Transcript for Video 3: 1D Schrödinger equation

[1] Welcome everyone to our third quantum mechanics video! Today I want to discuss with you the 1D Schrödinger equation, which means the Schrödinger equation of a particle travelling along 1 axis in position with co-ordinate "x". We'll talk about how to solve this equation in different circumstances: for particles enclosed by a square potential well, for particles contained by a harmonic oscillator potential, and for beams of particles which are incident on a potential step or barrier.

[2] In the previous video we saw that the solutions to the Schrödinger equation for particles of constant energy are stationary states, in which the particle's wavefunction is the product of an energy eigenfunction, which depends on position "x", and a complex exponential function which depends on time "t" and the energy value. We've labelled these energy states with an integer "n" to indicate there are multiple possible solutions with different energy values. The energy eigenfunction must satisfy the time-independent Schrödinger equation, which we can see on the slide. A common problem in quantum mechanics is to solve this differential equation for the energy eigenfunctions, given a particular potential energy function, "V(x)". Let's also recall that the time-independent Schrödinger equation is just the same as the eigenfunction-eigenvalue relation for the Hamiltonian or energy operator.

[3] The wavefunction in quantum mechanics must satisfy certain conditions, which help us find valid solutions to the Schrödinger equation. These conditions are known as boundary conditions, and such conditions are always needed when solving differential equations like the Schrödinger equation. For the Schrödinger equation there are two key boundary conditions. First, the wavefunction must be a continuous function of "x", meaning that there are no sudden jumps in the wavefunction. This is because the wavefunction represents a probability, and the probability must be well-defined at every point. A sudden jump in the wavefunction would imply that there are multiple values of probability, which is not allowed! The second boundary condition the wavefunction must satisfy leads from the first. If the wavefunction is continuous, then the form of the Schrödinger equation shows that the first derivative of the wavefunction must also be continuous. This is because the Schrödinger equation depends on the second derivative of the wavefunction, which can only be cleanly evaluated if the first derivative is continuous. The only exception to this second condition is where there's an infinite jump in potential.

[4] A classic example of applying these boundary conditions to solve the wavefunction, or energy eigenfunction, is for a particle enclosed in an infinite square potential well. Let's recap the solution to this problem. An infinite square well means that we have a potential function which is zero across the width of the well – we'll take that to extend across the range "x = -L" to "x = +L" – and infinity outside that range. To solve for the wavefunction, we first consider the time-independent Schrödinger equation inside the potential well, where the potential is zero.   This takes the form of a second-order differential equation for the energy eigenfunctions corresponding to energy "E", which has solutions of the form "sine k x" and "cosine k x". We can check these are solutions just by substituting them into the Schrödinger equation, after which we find a relation between "k" and the energy of the state. The constant "N" at the front of the solutions is the normalisation constant, which we

can set by ensuring that the modulus squared of the wavefunction integrates to "1" over the range. Next, we know that the particle cannot enter the outer region where the potential is infinity. This must mean there is zero probability of finding the particle in this region, hence the wavefunction must be zero in this outer region. However, we know from the boundary conditions that the wavefunction must always be continuous, and so the wavefunction is therefore tied to be zero at the edges of the potential well, where "x = -L" or "x = +L". Looking at our sine and cosine solutions, which oscillate according to "k times x", this implies that the value of "k" is restricted to certain discrete choices which mean that the sines and cosines perfectly fit inside the potential well, producing a value of zero at the edges. These discrete values of "k" lead to discrete values of energy, since the energy depends on "k". Putting this all together and determining the normalisation constant, we can find the set of possible energy eigenfunctions and eigenvalues shown on the slide, which are labelled by integer values of "n".

[5] Let's have a look at the shapes of these energy eigenfunctions: they are sines and cosines which are tied to reach zero at the edges of the potential well. Here's a plot of the first few energy eigenfunctions. Just for clarity, in this diagram the eigenfunctions have been offset along the y-axis to help distinguish them. Since these are energy eigenfunctions, particles which have these wavefunctions would have known, fixed energy values.

[6] Let's now consider a more complicated scenario: a particle enclosed in a finite square well. It's a similar set-up to the infinite square well, except the potential outside the well takes on the finite value "V_0", not infinity like before. We'll focus here on bound energy states of the particle, which are defined such that the particle's energy value is less than the height of the potential well. In classical physics, it would not be possible for a particle with such an energy to be found in the region outside the box, since this would violate conservation of energy. However, we'll shortly see that in quantum mechanics, the particle can actually appear in the forbidden region! This is a phenomenon known as quantum tunnelling. Let's now solve for the wavefunction of the finite square well and see how this situation can occur.

