Advanced Mathematical Methods for Chemistry

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Module - 02
Lecture - 05
Recap of Module 2, Matrices, Practice Problems

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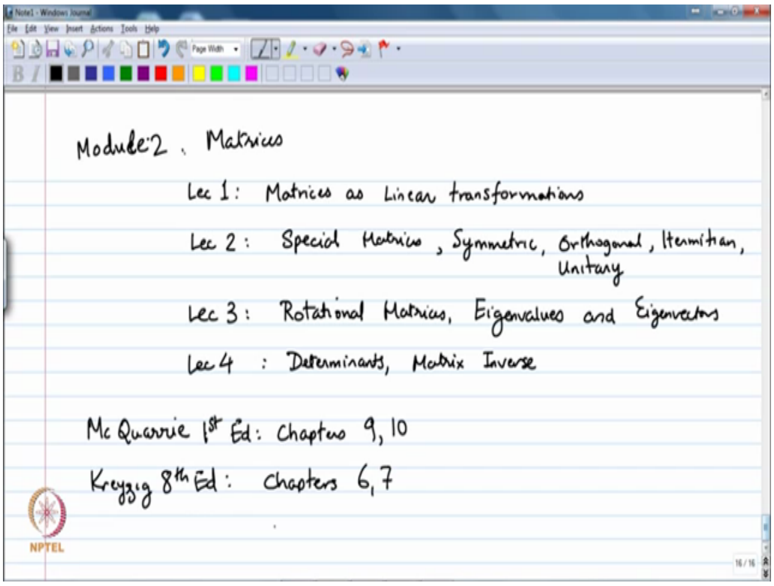

In module 2 we have discussed matrices and, so in the first lecture we talked about matrices as linear transformations of vectors. Then in the second lecture we talked about special matrices, we talked about symmetric, orthogonal, Hermitian and unitary matrices. Then in the third lecture we talked about rotational matrices and we talked about eigenvalues and eigenvectors of matrices, and then in the 4th lecture we touched on determinants and we talked about inverse of matrices.

So, now, this material you can find in Mc Quarrie 1st edition chapters 9 and 10 or Kreyzig 8th edition chapter 6 and 7. And let me emphasize that in both these books they do many more things with matrices, many more things with matrices and determinants and vectors such as change of basis, they look at transformations and so on. But, you should it is all these are, there are severally several useful tools involving these and we have just touched upon a few of them here.

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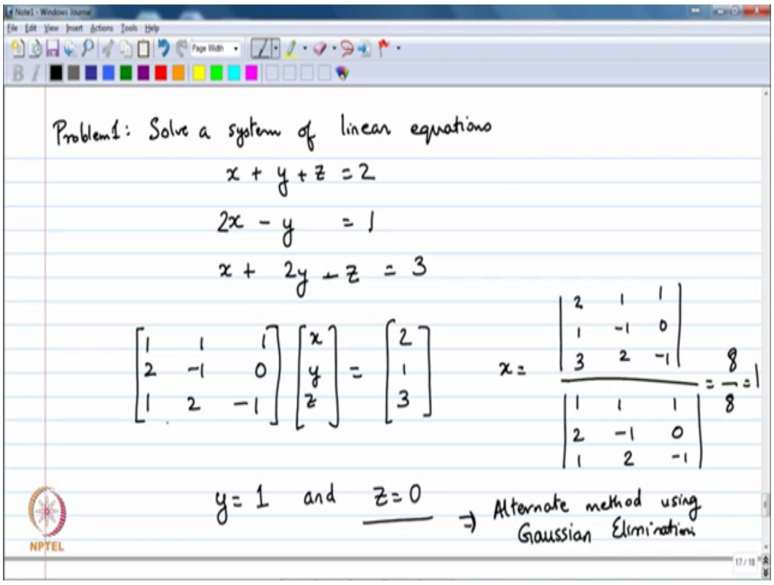

So, now I will do a few practice problems and the first one is to is solve a system of linear equations. So, let us take the system - let us say x plus y plus z equal to 2 and then in then we have x plus y or 2 x minus y equal to 1 and you have x plus 2 y minus z equal to 3. So, suppose you want to solve this system (Refer Time: 02:27) equations, so you want to solve them and get the values of x y z. So, what you do is you look at your matrix. So, the matrix of the; the matrix of coefficients is 1 1 1 the second row is 2 minus 1 0. So, I can this as 0 times z and then the third row is 1 2 minus 1. So, this is your matrix of coefficients. So, this times x y z this is equal to 2 1 3. So, I can write this in this form.

