**Time Dependent Quantum Chemistry**
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**Lecture 50**
**Master Equation of Light**

Welcome back to module 8, we have just introduced vector potential and we have said that and then we have also introduced scalar potential to represent this electric and magnetic field in terms of potentials. What we have seen is that vector potential is already an unknown potential, which is going to represent the magnetic field and if something is unknown, if we impose additional condition for that, it does not hurt.

And with that additional condition, then we will have to look for the actual formulation, actual expression of $\vec{A}$ that is the basic idea. So, we imposed one additional condition which is called selecting a gauge, and what gauge we have used? We have used coulomb gauge where we are assuming that the vector potential which is giving birth to this magnetic field, it is divergence less.

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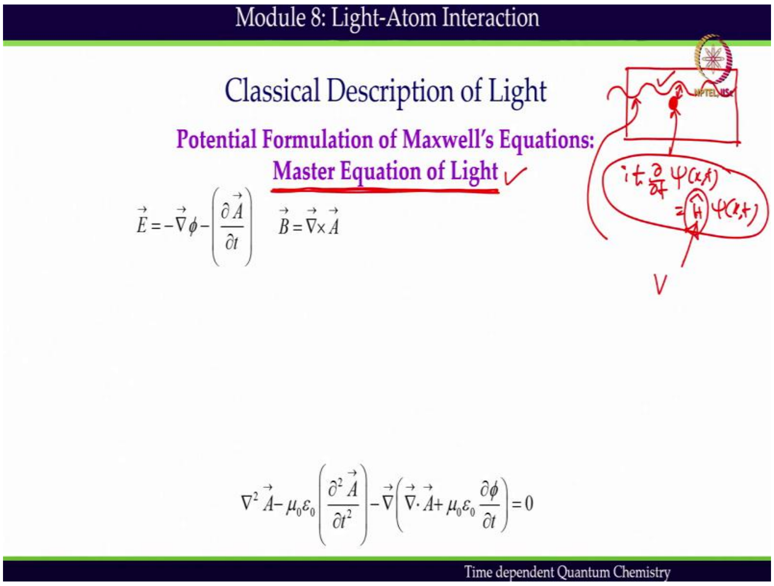


And with this extra condition, we can see, what would be the final expression if I combine all four Maxwell's equations, what would be the combined form because that combined form is going to give me the master equation of light, how I am going to represent light in terms of potential that is the representation we want, because it is all about light atom interaction.

So, I have an atom here setting here in vacuum and light is propagating through the medium. So, I know how to represent this atom, atom will be represented by quantum mechanically that is the Schrodinger equation. So, $i\hbar\frac{\partial\psi(x,t)}{\partial t}=H\psi(x,t)$. So, I have a clear idea now, how to represent this atom, but then question is, how do I represent this light going through the medium?

For that representation, I need the master equation of light which is representing the nature of the light, classical nature of the light and for that only all these formulations we are doing. Once I know this expression, how to represent it, I can know, I will be able to then find out the interaction between them by changing the Hamiltonian. Because in the Hamiltonian, we will have then a potential term which will be introduced as an interaction term. So, that is the ultimate motivation for doing all this formulation.

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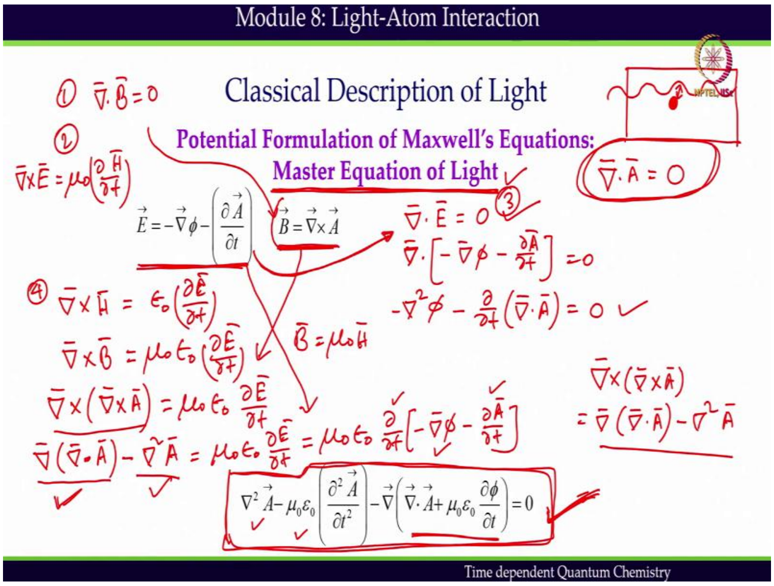


