Time Dependent Quantum Chemistry
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Module: 03 Lecture: 18
Stationary Gaussian Wavepacket

Welcome back to Module 3, of the course Time Dependent Quantum Chemistry, we have been discussing how to represent a particle in quantum mechanics and we have seen that the wave packet is the correct representation of a particle in quantum mechanics. And in terms of wave packet, we have got an analytical approach to solve the dynamics of wave packet. And for that first thing we need is that the initial Wavepacket has to be known. To find out how that known Wavepacket will move forward, or in other words how the particle will evolve.

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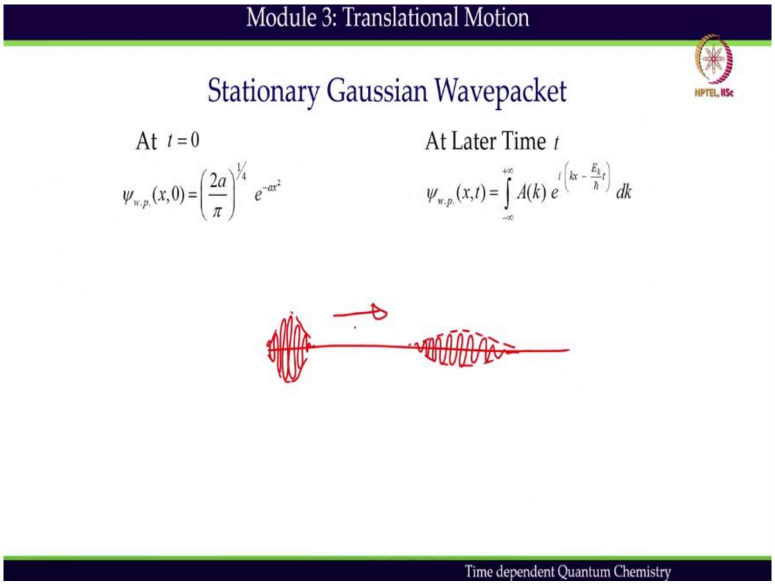

If I start with a Gaussian Wavepacket, then at different time it may so happen that it is moving but at the same time is broadening, when the particle is moving, which means that the shape of the particle is changing while it is moving, while it is freely moving, and that is something which we are going to now prove that what will happen with this analytical approach.

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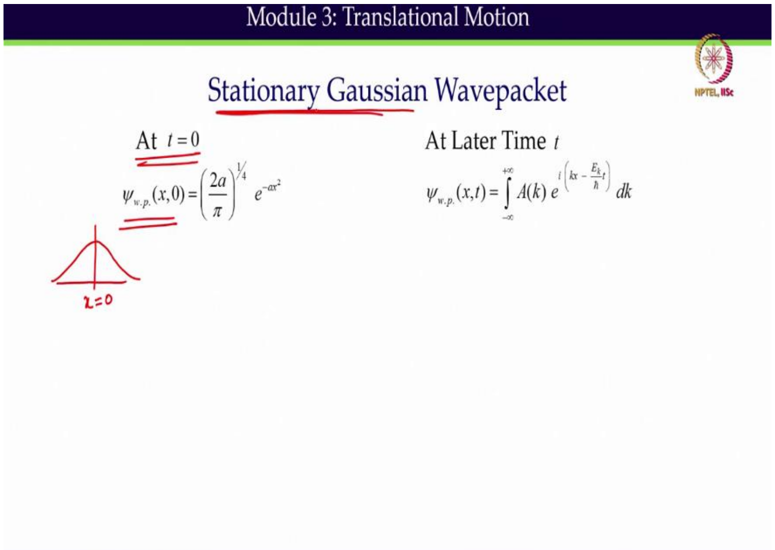

