Symmetry and Group Theory
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Lecture No. 25
Unitary Transformation

Today we are going to talk about unitary representation to start with in fact by and large we talk about unitary representation. And then you know what is reducible and irreducible representations are. What we will do if we will just talked a little bit about more formal definition of what is a reducible representation? And what is a irreducible representation? And that is where we stop today.

Now the logical next step is to derive the great orthogonality theorem which tells us about all the properties of irreducible representation ok. So, problem is if I start deriving this great orthogonality theorem on Friday I will not finish. So, what we will do it for the moment we will believe in it. After all it is written all books Bishops books Atkinson book all these books. So, for maybe one and half week we just take it asymmetrically. So, for we are not taking anything asymmetrically in this course but you will make we will have we will make an exception for great orthogonality theorem just for time being.

So what I will do it I will just write down the great orthogonality theorem and we will discuss what it means. We will talk about the five consequences of great orthogonality theorem. And using those we will learn how to construct the character tables that is something that is very easy compared to what we are doing now ok. Let us have something easy in the last class something that you do not even have to study.

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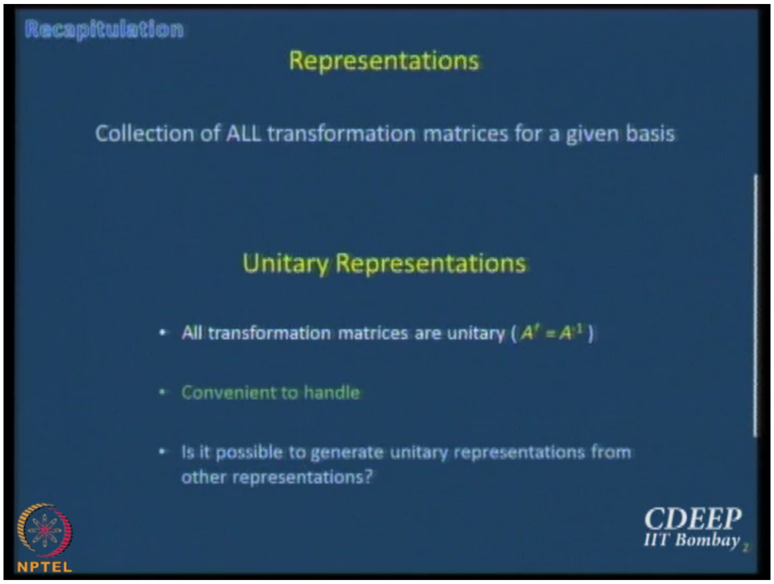

This is what we have been talking about that last couple of days we have been talking about representation and as we know by now. Representation is a collection of all the transformation matrices for a given basis. When I say all transformation matrices what does it mean? I mean transformation matrices for all the symmetry operations that have been there in the point group that we are talking about right. And of course representation is going to depend up on the basis. I think Rahul ask that question in the last class.

So what basis you choose governs what kind of representation that you get right. Couple of weeks ago we have gone through some examples where we worked out the matrix worked out the representation using different bases. Today we focus on a particular kind of representation. And that is unitary representation. And what are unitary matrices? A inverse is A dagger what is A dagger? Adjoint, what is adjoint? Transpose and each element is replaced by is complex conjugate.

What happens when I multiply the element with complex conjugate what do we get? Positive, positive quantity we are going to need it in a while so please remember that ok. So as you said correctly unitary representation is one in which all the transformation matrices are unitary A dagger is A inverse. Why do we even bother about unitary representation? Be bother about them because they are very convenient to handle. It is more often than not when you deal with matrices you need inverse.

If the transpose is the inverse or its adjoint is its inverse life becomes very simple. You do not have to worry about the annoying determinants stuff like that ok. Now the question that now we ask is it is possible to generate unitary representation from other representation.

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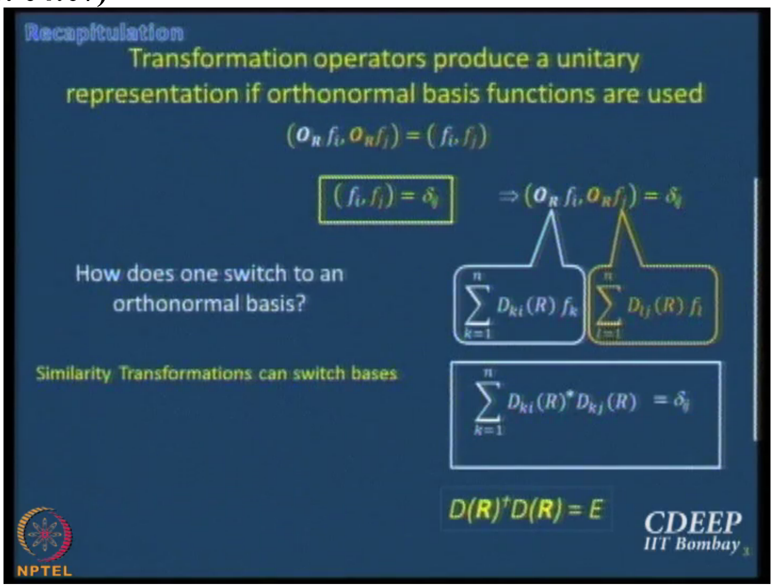

