Advanced Quantum Mechanics with Applications
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Lecture – 09
Rotation Operator and Invariance of Angular Momentum, Parity

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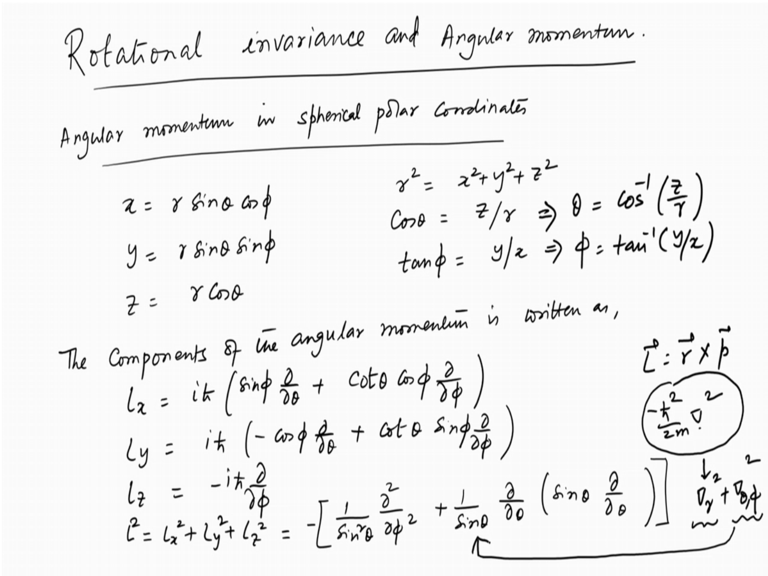

So, now ah, we shall talk about a rotational in variance of a system and it is relation to angular momentum; that is, if a system has a rotational invariance that is, it remains in variant under rotation in space, then the angular momentum is a good quantum number. Rather, the angular momentum is conserved and the quantum number corresponding to angular momentum is a good quantum number. And in order to a see that, we will study the rotational invariance; that is the rotation operator and when it acts on a wave function, etcetera and how it relates to the Hamiltonian of the system.

So, let us try to define angular momentum in spherical polar coordinates and we will see that in just a while that this is purely a function of the angular variables; namely, theta and phi ah. We know that the x coordinates in the Cartesian coordinate system x y and z coordinates. They are written in terms of r theta and phi. As this x equal to r sin theta cos phi y equal to r sin theta sin phi and z equal to r cos theta and r square equal to x square plus y square plus z square, this is known, this is the norm of the vector or the rather the magnitude of the vector.

Cos theta is given by z by r which that defines theta which is equal to cos inverse. So, that tells that theta is equal to cos inverse z by r and of course, tan phi equal to y by x which says that phi equal to tan inverse y by x. And these are the interrelationships between the variables in Cartesian coordinates and the spherical polar coordinates ah. This I do without proof the definition of L is equal to r cross p. So, where p is equal to minus i H cross del operator which can be written as i cap del del x plus j cap del del y and k cap del del z an r can be written as like this.

And, when we change it to the spherical polar coordinates, it is seen that they are purely functions of theta and phi just what I told a while back. So, L x is equal to i H cross sine phi del del theta plus cot theta cos phi del del phi L y equal to i H cross minus cos phi del del theta plus cot theta sin phi del del phi, and L z which as the simplest form which is minus i H cross del del phi. Now, these are the proofs you can easily do it yourself for any book on quantum mechanics. We discuss angular momentum; will give you these expressions.

So, the proton and the electron they are interacting via coulomb term coulomb repulsion or rather coulomb attraction here because of a opposite charges are being involved in this particular case.

And, if you write down the Schrodinger equation for a hydrogen atom ah, you will have the first term which is the kinetic energy term involves a minus H square by 2 m d 2del squared term and this del square term contains a del r square and the del theta phi square. And incidentally, this del theta phi square exactly apart from a small factor that is a constant factor is exactly this term, this angular dependence that is written. So which means that; the Eigen function or the angular Eigen function of the hydrogen atom problem coincides with the Eigen function of the L square operator.