And so now I can write x as this determinant of 2 1 3, 1 minus 1, 2 1 0 minus 1 divided by 1 1 1, 2 minus 1 0, 1 2 minus 1. You can easily calculate see the denominator is. So, this will give you 8 by 8 equal to 1. Similarly y is equal to is equal to 1 and z equal to 0 this is what you will find. So, you can verify that you get this as a solution and you can see that if x is 1 y is 1 z is 0 then x plus y is 2 2 x minus y is 1 x plus 2 y minus z is 3, solution using Cramer’s rule.

Now, the next problem that I want to do before I go that let me just mention that you know you can either solve this using Cramer’s rule. So, there is an alternate method using or equivalent method using a technique called Gaussian elimination and in this what you do is you do various operations various elementary row operations and convert your coefficient matrix to a diagonal matrix and once you convert it, once you convert it to a diagonal matrix you can immediately determine the values of x y z. So, I will not be doing gauss elimination, but I expect that you are familiar with gauss elimination.

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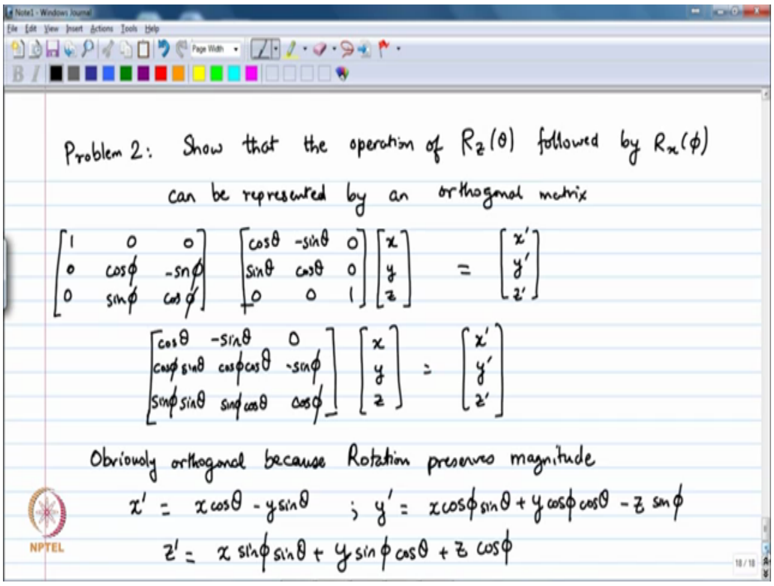

Now, the next problem that I want to do is this. So, show that the product of R z theta followed by R x phi show that the let me not call it a product, show that the operation of R z theta followed by R x phi can be represented by an orthogonal matrix and what I mean is you show it explicitly. So, let us try to show this explicitly. So, what you mean is you have a vector x y z, you operated on it by R z of theta. So, when you operate it operate on it by R z of theta you, so R z of theta is cos theta minus sin theta 0, sin theta cos theta 0, 0 0 1 and then you operate on this vector. So, this operation gives you another vector and you operate on this vector by R x of phi. So, what is R x of phi? That is 1 0 0 cos phi minus sin phi sin phi cos phi.

So, when you do this. So, you get, so let me call this x prime y prime z prime. Now I can write this, what I can do is I can write this I can do the 2 matrix multiplication first and then multiplied by the vector. So, suppose I do the 2 suppose I multiply these 2 matrices what will I get. So, 1 into cos theta, I will get a matrix minus sin theta 0, then this second column will be cos phi sin theta minus no will just be cos phi sin theta, this into this, this into this, this into this, this into this, now the third. So, then now the next element will be 0 into sin phi 0, so you have cos phi cos theta theta and the last one give me 0 0 and I have minus sin phi. Now in the last column will have 0 sin phi sin theta and 0 sin phi cos theta and I have 0 0 and I have cos phi.

So, this is what my this is what my this product of 2 these 2 matrices looks like and this when it operates on x y z will give me x prime y prime z prime. Now I want do this explicitly, but you can show that, you can show 2 things you can show that this is an orthogonal matrix. You can show that this matrix is basically orthogonal, by show I mean it is; obviously, orthogonal because rotation preserves direction preserves magnitude not direction preserves magnitude of a vector, but you can explicitly show this by showing by doing the following.

