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Presenter(s) James Binney
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Contributor So, we arrived yesterday at a statement of the fundamental dynamical principle of quantum mechanics; the time dependent Schrodinger equation here. I didn't offer any justification for this time. The justification or arguments which will make this seem plausible are about to come, but they have not yet come. However, we already, at the end of yesterday's lecture, realised that if upsi – if the state of our system is such that the energy is well-determined – the result of measuring energy is certain, then the tiny evolution of that state is absolutely trivial. The state evolves only in that its phase increments at a rate with an angular frequency, E upon hbar, which is typically very large because hbar is very small.

And we went on from that result there to show that the solution to this equation for any state Upsi, takes this form; that the state of the system at an arbitrary time is this sum over the states of well-determined energy where A N, as ever, is E N evaluated at. . .

So, if you evaluate these coefficients that time to equal nought – or indeed at any time at your convenience – then just by inserting into this sum, this ordinary sum, which we've seen a few time, of Upsi expanded in terms of a complete set of states; if we just insert these exponential factors, bingo! We evolve the state according to that equation.

So, that makes these states of well-defined energy of crucial operational significance. And the result of that is that we spent a great deal of time solving the defining equation of these states, which is that H E N is equal to E N E N. The states of well defined energy are by construction eigen states of the Hamiltonian operator. And this is the time independent Schrodinger equation. To distinguish it from the time dependent one up there.

So only states of definite energy solve the time independent Schrodinger equation. Any state – the state of our system – always has to `[[solve 0:02:37]]` off the time dependent Schrodinger equation.

So, the next item on the agenda fundamentally is to provide some justification; make it seem plausible that that is the correct equation of motion, and a good way to do that is to link that to classical mechanics. So, recall classical mechanics; classical physics is that limit where the uncertainty in the values of dynamical variables is sufficiently small that it isn't necessary to calculate the whole probability distribution. It's enough to know what the expectation value of the probability distribution is because the true value will be very close to the expectation value and we ordinarily don't distinguish between the expectation value and the true value when doing classical physics.

So, what we want to do is calculate D by D T of the expectation value of sum observable – I think we're calling observables Q. And let's put an I hbar in front of here, just in order to clarifysorry, in order to simplify the algebra. So, we're trying to calculate this; the rate of change of the expectation value of something. This something might be position, so this might be X; this might be momentum, it might be energy, it might be whatever you want to know about the angular momentum, whatever you want to know about the system, this would tell you the rate of change of the classical value of that variable. Because the classical value is the expectation value.

What is that? Well, this is just a product, so obviously in comes into three parts; I hbar, D Upsi by D T, times Q times Upsi, plus – let's take the last bit now – no, no – plus Upsi D Q, D Q by D T – sorry, these things should probably be – ah! Over there. Whether we make these things partial derivatives or total derivatives is of no significance. This is clearly a total derivative because the thing doesn't depend on anything expect time. Whether we make these partial or total is very unimportant.

So, here we have an I hbar rate of change of Upsi, so this can immediately be replaced by H Upsi. Here we have the `[[bra 0:05:18]]` Upsi and the original equation – we can take the hermition adjoint of the original equation – when it becomes minus I hbar D by D T of the bra Upsi. Curses! Bra Upsi equals Upsi H. Remember the rule when we take hermition adjoints is we reverse the order of the symbols and we take the adjoints of the individual bits. H is an observable, so it's a hermition operator. So, H equals H dagger. So, I can pop those into here and here. The first two terms give me – including the I hbar – this one is going to be minus Upsi H. So, that is I hbar D by D T of the bra Upsi times Q times Upsi. And this one, including the I hbar, this is going to be plus Upsi Q H, and then we have a trailing bit here which will be plus hbar Q – sorry; Upsi – Q by D T Upsi.

And these two can be handily combined together into a commutator because there's a minus sin here otherwise the order of the Q and the H are swapped around. So, this can be written as Upsi; the commutator Q comma H; Upsi; and then this is plus I hbar. Oops. This result goes by the name of Ehrenfest theorem and it's one of the more important results of quantum mechanics.

