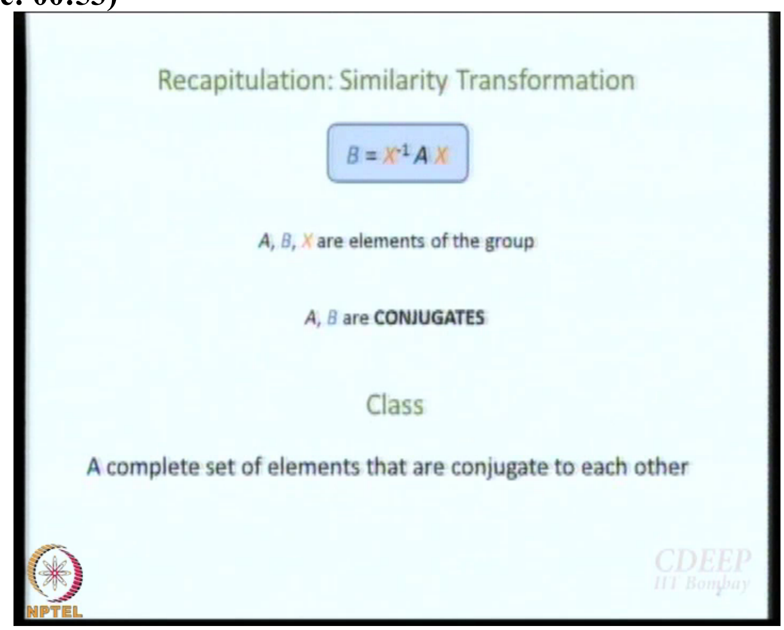
Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology-Bombay

Lecture-14
Application of Matrices in Solution of Simultaneous Equations

Today we will see how some of those matrices can be made to work for us. So slowly we are moving towards application. And when we do that we will also integrate this with something that we learn from group theory. So, before learning anything new let us recall what we have closed our discussion on group theory previously and what we have learnt so far in matrices. So this I think everybody remembers now, similarity transformation.

(Refer Slide Time: 00:53)

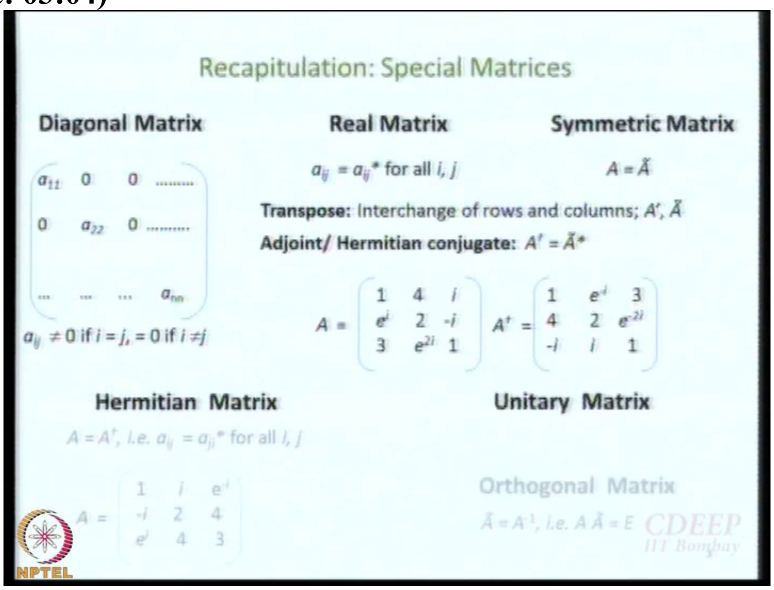


Similarity transformation is B = X inverse AX where A,B,X are all have to be elements of the group, of the group not the sub group, not the class, right. A and B are called Conjugates. And a class is defined as a complete set of elements that are conjugate to each other. I hope you know this already. Any chemical example of class that we have discussed, example from Chemistry of class from symmetry C, C3 and C3 square in C belongs to the same class and Sigma V, 3 sigma V belongs to another class and that as you saw in the previous day, confirms very nicely with a G62 kind of multiplication table that we had used, ok.