So, x prime is equal to. So, you say x cos theta minus y sin theta, then you have y prime is equal to x cos phi sin theta plus y cos phi cos theta minus z sin phi and and z prime is equal to x sin phi sin theta plus y sin phi cos theta plus z cos phi.

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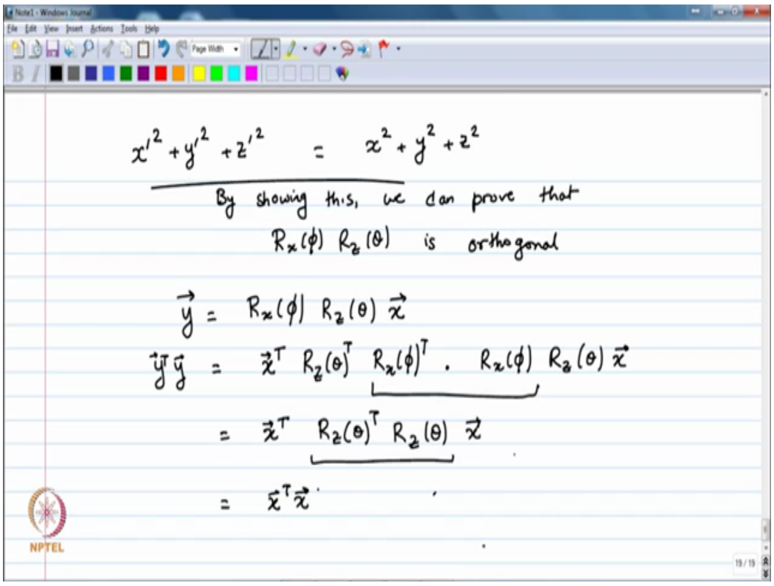

So, now you can show this explicitly by showing that x prime square plus y prime square plus z prime square is the same as x square plus y square plus z square can show this, this we can prove that R x of phi R z of theta is orthogonal.

So, so we sort of went a bit round about. So, we took I mean we intuitively know that a product of rotations should be an orthogonal matrix because a product of rotations will preserve the magnitude of the vector. So, if each rotation will preserve the magnitude.

So, the product should be an orthogonal matrix, but we can show it explicitly by doing through this procedure by seeing what the new coordinates are. So, this is a final coordinates x prime y prime and z prime, and we express them in terms of x y z. Now if you square this you will get various terms. So, will get x square cos square theta you will have y square sin square theta, you will have and you will have the cross terms x y 2 x y cos theta sin theta.

Similarly when you take y prime square you will get you get various terms and similarly z prime square will give you various terms and if you add all of them you collect all the terms you will get that this they satisfy this relation and by showing this you can prove that this product of rotations yields in orthogonal matrix, yields a matrix that is orthogonal.

Another way to do this yet another way to show this is to look at. So, if you say y is equal to R x of pi R z of theta y vector times x. So, if you take a vector x operate bit by R z of theta and by R x of phi. So, I can say I just call the corresponding vector y and what you need to show is that y transpose y. So, if you think of y as a column matrix and y transpose y is equal to, now, this is transpose of this whole thing, now when you take the transpose of this whole thing you have to take the transpose in the opposite order. So, it is x transpose R z theta transpose R x phi transpose times R x of phi R z of theta x. So, this is this is y, this is y, this is y transpose.

Now, now I can do this products in this way. So, I would multiply these 2 things first. So, R x of phi transpose R x of phi, now since R x is a rotation about x axis this is an orthogonal matrix. So, the transpose is nothing, but the inverse. So, this product is just the identity. So, I can write this as x transpose R z of theta transpose, this is just identity so I do not need to write anything and so, I just copy the R z of theta x I want to show the vector this. So, let me just put vectors onto all the x's, x's and y's.

So, now again I have R z of theta transports R z of theta which is nothing, but the identity. So, this is nothing, but the identity matrix, this equal to x transpose x. So, clearly this product is orthogonal. So, a third way to show it is this and so, if you take product of any 2 rotations you get another orthogonal matrix.