In most of our applications we can forget about this because what is this last term here? It's the expectation value of the rate of change of your observable. So, if the observable was, for example, X, it would have no rate of change. X is X is X; it's always the same operator. If you're observable with P, it would have no rate of change because the momentum is momentum is momentum; is doesn't change – our understanding of what momentum is doesn't change from moment to moment. If it were angular momentum, it doesn't change from moment to moment.

So, this term here usually falls away. If the Upsi – sorry; D Q by D T, which equals nought, which is the normal state of affairs, then we have that I hbar D by D T of the expectation value of Q, which is often written like this in short hand; notion, notation, alright? We've left out the Upsi either side, just leave the angle brackets, which means the expectation value in any state whatsoever, is equal to the expectation of the commutator `[[cube 0:08:38]]` comma H.

Okay. What does that tell us? It tells us immediately that if an observable commutes with the Hamiltonian – if Q commutes with H, that being the same thing as Q comma H equals nought – then clearly the expectation value of Q is always constant. And physicists are always very excited by quantities which are constant. So we call it – what do we call it in classical physics? – we call it a constant of motion. Famously Newton said that if you didn't go messing with particles the momentum was constant. Or maybe he said the velocity was constant, right? So velocity is a constant of motion. We would now reinterpret that as momentum is constant. We often know that angular momentum is – the angular momentum of the Earth – is almost constant insofar as it's not acted on too much by the moon. And so on and so forth.

So, physics is full of constants of motion, they're very important, in quantum mechanics there's a special notation around here, which is to say that Q, the eigen value of this is a good quantum number. If somebody says that angular momentum is a good quantum number then they're simply saying angular momentum is a constant of the motion.

We can go further than that though – so, we've shown that the expectation value of Q is constant. We could show, easily that the expectation value of Q squared is constant too. It's very straightforward. And it's obviously the case because Q squared is an observable. If Q commuted with the Hamiltonian then Q squared has to commute with the Hamiltonian, so Q squared is also a constant of the motion. That means that if you start – so this implies that if initially – if at T Upsi is one of the states of well defined Q – so, Q R; one of the eigen states of the operator Q, so we know for certain the result of a measurement will be Q R. Then what does that mean? That means that `[[apti 0:11:38]]` equals nought, and the expectation value of Q is obviously equal to Q R, and the expectation value of Q squared is equal to Q R squared, which implies that the variance of Q – so far implies the variance of Q, which is ever defined to be the expectation value of Q squared, minus the expectation value of Q – it's self-squared – vanishes.

So this variant expresses of course the fact that there's no uncertainty in the value that we get. But since this is the constant of the motion and this is the constant of the motion, if this variance vanishes at T equals nought, is vanishes at all times. And the only way that that can happen is if your system stays in the state that it was in originally. So, if it was in a state of well define Q at the beginning of T equals nought, it will be in the state of well defined Q at all subsequent times.

That's why people talk about good quantum number. If I know at some particular time that the angular momentum of this isolated body is hbar or whatever, then I know that at all later times, it's also hbar. It's a quantum number worth knowing because it's always valid information. So, we're very interested in quantities – in observables – that commute with the Hamiltonian.

Let's move over here for the next point. Yes. Okay, so we're interested in things that commute with the Hamiltonian in a trivial observation is that H comma H equals nought. Where I'm doing this is a bad place, isn't it? I'm not sure that there's anything we can do about it.

So, the Hamiltonian commutes with itself, which means that the expectation value of H is a constant if D H by D T equals nought. So, now we need to come back to this point that I said usually, it's going to be the case that the partial derivative of Q with respect to time – I've lost it, It's up there somewhere – the partial derivative of Q with respect to time vanishes. Now, the Hamiltonian is an interesting case where that isn't necessarily the case. There are very important circumstances in which the Hamiltonian does explicitly depend on time – the expression of the energy depends on time – for example, if you put a particle in a time varying magnetic field, the expression for the Hamiltonian – and the Hamiltonian's going to depend on the magnetic field – depends on time. And in those circumstances, the energy of the particle is not going to be constant. And the reason is that that time dependency of the Hamiltonian reflects the work that you're doing on the particle.

But if the Hamiltonian is independent of time, that will reflect you're not doing any work and the expectation value of H equals constant is conservation of energy. So, this condition, it will turn out, is intimately connected to whether or not you're working on the particle.