[7] Our recipe for determining the wavefunction is to solve the time-independent Schrödinger equation and apply the boundary conditions. I'll separate the solution into two separate cases for different ranges of "x". The first case is for inside the square well, for "x" values between "-L" and "+L". Here, the potential energy is zero. This is exactly the same situation as for the infinite potential well, so I can write down the same solution as before. I obtain a family of even solutions, or cosine functions, and odd solutions, or sine functions, where even and odd here refer to the symmetry of the function about the point "x = 0". Now let's consider the second range of "x" outside the well, where the potential is equal to "V_0". The Schrödinger equation here takes on an altered form because of the potential energy contribution, where the sign of the second term of the equation has changed compared to before, because for bound states the energy value "E" is less than "V_0". Because of this sign change, the sines and cosines we used as solutions inside the well will no longer work here. Instead, the form of the solution outside the well is an exponential function depending on a variable I've called "l", which can cause the exponential to either rise or decay depending on its sign. We can demonstrate this exponential solution works by

substituting it into the Schrödinger equation, after which we find a relation for "l" in terms of the energy and potential values. There's an important restriction on which of these types of exponentials are allowed. If the wavefunction represents a probability, it must be normalised across the full range of "x", from "minus infinity" to "plus infinity", such that it integrates to give "1". For this to work, the wavefunction must approach zero in the limits of plus or minus infinity, otherwise it could not be normalised. Therefore we always need to use the decaying exponential solution in each direction.

[8] I can now paste together the complete solution from these different regions and apply the boundary conditions. I'll focus here on the even solutions in the middle zone, using the cosine solutions. I'll also write down the form of the solution to higher "x" values, which is the decaying exponential. We can find the unknown amplitudes in these solutions using the boundary conditions. First, let's require that the wavefunction is continuous at "x = +L". This condition requires me to equate the wavefunctions at this point, obtaining a relation between the amplitudes. Also, the second boundary condition requires that the derivative of the wavefunction must be continuous, since we do not have an infinite jump in potential at this point. Applying this second boundary condition at the point "x = +L", we find a second relation between the unknown amplitudes. Dividing these two equations, the unknown amplitudes "A" and "B" cancel out, yielding a relation between "k" and "l". Since "k" and "l" both depend on the energy "E", this equation can be solved to find the possible energies of the particle in this finite square well. You can find the details of this solution in the textbook. Here's a picture of the first few energy eigenfunctions of the infinite and finite potential well that result from this process. These eigenfunctions have again been offset along the y-axis so you can more easily distinguish between them. A fascinating difference is that for the finite potential well, the wavefunction doesn't go to zero at the edge of the well, but transforms into a decaying exponential function which extends into the classically-forbidden region. The boundary conditions ensure that the different pieces of the wavefunction tie continuously together, to form the overall wavefunction.

[9] We'll now consider another important solution of the Schrödinger equation for a case known as the harmonic oscillator. A harmonic oscillator describes a particle moving in a quadratic potential as a function of distance from the origin at "x = 0", just like a mass on a spring in classical physics. In classical physics, the mass would oscillate to and fro, executing simple harmonic motion with an angular frequency "omega" related to the spring constant, and an amplitude related to the energy of the particle. This is also an important example in quantum mechanics, because it's a good model of certain atomic situations.

[10] When we solve for the wavefunction of a particle moving in a quadratic potential in quantum mechanics, there are some key differences compared to classical physics! The particle does not have a definite location and may be found outside the classically-permitted region. Also, its energy is restricted to certain discrete eigenvalues. These energy values can be found by solving the Schrödinger equation for the quantum harmonic oscillator, which we'll now demonstrate. The Schrödinger equation for this case includes the quadratic potential, as you can see on the slide. It's convenient to express this in terms of the angular frequency "omega" from the previous slide. By solving this differential equation, we can find the energy eigenfunctions and eigenvalues for the harmonic oscillator. The lowest energy eigenfunction actually has a Gaussian functional form, "e to

the minus a times x squared". I can verify this form is a solution by substituting it in the equation, after which I'll find that it has an energy value equal to one half, multiplied by h-bar, multiplied by omega. The substitution will also yield a value for the constant "a" inside the wavefunction. If you wish you can pause the video and give this a try. This Gaussian function turns out to be the energy eigenfunction with the lowest energy value, which is also known as the "ground state" of the harmonic oscillator.

