Symmetry and Group Theory
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Lecture No.13
Introduction to Matrices

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Corrective matrix think of a square matrix right if you take the trace some over i, aii that is the trace right that is also called that character and that will what will use, character is going to form a character of this course eventually right. Now now we will move on to familiarise ourselves about symmetry all we will do closure matrix, an array of elements that is fine, collection of numbers ok collection of numbers that is good enough.

Two dimensional collection of numbers if you want be more precise, can we have 3 dimensional collection of numbers I can I will take my son's blocks like 358 9 12 13 012 that is a matrix square matrix right shall I right it here and then I will move 2 inches and I start writing 359 12 15 1 13 0 3 and I will move 2 inches and another array like that. Then I have a 3 dimensional array of numbers what is that called.

She is very tensed over there, this called tensor that is all tensor is matrix is all about section of tensors and matrix is a rank 2 tensor right. So, do not be tensed about tensor, tensors are just arrangements of numbers you just cannot right it on a paper easily but you can take sections fine.

Come back to matrices that is a matrix everybody knows row matrix column matrix right just one dimensional array of numbers row matrix column matrix and they also called vectors right.

Now we know how to add matrices very simple subtraction is the special case of addition right. How many mathematical operations are there 2 what are they? I will say 1 multiplication is addition many times over. So, there is only 1 mathematical operation to be honest anyway. So, multiplication of matrices is known can I take any 2 matrices and I can multiply to them multiply them together? No.

What is the condition for multiplication of matrices number of rows should be equal to number of columns. Then how do we multiply matrices row multiplied by column that is enough if you say that you know I know what you are talking about no issue fine.

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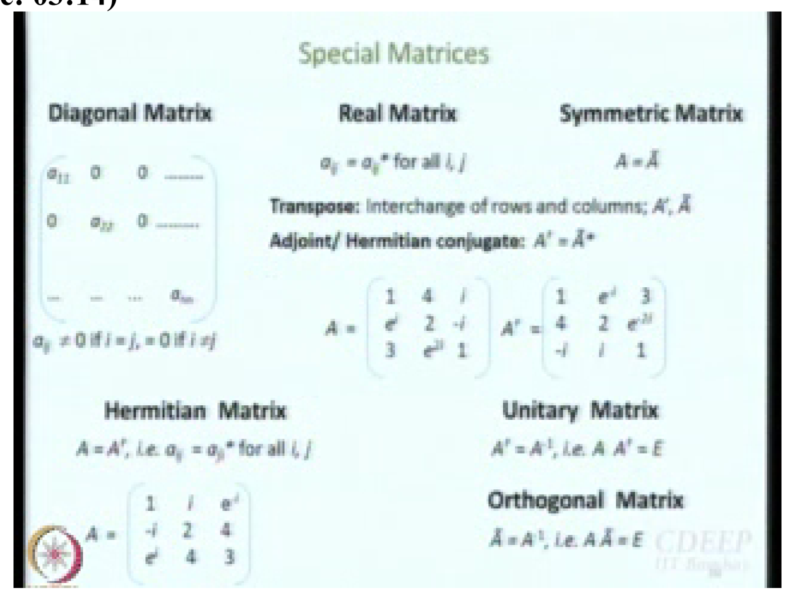

Now special kind of matrices and the matrices that we like very much are diagonals matrices what is the meaning of diagonal matrices, only the diagonal elements are non 0 rest is all 0, why do you like diagonal matrices and more fundamentally matrices represents complete uncoupled systems. Only ii is non 0 right that means what there is no interaction between i and j you have self sufficient set that is why very major problem whenever use matrices is to diagonalize the matrix. So, when you study a little bit those were studied already little higher level quantum mechanics you will see diagonalization of matrix is a very big issue.

They want to do it all the time because that is that is equivalent to what we have learnt already. Does it ring a bell what they would this be related to array, no, what I have in mind is separation of variables. When you diagonalize basically you have achieve separation of variables right.

Nothing else coupled with anything else fine diagonalize and you should not be scared if you write things in this notation aij what is i? And what is j? Row number column number fine aij is not equal to 0, i = j, and 0 if i not equal to j fine that is very easy.