Now. Let's have a look at the rate of change of the expectation value of any observable when we are in a state; when Upsi happens to be a state of well defined energy. Right? So, these states of well defined energy, we've explained that they're the key to solving the central equation of the theory. So let's ask ourselves a little bit about those states. So, the amplitude – let's have a look at Q E. Right? This is the amplitude to determine Q given that we're in the state E. Let's give it its N – Q N. So this is the amplitude to fine the value Q N if you would measure with the observable Q given that you're in a state of well defined energy E.

Let's work out the time derivative of this. I hbar D by D T of this quantity is equal to – it's very specific – D Q N by E T. I wonder if we should turn this off?

`[[Break in audio 0:17:01]]`

Okay, so we do the same thing. This has to be I hbar thing we get from the hermition adjoint of the equation and we get the time dependent Schrodinger equation, so we get a minus Q N H. So, that is that. And then we put P on to it. And this is going to be – Q N stands by while that, including the I hbar, produces the H E.

And this is nothing very much, right? Because H works on E to produce E, because that's an eigen state H; E times the ket E abandons this, reduces minus E times Q N E; and this H produces an E and so we get a plus E times Q N E. So, these two terms cancel and we've discovered that the rate of change of the amplitude to have the value Q N is constant. The rate change vanishes. This is amplitude Q N E is constant for any Q. So, in order to obtain a result, we didn't make any restriction, any restriction whatsoever on what the observable Q was. So, the remarkable fact, in these states of well defined energy, if your system has well defined energy, all its property – the expectation value of everything observable. And in fact it then follows with a couple of extra steps. The probability distribution of measuring any observable whatsoever is completely constant. Nothing ever changes.

So that leads to E being called stationary state. These states really forever; they are completely eternal or they're completely unchanging. They're not of this world. Right? And in particular, you can never get a system into – as far as this, you can never get a system into well defined energy. Because its going into there would imply something is changing. `[[?? 0:19:58]]` any other change. That's kind of a remarkable `[[?? 0:20:04]]`.

So, now we have a new topic; position representation. This will bring us much closer to the real difficult `[[world 0:20:19]]`. Requires a bit of `[[?? 0:20:20]]`

So, so far we've talked about – we've used abstract representation for a little bit like the energy representation. Let's say we've assumed that our observable has discrete spectrum. So the spectrum is made up of discrete numbers. The thing about the position operator – so this is the operator which encodes the states of well defined position on the X axis. It has a spectrum which is usually why it's continuous. Everyone's reminded of `[[?? 0:21:12]]` infinity. It's not discrete; it's continuous, and this requires some adjustment.

So we have been writing – let's divide the board – we have been writing Upsi is equal to sum A N, shall we say, E N – E is energy representation. Now we're going to write Upsi is equal in integral; that sum over the discrete set if possible, the values, numbers and spectrum becomes an integral over the possible values in the spectrum. So let's remind `[[?? 0:21:54]]` infinity; of some amplitude – the amplitude being X – times the state of well defined definitely being a `[[?? 0:22:03]]`. So this is the state – this is the `[[position 0:22:08]]` of where it is at X, when our particle or whatever is at X; and this is the amplitude to B and X, alright? Amplitude of B and X.

And this is the state at the beginning of X. We used to have that E M U N equals delta `[[?? 0:22:37]]`. What are we going to have now? Let's bra this thing through our X primed and we're going to have the integral; the X primed – sorry, the X – X primed X Upsi of X. This side – oops! – this side is clearly equal from sin – sorry. Sorry, sorry. And what do we want? What we want is this one – it's obvious that this thing vanishes except when X primed is equal to X because if it's definitely an X – sorry – yes, if it's definitely an X, then it certainly isn't an X primed if X primed is different from X.

So, this thing here is nothing except when X equals X primed. And it must be non zero and presumably rather large `[[?? 0:23:39]]`. Sorry, we can fill this in. What is this? This by definition, this is the amplitude to the X primed and I've already said that that is the amplitude to B and X primed. Sorry, X.

So, it's clear that this thing here is Upsi of X primed – the amplitude to B and X primed. So, we have that the amplitude – the Upsi of X primed our function is equal to D X of X primed X Upsi X N. I'm sure you've already met this relationship. And `[[professor 0:24:15]][[?? 0:24:16]][[lectures 0:24:17]]` that this can also be written as X delta with X Y minus X; Upsi of X. So, that result up there has been generalised or has morphed into this thing and then

X primed X is equal to a direct [[?? 0:24:36]] rather than Kroninger delta; delta of X Y Z, that's right.