And hence ah, things become easier and which we know as called as spherical harmonics. So, only we are left to solve this which is then obtained in terms of these are log w are polynomials. So, those things are known to you when you had gone through the first course of quantum mechanics. So, just to make you aware that this is the same as this a term that, we have found in your quantum mechanics or rather this hydrogen atom problem, all right.

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The Commutation relations are expressed as,

$$\boxed{\vec{L} \times \vec{L} = i\hbar \vec{L}} \qquad [L_i, L_j] = i\hbar \epsilon_{ijk} L_k$$

$[\vec{L}^2, L_{x,y,z}] = 0 \Rightarrow$ Thus there are simultaneous eigenfunction of $\vec{L}^2$ and any component of $\vec{L}$.

Angular momentum operators depend only on angular coordinates, then any radial function $f(r)$ commutes with $\vec{L}$.

$$[f(r), L_{x,y,z}] = 0 = [f(r), \vec{L}^2]$$

$$[L_x, L_y] = i\hbar L_z$$

So, there are computation relations. In fact, the L operators the components of the L operators do not commute with each other and they have a commutation relation which is in the most compact form is written as L cross L is equal to i H cross L ah.

So, that means, that there is a L i L j this is equal to i H cross epsilon i j k L k where epsilon i j k is a levi civita tensor ah. It is a symbol which takes a value 1 when you have i j and k to be it is taken in a sort of sequential manner and if you interchange the or rather if you break the sequence, then it breaks up a negative sign. So, this tells that. So, there is a L x and L y. So, that is equal to a i H cross L z and that is the computation relation. Now, if I take a L a L y and L x that of course, will bring me minus sign ah, that comes here.

Similarly, L square the square of the angular momentum operator at that of course, commutes with all of these components L x L y and L z. And so, they have similar or other same simultaneous Eigen functions which means that L square and any component of L has same simultaneous Eigen functions, there is same Eigen functions and they can be diagonalized simultaneously. However, in most practical cases 2 operators are chosen, that is L square and L z for no particular reason other than the fact that L z has got a particularly simple form and z is often taken as the preferred axis.

And the angular momentum operator depends only on the angular coordinates which is what we said. So, any radial function f of r that computes with any component of L. So, f of r and L x o r L y or L z will give you 0 and same as f r commuting with L square. So, these are things that simplify discussion concerning the angular momentum, all right.

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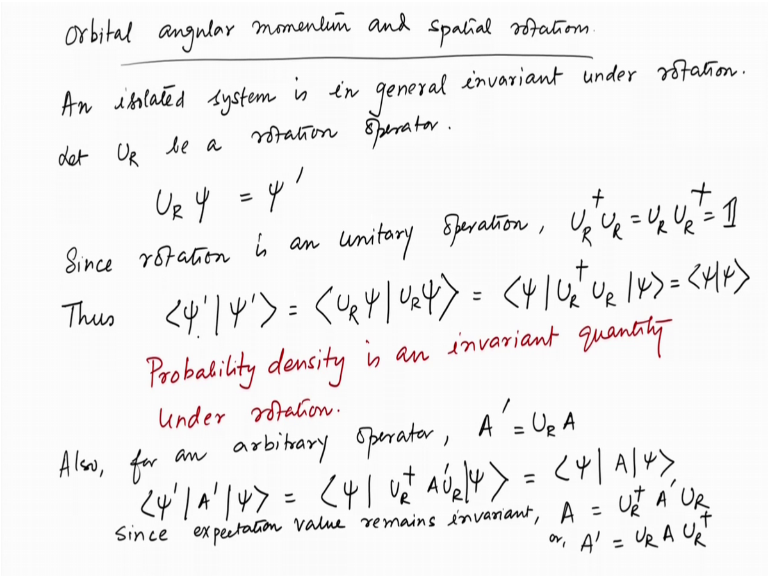

So, let us now see that the relationship between the orbital angular momentum and spatial rotations the rotations that happen in space. So, in an isolated system is in general invariant under rotation. And, let U R be a rotation operator, ok.

