Time Dependent Quantum Chemistry
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Lecture 51
Hamiltonian for Light-Atom Interaction

Welcome back to module 8, where we are discussing light atom interaction. And we have represented light so far classically and we are seeing that when light propagates through the medium actually, certain vector potential is propagating through the medium.

And vector potential is nothing but the plane wave and that is why we call it light is a plane wave. And we have seen the general form of that vector potential, which is propagating through the medium. Because that vector potential is going to contribute to the interaction potential which will be introduced in the time dependent Schrodinger equation.

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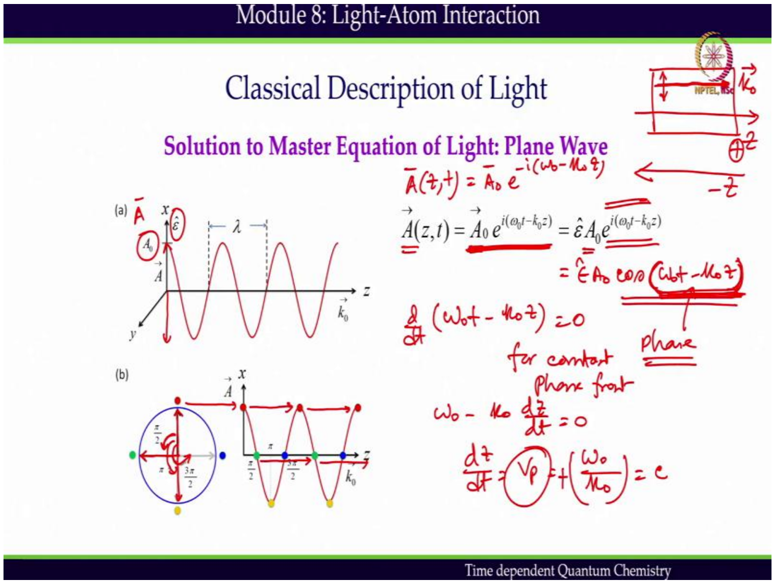

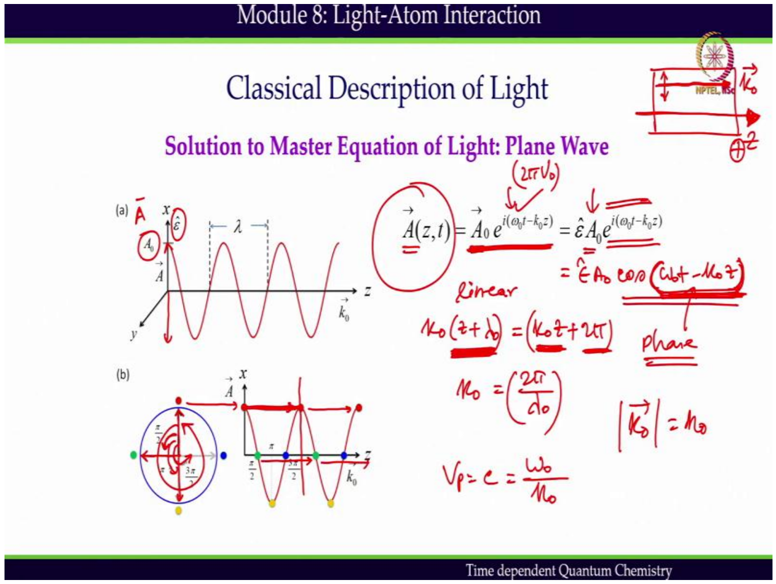

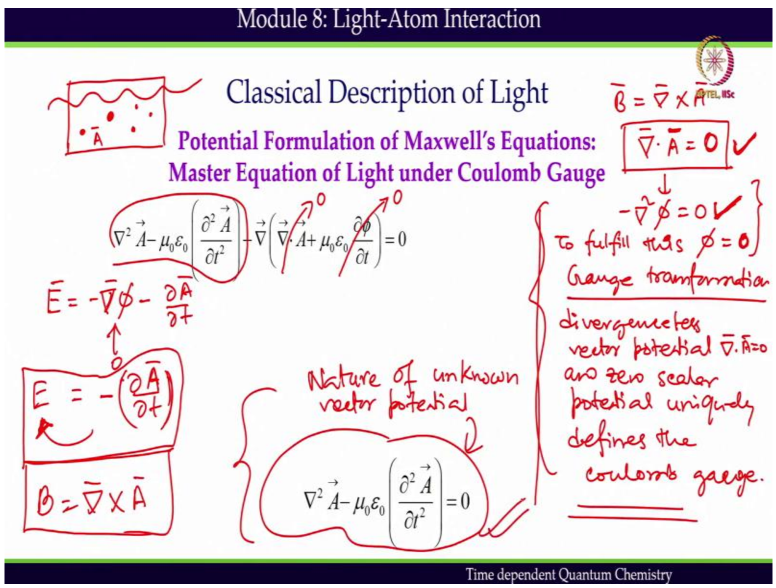

So, we will take a look at rigorously at the nature of the vector potential, if you are familiar with any plane wave propagating through the medium, it is quite it is actually the same as the plane wave propagating through the medium, but just the names the this new terms are we are using this vector potentials.

