Quantum Physics

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Lecture No. # 25

So let me complete this correspondence that I promised to bring out between the groups of rotation in 3 dimensions and a certain group of 2 by 2 matrices called SU 2 and the correspondence goes as follows.

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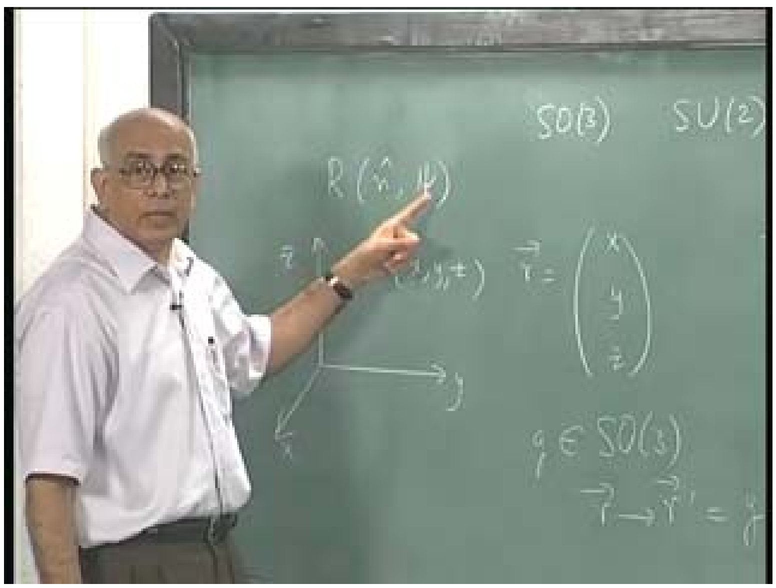

You recall yesterday we have got to a stage where we recognize that a rotation about some direction specified by the unit vector n through an angle psi lead to a parameter space, the polar angles specifying n and the angle psi which was not simply connected. This parameter space in fact was doubly connected and there were 2 classes of closed paths in this space which could not be reduced to each other. There were 2 inequivalent classes of close paths and I said that this is ultimately what was responsible for the fact that you had single and double valued representations of the rotation group. Because we also saw that the second class of closed path could be sent to a point.

It could be reduced to a trivial a transformation if you did 2 such closed paths; in other words, you did a rotation of 4 pi instead of 2 pi. And I mentioned that all those representations of the rotation group which transformed such that when you went through a rotation of 2 pi and you returned to the original state were called tensor representations and the others were called spinner representations. Today I want to show you very briefly in the beginning that you can look at rotations not in terms of 3 by 3 matrices which would act on the xyz components in some frame of reference but rather as 2 by 2 matrices which satisfy a certain property of unitarity. So the connection that we want to establish is between the group of physical rotations of SO 3; 3 by 3 unimodular orthogonal matrices and SU 2 which are the group of 2 by 2 matrices which are unitary and have determinant +1. And the way it goes is as follows. you see, instead of representing a point in space as a column vector, that is, an arbitrary point (x,y,z) in 3 dimensional space, instead of representing it as a column vector in this fashion and calling it the position vector r, its possible to represent it another way as a 2 by 2 matrix. All we have to do is to replace r by r dot sigma where is the Pauli matrices. and this stands for a 2 by 2 matrix and its components are trivially written down from the known values of what the sigma matrices are and it (z, - z, x – iy, x + iy) (Refer Slide Time: 04:27).

And now it's a trivial matter to verify that if you give me xyz, I uniquely have this matrix and if you give me r dot sigma, I can work back and find what xyz are. This is trivial because as you can see immediately by structure of the matrix. We have also pointed out that any 2 by 2 matrix can always be written uniquely in terms of the Pauli matrices and the unit matrix. So once you give me the components of the Pauli matrices; once you give me r dot sigma, I give you the vector r itself. So therefore, there is a correspondence between the vectors r and the matrices r dot sigma. Now on this, you would have a 3 by 3 element, so g, if its an element of SO 3 and if its stands for a rotation about the unit vector n through an angle psi, it is some 3 by 3 matrix and what you are end up getting is r goes under the rotation to r prime which is = this g acting on this column vector r. so this is a 3 by 3 matrix which acts on this column vector r and produces x prime y prime z prime.

In exactly the same way, there exists a 2 by 2 matrix which we will discover corresponding to this element g such that U acts on this 2 by 2 matrix with a U inverse here and this gives you r prime dot sigma. So therefore, this 2 by 2 matrix U which we are going to discover is a representative of this rotation here. And the question is what kind of relation is there between g and U. once that is specified, and then I might as well represent points in space by 2 by 2 matrices r dot sigma and rotations by U rather than g here. And the task is to discover what are the properties of this matrix U. what is the matrix U that corresponds to a rotation in SO 3? Obviously you would also be parameterized by theta phi and psi but what sort of matrix is it? It's a 2 by 2 matrix so that if the result is still a 2 by 2 matrix here.

So this is the mapping between one way of representing the rotations and another way of representing the rotations. These matrices U will turn out to be the group of 2 by 2 matrices which are unitary and which have got determinant +1. The original one was 3 by 3 matrices which were orthogonal and had a determinant +1 and also the elements were also real. There is not guarantee here that the elements are going to be real. They would have e to the i phi and things like that sitting there. So this is the program. The advantage is that the group Su 2 simply connected it's not doubly connected it's like a sphere and we will see what it is. So instead of proving the formal correspondence let me motivate it by telling you how this geometrical construction can be done. What one does is to say that you can make a mapping from the surface of unite sphere in 3 dimensions to a plane by something called stereographic projection.

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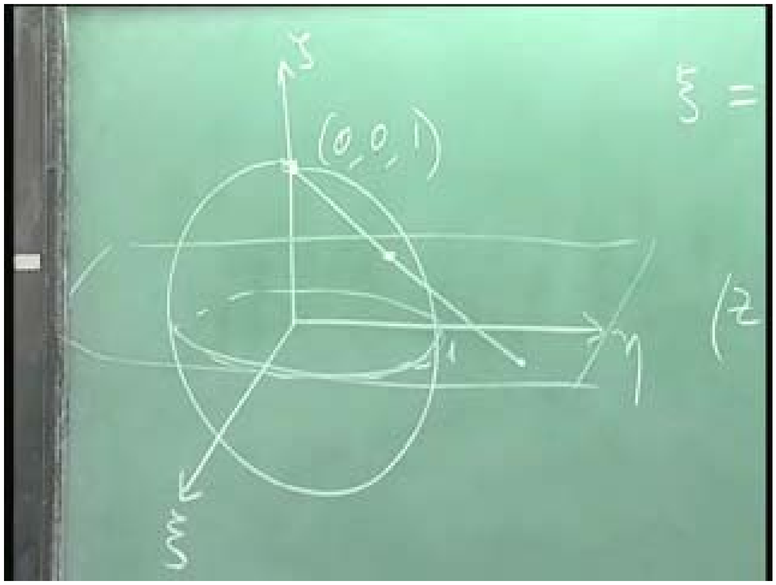

So let me specify 3 axis say xi, eta and zeta and put a unit sphere center at the origin such that this (Refer Slide Time: 08:54) is the equatorial plane and that's the unite circle and lets call this plane the xy plane (Refer Slide Time: 09:06). So the x direction is along the xi direction and the y direction is along the eta direction and this is the xy plane. In fact it's a complex plane. Then what is a stereographic projection? It corresponds to taking the North Pole whose coordinates are 0 01; xi and eta are 0 and zeta is1, and then drawing a line from there to intersect this sphere at some point and then to go and intersect the plane at some point. And the point where it intersects this sphere is mapped onto this point on the plane. And you can see that for a every point on the sphere, there is a point on the plane and vice versa. This is stereographic projection. The North Pole (Refer Slide Time: 09:59) of projection is mapped onto the point at infinity. The South Pole is mapped on to the origin in the complex plane; x + iy. The equator is mapped onto the unit circle. And what are these maps?

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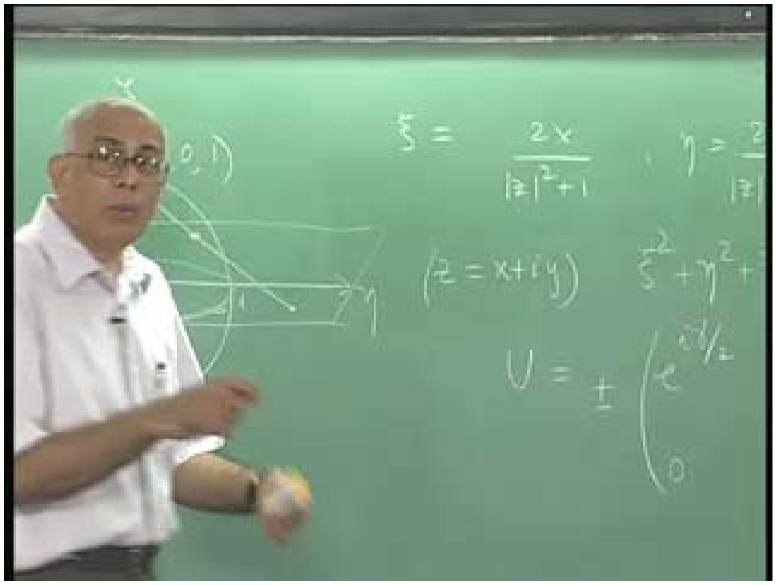

Well, xi is =2 x over mod z squared +1. z = x + iy; that's my complex z plane here. Eta =2 y over mod z squared +1 and zeta is = mod z squared -1 over mod z squared +1.

