Symmetry and Group Theory
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Lecture No. 24
Equivalent Representations

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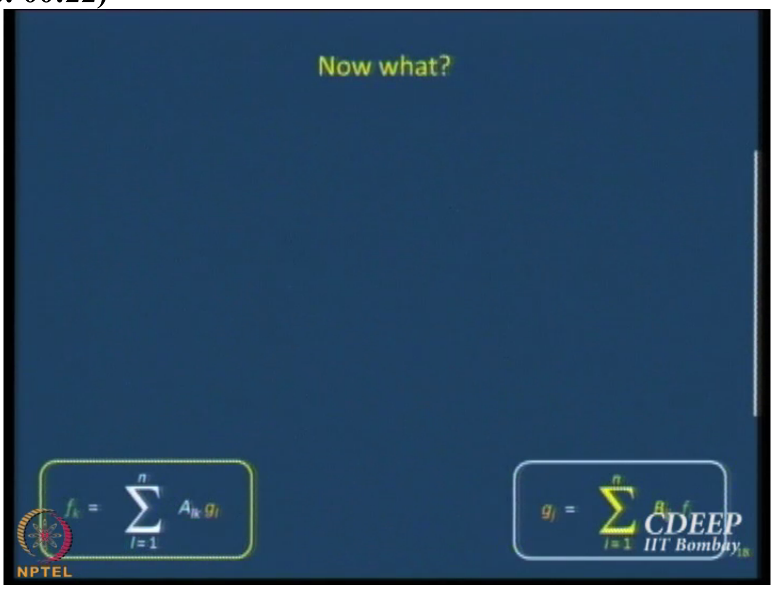

How we can switch basis let us see. So, what do you do now? So I come up to now what do you do now? See we have done whatever we could do with functions. Now it makes sense after all what are we trying to do, switch basis and then what? You want to switch bases and go from one set of transformation matrices to another set of transformation matrices that is what we want to do. So it makes sense that we invoke our old friend the transformation operator.

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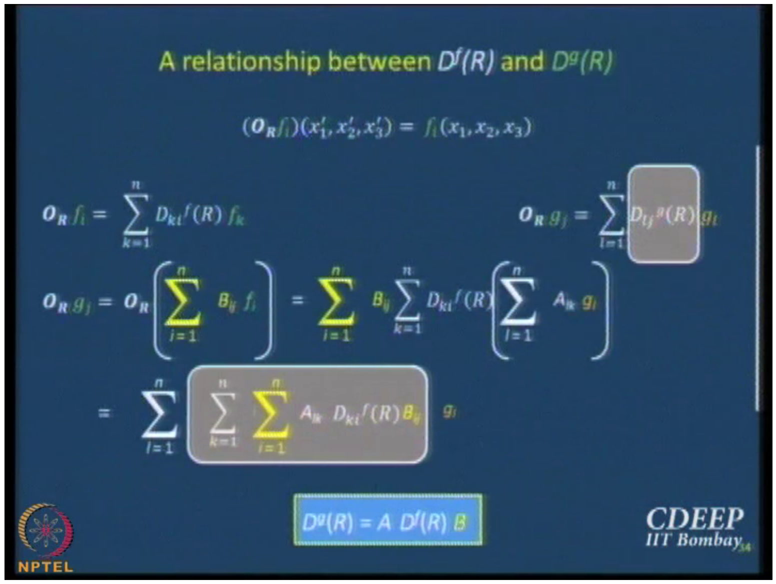

You remember transformation operator ORfi= ORfi x1 dash x2 dash x3 dash = fi x1 x2 x3 but that is not what is going to be useful for us at the moment. What is going to be useful is the relationship between OR and the transformation matrix. What is the relationship between OR and transformation matrix elements? That is something that you need to remember ORfi = k = 1 to n Dki superscript f of R fk for now neglect the superscript f. If I do not write the superscript have does that ring the bell.

Have you encountered expressions like this earlier ORfi = sum over k = 1 to n Dki R fk, that is what we are saying little while ago is it not, sum over k Dki means once again we are going down. Why are we going down? Because of D of R, what is D of R? Is the transformation matrix corresponding to the symmetry operation R, the D of R has been worked out using the coordinates and now what we are doing is transformation of basis that is why we are taken transpose. This is something that you know. Why we have written f here.

To denote that this transformation matrix that we are talking about is associated with the functions f, f functions not with g functions. Right now we are dealing with f functions and g functions right. So you have to label the transformation matrices as well. Matrices are actually going to depend on which basis you are work with you must label them f or g ok. Similarly I can write the expression for transformation matrix that work on the g functions.
That will be ORgj = sum over l = 1 to n Dlj then superscript g of R gl make sense. It is very important that you must write the super script f and g here. Because all we have are trying to do at this moment is that we are trying to see how you can transform Dl the DgR's to DfR's or vice

versa. When I say switching off basis what I mean? When I change the base from f to g then the matrices should also change from DfR to DgR for the same R. How to do that that is the whole purpose of this exercise.

