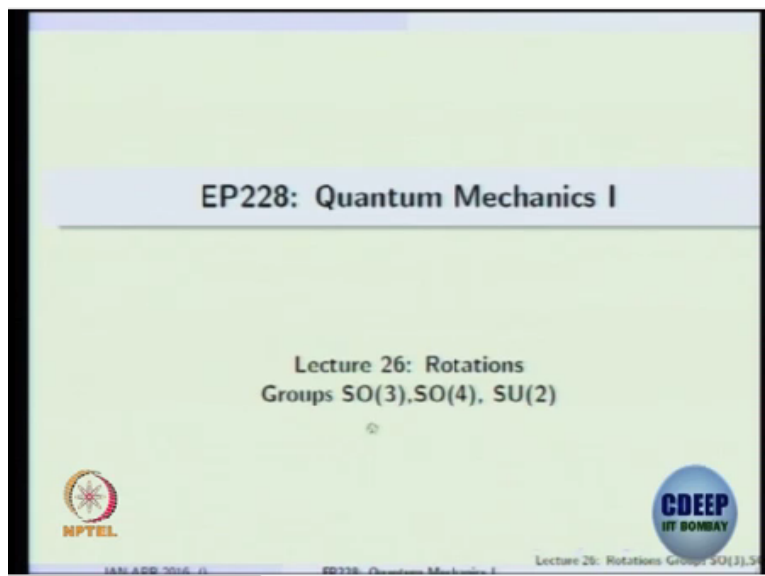


Quantum Mechanics
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Lecture – 57
Rotations Groups - I

Okay, so I was slowly bringing in to you these formal notations which you may see in any books on quantum mechanics, so you should at least be familiar even if you do not know the formal group theory, at least in the context of quantum mechanics, okay.

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So today the focus will be on groups. We discussed this in the last lecture explicitly on rotations. For completeness, I am going to go through it again. S it corresponds to proper rotation or determinant of the set of matrices which are 3×3 matrices. They have to be orthogonal, O is orthogonal, S is for determinant being 1 or proper rotation and in the 3 dimensional space. SO4 means determinant 1, you can assume that there is a fictitious fourth spatial coordinate even though you do not see it, okay.

So it is still a, research wise, we still feel that we may not be in 3 spatial. We may have higher spatial dimensions, okay. So just keep this in mind, as a mathematics problem, you can still put one more extra spatial coordinate. You can think it to be an abstract coordinate which you do not see, you only see x y z but you can still do the set of orthogonal matrices with determinant +1

and study that collection which you call that group.

It forms a group which is called $SO(4)$. I am not really telling you the axioms of a group or when does the set become a group. You have to give an operation typically since we are looking at matrices, they are matrix multiplications. And you need to say in that set, every element should have an inverse. If you take the product by the group operation which is matrix multiplication, you should get an identity matrix in that set.

So there are set of axioms which I am not putting in because this is not really a group theory course. But you can go and look it up, okay. Further, there are, we do study in quantum mechanics unitary operators and unitary matrices and if you look at unitary matrices which are 2×2 matrices with determinant $+1$, that collection of 2×2 unitary matrices with determinant $+1$, so that will constitute that will belong to a group which is $SU(2)$ in a context of rotations, specially the 2×2 matrices are required for spin half particle, right.

Spin half as 2 states possible. So you can write matrix representation in a 2 dimensional linear vector space as a 2×2 matrix. And what are those 2×2 matrices which you have been looking at? This is an exponential of Pauli matrices, okay. So this is what you have been seeing. So I am just putting it compactly here so that you get a feel of various jargons when you go open a book, you may see first.

As he pointed it out, rotation in 3 dimension, if you take a vector with the tip of the vector to be on the surface of an orange, if you do a rotation, the tip of the vector will always be on the surface of the orange, okay. So you can say that this symmetry on the surface of a sphere is $SO(3)$, the group symmetry, okay. It takes you a 1 vector, R vector to R prime but the magnitude of R and R prime are same.

