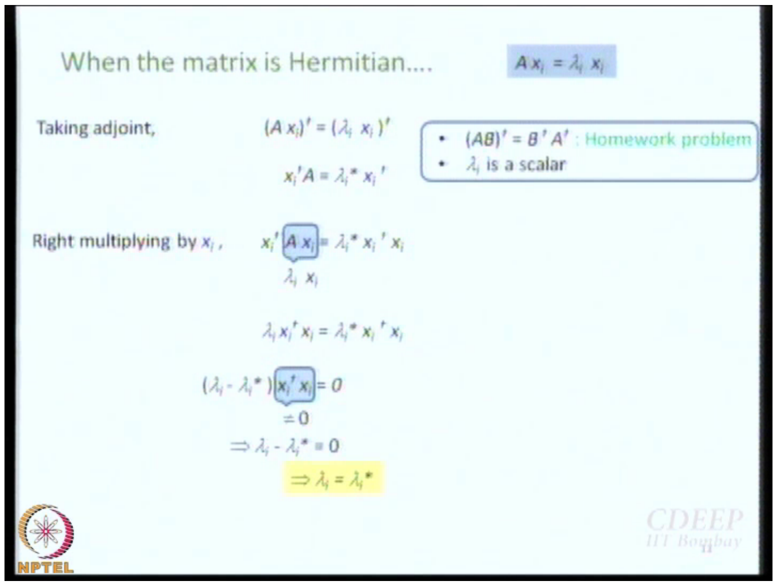
Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology-Bombay

Lecture No. 17
Similarity Transformation

(Refer Slide Time: 00:20)



Now let us repeat something that we discussed briefly but other aspects that we are going to bring up today. What happens when you have a matrix that is hermitian now I think you have understand the equation what is the meaning of i right. What is the definition of hermitian matrix? A = A dagger or A = A transpose A or A dagger equal to; A = A dagger. And what happens when A inverse = A dagger. It is unitary there is no reason to be scared. It is unitary fine.

Now what we have said is that you take the adjoint of the two side then you have dagger of Axi = dagger of Lambda Axi very simple. It is just put in a pair of brackets and in both sides and put in a dagger ok. And then the thing is you should work it out yourself that the dagger of AB = B dagger into A dagger not very difficult to work out leave that as homework problem. And do not forget now I think there no confusion Lambda A is scalar quantity right. So if that is the case will you agree with me the first equation yeah rather second equation goes on to become xi dagger A = Lambda i star xi dagger xi dagger right.

People are like me are going to be like Lambda i star right because he got an eigenvalue that is imaginary, complex ok. But then his neighbour is not going to worry about a dagger about star rather because they eigenvalue we got real Eigenvalue ok of course you know that star is going to go at the end. Now what do you do now it is that you write multiply by xi ok. Multiplying by xi this is what you get xi dagger Axi = Lambda A star xi dagger xi why do you right multiply by xi. Why not left multiply?

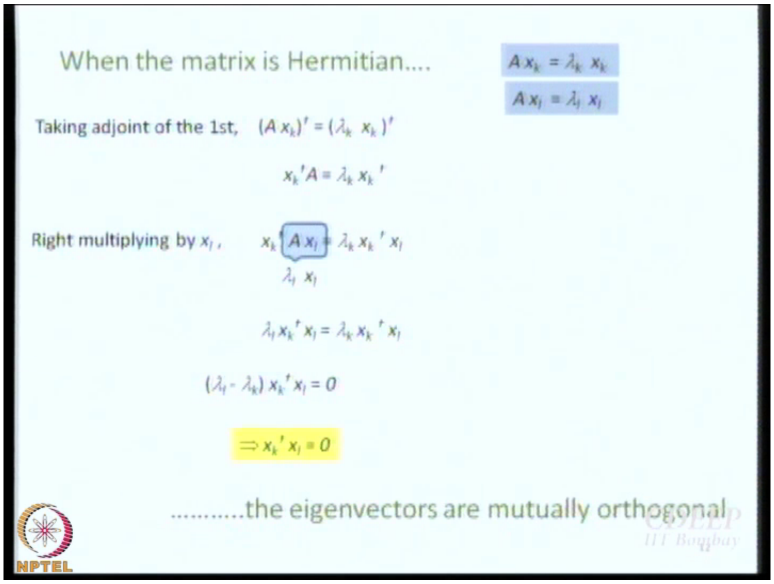
If I left multiply then I end up with not much. If I right multiply the good thing is it Axi is there and you know what Axi is. Axi is Lambda I Ax i ok so you can simplify little bit and I can write xi dagger Lambda Axi. And I can rearrange it write Lambda i xi dagger xi. Lambda is a scalar Lambda i xi dagger xi = Lambda i star xi dagger xi right. What is the next step make one of the sides 0 right Lambda i - Lambda star = Lambda i - Lambda i start multiplied by xi dagger xi =0.

