Time Dependent Quantum Chemistry

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Lecture: 49

Vector And Scalar Potential

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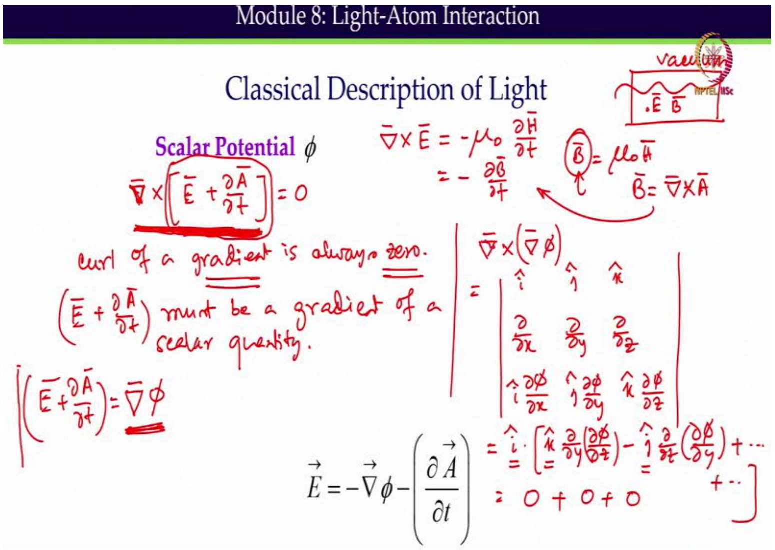

