Time Dependent Quantum Chemistry
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Lecture: 48
Vector and Scalar Potential

Welcome back to Module 8, where we are discussing light atom interaction. So, far we have given the classical description of light you using Maxwell's equations, and we have seen that Maxwell's equations are formulated based on electric and magnetic field. So, in a medium, if the light is propagating through the medium, then I have to check what is the characteristic of electric and magnetic fields I have in the medium.

Based on that characteristics I can explain the classical nature of light, but the problem is that in time dependent Schrodinger equation, which we will ultimately use time dependent Schrodinger equation to understand light atom interaction. In TDQC we use potential term or we use potential form. And that is why what we need to do is that this the field formulation needs to be converted to potential formulation to get the right form which we can include in the time dependent Schrodinger equation.

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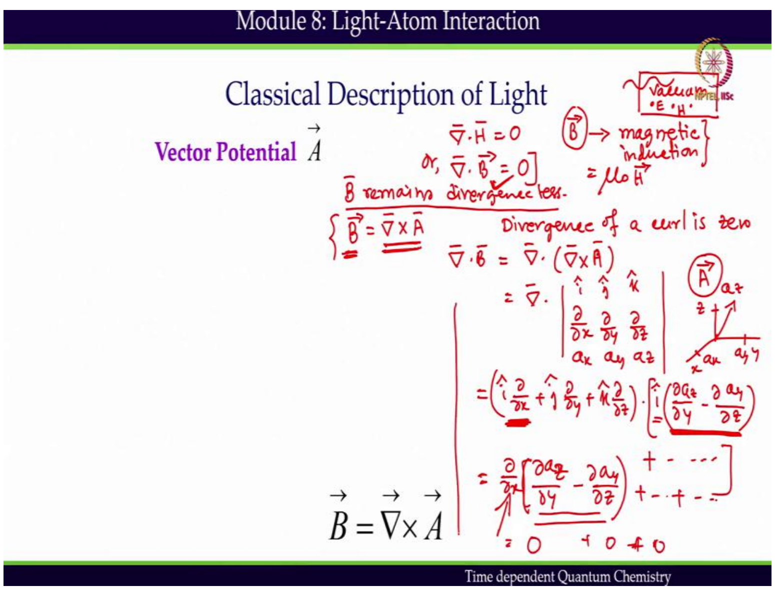

So, we will see how to get that potential formulation of Maxwell's equations, we have used four equations based on electric and magnetic fields, all four equations will be combined together in the potential formulation. And then we can use that potential formulation for the TDQC. So, we will spend little time on this formulation. In the following formulation, we will make use of rigorous vector algebra to obtain the potential formulation of Maxwell's equations.

Now, we already have seen that one of the equations of Maxwell's equations in vacuum. So, we are basically working in vacuum, in the vacuum, so as the medium is the vacuum which is the empty space and we are assuming that the light is propagating through the vacuum and when the light is propagating through the vacuum in the medium, different points, we can check what is the nature of E fields and H fields and we know that in the vacuum this is going to be divergence less, that is the characteristics we propose, I mean, revealed by Maxwell's equation this is going to be always 0, the dot product would be 0, mathematically it is the dot product with the del operator and, it physically it means that its divergence should be 0. And because it is the divergence is 0 one can also write down in the medium even in the vacuum medium we should represent this magnetic field more appropriately in terms of B that is there is called the name is given as magnetic induction, which is nothing but $\mu_0 \vec{H}$ that is the another more appropriate way of presenting the magnetic field in the medium we do not want to get into the more details of this derivation.

Because this comprises entire classical description physical optics part of and we do not want to get into that. So, in vacuum, this is we will present it in terms of B. So, in terms of B even this, the entire equation remains to be the same if the magnetic induction more technically it is called magnetic induction, but we can also say that it is a magnetic field in the vacuum.

So, magnetic field remains divergence less in the vacuum. So, $\vec{B}$ remains divergence less and if B is divergence less then mathematically one can propose that $\vec{B}$ is a curl of a vector and why I will prove that. So, if because $\vec{B}$ remains divergence less than one can write down $\vec{B}$ is nothing but curl of A vector, i.e., $\vec{B} = \vec{\nabla} \times \vec{A}$ that is the way one can represent and why it should be what is the basic reasoning behind this .