So, what we are going to do right now, we are going to combine all four Maxwell's equations in terms of potential and will represent the final equation of the light, how the light should look like mathematically. We will go ahead we have already seen that electric field can be expressed in terms of vector scalar potential, $\vec{E}=-\vec{\nabla}\phi-\left(\frac{\partial\vec{A}}{\partial t}\right)$ and magnetic field is represented by this , $\vec{B}=\vec{\nabla}\times\vec{A}$.

And we have also selected additional condition for $\vec{A}$, $\vec{A}$ is to be divergence less. Let us, assume that $\vec{A}$ is divergence less. In that case, we have to find out expression for $\vec{A}$ and we have to do this derivation. So, we will come back to this additional condition later, we will just remember that this is the gauge condition we are going to use.

First we will do one thing, we will just one Maxwell's equations we have seen is the dot product or so, divergence of E is 0, $\vec{\nabla}.\vec{E} = 0$. And if divergence of E is 0, one can plug that in, that is the here. So, I have now remember, $\vec{B} = \vec{\nabla} \times \vec{A}$ this equation was fulfilled by Maxwell's equation divergence less B,

$$\vec{\nabla}.\vec{B} = 0 \text{.........(1)}$$

. That is the consequence we have got here.

So, already we have fulfilled one equation. This equation we got from the fact that electric field is the time varying magnetic field was the source of electric fields. So, curl of E was represented by this, $\vec{\nabla} \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t}$ ...........(2)

So, equation (1) and (2) is fulfilled already by these two equations.

Now, we had other two equations and we have to combine them. One of the equations was this divergence less E and that is exactly what we are going to use. And now we are going to plug that in here, if we do that then we get $\vec{\nabla}.\left[ -\vec{\nabla}\phi - \left( \frac{\partial \vec{A}}{\partial t} \right) \right] = 0$ and $\vec{\nabla}.\vec{\nabla} = \nabla^2$

$$\text{i.e., } \nabla^2 = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right),$$

So, we get this del square operator, this is dot product, that is $\left[ -\nabla^2\phi - \frac{\partial}{\partial t}\left( \vec{\nabla}.\vec{A} \right) \right] = 0$ and then this is going to be the dot product of A, which is 0,i.e., $\vec{\nabla}.\vec{A} = 0$,. Now, this part we have taken to be 0, we will come back to this point later this is an additional condition we have imposed. So, something is unknown it is something like that we can take a metaphorical example from real life.

When you look for some, let us say furniture, let us say we are looking for a furniture it is something like the following metaphorical example, we are looking for a furniture and furniture is unknown, we do not know what kind of furniture we would like to look for. That is why we impose many additional condition.

Let us, say we are looking for a furniture which is white, which is 6 feet long, which is 7 feet width, these are the all additional conditions we are imposing. Because in the end, it is unknown, we have to look for an unknown and when you are looking for an unknown, even if I add additional condition, it does not hurt because when we will be looking for it, we will just look for the particular thing with those additional conditions only to fulfil my demand. So, something like that here going on.

We are looking for this $\vec{A}$ function, we will be looking for this to $\vec{A}$ function which is going to define my $\vec{B}$ field and because it is unknown, one can impose additional condition and this is the additional condition we are using, technically, it is called choosing a gauge and we are using coulomb gauge, why it is called coulomb gauge? That is something we will skip will not get into those details because that those details are part of electromagnetism or physical optics part and that part we are avoiding to represent here.