So, U R is an operator that rotates a wave function and we will see that R is another operator that does a rotation on the variables. So, U R is particularly reserved for the wave function. So, U R acting on a psi will transform it to psi prime ok. And the rotation is of course, unity operation which means that U R dagger U R equal to U R U R dagger and that should give equal to 1 1 means is an identity matrix. So now, let us see the overlap of the psi prime with itself which means that, we are talking about the probability density. So, it is a psi inner product of psi prime and psi prime each of these are written as U R psi and U R psi.

So, I can take this on the other side and write psi and U R dagger U R and which is eq and this is a psi again and which gives me because U R dagger U R equal to 1. It gives a A psi psi which means, the norm or the probability density that remains conserved; whether you take it in a rotated system or you take it in the original system which has main rotated. So, for an arbitrary operator; now, let us talk about an operator or an observable a prime which when it when the rotation operator acts on the observable. So, U R actually corresponds to rotation of both wave function and the observable of the operator.

So, A prime becomes U R A. Now, you see the expectation value is supposed to remain same whether you have done a rotation or not because expectation value is a physically observable quantity. So, if I take the expectation value of A prime between the rotated states, there should be rotated states. So, this is equal to I have left it simply equal to the A prime. I have left it same, but I have written that psi prime to be equal to psi and U R dagger and there is A U R psi. Since these are same ah, the operator A is equal to U R dagger A prime U R or the rotated operator A prime becomes U R A U R dagger, where U R is the rotation operator.

So, this is how formally rotation is done on a system. So, we have done it on the wave function and we have done it on any arbitrary operator as it is easily understandable that the arbitrary operator could as well be the Hamiltonian of the system. So, we know how to rotate or rather perform a rotation operation on the wave function and an operator.

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If $A \equiv H$ (the Hamiltonian for the system)

$$H' = U_R H U_R^{\dagger} = H$$

$\psi' = U_R \psi$

$\vec{r}\,' = R\vec{r}$

$$U_R H = H U_R$$

$$[U_R, H] = 0$$

It is worthwhile to find an explicit form of the unitary operator.

Let us consider a wavefunction $\psi(\vec{r})$. Under rotation, the wavefunction becomes $\psi'(\vec{r}\,')$ where $\vec{r}\,' = R\vec{r}$

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

$$\psi'(\vec{r}\,') = \psi(\vec{r})$$

Even if ψ differs from ψ', it must be by a phase factor

So, as just as I was saying that, if A is same as Hamiltonian of the system, then we have a relation that the H prime that is the Hamiltonian in the rotated frame is equal to U R H U R dagger which is equal to U R.

Sorry which is equal to H and this tells us that U R H is equal to H U R; so, which means that the U R commutes with the Hamiltonian of the system. And so, if this happens, then a U R and H have simultaneous Eigen functions. So, H is the Hamiltonian of a system which of course, has a rotational in variance. But, however, to solve for H or rather to find the Eigen functions and the Eigen values of H or you may have to solve a complicated a differential equation by some method which is usually a power series method. But instead of that, suppose we try to find the U R, because U R is an operator that computes with H.

So, they will have simultaneous Eigen functions. So, if you can avoid the complexity of solving a complicated differential equation in U of finding a form for this unitary operator that is worth of an exercise.

So, let us consider a wave function psi of r. So, under rotation, it becomes psi prime r prime. Now, remember that psi prime is being operates. So, psi prime 1 gets it by operating. So, U R operating on psi and r prime 1 gets it which are the variables of this. For this particular problem, it is the rotation operator is acting the R is acting on the variable r or the vector r and gives me a new vector which is r prime. So, that is this r prime now of course, what we have said earlier is true that is the overlap or the inner product should be conserved.

So, which means that a psi prime r prime should be psi of r they could at the most differ by a phase factor this is understandable because, a norm is conserved even if psi prime and psi they a differ by a phase factor because that phase factor will cancel out because you will take a exponential i alpha and then exponential minus i alpha that you cancel out, ok.

