Transcript for Video 2: How QM Works, Part 2

[1] Welcome everyone to our second video about quantum mechanics! This video is the concluding part of our summary of how quantum mechanics works, in which we're going over the basic principles, mathematics and structure of quantum mechanics. In this video we'll meet the operators corresponding to some different measurable quantities. We're also going to discuss the uncertainty principle, and what it means when two observables can be simultaneously known. Finally, we'll talk about how a wavefunction evolves forward in time.

[2] This first slide provides a quick recap of the measurement process in quantum mechanics, which we discussed in detail in the first video. The state of a particle is described by a wavefunction. Let's say we want to measure a particular observable quantity, such as position, momentum or energy. This observable has a corresponding operator, which possesses a set of eigenfunctions and eigenvalues. It's always possible to express the wavefunction of the particle as a linear combination of those eigenfunctions, and the possible results of the measurement are the corresponding eigenvalues of the operator. We don't know which eigenvalue will result, but we do know the probabilities of each result, which are determined by the coefficients of the eigenfunction expansion. Once we perform the measurement, obtaining one of the eigenvalues as the result, the wavefunction collapses to the corresponding eigenfunction. So, this is the way in which the world works in quantum mechanics!

[3] Now let's introduce some key observables and their associated operators. We'll consider the momentum, position and energy of a particle, which are all key physical properties. We'll go through which operators represent these quantities, and what this implies for their possible eigenvalues and eigenfunctions. And don't forget that mathematically, an operator is a mathematical instruction which acts on a function, to produce another function.

[4] Let's start with momentum. I'll state here the momentum operator for a particle moving in one dimension. This operator, which I'll write as "p" for momentum with a hat on top, differentiates a function with respect to "x", and multiplies the result by "minus i h-bar". The "i" that appears here is again the square root of minus 1, that is, an imaginary number. However, remember that the wavefunction in general can be complex, so that "i" can help ensure that our eigenvalues are real numbers. We can identify the eigenfunctions of this operator by using a trial solution. If we try an eigenfunction of the form shown on the slide, "e to the i p x on h-bar", and apply the operator for momentum, we'll end up with the same function multiplied by "p". You can try this out if you wish! Hence, this function is an eigenfunction of the momentum operator, with eigenvalue "p".

[5] How does this help us figure out, when we've given a wavefunction, which momentum values can be measured, with what probabilities? To answer this question we need to apply the quantum mechanics rules we've been discussing. The particle has a wavefunction, and we need to express that wavefunction as a sum over the eigenfunctions of momentum, weighted by some coefficients. This is always possible to do, since the eigenfunctions of an operator may be combined to construct any function. The momentum values appearing in

this expansion tell us which values can be measured from the wavefunction, and the modulus squared of the coefficients tell us the probabilities of obtaining each value. We need to remember to take the modulus squared, since those coefficients can be complex numbers in general, and the modulus squared produces a real number like a probability.

[6] Let's see an example of this process in action. We'll think about a particle which is in the ground energy state of an infinite potential well over the range "x = -L" to "x = +L", which has a wavefunction of the cosine form. If we look at this wavefunction, we can understand the "1 divided by the square root of L" term as normalising the wavefunction, to ensure its modulus-squared integrates to 1 over the range of the well. And the cosine function peaks at "x = 0", and reaches zero at the two edges of the well. To understand which momentum values can be measured for this particle, we need to express the wavefunction as a sum of momentum eigenfunctions – which are the complex exponential functions we met on the previous slide. There's some useful maths which we can use to convert between sines and cosines and complex exponentials. Applying this maths identity, we can transform the cosine wavefunction into a sum of two complex exponential functions. We can identify each of these two complex exponentials with a momentum value – by comparison with the form of the momentum eigenfunction, we can see that these momentum values are "plus or minus pi h-bar divided by 2 L". Hence, when we measure the momentum of a particle in this particular wavefunction we can obtain two values, which are equal and opposite: the particle's momentum can be directed to the left or to the right of the well.

[7] Now let's consider the operator for the position of a particle. This operator has a simple formulation when it acts on a function: its instruction is to multiply the function by the position co-ordinate "x", so the operator is simply the variable "x". We won't go into the eigenfunctions of the position operator in this video – these are called the "Dirac delta functions", whose maths is not part of our course – but we will need to use the position operator again over the next few slides, when we discuss the uncertainty principle.