So, when I say that light is propagating through the medium, it is actually what is going on, a certain vector potential is propagating through the medium and it has its maximum amplitude which is given by A_0 and it is actually varying along this x axis and that direction, along which vector potential is changing in the medium, it is the direction, called polarization direction of light, and this ε is the unit vector along that polarization direction.

So, vector potential is changing along this direction, but it is propagating through the medium like this way (see slide figures). So, this is the propagation direction, propagation direction is given by k_0 direction. So, that is the basic idea. So, when light is propagating through the medium, we will visualize as if a certain vector potential is propagating through the medium.

And what we have plotted here is the real part of this which is nothing but $\varepsilon A_0 \cos(\omega_0 t - k_0 z)$. We often represent a plane wave with the help of this kind of complex notation, because subsequent mathematics becomes easy to deal with. Otherwise, this complex does not mean anything, we have to convert it to the real part and the real part is going to be the cos part which is the cosine wave. So, vector potential is nothing but the cosine wave.

So, light is a is nothing but a cosine wave, plane wave in one dimensional problem. Now, if we look at this, what we see is that everything inside this bracket, $(\omega_0 t - k_0 z)$ this part is called phase, phase of the plane wave or phase of the light and what we see here is that, here the phase is depicted in terms of rotating dial.

So, what does it mean? I have this maximum amplitude here and now, it is rotating maximum amplitude is becoming 0, because it is aligned on this, then again maximum amplitude is increasing going to the maximum opposite direction. So, this phase at this point phase is 0, at this point, how do I define the phase? Phase is defined in terms of this rotating dial you can also define in terms of the length. So, this linear advancement is represented by this rotating dial form (see slide figure).

So, at this point, because everything inside this cos function has to be some kind of angle. That is why, when it is making and linear transform, linear transition in this in this z axis, axis let us say along the z axis when it is making linear transition, when it comes here, it is actually making $\pi/2$ phase. On the other hand, when it comes here, it is making π phase when it comes here, it making $3\pi/2$.

Similarly, here it is making again the it is making basically π phase which is nothing but the 0 phase it is repeating. So, what we see here from this rotating dial, this correspondence between the linear motion and the rotational motion, this correspondence suggests that after a certain time, the same phase will be repeated, if I am looking at this red colour, it will be repeated, if I am looking at this green colour, it will be repeated.

So, the same phase will be repeated and when the constant phase front repeats, it means that this total part if I take the time derivative, then this is going to be 0 and we if we make it 0, for the constant phase, front for constant phase front it is 0, which means I have $\omega_0 - k_0 \frac{dz}{dt} = 0$, $\frac{dz}{dt}$ is nothing but the velocity, this is called phase velocity, which is nothing but $\frac{\omega_0}{k_0}$.

So, phase velocity, we have got the velocity. So, we are saying that when light propagates through the medium, we do not know what does it mean by light, but in the medium will realize that certain vector potential is propagating through the medium and something is propagating through the medium it means that it should have a velocity, what is the velocity it has? It has the phase velocity and this phase velocity is going to be c in vacuum.

Also we see that this phase velocity, it is positive, which means that this equation is representing the light propagating along the positive z direction, increasing z direction, there can be another solution for the previous equation, this equation which we pointed out there is an equation this equation, we can have another solution and that solution corresponds to a light propagating along the negative or decreasing z direction. So, that is also possible we are not taking that solution, we are just considering one condition which is light is propagating along the increasing z direction.

And that is why this equation is valid for that particular plane wave. Another concept or idea we should clarify here is that, if we have the λ which is the wavelength, if I have this $z+\lambda$ advancement, $k_0\left(z+\lambda_0\right)$, λ is the wavelength of this wave. So, if I have $z+\lambda$ advancement, that means, I am going to have 2π angular advancement.