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Recap

- Action on angular momentum basis $|jm\rangle$

$$J_-|jm\rangle = \sqrt{(j-m+1)(j+m)}\hbar|j(m-1)\rangle$$

$$J_+|jm\rangle = \sqrt{(j+m+1)(j-m)}\hbar|j(m+1)\rangle$$

$$J_3|jm\rangle = m\hbar|jm\rangle ; J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle$$
- Angular Momentum algebra
$$[J_-, J_+] = 2J_3\hbar ; [J_3, J_\pm] = \pm J_\pm\hbar$$
- Associated with every continuous symmetry, we have conserved quantity-*Noether's Theorem*

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So let me recap what we did for angular momentum before we get to see the groups. So this is what we derived in the last lecture using Schwinger oscillator approach, right. So one of the ways in which you can remember that this is correct is that if the m was this j , then this is non-0. If m is $-j$, then it has to become 0. So that should be a coefficient with $j+m$, okay. This is one way of remembering it.

You can also derive it. So it is a ladder operator again or a lowering operator which takes the magnetic quantum number reduces it by 1 unit. Similarly, J_+ raises it by 1 unit and beyond $m=j$, it has to be 0 which means you will have a $j-m$ which will take care of and it becoming 0. You derive these things. I am just recapping it. And they are simultaneous eigen states of J_z and J^2 .

Sometimes we call it as J_3 . So this is eigen values $m\hbar$ and j with $\hbar^2 j(j+1)$. What was the angular momentum algebra involving these non-Hermitian, J_+ Hermitian conjugate of this is J_- . You can write the algebra, the commutative algebra involving J_3 , J_+ and J_- . And amongst them, they satisfy this problem. So that is what is called as an angular momentum algebra. And then we also saw that whenever you have a continuous symmetry like translations, state translations, time translations, or rotation, we have a conserved quantity.

And that conserved quantity is what we call it as, it comes under the heading of Noether's

theorem in classical mechanics which also goes through for quantum mechanics but on the matrix elements on expectation values, or in the Heisenberg pictures on the time evolutions of the operator, they satisfy this algebra, right. I am just trying to connect with what all you know so far. So just put it as a table here.

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Recap

- Action on angular momentum basis $|jm\rangle$

$$J_-|jm\rangle = \sqrt{(j-m+1)(j+m)}\hbar|j(m-1)\rangle$$

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$$J_3|jm\rangle = m\hbar|jm\rangle ; J^2|jm\rangle = j(j+1)\hbar^2|jm\rangle$$
- Angular Momentum algebra

$$[J_-, J_+] = 2J_3\hbar ; [J_3, J_{\pm}] = \pm J_{\pm}\hbar$$
- Associated with every continuous symmetry, we have conserved quantity-*Noether's Theorem*

Symmetry	generator	parameter
space translation: $\vec{r}' = \vec{r} - \vec{a}$	\vec{p}	\vec{a}
time translation: $t' = t + c$	\hat{H}	c
rotation: $\vec{r}' = R(\vec{n} - \theta \hat{n})\vec{r}$	\vec{L}_i	\vec{n}

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What is this symmetry? There is a translation which takes a vector r by a units. What performs this translation? The operator which helps you to perform this operation is the momentum, linear momentum operator and the corresponding parameter which shows up in translation is the a vector. So the linear momentum has 3, it is called generator which performs this slowly translation. p_x, p_y, p_z , there are 3 generators for translation.

Correspondingly, there will be 3 parameters which you can call it as a_x, a_y and a_z . So always you will see whenever you find the number of generators, you will have equal number of parameters. It will not be different. Time translation is just shift the time by a constant. Nothing happens. Most of the systems which you are considering as Hamiltonian is independent of time. So this is the generator of time translation and the corresponding parameter is c which is also 1 parameter.