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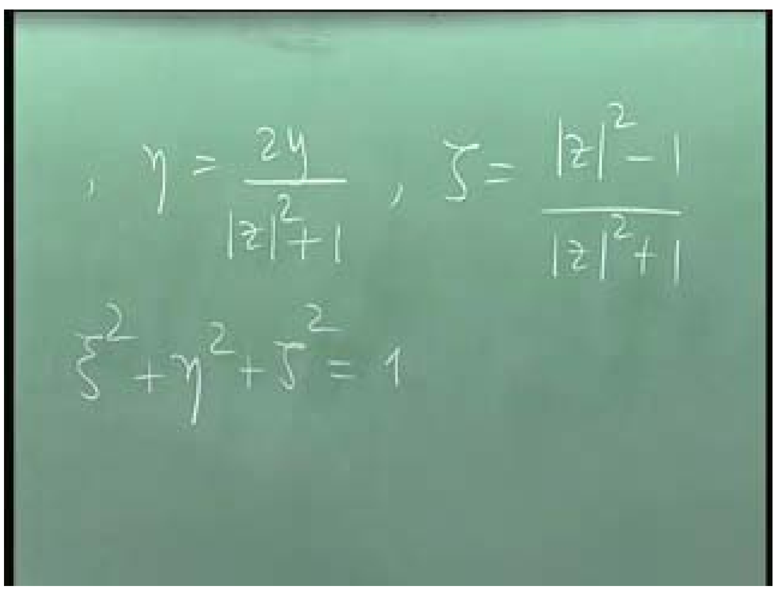

I leave you to figure out the inverse maps. Then of course, this is a unit circle. So you always satisfy xi square + eta square + zeta square =1. So you map this sphere called the Riemann sphere onto the complex plane by stereographic projections.

This projection has many interesting properties. For example it preservers it maps circles on the sphere onto either circles or straight lines on the plane because any latitude is clearly mapped onto the circle concentric with the origin. Any longitude is mapped onto a straight line passing through the origin. The map of the point at infinity is the point at infinity in the complex plane. Now a rotation in physical 3 dimensional space would correspond to rotating the Riemann sphere. And what does it do on the plane is the question. It induces a transformation on the plane as well and it's easy to check. I am not going to prove this specifically that in 3 dimensional space, if you rotate the xy plane about the z axis, then the rotation matrix is a very simple form.

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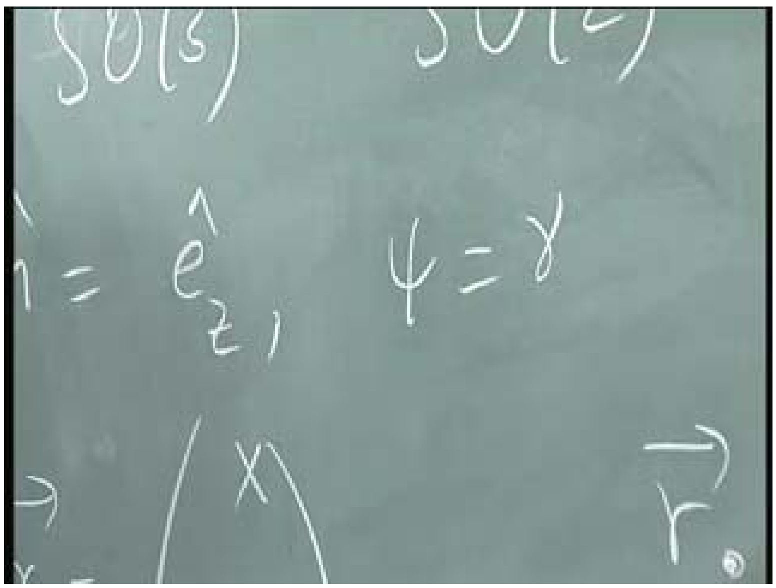

So if for example, n = ez about z axis and instead of psi = some angle gamma, I am imagining the 3rd Euler angle gamma. So I rotate in the xy plane about an angle gamma. then its clear that this element g of SO 3 is given by cos gamma, sin gamma, 0, - sin gamma, cos gamma,0 and 0,0,1 (Refer Slide Time: 12:57). Only the x and y coordinates change and the z doesn't. if you put that back here and I ask what does that transformation correspond to rotation in this plane about this z axis, then its easy to see that U is = e to the i gamma over 2, 0, 0, e to the - i gamma over 2. so this element g, the counter part of it, in this other way of looking at rotations is in fact the pair of matrices here (Refer Slide Time: 13:50).

Similarly no transformation or no rotation at all would mean the identity matrix here for g, just 1,1,1 and the diagonals. And that would correspond to setting gamma = 0 here. So it would be + or - the unit matrix in this language here (Refer Slide Time: 14:13). And that's not going to change. You can see if I put the identity matrix or - the identity matrix, i am going to retain just the same r dot sigma. Similarly for rotation about the zeta, xi and eta axes. They are a little more intricate but one can write them down because you know how to write it down in this case.

For instance, if there is a rotation in the in the y z plane, then its clear that the x thing would give me an unchanged value and you can compute what it does correspondingly new by those transformation rules. Then the question is, what kind of matrices do you have for U? it turns out that the matrices you have for U, the requirement that the matrices be of this form and that the magnitude of r be preserved suffices to ensure that these matrices U must be unitary and unimodular.

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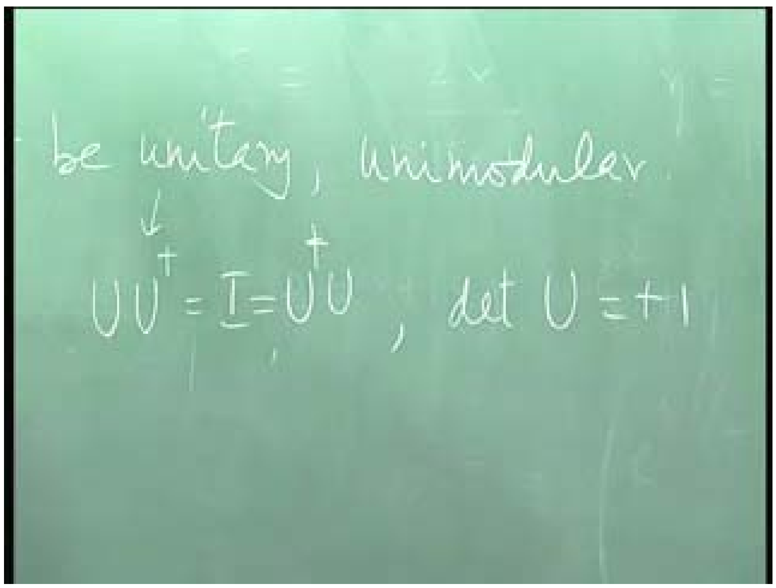

By unitary it means that the hermitian conjugate is the inverse of the matrix. U U dagger is = the identity matrix. Incidentally, this also implies U dagger U. it says U dagger U inverse. Orthogonal says O transpose is O inverse whereas that says complex conjugate transpose is the inverse. That is the difference unitary and the orthogonal. Orthogonal is what happens if the matrices have got real elements. The unitary matrix with just real elements is orthogonal. So all 2 by 2 matrices which satisfy these conditions would represent physical rotations in 3 dimensional space. And it's an easy matter to put these conditions in. start with the general matrix abcd with possibly complex entries and put in the requirement. How many independent elements for a complex matrix with 2 by 2 matrix are there? There are 4 elements; each of them can be complex. So you have 8 independent real parameters. Now you impose the condition that it should be unitary. There are 4 conditions and the determinant must be +1. So it becomes 5 conditions and you end up with 3 parameters. But 3 is precisely the number of parameters you have here to specify rotations. Therefore it's a very reasonable, plausible and provable exactly that in fact those are the correct matrices which would represent rotations but what is general 2 by 2 unitary matrix going to look like if determinant +1? It's going to be of the form alpha sum beta - beta star alpha star. That's what a general U would look like but the determinant must be +1. So it satisfies mod alpha squared + mod beta squared=1. Therefore these matrices; the real and imaginary parts alpha 1 alpha 2 beta 1 beta 2, none of them can exceed 1 in magnitude because a sum of the mod squares of alpha and beta must be =1. And written out in terms of components, what does it mean?