When you ask that question the background is already built because you know that unitary representation or unitary matrices are associated with orthonormal basis functions right. This is something that we have discussed earlier already and we have reminded ourselves yesterday as well. When you use the orthonormal basis function then you get unitary representation unitary matrices right. The question is how do I switch to an orthonormal basis? We have gone away in answering that question so far. What we have done until yesterday is that we have learnt how to switch bases? Orthonormal are not orthonormal that we have not discussed so far right.

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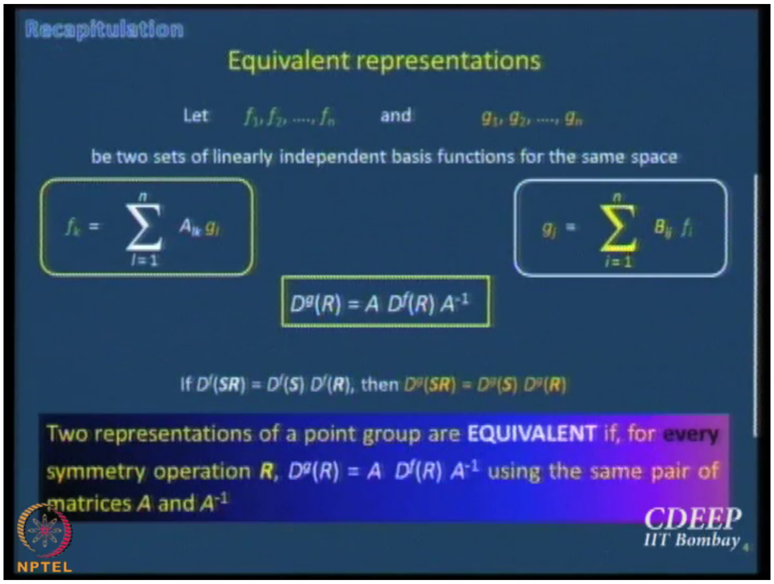

Orthonormal are not orthonormal that we have not discussed so far right. Until yesterday this is what we have done we have learnt what are equivalent representations. How does one switch bases? One switches basis by using an appropriate what, switch basis by an appropriate fill in the blank one mark question maybe half a mark question. Matrix will get one eighth similarity transformation right. Switch basis by using similarity transformation they even written there. Similarity transformation can switches bases ok.

Now what we did yesterday is that we worked with two different linearly independent basis functions. Did you say that orthonormal? Yesterday no, just linearly independent, you just worked with two linearly independent basis functions f's and the g's. And f's and the g's are related by system of linear equations like this fk =sum over l = 1 to n Alk gl right. The only trick here is going down; they are going down the column ok. And gj similarly sum over i = 1 to n Bij fi ok.

Then we have derived this also that if you take this matrix, this matrix can be used to perform the similarity transformation that can take you from the f domain to g domain. What is DgR? It is a transformation matrix corresponding to the symmetry operation R in g bases. What is DfR? It is the transformation matrix of the same symmetry operation R but this time in f basis right. By the similarity transformation A and A inverse I can go conveniently from f basis to g basis. That is what we have discussed yesterday.

And we can do that when we say that this representation consisting of all the DgR's is equivalent to the representation consisting of all the DfR's right. Already learnt how to switch bases, today what we do is we build up on that and then we try to switch orthonormal basis. Orthonormal basis function alright.