One operator and one parameter. The last one in this context, rotation takes an R vector to the r prime vector. R vector to r prime vector, let us rotate by an angle whose magnitude is θ about the unit vector direction \hat{n} . So you can call θ vector as $\theta\hat{n}$. So this rotation

matrix is a 3*3 matrix which operates on this r vector. So what were the generators of this? The generators of this rotation operation, it can be implemented by angular momentum.

I will go through those steps also again. And the corresponding parameters, so there are 3 angular momentum components. There will be 3 angle of rotation depending on whether you rotate about x axis, you call it as theta x; about y axis, you call it as theta y; and about z axis, you call it as theta z. So you see from this neat table for this simple continuous symmetry and these generators are the conserved quantities.

So d/dt of the p operator as a function of t in the Heisenberg picture will always be 0 or equivalently the Hamiltonian for a system which possess translation symmetry, should commute with the generator by the Heisenberg's equation, evolution equation. Is it correct? So everything falls into it.

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SO(3)

- Set of all 3×3 orthogonal matrices $\{R\}$ which includes the inverse $(R(\theta) = R(-\theta)^{-1})$ representing proper rotations ($\det R = +1$) form a group $SO(3)$ under matrix multiplication.
- Take an infinitesimal rotation represented by

$$R(\hat{n}\epsilon) = \begin{pmatrix} 1 & -\epsilon_z & +\epsilon_y \\ +\epsilon_z & 1 & -\epsilon_x \\ -\epsilon_y & +\epsilon_x & 1 \end{pmatrix}$$

For small rotation about x, y and z axes, if one retains terms of the order ϵ^2 , one gets the following matrices :

$$R(\hat{x}, \epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - \frac{\epsilon^2}{2} & -\epsilon \\ 0 & +\epsilon & 1 - \frac{\epsilon^2}{2} \end{pmatrix} \quad R(\hat{y}, \epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1 - \frac{\epsilon^2}{2} \end{pmatrix}$$

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So what is SO3? SO3 is a set of all 3*3 orthogonal matrices which includes the inverse. So the inverse of the R matrix is nothing but suppose you take theta to be about 1 particular axis, you just change the sense of rotation to -theta and they will be inverses of feature. Why? Then you take the product of this with this, it will be an identity operation. So representing proper rotation determinant R is +1, that forms a group SO3 under matrix multiplication.

You have to give an operation. So here the operation for the group is matrix multiplication. Just giving the set of R matrices or set of matrices which are orthogonal is not enough. You have to give the group operation and the group operation is just multiplications of matrices. And they are proper rotation that is why the determinant R is $+1$. So such a group is called $SO(3)$. You can take an arbitrary axis and look at an angle which is infinitesimal whose magnitude is ϵ .

You can write this $\hat{n} \cdot \epsilon$ as $\epsilon_x \hat{x} + \epsilon_y \hat{y} + \epsilon_z \hat{z}$ and you can write compactly for an infinitesimal in the sense that I do not want to keep anything higher than ϵ order. I do not want to keep ϵ^2 $\epsilon_z \epsilon_x$. I do not want to keep anything higher because they are already very small. Keeping only linear terms in ϵ , this is the most compact matrix you can write.

Suppose you take \hat{n} to be along x axis, okay. If you take \hat{n} to be along x axis, the one which will show up is the rotation which is ϵ_x and ϵ_x , right. And I am keeping terms. We will see why I am keeping terms up to ϵ squared later. You want to keep terms up to ϵ squared. Then you can write about the x axis in this fashion. Please verify this, okay.



Similarly, for the y axis rotation matrix, you will have terms in the first and the third column and the first and the third row to be altered. And you have this up to order ϵ squared. Will these 2 commute? They do not commute. For infinitesimal, they can be approximated because but if you want to keep up to order ϵ squared, you will see that it cannot commute. For workout this commutator of these 2, product of these 2, okay. Please do this.