To simplify this problem I can simply not simply I can substitute gj in ORgj by the expression that we know right. If I do that what will be the left hand side become OR this is what will become, we are working only with the left hand side not the right hand side. We will come back to the right hand side later. We are expert in simplification like this right. We are now working only with left hand side it becomes OR operating on sum over i from i = 1 to n Dij fi. How can I simplify this expression?

Summation can come out, why can the summation come out? Put it in a different way; it is linear, OR is a linear operator right. So it operates on something some number multiplied by a function then the result is the number multiplied by OR operating on the function this is what it is. OR is a linear operator so we can write it as sum over i = 1 to n Dij OR fi are you ok fine. What is your definition of a linear function? What did you write that if g = a into f, g is f is functions, a is scalar quantity.

Then ORg that is OR operating on a into f = a multiplied by ORf alright, can I write this and it is linear fine, are you all ok. What will be the next step? ORfi do you have ORfi somewhere else right I can substitute this. If I put it in what do I get sum over i = 1 to n Dij then sum over k = 1 to n Dki of R fk put it alright what more I can do. We know the expression of fk it is there somewhere on the slide, this. I can substitute for fk, I can write sum over l A1k gl, done ok. I have a little scary looking think but it is not all the difficult.

After all see what is there Bij Dki Alk these are all numbers is it not. What is the only function that is there in some words scary expression gl right? This is what it should be right sum over l = 1 to n something multiplied by gl ok and see there is a same functional form like right hand side this is almost there is it not. We are simplifying the left hand side we are getting something that is at the same form at the right hand side. What is there inside the bracket whatever summation does not matter right?

Where do we have to summations over i? L, one is l and other is i, I can did it from where maybe from a distance but it will be blurred. We cannot sum twice over i, see is the spelling mistake something like that. Here there is i and l ok. Now you see what is equal to what? Now if I compare the right hand side this expression is equal to this expression, E, I was wondering that why mike is frowning, all right now? No, that is what it between, that i is the spelling mistake yes.

I could not see that because I write down too light, please neglect that i that is not right. Now see what is this? This Alk Dki Bij, and what is there on the other side Dlj remember to do the matrix multiplication right. These coefficients seem to be cutting of cancelling each other. So this is a case when Dlj = Alk Dki Dij then what does it mean? That means this D is the product sorry Dg is the product of A Df and B. So I now go from matrix element to matrices.

Is it not the rule of multiplication of matrices? So I can write this oops I do not need them anymore. This is not too bright I hope Dg of R = A Df of RB, so see already you got a relationship between transformation matrices corresponding to the same symmetry operation R, but for two different basis one the f function and the other is g function right. When will this hold then can we do this, when we can express f is the linear combination of g the other way around.

Is that always the case for linear independent operators? Linearly independent operators you should be able to do that ok. Now but let us finish this story first there is no point in keeping B as B because you know very well that B is A inverse, remember. Now I see the smiles because the moment I replaced by A inverse then I have something nice. I have something familiar that is the similarity transformation.

Now see what similarity transformation does? The similarity transformation essentially switches the basis that is so important, it is not just some idle exercise you are doing. Similarity transformation takes you from one set of a linearly independent vector the base to another set of linearly independent vectors base right. That is the power of similarity transformation ok that is what transformation usually do. Have you heard of some other celebrated transformation?

What is the transformation that everybody has heard about, every chemist had heard about. No matter you know the meaning or not Fourier transformation right. Nobody has iR any more fti or ftR any more right. What is Fourier transformation? What does the Fourier transformation do? It will take you from time to frequency domain and vice versa. Please note the domain, you it takes it from time domain to frequency domain. Here also we are going from g domain to f domain are the other way around ok. That is what the similarity transformation does it switches the basis.

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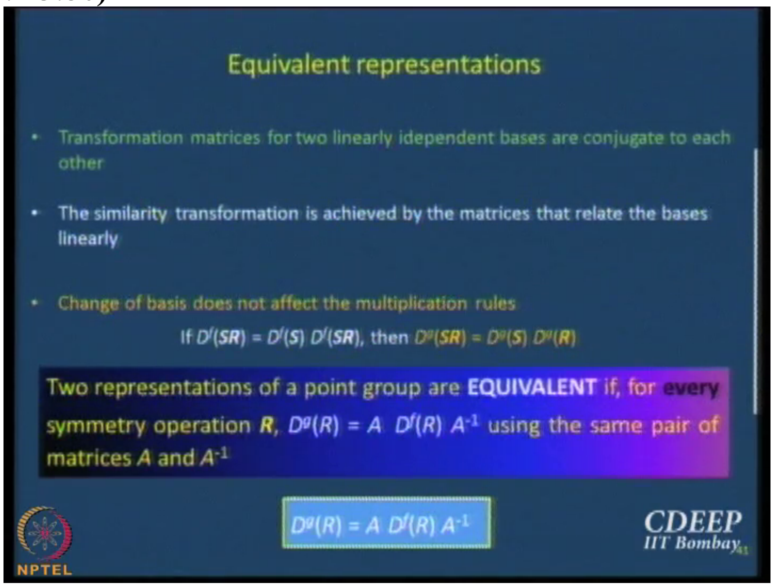