So, what we have is that this equation we get finally and another equation which is left. So, this is the third equation, Maxwell's equation $\vec{\nabla}.\vec{E}=0$....(3) and fourth Maxwell's equations was $\vec{\nabla}\times\vec{H}=\varepsilon_0\frac{\partial\vec{E}}{\partial t}$ ....(4). So, time varying electric field is producing the magnetic field that was the equation. And we can also write down this to be $\vec{\nabla}\times\vec{B}=\mu_0\varepsilon_0\left(\frac{\partial\vec{E}}{\partial t}\right)$ because $\vec{B}=\mu_0\vec{H}$ .So, we can write down this one and B is represented as cross product of A, $\vec{B}=\vec{\nabla}\times\vec{A}$. So, this is now I am plugging this in and what I am doing is that fourth equation Maxwell's equations, I am converting it in terms of the potential form and then I get

$$\vec{\nabla}\times\left(\vec{\nabla}\times\vec{A}\right)=\mu_0\varepsilon_0\left(\frac{\partial\vec{E}}{\partial t}\right)$$

We get this. So, again we will use a vector identity vector identity will not prove the vector identity we will use vector identity directly, this cross product $\vec{\nabla}\times\left(\vec{\nabla}\times\vec{A}\right)=\vec{\nabla}\left(\vec{\nabla}.\vec{A}\right)-\nabla^2\vec{A}$

So, we have again this kind of cross product, so, this cross product can be represented in terms of this. So, I can write down this to be gradient of this dot product this is this dot product is a scalar quantity and when del operator just acting on the scalar quantity it is called gradient. $\vec{\nabla}\left(\vec{\nabla}.\vec{A}\right)-\nabla^2\vec{A}=\mu_0\varepsilon_0\left(\frac{\partial\vec{E}}{\partial t}\right)$

So, we have already this electric field we have this electric field equation here. So, this part is having this potential part but here are still I have this field and I have to convert this field to be potential. So, what I will do I will insert this one again here. So, I will be able to get $\mu_0\varepsilon_0 \frac{\partial}{\partial t}\left[-\vec{\nabla}\phi-\left(\frac{\partial \vec{A}}{\partial t}\right)\right]$. So, this is the entire equation what I get. And if I little bit shuffle this equations then what I get $\nabla^2\vec{A}-\mu_0\varepsilon_0\left(\frac{\partial^2\vec{A}}{\partial t^2}\right)-\vec{\nabla}\left(\vec{\nabla}.\vec{A}+\mu_0\varepsilon_0\left(\frac{\partial\vec{\phi}}{\partial t}\right)\right)=0$ is this is the equation finally we get. We have this del square part here and then we have time derivative part this is the double derivative, second derivative with respect to time. So, this time derivative part is coming here and then the entire gradient part is here also I have a gradient and here I have also gradient. So, the entire gradient part comes here(see slide figure).

So, we get this this equation, this is very easy to do one can just go ahead and do this rigorous mathematical derivation. So, finally, what I get is that this is the equation,

$\nabla^2\vec{A}-\mu_0\varepsilon_0\left(\frac{\partial^2\vec{A}}{\partial t^2}\right)-\vec{\nabla}\left(\vec{\nabla}.\vec{A}+\mu_0\varepsilon_0\left(\frac{\partial\vec{\phi}}{\partial t}\right)\right)=0$ this is the final equation which is combining all four equations together to get me this equation. And this is the final expression for the how light should behave in terms of its vector and scalar potentials.

