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Contributor Shall we begin. So last term we discussed the dynamics of a harmonic oscillator which is a one dimensional system where the particle is bound by a potential v is a $\frac{1}{2}$ K x squared. And we found oh a number of important results, most obviously there was quantisation of the energy, so discreteness of the energy levels. And very importantly there was the phenomenon of zero point energy. That even when something was in its ground state it had uncertainty principle obliged it to have non negligible kinetic energy, and potential energy indeed.

So what we're going to do now is study a number of very simple one dimensional potentials, motion in a number of very simple one dimensional potentials which are themselves very artificial. These are step potentials so they change discontinuously at some values of x from one value to another value. So they're very artificial but the merit of them is that we can solve the governing, well the key equation the time-independent Schrödinger equation and obtain the states of well defined energy, from which we can, as we saw with the harmonic oscillator recover the dynamics of the system. We can solve this equation, this important equation simply for these rather artificial potentials.

And we'll discuss at the end, which of our results is artificial, you know reflects the artificiality of the potentials and which are generic and ones that we can believe in.

So this is what we're going to start with is the square potential well, which is this structure. This is potential energy being plotted vertically. The position being plotted horizontally. Here is the origin, this is going to be at distance a. It is going to be symmetrical. This is going to be a potential level v zero. And this is going to be potential level nothing.

Right so we set the zero as a potential energy to be at the bottom of the well. And then there's when you're more than distance a from the origin you have some potential energy v zero, which is a constant. So this is highly artificial but let's see what quantum mechanics has to say about motion in here.

So what we're going to look for is stationary states. That is to say states of well defined energy, which we write like that, right. So these are states of well defined energy. We're interested in these because they enable us to solve the time-dependent Schrödinger equation trivially. Once we know what all these things are, we can write down and we know – once we know what all these things are and we know how to, then we can express any arbitrary initial condition as a linear combination of these things and we can time evolve it in a simple way as we saw last term.

So we're going to find these things and they're going to have wave functions which we'll call u of x, so this is x, e is the wave function.

Now this potential is symmetrical – is an even function of x, right. So we have that v of minus x is equal to v of x, so it's an even function. The consequence of that is that we introduced the parity operator last term, we had that p, if you remember x, p is an operator, the parity operator, which makes out of state `[[upsi 0:04:01]]`, the state that you would get which has amplitude to be at minus x, well what is this?

This is the amplitude to b at x when you're in the state that p makes out of upsi, and this was defined to be minus x, upsi, in other words it was defined to be the amplitude to be at minus x, when you are in the state upsi. So the parity operator makes a state, which is the same as the state you first thought of, except if every point is reflected through the origin.

We discussed this operator, and because v is an even function of x. We have that pvx, pv upsi is going to be equal to minus x, v upsi. Which because v is a function of position, it's a function of the position operator, this is going to be v of x. x upsi. In other words it's going to be simply v of x, sorry, sorry, sorry, sorry I need a minus x and a minus x. So it's going to be v of minus x times upsi of minus x.

And because v is an even function of x. So v of minus x is the same as v of x, this is equal to. This is this and this could be written as p. So what does this mean? This means that because v is an even function of x it commutes with the operator p. In other words p, v equals nought. Because, this is rather a rigmarole I have to admit. P commutes with v because v is an even function. Which is a way of saying that the potential is symmetric about the origin.

This is the bottom line. If you have a potential which is symmetric about the origin as an even function of x, then it commutes with the parity operator. The consequence of that is, so the Hamiltonian is of course, is as ever p squared over 2m plus v of x. P squared is an even function if you write this in the position representation, it's minus h bar squared, d2 by dx squared. So this is an even function of x. So this commutes with the parity operator. We've just figured that this commutes with the parity operator. So we have p, h, so this implies that p, h is zero. So the parity operator commutes with the Hamiltonian whose stationary states we would like to find. Whose Eigen states, that is to say the stationery states we would like to find.

So what does that imply? When two operators commute remember the fundamental rigmarole is that this implies there's a complete set of mutual Eigen states of p and h.

That is to say we can if we wish, look for Eigen states of h, which are states of well defined parity and the wave functions of these states of well defined parity will either be even functions of x, if the parity is even, or they will be odd functions of x if the parity is odd.