So now we conclude this part of the story. I hope you all understood the transformation matrices for two linearly independent basis are conjugate to each other you just seen that Dg and Df are conjugate to each other not for any R both are to be for the same symmetry operation. You cannot have C3 on one side and Sigma V on other side. Secondly, we cannot just use any matrix right. You take any matrix under the sun and perform the similarity transformation you go from one base to another you would not.

What is the matrix that you have to use? What is the matter that we have used? We used A and B, what are A and B? They are the matrices they relate the base linearly, the conjugate actually but that something that leave it right now, right. Third is and this something that I like you to do yourself. Change of basis would not affect the multiplication rule this is what I mean this sum is very simple I think you can work it out. Can you work it out yourself not here later? It is very simple.

So now we conclude what we have done all the exercise that we have arrived at this very important concept of equivalent representation. But the take home message from this part which is going to be pretty much the part for today is the two representation of the point group are equivalent if next; what is very important if and each and every symmetry operation R. You can write a similarity transformation using the same pair of matrices A and A inverse. And you already know a and a inverse or not sum of arbitrary matrices.

These are the matrix that, correlate f functions and g functions ok so far so good. What we learnt so far? We learnt concept of equivalent representation. So this is very important equivalent when you take one side of transformation matrices and then you perform similarity transformation using the same pair of A matrices. So think of C3v what are the matrices De D3 D sigma C3 square D Sigma V1, D Sigma V2, D Sigma V3and what do the similarity transformation of each of these matrices using the same A and A inverse ok.

Then what you get if you get is another set of matrices. The representation that you generate that is equal to the representation that you started with alright this is the definition of equivalent representation.

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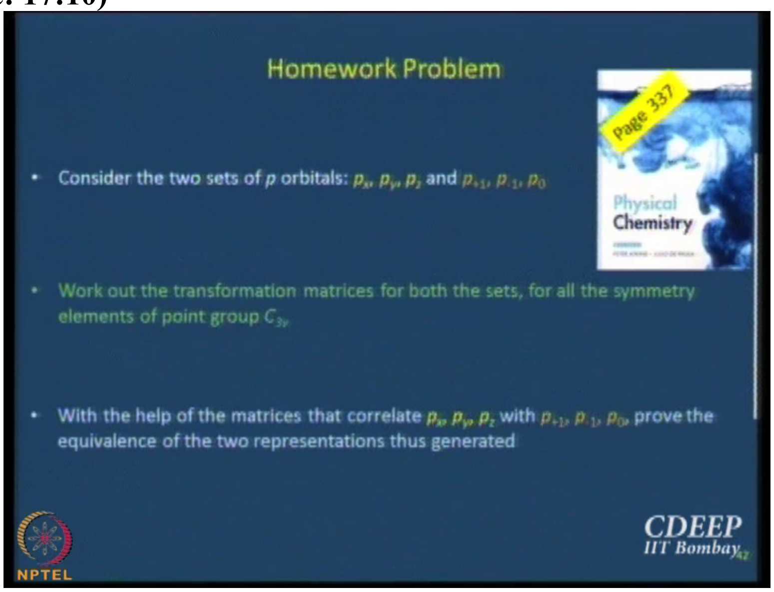

I want to give a home work problem I love to do it myself in case you are running so much behind schedule. Please work this out my request is work it out this evening, you are talking about lot of abstract terms right we are chemist we are not mathematician. So we only believe thing that we can work it out or something more tangible right. This is the problem consider two sets of P orbital's Px Py Pz and P+1 P-1 P0 ok. How they are related it is given in Atkinson physical chemistry book.

Not exactly the page 337 in the book but we have to start from one or two pages earlier 337 is the final page ok. You see how they are related. Now what I like to do is, workout the transformation matrices for both the set for all the symmetry elements point group C3v. So how many matrices do you generate? E C3 C3 square, E is very easy so I would not even count E. C3 C3 square Sigma V1 Sigma V2 Sigma V3, 5 into 2 is 10 plus the two bonus matrices E ok.

Then what will be the next step, in the first step what we have done. Next step is this with the help of the matrices which correlates Px Py Pz with P+1 P-1 P0, prove the equivalent two representations that is generated.