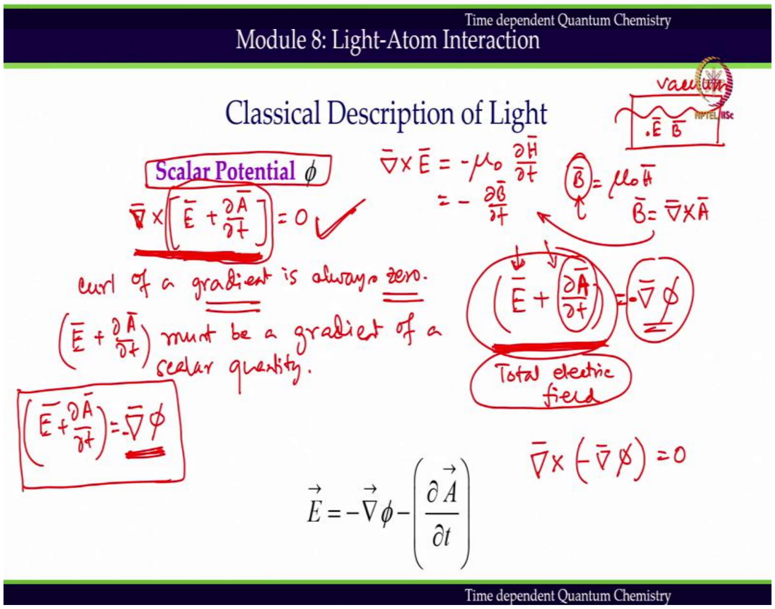

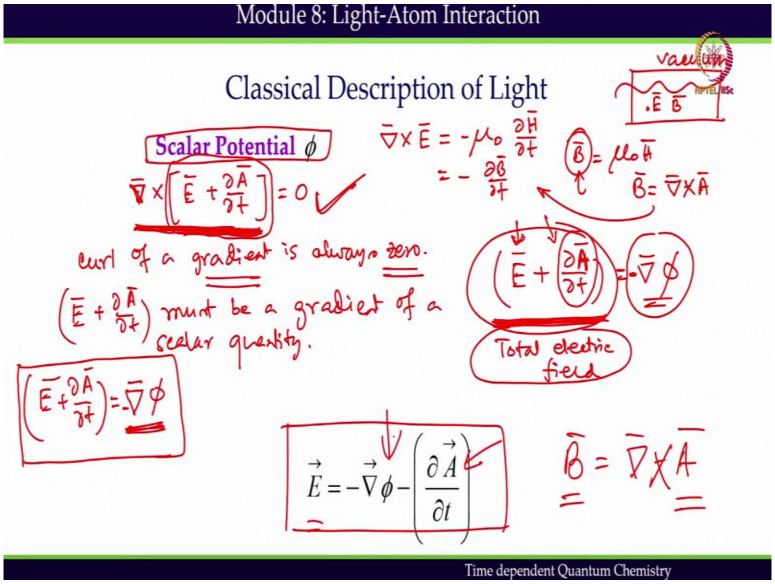

So, we know that now, because we had this equation, and now, we have another expression for B can be represented as the curl of A, $\vec{B}=\vec{\nabla}\times\vec{A}$ and that is why we can insert this here, if we insert it, then what I get here is that it is going to be $-\frac{\partial \vec{B}}{\partial t}=-\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{A}\right)$, this is a space dependent operator, one can easily write down $-\vec{\nabla}\times\left(\frac{\partial \vec{A}}{\partial t}\right)$

$$\text{i.e.,} -\frac{\partial \vec{B}}{\partial t}=-\frac{\partial}{\partial t}\left(\vec{\nabla}\times\vec{A}\right)=-\vec{\nabla}\times\left(\frac{\partial \vec{A}}{\partial t}\right)$$

One can take it out and one can easily write down like this way. Or in other words, we can combine these two, we can rewrite this as this cross product $\vec{\nabla}\times\left(\vec{E}+\frac{\partial \vec{A}}{\partial t}\right)=0$, one can write it down. So, if we can write down here is another interesting property is showing up and we are going to make use of that property of vector algebra.

We are not proving that properties how to prove that I mean in a general form, but we will prove it here in terms of electric and magnetic fields. So, what is the property we are going to make use of previously we have made use of the property that if a function is divergenceless then that function can be expressed that vector can be expressed as a curl of another vector.

Here, we are seeing that the curls itself is 0 this full quantity the entire quantity, the curl of this entire quantity is 0. And the moment curl often entire quantity is 0, which is a vectorial quantity is 0, it means that this curl of a gradient is always 0, another vector identity property. So, what we are seeing is that because this part, this curl, I mean, we know that cross product with the del operator is a curl. So, curl is 0 it means that this must be a gradient of a scalar quantity.

So, this $\left(\vec{E}+\frac{\partial \vec{A}}{\partial t}\right)$must be a gradient of a scalar quantity, this is just coming directly from the vector identities, there are many manipulations one can do these are the consequences of vector identities, one can prove this immediately here, we will prove it here, if we take the let us say, and gradient which means that it has to be represented like this way, gradient of a scalar quantity $\vec{\nabla}\phi$, ϕ is a scalar quantity.

So, this is the scalar quantity we have defining. So, this part has to be represented $\left(\vec{E}+\frac{\partial \vec{A}}{\partial t}\right)$ as $\left(\vec{E}+\frac{\partial \vec{A}}{\partial t}\right)=\vec{\nabla}\phi$,what we are noticing here is that we are just making use of pure mathematical concept to conclude something and then we are trying to find out the physical meaning of it we will find out the physical meaning later.

Right now, what we have shown that because this curl 0 and when the curl of a vector is 0. So, this entire quantity is a vector quantity, but it is a gradient of the scalar quantity. So, an gradient means it is the direction of change, which direction it is changing that is the called gradient or that is the meaning of gradient.

So, let us prove this that it should be 0. If I have a curl of a gradient like this, then I can represent it like as usual $\vec{\nabla}\times(\vec{\nabla}\phi)=\left|\begin{pmatrix} \hat{i} & j & k \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ \hat{i}\dfrac{\partial\phi}{\partial x} & j\dfrac{\partial\phi}{\partial y} & k\dfrac{\partial\phi}{\partial z} \end{pmatrix}\right|$. So, this is the representation of the curl and if

$$=\hat{i}\left[k\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial z}\right)-j\frac{\partial}{\partial z}\left(\frac{\partial\phi}{\partial y}\right)\right]+..+...$$

I explicitly do that simplify it so, it is going to be following it is going to be now $=\hat{i}\left[k\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial z}\right)-j\frac{\partial}{\partial z}\left(\frac{\partial\phi}{\partial y}\right)\right]+..+...$

Then, other two terms these two terms will come in now, look at this terms here I have a dot product with between i and k and i and j which means that the first term will be 0. Similarly, second term will be 0 and third term will be 0, so, enter term will be 0. So, we have proved that curl of a gradient is going to be 0.