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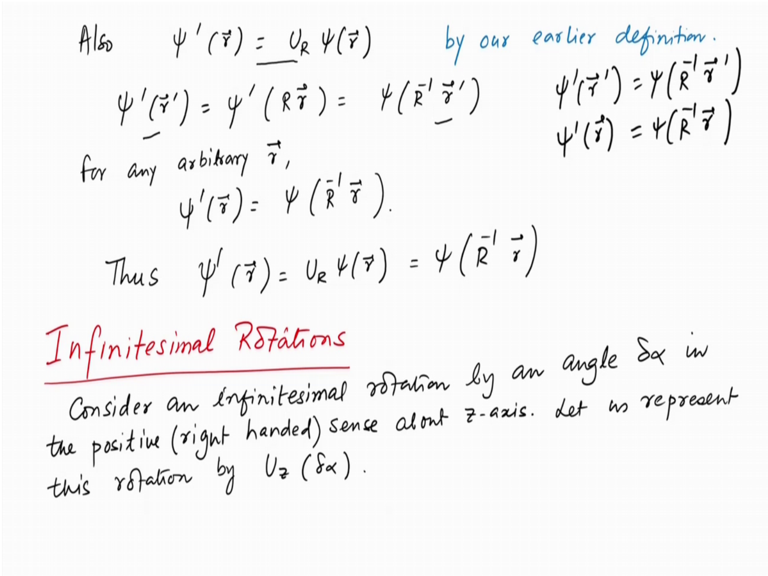

So, and of course, also that psi prime of r is U R psi of r. So, this has been given by our earlier definition. So now, let us look at psi prime r prime which is equal to psi prime r R which is a rotation operator on the variables acting on r and of course, and inverse rotation operator acting on the new variables r prime, that is the same thing.

So, if you just take simply the first part and the last part. So, we will have psi prime r prime that is equal to psi R inverse r prime. Now, since this acts for any R r prime is arbitrary. So, we can simply write it as psi R prime r equal to psi R inverse r. So, since this is r prime is dummy, we might as well as write it as r and this is what is written that psi prime of r equal to psi R inverse r. This is what appears here and the psi prime of r which is equal to U R psi R which is by our definition that is written here and that is equal to psi R inverse r.

So, psi prime r is equal to psi R inverse. So, these give you the relationship between the wave functions after rotation or the rotated wave function versus the original wave function. Now, let us discuss something called infinitesimal rotations and the reason that we do it is the following that usually rotations do not commute. So, successive rotations do not commute. What we mean to say is that, if we rotate a quantity or rather rotates an object.

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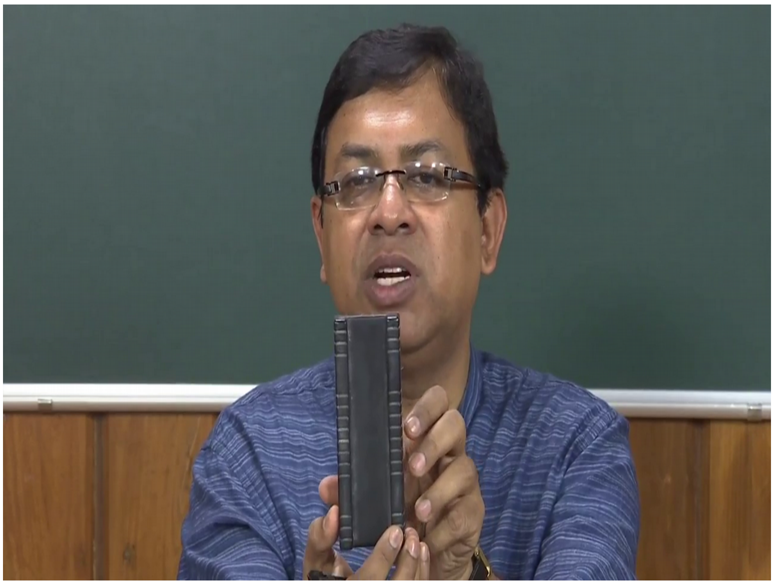

Suppose this is the object that we want to rotate and this is the z axis that is passing through this. So, if you rotate it about the z axis by an angle 90 degree and then we rotate it like this, and instead of that if we first; so, this rotation.