So what this means is we can insist or we can look for, so we can look for stationary states with wave functions u of x, meaning of course xe that are either even functions ux equals u of minus x or odd functions i.e. u of x is minus u of minus x.

And this observation, knowing that you're looking for an even function say, makes it much easier to find that function than if you don't know whether it's even or it's odd. This is a general observation and we'll just find a concrete example of it in a moment.

So, here is our potential again, a minus a. What do we have? We have here what is the time-independent Schrödinger equation. That is to say what is that, that is the equation which shows that h upsi is equal to e upsi. In the position representation what does this important equation look like here, well at this point here, where the potential is zero, h is p squared over 2m. So at this location here it becomes, this becomes p squared over 2m, which is minus h bar squared over 2m, d2 u by the x squared. So this is – I suppose I should change this sorry, in this context to u probably – Oh no let's leave it with e, that's what we were calling it. The state e.

So this left hand part now reduces to just this, in the position representation because we only have the kinetic energy at this location there is no potential energy. And on the right hand side of course we simply have e times u. So we're trying to solve this equation and we know all about the solutions of this equation. This is just the simple harmonic motion equation of classical physics essentially. It tells us, so we know that u is cos kx or u is sin kx, provides solutions of this equation. Cos kx is an even function so that must be the solution belonging to an even parity state. And sin kx is an odd function of x, so it's an odd parity thing.

So this has solutions u of x is equal to either cos kx or sin kx, depending on parity and we have that k, so right when you double differentiate this you're going to get minus k squared cos kx. So the minus sign deals with that. We're going to have that minus k squared. e is equal to this stuff here, in other words we're going to have that k is equal to – yes, no this is wrong, sorry, sorry, I've got this the wrong way up. What am I doing?

Sorry the double derivative is here, excuse me. So when we double differentiate we'll get minus h bar squared, k squared over 2m. We'll get a minus coming from the differentiation which will cancel this and we will have that k squared is equal to 2me over h bar squared, square root. Well k is that.

So we have determined what the wave functions are of the stationary states in that interval from minus a to a in terms of the energy.

What we now need to do is think about the state of affairs here. So this stuff is all true for mod x less than a. What about the case when mod x is greater than a, so another picture in this zone here, what does the time-independent Schrödinger equation look like. It still has kinetic energy minus h bar squared over 2m. D2u by the x squared. But now we have potential energy, how much, v zero so v zero times u. So this is the Hamiltonian operator operating on u. and that's equal to e u.

And let's now say we're looking for bound states, that's to say states where the energy e is less than the potential energy out here. So that classically the particle will be confined inside here. So we're going to look for bound states. There are other states too, but let's focus on the bound states. That means that e is less than v zero, so the particle classically is not allowed to get out of the well.

What happens then, well then this equation becomes d2u by the x squared is equal to, if we put this onto this side, since v zero is by hypothesis bigger than u, we have a negative right hand side. And we can cancel the minus signs on the two sides, so if we write it as we have 2m v zero minus the energy over h bar squared, times u.

So again we have a double derivative is equal to some constant times the function. But the difference is now that we don't have a minus sign here. So instead of having sinusoidal solutions we have exponential style solutions.

So the solution to this equation is that u is equal to a constant times e to the plus or minus k times x where big k is the square root of this stuff here.

What about this sign ambiguity here? Right there is a sign ambiguity here because it's the double derivative which has to be equal to a constant times u. If we go for the minus sign in taking the double derivative, two derivatives we get down two minus signs, we get a plus obviously, so that's why there's this ambiguity.

What do we do about that ambiguity? Well when x is greater than nought, we want the wave function to decrease as we head off to infinity. As x becomes larger and larger. Well in fact, right because we would like to be able to normalise the wave function. We'd like to have the wave function mod squared integrated over all space comes to one. And that's not going to be possible if we have an exponential divergence.

So the consequence of this is, that in this zone here we take that u is proportional to e to the minus kx, because x is positive over there and that means the bigger x gets the more we move over here, the smaller the wave function becomes.

If we're on this left side here where x is negative then we want to take u goes like either plus or minus e to the plus kx, because x is negative in this zone here. And the negativity of x gives the exponent of the exponential negativity, so that the bigger that x becomes in modulars the more we move over here, the smaller the wave function becomes.