Take $R_x \hat{\epsilon}$ and $R_y \hat{\epsilon} - R_y \hat{\epsilon}$ and $R_x \hat{\epsilon}$, please do that, okay. And see what is that non-0 quantity and write down on the right hand side, okay. I will leave it you to do this.

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$$R(\hat{z}, \epsilon) = \begin{pmatrix} 1 - \frac{\epsilon^2}{2} & -\epsilon & 0 \\ \epsilon & 1 - \frac{\epsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Upto to order ϵ^2 ,

$$R(\hat{x}, \epsilon)R(\hat{y}, \epsilon) - R(\hat{y}, \epsilon)R(\hat{x}, \epsilon) = \begin{pmatrix} 0 & -\epsilon^2 & 0 \\ \epsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = R(\hat{z}, \epsilon^2) - \hat{I}$$



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If you do that, you will find that the right hand side is this matrix and if you compare rotation of z of epsilon if you compare this with this, you can say that it is a rotation about z axis by an angle epsilon squared, okay. Just check this. -, you remove the diagonal elements or -the identity. So this is just to indicate that the matrices of SO3, they do not commute. This is non-0. Right hand side is non-0.

They do not commute if you keep up to order epsilon squared and the commutator has a unique form. In fact, we will see from here that the generators which are responsible for rotations are the angular momentum and you can show that the angular momentum commutator algebra exactly reproduces this relation. What is the commutator relation? $L_x L_y$ has to be $i\hbar$ cross L is that and you can get that out of this.

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Rotations in classical mechanics Vs quantum mechanics



- Rotation through an angle $d\Omega$ about an axis perpendicular to the plane of rotation transforms position vector \vec{r} to $\vec{r} + d\vec{r}$ where

$$d\vec{r} = d\Omega \times \vec{r}$$

so that

$$\vec{r}' = R\vec{r} = \vec{r} + d\Omega \times \vec{r}$$

- In QM, we need an operator $U_R(\theta)$, corresponding to a rotation R , which acting on a state $|\psi\rangle$ of the system, gives a state $|\psi'\rangle$.

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So rotations in classical mechanics versus quantum mechanics. So typically in classical mechanics when you did you rotate by an angle $d\Omega$ about an axis perpendicular to the plane, transform the vector r to $r+dr$, this is what you do where the change in vector for infinitesimal rotation, you can write it as a vector product. So that you can write r prime as $R*r$ vector and you can write that as a $d\Omega*r$.

This is exactly what we did in the earlier slide, writing the explicit matrix form but you can rewrite it in this fashion. This I am assuming you know from classical mechanics. In quantum mechanics, what we will want to do? We want to write a unitary operator for rotation for an angle θ , this subscript is for rotation, corresponding to a rotation R in physical space which when acts on a state ψ , takes it to a new state ψ' .

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$$|\psi\rangle \xrightarrow{\text{rotation}} U_R(\theta) |\psi\rangle = |\psi'\rangle$$

$$|\psi'\rangle = U_R(\theta) |\psi\rangle$$

$$\langle r'| = \langle r| U_R^\dagger(\theta)$$

$$\langle r'| \psi'\rangle = \langle r| \psi\rangle$$

$$\psi'(R^{-1}r) = \psi(r)$$

So you have a state ψ , you do a rotation and that is performed by U_R of θ . And that gives you a ψ prime, okay. Or how will I write this? ψ prime as U_R of θ on ψ , okay. So there is a unitary operator which can rotate the state and give me a new state. Similarly, I could also write r prime to be in the position basis which is U dagger of θ . So what will r prime ψ prime be?

So what is this? It is ψ prime of r prime = ψ of r . So you can try to shift what is happening to ψ prime by writing ψ prime of r to be ψ of $R^{-1}r$, you can write this to be the, you can invert the transformation, right. You have this as $R^{-1}r$. You can put an r inverse here and like this. Call $R^{-1}r$ as r , that is the case then r will become r inverse of it. Then what can you do here?

