

Quantum Mechanics
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Lecture – 54
Tutorial 9 - Part II

After these practice problems on Pauli matrices, we now move on to problems on particle, charge particle in an electromagnetic field whose Hamiltonian is given to us.

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$$\textcircled{a} \quad \hat{H} = \frac{1}{2m} (\vec{p} - e\vec{A})^2 + e\phi$$

$$\hat{p}^2 = p_x^2 + p_y^2 + p_z^2$$

$$\frac{dx}{dt} = \frac{i}{\hbar} [x, H]$$

$$= \frac{-i}{2m\hbar} [x, (\hat{p}_x - eA_x)^2 + (\hat{p}_y - eA_y)^2 + (\hat{p}_z - eA_z)^2]$$

$$= \frac{-i}{2m\hbar} i\hbar^2 [p_x - eA_x(x, t)]$$

$$\boxed{\frac{dx}{dt} = \frac{1}{m} (p_x - eA_x(x, t))}$$

And the Hamiltonian is given by, this is the Hamiltonian. So general representation of the Hamiltonian for a free particle we have seen is $p^2/2m$ and here we have a particle which is charged in an electromagnetic field and its Hamiltonian is $(p - eA)^2/2m + e\phi$, okay, +the scalar field, ϕ . So where A is the vector potential and this ϕ is the scalar potential which is given to you and p is the momentum.

So now we have to find out a quantum mechanical Lorentz force which is proportional to the d^2r/dt^2 . So you know classically how one writes the Lorentz force. You have to derive the quantum mechanical version of it. So let us start by writing the $d/dt = -i\hbar^{-1} [x, H]$. Recollect this we have been using several times, time evolution operator. So this is the Ehrenfest theorem which you are going to write for x which is the position operator or the position which has no explicit time dependent.

So we just have $\frac{dx}{dt} = -i/\hbar$ cross and the commutator of x with the Hamiltonian. We will not have the second term in this because x do not explicitly depend on time. So we can evaluate this by substituting \hbar over here which is, you can write this in terms of the 3 direction, p_x , p_y and p_z . So when I write this, what do I get. $i\hbar$ cross x , I will have $2m$ which I can take outside, okay. And when I operate, when I use this Hamiltonian operator, okay and try to evaluate this p_x , p_y and p_z , I can write separately.

So I will have $p_x - eA$ square, okay, +, I will have a p_y term, + p_z term, right. So I can take a commutator of just this term and the remaining term, $p_y - eA$, this is x , this will be y , okay, sorry, so this will be a +, +the same way we use to write for p square. Operator p square, how we wrote it as? We wrote it as $p_x^2 + p_y^2 + p_z^2$, correct. So here only this term will contribute.

That is why I am writing here this term and the remaining term would not contribute. So these would not commute. I mean these would give 0. They will commute sorry. And this will give you a non-0 result. So I can just take this term, p_x term and the commutator of $e\phi$ with x will also be 0. So only contribution comes from this through the entire Hamiltonian. So let us drop this term, $-i/2m$, commutator of this we know. $x p^2$ was $2p_x$.

So similarly, I will have a $i\hbar$ cross*, I will have $2p_x - eA_x$ which is the function of r and t , that is A is the function of x, y, z and t , okay. So this is what I have. So finally $\frac{dx}{dt}$ will be nothing but $p_x - eA_x$ r, t . Here I will have a factor of, this will be 1, this will be 2. So $1/m$, okay. So next step would be to calculate dV/dt , okay.

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4 A charged particle in an electromagnetic field is described by Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi$$

where \mathbf{A} and ϕ are the vector potential and scalar potential. Find the quantum mechanical form of Lorentz force proportional to $\frac{d^2\mathbf{r}}{dt^2}$.