So, this is linear advancement and as a result, I will have this angular advancement of 2π,. remember $k_0 z$ is representing an angle, but z is representing certain distance linear. So, this part is linear, but total part is an angle and that is we added 2π advancement. So, you see that from here , this is called λ and this in the linear scale it is λ but in the rotational scale it is going to be 2π .

So, 2π angular advancement is nothing but λ_0 linear advancement and if it is so, then I will have this $k_0 = \frac{2\pi}{\lambda_0}$ and the definition of k_0 we get. So, in brief the solution to the combined potential form of the Maxwell's equations in vacuum which is representing the light is featuring a plane propagating wave. So, light, what is light? Light is a plane propagating wave and in terms of the vector potential you can represent it in terms of field as well. And the similar conclusions you can make, but we are interested in terms of potential and that is why we are representing everything in terms of potential here.

So, in terms of potential light, what does mean by light? Light is a plane propagating wave, which is represented by this vector potential of the light and in the medium, it is actually creating this vector potential which is propagating through the medium. It has an angular frequency ω_0, this is the angular frequency, which is nothing but $2\pi\nu_0$, ν_0 is the optical frequency, k_0 is the magnitude of the propagation vector magnitude of the propagation vector is the k_0. So, propagation vector is this one along which we are assuming there is z direction is the propagation vector.

So, magnitude is k_0, A_0 is the maximum amplitude of the vector potential. So, A_0 is the maximum amplitude of the vector potential and this wave light wave propagates with a velocity V_p which is $V_p = c = \frac{\omega_0}{k_0}$ because we are working on vacuum. All these relations we get out of this as a consequence of the plane wave.

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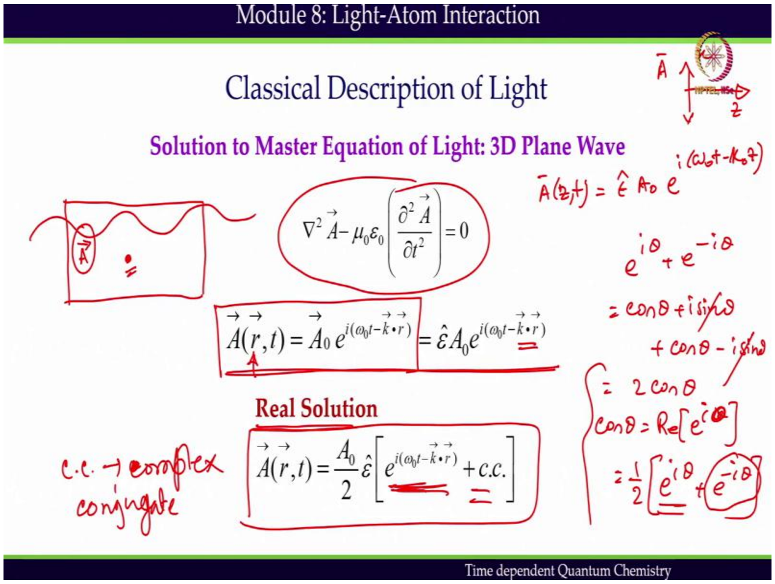

So, similar to the one dimensional problem. Now, we have to go back to this three dimensional issue and for the three dimensional problem, we get similar results, it can be represented by this way. So, previously we have represented $\vec{A}(z,t) = \vec{A}_0 e^{i(\omega_0 t - k_0 z)}$

And we said that, it is actually propagating along the z direction and A is changing along the x direction, which is perpendicular to the propagation direction and for the three dimensional situation if the position vector is represented by r, then this is going to be the dot product of r and if we find out the real solution, we know that $e^{i\theta} + e^{-i\theta} = \cos\theta + i\sin\theta + \cos\theta - i\sin\theta = 2\cos\theta$

$$\cos\theta = \text{Re}\left[e^{i\theta}\right]$$
$$\frac{1}{2}\left[e^{i\theta} + e^{-i\theta}\right]$$

. So, this is what we have used here, if the complex form represented by this, then the real form of the vector potential which is important would be represented by this c.c is representing the complex conjugate of this part.

So, this $e^{-i\theta}$ is the c.c of this part, that is the way we very conveniently represent c.c is the complex conjugate of the complex part. So, this is what the light looks like, I have vacuum, I have light propagating through the medium, it means the vector potential is propagating through the medium and I have an atom and this vector potential is going to now interact with this atom in terms of potential.

