x}$$



Note that these are not waves, but exponential functions.

We do not call it a k; we call it a k square because the equation, the simple harmonic equation, has this form that d square y dx square is equal to some minus omega square x, so that this omega is the angular frequency, and one can find out, you know, time period, etc., from this or the frequency of oscillations and so on. So, it is usually written as k square, where k is 2m E minus V0 divided by h cross square, square root of that, and for E greater than V0, that is when you have the energy of the particle to be larger than the barrier height. Suppose that there is a discontinuity like this, and so this is of magnitude V0, and the energy of the particle is larger than V0. Then the wave that is going to be propagating is written as A exponential ikx and B exponential minus ikx, with k equal to 2m E minus V0 by h cross square root. k is positive and real, and it's going to be a traveling wave here with k equal to root over 2 m E by h cross square, and it's going to be again a traveling wave here. Well, let me draw it inside, but it will be a traveling wave with a different k, where the k is reduced by 2m. I mean, this E will be reduced by E minus V0 inside that. So it will start, you know, propagating inside. I mean, I didn't mean to say that it's inside, but it's the wave; the particle will propagate as a wave even in the region. So let's say the discontinuity is at x equal to 0. So x less than 0, it's a wave with a wave vector.

This is called a wave vector, wave vector k, and it is going to propagate in the x greater than 0 region. So, this x less than 0 and this x greater than 0 with another k, which is this E reduced by E minus V0. Now, an alternative solution can also be written as A sin kx plus B cos kx. This is important to note that whenever you have a finite region of space to consider, which means if there is a discontinuity of this kind, where this is really a finite region between some minus a to plus a or from 0 to a or 0 to l, then we don't use the exponential solutions because the exponentials will oscillate even at infinity. Now, there's no infinity inside the box. You can, of course, use solutions which are exponential, which are on the left of the step. I mean, this kind of barrier and on the right of the barrier. But again, inside, one should use a sine or cosine, or if E is less than 0, then one uses a hyperbolic sine and a hyperbolic cosine. So, these are equivalent solutions to the exponential, the oscillatory solutions. These are called oscillatory solutions. And these are also oscillatory, but oscillatory in some confined region of space, because here the argument of sine or cos cannot be equal to infinity and so on.

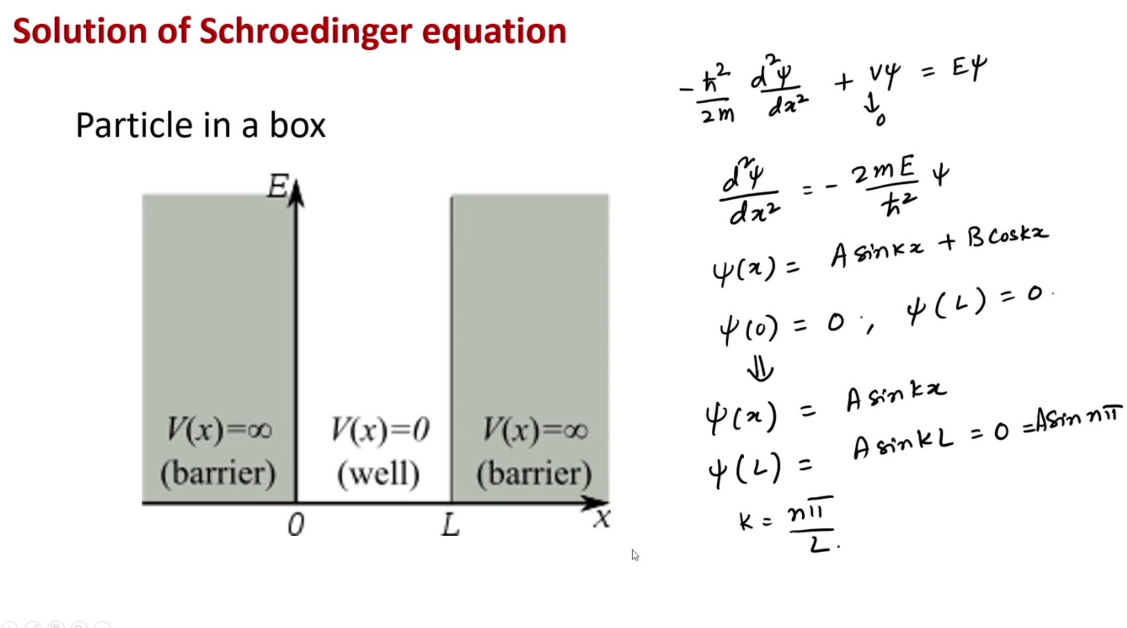
Now, when E becomes less than V0, let me complete one thing before I go on to E less than V0. Even at E greater than V0, you see that the particle will recognize that there is a barrier below its path of propagation, even if its energy is larger than V0. So, for a classical particle, it will not even recognize that there is a small barrier below its energy. But in this quantum mechanical sense, the wave vector recognizes that there is an E and an E minus V0 in the two regions you see here, okay. Coming to E less than V0, K becomes imaginary, okay. And what we can do is still use this notation where this is called a kappa equation. And this kappa is equal to the square root of 2m V0 minus E. So if you look at it, kappa is like i k and so on. So we'll still use kappa to be real and positive. But the solutions are no longer waves. They are exponentially growing or decaying solutions. And in some region of space, maybe one of them is prohibited due to the symmetry of the problem or the boundaries set by the problem.

But nevertheless, these are important solutions of the equations because they are needed to impose the boundary conditions, and the boundary conditions are important. Psi will be continuous or u is continuous u or Psi they mean the same thing and d psi dx is continuous and as I said that this is only true for finite discontinuity that is V0 having a finite value if it is an infinite value then of course the second condition is not satisfied. That is, d psi dx is not continuous but is discontinuous by a known amount. So we do not really use much information. We will show that in a while, if not today, then next class, okay. So, the simplest problem you do is the particle in a box, okay. This problem is quite well studied, and one talks about nanostructures and quantum structures, quantum confinement, and one really talks about this kind of picture where there is a potential well between 0 and L, where L is some length. And the potential is 0 inside the well. The potential has an infinite barrier height, so the particle cannot escape. The particle cannot escape is imposed by V equal to infinity. And this V equal to infinity, if you look at the second term in the Schrödinger equation, that is this term.

So, if your V is infinity, then the u has to be equal to 0, which means the wave function has to be 0, which means the particle is not allowed to escape from this region, which is there in between the particles. in between the two barriers, the two boundaries of this barrier that exists at x equal to 0 and x equal to L and this is that x, you know, there. So, we can write either, as I said, we can write either u or psi. Let us just write psi because we have written u and we are going to continue writing u later on. So, now, we are going to solve this equation. d square psi dx square now plus V psi this is equal to E psi. Now this term is equal to 0 because V equal to 0 inside the well. Outside there is no question of solving the system because the particle is not there. By solving the equation there is no particle there.