We used to have that Upsi Upsi was the sum of the A N squares with one, by conservational probability, that this was the sum of the probabilities to get the value E N, but since you had to get some value, that sum of probabilities had to be one. Now what do we have? What does this turn into? This relation here turns into Upsi Upsi – should be one – and how to we express it like this? We say that this is the integral; the X of Upsi X X Upsi. Here we're using the idea, sorry, that we used to have that the sums E N E N is the identity operator. Now we have that the integral X X X is the identity operator. So, all of these sums are turning into integrals so this relationship becomes this because this is the identity operator snuck into there.

And this is what is the amplitude to B and X, so we've call that the wave function of Upsi and X. This is the complex conjugate of that therefore the complex conjugate of this. So this becomes the integral DX of [[mod 0:26:36]] sin squared. So the integral of mod sin squared should be one in this continuous ring. But these are just natural transformations of what we've already done in the discrete case to the continuous case.

The one more thing that we need to write down; we used to have [[a different 0:27:02]] sin was the sum A N E N and phi was the sum of B N E N. Then the complex number phi sin was the sum of E N star A N sum of N. That's the result we have had was the analogous thing here is going to be that phi sin is going to be the integral. Into here we stick an identity operator; the integral D X of ket X primes. So this becomes the integral D X so we stick an identity operator into that [[Cross coughing 0:27:56]] of phi; X X Upsi. This is what we've been calling the wave function of sin of X is the amplitude to B N X which has appeared as a function – it is a function of X; it's a complex number depending on X. And by analogy we should call X Upsi – X phi, sorry. We should call the wave function phi X. That being so, this becomes the complex conjugate of it. And this becomes an integral of the X. So, both of these things of course become a functions of X.

So, this is precisely a transformation of that with the sum when N has been replaced by X and the sum of N becomes an integral over X. This is the stuff we have to do because the spectrum of X is continuous and not discrete.

Let's just do a little practice with this by asking ourselves how does the operator X work on an arbitrary state of sin in this representation? The thing to do is to ask ourselves what wave function represents that? Now, let's just say what is this complex number as a function of X? So, here's the operator X; here is an arbitrary value of X. I would like to know what the amplitude of B X is for this state that you get when the operator X works on [[?? 0:29:46]] wave function X.

When you see an operator X, the obvious thing to do is to stick into here an identity operator made up of the eigen functions of X. So, in order to understand what this is, what we do is we slide into here one of these identity operators. X is busy so my identity operator's going to have to be a sum of X primed; some independent value of X. X X, X primed X, primed sin. So here's the identity operator along with that. Now life is relatively straightforward because this is an eigen function of that operator with this eigen value. That's the definition of this [[?? 0:30:35]] here. So when X meets this it reduces X times X primed with the number times X primed. So this becomes the integral E X primed of the X primed. There's the eigen value of doubt. Then we have X, X primed, and this we recognise to be the wave function of sin evaluated on X primed.

But this we recognise now, we've see that this is the direct delta function of X minus X primed. So, when we do the integration over X primed, this ensures that we have no contribution except for split second where X primed is equal to X and we get the value of the integrand evaluated with these X primed turned into X. So, this is equal to X Upsi of X.

So, at the end of our long story, what have we discovered? We've discovered that the wave function associated with the result using the operator X on some state is simply X times the wave function of the original state. The way to remember that is to say that the operator acts on wave functions by ordinary multiplication. You don't usually go through this kind of performance; you know what's going to happen before you do it. But that's the logical basis with this state.

Let's introduce another very important operator, the momentum operator. Now I'm going to make an unsubstantiated claim about how this operator looks in the positional representation. I don't expect you to think, 'Aha! That makes sense.' It doesn't make sense; in a complete leap in the dark. You will understand later – considerably later – why these operators take the form that they do, but I hope soon to be able to build `[[?? 0:32:58]]` some kind of sense. But what we're going to do just about now is a complete leap in the dark.

