Welcome back to the lectures on introduction to quantum chemistry and molecular spectroscopy. This is a very short lecture in which my only purpose is to tell you how to get the time-independent Schrodinger equation from the time-dependent Schrodinger equation when the Hamiltonian is time independent. You see H of X tells you that H is only a function of the position variables that the wave function Psi is also a function of… Psi is a function of both position and time, the Hamiltonian is only a function of position, but it's independent of time, we say such Hamiltonian systems are conservative systems, but the language apart or definitions apart, the Schrodinger equation time dependent was introduced to you in the in a lecture earlier, as I H-bar or H by 2 Pi, the partial derivative of a function called the wave function of the system with respect to time Dou Psi by Dou T and that is equated to the action of the Hamiltonian H of X is the total energy function of the system and it's a function of the position, it's also a function of the derivatives of position, because of the momentum operator and so on. The Hamiltonian is an operator function and it acts on the wave function Psi of X T. Now if the Hamiltonian is time independent how do we get this equation H of X times a function, which is only dependent on position, a capital Phi of X ray, this is different from this, and that's equal to a constant which has the dimensions of the Hamiltonian namely the energy times the same capital Psi function.
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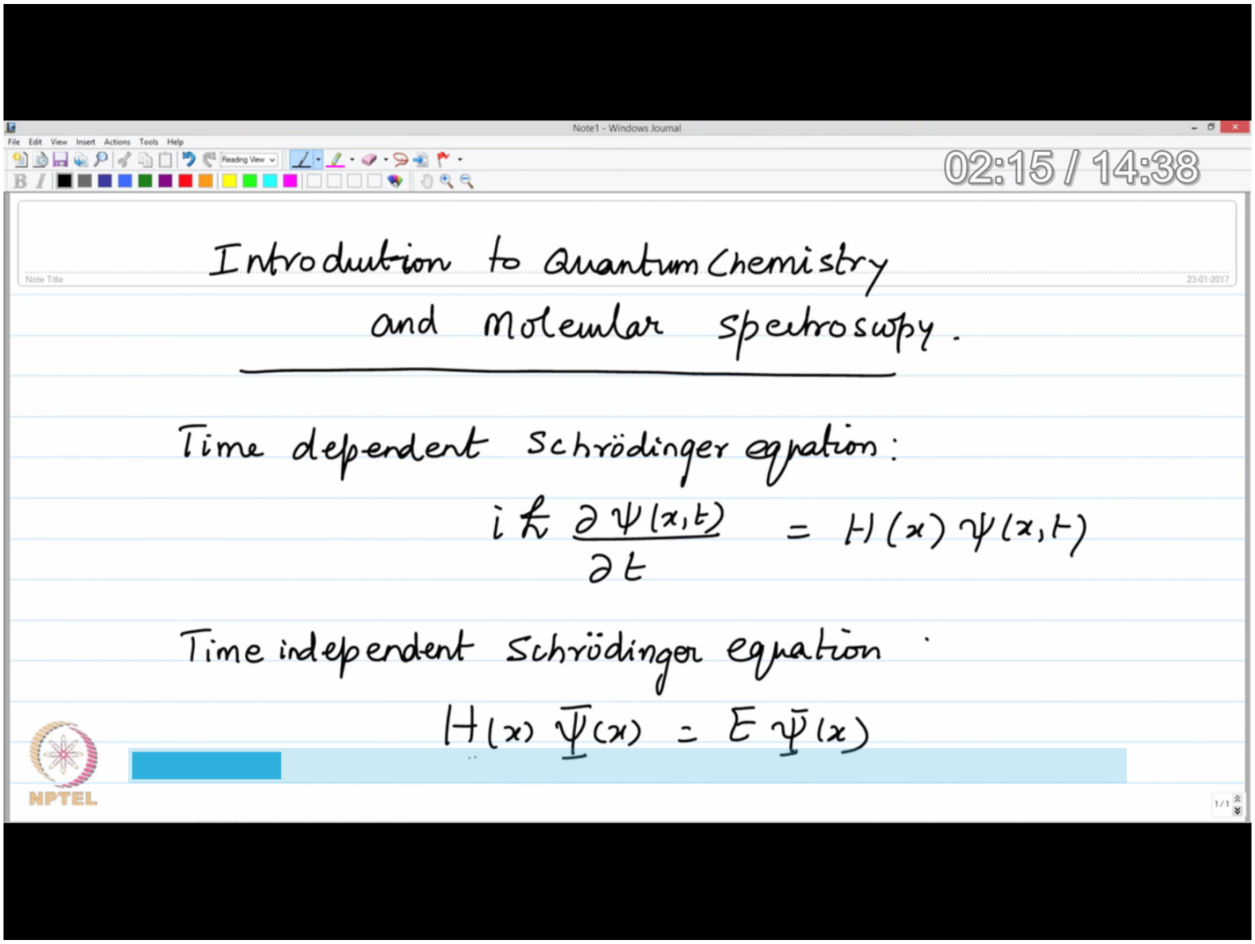

Now the process is to assume the existence of separability for such problems, namely to write Psi of X,T as proposed, we don't know what Psi of X of T is, but we propose that the variables of the function Psi, the wave function X and T can be separated in such a way that there is a function which only depends on the coordinate variable or the position variable and there is another function which is only dependent on the time variable and this is nothing but the product. Psi FX of T T of T is the product. This is called separation of variables. You have to be careful about what it means. I'll give you an example for what it is and what it is not. For example if we have a function cosine K X and sin KL of T, this if Psi of X for example is that then this is an example of a similar function that is the function here. The capital Psi of X is the cosine KX, the capital T of T is the sin L of T. They are... the variables are separator. Likewise if Psi of X of T is exponential I, for example Omega T some constant Omega and the time variable and another constant K and X if you have