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$$r' = R r = [r + d\vec{\Omega} \times r]$$

$$R^{-1} r = [r - d\vec{\Omega} \times r]$$

$$\psi'(r) = \psi(R^{-1} r)$$

$$= \psi(r - d\vec{\Omega} \times r)$$

$$= \psi(r) - (d\vec{\Omega} \times r) \cdot \nabla \psi$$

We know what is R on r . That is r prime which is $1 + d\omega \times r$ or $r + d\omega \times r$, right. So what will be R inverse? What is the R inverse? Inverse will change the angle by opposite direction, in the negative sign. So this will become. So what do we have? ψ prime of r vector is ψ of R inverse r . I can write this as ψ of r vector $- d\omega \times r$ for infinitesimal rotation. Can you do the Taylor series expansion here?

It will be ψ of $r - d\omega \times r$; something wrong here. ψ of r we can, can you do this Taylor series expansion and see whether you get ψ of r ? If I done it correctly? Yes, I have done it correctly. So then it will be, this is the correction. So that will be there dotted with ∇ of ψ , okay. This is the mistake I did. So this is $r +$ some correction and that correction is this. Now what do we do? What is the next step?

In quantum mechanics, what do we have to do? The ∇ operator has to be converted to a momentum operator. Put $i\hbar$ cross, convert it into momentum operator and it is a scalar triple product, play around, let us see what you get? Can you check it what do we get? You roughly know it should be the generator of rotation which has to be angular momentum, okay. So let me just go through the summary here and then in case you have not done it, you can take it from here.

So this changes the wavefunction which was initially ψ of r to ψ prime of r . If ψ is a scalar on rotation, this is what I said. ψ of r vector is same as ψ prime of r prime and you could rewrite this as ψ of r which can be rewritten in terms of rotation by an opposite angle in the opposite direction.

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Remove primes on r

$$\psi'(\vec{r}) = \psi(R(\hat{n}, -\theta)\vec{r})$$



i.e., the wavefunction of the rotated system at the position \vec{r} is the same as that of the unrotated system at the point

$$\psi'(\vec{r}) = \psi(R(\hat{n}, -\theta)\vec{r})$$

However,

$$\begin{aligned} \psi'(\vec{r}) &= U_R(\hat{n}, \theta)\psi(\vec{r}) \\ &= \psi(R(\hat{n}, -\theta)\vec{r}) \\ &= \psi(\vec{r} - d\vec{\Omega} \times \vec{r}) \\ &= \psi(\vec{r}) - (d\vec{\Omega} \times \vec{r}) \cdot \nabla \psi(\vec{r}) \end{aligned}$$

Note we have used a Taylor series expansion in the last step and approximated in the final rotation. Take $-i\hbar\nabla$ as the operator \hat{p} for momentum and rewrite the above equation.

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So this is what I did. This is R inverse and do a Taylor series expansion which I did already for you and take $-i\hbar$ cross as the momentum operator and rewrite the above equation. This is what I left it for your.

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$$\begin{aligned} \psi'(\vec{r}) &= \psi(\vec{r}) - \frac{i}{\hbar} (d\vec{\Omega} \times \vec{r}) \cdot \hat{p} \psi(\vec{r}) \\ &= \left[1 - \frac{i}{\hbar} (d\vec{\Omega} \times \vec{r}) \cdot \hat{p} \right] \psi(\vec{r}) \\ &= \left[1 - \frac{i}{\hbar} d\vec{\Omega} \cdot (\vec{r} \times \hat{p}) \right] \psi(\vec{r}) \\ &= \left[1 - \frac{i}{\hbar} d\vec{\Omega} \cdot \hat{L} \right] \psi(\vec{r}) \end{aligned}$$

where \hat{L} is the operator corresponding to the classical observable $\vec{L} = \vec{r} \times \vec{p}$, the orbital angular momentum. We have seen the need for spin angular momentum in quantum mechanics.

Here we will denote angular momentum as \vec{J} .