So, everything concentrated so far. So, how did we define the members of class so far? First of all, there has to be similarity transformation services to each other; secondly, I am talking about symmetry operations now, symmetry operations in the same class which we discussed, 3 ways of defining them. First is that they have to be similarity transformation for each other. Yeah, they should be transformable into each other by an operation outside the class. And what was the third property that we have discussed? Character should be the same.

Let us see today if we can have a more formal discussion of why the character should be the same, right. What we have done so far is of only demonstrated, right? We have taken matrix we have taken 2 matrices CN plus and CN minus and we have shown that the characters turn out to be the same in these two cases. Today let us see if we can have a more general derivation of this fact, right.

(Refer Slide Time: 03:04)



And then what are we doing is you are approaching the problem I do not know what has happened. It is supposed to be all invisible anyway as I have goofed up. So, anyway so you are going to do this as a tool of trade what we are going to use is matrices. As we saw earlier, the symmetry operations can all be represented as matrices and you had a glimpse of how you can block these matrices even manually and generate what are called representations. What are the representations but what is the definition of a representation?

When I say representation, what does, what do I mean? Sorry, representation is basically a collection of numbers or matrices ok spanning over the entire range of symmetry operations for a symmetric point group, ok. And representations arrives so far we have seen that we have use different basis as you are saying for what all we used is oxygen, hydrogen. Hydrogen b or we also used xyz, different bases; different basis sets if you want to call them.

And we have seen how they get transformed with respect to each and every symmetry operation and then we took a collection of those for all the symmetry operations that collection was called a representation. Representation is of a symmetric species of something which has a unique set of behaviour with respect to all the symmetry operations there are there in a particular point, right. That is representation, all the symmetry operations taken together.

What are the matrices or what are the numbers that tells you about a particular kind of behaviour, right. We will come back to that, when we talk about reducible representation and Irreducible presentation once again. But before that we need to know more about matrices and this is what we discussed in the previous class. Everybody knows what a diagonal matrix is. I think everybody knows what a real matrix is. In very simple terms, real matrix is a matrix in which all the terms, in which none of the terms are imaginary let me put it this way.

If I say all the terms are real and real matrix then, also it sounds very funny, is it not? Incidentally I saw this cartoon somewhere where i and Pi giving each other a hard time. This you have seen this. What does i tell Pi be rational and what does Pi tell i, get real, i is imaginary right, i for imaginary. What is the value of Pi you are diagonalising little bit by the way it will be useful but what is Pi? Pi = so if you did not say approximately you got you would have got a 0, Pi is not 22/7. Pi is irrational numbers do not forget.

If Pi is 22by 7 then it becomes a rational number so this 3.142 then, I do not remember after that. What is an irrational number? There is no value. It goes on. What is pi? How is it predefined? Originally, pi is an experimental quantity. Pi is an experimental quantity. Circumference = 2 pi r or pi d, right? Pi is basically circumference divided by diameter. But if you diameter is exactly seven 7.0, perimeter, circumference will never be exactly 22. It will be a little more or little less, right? So, it is not 22 by 7 fine. Let us come back to what we were talking about. The real matrix, the most formal definition is aij = aij star for all values of i and j, right.

