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

Lecture No.12 Classes, Similarity Transformations

So see you have already seen that we have to work with matrices lot of them when we talk about symmetry operations and at the risk of boring you by saying the same thing again and again the reason why we need matrices is that we want to translate what we see geometry into the language of algebra. Why do you need to translate into algebra to the language of algebra so that we can divide something which can be used like a black box eventually that is the goal right.

Now what we are doing is we are building a black box of course when you build it a black box it is not black we know very well what is in there because we are putting everything inside the box. Once it is done the idea is we do not; we can forget about everything and use it like a machine but to go there we have to digitise everything we have to put numbers and expressions for everything that is why we need matrixes.

And since we are going to use matrices in such a great extent it is imperative that is we know all about matrices that is the purpose of today's class on the next class the name is actually very accurate today is only get know our matrices what they do is going to come later on so that is what we do we just get familiar ourselves with some kind of matrices perhaps you already right. **(Refer Slide Time: 01:50)**



Even before that do not forget that we have some unfinished agenda from the previous class right. What is the unfinished agenda we just about started talking about similarity transformations and class ok. I might just go ahead and finish this discussion, whenever we finished the discussion like to bring in an example from the chemistry let us see whether we can do that as well so numbers just do not remind lifeless numbers but take some tangible form right. (Refer Slide Time: 02:29)

Similarity Transformation	
$B = \mathcal{H}^{1} \mathcal{A} \mathcal{X}$	
A, $B_{x} \times A$ are elements of the group.	
A, B are CONJUGATES	
Class	
A complete set of elements that are conjugate to es	ach other
(*)	

This is where we have stopped in the last class right with the correction typo in the last one here that is done. The similarity transformation is defined as E = X inverse AX and the condition is that ABX all of them to be elements of the group. So, if A and B are related in that way when you take A and then multiply it on the left side and right side with X and X inverse then you get B and then you say that A and B are similarity transformed at each other. And the other word is often used is conjugate A and B are conjugate of each other and they are related to thing called class because the class is defined as complete set of elements that are conjugate to each other alright this is something we have presented in the in the previous class right. (Refer Slide Time: 03:28)

Every element is a co $A = \Re^2 A$	njugate to itself
Left multiplying the LHS by A ⁻¹ ,	
$A^1A = A^1 X^1 A X$	$A^{\perp}X^{\perp}XA = E$
$= (\lambda A)^{\perp} (A \times)$	$\Rightarrow A^{\perp}X^{\perp} = (X A)^{\perp}$
But LHS = \mathcal{E} .: RHS = \mathcal{E} for LHS = RHS	
⇒ Either X = E	
or X commutes with A	

So, since we are talking about similarity transformation conjugates let us learn about couple of properties of conjugates. The first theorem is every element is conjugate to itself, A= X inverse AX and the question is what is X? Can X be anything any element in the group or is there any restriction on X let us see. So, whenever we have something like this, what we like to do is left multiply right multiply and simplify.

So, let us start with the left hand side and let us multiply it by A inverse why we want left multiply it by A inverse then it becomes E right it is always better to work with one things that is much simpler. So, if left multiply by A inverse what you will get A inverse A = A inverse X inverse AX right. Now what do we do now you need to work with the RHS A inverse X inverse AX, A is there X is there and their inverse is also there.

So, A inverse X inverse is inverse of X or not, let us see. Will you agree with me when I say A inverse X inverse is the inverse of XA right. It is very simple right X inverse X G then EA is A inverse E is A easy very simple. So, it is not very difficult to see A inverse X inverse is the inverse of XA, XA not AX alright. Let us take that and calculate that in right hand side to get XA inverse multiplied by AX. And hope you are not forgotten what is left hand side is, left hand side is E, so the left hand side is E and then right inside also as the E if this has to be correct right.

When is your right hand going to be E when XA is inverse of AX when will be XA inverse of AX, when A and X commute right is it necessary that you will have a element in the group which will commute with A for any group for any A, it is necessary that there will be one element in the

group that will commute with A, identity has to commute right nothing else X can be equal to E right.