[8] Let's complete our review of operators by considering the energy of a particle, which is a critical quantity in physics and also quantum mechanics. The energy operator is also known as the Hamiltonian operator, and has the symbol "H" (with our usual hat to indicate an operator). The form of the energy operator can be deduced by analogy. The energy of a free particle, which means a particle not moving in any potential well, is given by the kinetic energy, which can be written in the form "p squared divided by 2m", where "p" is momentum and "m" is the mass of the particle. To find the energy operator for a free particle, we can substitute the operator for momentum into this formula. Multiplying this out, we find the energy operator for a free particle. It's the second derivative with respect to position, multiplied by "minus h-bar squared divided by 2m". For a particle moving in a potential, we also need to include the potential energy term. To do this we just amend our Hamiltonian operator by adding in this potential energy function. So, this potential energy part of the operator simply multiplies the function acted on by the operator by "V(x)".

[9] The eigenfunctions of the energy operator are the solutions of the standard equation defining the eigenfunctions and eigenvalues of an operator. If I substitute in the formula for the Hamiltonian, or energy operator, I end up with this differential equation for the energy eigenfunctions "psi(x)" in terms of the potential energy function. You'll recognise this

equation from your previous studies of quantum mechanics: it's called the timeindependent Schrödinger equation. We'll shortly link this equation with the timedependent Schrödinger equation we met in the previous video, but it is an energy eigenfunction equation, where the "E" values are the energy eigenvalues or possible energy states of the particle. This time-independent Schrödinger equation is the typical starting point for many quantum mechanics problems, as we'll see in the next video.

[10] So, we've discussed the rules for measuring an observable in quantum mechanics. And we know that the results of this measurement must be an eigenvalue of the corresponding operator, but which eigenvalue we obtain is uncertain – unless, the wavefunction is an eigenfunction of the operator, in which case we'll always recover the corresponding eigenvalue. We'll now discuss the question of whether more than one observable can be simultaneously known – in other words, can a function be an eigenfunction of multiple operators? This is a central question in quantum mechanics: which set of observations can be simultaneously certain at a given moment. To answer this question we have to learn more about a mathematical idea known as commuting operators.

[11] What is meant by commuting operators? Two operators are said to commute if, for any function, the result of applying those operators doesn't depend on the order. So if I first apply "B" to the function and then "A" to the result of that, I'll get the same result as if I had first applied "A" to the function and then "B". Let's see some examples. An example of two commuting operators is the first derivative operator, and the second derivative operator. Regardless of the order in which I apply those operators. I'll obtain the third derivative of the function. Therefore, these are commuting operators. An example of operators which do not commute are the derivative operator, and the operator which multiplies a function by "x". In this case, the result does depend on the order in which we apply these operators, as you can see worked out on the slide, since the presence of the "x" creates an extra term to differentiate if it's applied first. Therefore, these are non-commuting operators.

[12] The concept of whether or not two operators commute is so important in quantum mechanics that we define a special symbol to cover it, known as the commutator. This symbol consists of square brackets containing the two operators, and it corresponds to the difference between applying the two operators in the opposite orders. So this commutator symbol is itself an operator, which can be applied to a function. If the commutator is formed from two commuting operators, then applying it to a function will always produce a result of zero, since the results of the two terms will cancel out. Returning to our examples, in the case where the two operators are the first and second derivatives, then I can determine the commutator of those operators to be zero, because it corresponds to subtracting identical third derivatives which cancel out. But if I evaluate the commutator of the derivative operator and the operator which multiplies a function by the position coordinate "x", this commutator can be evaluated to have the effect of multiplying the function by "1", that is, it leaves the function unchanged. I can derive this result by simply applying the commutator to a function, substituting in the operators, and expanding out the result, as you can see on the slide.