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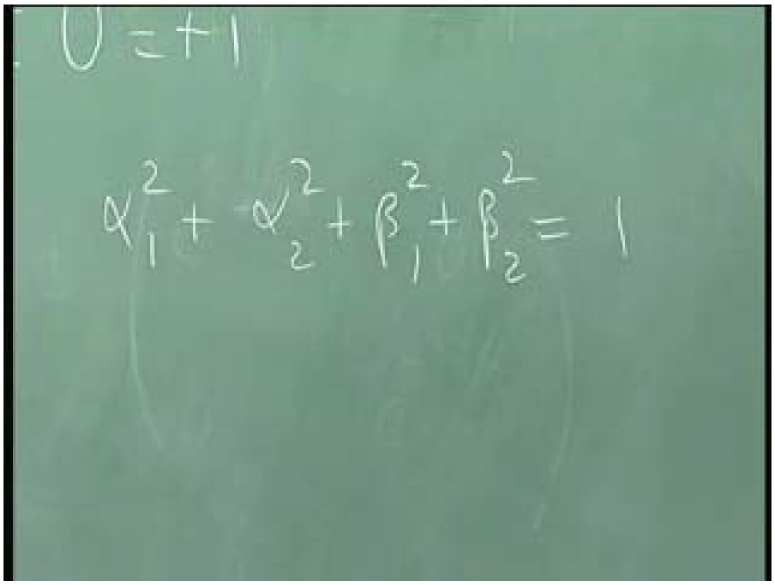

Therefore what is the parameter space of SU (2)? SU(2) is parameterized by 4 real numbers, alpha1 alpha 2 beta1 beta 2 satisfying the constraint that the sum of the squares of all these4 real numbers must be =1. Therefore, it's a sphere in 4 dimensions. The surface of a sphere embedded in 4 dimensions or S 3. So the parameter space of SU (2) is S 3. S 3 is simply connected. Phi1 of S 3 is trivial and is 0. On the other hand, SO (3) is not simply connected. So what is the connection between these 2?

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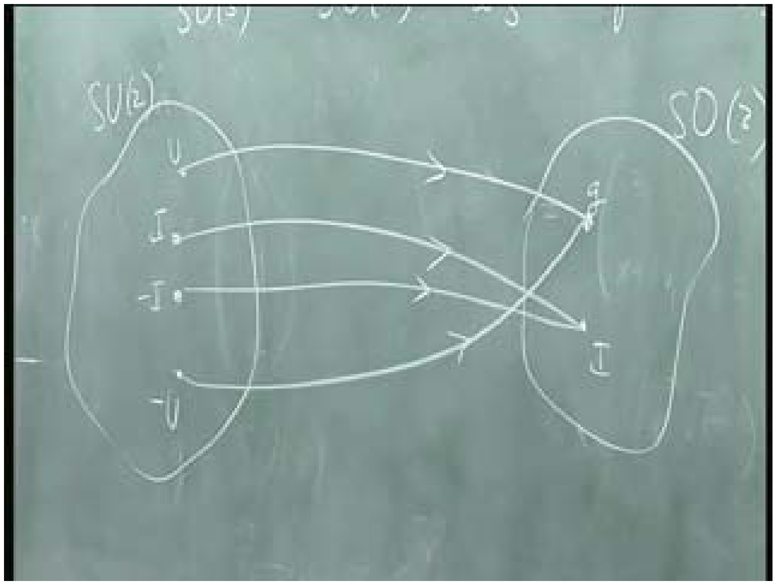

Well, you have 1 group. Here is a set of all matrices in SU (2). And here is a set of all matrices in SO (3) (Refer Slide Time: 19:57). For every rotation here; a point here is a rotation with some n and some psi, there are two SU (2) matrices which differ by a sign. So this gets mapped here and this gets mapped here (Refer Slide Time: 20:15). Some matrix U here gets map to sum element g here (Refer Slide Time: 20:20). And this is - U and that gets map to the same element. The unit element here (Refer Slide Time: 20:28) is mapped by both the identity and - the identity both these guys get mapped on to this (Refer Slide Time: 20:49). So this implies that there is not a 1 to1 mapping but a 2 to1 mapping. So it's the 2 to1 homomorphism from SU (2) to SO (3).

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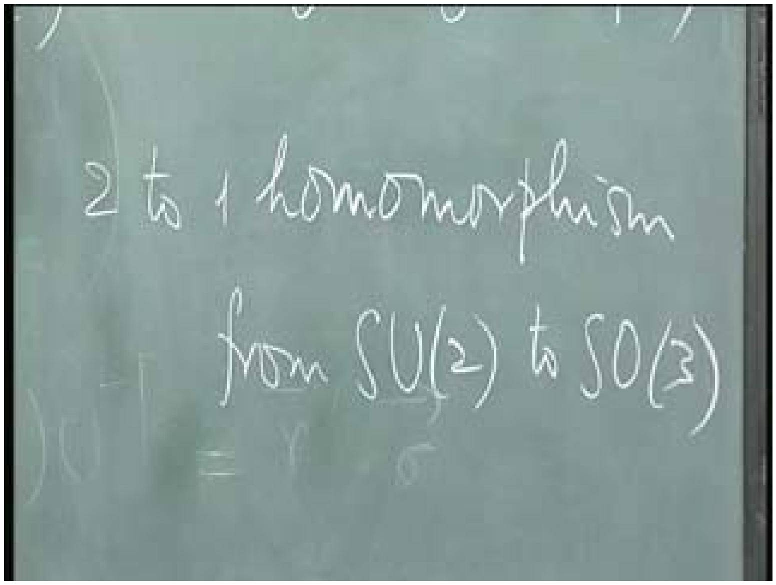

Now these 2 elements themselves which get mapped onto the identity element here are called the center of this group and what one writes in technical terms is that SO (3) is isomorphic to SU (2) quotiented with Z 2 because these 2 elements; the unit 2 by 2 matrix and - the unit 2 by 2 matrix themselves form a group under group operation of multiplication.

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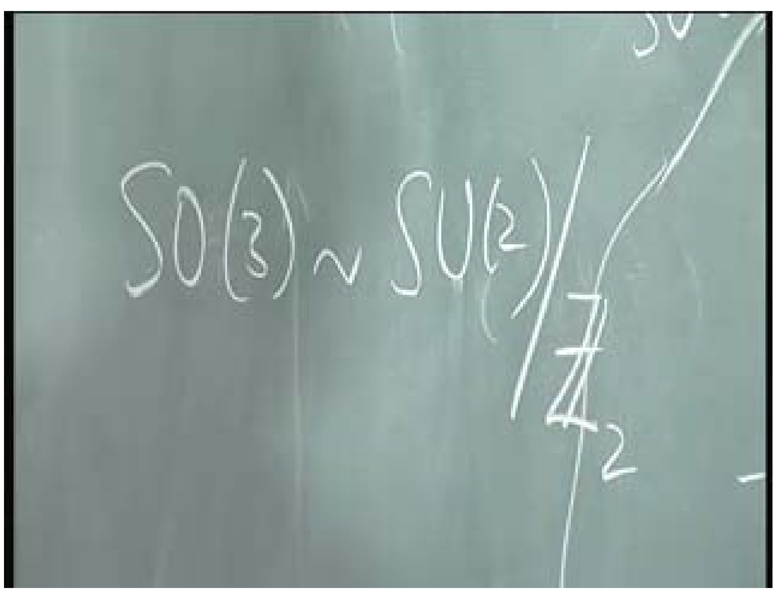

Because i times i is i, - i times - i is i and once again i times - i is – i. so they form a group among themselves. And it just the cyclic group of order 2. It is the group isomorphic to the set of integers under addition modulo 2. So you could identify this i with all even integers - i with all odd integers and the groups are identical. It’s the same z 2. So one says that SU 2 quotiented with Z2 is SO (3). the parameter space of this is S 3 and you do pi1 of this, S 3 is simply connected and you end up with z 2 along which is pi1 of SO (3). This group is called the universal covering group of SO (3). SU (2) is the universal.