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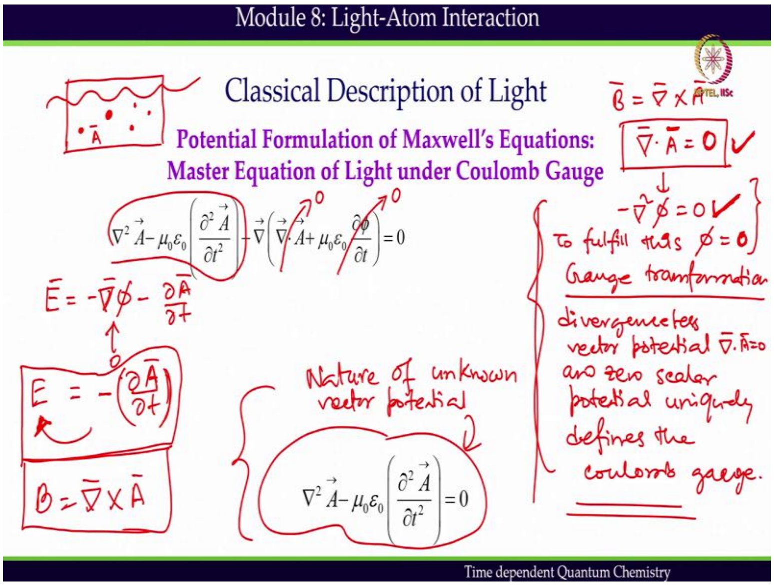

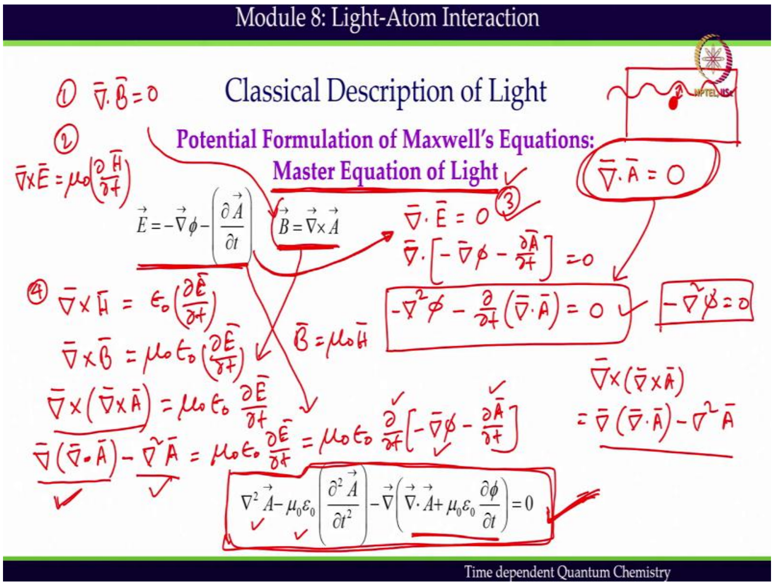


Now, using the additional condition, We have not imposed the additional condition yet, using the additional gauge condition where what we have assumed that okay of course $\vec{A}$ is unknown and $\vec{A}$ is representing $\vec{B}$ like this way and $\vec{A}$ is unknown because it is unknown already and I have to look for it, what about if I impose additional condition which is the selecting a gauge, selecting a particular pathway to solve the problem it is going to be 0.

So, this is the additional condition which we have used, $\vec{\nabla}.\vec{A} = 0$. So, this additional condition if I take then as we can see this equation from this equation, we are seeing that it is going to be then equals 0, $-\nabla^2\phi = 0$. So, with this additional condition, one can write down this del square operator, the second derivative of the scalar potential is 0, $-\nabla^2\phi = 0$.

And to fulfil this, we will assume that we will select $\phi$ to be 0 because if $\phi$ is 0, then this is this condition will be valid. If $\phi$ is constant, then also is valid, but we will just not go for the constant we will just simplify the problem by selecting this gauge. So, we will consider this $\phi$ to be 0, $\phi$ is a scalar potential, scalar potential is 0, which will satisfy my this equation which will satisfy this one also. So, we will be able to define it.

So, scalar potential is selected to be 0. In fact, here, the selecting gauge is more like an ADHOC selection. Suddenly we are just assuming let us assume like this way. But there are rigorous mathematical derivation which is called gauge transformation, which I am not showing here, gauge transformation, this kind of mathematical derivation can in fact support the fact that the divergence less vector potential which is represented mathematically as this and zero scalar potential uniquely defines the coulomb gauge.