that, this is again, it's exponential I Omega T times exponential I K X, so this is the T of T and this is the Psi of X, so here is the Psi of X and this is the T of T. So that such functions exist, is the assumption here for solving Hamiltonian systems which do not depend on time.

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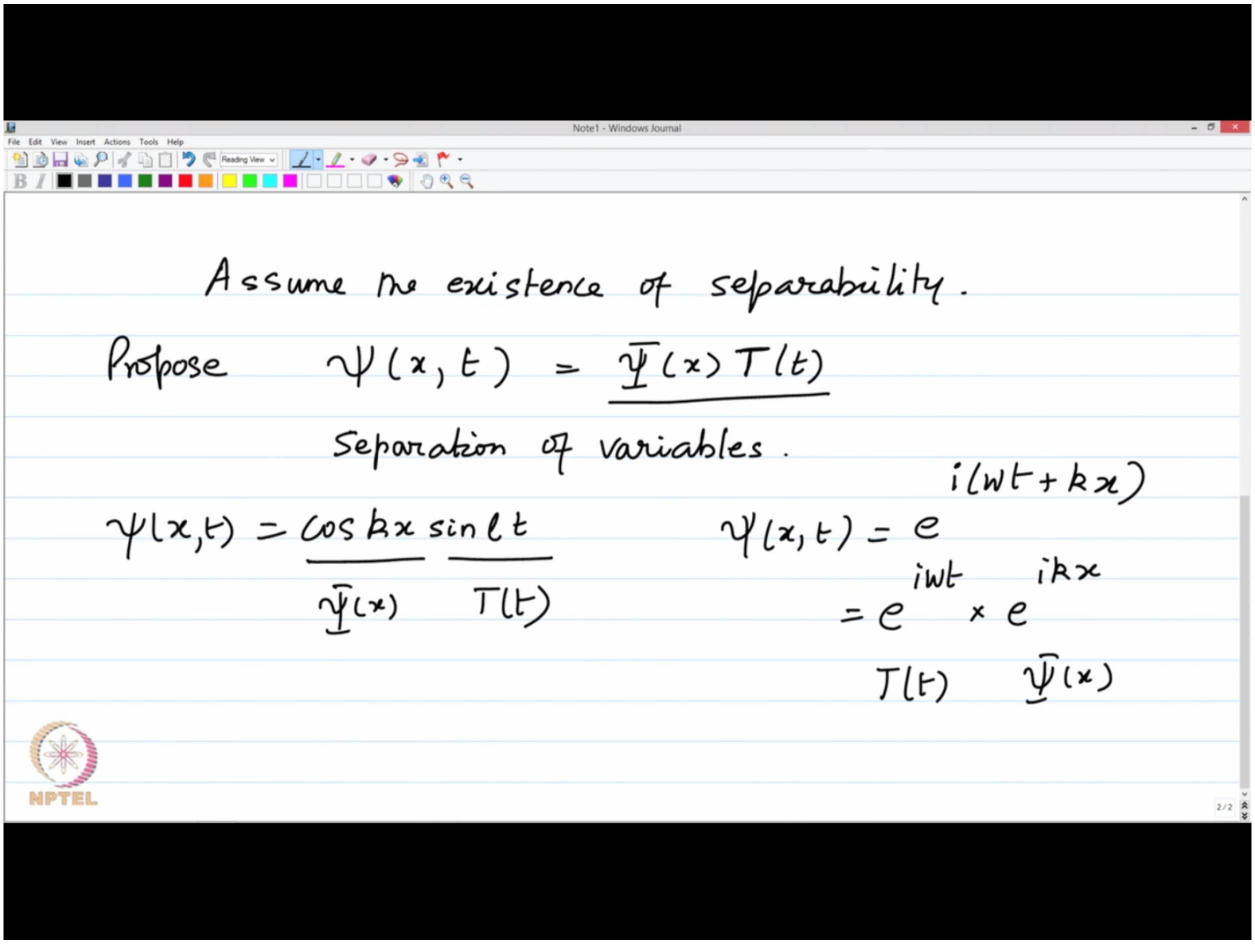

On the other hand a function such as cosine KX sin say LT + cosine let's... let's write some other example, sin KX cosine LT, which is nothing other than sin of KX + LT, okay. Now this is not separable. It cannot be written as a function that is only dependent on X and another function that is only dependent on T, it's a linear... it's a combination of multiple such functions, they cannot be expressed as a sin KX + L of T cannot be expressed as sine KX plus times some other function, therefore this is not separable. So this is the example of what may not be there, okay. Another example is if you do the same thing, if you do E to the I Omega T + KX, but suppose we have this function, then... with a square on it, then you know this is a problem too. It's E to the I Omega square T square plus K square X square plus 2 Omega K X T and if you write this it's E to the I Omega square T squar, a function of time only, a function of I K square x square, but it's also a function