Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology-Bombay

Lecture No. 26
Reducible and Irreducible Representations

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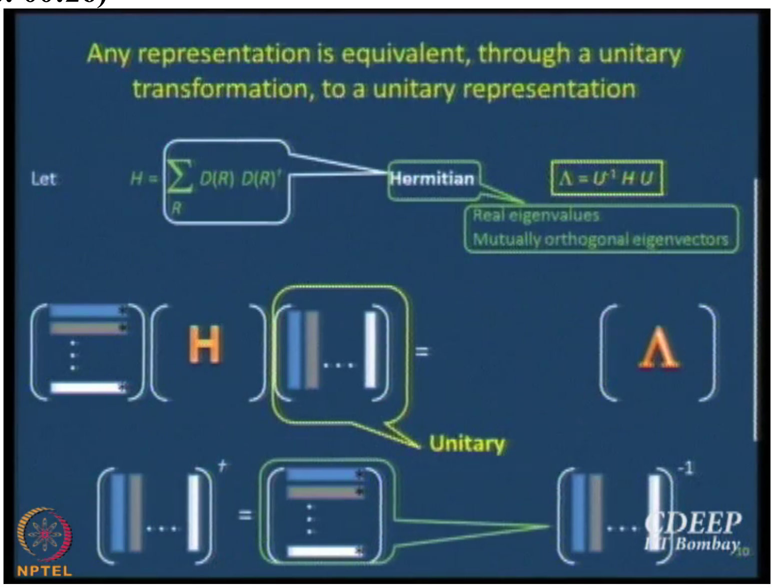

Here goes, so I have mind of made spoil sports and given you the answer to start with. Any representation can be seen to be equivalent to unitary representation through a unitary transformation. I should say through appropriate unitary transformation not just any unitary transformation. And we will see 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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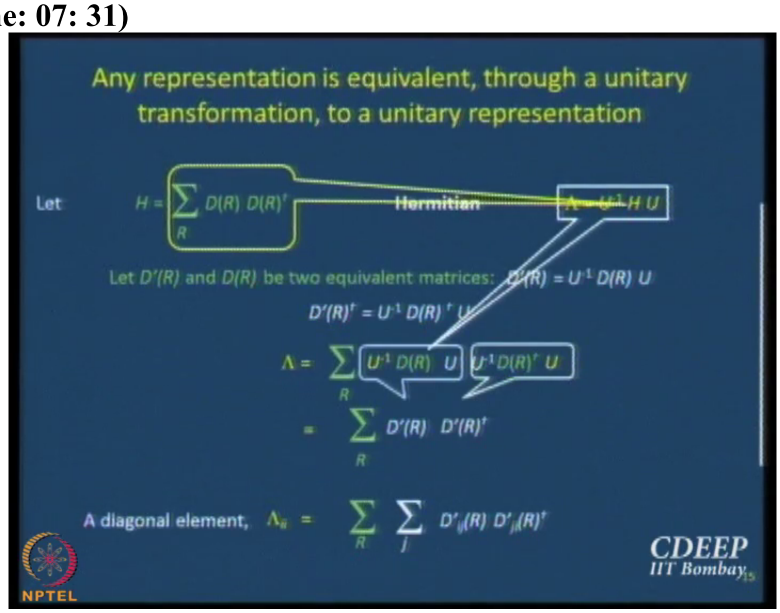

If not Let us clean the little bit this is what we will need H is hermitian matrix what are right this down the thing is at one point we will erase this also it is only so much we can write on the slide but we will need this. But it is very easy to forget what we are saying now in the maze that we get 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. The advantage of is that write this here what is the first elements is Dij prime R second one is Dij prime R star right multiplying complex conjugate.