So, coulomb gauge, and what is gauge? Gauge is just one pathway to solve the problem there are many ways one can solve the problem. So, this is selecting one particular pathway because that will simplify this particular problem. In some other problem it may show happen that the coulomb gauge would be difficult to solve. And that in that case, we have to go for some other gauge let say Lorentz gauge. There are other gauges also that is called length gauge, velocity gauges.

So, those are the things are part of discussion of electromagnetism and interaction of light with matter. We will not go into that will just follow this particular pathway, because it will simplify the problem and the pathway assumes that the potential, vector potential the unknown quantity is divergence less and the scalar quantity, the scalar potential is 0. So, if it is so, then one can readily write down, this $\vec{E} = -\vec{\nabla}\phi - \left(\frac{\partial \vec{A}}{\partial t}\right)$, the electric field representation and because we are saying that this part is 0, so, E is nothing but time derivative of the vector potential, $\vec{E} = -\left(\frac{\partial \vec{A}}{\partial t}\right)$.

So, electric field I remind the picture one more time I had an atom sitting in this vacuum and light is propagating through the medium, if the light is propagating through the medium electric field at any point of position, any point in the medium will be represented by the time varying vector potential at that point. So, at that point there will be time vector potential that is going to contribute to this electric field under the gauge condition we have used coulomb gauge condition.

And this is the kind of a representation of the electric field under the condition we have used gauge condition we have used and we see that because it is divergence less we have considered So, this is going to this part is going to be 0 and the $\phi$ is considered to be 0. So, this part is entirely 0. What I have finally, is this equation. So, how does the vector potential look like? This should follow this equation. $\nabla^2 \vec{A} - \mu_0 \varepsilon_0 \left(\frac{\partial^2 \vec{A}}{\partial t^2}\right) = 0$

So, what we have here now, in the medium due to propagation of the light, I have two potentials vector potential, scalar potential. Scalar potential is 0, So, it does not have anything, there is a vector potential which will show up in the medium due to propagation of the light. This vector potential, how does it look like? It should follow this. So, nature of unknown vector potential is represented by this equation we have to solve this equation, then I can get the nature of the vector potential. Once I know the nature of the vector potential, I will be able to get the electric field from there and magnetic field, of course, I will be able to get from here.

So, both fields are now can be represented in terms of the vector potential. And what does not mean by vector potential? The meaning is hidden within this expression and this is the way light would be described. So, that is the bottom line of this the entire story which I have represented.

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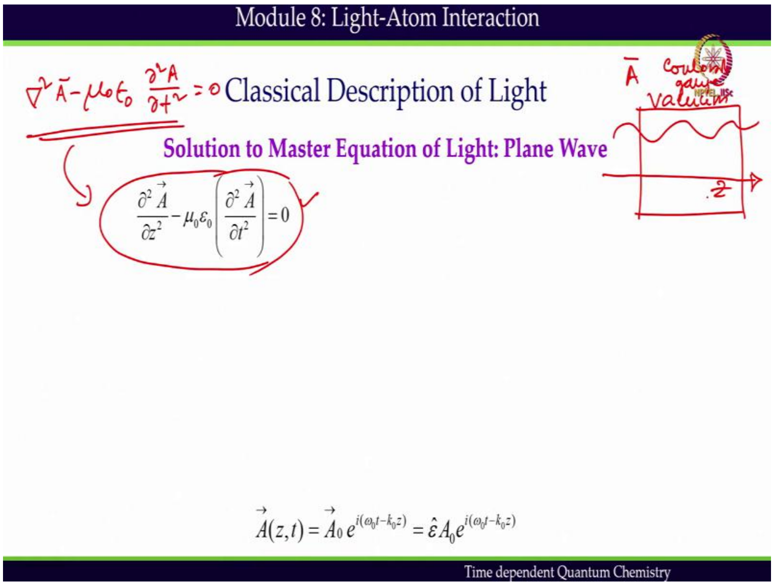