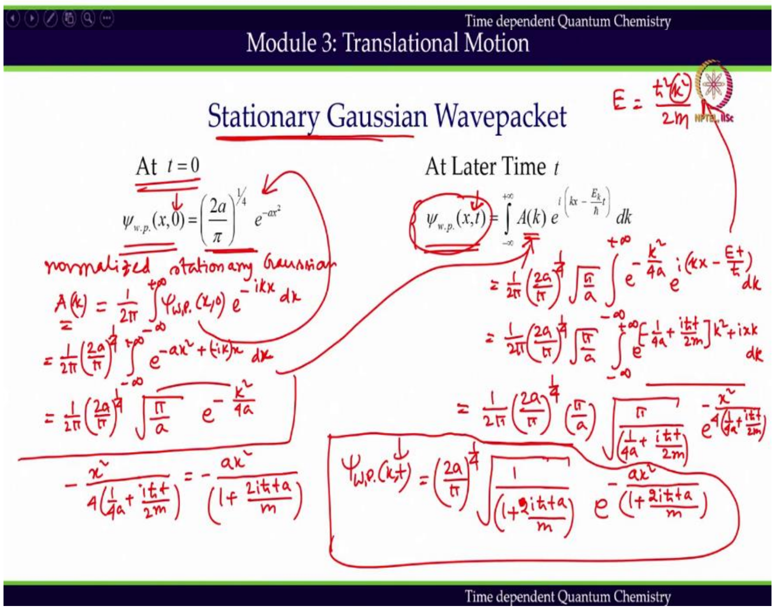

So, as we have mentioned before, at t equals 0, I have to make a good case for the Wavepacket. And here I have considered our normalized Stationary Gaussian Wavepacket. So, we are first looking at the Stationary Gaussian Wavepacket where I do not use e^{ikx} part.

$$\psi_{w.p.}(x,0)=\left(\frac{2a}{\pi}\right)^{\frac{1}{4}} e^{-ax^2}$$

So, then the particle would be presented by these Gaussian functions, which looks like this is just a Gaussian function which is centered at x equals 0. There is no fast oscillation, because oscillation comes because of this e^{ikx} term, this term is missing. And that is why it is representing stationary Gaussian function.

Why It is Stationary Gaussian function, it is Stationary Gaussian function because of that missing part that plane wave part here. And we have taken normalized Gaussian function that is also an requirement, we have to always begin with a normalized function in quantum dynamics. So, this is called normalized Stationary Gaussian function.

And then this is the final form of the Gaussian, final form of the Wavepacket at different time I will be able to find out. So, if I know at t equals 0 time, what I have, I will be able to find out at t equals at any time and any later time, I will be able to find out what is the typical shape of the wave function.

$$\psi_{w.p,}(x,t) = \int_{-\infty}^{\infty} A(k) e^{i\left(kx - \frac{E_k t}{\hbar}\right)} dk$$

So, for that I need to know A(k), and we have seen that A(k) can be calculated from this

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi_{w.p,}(x,0) e^{-ikx} dx$$

Where this initial wavepacket is given by this. So, I have to find out A(k) then we have to plug that in here I will be able to get the final form of the Wavepacket analytical form of the Wavepacket. And I will be able to get the time evolution how Wavepacket is evolving as a function of time, or in other words how the particle is evolving it is shape is changing where it is going every information, we will be able to get that. So, let us get this integration done first. So, if I plug that in here is going to be

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi_{w.p,}(x,0) e^{-ikx} dx$$

$$= \frac{1}{2\pi} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{-ax^2} e^{-ikx} dx$$

$$= \frac{1}{2\pi} \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\pi}{a}} e^{-\frac{k^2}{4a}}$$

$$\psi_{w.p,}(x,t)=\frac{1}{2\pi}\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{\pi}{a}}\int_{-\infty}^{\infty}e^{-\frac{k^2}{4a}}e^{i\left(kx-\frac{E_k t}{\hbar}\right)}dk$$

Where E is the kinetic energy given by

$$E=\frac{\hbar^2k^2}{2m}$$

I will rearrange this one, so that I can use the standard Gaussian integral.