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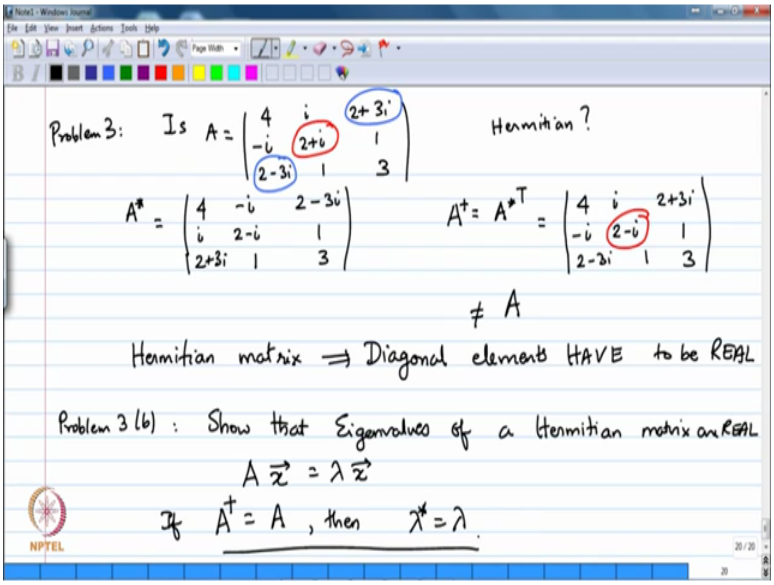

Next problem that I want to do has to do with Hermitian matrices and, this is problem 3 is this matrix 4 i 2 plus 3 i and since I want to talk about Hermitian matrices I am making it a complex matrix 1, 2 minus 3 i 1 3, is this Hermitian. So, if you call this as A equal to this then A star is equal to 4 minus i, so we take the complex conjugate of i is minus i complex conjugate of 2 plus 3 i is 2 minus 3 i, complex conjugate of minus i is i, this is 2 minus i 1 2 plus 3 i 1 3. So, complex conjugate of a real number is just itself and if you take a dagger this is nothing but it takes a complex conjugate and then you take the transpose. So, this is equal to, so you are just going to take the transpose of this matrix and transpose of that matrix is just given by 4 i 2 plus 3 i minus i 2 minus i 1 and 2 minus 3 i 1 3.

So, this is clearly this is not equal to A, and the reason it is not equal to A is because of this, everything else is the same it is only this 2 minus i and in this case you had 2 plus i. So, that was the difference. Now what I want to emphasize is that for a Hermitian matrix implies that the diagonal elements have to be real. So, the diagonal elements of a Hermitian matrix have to be real the off diagonal elements should be complex conjugates of each other. So, for example, you had a 2 minus I here or 2 minus 3 I then you should have a 2 plus 3 I there. So, that is the condition for a Hermitian matrix.

Now, next part of this problem, problem 3 b, show that eigenvalues of a Hermitian matrix are real. So, suppose you have a Hermitian matrix you show that its eigenvalues have to be real. So, suppose you have a matrix A and x equal to lambda x. So, if A dagger equal to A then lambda star equal to lambda. So, you have to show this, this is what you have to show, you have to show that if A is a Hermitian matrix then its eigenvalues are real.

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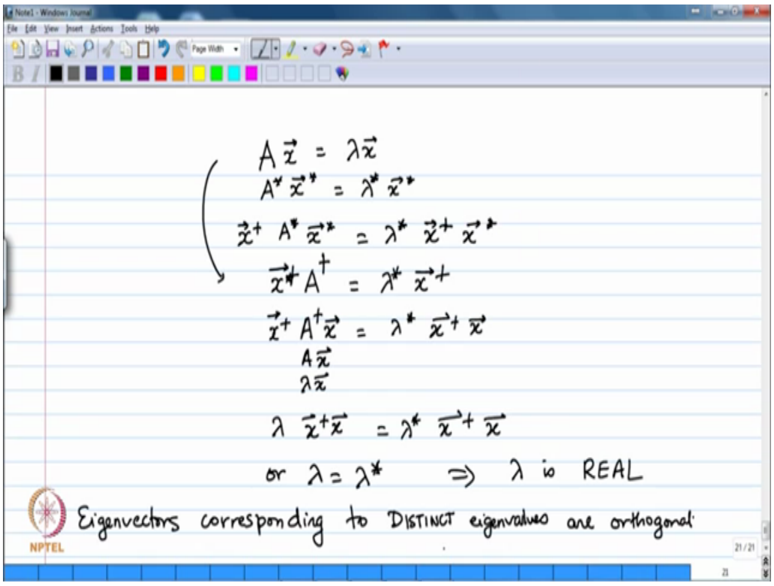