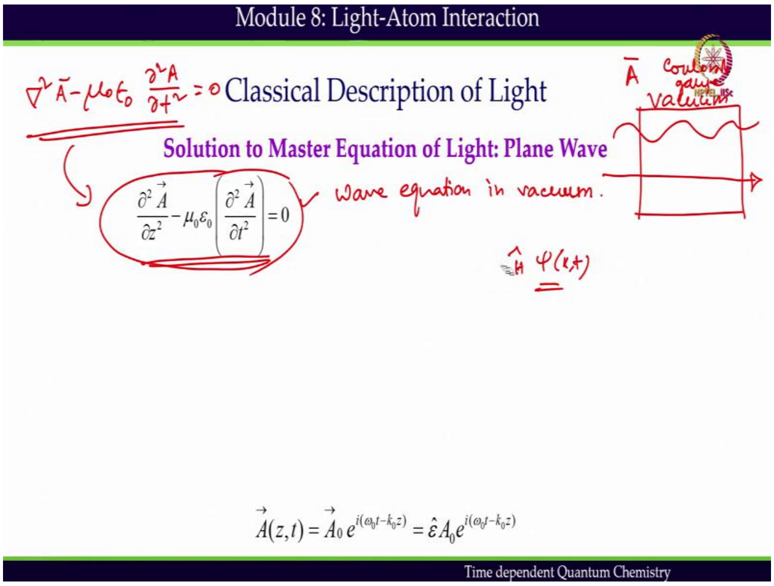


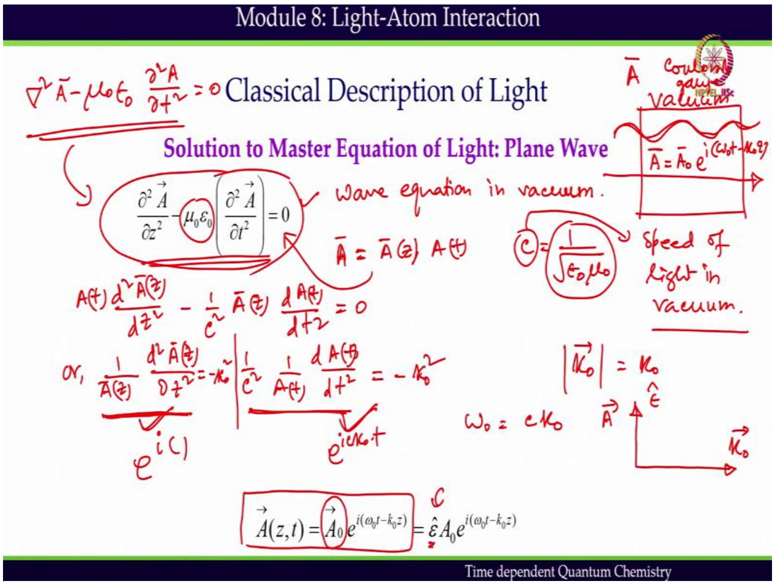

Now, I will go for the solution because finally, I have to find out how the light look like. Because through the medium( through vacuum medium), if light is propagating, then one way to understand this behaviour is to use the coulomb gauge, the coulomb gauge that is one way to look at light, how does it look like. And we will see that if we solve this equation, we will be able to represent light in terms of the vector potential.

So, in order to solve this, this is already one dimensional we have reduced it the equation was actually three dimensional. So, we have reduced it to one dimension to understand the meaning of it first equals 0. So, this was three dimensional equation, we have deduced to one dimensional equation which means the propagation direction is the z direction along the z direction this is the one dimension and the this equation is a one dimensional equation in vacuum and this is the wave equation basically.

So, this is actually a wave equation in vacuum, $\nabla^2 \vec{A} - \mu_0 \varepsilon_0 \left( \frac{\partial^2 \vec{A}}{\partial t^2} \right) = 0$. In terms of vector potential and general solution to this equation is obtained using the variable separation method. We have seen similar kind of equation we have seen for Schrodinger equation, time dependent Schrodinger equation. Time dependence Schrodinger equation has something like this $i\hbar \frac{\partial \psi(x,t)}{\partial t} = H\psi(x,t)$.