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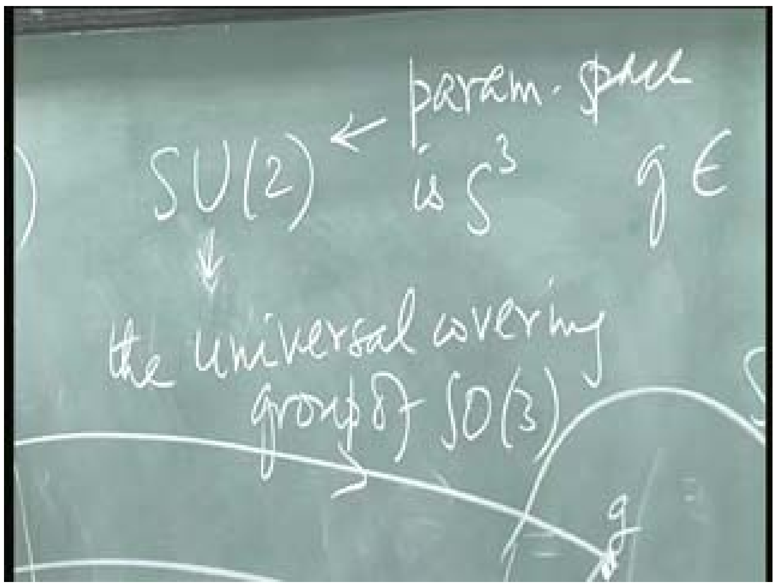

Every Lie Group whose parameter space is not simply connected is guaranteed to have a universal covering group whose parameter space is simply connected. And there is a homomorphism n to1 homomorphism between the covering group and the elements of the original group. so it’s not an isomorphism but a homomorphism. In this, you have the all the value representations of SU (2). It would include the single valued as well as the double valued representations of a SO (3). So really the fundamental group is SU 2 rather than SO (3) there because this is the bigger structure as you can see. Now the interesting thing is we discovered these properties of the angular momentum eigenvalues and so on by just the algebra of the commutators. The fact is that every Lie Group of this kind has an associated algebra of infinitesimal generators which when exponentiated would give you the elements of these matrices. Just as I take an infinitesimal generator of rotations and exponentiate it, I get a finite rotation. That algebra is called the Lie Algebra corresponding to the Lie Group. And the Lie Algebras are exactly the same.

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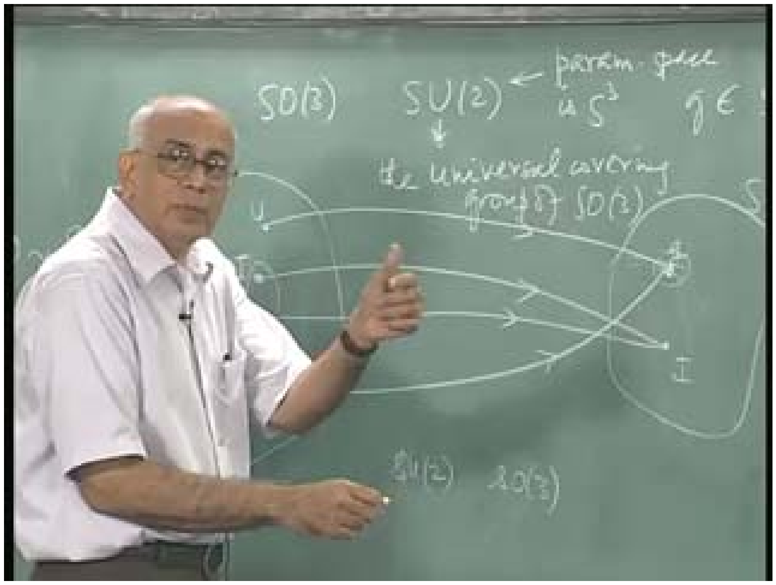

The Lie algebra of SU 2 which is written as su2 and so3 (in small letters), these are the lie algebras. The Lie algebras of the generators are exactly the same and each of them is just the angular momentum algebra. So these 2 groups locally look similar. so in a neighborhood of this g, if you look at infinitesimally different rotations, as compared to the parameters of g, you would get an infinitesimal neighborhood here as you would in an infinitesimal neighborhood here (Refer Slide Time: 25:36). And if you looked, only in this neighborhood or only in this neighborhood. But globally the group structure is different from that group there because there is a 2 to1 homomorphism. So the Lie algebras of a group and its covering group are always the same but the global structure is different.

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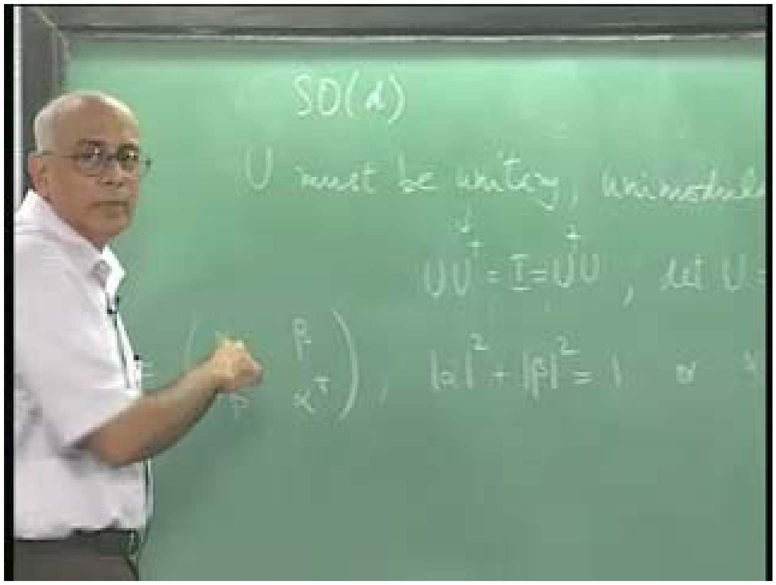

For any dimension, the group SO (d) in d dimensions, where d is 3,4, 5 etc, the covering group for it is called spin, d. that's the covering group. A spin 3 happens to be SU (2) for 3 dimensions. Otherwise it's called the spin group. Now the next question is the spin for the higher dimension, if you say 4, 5, etc is it SU d n -1? The answer is no. Now; there are some special relations SU (4) occurs as a covering group later on but not in general. It's just the spin group. A physical significance most important one in our present purpose is SU (2). So its worth understanding SU (2) very well and SU(2) has the advantage that its simply connected and every matrix in SU 2 has that simple form and you could easily represent it in terms of Pauli matrices. So you see why the Pauli matrices play such a fundamental role in understanding quantum mechanics, spin and so on.

This is because it is really connected with a rotation group and not just spin half. May be a few exercises on this and I will clarify some of these things. Let's now go back to our physical problem of a particle in a spherically symmetrical potential. We haven't done this. we talked about bound states in1 dimension, we looked at potential problems in 1 dimension but we haven't yet looked at the problem of a particle in a spherically symmetrical potential. So let's do that. You have already solved that hydrogen atom problem in the chemistry course long ago. Let me try and justify what was done there and generalize this a little bit. What is our task? We would like to motion in a central field.

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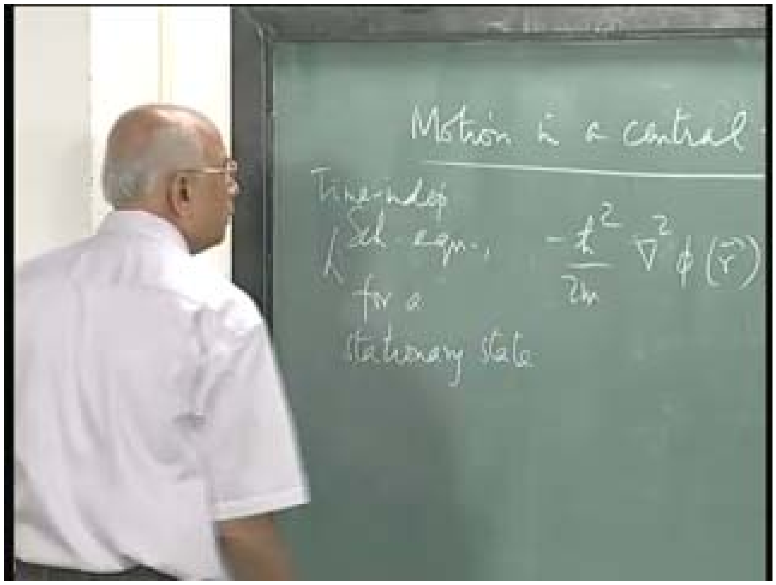

I have in mind the spinless particle. I am not going to look at spin now which is moving in a central field of force like the Kepler problem. Now classically I know that in such a situation angular momentum about the origin or the center of force is conserved. And that fact will remain true in quantum mechanics as well and what we need to know is what does it imply for the energy levels of the system. So here is a problem where in addition to the Hamiltonian, you are going to have other operators which commute with a Hamiltonian and therefore simultaneous eigenstates can be found and what is the consequence for the energy eigenvalues in eigenstates. So what is the Schrodinger equation? It's - h cross squared over 2 m del squared. That's the kinetic energy part and now I am writing it in the position basis and I am interested in stationary states. In other words, eigenstates of the Hamiltonian with specific energy is E. the Hamiltonian is just p squared over 2 m + a potential which is a function only of the radial coordinate, r. No theta. No phi.

