

Transcript for Video 1: How QM Works, Part 1

[1] Welcome everyone to our first quantum mechanics video! In this video I'll guide you through the first set of quantum mechanics slides. We'll focus on how quantum mechanics works: what are the rules, and the maths we need to describe those rules. We'll talk about the Schrödinger equation for the wavefunction, how physical quantities in quantum mechanics are represented by operators, and how the results of measuring those quantities relate to the eigenvalues and eigenfunctions of those operators.

[2] Let's start off by making some contrasts between quantum mechanics and classical physics. In classical physics we can determine the equation of motion of a particle using Newton's Laws: force is equal to mass times acceleration, or the gradient of a potential energy. The conditions of a particle's motion can be equivalently described by a conservation of energy rule: kinetic energy plus potential energy equals total energy.

[3] This same picture cannot apply in the quantum or microscopic world because particles can behave, in some circumstances, like waves. You can see this illustrated by the interesting results of the double-slit experiment. In this experiment electrons, which we classically think of as particles, can exhibit wave-like properties like interference and diffraction when passing through two slits. Since a wave is extended in space, this causes us to change how we mathematically describe a particle.

[4] In quantum mechanics, Newton's Laws are replaced by a beautiful relation known as the Schrödinger equation. Let's break down this equation and illustrate some pieces. The " m " is the mass of the particle, and " $V(x)$ " is the potential energy function across position. The " \hbar " with a line through it, also known as " h bar", is given by Planck's constant divided by " 2π ". This is a physical constant which is found everywhere in quantum mechanics. The Schrödinger equation is a differential equation for the wavefunction of a particle, whose symbol is the Greek letter " ψ ", and can be a function of both position " x " and time " t ". We'll discuss the wavefunction in more detail shortly. In the equation this wavefunction is partially differentiated with respect to " x " and " t ". We'll see in later videos how the Schrödinger equation is a direct replacement for the conservation of energy rule, where the sum of kinetic and potential energies equals the total energy. We can also see on the right-hand side of the equation an " i ", which is the square root of minus 1, hence an imaginary component. This seems like a strange variable to include in a physics equation! But this is fine because the wavefunction is also a complex number in general. So it's OK to have other complex numbers in the equation, and we'll shortly see how these imaginary values disappear when we make physical measurements.

[5] Let's talk more about the wavefunction. The wavefunction in quantum mechanics encodes a complete description of the state of a particle or a system at a particular instant of time. So we're no longer describing the motion of a particle by a fixed position changing with time, but rather it's always a state extending over space. In other words our classical picture of a point particle is smeared out into a quantum wave. This wavefunction depends on the co-ordinates of our system, which for our illustration here is just a position " x " and time, and it encodes all the information we can know about that system.

[6] What does the wavefunction mean? The wavefunction actually represents the probability of finding a particle at different positions in space. When we measure the position of a particle, the probability of this position being found in a tiny range between “ x ” and “ $x+dx$ ” is the modulus squared of the wavefunction at that point, multiplied by “ dx ”. Using this modulus squared, which means multiplying the wavefunction by its complex conjugate, is important. That’s because this operation always produces a real number with zero imaginary part, which is needed to represent a probability, whereas the wavefunction itself can be a complex number. This definition also implies that the wavefunction must always be normalised in such a way that this modulus squared integrates over all “ x ” to produce “1”, since the particle must always be found at some location in space, even if we don’t know exactly where. This probabilistic interpretation of the wavefunction is showing that quantum mechanics has a statistical nature – in the sense that we cannot predict the results of measurements in advance, only their different probabilities.

[7] A key fact about quantum mechanics is, when we make measurements of physical quantities, the possible results of those measurements are restricted to a set of specific or discrete outcomes, and we cannot obtain any arbitrary value. So this is like throwing a dice, where only a restricted set of numbers can be obtained. You’ll have seen this property of quantum mechanics before when you studied particles confined to an infinite potential well, and we’ll recap this case shortly. In this case, the possible energy values of the particle are restricted to certain allowed energy levels. Other famous examples involve cats!