of E to the 2I Omega K X T and this may not be separable into something called a function of X only and the function of T only, okay. Therefore there are examples for what is separable and... what are separable and what are not separable.

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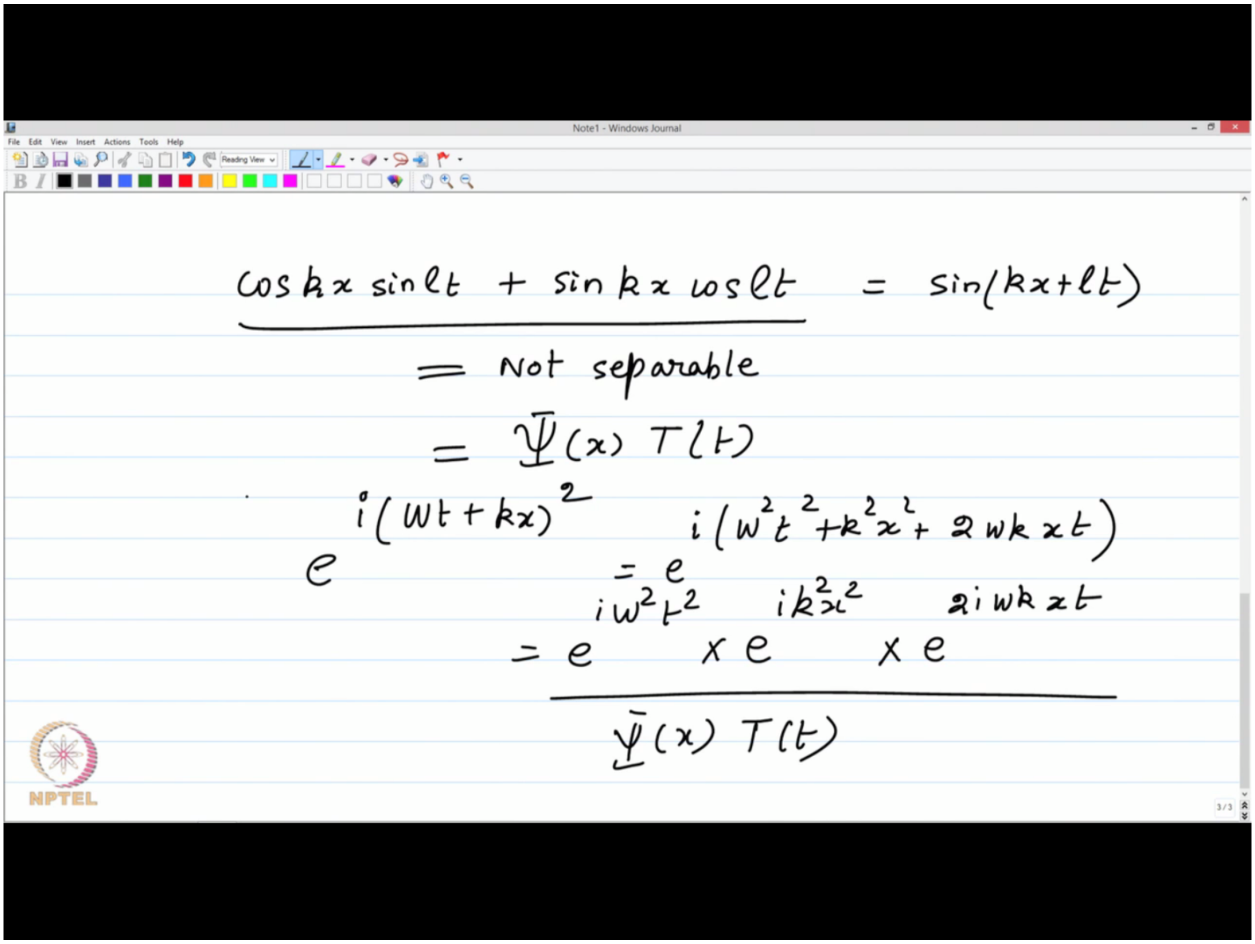

Let's assume that for our purpose that we can write the wave function in such a way that it's a product of a wave function that depends only on X, a wave function that depends only on T and then apply the algebraic tool.

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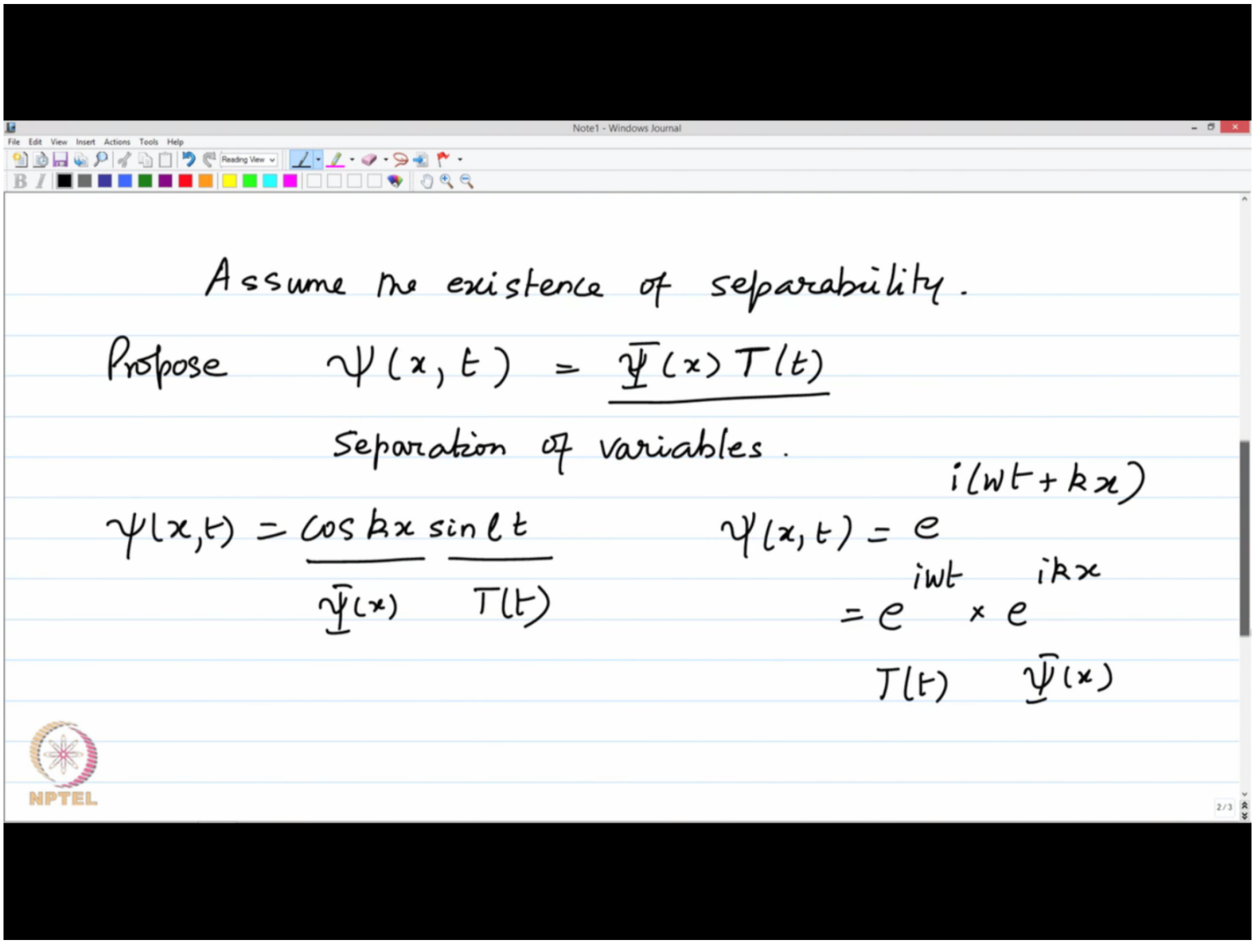

Therefore if we substitute that I H-bar D by Dou by Dou T of capital Psi of X T of T is equal to H the Hamiltonian operator with a hat on it, I forgot to write that earlier, H of X Psi of X T of T, the Hamiltonian operator which contains coordinate function X as well as derivatives on X will only have its action on Psi of X, it will not change anything to do with T F T, therefore this can be written like that, because the Hamiltonian doesn't have any derivatives or any others, which is a function of T, therefore it's only that. That's what I said, when the Hamiltonian is time independent. Now here it's a partial derivative with respect to time, therefore it's only going to act on the variables which... on the functions which contain time as the variable. Therefore this will also be written as I H bar Dou of T by Dou T and Psi of X okay. Therefore this is equal to H till Dou of X Psi of X and T of T. Now if we divide by the product, divided by Psi of X, T of T, then what we get, we get 1 by T of T, the Psi of X is gone, what we have is a H bar DT by DT because the partial derivative on a function with respect to time and the function is only, time dependent, then it's a total derivative, this is equal to 1 by capital Psi of X H of X Psi of X. Please understand that you cannot cancel the Psi with the Psi, because the Hamiltonian contains derivatives and therefore it has it has momentum operator P square, P momentum squared operator. Therefore the P operator is a derivative in the coordinates, position coordinates. The derivatives we change the function to something else therefore you can't cancel this Psi with that. So what is left over, here of course what we have done is very clearly, you cancel the Psi of X with Psi of X because this derivative does not affect the wave function, this does not affect to the time, therefore you have canceled the time, so this is what you have. Now please remember left hand slide depends only on time and the right hand side depends only on the position coordinate or the coordinate X, only on X.