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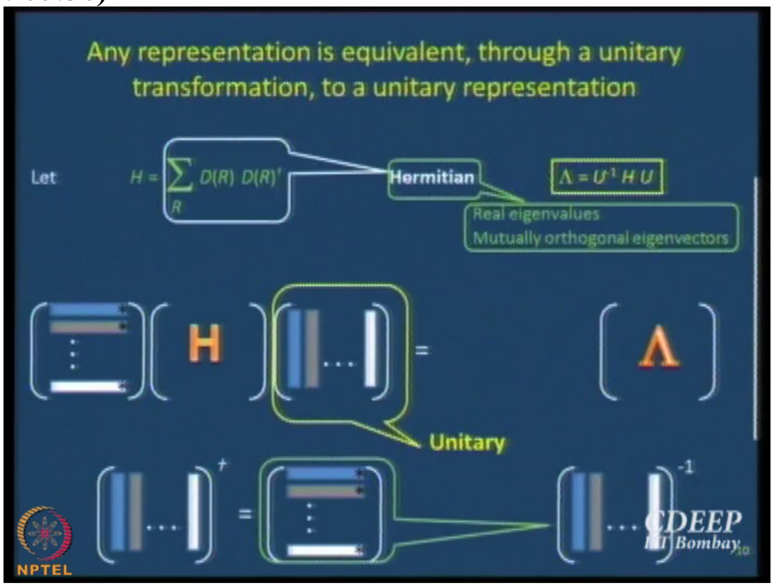

Here goes, so I have mind of made spoil sports and given you the answer to start with. Any representation can be seen to be equivalent to unitary representation through a unitary transformation. I should say through appropriate unitary transformation not just any unitary transformation. And we will see what that means ok. In other words you can generate a unitary representation from some other representation by using an appropriate unitary transformation. What is the meaning of appropriate? That we learn today.

What we will do then you are going through this little long derivation which is not difficult is long ok. Since it is long at the end what will do is write down the recipe how to go about doing this. The derivation itself is a just is a good exercise in remembering what we have discussed earlier on also. Where we are use lot of things that we have discussed few weeks ago. This is the nice topic to discuss before it ends midsem ok.

So, let us start with this let us say define a matrix H as sum over R into DR into DR adjoint. What am I doing here? For all the symmetry operation that are there C3v what are the symmetry operations? C3 C32 well do not forget E then Sigma V1 Sigma V2 Sigma V3 Sigma VA Sigma VB Sigma VC whatever we want to put it. How many symmetry operations? 6. Now let us say I am working with Ammonia how many atoms? 4, so I add this for atoms n HA HB HC using them as basis let us say we have constructed DE DC3 DC3 square D Sigma A D Sigma 1 D Sigma 2 D Sigma 3.

So I have all the DR's right, now that I have the DR's, if have any matrix I can work out its adjoint right, I work out the adjoint also. Now what I am doing it for E, what is the adjoint of the DE? Same entries right, so I take D I take the D adjoint and multiply them together. Then I take DC3 and its adjoint and multiply them together. DC 3 square is the adjoint and multiplying them together. D Sigma V for each Sigma V its adjoint and multiply them together. Then I add up all this product ok.

When I do that what should I get I should get another matrix right. What should be the dimensionality of the matrix I am working with the four dimensional basis how should I get 3 by 3 matrix, 4 by 3, 4 by 4 whatever it is the dimensionality of the bases. The dimensionality will be conserved right so this is the matrix right H = sum over R DR multiplied by adjoint of DR. Now H is a precious letter right we do not write H just for anything is it not. You see the enthalpy or it can be a Planks constant or it can be Hamiltonian right this has to be one of these otherwise why will I write H.

So what do you think H is? It is a Planks constant then what would it be? In fact this was the problem that you have I think worked out in assignment 2. There was a problem and assignment whereby you have to show summation R DR multiplied by DR adjoint is a hermitian matrix. Unless we said that do not have to work it out you have work this out ok. This is hermitian matrix H for hermitian. Ring a bell somebody work this out or not. It is not very difficult to work out you have not work it out then you work it out yourself.

But in case you have not work it out you are to believe me when I say that you not about to work out now, too many things are to be worked out anyway. So, that is hermitian matrix alright so just believe me. In case you are not done it yourself. So, if it is a hermitian matrix, what is a special about hermitian matrix right? So, do you have the 2 interesting properties that are associated with hermitian matrices? First is eigenvalues are real and second is eigenvectors that you get are mutually orthogonal I think that we discussed this right we drop this out ok.

If you are little lusty on this sit back and go to I think that Lothian matrices lecture 5. We must have discussed in lecture 5. No 6b, eigenvalue 6b right. So let me now knowing all this write down your familiar eigenvalue equation matrix eigenvalue equation in that expanded form that we have worked out. I hope you are not completely at the lost when I write this. What is Matrix eigenvalue equation? Hx = Lambda X, what we saw was that there is going to be a number of eigenvectors correspondingly eigenvalues right.