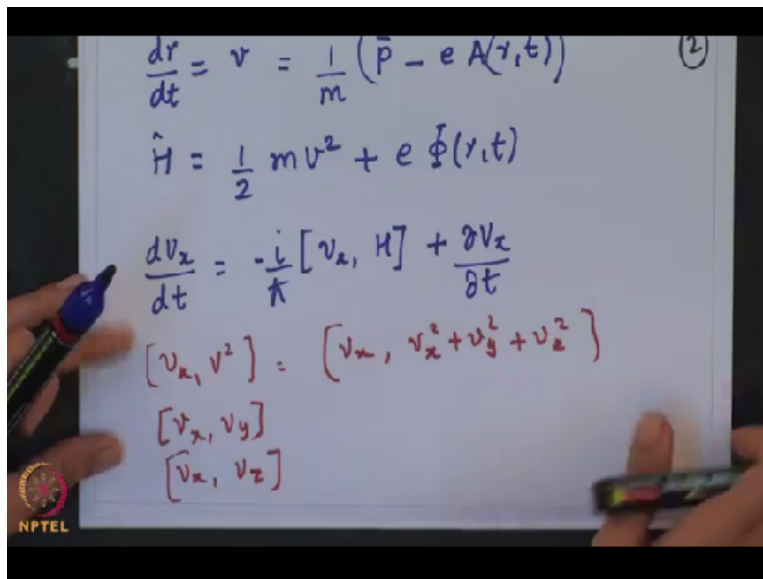
5(a) Prove that $[\mathbf{S}^2, S_z] = 0$ where $\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2$

(b) Show that the eigenvectors basis of S_z diagonalizes S^2 . Find the eigenvalues of S^2 . $[\mathbf{S} = \hbar\boldsymbol{\sigma}/2]$



Now we know this is the sample definition of V, velocity, will be dr/dt.

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So dr/dt will give me V. And this dr/dt, now this was for dx, right. So if I do it for dr, I will have p-eA, correct. So this will be nothing but this for the velocity. Now there will be a time-dependence which I can write it as p-eA r,t, correct. This is what I obtain from velocity. Now you know velocity. In terms of velocity, you can rewrite the Hamiltonian. So your Hamiltonian was, this is the square which I missed, sorry.

So Hamiltonian is 1/2m p-eA square+e phi. So this I can rewrite as V square. So 1/2m, there will be a m square, okay, coming from here. So this will become, in terms of p, so there will be m

square, $m^2 V^2$, this will be replaced. So I can rewrite the Hamiltonian operator as $\frac{1}{2m} V^2$, this term will remain unaltered. This is also a function of r and t which I have not written here but it explicitly, it means that it is a function of r and t . here also it is a function of r and t , the coordinates, space and time coordinates.

So now in order to calculate dV , so let us do it for x . Now velocity is time dependent. So we will have this modified as $-i\hbar$ cross, then I have $V \times H$ + the partial differentiation with respect to t . So this is what I have. For this you can, you just look carefully here. You have to evaluate few things. So that is V of x and V^2 .

This means you have to evaluate what is $V_x V_y$ and what is $V_x V_z$. $V_x V_x$ will not contribute, okay. So this you can write it as V^2 . This can be written as $V_x^2 + V_y^2 + V_z^2$, correct. That means you have to evaluate V_y^2 and V_z^2 . So that means you have to evaluate this. So going in the, doing back engineering, that is going from the bottom to the top to get the result.

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The image shows a whiteboard with handwritten mathematical derivations. The first equation is:

$$[v_x, v_y] = \frac{1}{m^2} [(p_x - eA_x), (p_y - eA_y)]$$

The second equation is:

$$= \frac{i\hbar e}{m^2 c} B_z \quad \text{and } \partial_x A_y - \partial_y A_x$$

The third equation is:

$$[v_x, v_y^2] = \frac{i\hbar e}{m^2 c} (v_y [v_x, v_y] + [v_x, v_y] v_y)$$

The fourth equation is:

$$= \frac{i\hbar e}{m^2 c} (v_y B_z + B_z v_y)$$

The fifth equation is:

$$[v_x, v_z^2] = -\frac{i\hbar e}{m^2 c} (v_z B_y + B_y v_z)$$

There is an NPTEL logo in the bottom left corner of the whiteboard image.

Let us evaluate what is $V_x V_y$, okay. So $V_x V_y$, you will substitute for V that is $\frac{1}{m} p_x - eA_x$. Similarly, for V_y , so you will have 4 terms. So the 4 terms would be, let me write $\frac{1}{m}$, square it will become. I have $p_x - e$, so there will not be a vector, A_x , this is the first term commuting with $p_y - eA_y$, correct. So this is what we have. Now commutator of p_x and p_y is 0, they commute and

$A_x A_y$, they will also commute.

So you will be left with the commutator of p_x with A_y and A_x with p_y . When you do this, what you obtain after doing all the substitution and everything. You will obtain \hbar cross. There will be e/m square c , that is what you will obtain by doing all the substitution, okay, $*$, you will have B_z . B_z is nothing but how will I write B_z ? It will be d , so z x and y , do $x A_y - y A_x$, it will be in this form, okay.