Now what is xi? Might sound like a foolish question at this point I do not want to wants to lose track what is xi? It is the ith eigenvector. Now if I take the adjoin of a eigenvector and multiply the original eigenvector what should I get? You work it out yourself what I am saying is that you are x1 x2 x3 so on and so forth. And since i is common I am not writing second i do you want to use it you can use it does not a issue. So I got a column x1 x2 x3 x4 etcetera right. If I take xi dagger and multiply it by xi what should I get is summation of square what kind of square? Square of user spectrum it is summation of square terms exactly or you want to modify the little bit.

xi star x1 star x1 + x2 star x2 + x3 star x3+ and so on and so forth what should that be equal to? That should be = 1, right. It has to be normalised better not to be normal but if you want normalise to a value of rather than one I have no issues write that happens many times. But you better not normalise to 0, to some; that is not a good idea rather you let us not do that. So the thing is whatever it is it is definitely not zero right.

If it is not 0 what does it mean Lambda i - Lambda star has to be equal to 0 or in other words Lambda i = Lambda i star right. Ho man and otherwise it becomes predictable he stole my line the eigenvalues are real ok. This is something that we encounter everywhere right and we use even mechanically if we have hermitian operator then you are going to get real eigenvalues and this is how it comes from mathematics algebra.

(Refer Slide Time: 06:21)



But we have not done with the hermitian matrices yet today. Now let us have some more fun we have said that these x values they are normalised right. Of this answer of this eigenvectors are orthogonal are these eigenvectors are orthogonal or not let us see. Of course the default answer keeping eyes closed is yes, you study in physical chemistry certain times yes in some case what is going on. Yours is not physical chemistry with whom we are discussing some problem in some context once and we have the sound dynamics problem you find delta H.

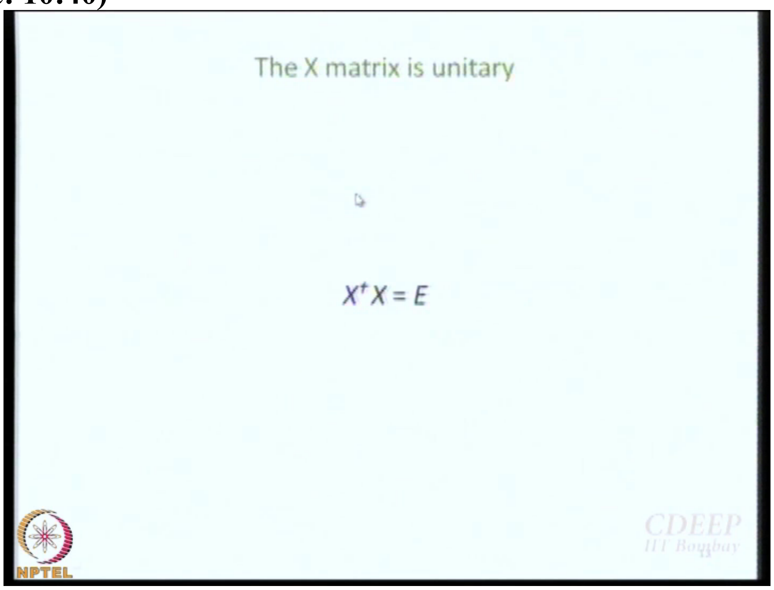
And this gentleman said if I were to write the answer I would have just written 0. (FL: 07:16) and as a locked the answer would have been only 0 so it is like that yeah. They are going to be orthogonal so let us see how it comes. So we will start with two if I want to talk about orthogonal orthogonality then I cannot work only with one I should take two vectors right. So let us say k and l xk and xl Axk = Lambda kxk and Axl = Lambda l xl right. Take this 2 and proceed more or less in the same manner as the previous derivation ok.