So, mathematically we are correct if we express it like this way, and the moment I express it like this way that this in entire quantity that is the electric field plus time derivative of the vector potential, this entire thing is represented by the gradient of a scalar quantity this ϕ is called scalar potential i.e., the definition of scalar potential is coming in. So, I have the scalar potential formulation which is nothing but $\left(\vec{E}+\frac{\partial\vec{A}}{\partial t}\right)=\vec{\nabla}\phi$. So, gradient of the scalar potential is represented by this vectorial quantity.

So, what we get in the end ? But, at the same time, we should remember that we have to be correct with the sign because here, there should be one negative sign, why this negative sign is coming up, we will understand it phenomenologically. This negative sign is coming up because this entire part is a vector, which is some kind of a field total field.

Let us say total electric field, $\left(\vec{E}+\frac{\partial\vec{A}}{\partial t}\right)$, why total electric field because this is electric field $\vec{E}$ and I am adding another quantity $\frac{\partial\vec{A}}{\partial t}$, if I am adding, two dissimilar quantities cannot be added. So, if this is electric field $\vec{E}$, this $\frac{\partial\vec{A}}{\partial t}$ has to represent some kind of electric field which is originating from the vector potential, but it is electric field.

So, two electric fields are combined together so, it is a total electric field. Now, total electric field, field is a force and the total electric field depends on the gradient of the potential but it is a negative gradient of the potential, why negative gradient of the potential, we know that if the potential is increasing this way, then the force or the field will be acting along this way.

That is the way they work they are acting in opposite direction always. So, because they are acting in opposite direction, we have to put this negative sign so, it is notational we should be correct for this representation. So, the basic idea of this negative sign is coming from the fact that the total electric field experienced by the particle, the field is the force and force is acting along this direction.

Because if the charged particle is left here, without any force, then it will just reduce its potential this way. And that is the way a force is acting. But this way potential is increasing, this is the direction potential is increasing (see slide) and this opposite directionality of the potential versus field is pointing out that we should have a negative sign it.

So, negative gradient should be there. And it is does not hurt the mathematics as well, because as long as this part is valid, even if it is negative, $\vec{\nabla}\times\left(\overrightarrow{-\nabla\phi}\right)=0$, it is still 0. So, this part is still okay with the Maxwell's equations, I am not violating Maxwell's equation but I have introduced this negative sign. So, that I am phenomenologically correct to make the two fields, the field and potential to be opposite in direction.

So, in the end, what I get is that the electric field can be represented like this (check slide image), where we have seen the magnetic field will be represented in terms of vector potential. So, magnetic field can be represented in terms of vector potential, electric field now can be represented in terms of vector potential and scalar potential, i.e., both are contributing to them electric field.

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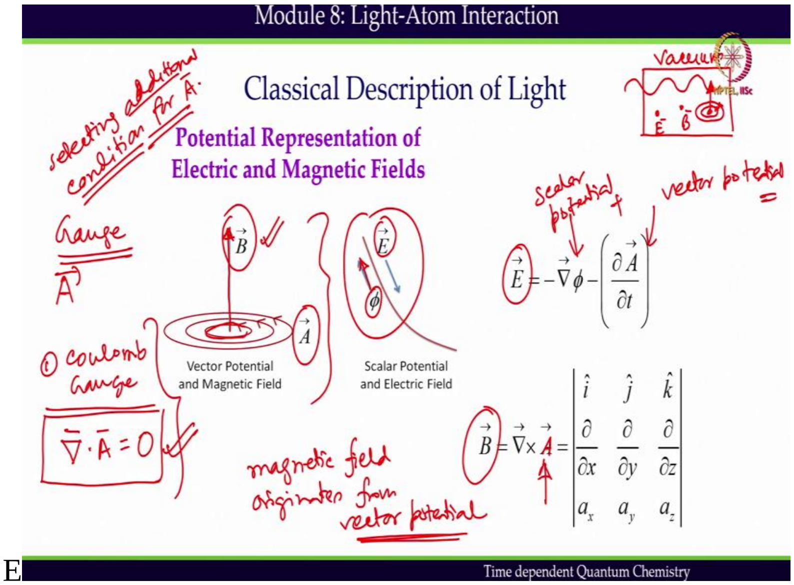

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So, there are two important realizations we have already got. When I have a medium and through the medium light is propagating, for the medium I have vacuum, I have selected vacuum to make things simple, and when light is going through this medium, then, to describe the nature of the light I have to find out electric and magnetic fields in the medium that is $\vec{E}$ field and $\vec{B}$ field specifically we are saying $\vec{B}$ field instead of $\vec{H}$ field.