[13] Let's now apply these ideas to quantum mechanics, using the operators we've introduced for position, momentum and energy. The commutator of the position and

momentum operators is very similar to the second example on the previous slide, since the position operator is equivalent to multiplying by the position co-ordinate, and the momentum operator is proportional to the derivative with respect to "x". Hence this commutator is not zero, but rather the result is to multiply the function by "i h-bar". By contrast, the commutator between the Hamiltonian (or energy operator) for a free particle and the momentum operator is similar to the first example on the previous slide, since the energy operator involves the second derivative of position, and the momentum operator involves the second derivative of these two operators is zero. We can express this situation by saying that the position and momentum operators do not commute, but the position and energy operators do commute for a free particle. So, we've seen that some pairs of operators have a non-zero commutator, and some pairs of operators.

[14] What does the difference between commuting and non-commuting operators imply for measurements? The important mathematical consequence is that when two operators commute, an eigenfunction of one operator is simultaneously an eigenfunction of the second operator. I've written a proof of this result on this slide, although you won't need to memorise this. This proof uses the expansion of a function in terms of eigenfunctions to show that when two operators commute, or in other words have zero commutator, these operators have an identical or simultaneous set of eigenfunctions. You can pause the video here if you'd like to study this proof more carefully.

[15] In this case, what happens when we measure the observables corresponding to two commuting operators? Suppose a particle has any wavefunction. We'll measure one of the observables, say "A", and obtain a result "a_n" which is one of the eigenvalues of that operator. The wavefunction now collapses, and the particle's new wavefunction is the eigenfunction corresponding to this eigenvalue. Now suppose we measure the second observable, "B". Since the operators corresponding to "A" and "B" commute, they possess a simultaneous set of eigenfunctions, so the new wavefunction is also automatically an eigenfunction of the second operator. Because it's an eigenfunction, we therefore know that when we measure the observable "B", we'll always get the corresponding eigenvalue "b n" with 100% certainty. Let's note here that the eigenvalues of the two operators are different values, even though the eigenfunction is the same. Let's now measure the first observable again. The wavefunction is still the same eigenfunction of the first operator, and so we'll again recover the same eigenvalue as before, "a_n". And if we now measure the second observable again, we'll also obtain an unchanged result. In other words, the result of measuring the two observables can be simultaneously predicted with 100% certainty, because the wavefunction can simultaneously be an eigenfunction of both operators. These two observables can be simultaneously known.

[16] Let's relate this scenario to our previous examples. The position and momentum operators do not commute, or in other words the commutator of these two operators is non-zero. This means that position and momentum cannot be simultaneously known: measuring one of these variables is always going to scramble the other variable in an unpredictable way. In contrast, the Hamiltonian (or energy operator) and momentum operators do commute for a free particle, which means a particle moving in a constant

potential. This means that the energy and momentum of a free particle can be simultaneously known.

[17] We can summarise the situation as follows: certain pairs of observables can be simultaneously known, such that repeated measurements of those quantities will always recover the same values. These observables, which are known as compatible observables, have commuting operators. Other pairs of observables can't be simultaneously known, and repeated measurements will produce values which change each time a measurement is made. These observables have non-commuting operators. It's important to remember this link between commuting operators and compatible or simultaneous observables.

[18] These considerations lead us to the famous uncertainty principle in quantum mechanics. The uncertainty principle is just another way of saying that a pair of observables can't be simultaneously known, if their corresponding operators don't commute. A good example involves momentum and position. If a particle has a precisely-known momentum, then its wavefunction is an eigenfunction of momentum, which we saw previously in this video takes on a complex exponential form. We can see that this eigenfunction is infinitely extended in space – if we calculate the probability density by taking the modulus squared, it's the same value everywhere. So precise information about the momentum, which we have because this is a momentum eigenfunction, implies no knowledge about the position.

[19] A nice conceptualisation of this issue is to imagine that the act of measuring one property, causes an uncertainty in another property. Suppose we want to measure the position of an electron, by bouncing a photon off it and using a microscope. This measurement process will perturb the electron and cause an uncertainty in the new value of the momentum. Hence, the act of measuring position, scrambles momentum.

[20] We can describe the uncertainty principle by precise mathematics using commutators and expectation values. I've written the exact formulation in the box, where the uncertainty is expressed as a standard deviation or spread in multiple measurements of both observables. The uncertainty principle states that the product of these standard deviations takes on a minimum value, determined by the commutator of the two corresponding operators. You can find a derivation of this result in the textbook. Since this limit is applied to the product of the two standard deviations, when the measurement of one of the observables becomes very accurate, implying a small spread, the uncertainty or spread in the other observable must become very large to compensate, and leave the product unchanged. Substituting in the commutator for position and momentum as an example, I recover the uncertainty principle that applies to these two observables: the product of the error in these two quantities must be at least "h-bar divided by 2".