Well animation gone wrong what to do what; but just I take the first one and take the adjoint this is what you get, really that is what you get xk dagger A = Lambda k xk dagger. I have not written star why not because I have benefit of Einstein because we have proved that hermitian matrix are going to have a real eigenvalues. So I have saved some ink by not writing star ok. Now what do I do? What did I do in the previous derivation I right multiply write this time also I will right multiply not by xk but by Axl that is right.

So I get xk dagger Axl = Lambda k xk dagger xl right. Once again you know very well what is Axl and we are using different substitute xl it sounds funny alright xl = Lambda Axl is it not and take that plug it in you get Lambda l xk dagger xl = Lambda k xk dagger xl yeah so transpose you get xl - Lambda l - Lambda k and also Lambda xl, Lambda l - Lambda k multiplied by xk dagger and our favourite xl = 0 alright. So what will be the next step xk dagger into xL is 0 When? When Lambda l and Lambda k are not the same, so if I write xk dagger xl =0.

Will you allow me to write the eigenvectors are mutually orthogonal right? So now we have to prove that eigenvectors are mutually orthogonal also. So that is why they are so useful in application in things the way the functions in quantum chemistry right so far so good even if it is = Lambda k it can be, but then they are not going to be mutually orthogonal they are mutually same vector actually ok it can be

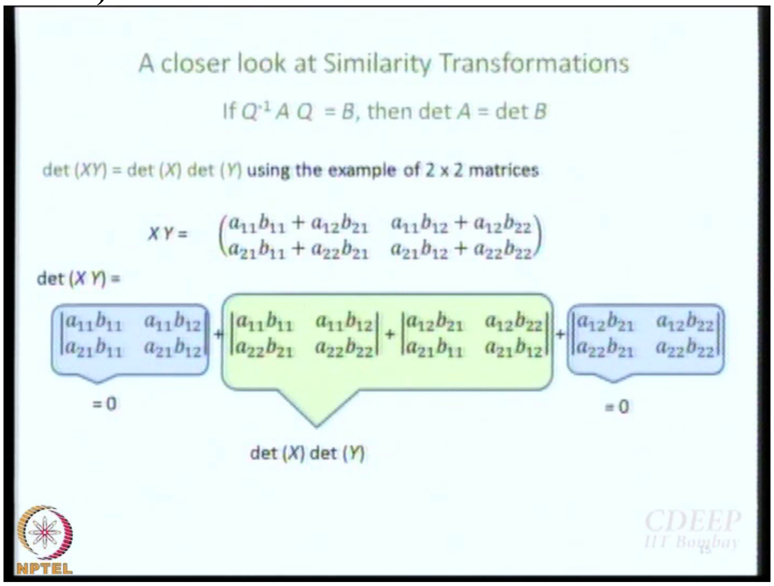
(Refer Slide Time: 10:40)



Now this is something that I will leave it to you, it is not very difficult, you want you to; I want you to figure out convince yourself 0 is not happy at all and then you work it out and then convince yourself that x the big X matrix is unitary. What is x matrix? So this eigenvector1, eigenvector 2, eigenvector 3 so on and so forth that matrix is unitary. How will you do it? You take the adjoint and then multiply the adjoint with the original matrix when you do that you have to keep in mind something, what do you have to keep in mind, this orthonormality condition ok.