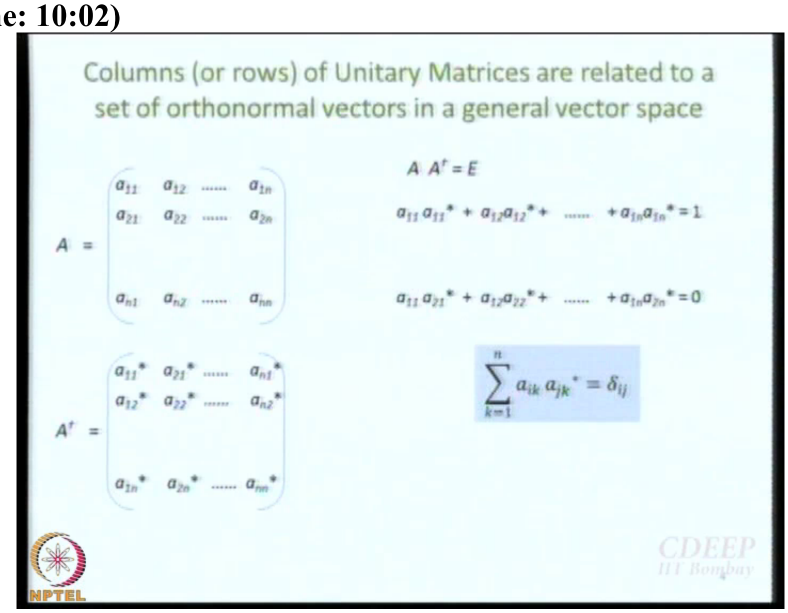
Then we talked about transpose and adjoin or Hermitian conjugate. Transpose is very easy just interchange the rows and columns, right? Essentially, it gives a 180 degree twist, with respect to the diagonal. If the class is symmetry you might understand it better this way to take the diagonal that is used C2 axis, turn the elements by 180 degrees, what you get, is a transpose. Interchange the rows and columns and it is called either A dash or A tilde. I do not know either it is really called A tilde. I call it A tilde. I do not know if it has a more proper name.

And what is an adjoin or hermitian conjugate? A dagger is A dagger is a dash star that means not only do transpose, you also take the complex conjugate of each and every element, alright? And Symmetric matrix is something which = its transpose = A tilde. That means in that case that C2 operation along the diagonals is a symmetric operation for those matrices, is it not right.

So, here we have worked out with given you A matrix and you had worked out what is A dagger. Remember? Then, we talked about hermitian matrix, what is hermitian matrix? Hermitian matrix is one in which A = A dagger. Please do not forget these two. In hermitian a = a dagger and in unitary matrix this is the only place where the cover as worked A dagger = A inverse. So if A dagger = A then A is hermitian if A dagger = A inverse then it is unitary, ok. Another way of putting it is that A, A dagger = E. And here we had given an example of hermitian matrix also, alright?

What is hermitian matrix? A = A dagger. Transpose is and take Complex conjugate of each and every element the matrix that you get is if it = the matrices that you started with, then A = A dagger, hermitian, and what is orthogonal matrix? Orthogonal matrix is one in which A transpose = A inverse. A transpose = A inverse that is what we worked for real matrices, right. You all know these definitions we are going to use them regularly in the subsequent discussions. If you do not know Unitary this is your last chance for it, remember.

(Refer Slide Time: 10:02)



And then this is where we have stopped. What we have done is we have taken away the matrix, a general matrix, and then you have worked out A dagger for it and then we said let us say that this is a unitary matrix. So if it is a unitary matrix then A dagger should be = E. So what we have done is you have worked out the 11 element and 12 element, 11 element would be 1, unit matrix; 12 element or 21 element for that matter would be zero and this is what you got, right. You got A 11 into A 11 star + A12 into A12 star + etcetera etcetera + A1n A1n star = 1.

And you are also got for the 12 element A11 A21 star + A12 , A22 star + etc etc + A1n A2n star = 0 right. Welcome back Sumithan I was worried that you have left us. So, see these metrics element then behave like a set of orthonormal vectors, right. To multiply an element by the complex conjugate or by itself and then add up all the products then you get 1. And then multiply an element by a complex conjugate of something else and add up all that whatever you have then you get 0.