Then what you did is this vectors are column matrices why not combine all the columns and make one square matrix and then we had construct a square matrix like that what I show you instead of writing like this X11 and all like this each of these columns is an eigenvector ok. Each column is an eigenvector ok. Now do you remember this equation we have written H matrix multiplied by capital X matrix into capital X multiplied by Lambda? What is Lambda matrix? Does it ring a bell, Vinod, this equation fine?

Now see what would be the adjoint of this X matrix columns become rows and then you have to take complex conjugate. So, everybody ok if I write it like this right. Since everybody ok with this will you agree with me when I say that this adjoint is also the inverse matrix, work it out. It is convenient if you multiply; left multiply this matrix by the adjoint. Let this be on the left and let this be on the right. Then what is the 11 element, what is this colour blue, so it is blue row complex multiplied by blue column.

What it should be? It should be 1, do not say blue, and it should be one. Orthogonal eigenvectors right mutually orthogonal eigenvector orthonormal eigenvector actually this should be one. Now the problem is when you want to see what is 12? What will be the 12 element blue star multiplied by what colour is this? Green I believe you. So what should it be? Either orthogonal you multiplying the elements and adding you should get 0, half diagonal elements all is going to be 0.

So what about 22? Green star multiplied by green that is also one. So what about the last one what is this colour? That is white that is white star multiplied by white that is one. So, all the diagonal elements will become one, all half diagonal elements become zero. So, the adjoint here is the inverse, so the adjoint is the inverse. Which matrix I am talking about I am talking about of quotes it is symmetry I am talking about matrix of eigenvectors right. I would have said correctly. The matrix of eigenvectors thus stands out to be unitary right.

As we discussed this earlier I do not think so, we have ok. This is unitary right, so now what I can do is next part definitely I remember we discussed earlier if I now left multiply the left hand side by the adjoint by the adjoint yes along the left hand side what you have similarity transformation. On the right hand side what will happen you multiply the matrix of eigenvectors by its adjoint which is also its inverse you get unit matrix right. So, this is the equation right. Now if you conciliatory of coloured column and coloured rows and all that you can write down the equation like this A = U inverse HU, I think earlier we did not sorry Lambda = U inverse HU.

Earlier we have did Lambda = X inverse HX right. Here I want to write stress you the fact that it is unitary number 1. Number 2, I think some what we are in line with Bishops notation ok. So if I read this if I try to speak this say this in English what will I say? Lambda matrix is obtained by unitary transformation of the hermitian matrix right. The Matrix which has the eigenvalues of the hermitian matrix along the diagonal and 0 will be whereas is obtained by a unitary transformation of the hermitian matrix ok. But while you say this you should not forget this just any unitary matrix. It is particularly a unitary matrix which matrix is that it is the matrix of the eigenvectors ok so far so good any question.

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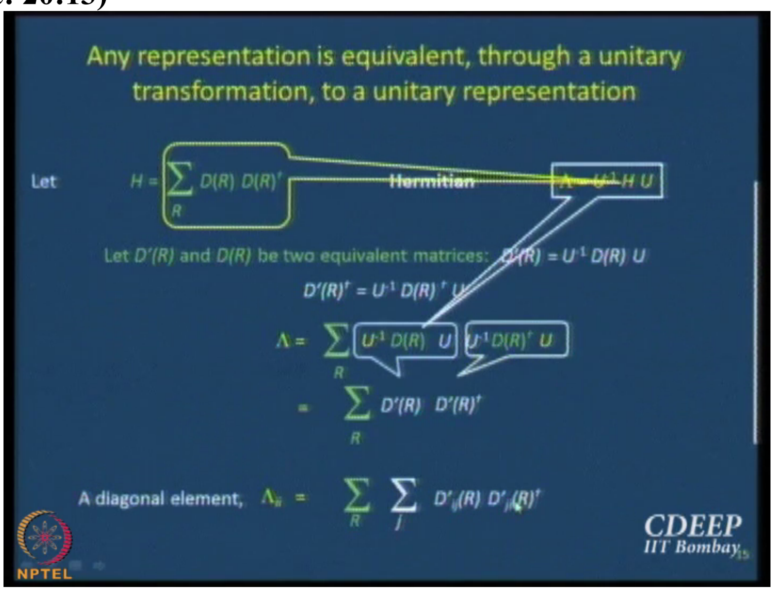

If not Let us clean the little bit this is what we will need H is hermitian matrix what are right this down the thing is at one point we will erase this also it is only so much we can write on the slide but we will need this. But it is very easy to forget what we are saying now in the maze that we get into. So please write down so H= sum over R DR multiplied by DR adjoint that is one. Second is Lambda = U inverse HU.