Let's investigate the operator. Right? I have to know the momentum `[[?? 0:33:09]]`. Let's investigate it; which is defined thus. Now let's just make sure we understand portionately what's happening here. And operator fundamentally is something which turns a state into another state. When we're in the positional representation we are working with functions. Our states are represented by their wave functions, which is the amplitude of B N X. So the X operator has to turn a wave function of sin into some other function and look X Upsi is another function. It depends on X in a different from what Upsi does.

So similarly, this momentum operator I claim is the momentum operator without any `[[paces 0:34:22]]` we're going to try `[[E 0:34:23]]`. This momentum operator is turning the wave function of sin into its derivative. A derivative is a function different from the function we first thought of. So indeed it's turning a function into a function. So means it is at least a valid operator. Is it hermition? It's not obvious that it's hermition and if it is a hermition, it certainly can't be the momentum operator. So, let's check that out.

Let's write down the complex number of phi P hat Upsi. Let's evaluate this by using this hocus pocus here, alright? So, this is the integral D X. What am I going to do? I'm going to put an identity operator just in here made up of Xs, right? Why? Because I defined P in terms of what happens when it has an X on the left of it. So this is going to be phi X X P hat Upsi. And now we can turn this into wave function language; this is the complex conjugate of a wave function phi. So, this is the integral of the X phi star of X. And we defined what that is; it's minus I hbar D by D X Upsi.

So, we can now integrate by part – we're integrating `[[?? 0:36:18]]` with infinity – so we can integrate by parts – this part of the derivative – to get this part of derivative of phi and on to the phi. So, what does that give me? We get a square bracket term; we have a phi star – oh, and that wretched minus I. Put the minus I hbar outside some vast bracket, right? So, we're going to have a square bracket term now. We're going to have an Upsi star – sorry, a phi star Upsi – of minus infinity infinity. And then we're going to have minus the integral D X D Upsi – sorry; Upsi D phi star by E X. Close the big bracket.

So we can operate under the assumption that this thing vanishes. Now, this is a rather hairy 'don't-press-too-hard' as to whether this really does vanish, but the general idea is that the amplitude to find your particle on the edge of the universe is zero. So, we dispose of this on the grounds that it is the amplitude to find the particle infinitely far away. We're going to say that that's zero. We will actually be working, you'll see quite soon, with some wave functions where that doesn't vanish, and this is an example where physicists are rather fast and loose. But fortunately, this doesn't lead to any bad effects.

So, this we put in the bin, and this we can see is more or less what we want. Let's just tidy up a bit; so what is this that survives including this minus I hbar? So, we're going to have a minus – let's leave the minuses out – yes – D X of Upsi and then we can have an I hbar D phi by D X. Supposing I take the star of all that? Then I think I need a minus sin. Because this minus will cancel on this minus. So, we'll have an I hbar times this stuff with Upsi starred. If I take that Upsi

– that star – and put it around the whole caboodle included the I, I'll need an additional minus sin to cancel the minus sin that will arise when that star is evaluated on here.

And I can say now that that is the integral D X Upsi star, minus I hbar D phi by the X; star. So if I take this star completely outside the whole thing, then sin will need a star, which will be cancelled by the global star and otherwise we can be okay. And what is this? This that we have in here in Dirac notation is Upsi P hat phi. And that star sits outside. What's inside the star is by definition this. So, there we are; the answer is, it is hermition. Provided we get rid of that surface term, that minus infinite in square bracket.

One more. Okay. Let's calculate the commutator X hat comma P hat. We're going to calculate it like this. So what we're going to do is calculate the action. So all we know at the moment is the action is P hat on any wave function, and we know the action of X on any wave function, so I want to work with wave functions which means I put a bra at this end here. A bra X at this end here. And what does this give me? So, this is going to be obviously X; X hat P hat Upsi; minus X P hat X hat Upsi. No prizes for that.

Now, this we discovered X on this – we discovered that X on any wave function on any object gives you X times the wave function you first thought of; the wave function you were operating on. What is the wave function that this produces? The wave function that this produces is minus I hbar D Upsi by D X. So, we merely have to take that and multiply it by X and then that's what you get there, right? This is a complex number depending on X; this is a complex number depending on X. So, P on this is a certain wave function. It's this. And then X hat on that produces X times that wave function so that's it.