[11] How can we find the other energy eigenfunctions, with higher energies than the ground state? One approach to this problem would be to carry out a general solution to the Schrödinger equation for the harmonic oscillator – this is a somewhat arduous exercise that you can find in the textbook! However, there is a quicker approach which makes use of operators. Here I'm going to introduce two new operators, "A plus" and "A minus", which are called ladder operators for reasons we'll soon see. These ladder operators are combinations of the quantum mechanical position operator "x-hat" and the momentum operator "p-hat", and by substituting in their known forms, I can find the expressions for these ladder operators shown on the slide. Here, I'm using the same constant "a" I introduced on the previous slide, which helps parameterise the ground-state wavefunction.

[12] Operators act on functions to produce other functions. Let's calculate the result of applying the "A-plus" operator to the ground-state energy eigenfunction, which I'll call "psi_1". When I do this calculation, I find another wavefunction which I've called "psi_2". It turns out, which I can show by substitution in the Schrödinger equation, that "psi_2" is another energy eigenfunction of the Schrödinger equation, with energy eigenvalue "three halves h-bar omega". Similarly, I can show that if I apply the "A-minus" operator to "psi_2", I'll get back the ground-state eigenfunction "psi_1" – and also that "psi_1" and "psi_2" are orthogonal. We learn from these calculations that when we apply the operator "A-plus" to an energy eigenfunction, we obtain the next eigenfunction of higher energy. And when we apply the operator "A-minus" to an energy eigenfunction, we obtain the next eigenfunction of lower energy. Hence "A-plus" and "A-minus" are called ladder operators, because they move up and down the ladder of energy states.

[13] We've seen that the first two energy eigenvalues of the quantum harmonic oscillator are "one half h-bar omega", and "three halves h-bar omega". In fact, all the energy eigenvalues of the harmonic oscillator are evenly spaced by intervals of "h-bar omega", as you can see in the general formula listed on this slide and this gratuitous picture of a cat!

[14] Let's make a graph of the first few energy eigenfunctions of the quantum harmonic oscillator, as a function of the position coordinate, where the bottom of the potential well is located in the middle of each graph. On the left-hand side we can see the wavefunction against position, and on the right-hand side the wavefunction has been squared to obtain the probability density against position. The different rows of graphs show different energy states, starting from the ground state eigenfunction at the bottom, which we have already seen is a Gaussian function. As we move up the energy states, the eigenfunctions alternate between even and odd functions of "x", and become more "wiggly" as we add in new polynomial orders.

[15] Here is a general proof that when the "A-plus" operator is applied to an energy eigenfunction, it always produces another eigenfunction of higher energy. I won't go through this proof in detail and you don't need to memorize it, but I've included it in case you are curious whether the cases we've demonstrated on the previous slides hold more generally. Please feel free to pause the video here if you'd like to check it in more detail.

[16] In the final section of this video we'll discuss unbound particles moving in one dimension, which means particles which can escape to infinity because their energy values exceed any potential step which might limit them. We'll first consider a particle which is completely free in space, moving in a region of space where the potential is zero. The solution of the time-dependent Schrödinger equation in this case is a complex exponential function, which we can demonstrate by substituting this solution form into the Schrödinger equation. The "e to the i k x" term in this wavefunction describes a wave travelling in the positive "x" direction. If a particle was moving in the negative "x" direction instead, I would have to take the form "e to the minus i k x" instead. I can understand this difference by noting that these complex exponentials are eigenfunctions of momentum, with positive and negative momentum values depending on the sign. After substituting this wavefunction in the Schrödinger equation, I can also find relations between the energy of the particle and the values of "k" and "omega". This complex exponential wavefunction represents a wave – that is, a beam of particles with definite momentum, but no definite position.