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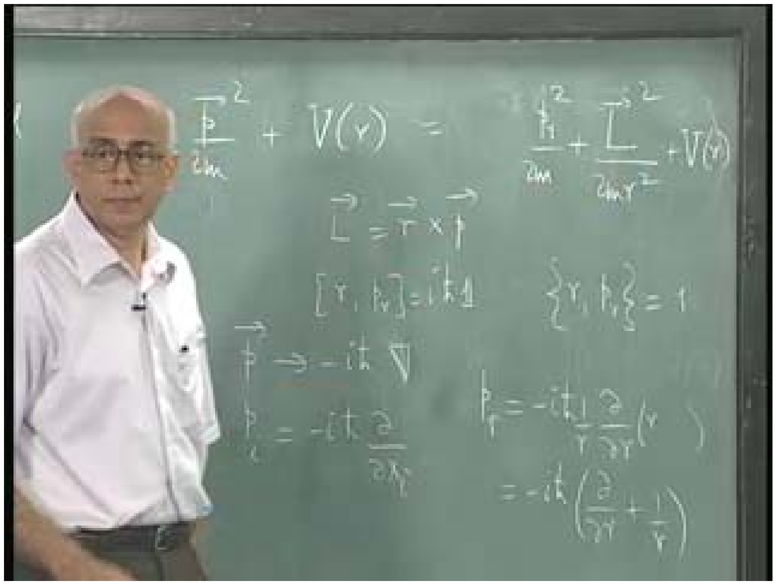

Now just to recall what happened in classical mechanics that p squared was the square of the linear of the momentum. It could therefore decompose into the radial momentum and the angular momentum. So you could also write this classically as = p radial momentum squared over 2 m + angular momentum squared over 2 m r squared, that's twice the moment of inertia + V (r). And we know it's easy to prove that L is a constant of the motion, dl over dt was 0 or the Poisson bracket of L with the Hamiltonian was 0. Classically there was nothing to forbid you from simultaneously finding sharp values for Lx and Ly and Lz. but quantum mechanically, they don't commute with each other and therefore you can't do that and quantum mechanically, we expect we would be able to diagonalize any 1 component of L.

So the Hamiltonian is exactly the same. The definition of L remains unchanged. L is r cross p. r and p doesn't commute with each other. The cartesian components of r don't commute with the counter parts of p. on the other hand, I write L as r cross p and r p are Hermitian operators. So shouldn't I symmetrise this or something like that? xi and pj commute with each other unless i = j and since in the cross product, you never have a Cartesian component of the coordinate and the same component of the momentum, this commutation problem isn't there.

Otherwise, suppose that one is the case, what should I have done? I should do r cross p - p cross r and take it divide by 2 but i don't need to do that here. What would be the radial momentum by the way? Because classically, I would have {r, pr} =1 and quantum mechanically that should translate to [r, pr] = ih cross times the identity operator. Now my general rule is that in the position basis p goes to - ih cross del. and this is fine for each Cartesian component but i have to be little a careful about the radial component. Normally classically I would define the radial component, pr as simply r dot p divided by r itself. It’s the unit vector along the radial direction dotted with p to give me pr. what should I do quantum mechanically, these operators don’t commute? pr classically is r over r dot p. it’s the component of p dotted with the unit vector in the radial direction. That’s my definition of the radial momentum.

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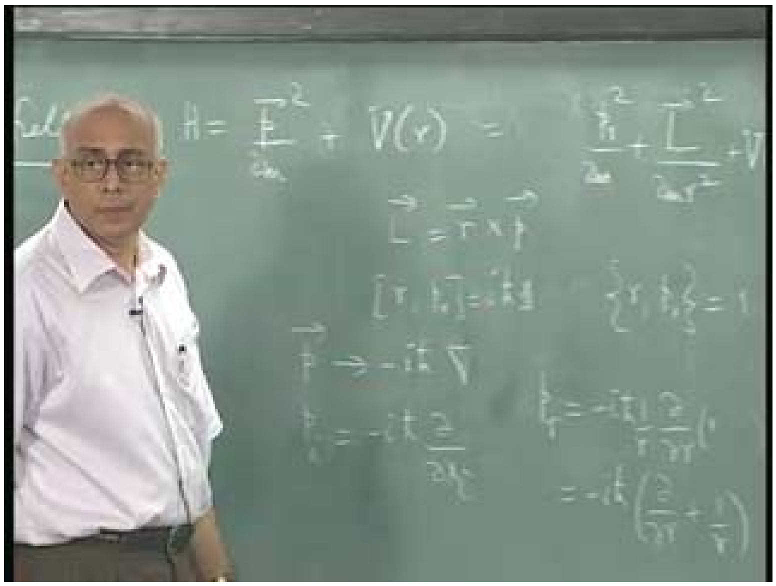

But I could also have written this as p dot r over r. There is no commutativity problem classically. Quantum mechanically what should I do? Which1 should I choose? But you can’t choose either one of them because if you choose this or that, you will have a trouble with hermiticity. It should be hermitian. If you got a product ab, the hermitian conjugate is ba. If b and a don’t commute with each other, you are in trouble. So what should the quantum mechanical thing be? pr would be p dot, notice I can’t bring this r out here, r over r + r over r dot p, that would be a good compromise but it should become hermitian which this is , so I need this + sin and then I have to make a half here.

By doing this I ensure that pr is actually hermitian as it should be so that the eigenvalues are real. More technically self-adjoint but this is guaranteed to give real eigenvalues. So that is the right way to write it. So what would the quantum operator be? p Cartesian is - ih cross delta over delta xi. There is no problem with that. But pr is not - ih cross delta over delta r. that will not satisfy this condition here. So it turns out that 1 over r delta over r r satisfies the conditions that you need. You can work it out by putting p as - ih cross del there.

So this becomes = - ih cross delta over delta r +1 over r. that’s the operator corresponding to the radial momentum. and then indeed, in quantum mechanically also one can write V(r) in this form here where pr in the position space has this representation (Refer Slide Time: 36:24). So we have to make sure it’s actually hermitian. Then what does the

Schrodinger equation become? by the way, I am assuming that you are familiar with the fact that the way you arrive at a particle moving in a central potential originally for physical problems is when you have 2 particles which experience a certain interaction which depends only on the distance between them, the centre of force and then you go to the center of the mass coordinates eliminate the center of mass and then relative coordinates you get a1 body problem in a central potential. So I am assuming this job has already been done. So the Schrodinger equation now can be written down. its just H acting on psi = ih cross delta psi over delta t and for stationary states which are eigenfunctions of the Hamiltonian, then the time independent Schrodinger equation is del squared phi(r) + V(r) phi (r) = E phi (r). This is the time independent Schrodinger equation for stationary states. That is the equation we have to solve.

Let’s write it out in the position basis and see what happens explicitly. In the position basis, all we have to do is to take del squared and write it out because that’s what p square is.

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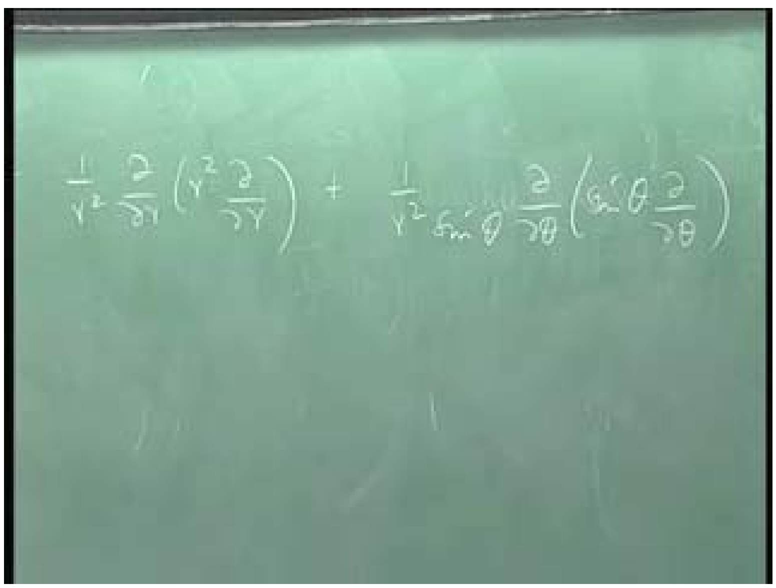

It’s 1 over r square delta over delta r r squared delta over delta r +1 over r squared sin theta delta over delta theta. There aren’t too many things worth memorizing but delta squared in spherical polar coordinates is worth memorizing. Otherwise you have to work it out each time which is a nuisance. +1 over r square sin squared theta delta 2 over delta phi 2. So if I use this (Refer Slide Time: 39:50) prescription, then it is clear that what I have is p squared = - h cross square delta squared. And I am writing this as = pr squared + l square over r squared. So what is L squared? We can identify L squared here in the position basis. It’s quite clear from here that L squared is 1 over sin theta delta over delta theta sin theta delta over delta theta +1 over sin squared theta delta 2 over delta phi 2. That’s L square in the position basis written in spherical polar coordinates.