$$=\frac{1}{2\pi}\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{\pi}{a}}\int_{-\infty}^{\infty}e^{\left[-\frac{1}{4a}+\frac{i\hbar t}{2m}\right]k^2+ikx}dk$$

$$=\frac{1}{2\pi}\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\left(\frac{\pi}{a}\right)\sqrt{\frac{\pi}{\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)}}e^{-\frac{x^2}{4\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)}}$$

We can write down,

$$-\frac{x^2}{4\left(\frac{1}{4a}+\frac{i\hbar t}{2m}\right)}=-\frac{ax^2}{\left(\left(1+\frac{2i\hbar ta}{m}\right)\right)}$$

We can write down this way. So, if we can write down I will be able to write down

$$\psi_{w.p,}(x,t)=\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{1}{\left(1+\frac{2i\hbar ta}{m}\right)}}e^{-\frac{ax^2}{\left(1+\frac{2i\hbar t}{m}\right)}}$$

That is the final expression for the stationary wave packet at any time t. And finally, we are interested in density because that can be connected to the experiment.

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$\frac{2\hbar t a}{m} = b$

Stationary Gaussian Wavepacket

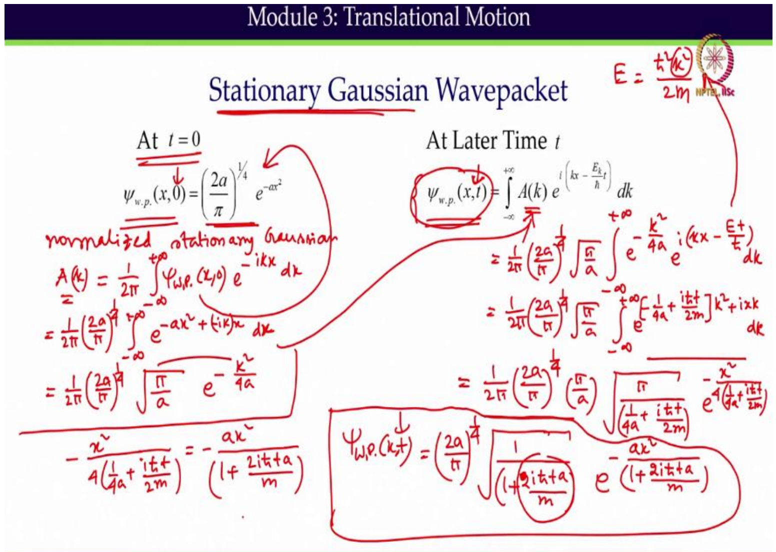
Time Evolution of Probability Density

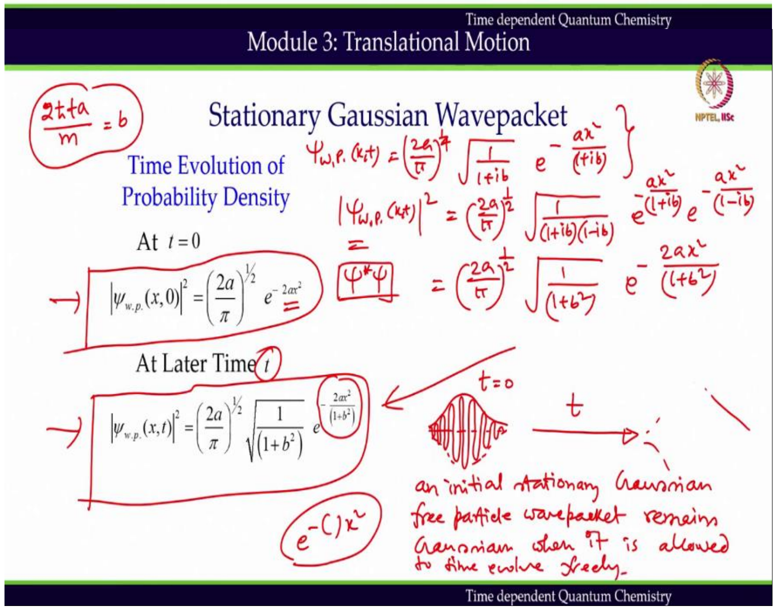
At $t = 0$

$$\left|\psi_{w.p.}(x,0)\right|^2 = \left(\frac{2a}{\pi}\right)^{1/2} e^{-2ax^2}$$