So, you can write down this second order differential equation equal to minus 2 m E by h cross square psi and the solution is psi is equal to A sine kx plus B cosine kx following the advice or the suggestion that has been given earlier, that because it is a finite region in space, one can use the sine and cosine solutions, even though mathematically both are valid solutions, that is a superposition of I mean, sine is a solution, cosine is a solution. And because it is a second order linear differential equation, we can linearly superpose these two solutions to bring out a new solution, which is a sine kx plus b cos kx. And that is the general solution for the problem. But now you see there is a problem that the psi has to be 0 at x equal to 0 and psi also has to be equal to 0 at L. So, at x equal to L, the psi has to be 0. At x equal to 0, the psi has to be 0. Now, the first condition sort of prohibits the cosine solution to exist because the cosine solution will not be equal to 0 at x equal to 0.

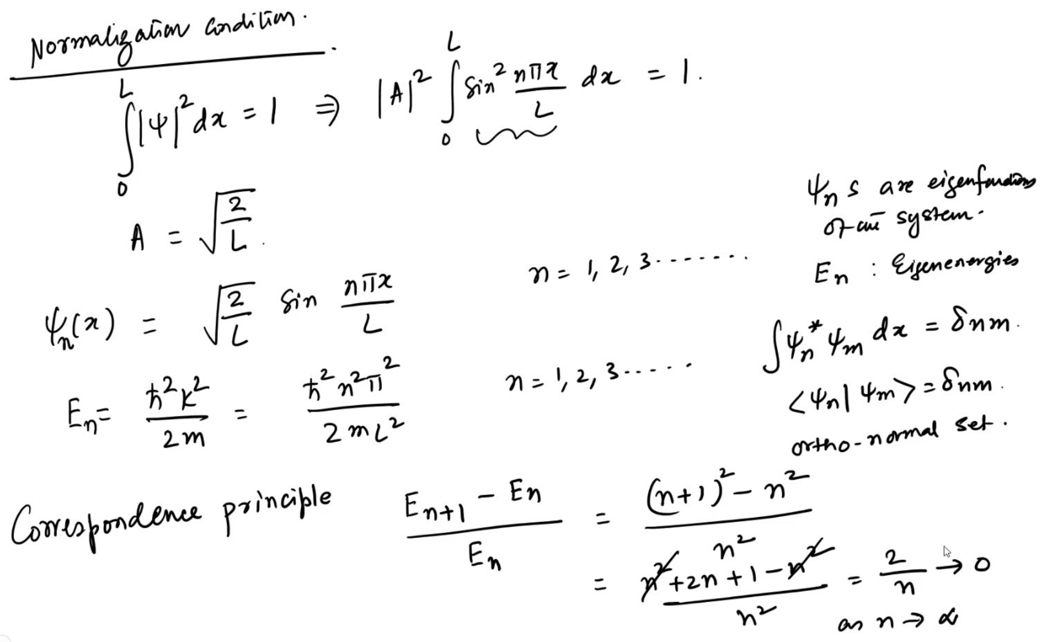
In fact, it becomes just a constant B, which is what we do not want. So, we only keep the sine solution because the sine goes to 0 at x equal to 0. And so, my first condition, we really do not need the d psi d x condition because we have these, you know, infinite discontinuities there. But these two boundary conditions here, they are good enough for us to have a complete solution for the problem. Okay, so this is the solution for this and I will use now the second condition which is psi of L which I will write A sine KL and that is equal to 0 means that is equal to sine n pi. Okay, for any value of n, n equal to 1, 2, 3, do not take 0 because 0 would mean that the particle is not there. Then of course, there is no point in talking about the solution. So, this say A and so K becomes equal to n pi over L. And what else can be found out?



We still do not know what is A and that can be found out from the normalization condition and the normalization condition is is in principle minus infinity to plus infinity psi mod square dx is equal to 1 but however these two limits do not make sense because everywhere the wave function is equal to 0 and if it is non-zero it is only in this region 0 to L so we will write it as 0 to L psi square dx and if you use this as a square which is in general, a complex constant, not in this case, but in general, a complex constant is equal to a sine squared n pi x by L dx from 0 to L, which is equal to 1. I leave this integral to be done by you. You can just multiply and divide by a factor of 2 and then use it as a cosine 2 n pi x by L and then perform this integral. This integral is going to give a equal to the square root of 2 by L. And then, of course, what you get is that the wave function, then the full solution of the wave function is root over 2 by L sine of n pi x by L with n equal to 1, 2, 3 and so on, all these numbers, integers. And what is E in this case? What do the particles, what energies do the particle have? The energies are given by h cross squared k squared over 2m. That's the only the kinetic energy. There's no potential energy there. So this is equal to h cross squared k n square pi square by 2 ml square, again, n equal to 1, 2, 3, and so on. Now, you see that the energy levels are not equidistant. They, in fact, grow as n grows as a square of that. So, another thing you need to notice here is that 1 over L squared sits in the denominator.

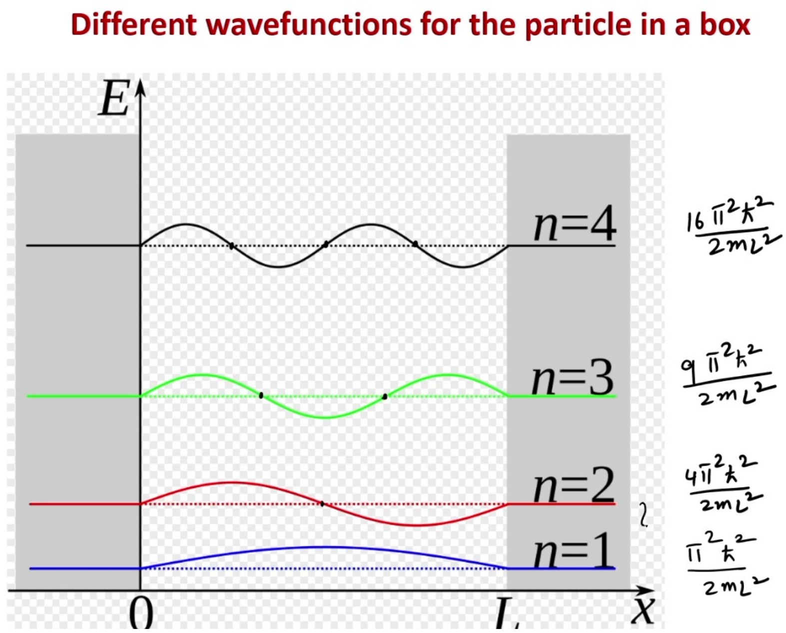
And because of this term, if you decrease L, the spacing between the energy levels will go up, and that is an important concept we use in quantum confinement. So, if you confine a particle more and more, the energy levels that will become more and more discernible, they are identifiable and because they are, you know, the distance between the successive energy levels become that increase, okay. All right. You can also see the correspondence principle from here. So, what's the correspondence principle? We'll use this. Let's call this E n and call this psi n. So, psi n's are called the eigenfunctions of the system. And E n are called the energy eigenvalues, eigenenergies, or energy eigenvalues —anything you can call them by. And each of these psi n's forms a complete set of states because of these psi n star psi m dx that is equal to delta. n m, okay, which means that this can really be written in your bra-ket notation as this delta n m. So, if n is not equal to m, this overlap or the inner product is 0. If n is equal to m, then it is equal to 1, which is what we have used for our normalization, okay.