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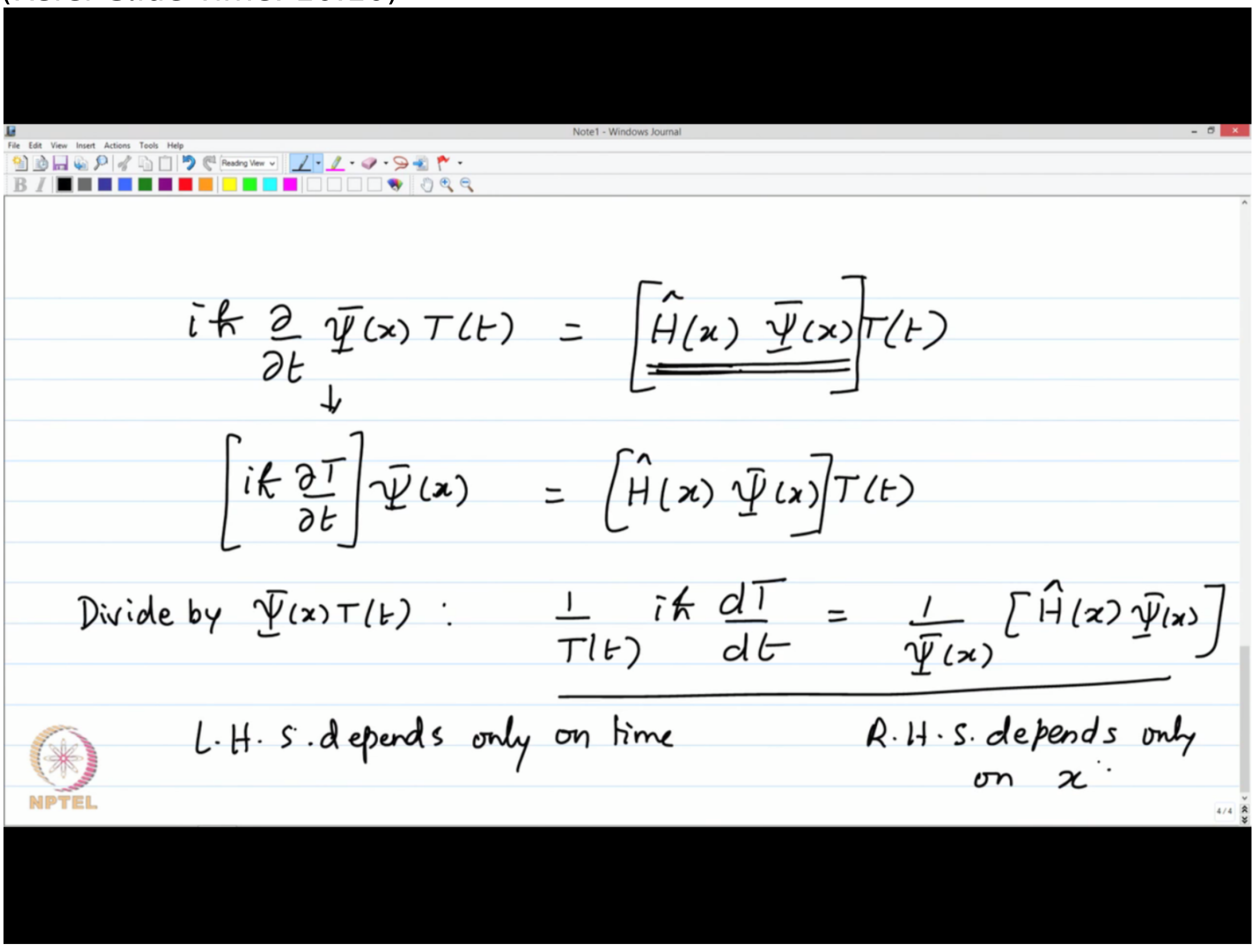

Therefore if we go back and write this 1 by Psi of X H of X Psi of X is equal to 1 by T of T by H bar DT by DT only on X only on T they both have to be equal to something which is independent of both X and the T and therefore constant with respect to X and T, and that constant may be written by a symbol E. Now what is the dimension of this constant, please remember whatever is the dimension of the wave function is cancelled by the dimension of this wave function. So here it's a dimension of energy. H bar is the energy into time divided by 2 Pi and the derivative D by DT is 1 by time and the dimension of T of T is cancelled by this T of T, therefore both sides you have energy as the dimensioned quantity, and therefore E has to have... has to be energy dimension, okay. Now it's easy to solve this and the fact that they have to be independent of each other is because of the fact that this does not depend on T and therefore this cannot depend on T, this doesn't depend on X therefore whatever is on that side, this cannot also be dependent on X, therefore E is to be independent of both X and T. Now the solution is therefore H of X Psi of X is equal to E times Psi of X, when you multiply and also I H bar DT by DT is equal to E T of T. See this is a partial derivative here with respect to X and this is the partial derivative with respect to time which is a total derivative here, this is the time independent Schrodinger equation and the wave function Psi of X of T is of course the product Psi of X times T of T.