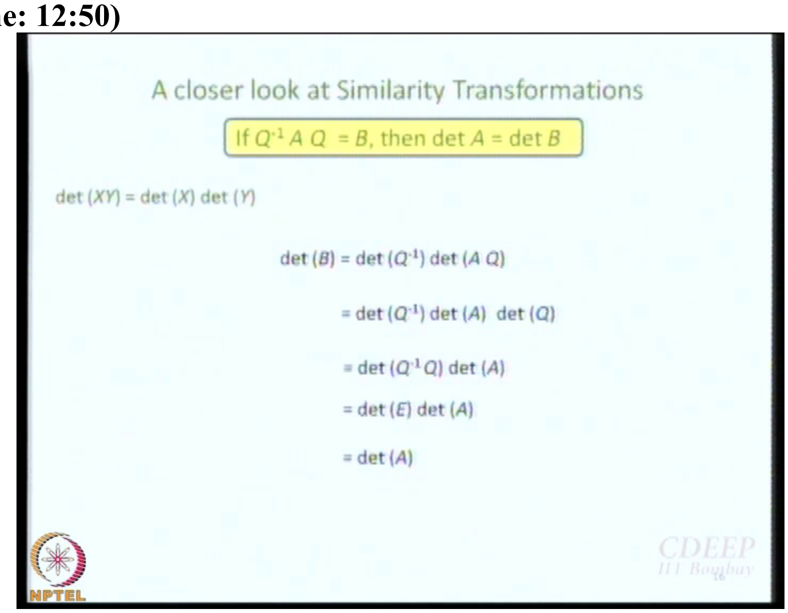
You keep that in mind and see what should be the product to be if it is unitary the product of the adjoint and the matrix itself what should it be if it is unitary, should be a unit Matrix now ok. What is the definition of unitary matrix? It is A inverse is A dagger right. So this is what you have to show X dagger X =E, I will leave it you, to do it, it is not very difficult. Just do not forget the orthonormality then you got a problem ok.

(Refer Slide Time: 12:04)



Now let us; May be last few weeks we have done this once already so if Q inverse AQ=B then det A = det B this is what we want to prove. We start with this let det xy = det x det y right how do you do it? You do it using an example of 2 by 2 matrix and it is ok we have discussed it earlier also xy is this. What is det xy as for you trouble, I will write it myself and but then perhaps you can figure it out these two determinants are going to be 0. It is not very difficult to see this it is; this gets you det x into det y ok.

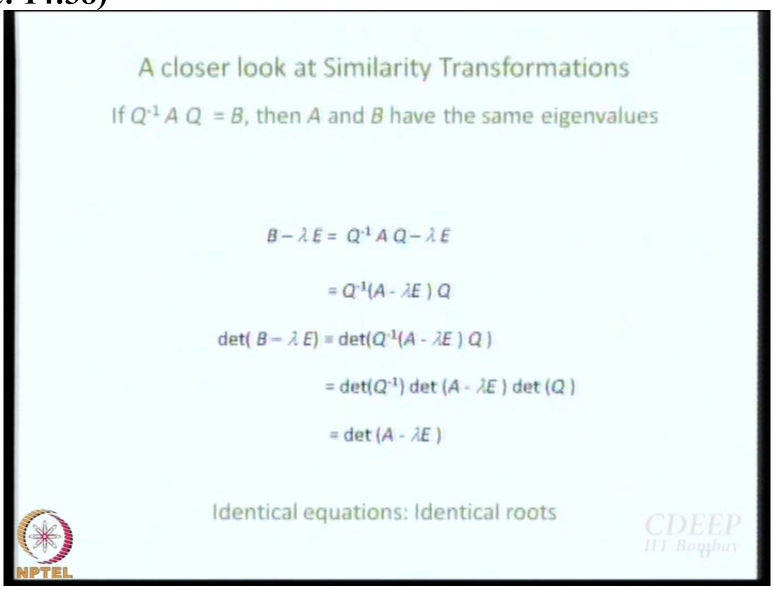
(Refer Slide Time: 12:50)



With that we need to see if this is correct or not. If Q inverse AQ=B then det A =det B. I am doing this again because there will be confusion last day and then we are going to use this in what you are going to say today also almost very 10, 15 minutes more almost done do not be impatient ok. Do you agree with this det B= det Q inverse det AQ. You started with B = Q inverse AQ right. So I can write it like this expand det AQ and I get Q inverse det A det Q and determinants are just numbers it does not matter in which order you will write.