So, that is why they are called as orthonormal They are both orthogonal and normalized. So, that is called as an orthonormal set. And now, you notice that n can be any of the integers that is n equal to 1, 2, 3, 4, 5, anything is allowed. I mean, very large numbers and so on. And so, we were talking about the cat being dead or the cat being alive, which really gives us only two states, or the coin being tossed giving you heads or tails—there are two solutions or rather two situations that can arise. But here, for each value of n with n unbounded, any of these are actually the eigenstates of the system. And that's why this entire linear vector space that we are dealing with is called a Hilbert space. So, in that connection, we want to understand what is E n plus 1 minus E n divided by E n, say for example. So, this is like n plus 1 whole squared minus n squared divided by n squared, and this is like E. n squared plus 2n plus 1 minus n squared divided by n squared, and the n squared will cancel. And if n is large, then of course we can neglect 1 in front of 2n, so this really goes as 2 over n and will go to 0. This energy spacing will go to 0 as n tends to infinity.



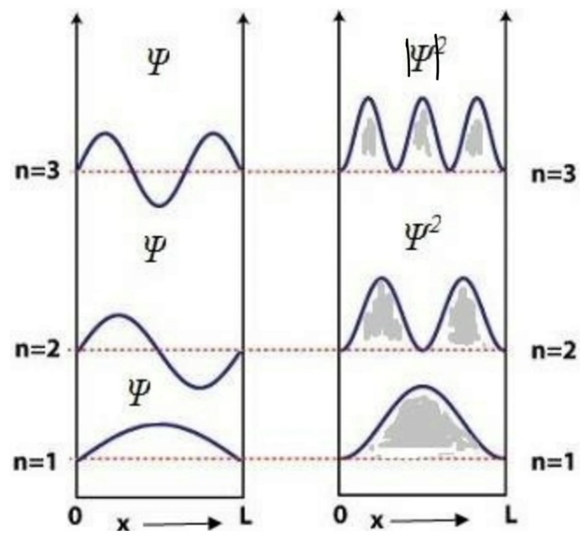
And that is the correspondence principle, Bohr's correspondence principle, that we have learned earlier. Let me add a little trick to this problem. Before that, let me show you these different energy eigenmodes or eigenvalues, rather eigenfunctions. So, n equal to 1, which is called the ground state. That is the lowest energy state which has got an energy which is equal to pi square h cross square by 2 m L square. So, this has only nodes at the two edges at 0 and at x equal to L. Then the red one which has got energy which is 4 pi square h cross square by 2 m L square because n equal to 2, so it goes as n square, n square is 4 and then it has a 9 pi square h cross square by 2 m L square. Now, you see the red one, which is n equal to 2, has two nodes at the two edges. Nodes mean the wave function goes to 0. The wave function must go to 0 at the edges because the particle cannot escape, and the wave function should be continuous everywhere. There is also a node at L equal to 2, okay? So, that is at the midpoint and then you have for n equal to 3, there are apart from the two nodes at the edges, there are two more nodes at these points and these points and so on. So, maybe L by 4 and 3L by 4, n equal to 4 has more nodes here, here. So as you go to larger and larger n, the wave function starts oscillating rapidly, okay.

I’ve just plotted four of them, but you can plot more. One more thing we’ve said is that the energy levels are not equispaced. This is small, then this is larger, and it will be progressively larger because it varies as the square of the quantum number, okay?



And then going on to the probability density of these things for each of these states, we are showing three of them. You see that the probability density, which is psi square, is for the lowest state, it is the probability density peaks at the middle of the well. So the particle is most likely to be found at the middle of the well. And as you go to n equal to 2, it is equally likely to be in the left half, the middle of the left half and middle of the right half. And then as you go to n equal to 3 and so on. So you go to larger and larger and these oscillations will increase because you're taking psi square or rather this is actually psi mod square here because we are, We did not write $|\psi|^2$, but in principle, one should use $|\psi|^2$. Because it is $|\psi|^2$, it does not go negative but always takes positive values and oscillates wildly as n increases. At large n, the particle is likely to be found anywhere between 0 and L, okay? That is what it means. All right, let me do one more problem. It says the particle is likely to be found anywhere for large n, which we’ve talked about in connection with the correspondence principle.

Probability Density: Stationary States



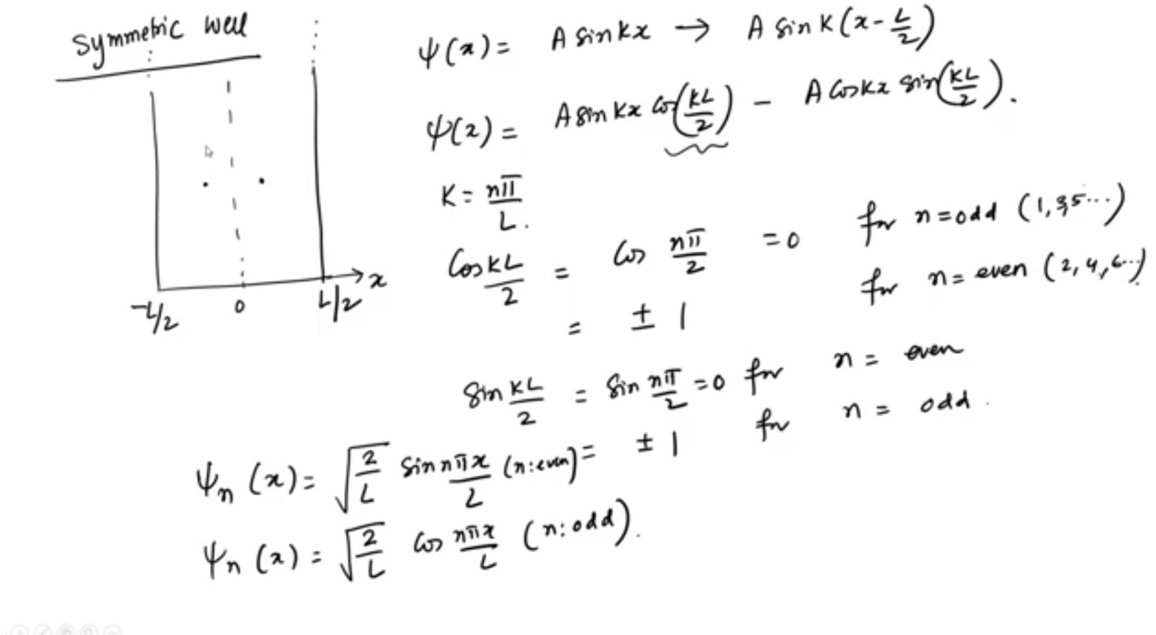
The particle is likely to be found anywhere for large n.