And whether we want to take a plus sign, if we're looking for a state of positive, of even parity, then we want to take this plus sign, so the wave function over here has the same numerical value as the wave function at the corresponding point over there. If we're looking for a state of odd parity we take this minus sign, so the wave function at negative x becomes minus the wave function at the corresponding point of positive x.

So that's where we are so far. So we've now solved, what have we done? We've solved the time-independent Schrödinger equation everywhere except at x equals a and x equals minus a. But we haven't solved it at those points because at those points, if you go a bit to the – for example at the point x equals a, if you go to the bit to the left of that point then the wave function is supposed to be cos or sin kx and if you go a bit to the right it's going to be this exponential function. But at that point we must still have the time-independent Schrödinger equation satisfied.

So what does that require? Well, for the time-independent Schrödinger equation to mean anything even, the second derivative of the wave function has to be well defined at that point because the time-independent Schrödinger equation equates the second derivative to some stuff.

So what we can say is that at x equals plus or minus a, we need that d2u by dx squared is defined. Or we can't solve the `[[tize 0:19:32]]` there. Satisfy the tize there.

Well this is the rate of change of the gradient that is certainly not going to be defined if the gradient isn't continuous. So that implies that u by dx is continuous. And that's a non trivial requirement because at the moment we've got the wave function in pieces and there's no obvious reason, unless we do some engineering on our pieces, why the gradient is defined by one piece or one side of the barrier of the transition should equal the gradient from a completely different function on the other side.

Okay, so the gradient has to be continuous. The gradient is certainly not going to be even – is not even going to be defined unless the wave function itself is continuous. So we also require similar reasons, that u is continuous at these points.

So we have to insist that u of a minus some tiny bit is equal to u of a plus some tiny bit and we have to insist that the u by dx evaluated at a, minus the tiny bit is equal to the u by dx evaluated at a, plus a tiny bit, called Epsilon.

That's what we've got to insist on. What does that amount to? That amounts to here if we're just to the left of a we have for the even parity solution we have that u is equal to cos k, x and x is a minus epsilon but epsilon's as small as we like, so let's just make it equal to cos ka. That's got to equal the wave function on the right hand side, which is some constant. We call that constant big a times e to the minus big k times x, plus the tiny bit. Let's forget about the tiny bit because this is a continuous function.

So we require that, that's the continuity of u of x.

Similarly the gradient just to the left of x equals a is given by the derivative of cos kx, so we're looking at minus k sin ka and that's got to equal to the gradient of a e to the minus kx, evaluated at x equals a, so that's minus big k a e to the minus ka. At that's the continuity of the u by dx.

And we also have to satisfy these continuity conditions at x equals minus a. But the nice thing about choosing, deciding that you're going to look for a wave function of well defined parity, either an even function or an odd function is that it's easy to persuade yourselves, you probably want to sit down quietly and do this afterwards, that if you satisfy these conditions on the right hand side at x equals plus a of the origin, then you've also satisfied these conditions to the left of the origin. These equations suffice to fix up the arrangements on both of the discontinuities. And you don't have to deal with them separately, that's the great advantage of choosing wave functions of well defined parity.

So what do we have here? We have a pair of equations and we have a number of unknowns. As it stands we do not know what little k is or big k is, and we do not know what a is. Big a is, right. Those are all unknowns.

We've two equations and we need fundamentally to determine these unknowns.

Most important is to determine little k and big k because they're related to the energy by formulae which are, there's little k right at the top there is the square root of 2me over h bar squared. And big k half way up is 2m v zero minus e.

So little k and big k are both related to the energy and once we've found the energy we'll know what both big k and little k are and it's the energy that we're fundamentally after. So that's what we want to focus on.

Big A is of less interest. So let's get rid of big A by dividing this equation through by this equation. Then we will find – so we divide equation two basically by equation one. And that leads to the conclusion that minus – do it down here – minus k tan ka, from sin over cosine is equal to minus big k everything else goes because we have an ae to the minus big ka in both equations.