And then if anything else then you remove the barrier, it does not matter but the point is that even if there is no other element E serve the purpose. E inverse AE = A is that correct what is the inverse of E, E itself, EAE what is that that is still A right and as you are said that identity is essential property essential condition for formation of group so E as to be there you cannot do without E alright. So, every element is conjugate itself now let me have done the proof it sounds kind of silly, trivial right but when you started sating is perhaps you did not, fine. (Refer Slide Time: 07:14)



The next one is somewhat the 0th law of thermodynamics, if A is conjugate to B and C then B and C are conjugate with each other. If I just write down this line in a mathematical form is going to be A = X inverse BX and A = let us say Y inverse CY where X and Y may say they are different I do not know it ok. Same is this special case of different, so it is better to start with different fine. So, now will you agree with me if I write B= AX inverse what I have done I have left multiplied by X and right multiplied by X inverse right.

Left multiplied by X, XX inverse becomes E right multiplied by X inverse X X inverse becomes E, so I am left with B and here it becomes X inverse AX A inverse all right. Now what will I do I can plug in this value of A into this right A = Y inverse CY right what I am trying to find? I am trying to find the relationship between B and C ok. So, it makes sense to eliminate A from the expression of B and substituted it by C. So, I am doing that what do I get, I get X = XY inverse CY X inverse alright.

Now will you agree with me if I say XY inverse is of YX inverse just multiply XY inverse YX inverse Y inverse Y is easy do not you want to write it let it XX inverse that is also E. So, XY inverse is inverse of YX inverse alright and just for the sake of simplicity I will write Z = YX inverse right. So, what do I have here, what does it become B = Z inverse CZ and therefore what we are stated to start with is proved if A is conjugated to BC and B and C are conjugate with each other right simple. (Refer Slide Time: 09:52)



So now that we know little bit of a conjugate let us talk about class, class as you said earlier is a complete set of elements that are conjugate to each other alright and this is best understood by taking example. So, let us refer to our old friend G62, G6 number 2 and this is a multiplication table shown in the previous class and in what context we discussed G62 subgroups right. So, what are the subgroups here EA EB EC and then ED they form another subgroups and what is this related to what was the chemical example that be used, yeah.

But I did not talk about G6, did I ok fine. We will do it today right now let us see find the complete set of elements which are conjugate to each other what will I do, the only thing I can do this group force I Take every element work it out right. Since it has lot of work I will not I will do it you will do it, I will only ask a question you will be giving me the answer. Here goes the first question, what is E inverse AE? Stupid question we know already what is the answer A very good. Next one A inverse AA that is also easy A inverse A is E so its needs lot of work maybe it is not A.

But then it is not also the as easy as you might seem so far, it is a very common strategy of marketing right show the good points first and then attack people and then make them do things that people might may not want to do. So, let us do this B inverse AB this out workout, what is B inverse? B inverse is D, BD then it is easy and then what is AB or BA, AB will be what AB that is F and B inverse is BFC. So, now comes the first, useful information something that you did not know right that A and C are conjugate to each other ok A and C will belong to a class.

Next C inverse yeah they belong to a class let us just skip it there then we will see of course since it is a similarity transformation some similarity as to be there what will see what that means C inverse AC further doubt B ok good. Next is D inverse AD you see that what we are doing you have taken A then we are using all other elements right to similarity transformation and see what we get D inverse AD rapid fire does not work finally F inverse AF, C, so what does it mean ABC form a class will you agree with me.

ABC are conjugate to each other and they form a class do you agree with that that ABC are conjugate to each other but here I have shown that A and C are conjugates and A or B conjugates how do you know that B and C are conjugate just now you have proved, do not forget column first row second in a product column first row second you have any confusion I had the confusion long time even now I get confused time to time so you are in good company.

I think it is G62 we did not discuss G61 we did not work out G6, we have I just taken it from Carton's book alright so using the theorem that we know already that if A and B are conjugate and A and C are conjugate and B and C also have to be conjugate we see that here AB and C form a class of order 3 alright. Now what is left D and F do not think that D and F must necessarily form a class they might be classes of their own we never know right let us see.

E inverse DE is D, A inverse DA what is that A inverse DA, F, so D and F are conjugate to each other and I think you can guess the remaining part of the answer no matter what you do if start with D you will get either D or F, B inverse DB is F what is the C inverse DC, what is the D inverse DD that is very simple yeah D ok, F inverse DF, D alright G inverse DG there is no G. So, there is no point in talking about G inverse G so, what does it mean that means that D and F form a class of order 2 right.