What happens if the well is symmetric? Which means that the well is not between 0 to L, but it is between L by 2 to minus L by 2 to plus L by 2. So, this is 0. So, this is the x axis. And the same problem remains. These are infinitely large walls. The particles cannot escape. And you just think that maybe, you know, the well is simply shifted to the left by a distance L by 2. How would the particle, you know, react to it or how would it know or what would be the change in wave function? There shouldn't be any change in wave function. But unfortunately, there is a big change in the wave function. In fact, what we can we can show is that your psi of x was nothing but a sine kx earlier. And now what you do in this particular case is that you write it as A sine kx. minus L by 2 because all the x coordinates have been shifted towards, you know, by this x minus L by 2. So, what we can do is that we can expand this sine of, you know, C minus D kind of thing and we can get it as A sine K x cos K L by 2, and minus A cos kx sin kL by 2. That's what you get when you expand the sine function. So, you have $k = n\pi/L$.

which is the same quantization that we use, we can use a k of n and then the cos of k L by 2, let me just remove this, k L by 2 to be equal to cos n pi over 2, which is equal to 0 for n odd, for example, 1, 3, 5 and all that. And similarly, for the other one, so this is for the first term. For the second term, also KL by 2, which is sine n pi by 2. Now, this is also true that this is equal to plus minus 1 for n to be equal to even. which means that 2, 4, 6 and so on. Now, similarly, for the sine, one still has KL by 2 is equal to 0 for so sine n pi by two. two for n equal to 0 for n equal to even and this is equal to plus minus 1 for n equal to odd. So that tells you that the first term would be not an applicable solution for n equal to odd because the associated coefficient is 0.

While the second term, which was earlier not the solution, which is a cos kx, is actually going to give you the solution for n equal to odd. So, the solution, so psi of n x is equal to again the same normalization in sine n pi x by L for n even and psi n x is equal to root over 2 by L cos n pi x over L for n to be equal to odd. So, you see the change in the stand of this that instead of simply a sine and cosine solution. I mean, it's simply a sine solution, which was there for the well that we have seen earlier. This is not only a sine solution, but also a cosine solution, depending on whether n is even or n is odd. So this is the for the symmetric well. We have both the solutions allowed. And so the sine solutions will be n equal to even for even values of n and the cosine solutions will be n equal to odd and put together they would define the entire vector space for the problem.

So, what is important here to note is that there is another additional symmetry that is present in the system because if you put x to minus x or rather if you draw a line at this dotted line that you see at x equal to 0, so there is a symmetry, a left-right symmetry and this is called as a parity. So, this because of this parity symmetry the wave function has a left vector or it has a left property and a right property. The entire vector space actually fragments into left and right and this is a property special property of systems with a parity or the inversion symmetry, okay, because any x corresponding to x here, there is x minus x here. So, for any x, there is a minus x and this symmetry is called as an inversion symmetry. If a system has an inversion symmetry, then the eigenvalues will be either even or odd and they would put together would define the entire space, entire Hilbert space, okay. So what we are going to say is that not only we got the solutions, but how do we make use of these solutions? Can we make something useful along with this what we have already discussed? And it turns out that yes, it is of a lot of use. Let us, you know, sort of derive or rather verify, not, is confirm the Heisenberg's uncertainty principle. How do we do that? I will not do that. I will tell you how to do it so that you can do it.



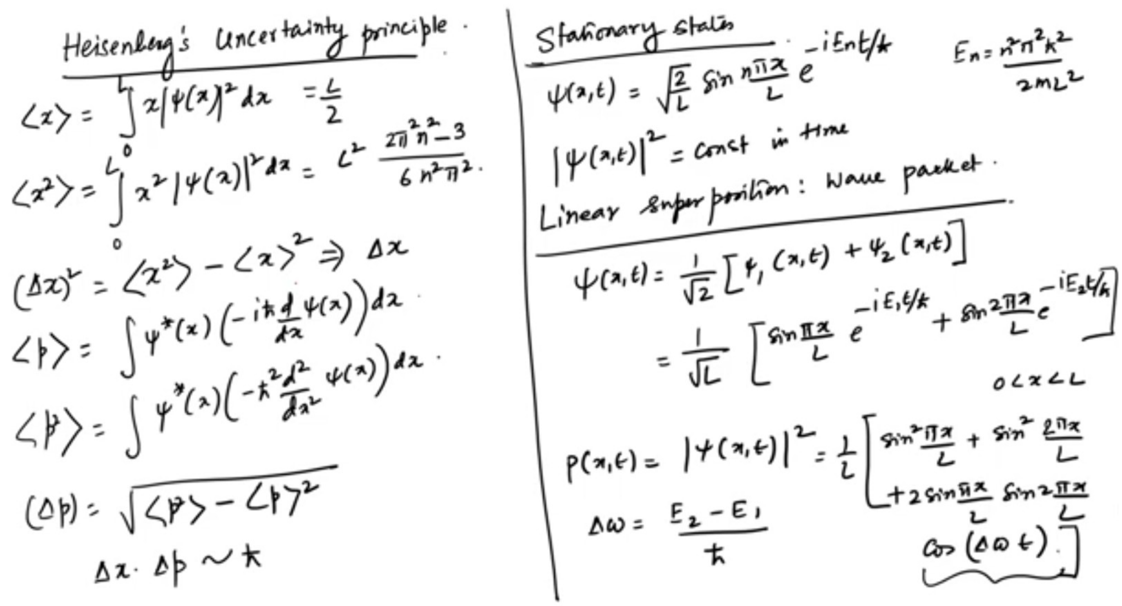
And what you can do is calculate x, and x is nothing but x, and then a psi square x dx from minus infinity to plus infinity. But here, you know that the only relevant region of space is 0 to L, and this is nothing but equal to L by 2. You can also calculate x square. So, with, you know, I go back to the old problem, which is 0 to L. The solutions are sine n pi x by L. So, 0 to L again, x square, psi of x mod square, and you can again calculate this. This is equal to some L square and 2 pi square n square minus 3 divided by 6 n square pi square, and so on and so forth. And then you can calculate delta x square, which is equal to x square average minus x average square. And you can also calculate p, but for calculating p, you need to be a little more careful. You have to use this psi star x minus i h cross d dx of psi x.

So, do not take the psi star and this, and you can also calculate P square, which is equal to psi star x and so minus h cross squared d2 dx2. And Psi of x and dx, and you can calculate a delta P square as well by taking, you know, so delta P square. You don't have to take a square root because, well, I mean, from there you calculate delta x. So, let's talk about this delta P, which is the square root of P square expectation minus P expectation square. And now you see whether delta x, delta p gives you the value that you want. It should be of the order of h cross. So, this is the uncertainty principle that you can test, okay. And let us understand what the stationary states would be. So, these, if you want to evolve these states, wave functions in time, what you would do is that psi x t is equal to root over 2 by L sin of n pi x by L exponential minus i E n t by h cross, okay, where e n is given by n square pi square h cross square. By 2 m L square. Just to remind you that even for the symmetric problem, even though we have sine solutions and cosine solutions, both are acceptable ones. Energy is still given by this n square pi square h cross square by 2 m L square.