Next is real matrix that is also extremely easy, real matrix means matrix of all real numbers that is all, aij = aij star for all ij. What is aij star complex conjugate aij into aij star not necessarily 1 right mod of aij. Do not forget that it is not necessarily 1 right mod of aij square good ok. You know what is the minimum of transpose just interchange the rows and columns right. Interchange the rows and columns and it is written in 2 ways sometimes it is written as a dash easier to right.

But then theoretical it comes to complicate things always so it is also written as a with a Tilde on top whatever it is called, I can call it a tilde the sine wave thing that is called tilde. I will call it as a tilde but may be supposed to be written in another way I do not know to be honest fine. So in a symmetric matrix what will happen is that a is going to be equal to a tilde or a dash right. What is the meaning of symmetry matrix that if you interchange the rows and columns nothing will change you get the same matrix ok?

So, a = a Tilde so far so good very easy everybody knows everything. Now let us slowly go up the complexity ladder by bringing in complex numbers right at adjoin hermitian conjugate is defined as a tilde star what does it mean it is written as a dagger, what we have to do if you start with matrix first transpose it and for every element that you get right the complex conjugate that is what it means understood sure.

Do not confuse transpose with adjoins please adjoins is transpose + complexifing the problem right. Adjoins are sometimes it is also called hermitian conjugate this I showed a little but this entire part of matrices you consult Bishop book on that there are many goods for matrix algebra you start reading from there then not remains a course in symmetry it become a course in matrices.

That will become a too much Bishop book is good enough now adjoin and hermitian conjugate a dagger is a tilde star so far so good no confusion about adjoin will you ok. Now since there is no confusion let us workout and adjoin a is given 14i e to the power i 2-i 3 e to the power-2i1, I want you to work out a dagger. Let us finish this column 14 -i now let us go to the top what is the next element after 1, e to the power -i right then you are giving the bottom one. Now you are going left to right ok 3, next you have no issue with that, next below 2 last one is unchanged right which are the elements that remains unchanged, the diagonal ones right.

Diagonals remain unchanged provided they are real if there are complex numbers then you have got the complex conjugate but they do not change places right so it is right. What symmetry operation is it? What operation it is not a symmetry operation here, it would have been a symmetry operation if it was a symmetric matrix. What is the operation that you are performing, that is rotation right a square matrix right. You take this diagonal that is your axis and you perform rotation by what is the angle 180 degrees not 45 ok.

So, we know how to work out a dagger right adjoin it is the; what you do is first transpose and replace each element by its complex conjugate fine. Next is hermitian matrix, have you heard the term hermitian anywhere? So now tell me in what context you have heard this term hermitian operators, what are hermitian operators? They will give real eigenvalues right everybody knows that hermitian operators will give real eigenvalues.

Who has said that other than the real professor Datta and that is clearly what I have got written on a stone integral of fire where does it come from. Let us see if we learn in this course whether you can prove in this course that hermitian matrices have real eigenvalues. This hermitian that hermitian or not very, very different hermitian matrix, what is hermitian matrix? a = a transpose that means aij = aji star for all values of i and j this is the definition of a hermitian matrix. Have you learnt hermitian matrix earlier which course linear algebra yeah that is right.

But what you do in this course is that we develop a connection between linear Algebra and Quantum chemistry ok they are not diverse from each other, is the definition is correct a = a transpose, hermitian matrix, a dagger sorry adjoin a dagger. An example of that is these convince yourselves that this is correct. Work out a dagger so what you have to do, you have to take this elements in the row into the column and then take complex conjugate 1 remains 1 – i goes here what is the complex conjugate of -i is i, it becomes i here, e to the power i goes to first row first column third row, first row third column.

And e to the power of i becomes e to the power-i so what was the first row is what we have got. Now second row take second row i where will this i go to 21 position and it will become -i complex conjugate 2 does not change place and it is a real number no issues 4 goes here right then e to the power-i should come to 31 and it become e to the power +i 44 well this 4 earlier I got confused between these two 4's so 3 remains in is old place. This is an example of a hermitian matrix right.