So, this is my x axis and this is my y axis and this is my z axis. So, we have done first rotation through the through the z axis and now, while do a rotation about the y axis. So, it takes a form like this. So, the white part of the duster which is this one is towards me and the black part of the duster is facing you. But, however, if we do it; so, we first do it rotation about z ax y axis. So, that is your y axis. So, this is your ah. So, this is your y axis. So, we take we do a rotation about this and then, we do a rotation about the z axis which is this.

Then, of course, the final configuration of the duster does not remain same and hence, the successive rotations do not commute. And, in order to see that, we can talk about initially infinitesimal rotations and see that actually infinitesimal rotations by an amount delta alpha, where delta alpha is very small that commutes and let us do a rotation by an angle delta alpha to a system in a positive direction or it is right handed sense. So, if you do a right handed rotation about z axis. So, it rotates the anticlockwise and this is represented by a U z delta alpha. U z is a rotation operated delta alpha signifies that it is rotation about term by an angle delta.

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To first order in $\delta\alpha$, the coordinates (x', y', z') of $\vec{r}\,'$ $(= R\vec{r})$ are given by,

$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$

$f(x) = f(x_0) + (x-x_0) f'(x)\big|_{x_0} + O(x-x_0)$

$$x' = x - y\,\delta\alpha$$
$$y' = x\,\delta\alpha + y$$
$$z' = z$$

in general, $\underline{\vec{r}\,' = R\vec{r} = \vec{r} + \delta\alpha\, \hat{n} \times \vec{r}}$

The coordinates of $R^{-1}\vec{r}$ are obtained by changing $\delta\alpha$ to $-\delta\alpha$

$$\psi'(\vec{r}) = U_z(\delta\alpha)\psi(\vec{r}) = \psi(R^{-1}\vec{r}) = \psi(x + y\delta\alpha,\ x\delta\alpha - y,\ z)$$

Doing a Taylor expansion and retaining terms till first order in $\delta\alpha$, we find,

$$U_z(\delta\alpha)\psi(\vec{r}) = \psi(x,y,z) + y\,\delta\alpha \frac{\partial \psi}{\partial x} - x\,\delta\alpha \frac{\partial \psi}{\partial y} + O(\delta\alpha^2)$$
$$= \left[1 - \delta\alpha\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right]\psi(\vec{r})$$

So, to the first order in delta alpha which means that if delta alpha is small the coordinates x prime y prime and z prime of the r prime vector which is equal to R r which R operating on r. So, x prime becomes x minus y delta alpha and x a y prime becomes x y plus x delta alpha. You should you should convince yourself and z prime equal to z because, we have rotated it about the z axis. So, z coordinate remains the same and the in general, this you might have learnt in your classical mechanics course that r prime or the variable the rotated variable is related to the original variable before rotation by his r plus this angle delta alpha and this n cap is the axis about which the rotation has taken place crossed with r.

So, here delta alpha is of course, delta alpha it is a n cap is z cap. So, it is a z cap cross r. So, x prime will be x plus delta alpha z cap cross r and similarly, y cap equal to y y plus delta alpha z cap cross y y component. I mean, R means x component y component and z component and you will see that because z cross z equal to 0. So, that is. So, z prime becomes equal to z and this other things will remain will it will be written as something like this and of course, you got a minus sign because you get a z cap cross x which is x x x cap ah, ok.

So, R if you just simply write it with x x cap plus y cap plus z z cap, you would get apply. This you would get these relations between the rotated variables and the original variables. So, the coordinates of R inverse r are obtained by changing. So now, I am a doing it now. Here, I have done it with the rotating it by R.

If we rotate it by r inverse ah, that can be obtained by simply changing delta to minus delta alpha 2 minus delta alpha and your psi prime which is rotated wave function psi prime of r is U z delta alpha psi of r and the by a earlier definition this is equal to psi R inverse r and we have simply change the signs in between. So, it became x plus y delta alpha and x delta alpha minus y and z.