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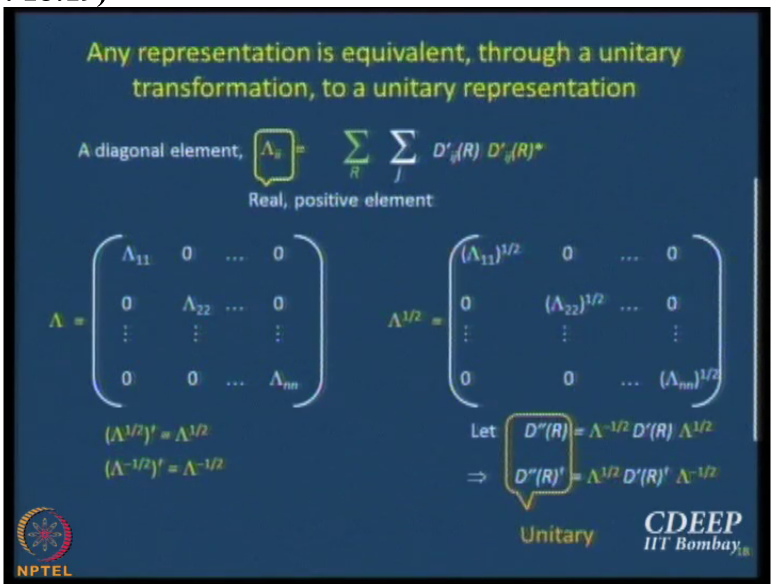

Before multiplying Complex conjugate then what should I get? I would said you should get the Mod value you should get the positive value you cannot get negative value. So the point is Lambda A is real and positive value you are right is just that we are going to prove it, fine. Now what do I do? How does it help? If it is real and positive what are the things that we can do with real and positive number that we cannot do with real and negative numbers. We can happily take square root without having to bother about annoying i coming right that is what we are going to do ok.

This is Lambda this is the Lambda matrix right Lambda 11 Lambda 22 etcetera up to Lambda nn these are the non zero elements and as we have seen these are all positive quantities positive and real quantities all of diagonal elements are zero. See what is this Dji R dagger what is the meaning dagger? I transpose and I take Complex conjugate ok. Now see ijth what is this see jth and ith element of the transpose is the ijth element of the original matrix right that is what I have written.

Instead of; if I write ij then I can lose the transpose sign but I still have to have star it is adjoint not transpose. Dagger means transpose not adjoint. You transport and as well as write the complex conjugate ok. So now what I am doing is that I am kind of transposing back but keeping the complex conjugate and the advantage is that now you are multiplying each number with its own Complex conjugate so you know what the sum is going to be. The song is going to be real positive quantity right ok.

So this is Lambda Now since all this Lambda ii value is real and positive I can happily take square root. Although you might ask why you would you want to take square root in the first place. Two things first is the hint secondly I have the benefit of my insight. What is Lambda to the power half? How will I define Lambda 2 to the power half? Lambda to the power half multiplied by Lambda to the power half = Lambda ok. What is Lambda 2 to the power half? What will be the matrix? What will be the matrix elements?

What is the 11 element of the Lambda to the power half? Lambda 11 to the power half what is the 22 element? Lambda 22 to the power half, it is as simple as that ok. Now that you have written the matrix are you convinced that it is actually Lambda to the power half? Multiply with yourself do not you get Lambda right, no issue with that? What is Lambda to the power minus half? Just changed half to minus half nothing else trivial but it is going to come handy.