This is not just ideal worship these matrices actually come very, very useful for us in application chemistry as we work to see in near future. From now let us not forget what are hermitian matrices are. What id hermitian matrix, a = a adjoin welcome to the club, thanks for making the same mistake which I made and last not last second last this is the last and may be this is last 1 after the last right, one for the road this is very important for us in this course unitary matrices.

So, we need to understand what are unitary matrices are? Unitary matrices are little more complicated than hermitian matrices here we have A dagger = A inverse. The adjoin of the matrix is its inverse as well when that is the situation then we call it unitary matrix A dagger = A inverse or A into A dagger = E that is the definition of unitary matrix. One way of remembering it is when a gets unitary right unit so when A gets multiplied by A dagger it gives unit matrix. I do not know it helps or not, A A dagger = E ok alright.

These are very important for us we learn little bit of that before we close but before that let us for the sake of completion another kind of matrices that is called orthogonal matrix. Orthogonal matrix is a matrix where the transpose of a matrix is its inverse A tilde = A inverse. So, do unitary matrix and orthogonal matrix are something to do with each other or not, if A is a real matrix then exactly, so unitary matrix is more general case orthogonal matrix is a special case when you are talking about real matrix right.

So, orthogonal matrix is really subsets of unitary matrices ok when all the numbers are real then life becomes very simpler. So, the point these orthogonal matrices or unitary matrices in when but the only difference is that you do not have to worry about Complex conjugate you are working with real numbers through out ok. So, unitary matrix is a general case orthogonal matrix is the special case why are we so bothered about unitary matrices

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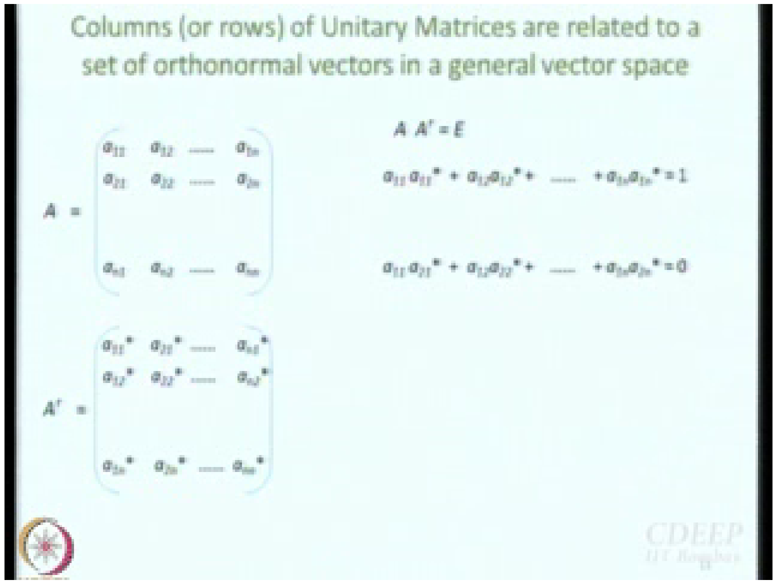

Unitary matrices have these very special properties that columns or rows for that matter of the unitary matrices are related to a set of orthonormal vectors in general vector space. You can maybe not even think about in general vectors part of it just let us focus on first part columns or rows of unitary matrices are related 2 set of orthonormal vectors. Have you encounter the set of orthonormal vectors anywhere, did you not study that the orbital what is an orbital, whether one way different function it is not a region or space of finding probability of the electron maximum.

That is there most popular wrong answer is acceptable 1 electron main function ok. Now all those behave like orthonormal vectors right so orthonormal vectors are unit vectors in quantum mechanics you could encounter them everywhere alright. That is there connection with the unitary matrices. Columns or rows of unitary matrices are related to a set of orthonormal vectors looking at this innocuous matrix it is very difficult to believe what I am saying. I will give you a break an array of numbers and you want to build a story that there is an orthonormal vector hiding somewhere.

So, it is only human to not believe what I am saying but before you discount what I am saying please do not forget not talking about the general case. I am talking only about the unitary matrices ok and the proof of putting in the seating's. So, let us see if we can arrive at what you are saying. So, let us say this is a general matrix unless it is a unitary matrix right is a square matrix in its general form right N by N matrix.