And let's ask what this is. Let's try and relate this, so big k and little k are both related to the energy from which it follows that I could express big k as a function of little k, so let's do that. This is minus the square root of 2m v zero minus e over h bar squared. Which is equal to minus square root. Now 2me over h bar squared is actually from, we've maybe just lost it unfortunately, let's bring it back into focus right at the top there, it's 2me over h bar squared is in fact k squared.

So 2me over h bar squared is k squared. So what we want to do is write this as 2m v nought over h bar squared minus k squared.

So here we have an equation now that this is equals this, which has only one unknown, namely k. So the left side is a function of k. The right side is a function of k. Any values of k for which these two sides are equal are – provide solutions to our time-independent Schrödinger equation and provide wave functions for stationary states, for states of well defined energy.

To solve this equation the way to go is to divide through by this, well obviously cancel the minus signs. Divide through by k both sides and this then becomes tan ka is equal to the square root of 2m v nought over h bar squared, k squared minus 1. And it's good now to multiply the top and the bottom of this by a squared and write this as the square root of w over ka squared minus 1, where w is 2m v zero a squared over h bar squared. Why do I want to do that? Ka is obviously dimensionless because you know this is a wave number, the wave function was sin kx, the argument of a sin must always be dimensionless, so this is dimensionless. That's obviously dimensionless therefore this must be dimensionless, you can explicitedly check that it is dimensionless. So the reason I would define w is that this thing is dimensionless.

And it's a dimensionless measure of the depth and width of the potential well. Right it depends on the depth of the potential well, it depends on the width of the potential well. And it's the dimensionless – the mathematics is telling us that this is how you quantify, how you know what kind of potential well that you've got. Whether you've got a very deep one or a very shallow one.

So how are we going to solve this equation here? Well the way to go is to plot both sides of the equation graphically alright. So the tangent is to plot both sides of the equation graphically and see what you get. See at what points they meet.

So if this is a plot, this is ka being plotted this way. Then if I plot tan ka, it starts off at zero and rises like this. And when ka becomes equal to pi over two, it zooms off to infinity. Right that's what tangents do and down here it goes symmetrically.

What does this thing do? When ka is nothing that thing is obviously infinity because it becomes w over nothing square rooted. So this is the left hand side. I better write that down. So this here is the left hand side, its tan ka.

The right hand side is coming down from infinity and it's going to go to zero when ka is equal to or k squared is equal to w. So this right hand side is cruising down from infinity and it's going to go to zero when ka is root w.

And from this we see, it's obvious now that no matter what the value of w is, so as you change the width and depth of the potential you move this point to the right or left, but no matter where you put it from nowhere to infinity, it will cross, there will be this intersection here. These two curves always cross. And where they cross gives you a value of ka and therefore a value of k, which is a solution to the time-independent Schrödinger equation.

So what we've just learnt is that this well always has a bound state. It doesn't matter how shallow the well is or how narrow the well is, it always has a bound state, because these two curves always cross.

This tangent on the left, right, has other branches. There's also a branch – so tangent comes along here, goes off to plus infinity and then somewhere down here, when ka is equal to pi upon 2 plus bit, it becomes minus in points, it comes in from minus infinity and repeats itself. So this is the LHS second branch. And this second branch may or may not cut this curve of the right hand side again, right. So if we made ka smaller than here, this is where ka, this is the place pi, if we would make this less than that we wouldn't get a second solution. But if we have ka bigger than this we do get a second solution.

So it may have other even parity stationary states. So depending on the depth of the potential we have one, two, three, four etc. stationary states of even parity. We've only dealt with the even parity case.

If we want to look at the odd parity states, let's just begin to do this but this is basically an exercise for the problems. Then our conditions are a wave function for the odd parity state. We've lost it somewhere but it's a wave function for the odd parity states is the sin kx right up there, right. So in the middle it's sin kx, at the edge it's still ae to the minus kx. So our continuity conditions become that sin ka is equal to ae to the minus ka. And that's the continuity of the wave function itself, at x equals a. The derivative of this is going to give me k cos ka is equal to minus big ka, e to the minus ka. If we divide this equation by this equation analogously to what we did before, we are going to get k co tangent of ka, is equal to minus big k. So now we have only one minus sin. Previously we had a pair of minus sins which cancelled. Now we have only one minus sin because we differentiated a sin, we didn't differentiate a cosine. And correspondingly we have a co tangent instead of a tangent. So this equation can be graphically solved. That's the exercise. And we find that we may get nought, one, two solutions for k. And for every solution we have an odd parity, we have an odd parity stationary state.