Questions yeah ask E is a class of its own because we can prove X inverse EX what will that be EX is X then you have X inverse, X inverse X is E. So, no matter what you use A B C D X Y Z P Q R S, E will always transform into E. So, E is a class of its own, column first row second top first side second in the product right. And see now look at the numbers what is the order of the group? Order of the group 6 and what are the order of the classes? 3 and 2, 3 into 2 = 6 all this is almost becoming numerology right.

Orders of classes are integral classes of order of the group pretty much like the order of the subgroup we have to prove it in the same way alright. But now the question is what is this ABCD does it make any sense. Let us see whether it make any sense can you think of some point group which could be G6. G6 means how many symmetry operations 6 including E have you discussed any molecule any point group that has 6 symmetry operations C3v right and C3v happens to be belongs to G6.

So here you see what are the operation that belongs to the class can you now substitute in this multiplication table and convince yourself that C3 multiplication table in did like G62 instead of ABC you can write Sigma vA Sigma vB Sigma vC instead of D and F you can write C3 and C3 square of course I am dictating this order because of I know the answer ok. If you do that at least take some elements ok what do you say? You said that DU C3 and C is one of the planes let us make it even simpler.

D is C3 and F is C3 square right what is the product D and F, E let us see D and F is E, F and D is E, ok that is why I said that now what about this three EAB, A what is the inverse of A? A, what is the inverse of B? B what is the inverse of C? C. Now think of reflection plane what is the inverse of a reflection operation? Reflection in the opposite direction basically they are same. So, that is why it falls in place. So, we have 3 deflection kind of operation here and 2 operations are like rotation C3 and C3 square ok.

Work out the multiplication table of ammonia C3v you see you will get the exactly the same answer all right. Now see now what are you saying you are saying that ABC form class of order 3 what is ABC? What did you say 3 planes right ABC the 3 Sigma's belong to a class and C3 and C3 square belong to a class. I think have mentioned class of symmetry operation in one of our previous classes I say in class too many times on the previous sessions days whatever. So, this is what is the meaning of class even the symmetry operations.

So, what does it mean, It means that if you take the reflection operation of any plane and perform a similarity transformation what should you get, let us say what are the elements A B C right if you take A and perform similarity transformation using the other planes or using C3 or C3 square operation or using identity what should you get? What would you get itself, no remember so see when you use E to perform the similarity transformation you get A when you use A itself that also you get A ok.

When you get used anything else do not forget ABC are the planes right D and F are the rotations even when you use rotation you get some plane alright even when use the rotation to perform the similarity transformation you start with the plane you get a plane or you get a different plane yes with rotation. And same is true for other rotations do not forget ABC are the planes even if you use the planes to perform the similarity transformation you do get some rotation only nothing else alright. This then is the chemistry example right.

So, A B C 3 planes belong to 1 class D and F belongs to another class ok. Earlier we have defined classes in little different manner, what did we say what are the definition of classes that we used earlier classes of symmetry operations, when the symmetry operation belongs to the same class yeah that is now, whatever earlier also we said something right. When we are talking only about symmetry innocent if the knowledge of all these numbers, how did you define symmetry operations in the same class equivalent symmetry operations, same character will come but same character something that we have demonstrated already right but even easier example.

When you apply another symmetry operation then this symmetry operation gets converted to another symmetry operation of same class right. What is the when you apply C3 A becomes B and B becomes C and C becomes A and ABC are the 3 planes. Similarly when you apply one of the planes then C3 will become C3 square right. So, this then is the 3 different ways in which you can think of a class of symmetry operations.

First is do they interchange upon some other symmetry operations very simplest. Second is when you look at the matrices and look at the character of the matrices do they have a same character then of course something that we are proved only that we have demonstrated not proved right yeah only demonstrated using only one example that the operations belonging to the same class at the same character.

And now we learn the most formal most formal group theoretical definition that symmetry operations or anything belong to the same class when they are similarity of transformation of each other of course this definition is not restricted to symmetry operations alone it is true for everything. If you have a set of numbers in which you can do symmetry operation I mean similarity transformations like this they belong to the same class alright fine.