So now tell me why shouldn't I bother about the order between little r and L squared? They have nothing to with each other because they are independent coordinates. This is entirely radial and that's got only the angular variables. So they commute with each other. Therefore it doesn't matter whether I wrote this as L square over r squared or 1 over r square L square or L square times1 over r square it didn't matter. But one is right to be cautious. now this equation suggests immediately that you can simplify it because this coefficient V (r) which is a hard part, you don't know it's a general potential and depends only on little r.

So it at once suggests that you try to solve the problem by the method of separation of variables. And then you have to use uniqueness theorem to show that that is a unique solution. If you get more than1 solution for the same boundary conditions then you have to superpose all these solutions with appropriate normalizing constants to get a physical solution. And so far I haven't said whether E is positive or negative. It's only an energy eigenvalue. So since the Hamiltonian is Hermitian, you are guaranteed this E is a real constant and now what values of E are physically acceptable depends on V (r), the boundary conditions and what you require of the solution.

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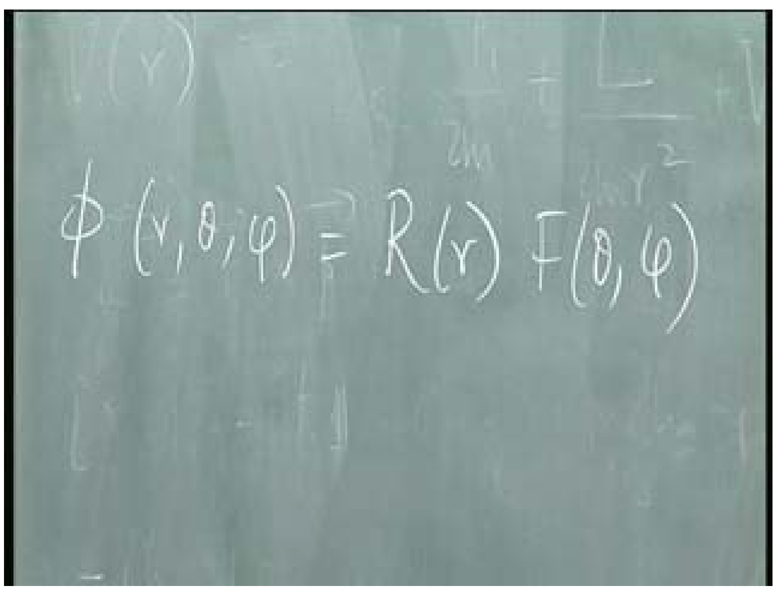

So the first step is to put phi(r, theta, phi) = R (r)multiplied by an angular function which depends on theta and phi alone. So some F (theta, phi). Substitute it in here. use the fact that the radial part delta over delta r part acts only on capital R and the angular part, the sin and the derivatives with respect to theta and phi act only on the F. now to cut a long story short, we know that in this problem and this is true classically.

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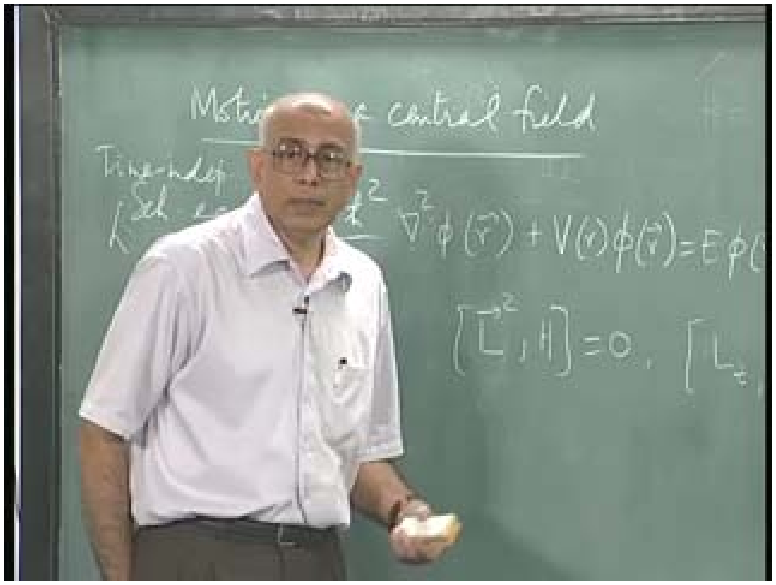

And quantum mechanically, you know that L squared with H is 0. That's simple to prove that angular momentum is conserved in this problem. The only difficulty would have been if this V(r) had dependent on other coordinates as well on the theta and phi. That's not true here. [Lz, H] = 0. You could have chosen any component but I just choose this z axis because once I have chosen spherical polar coordinates, I have singled out an axis the polar axis. So let me quantize along that direction. So I have a situation where I have a set of 3 mutually commuting observables H, L squared and Lz.

Therefore I expect that they have a common set of eigenvalues. I expect therefore that the eigenvalues would be labeled by the quantum numbers corresponding eigenvalue of H L square and Lz. I therefore 3 quantum numbers. Let me call them the radial quantum number, the angular orbital momentum quantum, l and m. now what sort of equation, once you go through this rule, what sort of equation would this function F satisfy? It has to be an angular momentum eigenstate and F is only the portion which carries the angles. So the equation it would satisfy is precisely this.

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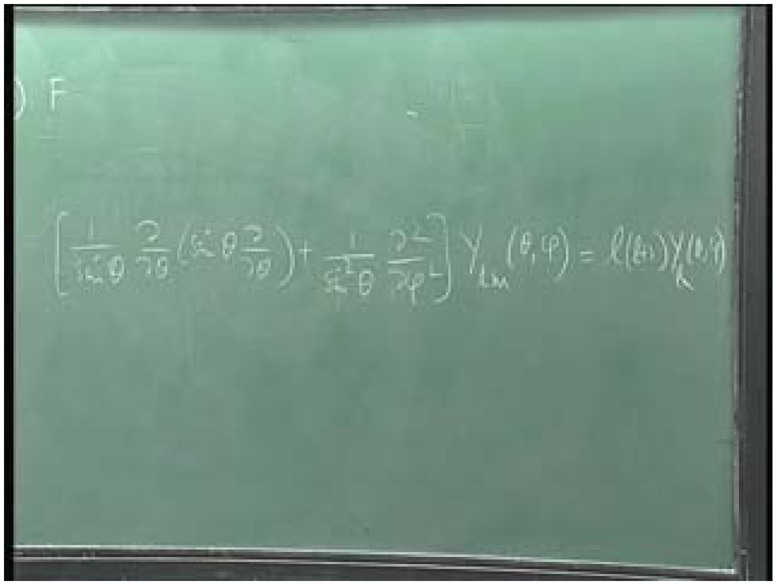

L squared acting on this F must be = the angular momentum eigenvalues which would be this (Refer Slide Time: 45:40) because you already know that the square of the angular momentum has eigenvalues h cross times l times l +1. So essentially these functions this function F would be labeled by the eigenvalues little l and little m too. So what is the equation it would satisfy? It's conventionally denoted as Y_{lm} and it's labeled by l and m. it's a function of theta and phi out here. This would be = -l times l +1 Y_{lm} (theta, phi). Now the next thing to do is to assume that this Y_{lm} of theta and phi is a product of a function of theta and a function of phi, again separation of variables and it is suggested by the form of that equation there. So let me write the solutions down.

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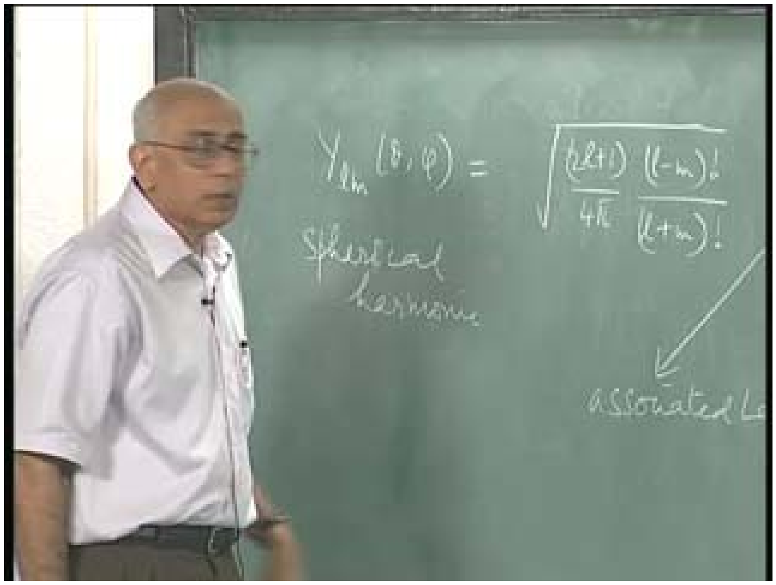

Y_{lm} of theta and phi are the following and then it becomes a standard equation. Once you separate out the phi part and require that it be single valued in phi which we already know that m must be an integer running from - l to l, then the equation that you get is called the differential equation satisfied by the associated with the Legendre polynomials. And the actual solution looks like this. Y_{lm} of theta and phi has got a normalization constant which I remember is 2l +1 over 4 pi (l-m) factorial over (l + m) factorial (refer Slide Time: 49:50). This is for m greater than or equal to 0.that - L less than = m + L itself is 01 2 etc. at the moment, this is all we know. We don't know that it stops at some principle quantum number n -1. We are just solving the angular part and that's just a standard in solving the problem of the orbital angular momentum. This is nothing to do with V (r). We don't yet know what V (r) is. So this is the definition of Y_{lm} (theta, phi). It's called spherical harmonic. And incidentally, for m less than 0 because m can take on negative values as well, you need a definition and that definition is as follows.