[8] Let’s recap the case of a particle enclosed in an infinite potential well, which you have previously studied. An infinite potential well means a potential energy function that is zero within a fixed range, and infinity outside of that range, effectively confining the particle to a box. You’ll remember that the energy of a particle in such a box can only assume certain discrete values, and when the particle is in those energy states, its wavefunction takes the form of sine waves which reach zero at the edges of the box. Please check back the previous quantum mechanics unit if you can’t remember this well – and we will also recap these details in a future video.

[9] Physics is always represented by the language of mathematics, so now let’s talk more about the mathematical ideas which underpin these concepts we’re describing. We need a mathematical structure in which a set of discrete values – which are the results of measurements – naturally appear. This leads us to our new friends: operators, eigenfunctions and eigenvalues. We’ll get to know them well over the next few weeks! The key mathematical statement of quantum mechanics is the following: each quantity we can observe is represented by a corresponding operator. If we measure that observable, we’ll always obtain a result which is one of the eigenvalues of the operator. Let’s go through what these words mean!

[10] We’ll start with the idea of an “operator”. An operator is a mathematical instruction which acts on a function, to produce another function. Here is a symbolic representation. An example operator is the derivative operator, which acts on a function to produce a second function which is the derivative of the first function. Another operator might contain the instruction to multiply a function by “ x ”. This produces a second function which

is “ x ” multiplied by the first function. Both of these mathematical instructions are examples of operators.

[11] Each operator is associated with some special functions called “eigenfunctions”. These functions are special because when we apply the operator to an eigenfunction, it returns the same function we started with, multiplied by a constant. This constant is called the eigenvalue. We can write this idea mathematically using this equation on the slide. In this equation, the upper-case “ A ” is the operator, and we like to write the operator symbols with a hat on top, to identify the fact that it’s an operator. When this operator acts on an eigenfunction, which we have written as the Greek letter “ ϕ ”, it produces the same eigenfunction scaled by a number known as the eigenvalue, which we have written using a lower-case “ a ”. The label “ n ” indicates that there are multiple eigenfunctions and eigenvalues for which we can use different values of “ n ” such as 1, 2 and 3. So in summary, when I apply the operator to the eigenfunction, I’m getting back a scaled version of the same function.

[12] Here’s an example: let’s consider the operator which takes the derivative of a function with respect to “ x ”. It turns out that the function “ e to the power of a times x ”, where “ a ” is a constant, is an eigenfunction of this operator. That’s because when I apply the operator by differentiating this function, I get back “ a ” multiplied by the original function. Therefore, this function is an eigenfunction of the derivative operator with eigenvalue equal to “ a ”.

[13] Let’s recap our key mathematical rule of quantum mechanics: each quantity we can observe is represented by an operator, and the result of an observation will always be one of the eigenvalues of the operator. Some of the physical quantities we’ll be considering to be represented in this way include momentum, position, energy and angular momentum. We’ll meet the precise operators representing these quantities in the following videos. In this video, we’ll speak about things generally so we can understand the mathematical rules which always apply.

[14] The operators which represent physical observables must possess some important properties for these mathematical rules to work. Let’s list the three key properties. First, the eigenvalues of the operator, which correspond to the results of physical measurements, must be real numbers with no imaginary component. Of course, that’s because such measurements of the world do not result in complex numbers. The second key property is that eigenfunctions of these operators form an orthogonal set. This is a mathematical property such that when two different eigenfunctions are multiplied together and integrated over all space, we always obtain an answer of “0”. In this operation, we’ve taken the complex conjugate of the first eigenfunction. When we apply this procedure to a pair of the same eigenfunctions, we end up integrating the modulus squared of that eigenfunction, which will produce an answer of “1” if the eigenfunctions are normalised. The third key property is that any function may always be expressed as a linear sum of these eigenfunctions. Here is the mathematical relation expressing this property, where the coefficients “ c_n ” are numbers multiplying the different eigenfunctions in the sum. We’re going to discuss these properties in more detail over the next few slides.

[15] Let's first see an illustration of the property of orthogonality using the energy eigenfunctions of the infinite potential well, which we previously recalled were sine waves. If I multiply together any two of these sine waves, and integrate the product over the interval of the potential well, I will always get zero because the positive and negative contributions cancel out to produce an average of zero over the full range. Hence, these sine waves are orthogonal. Also, if I take the same eigenfunction twice, setting "m equals n" in this formula, I recover the normalisation condition for these eigenfunctions.