And so, this Psi x t, that is the probability density, is constant in time. Constant in time, I am not saying that it is constant in space because we have already shown these variations within the well. So, constant in time for all time because the time goes away. Now, let us look at the linear superposition and form a wave packet, which is what we have learned as well. And wave packet, okay, so let us say we have, A wave packet comprising the linear superposition of this psi 1 x t plus a psi 2 x t. So, the particle is in a superposed state of the ground state and the first excited state. So, it's like saying that we are removing all the other possible eigenstates and we have prepared the system in such a way that it can be either in this ground state or in the first excited state, just like a head or tail problem. Now, this is, it is a 1 by root 2 and so on. So, it is, so there is a root 2 by L. So, the root 2 cancels and there is an L here, and then we have a sine pi x by L, that is the ground state, exponential minus i, say for example, e1 t by h cross.

and plus sine 2 pi x over L exponential minus e 2 t by h cross L. So, that is the wave function. Now, this is between, of course, 0 to x less than L. Otherwise, it is equal to 0. That is very easy to see. Now, one important thing is, how do we interpret this, or rather, what is the probability density? Is it still a stationary state and so on? No, it is not a state whose probability density is independent of time because it does not have definite energy. If you make a measurement, it will collapse onto one of the states, either in the ground state or the first excited state. But it still has the energy to be with certain probability you will get if you make a measurement before you actually make it. you would get the ground state energy with certain probability and the first excise state energy with certain probability, which were respectively given by pi square h cross square by 2 mL square and 4 pi square h cross square by 2 mL square. So, this probability density is going to be oscillating with time and if you calculate this P x t which is nothing but equal to mod of Psi x t square and this will give us you know equal to 1 over L.

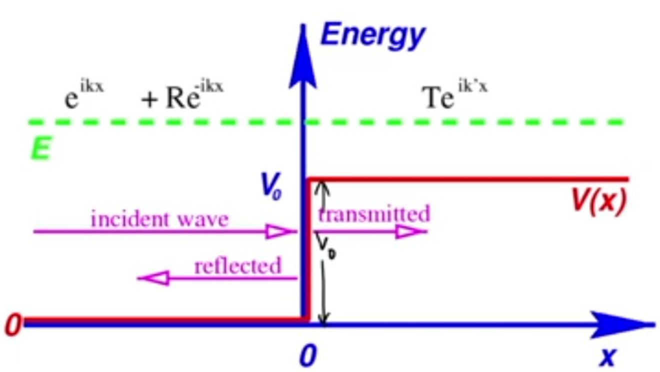
And then you have a sine square pi x by L plus sine square 4 pi, I mean there is a sine 2 pi, sine square 2 pi x, not 4 pi, 2 pi x by L. And, and then we have a 2 sin pi x over L, sin 2 pi x over L and then there is a cosine of a delta omega t, that is the time part which is coming from the interference where delta omega is nothing but E2 minus E1 divided by h cross, okay. That is the time part with which it will oscillate, and I have made a video where L is varied from 0 to 1, 1 is some unit of length, and then T has been taken in unit of ω such that, you know, this cancels out, and you see that as time increases, it changes from being in the left part to the right part, then it comes and gets reflected on the left boundary of the well and then it goes to the right boundary and so on so forth. So, it sort of gets reflected from here and go to the, so this is the initial time you have it in the left side or left half of the well and As time progresses, it sort of evenly distributes or rather equally distributes, you know, both sides of the well. Then later at larger times, it goes to the right half, gets reflected from the boundary, again reappears at the, you know, at the left edge and so on. So, this is the animation for the probability density at different times, okay.



All right. Let us now do a number of problems and sort of keep this thing a little quick now because now you are familiar with how to handle this and what the boundary conditions are. All you have to do is write down the Schrödinger equation and match the wave function or match the solutions at the boundary. First, you have to get the wave functions. So, what we did is that here there is a potential step. The step is of height V_0, okay? And a particle is coming from the left whose energy E, shown by the green dashed line, is greater than V_0, okay? And we want to calculate what are these R and T, which are called the reflection and transmission amplitudes. R is the reflection amplitude, and T is the transmission amplitude. Okay, so there are a few comments that will help you to solve this problem. There are two cases. One is E greater than V0. We are showing at this moment by the green line E greater than V0. That is shown here. E less than V_0, which should be more interesting, that is a particle which would, you know, appear with lesser energy and has energy lower than the barrier height. A classical particle can never jump over to the other side or get into the region which is classically forbidden. Say a high jumper would never be able to cross a barrier which is more than what he or she could jump.

So, but here any particles such as an electron or photon and so on, they will go into the classically forbidden region. 'Go into' means there will be a sort of wave function that would be finite, but it would not correspond to any propagating wave. Maybe those are called evanescent waves. But the wave function would still exist, which means that there is a probability of the particle to be found in the classically disallowed region or the forbidden region. It will still be found. And we will have to match the boundary conditions at x equal to 0, and the reflection and transmission amplitudes R and T will have to be calculated. And sometimes, you know, in questions, you are not given this figure, but you are given it in writing that V of x equal to 0 for x less than 0 and V of x is equal to plus V0 for x greater than 0.

The potential step



Comments:

1. There are 2 cases:
   $E > V_0, E < V_0$
2. The wavefunctions have to be matched at the boundary at $x = 0$.
3. The Reflection (R) and Transmission (T) have to be calculated.

$$V(x) = \begin{cases} 0 & x < 0 \\ +V_0 & x > 0 \end{cases}$$

R: Reflection amplitude
T: Transmission amplitude.

They mean the same thing. You will have to picturize this and draw your own, you know, schematic diagram. So, as we said that we are first doing it at e greater than V0. So, for x less than 0, we have this u of x, which is the solution. We again go back to the notation u, but they mean the same thing if you write it as psi. It's exponential ik x, so which has a coefficient equal to 1. And in keeping with what we have said, because it's an infinite extent, both on the left and on the right, we write exponential solutions.

So there's an amplitude 1, part of it is reflected, so we call it R, and a part of it is transmitted, we call it T. So k is given by, so this amplitude is equal to 1, that's why it's not written there. And so this R is the reflection amplitude, k is equal to root over 2mE by h cross square here. For x, sorry, this has to be x greater than 0. So, x greater than 0, you have u prime, which is the solution in the classically, you know, not classically forbidden here because E is greater than V0. It is in the right region, right of the discontinuity. You have 2m(E minus V0) by h cross square and the transmission amplitude and exponential ik prime x and so on. So, that, you know, the current is conserved. The solution is written in this particular fashion. There is no reflected wave because in the second solution, that is x greater than 0, you see that there is nothing to reflect it back. So, it is only a solution which is exponential ik prime x, even though mathematically, it is possible to write exponential minus ikx.