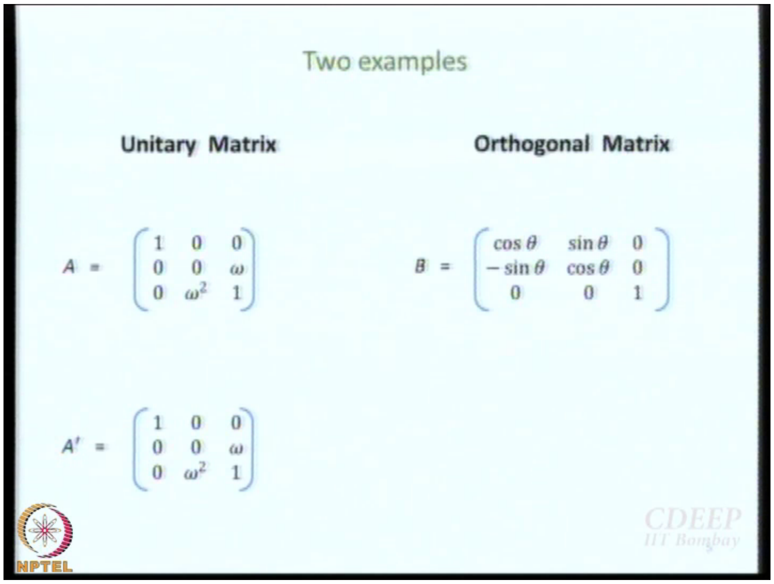
So that is the property of a set of orthonormal vectors and in quantum physics, quantum chemistry, you encounter this orthonormal vectors, all the time. They come back and haunt you everywhere. That is why these unitary matrices are so useful. Anybody who works in quantum mechanics or quantum chemistry actually loves unitary matrix we can use it all the time.

This is where we stopped and this is where we will start today. Now I asked you to try and write down the general expression.

I will invoke A as well. So some over will work K = 1 to n, a i k a j k star = del k z. It will be easier to write if you invoke A, ok, right? What is delta i j? It is Kronecker delta, when it is same then it is one; when they are different then it is zero. What is zero, each element is zero, and then the sum of the products is zero. Do not forget that please. The sum of the products is one if you are multiplying each element by Complex conjugate as well, sum of products is zero if you multiplying the complex conjugate of anything else with an element.

It does not imply in any way that each and every vector is zero. Please do not have that confusion. You have to invoke otherwise it is very difficult right ok.

(Refer Slide Time: 13:13)



Now let us move on. Here are two examples, one of a unitary matrix and one of an orthogonal matrix. But of course just because I say that this is unitary and that is orthogonal there is no reason why you should believe me, right? Max Planck had said experimental results are the only truth. Everything else is poetry and imagination, right? So now workout the adjoints and prove to yourself that this is unitary and the second one is orthogonal.

Now let us start with the first one. What is the adjoint of the first one? Everybody knows that omega and omega square are same, right? What are they? Cube root of 1 and how is omega related to i? Is omega related to i in some way? It is not related i at all, your homework problem number 0. Find out relationship between, among Omega, omega square and i. Is there relation or is there no relation. I mean omega and i, omega square will follow. Is omega in somewhere related to i or not.

If it is not, then you are going to have another number line, is it not, you have a real number line and then you multiply by i what happens is that you get a perpendicular imaginary number line. So, if you need another number line in omega then you got a problem. Omega, omega square definitely cannot be real. If they are real then they have to be one, right? So it is better it is related to i in some way or the other. Please find out how they are related to i, fine.

But let us move ahead anyway. What is a complex conjugate of omega, so Avinash tell me that what is the conjugate of omega, omega square, very good? So now work out the adjoint. First one 100 there is a first row what is the second row? What is the second row? 0 0 omega squares does the transpose, I want the adjoint, 0 0 omega. What is the third line 0 omega square 1, right? It is 100 00omega 0 omega square 1. Have you seen this matrix somewhere?

Yeah you have seen that matrix right here on the same page. Same matrix so what is it A = A dagger right? So, if A = A dagger what kind of matrix is it? Dalmation what hermitian matrix speaks loudly and clearly? Do not be scared. If you say anything wrong will just say it is out. Do not worry. It is a hermitian matrix, right it is also unitary. Multiply and see. What is the condition for a matrix to be unitary? A into A dagger = 1. You know A, you know A dragger. So, multiply them together and see what you get.