So this B_z is proportional to this. I mean we have got it from here. We wrote B_z in terms of B , okay. So this is what you have when you do the, when you solve this. So you will have 4 terms. Again I am repeating, only the cross terms, these 2, these 2 will contribute, this and this, this and this. This will give me p_x . So this is $p_x A_y$. Here I will have $p_y A_x$. This will give me term proportional to B_z , okay, z component of (\mathbf{L}) (10:58).

So similarly, you can write what will be $V_x V_y$ square. $V_x V_y$ square is simple. You will, you can rewrite this and use the relation V_x , this one, V_y . I will have square, I can write here V_y , $+V_x V_y V_y$. This is the standard way of solving. So \hbar cross e/m square c , this we have already, okay. This is nothing but, okay, I wrote this beforehand only, sorry. This will be written as $V_y V_x +$, commutator of $V_x V_x$ with the V_y on the left, commutator of $V_x V_y$ with V_y on the left.

So after substitution, you get B_z . So $V_y B_z$, this will give me B_z , $+B_z V_y$, okay. This is what you obtain on substitution. Similarly, now you can guess what will be $V_x V_z$ square. No need to repeat this exercise. You can just make a guess. So everywhere when you have x and y square, you will have $V_y B_z$. So now I will have $V_z B_y$, correct or $V_y B_z$. So here I have z , right. So now here I have z .

So now here I will have y , $B_y V_z$, okay. So this will give me $V_y B_z$ and this will give me $B_z V_y$, correct. Similarly, you will have a swap term, okay. So here I have got this contribution, okay. There will be $-$ sign here because here you have $V_x V_z$. So when you are doing this, be careful with the sign, $x y$, $y z$, $z x$. So here it has to be $z x$ to have a $+$ sign. But I have $x z$. So I will have a $-$ sign. So now going further, you have to add these 2 to get $V_x V$ square, okay.

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$$\frac{dv_x}{dt} = \frac{e}{2mc} [(v \times B)_x + (B \times v)_x] + \frac{eE_x}{m}$$

quantum mechanical force force
in x direction

in general,

$$\frac{dv}{dt} = \frac{e}{2mc} [(v \times B) - (B \times v)] + \frac{eE}{m}$$

When you do this addition, you will simply obtain dv_x/dt is nothing but $e/2mc$ $V \times B$ x component + $B \times V$ x component + eE/m , okay. So this let us go back here. So here we had this. We have to find out $V \times V$ square. And $V \times V$ square, we have broken in steps wherein here we obtain V_x . V_x square + V_y square + V_z square, you add these 2. So here we have $V_y B_z - V_z B_y$. So this will be V cross B term.

One V cross B term will give me $V \times B$ x, x term, $V \times B$ x and $V \times B$ x. So we have resolved this part. In the second part, that is the second term, what we have done is, do $V \times dt$, you can just rewrite this in terms of ϕE , in terms of ϕ and obtain this. This is nothing but quantum mechanical Lorentz force, okay in x direction. This is for x direction. Now in general, you have, what you can do is when I rewrite in general, I will have, so this will be again x component, okay, remember.

So when I have to find out internal dV/dt will be $e/2mc$ $V \times B$, okay, $-B \times V$, this is the term, $+E/m$. So this is nothing but the quantum mechanical Lorentz force which is proportional to; this dV/dt , you can rewrite this, this is nothing but $d^2 r/dt^2$ which is asked in the question. So it is proportional to this in terms of the quantum mechanical Lorentz force. And I think this part was also discussed in the lecture.

So it will help you to understand better if you try your hands on and do the exercise by yourself which I have been telling in all my tutorials. But it is very helpful when you do it yourself at least once. And the fifth problem after the exercise of commutator bracket for; and the Pauli spin matrices which was there in the previous tutorial, fifth tutorial you will find as very simple one.