Will you agree with me if I say that the adjoint of Lambda to the power half is also Lambda to the power half. It is very obvious that it is a diagonal matrix no issues. Similarly the adjoint Lambda to the power minus half is Lambda to the power minus half right. So now let us write it like this let us say D double prime R is Lambda to the power minus half D prime R Lambda to the power half do you agree with this same thing holds for the adjoins right. Somehow we are going to prove that these matrices double prime matrices are unitary. That is the final rule.
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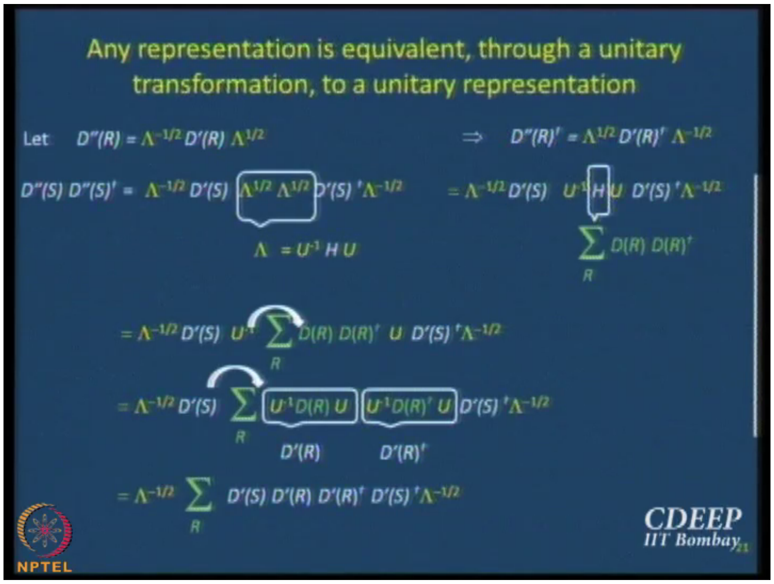

Let workout this now so see R is the general operation let us focus on one operation, yes. What is D Prime D double Prime S dagger D double Prime S adjoints what is that? Lambda to the power half D prime R Lambda to the power half then Lambda to the power half D prime S dagger is correct. We will go back to the earlier one, Lambda to the power minus half. Earlier one does not matter right. Because when you do that manipulation instead of writing U U inverse we have to write U inverse U and I think that work out, let us see.

But let us finish this first ok this is fine. What is the next step? What is the next up here? Yes what is Lambda? U inverse HU right, so I can write it like this Lambda to the power minus half D prime S U inverse HU then adjoint of D Prime S Lambda to the power minus half. What do we do next? What can I do next? H, what is H? Sum over R DR DR dagger we put that in and this is what we get Lambda to the power minus half D prime S U inverse sum over R DR DR dagger U D prime S dagger Lambda to the power minus half.

What do we do next? Without losing any generality can bring in U inverse inside right because what am summing over? We are summing over all R. Is U define is U different for every R? No, where did you get U from? What is U? It is a matrix of the eigenvectors of H. How did you get H? What is your H? Sum over R DR DR dagger write it does not matter what symmetry operation you are working with ok is the same. Bring you inverse inside this is what I get what do I do now?

What is U inverse DR U that is D D prime R and this is D prime R dagger what we have said right and that is the contradiction ok alright. I will have to work on this let us go ahead with this fine. So again let us bring the prime S in and this is what we get Lambda to the power minus half sum over R D prime S is D prime R D prime R dagger D prime S dagger Lambda to the power minus half what do I do next.

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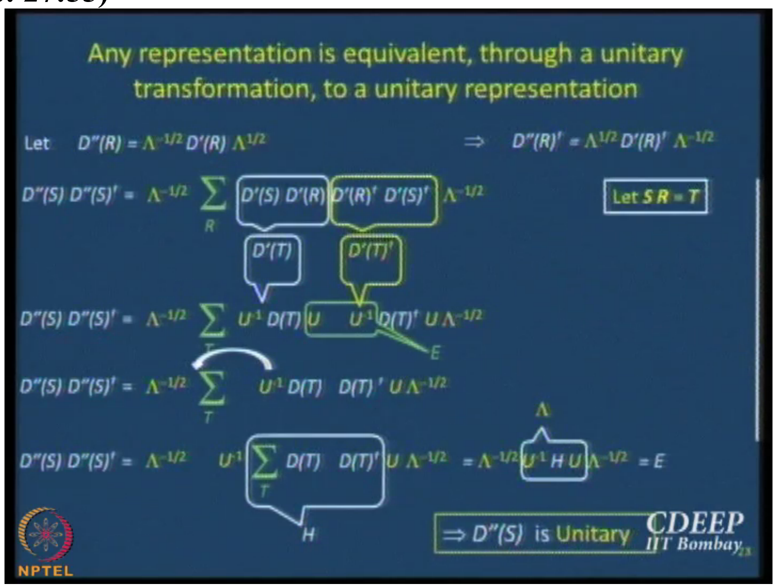

This is what it is, what do I do next? Yes after all you are talking about the product right D prime S multiplied by D prime R D prime R multiplied by D dagger D prime S dagger what is R and what is S they are symmetry operations. S particular symmetry operation R is a general notation. So, we can have different symmetry operations substituting for R right. So let us say SR =T is T a variable or a constant? T is a variable because R is a variable. So if SR = T then this is going to be D Prime T and this is going to be D Prime T adjoint.