So, here same stuff; X on this is going to produces X Upsi X Upsi. And then P on that is going to produce minus I hbar D by D X of that stuff, and there's a minus sin floating here. This minus sin is this, that minus belongs to the P operator.

So, I think you can see that the X – the Upsi by the X terms. When you differentiate out this product you'll get two terms; you'll get X `[[D Upsi D B D X 0:41:46]]` which will cancel on this because of the two minus sins and you will also get an Upsi times the derivative of X in respect to X which is obviously one. So, we're going to get I hbar Upsi of X, which can also be written I hbar X –whoops – Upsi.

So, what have we learnt? What we've learnt is that for any state of sin whatsoever – we never said what it was – the wave function associated with X P Upsi is simply I hbar times the wave function of sin. So that means that we can now write down an operator statement with X hat comma P hat is equal to I hbar. So the commutator of these two operators is a constant. A small constant, but constant. And a commutation relation of this sort is called a canonical commutation relation.

We will meet other relations of this type where the commutator of two operators is equal to I hbar and they will be declared canonical as well. This canonical of course comes from classical mechanics – Hamiltonian mechanics – and this arises because, in classical mechanics, momentum is canonically conjugate - quote, unquote – to X.

Right. So now that we've done that, let's – yes, we've just got time I think to do this – let's apply Ehrenfest's nice theorem to – let's work out this; I hbar D by D T of the expectation value of X. What do you think this should be? The rate of change of the expectation value of X should be the speed. Right? Did I say that right? The rate of change of the expectation value of X should be the speed. Velocity, whatever. So we're hoping that this turns out to be I V which should be I P upon M if we're doing this right.

According to Ehrenfest, what's this equal to? It's equal to Upsi X hat comma Hamiltonian Upsi. Right, that's Ehrenfest's theorem. Concrete example of; application of. So in order to go further, we need to say, so what's H? H is the energy operator. What do we know about the energy of a particle that's moving in – possibly with some potential present, alright? So, the energy should be a half classically – class-ic-ally – perhaps if we're doing this classically I should replace this with and energy – should be a half M V squared plus the potential energy depending on X. Which could also be written as the momentum squared over two M plus the potential energy. Right, because P is classically M V.

Let's suppose that we can carry this forward into the quantum domain, and say that the Hamiltonian operator is the momentum operator over two M plus V. The function V evaluated on the position operator. Then we're going to have that I hbar D B D T of the expectation value of X hat is going to be the expectation value of X commuted with P squared over two M plus V. But this commutator can be broken down into a sum of two commutators; the commutator of X with P and the commutator of X with V. But V is a function of X and therefore X – the position operator – is going to commute with this. So, we're going to have that X comma V equals nought because V is a function of X.

So, what we're left with is the expectation value of P P – sorry; expectation value of the commutator of X – with P P Upsi over two M. Okay, I can take the two M out of the commutator because it's just a number, and I can express P squared as P P, but we discussed – probably yesterday – how we took the commutator of a product; we used a rule analogous to differentiation of a product – so this is equal to sin onto X comma P commutator P standing idly by, plus the first P standing idly by while X commutes with the second P.

But we've discovered that this animal is I hbar, right? This is I hbar and this is I hbar. I hbar's just a boring number, so it can come out front, so that becomes I hbar over two M. And then we have P plus P - which is two P, so I can rub out that two – times…

So what have we discovered? We've discovered that we can cancel this I hbar on the right side with what we had on the left side and say that D B D T of the expectation value of the position is in fact equal to the expectation value of the momentum – what I claim is the momentum anyway – over M, which is exactly what we were hoping for, right? So we have recovered the definition of – well, the relationship between velocity and momentum, which in classical Hamiltonian mechanics is a rather – those of you who've done S seven will realise that the connection between momentum and velocity is not as simple as elementary Newtonian mechanics would lead you to believe. It can be quite subtle, and it's determined by this; this is one of Hamilton's equations.

What we've done is we've derived one of Hamilton's equations which supersede Newton's laws of motion in classical physics. So we've derived from quantum mechanics a classical result, which was already known, but this is the justification for Hamilton's equations. Because this is true, then Hamilton's equation is true.

And we'll leave it on that and tomorrow morning I'll start by deriving the other of Hamilton's equations which is analogous to F equals M A.