Can you right down the, adjoin, what do you want to do transpose or adjoin of something else when you want to get the unitary matrices adjoin or transpose sure then work out the, adjoin.

How will you work out the adjoin interchange rows and columns and then put star wherever there is no star put the star whenever there is a star remove star, very easy, done. What is a dagger? Is this right or is this wrong right you got it right ok great, this is right what was the row a11 a12 etcetera, etcetera a1N.

A11 a12 etcetera, etcetera a1N show first row has become first column and additionally I put stars all over. My younger son will be happy to see this he passed stage when I get star in his class work and homework still the fascination remains. Second row a21 a22 etcetera, etcetera a2N second column a21 a22 etcetera, etcetera a2N with the stars and then it etcetera, etcetera, etcetera so let us go to the last row aN1 aN2 dot, dot, dot, aNN here aN1 star aN2 star dot, dot, dot aNN star ok you are convinced that this is the transpose, no that is adjoin right.

Now what is the property of the unitary matrix property is written right here a a transpose = E what does it mean if I take a and multiply with a dagger then I should get unit matrix right what does unit matrix look like, in this case N by N square matrix diagonal elements are all 1, half diagonal elements are all 0 right. So, just workout we will talk about the general notation later work out the 11 element in terms of this a's. What is the 11element in terms a tou a a dagger.

Yes then plus you are working out a dagger a do it a a dagger so that you get the same answer your answer is also be going to be correct. But it is just a little all the 1 ones and 2s will be interchanged a11 a1 star + a12 a12 star + a13 star do you see the pattern, what is the pattern? This is what it is a11 a1 star + a12 a12 star + whatever, whatever, whatever +a1i a1i star +again lot of elements then +a1N a1N star and that has to = 1first element 11 that is =1. Do you see the pattern in the left hand side, do you see the pattern every element is multiplied by its own complex conjugate right. You added all of them what are we got 1 right.

Now suppose I do not write 1, I write i any integer between 1 and N this will be perfectly valid right so till that thought. Now let us work out something else first row into second column we want 2 element even before start working what is the 12 element going to be 0 right unit matrix. First row multiply by second column what will it be a11 a21 star + a12 a22 star and so and so forth and finally a1N a2N star that is = 0 right.

Ring a bell does it ring a bell does that remind you something not only orthogonal, orthonormal when you multiply an element with itself not itself with with conjugate of itself right and you add everything in the set then you get 1 right that means the normalisation is 1 sum of square is normalised 1. When you multiply this by complex conjugate of something else and then you add up then you get 0, is that not worth you get in a set of orthonormal vectors right. So, see all of a sudden this innocuous matrix has taken up this magical property.

That you can associate with sets of orthogonal factors ok. Now things get interesting now you can use it in quantum mechanics now you can use it in symmetry. How do you write it in general sum over i aij combine both I am right combine both see instead of 1 already we have put i instead of the second digit let us put j. So, first 1 is what sum over i sum over j aij aij star sum over j from j= 1 to n aij aij star that = 1 leave it there.

Then next for the second 1 right so now can we combine 2 in 1 statement in the first case it is = 1 in the second place it is = 0 right either 1 or 0 what is that somebody gave that answer right in some other context is Kronecker delta can I combine the 2 line into one statements right and equal to can I write Kronecker delta ok work it out difficult to say too and I was not intentionally I want you to work it out, work it out and this is what it will start with on Tuesday alright.

But the take home message today is see that is not get any matrix when you work with unitary matrices then you have the magical transformation into collection of sets of orthonormal vectors which are ubiquitous in quantum mechanics that is why we can now use this matrices in quantum mechanics. In next day we try to learn something more we try to see; everybody knows about the eigenvalues equation right.

Somebody says eigenvalue equation what is eigenvalue equation? Eigenvalue equation an operator on side gives you some number multiplied by the same side that is called eigenvalue equation function is Eigen function the number that you get his call Eigen value. Now next what we learn is that using matrices you can right eigenvalue equations, Matrix Eigen value equation right so that from then so we take go on forever and eventually we will be able to understand where this great orthogonality theorem comes that is the ultimate goal of the session of the course.