Let's have a look at the uncertainty principle in this example. Just to remind you last term quite early on, we showed, we considered the case, so this is a summary of last term. We considered the case where upsi of x is proportional to e to the minus x squared over four sigma squared. So we considered a wave function whose spatial form was a gaussian. Such that when you mod squared this in order to get the probability distribution you found that it was a gaussian with dispersion sigma, so this thing here is the expectation of x squared, right. That's what sigma squared is from that formula.

And what did we find? We found fundamentally by doing a Fourier transform, that if that's what the wave function looks like then the probability, while the amplitude to find – so this is x upsi right wave function looks like that. Then the amplitude to get a certain momentum, if you would make a momentum measurement was looking like e to the minus p squared over 4 sigma p squared. Right, where this thing becomes the expectation value of p squared. So the variance. The expectation value of momentum in this state is zero. The expectation of the square of the momentum is going to be this sigma p squared.

And what we found was that sigma times sigma p is equal to h bar on 2. This was a concrete example of the uncertainty principle, where the smaller the uncertainty in x is, the bigger the uncertainty in momentum and correspondingly the smaller momentum in p is, the bigger the uncertainty in x has to be, because the product is always the same, in this particularly gaussian example.

So we have some idea that the uncertainty in x times the uncertainty in p, we say to ourselves is inherently never smaller than this number h bar upon 2. It may be bigger than h bar upon 2 easily. It often is bigger than, it usually is bigger than h bar on 2. But this is kind of as small as it gets. So that was what we did last term.

So let's have a look at it in this particular case right. So let's look at the ground state. Oh yes another point to remind you is that the ground state wave function of the harmonic oscillator. So the ground state of a harmonic oscillator actually has a wave function which is the gaussian. At the time that we did this calculation this gaussian was just picked out of the air. But for the ground state of the harmonic oscillator actually does have this thing here. Fits this example.

So let's have a look at the wave function of the ground state of this that we have here. What you might argue to yourself, you might say "Okay so what we can say is that p is less than or on the order of - well p squared over 2m the energy is less than v zero right? Because it's bound. So it's less than v zero. So what we can say is that p squared is less than 2m v zero. Yes, sorry that's meant to be a less than. Seems reasonable doesn't it? The particle can't have any more kinetic energy than the energy it requires to escape because we know it's bound.

The next thing you might say is "Well so what's x squared?" What's the uncertainty in x. Well you might say to yourself "Well look this particle is trapped in this potential well that goes from plus a to minus a, so what's the uncertainty in x squared?" Well this must be on the order of a squared. Seems reasonable doesn't it? Less than on the order of. Well I'll put in a factor 2 or 4 or just to be sure than less than is holding. Because the thing is trapped by a potential well that extends only from plus a to minus a. So it has a range of 2 a's that it can run in. So we say x squared is definitely less than 2a squared. It's almost certainly. It's clearly less than that. Significantly less than that.

So what does that give me, oh and this square of the momentum is so, we have that x squared, p squared. I mean I can put expectation values around that too I think. Is less than on the order of whatever it is, 8m v nought, a squared. But that is w isn't it somewhere. Yes, look w, this is basically w because that was 2m v nought. So this v nought a squared is – it is something like 4 mv nought a squared is h bar squared.

Have I done this right, because I'm getting an answer which I'm – times w, yes exactly, that's right. The dimension is another w, right.

The point is right that w could be made as small as you like we've agreed and it's not a bound state. So this naïve argument suggests that we are going to violate the uncertainty principle because we can make this as small as we like. So what's the problem. This argument's bogus, what's bogus about it? It's not all in the well.

As you make w smaller and smaller. Let's draw what the wave function looks like.

So if we have, let's have a nice big value of w. A big value of w means a nice spacey well with right high walls. And then we will have a ground state wave function which is a cosine and some little bits like this.