Because, the, because divergence this is a very frequently used vector identity I told you that we are going to use vector algebra rigorously here. So, one of the identity, vector identity is that divergence of a curl is 0 and that is exactly happening. So, if $\vec{B}$ is represented as curl of a vector, let us say $\vec{A}$ something so far, let us say then it is divergence is going to be 0.

So, it is just a mathematical consequence and we will begin with this pure mathematical idea and try to understand the physical meaning later. So, one can prove this if it is a $\vec{B}$ is represented as a curl of $\vec{A}$ then it is divergence is going to be 0. And one can prove it like this way this is nothing but $\vec{A}$ that is the way we are representing and if it is, so, then I can represent it like this way.

Curl is represented by I have shown curl is represented by this and then $a_{x,}a_{y,}a_z$. So, what is going on these $a_{x,}a_{y,}a_z$ are the components of the vector along the x, y and z directions respectively. So, this vector we have considered and what is the meaning of this vector? We will come later. But right now, we are just saying that if $\vec{B}$ is a curl of a vector, then immediately this relation holds. So, that will be satisfied immediately.

$$\vec{\nabla}.\vec{B} = \vec{\nabla}.(\vec{\nabla} \times \vec{A})$$
$$= \vec{\nabla}.\left|\begin{pmatrix} \hat{i} & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ a_x & a_y & a_z \end{pmatrix}\right|$$

And that is the reason why we have written this $\vec{B}$, as a curl of vector $\vec{A}$. And $a_{x,}a_{y,}a_z$ it is just if $\vec{A}$ is the vector then in 3-Dimension, one can represents its components, components is going to be x, y, z components. So, this component is going to be $a_{x,}$, this component would be $a_{y,}$ and this component would be a_z, those are the components we have written. Now, if I explicitly do this, then this is a del operator.

So, I will write down its explicit form of the del operators of vector differential operator and then it is going to be dot product with this one and this part this determinant can be written in a following way. This is $\left(\hat{i}\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + k\frac{\partial}{\partial z}\right)\left[\hat{i}\left(\frac{\partial a_z}{\partial y} - \frac{\partial a_y}{\partial z}\right) + ...\right]$

But one thing we see that this dot product will exist only when we take the derivative this part this is associated with the i vector, this unit vector and this is associated unit vector. So, only this term will exist other terms will not exist because dot product does not give you, the dot product becomes 0, such as $\hat{i}.j = 0$, it will be 0.

So, other dot products should be 0. So, only dot product which will exist is the, which is continuing the same unit vector. So, it is nothing but this is $\frac{\partial}{\partial x}\left(\frac{\partial a_z}{\partial y} - \frac{\partial a_y}{\partial z}\right) + ... + ...$ There are two terms will be there. Now, what you see that this is with respect to x, this is the derivative with respect to x, but these terms does not have any x dependency. So, this entire term will be 0.

Similarly, other terms will be 0 also, other two terms should be also 0. So, entire analysis shows that if I can represent this $\vec{B}$ as a curl of a vector $\vec{A}$ then its divergence would be 0.

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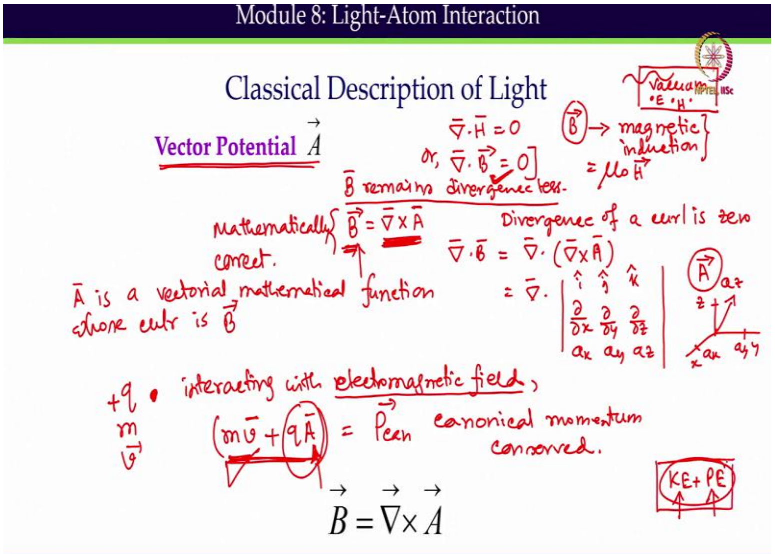