At Later Time t

$$\left|\psi_{w.p.}(x,t)\right|^2 = \left(\frac{2a}{\pi}\right)^{1/2} \sqrt{\frac{1}{(1+b^2)}}\; e^{-\frac{2ax^2}{(1+b^2)}}$$





So, will get the density also. And for getting the density what we will do. So, this part can be represented in terms of b, this part also can be represented in terms of b, and that is the representation we have.

$$\frac{2\hbar ta}{m} = b$$

So, we have not reached there yet. So, first we have to represent in terms of b. So, we will represent it wave function, this wave function in terms of b

$$\psi_{w.p,}(x,t)=\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{1}{(1+ib)}}e^{-\frac{ax^2}{(1+ib)}}$$

So, the density is going to be

$$\left|\psi_{w.p,}(x,t)\right|^2=\left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\sqrt{\frac{1}{(1+ib)(1-ib)}}e^{-\frac{ax^2}{(1+ib)}}e^{-\frac{ax^2}{(1-ib)}}$$

$$\psi^*\psi=\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\sqrt{\frac{1}{(1+b^2)}}e^{-\frac{2ax^2}{(1+b^2)}}$$

So, we get this expression. So, what we have presented is that this is the density, probability density distribution of that particle at t equals any time later time and initial density distribution was this. So, this is a two different expressions, we have four different time, this is the initial time and this was the final this was the initial time and this was the final time the density distribution.

One thing is quite clear from here is that if I start with a Gaussian Wavepacket. A particle which is represented by a Gaussian Wavepacket, if we start with this Gaussian Wavepacket this was at t equals 0, this is Gaussian, we see that after even many times when the particle has propagated, it is still remaining to be Gaussian there are some changes going on we have to find out what kind of changes.

But still this form e to the power minus something multiplied by x square form is still maintained. So, it is still a Gaussian function so, good thing about this is that an initial stationary Gaussian free particle Wavepacket remains Gaussian when it is allowed to time evolve freely. It will maintain that the Gaussian form even after certain time.

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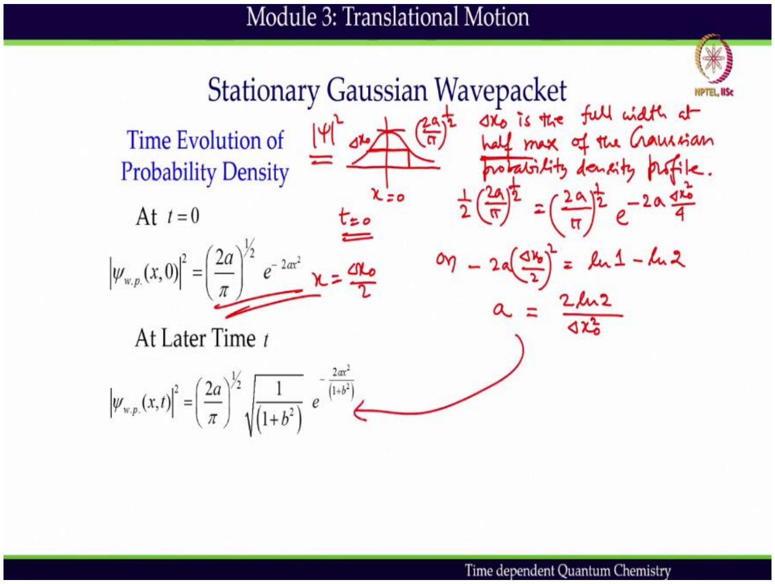

So, next what will do, we will try to understand what are the changes will expect for that Gaussian, for that we will find out the width of the Gaussian. So, I started with this which is centered at x equals 0 and the wave function this was the density maximum is $\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}$ to the and initial width was Δx_0 that was the initial width.