However, we see that that solution will not be an acceptable solution because there is nothing that is reflecting back the wave to move in the direction towards the barrier or towards the potential discontinuity. So there is no reflected wave for the second one. And so what we have to do is match the boundary conditions for x equal to 0 for the wave function. I mean, and x greater than 0. So, the boundary condition is for x equal to 0. So, it really does not make sense. So, we can just simply write x equal to 0. So, this is not acceptable. So, these boundary conditions have to be matched. We have written down the solutions, put x equal to 0, and match u and u prime, and that gives 1 plus R equal to T. So, if you put x equal to 0, The first term on this becomes 1, this becomes R, and this becomes T, so it is 1 plus R equal to T.

$E > V_0$

For $x < 0$, $u(x) = e^{ikx} + Re^{-ikx}$

$$k = \sqrt{\frac{2mE}{\hbar^2}}.$$

For $x > 0$,

$$u'(x) = Te^{ik'x}$$

$$k' = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

There is no reflected wave!!

The boundary condition at $x = 0$ for the wavefunction is:

$u(x = 0) = u'(x = 0)$ yields $1 + R = T.$

And then the other boundary condition, which is the derivative of the wave function at x equal to 0, is also continuous. Take the derivative and then put x equal to 0. If you write them down and then put x equal to 0, and then you eliminate T and write it in terms of R. Now, finally, you solve for both R and T. They are (k minus k prime) divided by (k plus k prime), and T is equal to 2k divided by (k plus k prime), with all these k and k prime given in terms of E and V0 and also, of course, m and h cross square. They have to be there along with the mass of the particle and Planck's constant.

$$\frac{du(x=0)}{dx} = \frac{du'(x=0)}{dx} \text{ gives } [ike^{ikx} - ikRe^{-ikx}]_{x=0} = [ik'Te^{ik'x}]_{x=0}$$

Eliminating T,

$$k(1 - R) = k'(1 + R)$$
$$(k + k')R = (k - k')$$

Solving for R and T

$$R = \frac{k - k'}{k + k'}$$
$$T = 1 + R = \frac{2k}{k + k'}.$$

So, the wave functions in the two regions are now because we have calculated R and T can be written as exponential i k x k minus k prime divided by k plus k prime which is the amplitude exponential minus k x for x less than 0 and for x greater than 0 it is 2 k divided by k plus k prime exponential i k prime this is equal to 0. So, this transmission amplitudes and the reflection amplitudes can be you know squared up to get the probabilities for reflection. Sometimes you will see that in some books, this R and T, capital R and T are written as small r and small t. And the P reflection and P transmission are written with capital R and capital T.

The wavefunctions in two Regions:

$$u(x) = \begin{cases} e^{ikx} + \frac{k-k'}{k+k'} e^{-ikx} & x < 0 \\ \frac{2k}{k+k'} e^{ik'x} & x > 0 \end{cases}$$

The probability of Reflection and Transmission now are finite (unlike classical mechanics!!)

$$P_{\text{reflection}} = |R|^2 = \left(\frac{k-k'}{k+k'}\right)^2$$

$$P_{\text{transmission}} = 1 - P_{\text{reflection}} = \frac{4kk'}{(k+k')^2}.$$

But nevertheless, they mean the same thing. So this reflection probability or this is the. A reflection coefficient at times it is called. So, reflection coefficient and transmission coefficients are given by these k minus k prime whole square divided by k plus k prime whole square and 4 k k prime k plus k prime whole square. You can simply see that they obey that 1 plus, you know, so this reflection plus transmission, if you, you know, add up, you would get it. So, there is, so P R, let us call it, and a P T, that is the one that you see here. So, you have a k minus k prime squared.

Do it for $E < V_0$.

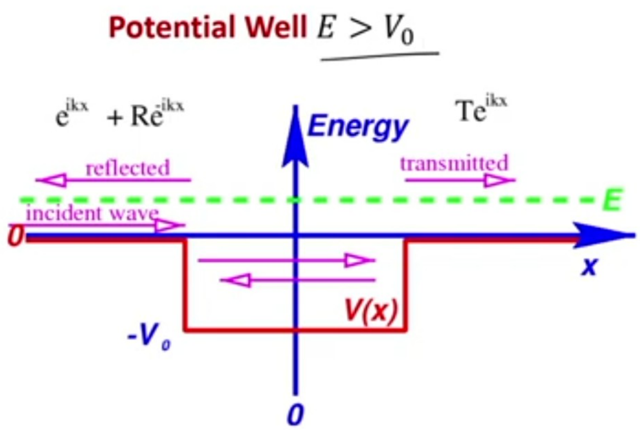
Hint: The wavefunction for $x > 0$ will be $u'(x) = Te^{-\kappa x}$, where $\kappa = ik' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

Result: $P_{\text{reflection}} = 1$. So the particle will be totally reflected back. Although the region $x > 0$, has a finite probability of the wave to exist. $u(x > 0) = |T|^2 e^{-2k'x}$

plus 4k k prime and this is equal to k plus k prime square and this is equal to k square minus 2k k prime plus k prime square plus 4k k prime divided by k plus k prime square this is equal to 1 which means that the reflection coefficient or probabilities of reflection and probabilities of transmission add up to 1 which they should. The wave is not getting lost, it is not going anywhere. So, these two probabilities should become equal to 1. And I leave it to you to do E less than V0. The hint is that for x greater than 0, which is in the now you have the particles energy to be, you know, lesser than this barrier height. So, you will have this k prime to be actually a complex quantity and you write it as kappa the way we have shown and so on and you get it as exponential minus kappa x and where kappa is equal to i k prime which is equal to 2 m V naught minus e by h cross. And you will see that the result is that the reflection, this coefficient or probability of reflection is equal to 1. So, the particle will be totally reflected back.

Although this region, which is classically forbidden, has a finite probability of the wave to exist and this is actually given by this. So, there is no current associated with it because it is fully real remember the current density is these h cross I mean h cross by 2 mi psi star del psi minus psi del psi star that is equal to 0 because there is no difference between the first term. So, the current is given as you know h cross by 2 m i And psi star del psi minus psi del psi star, that is equal to 0. And the reason it is 0 is that because psi is real here, so it should not have, the first term will cancel exactly with the second term. And what you see is that it is a traveling wave in the region that is or it's called as a standing wave in the region which is left. And then it's an evanescent wave and falling off to a value which is called as a, you know, this value at which it falls to a value one over e n side is called as that exponential minus kappa x. So, kappa equal to 1 over x is called this skin depth.