And we have to find out what is the nature of these fields and we have seen that there is a particular way it is behaving it is divergence less it curl exists and time varying one field is generating the other field that is the way we have seen already. But then we would like to convert it to the potential formulation the moment we get the potential formulation, it gives you the origin of those fields in the medium, due to propagation of the light. Now, the origin is following what we see that the $\vec{B}$ field, this is the magnetic field, magnetic field originates from the vector potential, so magnetic field originates from vector potential, and electric field, in this medium, originates from scalar potential plus vector potential.

So, these are the two realizations we have and we have to use that. Now what is the pictorial representation? We have said that in the first step, one mathematical derivation of potential formulation of Maxwell's equations, $\vec{A}$ is proposed to be an unknown function, we said that $\vec{A}$ is an unknown function, and later we said that it is the vector potential.

So, how does it look like now, one can say that the electric field is the force, force is acting to reduce the potential electric field. On the other hand, the scalar potential is increasing in the opposite direction of the field. So, this is the pictorial representation of the scalar potential, very nice pictorial representation of the scalar potential.

So, scalar potential is increasing in a particular direction and the field, total electric field would be acting in the opposite direction. On the other hand, the pictorial representation of the vector potential is following vector potential, $\vec{A}$, $\vec{A}$ is rotating in nature like this way (see slide figure). So, this rotation or rotating field (this rotating potential field) basically is originating the giving birth to the vector field which is perpendicular direction because it should follow the right hand rule. So, if rotating like this way (see slide figure), then it should point along this direction. So, that is the way one can imagine how this fields are correlated with the corresponding potential. Scalar potential is easy to understand is easy to visualize this is something gravitational potential let us say as we go up, gravitational potential is increasing, but at the same time forces is increasing but gravitational potential is in a opposite direction. So, something like that, it is actually trying to reduce the potential.

On the other hand, this vector potential because it is a vectorial quantity, it takes some time to understand what is the meaning of it? Now, $\vec{A}$ is unknown function, one may conveniently impose additional condition to define it because, if something is unknown, we have to figure it out what is that unknown and when we have to figure out what is unknown, we can impose many other constraints and then figure out what is that unknown.

So, that is the basic idea. So, because it is an unknown function, one can conveniently impose additional condition to define it. And technically, when we do that it is called choosing our gauge to define this $\vec{A}$ and selecting additional condition for $\vec{A}$, that is called selecting a gauge. Two commonly used gauges include coulomb gauge, we very frequently use these two gauges coulomb gauge, And other gauge is Lorentz gauge, these are the two gauges we use very frequently and what is the difference between these two gauges it is just the defining conditions are different. So, what kind of $\vec{A}$, it should be we are just defining it and then because it is unknown, we have to look for that with that condition.

When the problems associated with light matter interactions are solved using different gauges, each gauge may render different mathematical derivation steps with varied difficulty levels. However, ideally they should not change the final outcome. That is the point. So, if we use a particular additional condition for $\vec{A}$ to define $\vec{A}$ before we start describing the light atom interaction, the final outcome should be the same ideally.

Therefore, selecting a suitable gauge for a given problem of light matter interaction or light atom interaction is mostly our discretion it is our freedom to decide what should be selected for a particular situation if a particular gauge or particular additional defining condition is helping me to get a simplified mathematical derivation. So, we should follow that so, that is the basic idea.

In our discussion, we will use this coulomb gauge because that is easy to percept and when I say coulomb gauge it means that I will assume that this unknown function is divergence less, it is purely rotating in nature and this is the additional condition we are imposing and then we have to find out what kind of $\vec{A}$ it is going to be if I have this condition.

So, if it is divergence less it is purely rotating in nature. And that is why we have shown this figure, it is purely rotating in nature and that is the curl, which is represented by the $\vec{B}$ field, curl of $\vec{A}$ is going to be $\vec{B}$ field. And that is the way it is representing. So, in every point, we have in this vacuum, every point we have a rotating vector potential field and the magnetic field would be just perpendicular to that to the plane of this vector potential field.

So, this is the meaning of vector potential and additional condition we will use this one for getting the solution of Light-Atom Interaction. We will stop here and we will continue this module in the next session.