[16] Let's discuss further this idea that any function can be expressed as a linear combination of eigenfunctions, using the formula shown on the slide. In this formula, " $f(x)$ " is any general function, the " $\phi(x)$ " are the different eigenfunctions labelled by " n ", and the " c_n " are the coefficients multiplying these eigenfunctions in the sum. The question is, how can I determine these coefficients? Actually, I can find them using the orthogonality property we have just been discussing. Here's a short derivation. I'll multiply both sides of this equation by one of the eigenfunctions, the complex conjugate of " ϕ_m ", and then integrate both sides over all space. On the right-hand side I can exchange the order of the integral and the sum, whilst leaving the value of the expression unchanged. After applying this step I have created an integral which is the same as the orthogonality integral, which is hence equal to zero (if " m " is not equal to " n "), or otherwise equal to "1". After this substitution, the sum reduces to just one term, the coefficient " c_m " we are trying to find. This relation then provides the recipe for finding the different coefficients of an eigenfunction expansion, given a function " $f(x)$ ".

[17] Let's now focus on the process of measurement in quantum mechanics, and how this process relates to the mathematical rules we've been discussing. This issue is at the heart of quantum mechanics: when observing a property from a given wavefunction, what can I say about the measurements I can obtain, and their respective probabilities? Suppose we want to measure a particular observable such as momentum, position, energy or angular momentum. As we know, this observable is represented by a corresponding operator. We'll discuss the exact form of these operators soon, but let's leave our discussion general for now. Let's first suppose that the wavefunction of the system happens to be an eigenfunction of the operator in question. It doesn't have to be, but let's suppose that it is. In this case, the result of the measurement is always the corresponding eigenvalue of that eigenfunction, with 100% probability.

[18] But what happens if the wavefunction is not an eigenfunction of the operator? As we just saw, even if the wavefunction is not an eigenfunction, it can always be expressed as a linear combination of different eigenfunctions. This was our third key property of the operators representing physical observables. In this case, when we measure the property in question, we can obtain any of the eigenvalues as a result. We don't know which eigenvalue we will find, but we do know the probabilities of obtaining each one. Those probabilities are determined by the coefficients in the linear combination, which have the symbol " c_n ". In fact, the probabilities are the modulus squared of " c_n ", which is always guaranteed to produce a real number, whereas the coefficients could be complex numbers. Importantly, following the measurement the wavefunction changes – we say the wavefunction collapses – and it becomes the eigenfunction corresponding to the eigenvalue I just measured. This is the central measurement rule in quantum mechanics. It's important

that the collapse of the wavefunction takes place because, were I to measure the same observable again, the current wavefunction would now be an eigenfunction of the operator and by the previous rule, I would be bound to obtain an identical result as before, for the repeated measurement. Hence, this rule ensures that if I measure the same quantity repeatedly, I will obtain the same result each time.

[19] Summarising all this: in quantum mechanics, the process of measurement changes the wavefunction – that is, changes the state of a system – causing it to collapse into an eigenfunction. This ensures that future measurements of the same quantity produce the same result. It's equivalent to opening the box containing Schrödinger's cat and seeing what's inside! Having seen the contents, we can't go back and change them!

[20] Let's go through this measurement recipe again, because it's so important. This time I'll represent it on a flow chart. To start off, the state of a particle is described by a wavefunction. Let's say we want to measure a physical observable. We start by asking: what is the operator corresponding to that observable? And what are the eigenfunctions and eigenvalues corresponding to that operator? Then, we're going to express the wavefunction as a linear combination of these eigenfunctions, multiplying each eigenfunction by particular coefficients. The possible results of the measurement are then the corresponding eigenvalues, and the probabilities of each result are given by the modulus squared of these coefficients. I'll then perform the measurement, and obtain one of the eigenvalues as a result. At this moment the wavefunction collapses into the corresponding eigenfunction. Please study this slide and make sure you're happy with this process.