So, we had time dependency, we had space dependency and we have used this variable separation method. So, here also we can use the variable separation method the way we can do this this A will be represented as function of z because here z coordinate we have taken as one dimensional space coordinate, and then I have this time dependent part as well, time and space will be separated. $\vec{A} = \vec{A}(z)A(t)$

And we will say that $c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}$. We will see that c would be finally representing the speed of light in vacuum. So, if we now insert this $\vec{A} = \vec{A}(z)A(t)$ one into $\nabla^2 \vec{A} - \mu_0 \varepsilon_0 \left( \frac{\partial^2 \vec{A}}{\partial t^2} \right) = 0$, here, then what I get? We get $A(t)\left( \frac{\partial^2 \vec{A}(z)}{\partial z^2} \right) - \frac{1}{c^2} \vec{A}(z) \left( \frac{\partial^2 A(t)}{\partial t^2} \right) = 0$

Now, this cannot be a partial derivative anymore. $A(t)\left(\frac{d^2\vec{A}(z)}{dz^2}\right)-\frac{1}{c^2}\vec{A}(z)\left(\frac{d^2A(t)}{dt^2}\right)=0$

$$\text{Or, } A(t)\left(\frac{d^2\vec{A}(z)}{dz^2}\right)=\frac{1}{c^2}\vec{A}(z)\left(\frac{d^2A(t)}{dt^2}\right)$$

So, you can see that this left hand side I have I can further manipulate it conveniently and this one will be written as $\frac{1}{\vec{A}(z)}\left(\frac{d^2\vec{A}(z)}{dz^2}\right)=\frac{1}{c^2}\frac{1}{A(t)}\left(\frac{d^2A(t)}{dt^2}\right)$.

So, what we see that in the left hand side I have this two are equal and left hand side I have one particular variable right hand side I have another variable, two variable dependent, independent variable the two terms which are which depends on two different independent variables they are equal these two terms has to be equal and that can only happen when this is constant. The same logic we use previously and the constant we are selecting to be $-k_0^2$

$$\frac{1}{\vec{A}(z)}\left(\frac{d^2\vec{A}(z)}{dz^2}\right)=\frac{1}{c^2}\frac{1}{A(t)}\left(\frac{d^2A(t)}{dt^2}\right)=-k_0^2$$

We are selecting it and later we will find out that $\vec{k_0}$ is actually representing the wave vector or magnitude, $\left|\vec{k_0}\right|=k_0$. So, if we do that, then finally, we get two equations, one equation is

$\frac{1}{\vec{A}(z)}\left(\frac{d^2\vec{A}(z)}{dz^2}\right)=-k_0^2$ and $\frac{1}{c^2}\frac{1}{A(t)}\left(\frac{d^2A(t)}{dt^2}\right)=-k_0^2$.

There are two equations we get one equation z dependent another equation t dependent and these equations can be solved by the exponential function like here it is going to be exponential, complex exponential function of something, this $k_0 z$ and this would be complex exponential function, some time dependent complex exponential functions.

And if we combine them together then what I get is this general solution. This is a general solution we get for the vector potential. So, what we see that due to propagation of light in the medium, in the medium there is a potential which I will create that is the vector potential and the nature of the vector potential is nothing but a plane wave which represents which is represented by $\vec{A}(z,t) = \vec{A}_0 e^{i(\omega_0 t - k_0 z)} = \varepsilon A_0 e^{i(\omega_0 t - k_0 z)}$

Where $\omega_0 = ck_0$ and this $\varepsilon$ is the polarization direction where we are showing that along this along the direction where $\vec{A}$ is changing along that direction. So, $\vec{A}$ is changing along that direction, this is the propagation direction and this unit vector is along this direction where $\vec{A}$ is changing, it is called polarization direction.

So, the unit vector along the polarization direction is the $\varepsilon$. So, we get the final form of this vector potential and meaning of the final form of this vector potential we will go over it. We will stop here and we will continue the discussion of this representation of light in terms of vector potential in the next session.