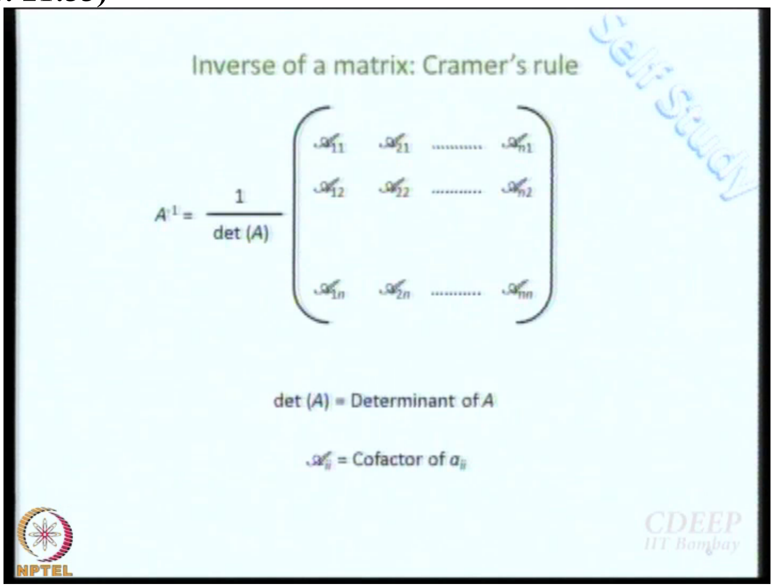
We have already established that this is a hermitian matrix (Foreign Language: 17:01) what is the point in saving so much of paper. Multiply them together what you get? It is the typing mistake. Last one has to be zero 3333 element, if it is zero. If it is zero then, it will works out, right? So, I have to changed that ah now but then the point is this still a hermitian matrix, it is hermitian and it is also your unitary, right.
If it is 0, if the last one is not one this has to be 0. This is just once again perils of copy paste, alright hermitian as well as unitary. So, what we learn is that there is no problem for hermitian matrix to be unitary; they are not mutually exclusive. And also what are you getting your way, we take a matrix multiplied by itself and get unit matrix. Such matrices have another name A square = one what is it called? It is also A square not = one it is it is. So, if A square = 1 what is such a matrix called Idempotent, that is right.

Idempotent and if it is zero, null-potent, so, see this one matrix is so many things; is an all rounder matrix, right? This device can be processed be isothermal as well as adiabatic, like this matrix. We know of isothermal expansion, we know of adiabatic expansion. Is it possible to have a process that is isothermal as well as adiabatic? Free expansion is isothermal as well as adiabatic. Results are not reversible ok.

Let us move on. Instead of going of orthogonally to our discussion into thermo dynamic and all let us rather talk about orthogonal matrix. B, what is the transpose of B? And hoping that there is no further typo here, what is the transpose of B? Cos theta minus sin theta 0 sin theta cos theta 0 001 right. Can you multiply them together and see what you get. B multiplied by B transpose what do we get? Do you get the unit matrix? If you get the unit matrix it is orthogonal matrix, ok. So, here we have taken two examples.

There is a little mistake in the first one but then that is not such a big deal. We will correct it here before I forget. Now it is ok. Yes sir, yes. That is right xyz with xyz as a basis. That is right. Rotation by theta, plus and minus, so, they are orthogonal ok fine.

(Refer Slide Time: 21:33)