What is D Prime T? U inverse DT U as you have defined it right. This is U inverse adjoint DT U as you have defined it. So this is what D prime D double Prime S D double Prime S dagger is what do I do now? Earlier I am putting U inverse now you can eliminate right this is what you get what do I do next. I can bring U inverse outside it is a kind of going in a reverse direction right. This is what we have D double Prime S D double Prime S adjoint = Lambda to the power minus half U inverse sum over T DT DT dagger U Lambda to the power minus half.

What is this? This is H right. Why it is H? H is sum over R what do I have Lambda 2 to the power minus half U inverse HU Lambda 2 to the power minus half. What is this? What is Lambda 2 the power minus half Lambda Lambda 2 the power minus half E, so D Prime is unitary because D double prime is multiplied by its own adjoint gives you E right.

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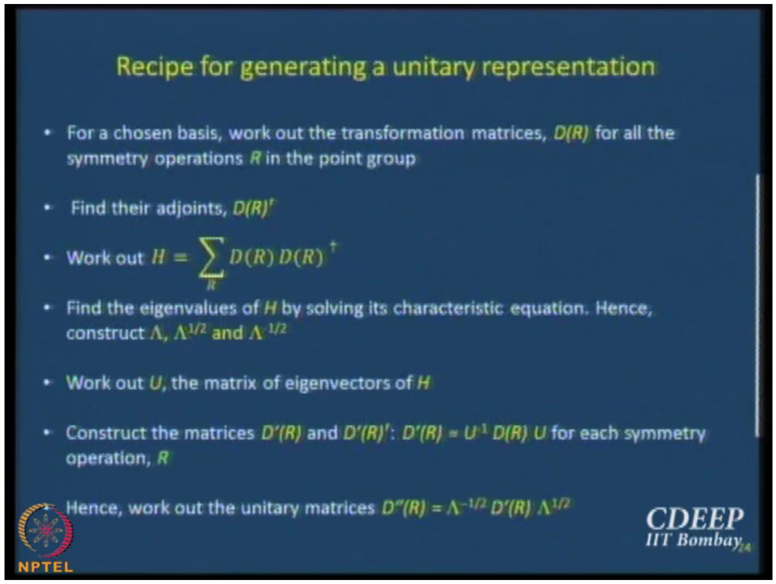

Of course and which what you want to know what we really want to know after all this is that how do generator unit representation what is the recipe? That is something going to come handy. So the recipe is this; choose whatever basis you want to work with and for that basis you work out the transformation matrices for all the symmetry operations in the point group. They are going to be DR right. Then you find adjoint for every matrix that is DR dagger, next workout the hermitian matrix sum over R DR DR dagger.

Next is what you need to do if we need to work out the eigenvalues first right you have done this earlier with the example of a matrix. You work out the eigenvalue first. How you workout the eigenvalues? By solving the characteristic equation, what is the characteristic equation? Yes, that is equal to zero. So when you solve that get all the values of Lambda, I mean you get Lambda 11 Lambda 22 so on and so forth. You construct matrix Lambda if you know what is Lambda you can construct Lambda to the power half Lambda to the power minus half.

Next you can work out U, which is the matrix of eigenvectors. Once again this is something that we did few weeks earlier. Not for hermitian matrix maybe for some other matrix. And then once you got U you can work out D prime R matrices by performing the similarity transformation. And finally since you know land already you work out the unitary matrices by performing the second similarity transformation on the D prime R. So now irrespective of what basis I started with I can convert all the matrices to unitary matrix and thereby generate unitary representation ok. That is something you should able to do.