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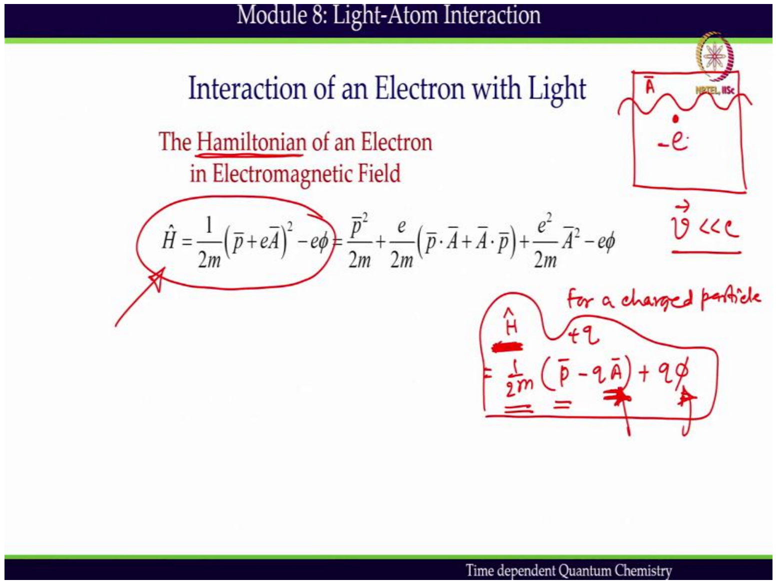

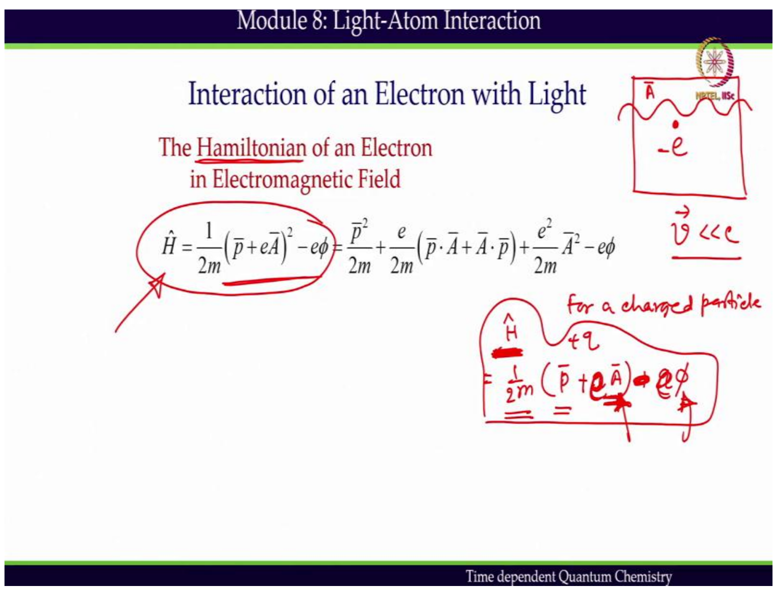

So, we are now ready to look at the interaction of an electron, I will first assume instead of presenting the light and atom interaction will consider that I have an electron light is propagating through the medium, that is why it has created vector potential and this vector potential will interact.

So, with the classical description of light given already. One may write down the Hamiltonian in the end always to solve any quantum mechanical problem I have to get the Hamiltonian associated with this problem. So, the Hamiltonian of the of an electron which is the electron is assumed to be non relativistic, which means that its speed or its velocity of electron is much less than c. When this kind of electron, non relativistic electron interacting with the light in vacuum, then the Hamiltonian one can represent the Hamiltonian as this form. $H = \frac{1}{2m}\left(\overline{p} + e\overline{A}\right)^2 - e\phi$

Actually general form of the Hamiltonian for a charged particle. So, for a charged particle with a q charge, the Hamiltonian would be $H = \frac{1}{2m}\left(\overline{p} - q\overline{A}\right)^2 + q\phi$ m is the mass of the charged particle, then P there is the momentum operator q is the charge and scalar potentials, one can represents total Hamiltonian for the interaction for the charge particle interacting with the light. Now, it is not an easy task to show how we get this Hamiltonian.

We will just for that, we have to know classical mechanics, we have to use classical mechanical equations, Hamilton equation, and we can prove that. But those rigorous methodologies will not use here, will just make use of the final form. The final form of a charged particle, we can remember that, if a charged particle q, if a nonrelativistic charged particle q is interacting with light its vector potential, then the Hamiltonian of the total Hamiltonian would be represented by $H = \frac{1}{2m}\left(\overline{p} - q\overline{A}\right)^2 + q\phi$, ϕ comes into the Hamiltonian.