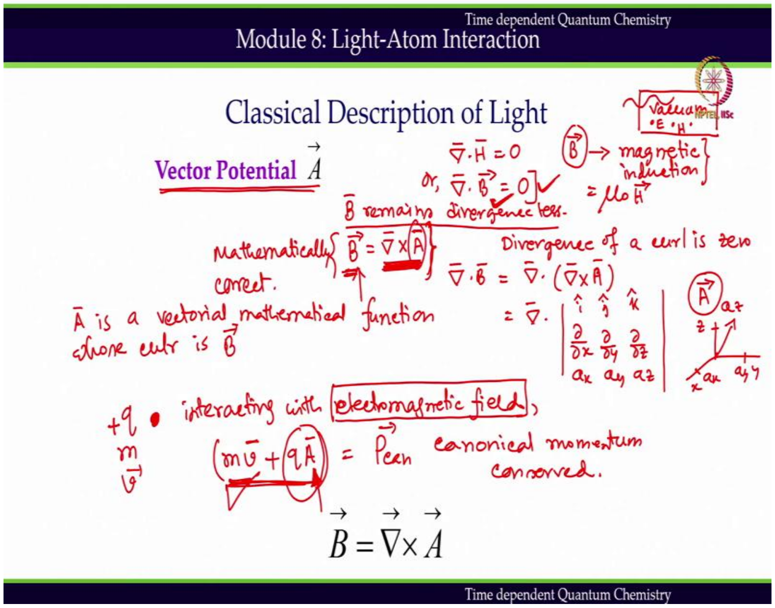

So, this is proved, so this is mathematically correct, but physically what does it mean we will come back and remember this physical meaning of this part this particular and this $\vec{A}$ is will be called vector potential, this is the first time we are introducing this vector potential it so, far we have shown its origin mathematical origin in terms of the vector what is its mathematical origin it comes from the fact that because $\vec{B}$ has to be divergence less than $\vec{B}$ can be expressed in terms of a Curl of $\vec{A}$.

So, it is mathematically correct and this $\vec{A}$ is called vector potential, which is representing the magnetic field. So, the potential associated with the magnetic field is vector potential. And, at this point we can assume that $\vec{A}$ is just a mathematical function whose curl is B. So, $\vec{A}$ what is $\vec{A}$? $\vec{A}$ is a, vectorial mathematical function definitely.

$\vec{A}$ is a vectorial mathematical function whose curl is $\vec{B}$. So, it is representing $\vec{B}$ basically in terms of this curl notation. But later we will find out that, this has many insignificance actually this $\vec{A}$ vector potential, vector potential has many significance. So, one can imagine it is something like this, $\vec{B}$ is a magnetic field and field is nothing but a force a nd force originates from certain potential. In this case force this magnetic force is originating from vector potential that is the way one can imagine, but there are many other significance of $\vec{A}$ and one of the challenging part of physical optics is that, to give a pictorial, view of vector potential, vector potential the concept to understand the concept vector potential it takes a long time.

For somebody who is not familiar with this, with the electromagnetism, but we will try to give some pictorial meaning of vector potential. One of the physical significance of representing $\vec{B}$ in terms of, vector potential is that, for a charged particle if I have a charged particle +q charged particle with mass m, and velocity, let us say $\vec{v}$.

If this particle is interacting with electromagnetic field, if it is interacting with electromagnetic field, then the inertial momentum is going to be definitely m$\vec{v}$, but this we know that m$\vec{v}$ is the momentum which is conserved in classical mechanics but when a charged particle is interacting with electromagnetic field then its inertial momentum is not conserved, it is generalized momentum, is conserved that is called canonical momentum and canonical momentum is expressed by this m$\vec{v}$ + q$\vec{A}$.This entire thing is called this $\vec{P}_{can}$, this is conserved. So, this is called canonical momentum, this is something which I am introducing and this concepts are taken from electromagnetism.