So, doing a Taylor expansion and retaining term till first order in delta alpha, one can find that U z delta alpha that is this thing is x x y z. So, doing a Taylor expansion of this, so, this y delta alpha del psi del x and minus x delta alpha del psi del y just to remind you that function f of x is done at Taylor expansion about some x 0 ah. This is equal to x minus x 0 f prime evaluated at f prime of x evaluated at x 0 and so on and then, there are terms which are you know of the order of this x minus x 0 whole square and that is what we have done here. So, if you do a bit of simplification, it becomes 1 minus delta alpha x del del y minus y del del x and psi of r.

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Remember: $\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = iL_z$ $L_z = (\vec{r}\times\vec{p})_z$

Thus $U_z(\delta\alpha)\psi(\vec{r}) = \left(1 - \frac{i}{\hbar}\delta\alpha L_z\right)\psi(\vec{r}) = \psi'(\vec{r}\,')$

$e^{-i\alpha\hat{n}\cdot\vec{L}}$

So the operator $\boxed{U_z(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha L_z}$

Similarly for rotations about x and y axes,

$U_y(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha L_y$; $U_x(\delta\alpha) = 1 - \frac{i}{\hbar}\delta\alpha L_z$

In general about a arbitrary axis $\hat{n}$,

$\boxed{U_{\hat{n}}(\delta\alpha) = \mathbb{1} - \frac{i}{\hbar}\delta\alpha\,\hat{n}\cdot\vec{L}}$ This is called the infinitesimal rotation operator in space.

Thus $\vec{L}$ is called as the generator for infinitesimal rotations.

So, if you remember that h cross x del del y minus y del del x, that is the definition of i L z which simply comes from L z equal to r cross p and the z component of that where x equal to x x cap y y cap z z cap and p is equal to minus i h cross del del x x cap minus I mean plus del del y y cap and del del z z cap and then, you take the cross of that. So, U z of delta alpha which is here which is here can now be written as it is equal to U z delta alpha psi of r equal to 1 minus i by h cross delta alpha L z and there is a psi of r which is psi prime r prime. So, the operator U z delta alpha is equal to 1 minus i by h cross delta alpha L z.

So, this is the form of the operator. This is what we were trying to find because, just to remind you that you know that U R or here U z commutes with h. So, they have simultaneous Eigen functions. So, instead of solving for h, we are solving for rather trying to find a form for U R which is U z here and similarly, U y delta alpha is equal to this and U x delta alpha is equal to this ah. So, is very clear that the U y goes with L y U x goes with L x and U z goes with L z.

So, U n cap where n cap is a an arbitrary axis about which is the rotation takes place by an angle delta alpha is equal to 1 minus i by h cross delta alpha n cap dot L. It is almost clear from this part that if we have included a term which is quadratic and delta alpha will would have gotten a delta alpha square by 2 factorial and then all these things square.

So, all these terms or the parts of the series which is exponential minus i and so on which is what we are going to see. So, it is exponential minus i alpha n dot L that is a part of the series. But, we will see that clearly later. Thus, L is called as the generator for infinitesimal rotations. So, it is a generator for rotations ah. And so, which means that you know if some operator commutes with U z or U n cap U R. It also commutes with the all components of L.

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In general rotation operations don't commute unless it is done about the same axis. Now it must be pretty clear that the non commutability of rotation is due to the non-commutability of components of the angular momentum.

Let us check this:

use $\vec{r}' = R\vec{r} = \vec{r} + \delta\alpha\, \hat{n} \times \vec{r}$

$$U_y(\delta\alpha)\, U_x(\delta\alpha)\psi(\vec{r}) = \psi\left[\vec{r} - \delta\alpha\, \hat{y} \times \vec{r} - \delta\alpha\, \hat{x} \times \left(\vec{r} - \delta\alpha\, \hat{y} \times \vec{r}\right)\right]$$

simly,

$$U_x(\delta\alpha)\, U_y(\delta\alpha)\psi(\vec{r}) = \psi\left[\vec{r} - \delta\alpha\, \hat{x} \times \vec{r} - \delta\alpha\, \hat{y} \times \left(\vec{r} - \delta\alpha\, \hat{x} \times \vec{r}\right)\right]$$

$$\left[U_x(\delta\alpha), U_y(\delta\alpha)\right]\psi(\vec{r}) = \psi\left[\vec{r} - \delta\alpha\, \hat{x} \times \vec{r} - \delta\alpha\, \hat{y} \times \left(\vec{r} - \delta\alpha\, \hat{x} \times \vec{r}\right)\right] - \psi\left(\vec{r} - \delta\alpha\, \hat{y} \times \vec{r} - \delta\alpha\, \hat{x} \times \left(\vec{r} - \delta\alpha\, \hat{y} \times \vec{r}\right)\right]$$