Let us say at t equals 0, we had an initial width of the Gaussian Δx_0 and Δx_0 is defined as the full width at half maximum of the Gaussian probability density profile. It is not the wave function it is the probability density full width half max. We have to remember that it is not the wave function full with half max.

It is not that it is the full with half max of the density profile. And if it is so, then I can find out this a-value because by definition, it is going to be half full width at half maximum. So, half of its maximum value that is $\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}$ it occurs when the function takes the value, this function takes the value when $x = \frac{\Delta x_0}{2}$.

$$\frac{1}{2}\left(\frac{2a}{\pi}\right)^{\frac{1}{2}} = \left(\frac{2a}{\pi}\right)^{\frac{1}{2}} e^{-2a\frac{\Delta x_0^2}{4}}$$

$$-2a\frac{\Delta x_0^2}{4} = \ln 1 - \ln 2$$

$$a = \frac{2\ln 2}{\Delta x_0^2}$$

I get the a value, why I need this a value. Because I have to then plug that in here, so, that I can get the final expression for the later time.

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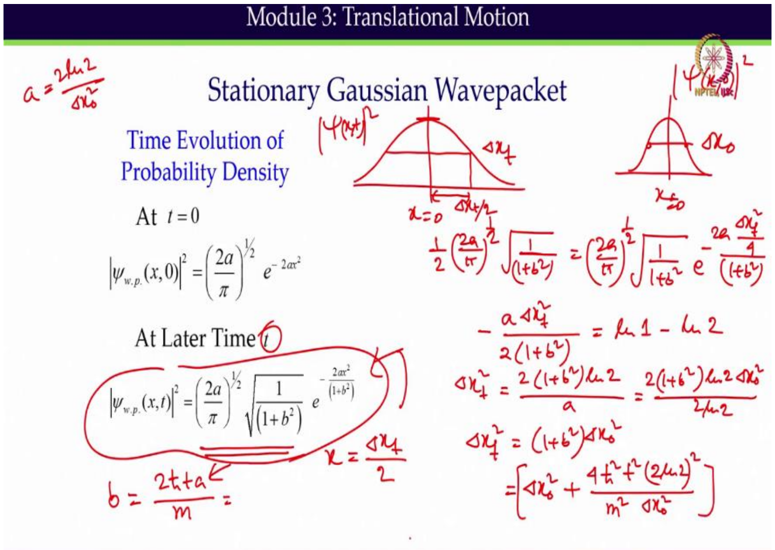