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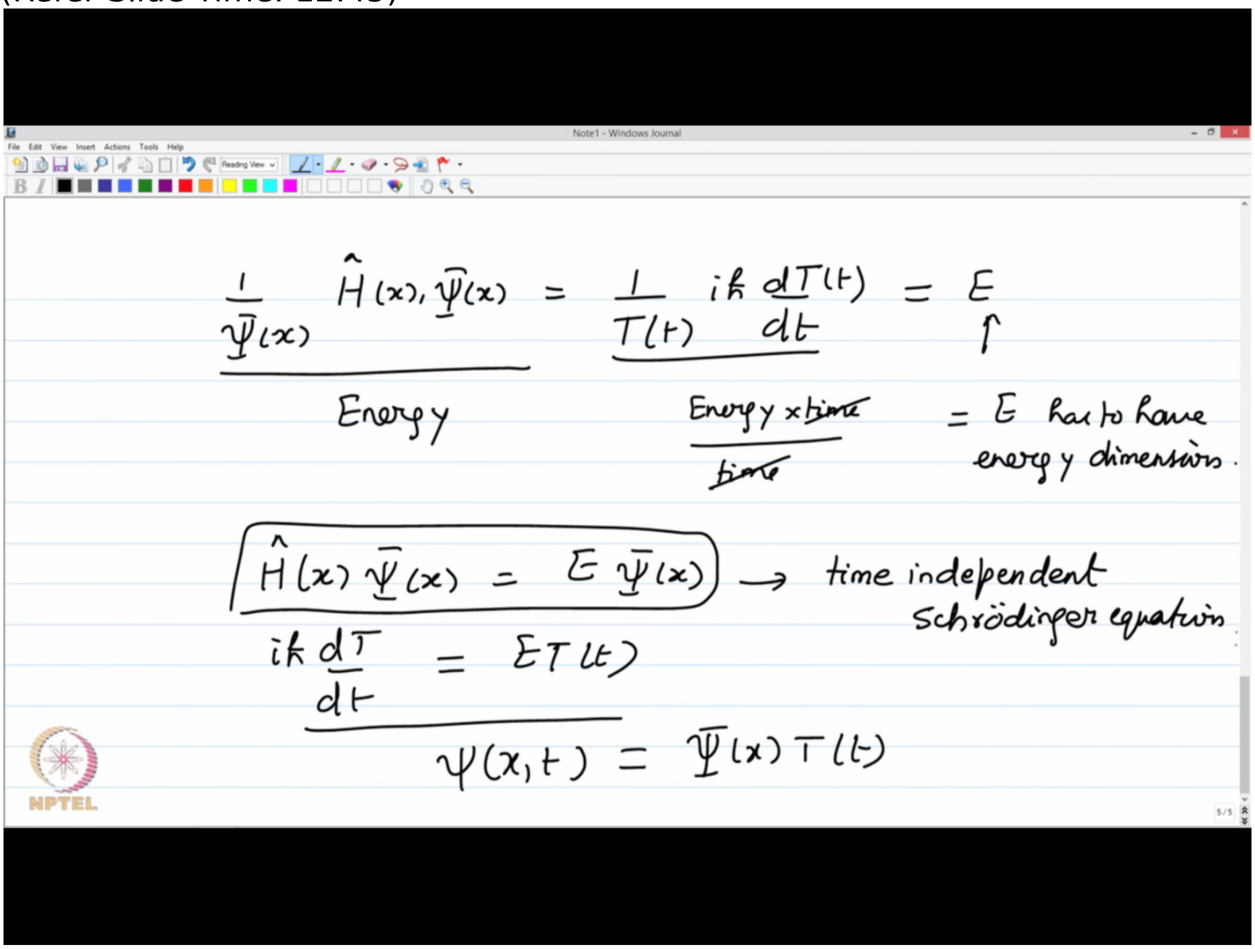

Therefore the wave function for the time independent Schrodinger equation is of course time independent itself, but the wave function for the time dependent Schrodinger equation… the wave function for the time dependent Schrodinger equation is a function of both X and T, even when the Hamiltonian is not a function of time. So this is therefore important immediate step in the models that we want to solve. All the models that people solve will not have time dependent Hamiltonian. We do have a part of the course containing spectroscopy, but we are not going to look at anything called the time dependent spectroscopic Hamiltonian ended solution, but we are only going to look at the molecular energy levels in spectroscopy, therefore there also we will not use the time dependent Schrodinger equation. Therefore this step of changing the frame dependent Schrodinger equation to a simple time independent Schrodinger equation for solving problems related to this course is something that you have to keep in mind. There will be some examples of this in your assignments or in tutorials and in the next lecture… from the next lecture onwards we will start looking at the model problems for the quantum mechanics starting with the particle in the one dimensional box, a free particle in the one dimensional box and with infinite potential barriers, until then thank you very much.