And for e, because it is an electronic particle -e charge, I have now this is e and this part becomes -e and that is exactly what I have written here. So, there is a rigorous mathematical derivation to obtain this kind of Hamiltonian we will just use that final result will not show how to get that, one thing is clear here is that Hamiltonian now, I have for the charged particle interacting with this or electron interacting with this electromagnetic field.

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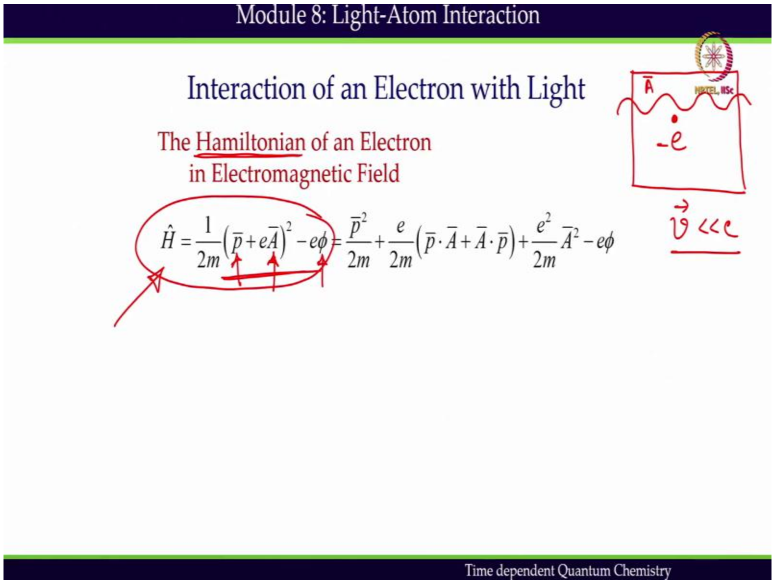

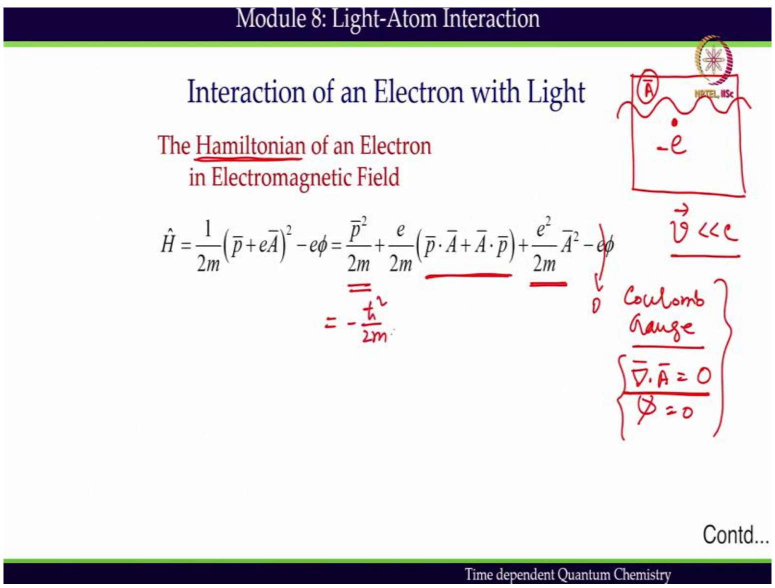

For that Hamiltonian, I have Hamiltonian depends on its momentum operator, that should be, we know, but in addition to that, it depends on vector potential and scalar potential in the medium, which is originated due to propagation of the of the light. So, one can simplify this equation by writing this as square. $H=\frac{\bar{p}^2}{2m}+\frac{e}{2m}\left(\bar{p}.\bar{A}+\bar{A}.\bar{p}\right)^2+\frac{e^2}{2m}\bar{A}^2-e\phi$

So, first we are taking this p square then we are taking this term and then we are taking this term this is just simplifying it and because, we have already said that certain procedures or certain additional condition will use to define A. There is an A which is originated due to propagation of light in the medium, but, we are going to define A in a certain way and the gauge condition we have used is that for the coulomb gauge we have used A to be divergence less and ϕ to be 0, this is the gauge condition we have used.

Under these gauge condition or in other words following this particular pathway, we try to get the solution. Because if we follow this pathway, then we can get a simplified solution. So, definitely ϕ is 0 which means that this term would be 0 from the Hamiltonian and then we will see what is the consequence of this divergence less A, that we will see. The consequence is following we will be able to write down these to be $-\frac{\hbar^2}{2m}$ ....(continued in the next lecture-Lec 52)