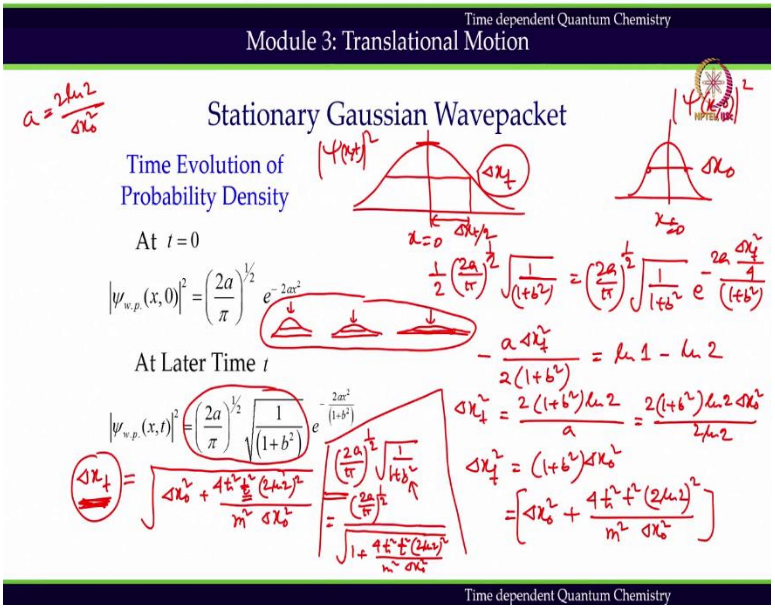

What is going on at the later time, for the later time here I will do the same thing this profile can be plotted let us see, this profile is something like this, which is centered again x equals 0, and it is width, I will call it Δx_t , because at time t it is width and I will compare with it is width which I have got at this is again $|\psi(x,t)|^2$ density plot.

And this is also $|\psi(x,0)|^2$, density plot this was Δx_0 . So, I started with Δx_0 I will check what is going on width Δx_t width after the time evolution for t-time. So, by definition of full width half max, again half of it is intensity, maximum intensity, this is the maximum intensity half of its maximum intensity is obtained.

When the $x = \Delta x_{\frac{t}{2}}$

Because this is $\Delta x_{\frac{t}{2}}$.

$$\frac{1}{2}\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\sqrt{\frac{1}{(1+b^2)}} = \left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\sqrt{\frac{1}{(1+b^2)}}e^{-\frac{2a\frac{\Delta x_0^2}{4}}{(1+b^2)}}$$

$$-\frac{a\Delta x_t^2}{2(1+b^2)} = \ln 1 - \ln 2$$

$$\Delta x_t^2 = \frac{2(1+b^2)\ln 2}{a} = \frac{2(1+b^2)\ln 2\Delta x_0^2}{2\ln 2}$$

$$\Delta x_t^2 = (1+b^2)\Delta x_0^2$$

And we know that b

$$\frac{2\hbar ta}{m} = b$$

We know a, we can plug that in. So, finally, if we insert all these values b value then I get this expression

$$\Delta x_t^2 = \left[\Delta x_0^2 + \frac{4\hbar^2 t^2 (2\ln 2)^2}{m^2 \Delta x_0^2}\right]$$

Final expression for the width this delta x t at particular time t.

$$\Delta x_t = \sqrt{\left[\Delta x_0^2 + \frac{4\hbar^2 t^2 (2\ln 2)^2}{m^2 \Delta x_0^2}\right]}$$

So, what we observe from here is that Δx_t is proportional to it will depend it is not directly proportional, but it will depend on time.

So, more time it spends during the evolution it will just spread out more. It is just increasing Δx_t it will increase the width of the Stationary Gaussian. So, let us say I started with this Gaussian slowly it will spread out it will more spread out and when it is spreading out its amplitude will go down definitely.

Because total integration has to be 1, so area under the curve has to be constant. So, width this slowly increasing and amplitude will go down amplitude going down can also be proved.

$$\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}\sqrt{\frac{1}{(1+b^2)}}=\frac{\left(\frac{2a}{\pi}\right)^{\frac{1}{2}}}{\sqrt{1+\frac{4\hbar^2t^2(2\ln 2)^2}{m\Delta x_0^2}}}$$

This part is the amplitude of the Wavepacket at time t What we see here is that amplitude will be inversely proportional with t and width is directly proportional width t.

So, as we increase the t amplitude will go down just what we have presented here amplitude will go down slowly and its width will slowly increase. So, that is the basic idea of Stationary Gaussian Wavepacket Motion. We will continue this session and we will see how this wave packet will behave if it is traveling Wavepacket so far we have said that the Wavepacket which is present is a stationary Wavepacket.

So, the Wavepacket which is staying in a place it is not changing, the position is staying at the same position. But if it is staying here as the time progresses it will just spread out and its amplitude will go down that is the behavior of a particle in quantum mechanics we will meet again in the next session.