And you can show this quite easily. So, suppose you take A x equal to lambda x now this implies that A star you just take complex conjugates on both sides. So, you get A star x star is equal to lambda star x star, now if you pre multiply by A by x dagger, you do x dagger A star x star is equal to lambda star x dagger x star. So, now, if you do another thing, let us say you take the first equation and you take its Hermitian conjugate. So, if you take this equation and take its Hermitian conjugate you will get, so you will be taking both the transpose and the complex conjugate. So, what you will get is x dagger A dagger. So, the order changes because when you take the transpose of a product, you get the product of transpose in the opposite order.

Now, lambda is just a scalar. So, I can just write lambda star and x dagger I should write x dagger. So, now, if I post multiply by if I post multiply by x star yeah. So, now, if I use if I post multiply by x by just post multiplied by x what I will get is x dagger A dagger x is equal to lambda star x dagger x and A dagger x is nothing, but A x. So, this is A x. So, this is equal to A x this is equal to lambda x. So, what I get is that lambda times x dagger x is equal to lambda star times x dagger x or lambda equal to lambda star, so implies lambda is real.

So, Hermitian matrix has real eigenvalues further. So, distinct, so eigenvectors corresponding to distinct eigenvalues are orthogonal and what we mean by this is that.

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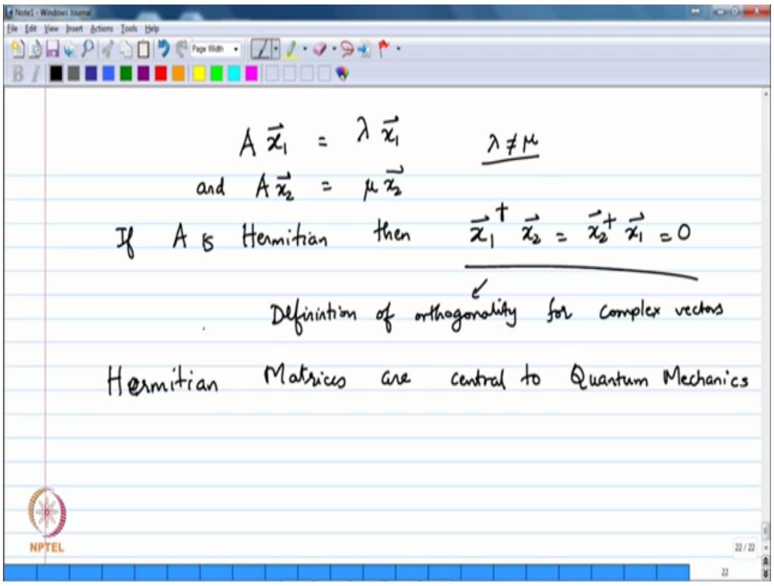

Suppose you had A x 1 is equal to lambda x 1 and A x 2 equal to mu x 2. If A is Hermitian then x 1 dagger x 2 is equal to x 2 dagger x 1 equal to 0. So, x 1 dagger x 2 is a scalar and you will show, you will be able to show that if this of course, we are assuming that lambda, lambda not equal to mu. So, they are distinct eigenvalues. So, the eigenvectors corresponding to distinct eigenvalues are real, this is oh sorry, eigenvectors corresponding to distinct eigenvalues are orthogonal.

Now, now notice that the definition of orthogonality, definition of orthogonality for complex vectors. So, this involves transpose and conjugate. So, whenever you are dealing with complex vectors or complex matrices then instead of just doing the transpose you should do a transpose followed by the complex conjugate. So, this illustrates 2 properties of Hermitian matrices which are actually extremely important. So, Hermitian matrices are central to quantum mechanics.

So, Hermitian matrix you can write a differential expression for an operator and so, you can define something called a Hermitian operator or you can write a matrix representation of an operator and that involves Hermitian matrices. So, the idea of Hermitian quantities are central to quantum mechanics because they have real eigenvalues, eigenvalues corresponds to observed values. So, if you have an observable then its value should be real. So, it should have real eigenvalues and the matrix that has real eigenvalues are the Hermitian, is a Hermitian matrix.

So, this idea of Hermitian matrices plays a very important role in quantum mechanics. So, with that I will conclude module 2.