And in optics, this would correspond to a denser medium to a rarer medium, which means that n1 is greater than n2 in terms of the refractive indices, okay. All right, so continuing along that line, we have these potential wells that are shown like this, where you have exponential ikx, r exponential minus ikx, and again t exponential i k x now is greater than V0, which is an easy thing to do. The results for these reflection amplitudes and transmission amplitudes are a bit complicated, but one can simply write down the solutions in the three regions. Now you have region 1, region 2, and region 3, and you have these discontinuities at, you know, at 0 and a and so on. So, you have to match the boundary conditions at x equal to 0 and at x equal to a for both the psi being continuous and d psi d x being continuous. So, if you square them up and add them, this will give you the total probability. There is something interesting that happens if you look at it, you know, if you look at the reflection coefficient, which has a sine 2k prime a in the numerator and sine being, you know, a harmonic function.



$$R = ie^{-2ika}\frac{(k'^2 - k^2)\sin(2k'a)}{2kk'\cos(2k'a) - i(k'^2 + k^2)\sin(2k'a)}$$

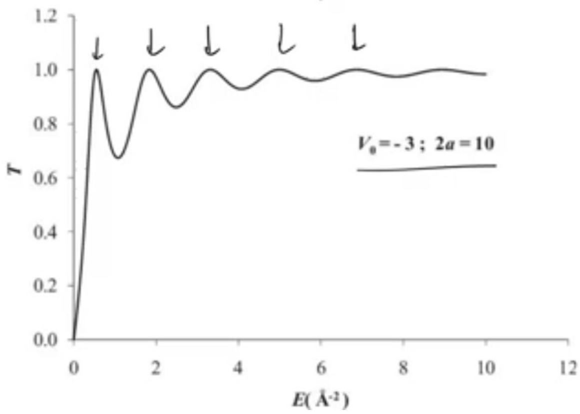
$$T = e^{-2ika}\frac{2kk'}{2kk'\cos(2k'a) - i(k'^2 + k^2)\sin(2k'a)}.$$

It will tell you that this reflection will go to 0 for certain values of this k prime, and k prime is a variable because k prime is related to energy as 2m E minus V naught and so on. So because it's related to energy, k and k prime are the two wave vectors which are written here. You know, these wave vectors that you see on the screen. And so this is, you know, so this sine 2kA that you see here. It will make the reflection amplitude go to 0, and you see that for those values when 2k prime a becomes n pi with k prime equal to this, you have a complete transmission because the reflection goes to 0, and these are the values and so on, okay. And this is for a particular value of V0 and the width of the well. And it is plotted as a function of E in terms of 1 by length squared, that is in angstrom. And this plot is adopted from an Am. J. Phys article in 2010 by Uma Maheshwari et al. The energy is still given by minus V0 because it has a minus V0 energy. You see that it's minus V0. So it's a potential well. Okay, so this is V0 and so on. So it's minus V0 n square pi square h cross square by 8 m A square and so on. And E less than V0 are called the bound states. I'll sort of do it quickly and explain. So, we have these solutions; you can again write down these equations and do the necessary simplification of that.

Something interesting happens!! $R \to 0$ when

$$2k'a = n\pi$$

$$k' = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$



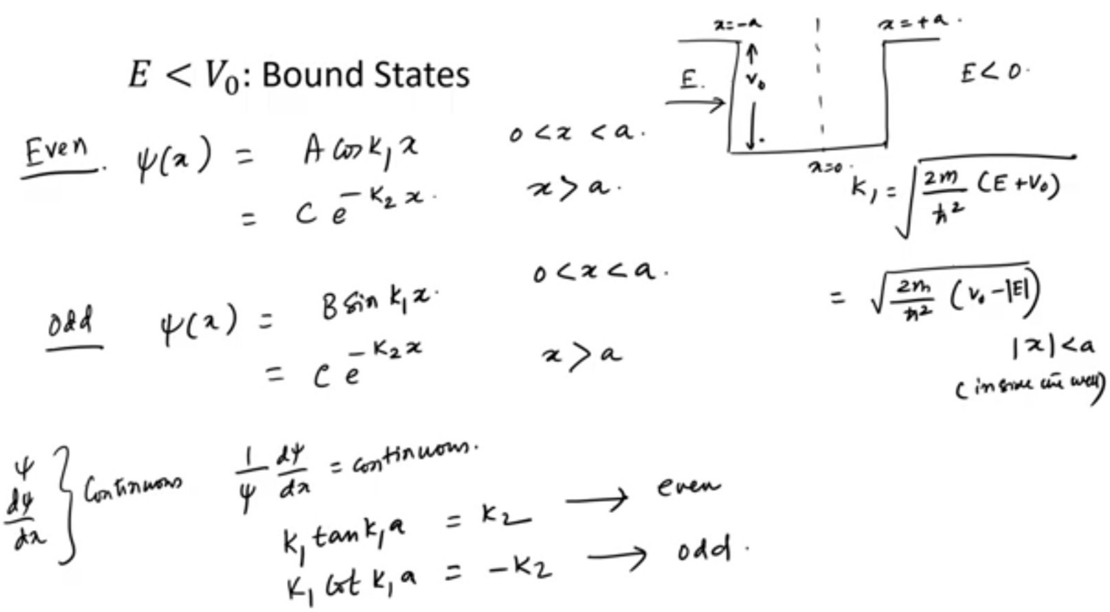
$$E = -V_0 + \frac{n^2\pi^2\hbar^2}{8ma^2}$$

Plot adopted from U. Maheswari et al. Am. J. Phys. 2010.

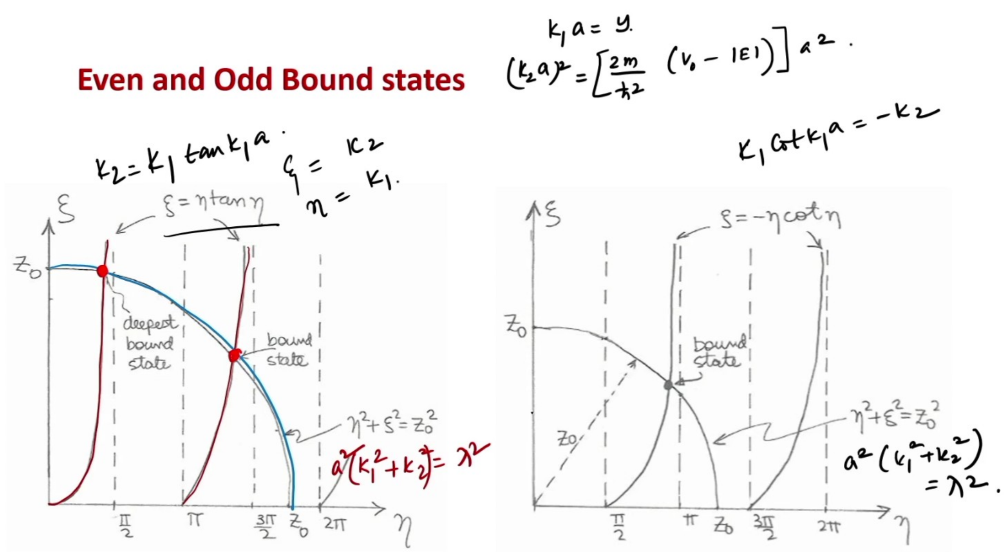
So, psi of x is equal to, you know, it is a cosine k1 x, and just to make it a little more interesting, I put these discontinuities at x equal to minus a and x equal to plus a so that these even and odd solutions would arise, and so it is A cos k1 x for 0 less than x less than a. And this is equal to, well, I mean, I am writing it as k1 and k2 instead of k and k prime, but I will define what k1 and k2 are. So, this is C exponential minus k2 x. By hand, it is a little difficult to write this kappa, or you may actually misunderstand it as k. So, that is why I am writing k1 and k2. So, this is for x greater than a. With these k1 to be equal to 2m by h cross square e plus V0 because V0 is negative here, a square root of that, and you can also write it as this one as 2m by h cross square E.