[21] Let's look at an example of how this works in practice. We'll consider a particle which is confined to an infinite potential well in a range between " $x = -L$ " and " $x = +L$ ". This particle has been prepared with the particular wavefunction shown on the slide, and we want to know what energy values can be measured for the particle, and with what probabilities? Let's describe the steps involved when answering this question. First I want to note that the factor at the front of this wavefunction – that is, one divided by the square root of 5 times L -- is playing an important role. It ensures that the wavefunction is normalised, meaning that the integral of the modulus squared of the wavefunction is equal to "1", as it always must. If we're making a measurement of energy, we need to express the wavefunction as a sum over the energy eigenfunctions, which we know are sine waves for the infinite potential well. And we can already see that the given wavefunction is a sum over two of these sine waves. In other examples it could be more complicated to determine this sum, but we're starting with a simple case where it can just be done by inspection. Substituting in the exact form of these normalised eigenfunctions, we see that we can write this wavefunction as a sum over the first two eigenfunctions with coefficients equal to 1 divided by the square root of 5, and 2 divided by the square root of 5. By the measurement rules of quantum mechanics, this expansion means that the possible results of measuring the energy of the particle are the first two energy eigenvalues of the infinite potential well. And the corresponding probabilities are given by the modulus squared of the coefficients, which gives one fifth for the first energy, and four fifths for the second energy. As a check on our answer, we can see that these probabilities sum to give "1", which is good!

[22] Let's now introduce the concept of the expectation value of a measurement. Although we can't predict the exact value resulting from a measurement in quantum mechanics, we can predict the average or mean value of the result, which is known in the language of quantum mechanics as the expectation value. It's as if we carried out the experiment many times, preparing the wavefunction in the exact same initial condition each time, and took an average of the results. The expectation value of a quantity is mathematically denoted using the angled brackets you can see in the formula on the slide, and it's obtained mathematically using the formula for the mean: we weight each of the possible results, which are the eigenvalues in this case, by the probabilities of obtaining those results. As an example of this calculation, imagine throwing a dice. We know that we can obtain any value on the dice from 1 to 6, with equal probabilities of one sixth if it's a fair dice, but we don't know which value will result from any given throw. However, we can calculate the average value over many throws, which is the expectation value, by summing up our possible results weighting each by one sixth. Performing this calculation, we find that the expectation or average value of the dice throw is equal to "3.5", even though this is not a value that can be obtained for any individual throw!

[23] In quantum mechanics we know that the probability of obtaining each of the eigenvalues of a measurement is equal to the modulus squared of the coefficients in the eigenfunction expansion. Knowing these coefficients, we can determine the expectation value using the formula on the slide. In the example of the particle in the infinite potential well that we discussed a couple of slides ago, the two coefficients were one-fifth and four-fifths. Therefore, the expectation value for the energy is given by one-fifth of the first energy eigenvalue plus four-fifths of the second energy eigenvalue. This is the average energy measurement that would be obtained when measuring the energy of many systems with the same wavefunction. So after each measurement the wavefunction collapses, and we have to reset it in the same original state. We can also find a more general formula for this quantity involving the original wavefunction. To do this, we can substitute in for the expansion coefficients using the formulae we previously derived, in terms of the wavefunction and eigenfunctions. I won't show the full derivation, but here is the important formula we obtain for the expectation value of measuring a given quantity from a specified wavefunction, where the capital "A" with the hat is the associated operator.

[24] Let's end this video by re-capitulating the rules of quantum mechanics we've covered today. The state of a particle is described by a wavefunction, which satisfies the Schrödinger equation. The wavefunction tells us the probability of finding the particle in different regions of space at a given moment in time. The quantities we can observe are represented by operators, and the results of measuring those quantities are the eigenvalues of those operators. Any wavefunction can always be expressed as a linear combination of the eigenfunctions of an operator, and the coefficients of this sum tell us the probability of obtaining each value. And when a measurement produces a particular result, the wavefunction collapses into the corresponding eigenfunction. That's all for today. I hope this video provided a useful rundown of the mathematical rules of quantum mechanics, and in the next video we'll develop this further by considering some specific examples of observables, and their corresponding operators. Bye for now!