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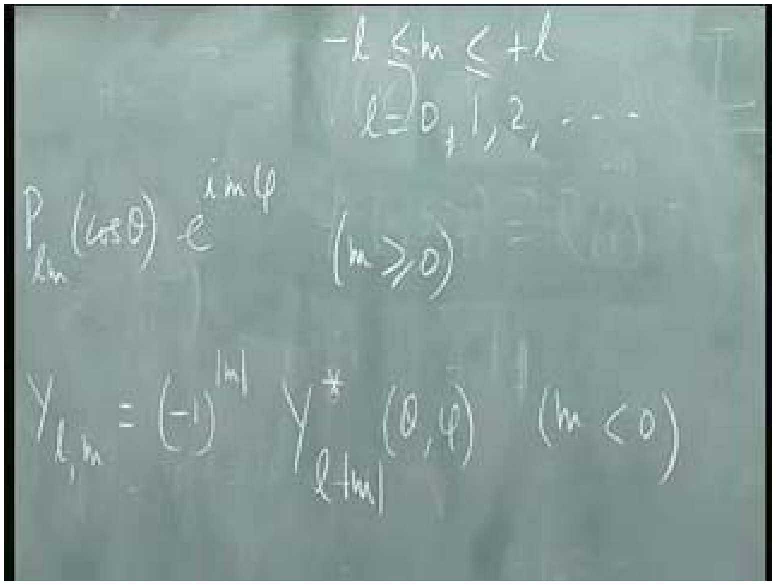

Y_l m = -1 to the power mod m Y_l mod m star of theta phi. So it just differs by a phase factor and then that the e to the im phi complex conjugate. These quantities are the associated Legendre polynomials and they are tabulated. They are derivatives of the general polynomials themselves.

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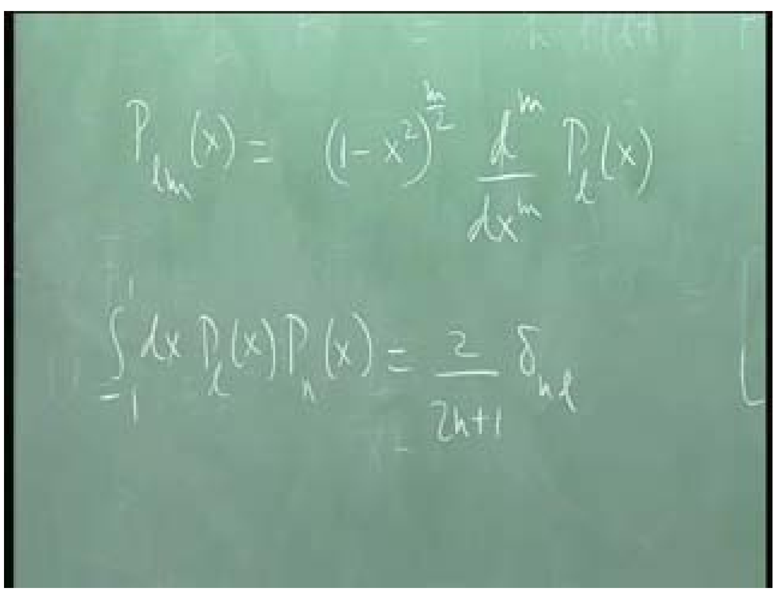

So if recall the definition, P_{lm} (x) is = (1 – x squared) to m over 2 d m over d x m P_l (x). There may be some normalization factors I have left out. But as I recall it, it is the derivative of P_l (x). Pl of x itself is the ordinarily Legendre polynomial. P $_0$(x) is1, P_1 (x) is P_1 x is 1/2 of 3 x squared -1 and so on and so forth. So P_l (x) has got parity -1 to the l. it's a polynomial of order l. and its got a nominalization rule. So if you recall that's (Refer Slide Time: 53:14) = 2 over 2n+1 delta nl. So those factors have been put in here and you end up with a similar normalization condition here. If you integrate this multiplied by its complex conjugate and you integrate over theta and phi, over all solid angles then you would get Kronecker delta in mm prime.

So I am not going to bother to write it down in that case but one can derive it fairly trivially. So these functions are already normalized. We have already formed an orthonormal basis for the angular functions. The question is what happens to the radial part. Now notice that once you have taken care of the phi dependence which came from here by that e to the im phi, then matters become very simple. You can go back and ask what it does for the radial equation itself. What is the equation obeyed by R? And then something very simple happens. The equation obeyed by capital R is what we want to discover.

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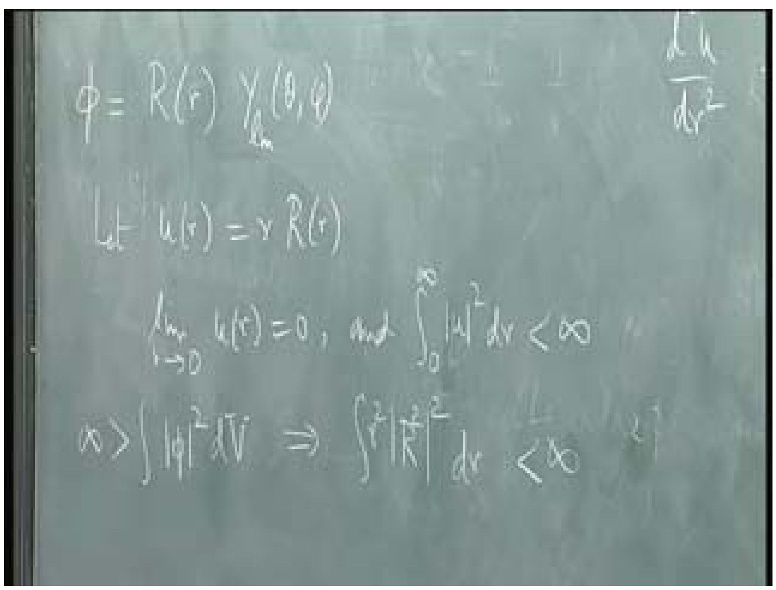

Remember that I put phi = this times now it is Ylm of theta and phi and I would like to know what is the equation obeyed by this. now that equation will have the radial part which is the - h cross squared over 2 m 1 over r square d 2 over dr 2 etc but this part of del square which involves d 2 over dr 2 has also a d over dr part. And the disadvantage of that is that d over dr is not self-adjoint. d 2 over dr 2 is. So, one would like to get rid of the first derivative always. And this is done in a standard form by saying let U (r) = rR (r) and then you write differential equation down for U . But before I do that, lets go back and ask what is the equation obeyed by this a capital R. it was - h cross square over 2 m1 over r squared d over dr of r squared d over dr R, that was a kinetic energy part + V (r) times R that came from the potential energy.

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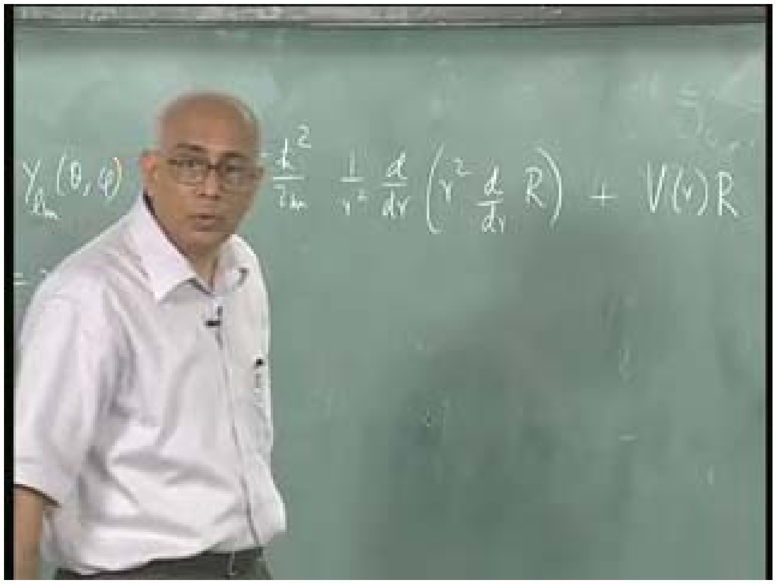

And then there was portion which came from the angular portion which was - h cross squared over 2 m r squared and L squared, but L square is + h cross square l times l +1 over r squared, this also acts on R in this fashion = E times R and the Y_{lm} canceled out on both sides. Now take a look at this equation. If this potential V (r) is finite everywhere, then so should the wave function also be finite everywhere. So what is the boundary condition I require on this R, especially R = 0, what should I expect? What should happen to this at R = 0. I expect it to be finite. So if I want to get rid of the first derivative term by putting a U (r) here, this is finite at the origin which would imply that U (r) must vanish at the origin. So the boundary condition I require is that they should vanish at the origin. Is there anything I require of the potential at the origin because remember, that even though it looks like a1 dimensional problem now, there is a huge difference in the fact that little r runs from 0 to infinity rather than - infinity to infinity.