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Handwritten mathematical derivations on a whiteboard:

$$\begin{aligned}
 & \text{(a)} \quad [S^2, S_z] = 0 \qquad [L^2, L_z] = 0 \quad \text{(b)} \\
 & [S_x^2 + S_y^2 + S_z^2, S_z] \qquad \hat{S} = \frac{\hbar}{2} \hat{\sigma} \\
 & [\hat{S}_i, \hat{S}_j] = \frac{\hbar^2}{4} [\hat{\sigma}_i, \hat{\sigma}_j] = \frac{\hbar^2}{4} \epsilon_{ijk} \hat{\sigma}_k = \frac{\hbar^2}{2} \hat{S}_k \\
 & [\hat{S}_x^2, \hat{S}_z] = \frac{\hbar^2}{4} [\hat{\sigma}_x^2, \hat{\sigma}_z] = \frac{\hbar^2}{4} (-\sigma_x \sigma_y - \sigma_y \sigma_x) \\
 & [\hat{S}_y^2, \hat{S}_z] = S_x S_y + S_y S_x = -S_x S_y - S_y S_x
 \end{aligned}$$

So in this you have S square. We have to prove that S square Sz commutes, okay. What will happen if S square and Sz commutes? If S square and Sz commutes, then they form simultaneous eigenket. You have also seen the same thing for angular momentum operator, L square Lz is commuting. So you can form a simultaneous eigenket for L square and Lz. Lz and here Sz form has a diagonal, is a diagonal matrix.

So it is easy to calculate the eigen values in eigen vector. And once we know the eigen vector of Sz, we can have simultaneous eigenket for S square also. So the eigen vectors of Sz will also be the eigen vector of S square. And that simplifies the calculation. So let us start by doing Sz, you can write it as Sx square+Sy square+Sz square, correct. You have to find the commutator of Sx square with Sz, okay.

So you have seen already and in general also you have Si, Sj; you can write it as, remember, just recollect that S operator, spin operator can be written in terms of Pauli matrices which we have discussed already or you might have seen in the class at least once. So in terms of Pauli matrices,

you know what is the commutator of sigma i sigma j which we discussed last time. So this will be \hbar cross square/4, correct, sigma i, sigma j.

And what is sigma i sigma j? If I write in terms of epsilon ijk sigma k, okay. So when i and j are equal, this will be 0. You all know this tensorial notation. So using this with the help of this, you can actually calculate what is S square Sz, right. S square Sz will be sigma x square sigma z which will be, which will give me, what it will give me? Sigma/, this will give me, and so the same relation actually you can rewrite this again. I will just come here back to; this you can rewrite again as, okay, this relation.

So either you substitute for this and check the result or you keep these in terms of Sz notation if you know the commutator of S. So if I substitute for this, I will have, I can rewrite this as, I will have sigma x, so I will have a y, okay, so -y, -sigma, this will be y sigma z, okay. So when I am rewriting this, I will have the fall, -SxSy-SySx, okay. And what do I obtain for Sy square Sz? It will be; now you have a y z. So you will obtain SxSy+SySx. And for square Sz, you know the commutator is 0. So when you add these, what you obtain the final answer as?

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$$[S^2, S_z] = 0$$

S^2, S_z form a simultaneous eigenket

(b) $S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$S^2 = \frac{\hbar^2}{4} (S_x^2 + S_y^2 + S_z^2) = \frac{3}{4} \hbar^2 \mathbb{1}$

e. vector $|+\rangle$ $|-\rangle$
 e. value $+1$ -1
 $S_z^2 = 1$

Commutator of S square with Sz is 0. This is the important result and this result means that S square and S form a simultaneous eigenket, okay. So eigen values of Sz and eigen vectors of Sz can help you to find out the eigen vectors of S square. So in the second part, you are asked that

show that the eigen vectors bases of S_z diagonalizes S^2 , okay. And you have to find the eigen values of S^2 also. So b part.

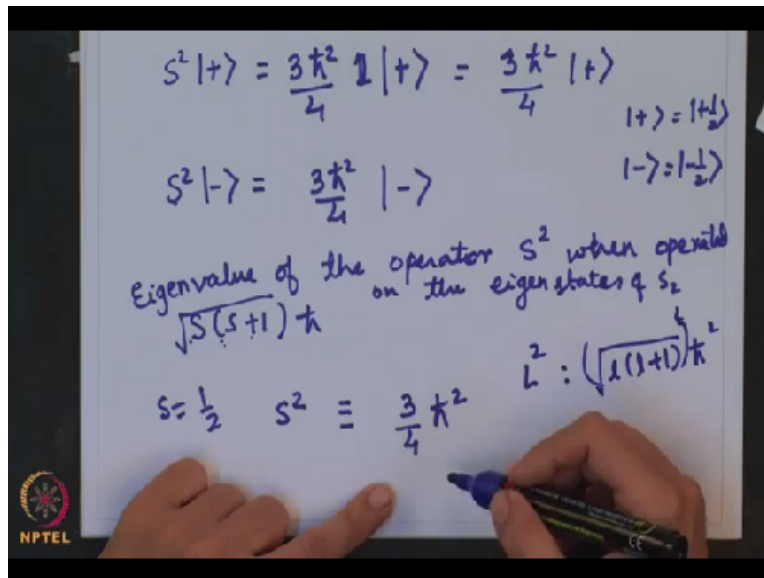
Now you can write S_x in terms of Pauli matrices, we have seen that $\hbar \sigma_x$ is $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, correct. S_y is $\hbar \sigma_y$ is $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and S_z is $\hbar \sigma_z$ is $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. See S_z is a diagonal matrix. So you can see from here, you can infer from here that it will have eigen values 1 and -1. And the eigen vector will be of the form $|+\rangle$ and $|-\rangle$, right. So these will be the eigen vectors or eigenkets.