However, the components of L do not commute amongst themselves. So, in general, rotation operators do not commute unless it is done about the same axis. This is what we have demonstrated and explains this value. So now, it must be pretty clear that the non-commutability in rotation is due to the non-commutability of the components of the angular momentum, ok. So, because the different components of angular momentum do not commute; so, the rotations about different axis they do not commute. However, this is untrue at least for infinitesimal rotation. Let us check this.

So, we have r prime equal to R r. So, r plus delta alpha n cap cross r U y delta alpha U x delta alpha psi of r psi of r minus delta alpha y cap cross r which is delta alpha x cap cross r minus delta alpha ah. So, this is that second rotation. So, I am doing I am trying to find a commutation between U i delta alpha and U x delta alpha. So, I reverse the order. So, which is U x delta alpha U y delta alpha acting on a psi of r and then everything is same excepting that you change your y by r and now, you take the difference between the 2 that will give me a commutation of U x delta alpha U y delta alpha and psi of r.

Now, this is a. So, this is the second term minus the first term and these are this can be the bracket can be open.

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$$[U_x(\delta\alpha), U_y(\delta\alpha)]\psi(\vec{r}) = (\delta\alpha)^2 \left[\hat{y}\times(\hat{x}\times\vec{r}) - \hat{x}\times(\hat{y}\times\vec{r})\right]\vec{\nabla}\psi(\vec{r})$$

$$= (\delta\alpha)^2 \left[y\hat{x} - x\hat{y} \right]\vec{\nabla}\psi(\vec{r})$$

$$= (\delta\alpha)^2 \left(\hat{z}\times\vec{r}\right)\vec{\nabla}\psi(\vec{r})$$

$$= (\delta\alpha)^2 \left[z\cdot(\vec{r}\times\vec{\nabla})\right]\psi(\vec{r})$$

$$= (\delta\alpha)^2 \frac{i}{\hbar} \underline{L_z}\, \psi(\vec{r})$$

Since $i\hbar L_z = [L_x, L_y]$

$$[U_x(\delta\alpha), U_y(\delta\alpha)]\psi(\vec{r}) = -\frac{(\delta\alpha)^2}{\hbar^2}[L_x, L_y]\psi(\vec{r})$$

$= 0$ if we ignore $(\delta\alpha)^2$

Thus infinitesimal rotations commute, but not finite rotations.

And some simplifications can be done and once you are keep a following these steps ah, if it is very straight forward, you follow the steps. It becomes equal to delta alpha square i by H cross L z psi of r. So, this commutation has only non 0 values up till order delta alpha square. So, if delta alpha is small delta alpha square. If that can been neglected this, then this is equal to 0 and this thing can be you know, I mean since it came out as L z; if you follow this simple few steps.

So, this is equal to L x L y computation and this is equal to the commutation of L x L y and so on and that is equal to 0. If we ignore terms of the order of delta alpha square, so, infinitesimal rotations commute ah, but not the finite rotations and as I told you earlier that the finite rotations do not commute because, they have the components of the angular momentum do not commute among themselves. So, let us go to the finite rotations.