So 0 less than = r less than infinity. That's very important. So I need to specify now some conditions at the origin as well as + infinity whereas in a 1 dimensional problem on the line I just specified it at - and + infinity. Now we have to be careful about the origin. Now for this equation it's a second order differential equation, the most singular part is going to come from this 1 over r squared everywhere. So it is clear that this 1 over r squared is going to play huge role near the origin and you don't want in a second order differential equation, if you recall the Forbenius theory of second order differential equations, you would like the singularities to be ordinary singularities. You want this to be Fuchsian equations only then you would have respectable spectrum and so on and so forth. Now these statements can be made fairly rigorous but I don't want to get into the technicalities of differential equations here. You don't want a singularity worse than1 over r square at the origin. So the assumption i am going to make, we will relax this assumption and i will tell what happens relax it is that limit as r goes to 0, r squared V (r) = 0. In other words, V (r) does not have a singularity worse than 1 over r squared. You could ask what happens V (r) is exactly =1 over r squared. That is the limiting case and we will come and look at it specially. So, as long as V (r) if it blows up at the origin, it blows up no worse than1 over r to the 2 – epsilon. If this limit is finite, that would imply that V (r) goes like 1 over r squared near the origin. Then this is a limiting case. It will turn out that if the strength of this1 over r square is some number alpha, for alpha less than a certain critical value you would have respectable bound states, for greater than, that thing will fall into the origin. They will be collapsed. And if that limit is infinite, if its unbounded, then the V (r) goes to 0. It blows up worse than 1 over r squared at the origin.

Then it is collapsed with the origin. So the1 over r squared potential is the marginal case. On the other hand, the potential which we are interested in, the Coulomb potential is 1 over r and that's very safe already. So we will relax this and come back to this later. Now on the wave function, I am going to put in the condition, limit r tends to 0 U(r) = 0. So that's my boundary condition at the lower end. And at that upper end, the boundary condition should be normalizable. Now what is the normalization condition on phi? It says integral mod phi square dv should be finite.

That's all you need and after that we will fix the constant so that the thing comes out to be1. Now the angular part is already normalized to1. So this would imply that integral mod R squared less than infinity is r squared dr. and integral 0 to infinity mod U squared dr less than infinity .that's all you need here because r times r is in fact U by definition. So this sets our problem. this is a boundary condition under which I am going to solve the equation for U. limit U goes to 0, U(r) is 0 and U (r) should vanish at infinity sufficiently fast that this integral is finite (Refer Slide Time: 01:03:00). Please notice that this requires this requires for bound states I want this normalization this requires that U goes to 0 as r tends to infinity sufficiently rapidly, for bound states for normalizable solutions. Now what is the equation for U itself?

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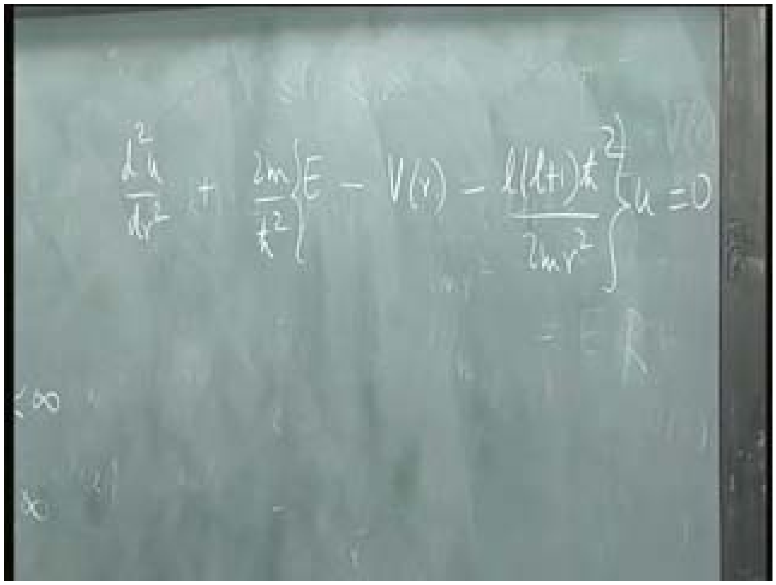

The equation for U itself is d 2 U over dr 2, the first order term has gone away + 2 m over h cross square I bring the e to this side - V (r) - l times l +1 h cross squared over 2 r squared on U = 0 . That is the second order equation obeyed by U. but it's showing us something very interesting. Again I call your attention to the fact that 0 less than equal to r is less than equal to infinity. It's a like a 1 sided problem. Not a full 1 dimensional problem but a 1 sided problem with a barrier at the origin because I want to put this boundary condition u of r = 0. That would be the case in a1 dimensional problem if I put an infinite barrier at the origin. Then the wave function is 0 at the origin. So it's like saying I have a potential on a line, - infinity to infinity, the physical region is 0 to infinity but I have an infinity barrier at R = 0. No negative r allowed. And what is the effective potential?

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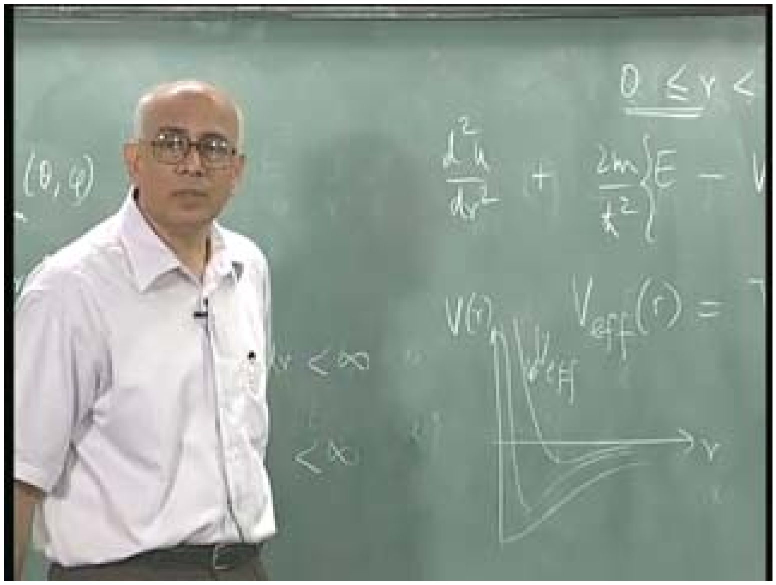

It's a function of r. it's the actual physical potential + l times l +1 h cross squared over 2 m r squared. So it's as if there is an extra potential due to the orbital angular momentum of the particle and that's called the centrifugal barrier because this potential as you can see, is 1 over r square with the positive sign. Therefore it's always a repulsive potential. so if I have a potential, here is r, here is V (r), if this potential was some nice bound state kind of potential (Refer Slide Time: 01:06:00), suppose this was the potential, then I would expect some bound states inside here. Now with the advent of this extra term here which blows up at origin at l = 0, this isn't there at all. This is what will happen in the ground state but for higher excited states, when l is not 0, that offers a repulsive potential and therefore this potential would start looking like this (Refer Slide Time: 01:06:26). With increasing l, it becomes shallower and the minimum shifts to the right. This is exactly the classical counter part of the fact that when you have a bound state, the higher the angular momentum, the further the orbit is.

And that is precisely what is happening and the potential is getting weaker. It's getting less and less strongly bound. It's getting more and more weakly bound and that's exactly what increasing l would be. Now you begin to see why the 1 over r square potential is so critical. It depends on the relative signs of this and that's because if you had a1 over r squared potential, depending on what the l value is, you may or may not be able to support a bound state. It may fall into the origin or it may get kicked out completely. So that's why the1 over r squared behavior of this near the origin is like a kind of marginal case. It divides 2 classes of potentials. So I will stop here and we will take it up from this point. We will try to solve this for various cases. I want to explicitly write down the solution because this involves special functions of various kinds but I will point out what happens if you have, for example, a free particle or harmonic 3 D oscillator or in the

Kepler problem and what is special about the Kepler and oscillator potentials, and then it brings us to the idea of degeneracy here. So we will take this up tomorrow.