So, V naught minus E, where this E is actually negative. So, I have taken the mod of E, and this is for within the well. So, that is like mod of X is less than A, which means that we are talking about inside the well. So, these are the solutions, and these are the even solutions because now we have these even and odd solutions. Then, these odd solutions would look like Psi of x is equal to B sine k1 x. I mean, in the sense that what I meant to say by even and odd is that, you know, if x changes to minus x, cosine does not change its value—cosine is an even function. So, it is in that sense that we talk about even and odd, whereas sine changes. Of course, if you change x to minus x here in the second solution with the C exponential minus k2x, that will become plus k2x, which is not a physically acceptable solution. So, our even and odd notion is based on the harmonic solutions, which are either cosine or sine. These even solutions are truly valid for odd n, and odd solutions are in fact applicable to even n. But this even and odd is with respect to changing x to minus x, which is why we call them odd and even.

So, this is for 0 less than x less than a for the odd solutions in the same region—that is, you know, this is your x equal to 0 and so on. And so this is V0, and the energy is negative. So, the energy is negative, but it is greater than this V0, minus V0. It is greater than minus V0. All right, and this is equal to some C exponential minus k2x for x greater than a. So, these are the solutions. Now, what we can do is a smart thing: combine the two conditions—Psi being continuous and dPsi/dx being continuous. So, these two can be combined into a single condition, which is that 1/Psi dPsi/dx is continuous. So, instead of writing the two conditions, we can also use this 1/Psi dPsi/dx being continuous. That gives us two conditions: one is k tan(k1a) equal to k2, and k1 cot(k1a) equal to minus k2. So, this corresponds to the even problem, and this corresponds to the odd problem. Now, you see that there is a problem in solving these equations because k1 and k2 correspond to energies, which are on both sides of the equation and cannot be solved so easily. These are called transcendental equations.



So, one way is to solve them numerically, which is what we are not going to do here. But what we can do is write or plot these solutions. And these solutions—the intersection of the left-hand side and the right-hand side—will give us the solutions we are looking for. So, you know, a little bit of different language. Let me sort of give you that. If you say k1 a is equal to y. Then, k2 a whole square, this is equal to 2m by h cross square V0 minus mod of E and so this into a square. And let me actually create another page so that it is easily understandable for you. So, what we do is call k1a equal to y. We have used different notations for plotting, but I will tell you what these are. And now you have a k2 a square is equal to 2m by h cross square V0 minus E and this multiplied by a square. So, that tells us that k2 a square. is equal to 2m by h cross square V naught a square for a given problem that is a constant and minus 2m mod E divided by h cross square a square and this is nothing but let us call this as lambda square minus k1 square a square.



So, k2 square a square equals lambda square minus k1 square a square, and call this lambda square minus y square. So, k1 and k2 are positive, and also we have a k1 plus k2 square. k1 square plus k2 square and a square equals lambda square because you can add both of them, and then where lambda equals nothing but this 2m V0 a square divided by h cross square whole to the power half, and here let us, you know, sort of show. So, these are the solutions of these xi tan xi where, you know, we have probably the calculations done on the last step were not that necessary. So, this k1, so k2 equals k1 tan k1 a. So, your xi equals k2 and eta equals k1, and A could have been taken as 1. So, if you plot this xi and eta tan eta, then these lines that you see here, let me sort of redraw them like these ones are the tan solutions. Okay, and these solutions that you see are these ones that are given by these k square, k1 square plus k2 square equals some lambda square, which is what we have derived here. I mean, the a has been taken equal to 1, but you can just add this. I mean, there is a square.

Call $k_1 a = y$.

$$(k_2 a)^2 = \left[\frac{2m}{\hbar^2}(V_0 - |E|)\right] a^2 \Rightarrow (k_2 a)^2 = \frac{2m}{\hbar^2} V_0 a^2 - \frac{2m|E|}{\hbar^2} a^2$$

$$= \lambda^2 - k_1^2 a^2 = \lambda^2 - y^2$$

k_1, k_2 are positive,

$$(k_1^2 + k_2^2) a^2 = \lambda^2$$

$$\lambda = \left(\frac{2 m V_0 a^2}{\hbar^2}\right)^{1/2}$$

So that's equal to lambda squared, which is nothing but a circle. So you see that you now plot the circle, which is, say, the blue line, and the tan hyperbolic. So you see these solutions emerge at, say, for example, these lines. These bright red points, these are the solutions where these are the bound states. So this is the deepest bound state, and this is the bound state for, you know, some other bound states and so on. We have shown two of them. The more the depth of the well is, you have these, you know, there will be more and more number of bound states there, and for the odd problem which corresponds to this. k1 cot k1 a equals minus k2. Now, it is a cot solution which does not go to 0 at or does not start from eta equal to 0 or k1 equal to 0. In fact, it starts from pi by 2, and one can actually see that, so there are. So, these it starts from pi by 2 there, and if you have a circle which is nothing but this eta square plus i square equal to z0 square, which in our language is nothing but a square k1 square plus k2 square equal to lambda square. So, if this circle is like this, then there is no bound state. So, for having a bound state, an odd bound state, you need to have a certain depth of the potential. So, for any infinitesimal potential, you can only have an even bound state, but for having an odd bound state, you need to have a particular depth for the potential. And so, there is a solution that emerges here which we have shown in color.

So, there is a solution which is here, and we have just shown one solution, and this is the part of the circle of length either you call it z0 or you call it lambda. So, z0 is nothing but this lambda, okay. So that's the solution that we have for these bound states. And, you know, there are these bound states that are formed, and you can be given a certain depth of the well, and you can calculate the number of bound states present from these conditions. That is how many times this circle crosses. If you are talking about an even bound state, then any infinitesimal depth of the well will give rise to a bound state. However, that is not true for the odd bound state. You need to have a critical depth to have at least one bound state. So, we stop here for now, and so this is what is written there or no odd bound state below a critical depth of the well. So, we will stop here and start with some more problems in quantum mechanics involving perturbation theory and Stark effect and so on. So, we will start with time-independent perturbation theory and then go over to this time-dependent perturbation theory. Thank you.