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What will that be? There are these in between steps, you can take the scalar triple product, write it as $d\vec{\Omega} \cdot (\vec{r} \times \hat{p})$, $\vec{r} \times \hat{p}$ is the angular momentum, orbital angular momentum. Physical rotation when you do in physical space, what you have is only orbital angular momentum and you get automatically the change in ψ at the position \vec{r} . So this only gives you the unitary operator which takes ψ to ψ' at the same position \vec{r} .

Wavefunction changes at a position r to ψ prime and how it changes is the unitary operator and this is unitary for an infinitesimal angle. If you make the angle to be, if you increase the angle, finite angle, then what you have to do? Keep taking more pieces. You can multiply this thing because it is a continuous symmetry, any finite rotation can be treated above the same axis, can be treated as product of infinitesimal rotation about the same axis, okay.

So even though I did it for a physical rotation, you have seen from Stern-Gerlach experiment and many of the experimental data that you need to put in another quantum number whose properties are similar or the angular momentum algebra are similar to what you see for the orbital angular momentum and we compactly call angular momentum as vector J or operator J in quantum mechanics.

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Rotation operator

- The unitary operator $U_R(\hat{n}, d\theta)$ defined as

$$U_R(\hat{n}, d\theta) = 1 - \frac{i}{\hbar}(\vec{J} \cdot \hat{n})d\theta$$

where \vec{J} is the angular momentum operator. A finite rotation may be built from infinitesimal rotation

$$U_R(\hat{n}, \theta) = \lim_{N \rightarrow \infty} \left[1 - \frac{i}{\hbar}(\vec{J} \cdot \hat{n})\frac{\theta}{N} \right]^N = \exp\left(-i\frac{\vec{J} \cdot \hat{n}}{\hbar}\theta\right)$$

- Note the components of J_x, J_y, J_z are generators of infinitesimal rotations.

Recall p_x, p_y, p_z are space translation generators and their commutators $[p_i, p_j] = 0$. We know $[J_i, J_j] \neq 0$ for $i \neq j$.

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So we can try to write unitary operator for a spin J in general particle under rotation by an infinitesimal amount is this. And if you want to do the finite rotation about the same axis; about the same axis, the matrices commute. You all know that, right. If I do a rotation about z axis by an angle, let us say 20 degrees and then do a rotation about z axis by 30 degrees, then it will be like a rotation about the same axis by 50 degrees.

Is that right? So they commute. The order really does not matter there. So you can try to write the product of unitary matrices for infinitesimal rotation which you can write it as a finite rotation by

n as the $d\theta$ and do it n number of times. And this is the formal definition for an exponential form of it. So there is a unitary operator in quantum mechanics which performs rotation not only in physical space.

But it could also be in the spin space or some internal space which we call it as a total angular momentum J where the generator is the angular momentum J , okay. So this is what we call it as a rotation operator even in the spin space. So we have been doing this many times the $J_x J_y J_z$, now I have tried to motivate you in quantum mechanics even in the abstract space, they can be treated in the abstract space which is like a spin space.

Spin half will have a 2 dimensional linear vector space in that space. Also it is a rotation and that rotation can be generated by $J_x J_y J_z$ which are generators and there is one certainty which you should compare between translations and rotations. In translation if I do translation along x and then do a translation along y or if you do y and then x , the final result will be the same. Final destination will be the same, right.

What is the reason? Generators of the translations which are P_x and P_y , the commutator is 0. But if you do a rotation about x axis and then a rotation about y axis, and reverse the order, you know they do not commute. Another way of saying is that generators of such a rotation should not commute. So the group of these matrices which do not commute, they are in general called non-abelian group.

If you do a rotation about one axis, only one axis, will they commute or no? They will commute. So that is called abelian group, the group of matrices which you write about only one axis will be an abelian group but if you have 3 axis, 3 independent, linearly independent axis, the rotation matrices in general do not commute. Reason for them not commuting is that the generators which are angular momentum, they do not commute, okay.