You are going to need this letter on of course you are all masters of manipulation you know how to take square of all whole sides and transpose and take cube root and get the answer that is basically what you are trying to do after this. Please write this ok can I go ahead now Lambda = U inverse HU ok. So now let us now talk about two equivalent matrices DR D prime R. DR is any transformation matrix that you get you have used some basis without bothering about whether they are orthonormal or not right.

You use some basis and you have got the transformation matrices. Using the transformation matrices you building representation, so, DR is that a kind of transformation matrix right. DR is this innocent transformation matrix you do not bother about what the basis. You just use some basic as you like and you got the DR you know nothing more right. D prime R it is less innocent because D prime R is obtained by similarity transformation of DR right. Of course anybody can call my bluff at this point and say that DR is also; it is also possible to get DR by a similarity transformation of D prime R that is right.

What we are saying yes you start with DR perform a similarity transformation and get D prime R and if you notice you performing the similarity transformation particular unitary matrix. Which matrix is that? It is the matrix of the eigenvalues of H eigenvectors not eigenvalues sorry it is the matrix of the eigenvectors of the H matrix ok. What is H matrix? This is how you get H matrix everything is correlated ok. Please it is important to understand here we are not really taking arbitrary matrices and multiplying left right and centre ok.

You start with DR alright you performer similarity transformation and you are going to get D prime R. On the other hand take all the DR's and the adjoint multiply and sum over all symmetry operations then you generator matrix H. From there you get the matrix of eigenvectors U. D prime R is the similarity transform of the DR using this matrix of eigenvectors ok. So this is a correlation this is not D, D Prime, H are all uncorrelated scattered everything is correlated alright come back to this.

This also please take down you will forget later on D prime R= U inverse DRU ok. So our basic first matrix is DR. Will you believe me if I write this the adjoint of D prime R is the similarity transformation of the adjoint of DR; yes, H; U cannot be a diagonal matrix right Lambda is diagonal matrix. I mean we should not say that cannot be diagonal matrix but in most general case it is not alright. Adjoint of D Prime R is also similar similarities transformation of the adjoint of DR ok so far so good. Now with this, what you do is we can start playing. What do I do? You know what H is? H is sum over R DR DR dagger so what I can do is I can take this definition and substitute there right.

This is what it is, so it might as well expand H in the definition of Lambda ok see where we are going. We are going a long way but the destination is interesting this is what we write. Lambda = sum over R U inverse DR DR dagger U. What can we do next? What should I do next? Replace by what by which equation. Eventually we will do that also but then see this second equation relates DR dagger with D prime R dagger ok. What we can try to do is this we have to get to D prime R of course.

So we need to convert this into a product of similarity transformation. Here you see DR is left multiplied by U inverse DR dagger is right multiplied by U. So you can put in E and E can be obtained in many different ways. So this time we choose to obtain E by writing U and U inverse right, U inverse; this was U and this was U inverse it would have been written as U inverse U no problem ok. When I write that what do I get U inverse DR U U inverse DR dagger U right, first one is a similarity transformation what does it gives me? It gives me D Prime R. Second one is also similarity transformation D Prime R dagger ok nice I can write this.

What I can do is if I sum this up over R then I get Lambda right. Here what we did that is we just wrote the terms and if we summit over then we get Lambda once again ok. What do I do next? Let me see what the diagonal element is to start with? You remember Lambda is a diagonal matrix right. See this is what the diagonal matrix element is going to be. Lambda jj will be once again sum over R sum over j Dij prime R multiplied by Dji prime R dagger is that correct. Let us see what is Lambda 11 what is Lambda 11, D11 prime R multiplied by D 11 prime R dagger + D12 prime R D21 prime R.

D12 prime R right, so the summation is on j the second one D12 prime R multiplied by D21 prime A dagger summation is on j. So, j is the first element here and so on and so forth you sum j = 1 to n, is that, are you all comfortable with this. It is a diagonal element. I do not care about half diagonal element because I know already that diagonal element half diagonal element are all zeros right. I only care about diagonal elements. What are the diagonal elements? Or they are all one then what are they Lambda values the eigenvalues.

So what are the eigenvalues they are real right. Why? Hermitian, are they are all positive? I do not know, maybe or may not be the probability is 50%. Since they do not know anything else ok but then real numbers that much is sure ok, are you all ok with this notation sum over j Dji prime R multiplied by Dji prime R dagger ok with this.