And eigen values will be + and -1. It is very simple to infer from this. Now you need not solve, use the eigen value equation. You are very familiar and just by looking at the matrix, if it is diagonal, the diagonal elements would correspond to the eigen values. And eigen vectors, you can easily write them in terms of $|+\rangle$ and $|-\rangle$ ket, $|+\rangle$ ket $|-\rangle$ ket or 2-dimensional or 3-dimensional, we write in terms of $|+\rangle$ $|-\rangle$ ket 0, okay.

So this we know already. So now S^2 will be; S^2 , how will you calculate? It will be $\hbar^2 (\sigma_x^2 + \sigma_y^2 + \sigma_z^2)$, correct. So if I make this substitution in terms of sigma matrices, what do I obtain is; so here I will have to write sigma x sigma y and sigma z, because I wrote already the $\hbar^2/4$, okay.

So when I square this, this square+this square+this square, we know that sigma i square is 1. So this will give me $3\hbar^2/4$, identity+identity+identity which is nothing but identity matrix, okay. So this identity matrix would give me, now this when you operate an eigenket, $|+\rangle$ on this, what do you obtain?

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When I operate S^2 on the $|+\rangle$ state, what do I obtain? $\frac{3\hbar^2}{4}$ and if you have an identity operator, when you operate a $|+\rangle$, it will project out the $|+\rangle$ component which will be nothing but $\frac{3\hbar^2}{4}|+\rangle$, okay. In some places, you will find that this $|+\rangle$ ket is represented as $|+\frac{1}{2}\rangle$ and $|-\rangle$ ket is represented as $|-\frac{1}{2}\rangle$. So this notationwise, I mean here the same thing as what here you have that is when you write the eigen vectors as $|1\ 0\rangle$ or $|0\ -1\rangle$, they would correspond to $|+\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$, this you should remember.

So this is called as spin upstate. This is called as spin downstate. These things you must remember. S^2 when operated on $|-\rangle$ ket, this will give you $\frac{3\hbar^2}{4}$ and $|-\rangle$, this is nothing but downstate. So it will project out only the downstate when you operate this on. You can work out each step if you are not very much convinced with what I have written here. So from this you can see or you can also think in another way like S^2 when operated on these eigen vector, gives me the eigen value of the form $S(S+1)\hbar^2$.

So this forms a simultaneous eigenket but it gives you the eigen value. So this will be the eigen value of the operator S^2 when operated on the eigen states of S_z . The eigen states which we have inferred from your $|+\rangle$ up and down state. So when you substitute for S as $\frac{1}{2}$, what do you obtain? You get the eigen value, sorry $S(S+1)\hbar^2$ actually, \hbar^2 , okay, square root of $S(S+1)\hbar^2$.

So when you do S^2 , you will have $S(S+1) \hbar^2$ cross square. So the eigen value of S^2 will correspond to, S is $1/2$, $1/2+1/2$, so this will be $3/4 \hbar^2$ cross square. You remember this is the same result as we got for orbital angular momentum which was $l(l+1) \hbar^2$ cross square root of $l(l+1) \hbar^2$ cross for L . So L^2 it was square of this, square of this, okay. So with this we can end here.

And there will be more problems which you will discuss in the later tutorial but I hope you must try your hands on each and every problem to ease yourself with the assignments. The assignment problems would be objective, maybe but they would give you, there will be a better chance to understand the assignment and get all your problems right if you are going in hand and hand with the tutorial and the lectures.