[21] In the final part of this video we'll focus on the time-evolution of the wavefunction. Let's return to the time-dependent Schrödinger equation we met in the previous video, which is the equivalent of the equation of motion for a particle in quantum mechanics. Substituting in the form of the Hamiltonian or energy operator, this equation can be written in the form shown on the slide, where we saw previously that the Hamiltonian includes terms corresponding to the kinetic and potential energies of the particle. There's an important technique for solving equations like this, in which we look for a separable solution. This means that we consider solutions in which the dependence of the wavefunction on "x" and "t" is separated into a product of two different functions, each depending on only one of these variables. We can use this separable form as a trial solution to the equation.

[22] After substituting in this separable solution to the time-dependent Schrödinger equation and re-arranging, we find the equation you can see on the slide. We have rearranged this equation such that all the functions depending on "x" are on the left-hand side, and all the functions depending on "t" are on the right-hand side. The key to the solution is that both sides of this equation can be set equal to a constant, which I've called "E". That's because I can already see from the left-hand side that this equation is just the energy eigenfunction equation, in which "E" is the eigenvalue. I can now use the right-hand side of the equation to solve for the time function. This is a relatively simple differential equation whose solution is a complex exponential in time. Now putting the position and time components back together, the separable solution takes the form of the energy eigenfunction multiplied by a complex exponential in time which also depends on the energy eigenvalue. This wavefunction is a solution to the time-dependent Schrödinger equation which has a definite total energy, because it is an energy eigenfunction evolving forward in time. This wavefunction is also called a "stationary state", because when I compute the modulus squared of the wavefunction, which describes the probability of locating the particle as a function of position, this probability does not depend on time, because the complex exponential cancels out when taking the complex conjugate. So the "stationary" refers to the fact that the probability distribution of position does not vary with time.

[23] How do we apply this solution form in a practical case? Let's say we're given the wavefunction of a particle at time zero, and we want to know how this wavefunction evolves to later times. We can use stationary states to solve this problem, and we'll express the solution as a series of steps. The first step is to express the wavefunction we've been given, at time zero, as a sum of energy eigenfunctions. We can always do this for any wavefunction. The second step is to remember that each energy eigenfunction evolves forward in time by multiplying it by the complex exponential factor depending on the energy of the state. The third step is to combine these time-evolving eigenfunctions using the same coefficients as in the first step. This produces the time-dependent form of the wavefunction.

[24] Let's consider an example of this, using the same case we considered in the previous video, of a particle in an infinite potential well with a wavefunction at time zero equal to the sum of two sine waves. We'll apply our 3-step method to find the wavefunction at later times. First, we saw previously that this wavefunction can be expressed as a sum of the first two energy eigenfunctions of the infinite potential well, with coefficients equal to "1 divided by the square root of 5" and "2 divided by the square root of 5", which ensure that the wavefunction is normalised. Moving to the second step, if the two eigenfunctions have associated energy values "E_1" and "E_2", we can introduce the time evolution by multiplying each eigenfunction by a complex exponential function depending on these energy values. And in the third step, we recombine these time-evolving pieces using the same expansion coefficients as in the first step. We can also check that the modulus

squared of this new wavefunction will be equal to "1" at all times, ensuring that normalisation holds true at all times. I'll leave that for you to check based on the given equationif you wish to do so!

[25] Here's a summary slide to recap the principles we've been discussing in this video. We've introduced the different operators for momentum, position and energy, and identified the time-independent Schrödinger equation as the energy eigenfunction equation. We've also introduced the idea of commuting operators, and their significance in understanding whether or not two observables can be simultaneously known, which is related to the famous uncertainty principle of quantum mechanics. We've also studied the time-evolution of the wavefunction, and how the time-dependent Schrödinger equation can be solved by writing the solution as a sum of stationary states, which are the energy eigenfunctions multiplied by time-dependent complex exponentials depending on each energy value. I hope this was a useful guide to the slides, and I look forward to chatting with you again soon!