So I can write det Q inverse det Q det A and det Q inverse det Q as we have seen earlier det xy= det x det y. So this becomes det Q inverse Q. What is Q inverse Q? Unit matrix, so it becomes det E and what is det E? 1, this becomes det A and hence proved. And if B and A are conjugate to each other. Do not forget the term conjugate. Similarity transforms also go by the name conjugate. If A and B are conjugate to each other then the determinants are the same and this is only the first of list of things that are same for conjugates, the determinants are the same.

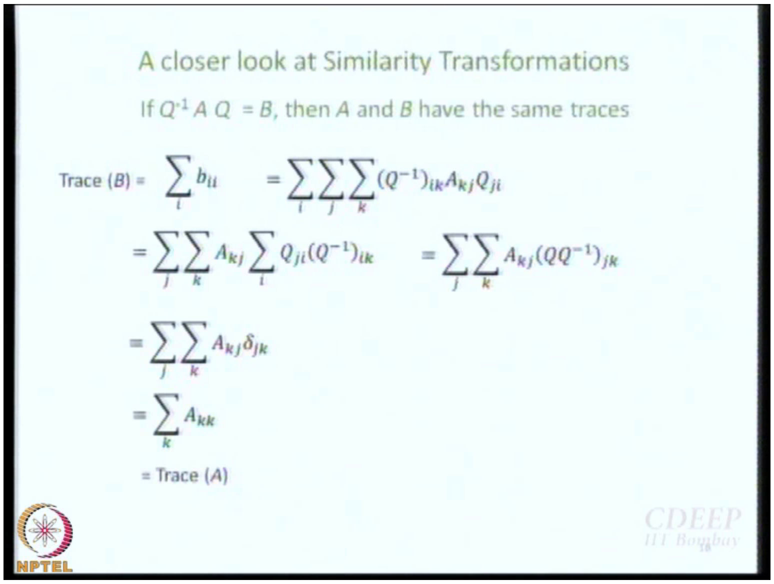
(Refer Slide Time: 14:38)



Next what you want to show is that conjugate have the same eigenvalue. If A and B are conjugate to each other then they should have the same eigenvalue. Start with this B = Q inverse AQ and then let us write -Lambda E on both sides. So now, from there will you allow me to write Q inverse A - Lambda EQ, can you do that? Lambda is this scalar and E is unit matrix that is why I can do it right. So then you get det B - Lambda E = Q inverse A - Lambda Q which gives you det Q inverse det A - Lambda E det Q.

And then again you can write Q inverse and Q together and finally you are going to get determinants of A - Lambda E right. So, since they are identical equations you get identical roots if you get identical roots then you have same set of eigenvalues.

(Refer Slide Time: 15:57)



Next second last today is if A and B are conjugate to each other then they have the same traces and this is of utmost importance in our discussion in chemistry in symmetry. Because if A and B are conjugate to each other then they belong to the same class right. What is the definition of a class? It is a set of elements they are conjugate of each other are conjugate to each other. So what we are going to show that here they have the same traces.

So trace B is sum over i bii ok and I do not mind mixing capital letters and small letters here somehow I felt that I could not write small q inverse just I did not sound right. So you could understand what I mean. So instead of bii I can write Q inverse AQ and in order to get ii this is how subscripts have to be ik kj ji that something that comes from basic mathematics algebra I think All of you know. So I am going to get Q inverse ik, what is the meaning of Q inverse i k, which element, ith row kth column or ith column kth row, ith row kth column.