And indeed the probability to find the particle outside the well, outside plus or minus a will be not very much. But as you make this smaller and smaller and smaller, you bring this in making a smaller and/or you lower these, making this curvature smaller. So that curvature of that wave function is a reflection of the kinetic energy which is a reflection of v nought. We have a narrow, a titchy witchy thing like this. Then we have barely – you have almost a straight line across here. I can't draw it well. Almost a straight line across here and then enormous long exponential decays. And the particles almost certain not to be in the potential well. That's a very remarkable conclusion to come to right? That you can trap a particle with a potential well which is almost – it has very little probability of actually being in. But that's what the theory says.

Something else we can show is we can say, we can argue as follows. Supposing we're given some other potential well right, and here is some other potential well. Sorry it's meant to be an even function of x right, so it's meant to be the same on both sides, symmetrical. And somebody asks you "So does this potential well have a bound state?" Then you reason as follows. Let us inscribe a nice square potential well. There are many square potential wells you can inscribe into it right, but there's one.

Then you can argue that this potential well is narrower and shallower than the one you were given. So less likely to trap a particle. But this potential well has a bound state. So this well is shallower, narrower but it has a bound state. At least one bound state, because it's a square well and we understand about square wells.

So you reason that this wider and deeper well also has a bound state. So we're making an inference from this very special rather artificial square well potential about all one dimensional square wells.

What happens now – let's conclude with a special case. An important special case, which is the infinitely deep well. Whoops. So now we let v zero become arbitrary large and we have a well that looks like this. It just goes up and up and up and up and up and up. What happens then? Well let's go to our graphical solution. What have we done? We've left a constant. I mean we've left a at some values. And we've allowed v zero to become arbitrary large, which means we've made w arbitrary large. What's the implication of that for our solution of this equation? So we're solving this equation for w arbitrary large. So we're saying that the roots are going to become where tan k a, the even parity roots are going to be where tan k a equals infinity. And we know what that means. We know that k a must be pi upon 2, 3 pi upon 2 etc. So we've made w goes to infinity, which implies that the governing equation, the equation that determines k becomes tan ka equals infinity. Which implies that ka is equal to either pi upon 2, or 3 pi upon 2 etc. etc. etc. And all of these values are going to be okay.

Graphically what's happening is that this curve, right this was the curve of the right hand side for finite w, is going to just become a line along here at infinity. And it's going to cross these various branches of the tangent at infinity. Which means at these pi upon 2, 3 pi upon 2 points. And it's going to cross every single one of them, all the way out right. So we're going to have an infinite number of even parity stationary states, and they are going to have those values of ka.

And when you study the corresponding problem for the odd parity states, which we just vaguely discussed here, it's going to be the same deal. We're going to be solving an equation which says that cot k a is going to be infinite and that means that k a is going to be pi, 2 pi, 3 pi, so on. So these are going to be the even parity states and then we will find that k a is equal to pi, 2 pi, 3 pi, etc. for the odd parity states.

So the infinitely deep well will have an infinite number of solutions and what do the wave functions look like? Well the wave functions are going to be cos k x where k a is equal to some number of odd pi by 2's. So the wave function of the even parity states is going to vanish. This is going to be cos k x, and the wave function is going to vanish here and here by virtue of these conditions there. And the same thing will happen for the odd parity states. For example the first odd parity state is going to have a wave function which looks like this. It's going to be sin k x – I need a better piece of chalk – it's going to be sin k x where k a is equal to a number of pi's and therefore the sin vanishes. So it's going to vanish. So this is a concrete example but it leads to the general – it inspires the general principle that a wave function vanishes adjacent to an infinite, region of infinite potential.

Physically what's happened is that well this big k has grown bigger and bigger and bigger and bigger and therefore this exponential has grown steeper, the curvature of it has grown larger and larger and larger and larger, so we've gone through a – as we raise the walls the transition at the edge of the well goes from being nice and easy, with a small value of k, through a bigger value of k, to ultimately an infinite value of k, which allows it to discontinuously go from a finite slope right round to no slope. And that's why it's a general property of these solutions, of the time-independent Schrödinger equation, that as you approach the edge of a region of infinite potential, the wave function vanishes in anticipation of that infinity.

So another strange aspect, another physically strange thing that the theory is telling us is that the wave function, the particle has negligible probability of being found in the neighbourhood of this region where it's strictly forbidden. It anticipates the fact that it's going to be forbidden. And you won't find it even near this dangerous place.

Okay, it's time to stop.