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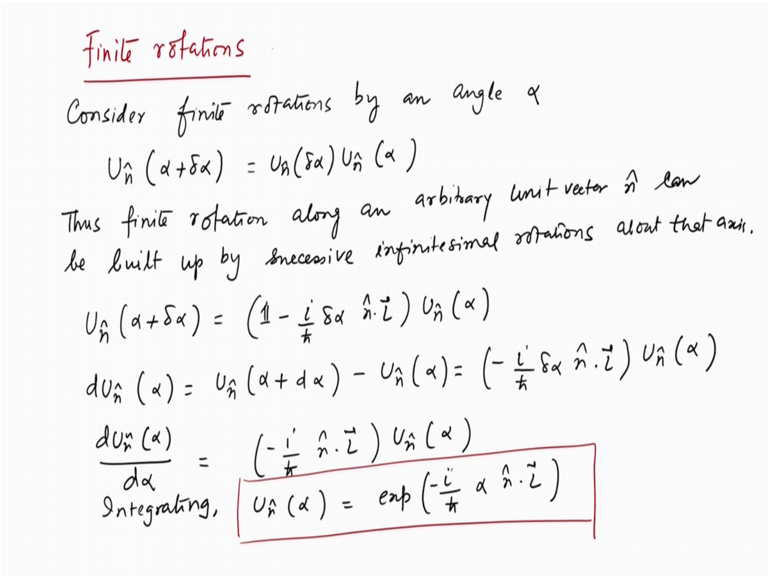

Then, because infinitesimal rotations are really idealized concepts, but; however, you can build up finite rotations starting from a large number of infinitesimal notations.

So, finite rotations by an angle alpha can be defined as U n alpha plus delta alpha which is U n alpha and then U n alpha. So now, this of course, you know you can write it in any order you want because, it is a rotation about the same axis. So, the finite rotation along any arbitrary unit vector n cap can be built up by a successive infinitesimal rotations about the axis and you n cap alpha plus delta alpha equal to 1 minus i by h cross delta alpha n cap dot L and U n alpha. Now, if I do this so, d U n which is equal to U n cap alpha plus delta alpha and U n alpha, this becomes equal to this and if I do the simplification, I get a differential equation which is for the rotation operator which is d U n cap alpha by d alpha is equal to this.

And then, if we integrate you get U n alpha is equal to exponential minus i h cross alpha n cap dot L. This is what I was saying that the expression that we got here is actually the limiting expression for this one as a exponential. So, if you expand the exponential, the first 2 terms you will get it as 1 minus that term that was written which is delta alpha n n n cap dot L.

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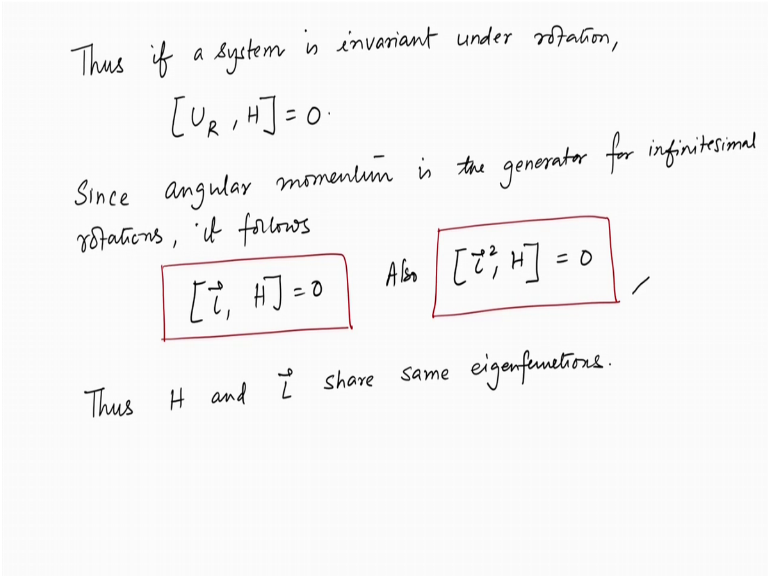

So, if a system is invariant under rotation finally, we get that the U R and H would commute and since angular momentum is a generator for infinitesimal rotation, it follows that L commutes with H and also, L square commute with H and we have the same set of Eigen functions.

So, we will see examples or applications of this rotational invariance of systems ah. I am sure that you have studied hydrogen atom which is as I said that is the simplest atom with 1 electron and 1 proton and your solve the Schrodinger equation for that and luckily, because of this relation, we did not really have to solve the theta phi part of the angular part of the Hamiltonian which coincided exactly with apart from a constant factor with L square. And that is why; they had the same set of Eigen functions which are known to be the YLM functions or the spherical harmonics.