Latitude and longitude is important if you mix up with latitude and longitude then instead of coming to Bombay you could have reached I do not know. So the ith row kth column element of which matrix, Q inverse and similarly you know what is akj and what is qji right. So now I separate A, because Q is there Q inverse is there so I can easily get rid of them. So it is some over i some over j akj sum over i qji q inverse ik right, will you agree with this now.

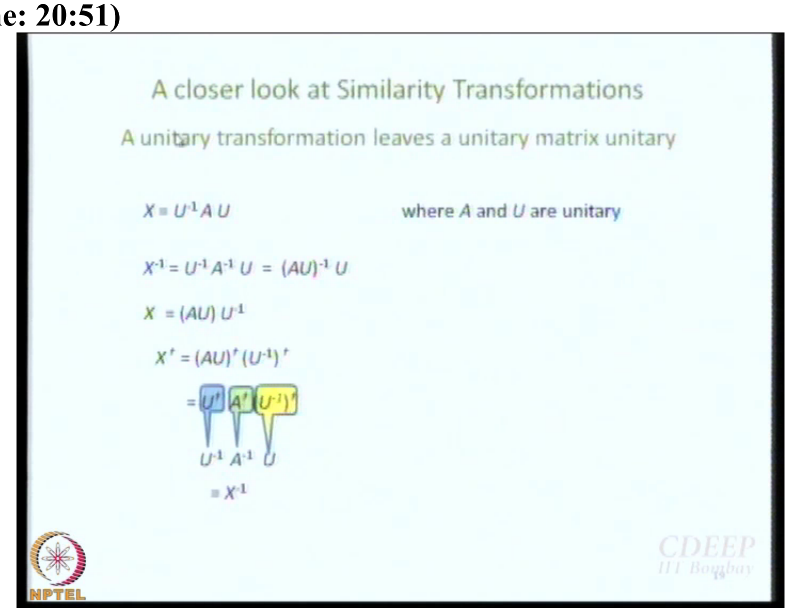
Can I combined this as Q Q inverse jk, I am multiplying right, I am multiplying qj q with q inverse not only that I am multiplying this qji with q inverse ik, so what I get is that once again I suggest is that second subscript of the first and first subscript of the second cancel they do not actually cancel but it is easy to remember that way ok. When you multiply together what you can write is you can write q q inverse and the subscript are going to be jk alright.

And what is Q Q inverse? E spoil sports again q q inverse is E, so now in E what happens when j = k that element is 1, and when j is not = k the element is 0. So, I can write our favourite Kronecker delta, delta jk right, Akj delta jk is over j right. What do I get then? Once again multiplying this jj cancel of and you left with kk, some over k Akk, what is that? The trace right or the name that we are giving used earlier we are talking about the transformation matrices is character.

Now we have thought about reducible representation and we have talked about irreducible representation so on and so forth. So does that depends upon whether the matrices is that we are working with belongs to a reducible or irreducible representation? No right. Who has talked about reducible or irreducible representation here nothing I only talk about some matrix right. I am only talking about two matrices A and B the only condition is that A and B are conjugate to each other.

So no matter whether the representation is reducible or irreducible it does not matter the traces of matrices that belong to the same class are going to be the same right. This something we will use extensively when we discuss character tables ok.

(Refer Slide Time: 20:51)



Last topic of discussion this is also something that keeps coming back haunt us in many case. This is very important sounds a little funny. A unitary transformation is a unitary matrix unitary it is almost like poetry, to many unitaries right. Unitary transformation is a unitary matrix unitary let us see. Let us say then I start with this X is U inverse AU where A and U are unitary. Alright we start from here that is the meaning of unitary transformation. What is the meaning of unitary transformation?

Yeah, no, but what is the unitary transformation? When I say unitary transformation what does it mean? So that the matrix that is used to for transformation that is U inverse U that matrix is unitary that is what it means. Now what you are saying is that if A is also unitary then X should be unitary as well. Unitary means too many times please do not get confused; unitary transformation is got to do with the U's ok. When I say unitary suppose A it was some matrix B which is not unitary. Even then it would have been a unitary transformation is that I am in little clear now what I am trying to say. The U's have to be; this U and this U, if I say U then once again it will confusing.