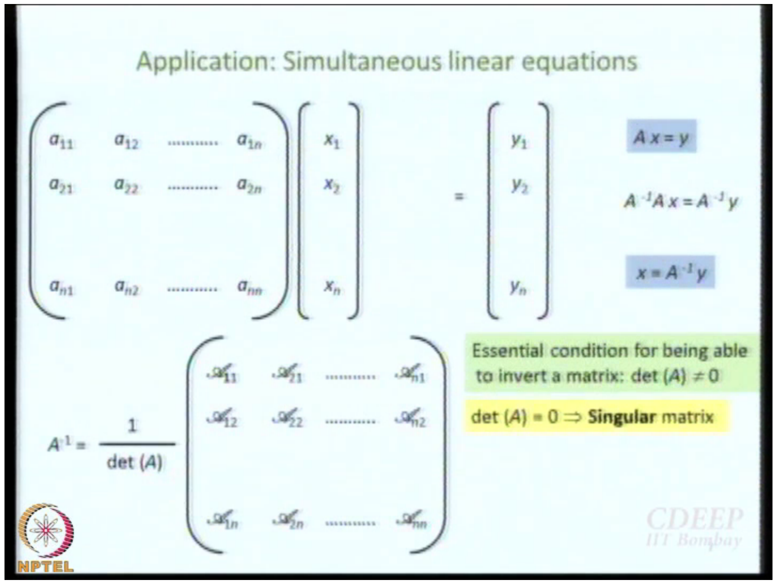


Next I think this is something you have studied in matrix whatever matrix algebra you have done. I am not going to spend 20 minutes deriving it actually. Please read it by yourself just to remind yourself how it came and I think this relationship is not very unfamiliar. How do you get inverse of a matrix? What is the inverse of a matrix? What is the definition of inverse? Inverse of a matrix is a matrix which when multiplying by itself gives you E.

On the compute with each other, fine. So, this is inverse 1 by determinant of A outside and then what is this Matrix called? What are all these stylish A's, cofactors. Cofactor is there in Biology where did cofactors come from in matrix. Cofactor is biology, right. Ah enzyme, cofactor, cofactor is there. So what is this mathematical cofactor? How is cofactors defined, come on? What is cofactor? When I say A11 stylish A11 what do I mean yeah ok right.

Yeah I can ok right. Take out A take out the first row and take out the first column whatever is there make a determinant of it that is cofactor and what about the sign? So det A is a determinant of A and the stylish A's are the cofactors of the matrix elements, right. Now where do you us an inverse. All of a sudden why are we started talking about inverse?

(Refer Slide Time: 23:26)



The biggest use of the inverse of a matrix, right is in Simultaneous Linear Equations. All of you know that we can write a set of simultaneous linear equations in the matrix form. They have already written one or two already right. This is General form A11, A12 etc up to Ann and then column rows A11 A21 all the way up to A1n and then you can fill in all the n y and elements. When this matrix operates on x1 x2 up to xn, then you get y1 y2 etc up to yn.

I hope you are all familiar with this. Can you write the equation actually? What will be the first equation here? A11 x1 plus A12 x 2 plus A14 x4 = last is A11 xn. = y1 + y2 + y3, no only y1. Ok. Good. So in that case what is y1? A linear combination of the x1's or if I may put it that way it is a mixture of the x1's, right. Yeah of course wherever I say mixture, you think of a function, that is right fine.

So now ax = y if left multiply both sides, by A inverse what will happen? The left hand side you will get E unit matrix and you get x = A inverse y. You work it out and you already know what A inverse is, is it what? So, I was saying that every square Matrix that is there we restrict ourselves to square matrices. Every square matrix that is there, that I can write is it going to have any inverse? So, what is the condition for having an inverse, this right?

If you have a zero it is going to be a problem. So, the essential condition to be able to invert a matrix is that the determinant should not be = zero. As you will know this if the determinant should not be = 0. If the determinant of square matrix = 0 then it is a weird matrix then weirdo right it is a renegade, outlaw. But since we do not want to use such impolite terms we use a polite terms and call it a singular matrix.

If the determinant = 0 then, it is called singular matrix. What is the meaning of singular? You can actually guess even if you do not know singular, one of a kind. Singular is one of a kind not in a positive sense. If you guys read Sherlock Holmes stories in original, in English, Sherlock Holmes keep saying all the time is it is what can I see a singularity; singularity was very pet word of Sherlock Holmes or the writer of Sherlock Holmes rather. Singularity means something that stands out, exceptional ok. So, these are exceptional matrixes.

Singular matrixes, problematic matrixes ok. Another more formal definition of singularity right is to do with a breach in space time that is also called the singularity in astrophysics. But here singular just means a matrix that cannot be inverted and the reason why it is called singular is there it is weird it stands out it is not regular, an outlaw, Phoolan Devi kind of matrix, ok. Now we talked about simultaneous linear equation one particular kind of equation simultaneous linear equation that keeps occurring in quantum mechanics is called the matrix Eigenvalue equation.