The classical theory of charge particle interaction with electromagnetic field. And we are just picking up the useful information which will be used in the context of light atom interaction. So, just one thing we should remember when a charged particle is present and interacting with electromagnetic field its inertial momentum is not conserved, it is canonical momentum (total canonical momentum) or generalize momentum is conserved.

So, this is conserved and that can be proved, we are not going to show the proof for this, but what is interesting to note that this q$\vec{A}$ term needs to be added to the inertial momentum m$\vec{v}$ to fulfill the momentum conservation law of a charged particle in the electromagnetic field.

So, $\vec{A}$ has a big significance this vector potential comes into the momentum conservation law, it is more like when I do not have electromagnetic field or neutral particle is moving, then we say that it is kinetic energy + potential energy part, total energy is conserved, something like that so, in a conservative force field.

We say that, potential energy part has to be added to the kinetic energy part, then total energy is conserved. That is the way we say, in a similar sense, when a charged particle interacting with electromagnetic radiation remember electromagnetic field, in order to interact with electromagnetic field the particle has to be charged.

If the particle does not have any charge, then it cannot interact with the electromagnetic field. And I mentioned before that when a charged particle is not moving, it is static at standing at a single point, it is not moving with a velocity. So, velocity is 0, then electric field can act on it, but magnetic field cannot act on it.

In order to have some action from magnetic field or in order for the charged particle to experience magnetic field it has to move it has to have some velocity. So, these are the different consequences, we are picking up randomly, but removing the fact that they are useful in the context of light atom interactions, but we are picking up those information which will be useful for the present discussion of light atom interaction.

So, we will move on so, we see that vector potential has a big role in the Light-Atom Interactions and but its origin was pure mathematical, because it is divergenceless, one can immediately express as a curl of this function and this function is called the vector potential.

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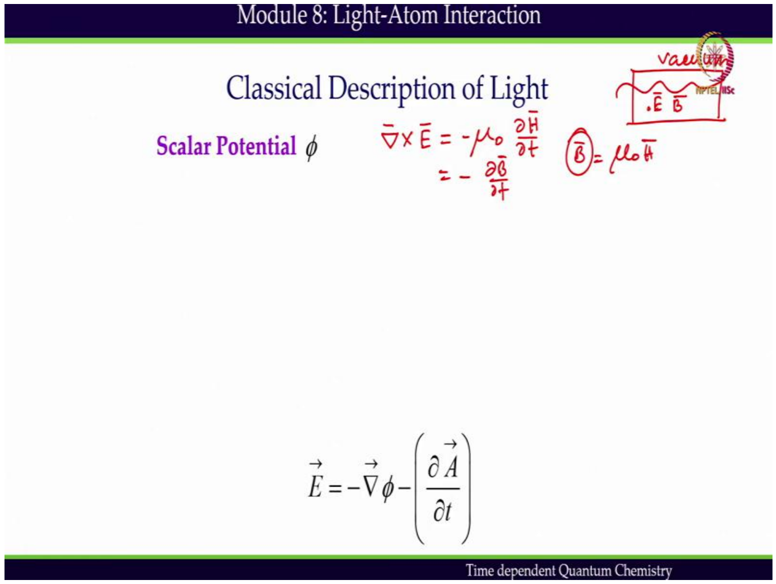

Now, if we have that, then one can insert, So, previously, we had this equation, this curl equation, we said that when the light is propagating through the medium, and because it is vacuum, in vacuum, we are looking at it, so, we have this electric field and magnetic field. And we have to check the nature of the electric and magnetic field in the vacuum.

And we have seen that although they are divergence less but they are curl exist and this is the way we got another equation Maxwell’s equation $\vec{\nabla}\times\vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t}$. So, we can also write down this as $-\frac{\partial \vec{B}}{\partial t}$, because we have defined $\vec{B}$ as $\vec{B} = \mu_0 \vec{H}$ is another physical quantity which is describing technically better way of presenting the magnetic field in terms of $\vec{B}$ that is all I mean that is the way we can think of it right now.

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