This U and this U, second U actually U and U inverse that is a unitary matrix, U for unitary ok. That is the meaning of unitary transformation and when you perform a unitary transformation on a unitary matrix A then our contention is that the matrix X that you get it is also unitary that is what we are going to learn alright. Unitary transformation is a unitary matrix is unitary let us see.

Will you agree with me that X inverse is U inverse A inverse U how? Start left multiplying X = X inverse AU is it not. So if I want to keep on left multiplying what should I get? If I want inverse of X then I should left multiply by the inverse of the first element first so that gives U next will come A inverse and finally you get U inverse. So you get U inverse A inverse U. Are U ok with this sometimes the order becomes confusing ok with U inverse A inverse U. Are you convince that it is X inverse, sure.

Now if you are convinced then allow me to write it as inverse of AU multiplied by U right. In that case next step is easy then X is AU multiplied by U inverse. I multiply AU first A and U together then multiplied by U universe. So, what is the adjoint of X? X dagger, it will be dagger of AU multiplied by dagger of U universe right. That is going to be U dagger A dagger, dagger of AU, AU you inside the bracket is U dagger A dagger, I think you asked workout or something. U dagger A dagger multiplied by U inverse dagger and we are done.

We are done, U dagger A dagger or dagger of A inverse are we ok with this so far. If you are ok with this then we are done because U dagger is U inverse do not forget that U for unitary right. A dagger is A inverse, now U - dagger is most interesting because U - dagger means inverse of U inverse. Inverse of U inverse is U. If I want to just touch my nose I will go around my head and touch that is that kind of thing. So that is U right and what is U inverse A inverse U? Will you not agree with me if I say it is X inverse right.

Because you have started with X inverse AU, so what do we get? We get x dagger = X inverse is that not the condition for X to be unitary right. So, we have proved this somewhat funny sounding theorem that the unitary transformation leaves a unitary matrix, unitary ok. We stop here today because yeah I was also thinking that but I do not think so you work it out let me also work it out myself I do not think that it is a problem.

And then what we do it from this fitter we go on to something that is perhaps a little more abstract perhaps not. It starts about functional spaces, have you; functional space. Have you studied is in some other course or the other, in what ok yeah. The function space sounds scary but no reason to be scared about. I should be scared because while teaching first year B Tech course one side say let us say I have n dimensional space and they smart Alec stand, sir I say no you cannot talk about n dimensional space, Why?

Space in 17 dimensions, what are you talking about yes space is 17 dimensional we have been taught in Physics we used to study in relativity that time. I do not know exactly these 17 dimensional things. But present Dean I said who has taught them that. So I do not know what is that 17 dimension are. But anyway the thing is when we talk about space we will think of 3 dimensions is it not, X Y and Z. But then suppose I have something that is dependent on more parameters.

Basically I am talking about the relationship like Y=x1 A1+ x2 A2 + A3x3 and so on and so forth. Can we not have equations like that, you already add equations like that, you encountered today also write. So, that what spaces to n dimensional space right the space is not face space it is just an analogue of space that we are talking about. Now say think of a position vectors, you know position vectors? Right, if I am the origin this is the. This is the position vector right.

Well everybody is origin with respect to himself or herself this is another position vector this is another position vector how many position vectors are there? Infinite, so these position vectors constitute function space. But then the point is this all this position vectors can be represented as something into X and something into Y and something in to Z right. So those are the normal modes, orthogonal modes of the functional space that is defined by position vectors ok.

So that is what we start talking about and then we need this concept to develop orthogonality theorem. And we talk about something called OR, transformation operator that will need one class and from there we move on to reducible and irreducible representation that will be next week. Week after that finally get to our orthogonality theorem the great. After that it is very, very simple it is just using orthogonality theorem to derive character tables using character tables you figure out lots of stops of whatever molecule you want. That is how this course is used to go from here.