[17] How should we think about the normalisation of this wavefunction? We normally aim to normalise a wavefunction by fixing the integral of the modulus squared of the wavefunction over all space to give a value of "1". However, we can see that for the free particle wavefunction represented by a complex exponential function, this integral actually gives us infinity! So in this case, we have to think about normalisation in a different way. We'll imagine that this wavefunction represents a beam of particles, not a single particle, and we'll consider that the normalisation indicates the average separation of particles in the beam, which we can also think of as the intensity of the beam. Here's a picture of this situation in which particles are separated by a distance "L", remembering that this is a classical representation of a function that is actually a wave! After normalising the wavefunction over a range "L", rather than over infinity, we deduce that the normalisation constant "N" is equal to "1 divided by the square root of L". Hence the intensity of the beam, which is proportional to the number of particles per unit length, is proportional to the modulus squared of this normalisation constant.

[18] Let's now use these free particle wavefunctions to study what happens when a beam of particles is incident on a potential step. We'll assume here that the energy of the particles exceeds the height of the step. A certain fraction of the incident particles will be transmitted across the step and propagate to positive infinity, and a certain fraction of the particles will be reflected back from the step and propagate to negative infinity. Our aim in this problem is to find these transmitted and reflected fractions. The solution method is to split the wavefunction into three different terms: an incident, transmitted and reflected beam. I can use the free particle wavefunction to write the forms of these different contributions. First, the incident beam takes on the complex exponential form we discussed on the previous slides, where the "k" value is related to the energy. The reflected beam takes on a similar form to this, where I've changed "plus k x" to "minus k x" because

the beam is moving in the opposite direction, and I've also changed the normalisation constant from "I" to "R" because only a fraction of the beam is reflected, which we still need to determine. Finally, for the transmitted beam, the variable "k" changes its value and I've called it "l", since if I substitute in this transmitted solution to the Schrödinger equation in the region "x greater than 0" containing this potential function, I'll find a relation for "l" in terms of both the energy and the potential "V_0". I've also included a different normalisation for the transmitted wavefunction, "capital T".

[19] How can I find the relations between these normalisation constants? In the region of negative "x", to the left of the potential step, the total wavefunction is a sum of the incident and reflected wavefunctions, which I've combined in the equation on the slide. In the region of positive "x", to the right of the potential step, the total wavefunction just consists of the transmitted particles. We now apply the boundary conditions on the wavefunction at the join between these regions, at "x equals 0". Since the wavefunction must be continuous at this join, substituting "x equals 0" in the trial solutions, and cancelling the term involving time, produces the result that the incident coefficient plus the reflected coefficient must equal the transmitted coefficient. However, this equation doesn't give me enough information to separately solve for "R" and "T". The second condition comes from the fact that the derivative of the wavefunction must also be continuous at this join. Differentiating the trial wavefunctions with respect to "x", and again substituting "x equals 0" and cancelling out some terms, I obtain this second relation linking the different coefficients. I now have two equations for two unknowns, which I can re-arrange to obtain the values of "R" and "T" in terms of the incident amplitude "I". In these equations I have also substituted in the relations for "k" and "l" in terms of the energy of the particle "E", and the height of the potential step "V_0". You can see that these reflected and transmitted coefficients depend on the height of the step compared to the energy of the particle – for a low step the reflection coefficient reduces towards zero.

[20] An interesting case occurs when a beam of particles is incident on a potential barrier which has a height greater than the energy of the particles. Classically speaking, all the incident particles should reflect from this barrier and not be transmitted, since they don't have enough energy to cross the barrier. However, quantum mechanics says differently! In a phenomenon known as quantum tunnelling, some particles can still reach beyond the barrier and propagate to plus infinity. The key point is that the wavefunction inside the barrier region is not zero, but rather we can assume a trial wavefunction involving simple exponential functions, rather than complex exponential functions like for the incident beam. But the solution method is the same, and involves applying the boundary conditions at the two joins "x equals 0" and "x equals L". We'll go through this case in more detail in the class activity.

[21] I'll end with a summary of this video. We started by discussing square potential wells or bound particle states. The energy eigenfunctions satisfy the time-independent Schrödinger equation, and we mentioned the key boundary conditions on the form of the wavefunction which must apply at any change in the potential value. We also introduced the quantum harmonic oscillator and the ladder of resulting energy states separated by intervals of "h-bar omega". Ladder operators can be used to convert between the different energy eigenfunctions. Finally, we discussed the wavefunction representation of a beam of

free particles, and how boundary conditions can be used to determine the reflection and transmission coefficients of these beams at potential steps and barriers. This ends our summary of the different applications of the Schrödinger equation in 1 dimension, and in the next video we'll build on this by extending our discussion to the full 3 dimensional world!