Chemistry Atomic Structure and Chemical Bonding
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Lecture - 05
Elementary Mathematics: Introduction to Matrix Algebra
Part I

Welcome back to the lectures in Chemistry and the topic being Atomic Structure and Chemical Bonding. I am Mangala Sunder from the Department of Chemistry, where I am a professor in the Indian Institute of Technology Madras and my email addresses are given here ok.

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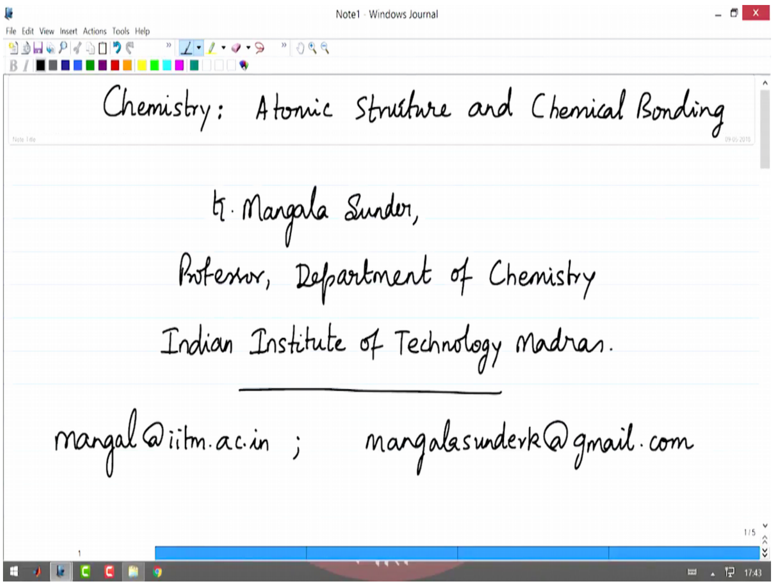

Now, this lecture is the first of several lectures on introductory matrix algebra. Matrices are extremely important, quantities for understanding principles of quantum mechanics and also for applications calculating and computing large scale applications in quantum mechanics.

When quantum mechanics was first discovered within a year there were two formulations the one by, professor Max Born Werner Heisenberg and Pascal Jordan proposed quantum mechanics, using matrices the other formulation of quantum mechanics was proposed by professor Erwin Schrodinger, where he employed the differential equations. A third formulation of quantum mechanics came much later, due to professor Richard Feynman from Caltech and that is known as the path integral formulation of quantum mechanics, which we will not consider in this course.

The preliminary part on matrices is very important for our calculations and also some of the applications and we have to learn what are called the eigenvalues and eigenvectors and how the Schrödinger equation itself is an eigenvalue equation and so on. Therefore, introductory matrix algebra is part and parcel of this course and of course, I will take you through fairly elementary parts of matrices. Later courses, I will do somewhat more advanced matrix algebra.

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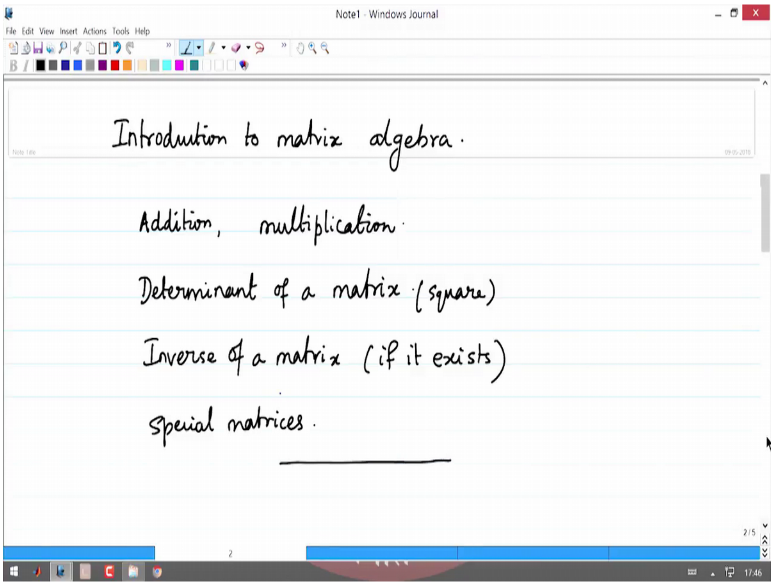

Now, in this lecture what are we going to look at? I have them here, it is an introduction and let us just go back and just revise the basic ideas like; addition between addition of matrices multiplication. We will also talk about determinant of a matrix, particularly when the matrix is a square matrix. We will see that and we will also see an example, true for finding the inverse of a matrix, wherever the inverse exists and then we shall define a few special types of matrices, which are important for quantum mechanical studies ok. So, let us start with the first one; namely the addition of matrices.

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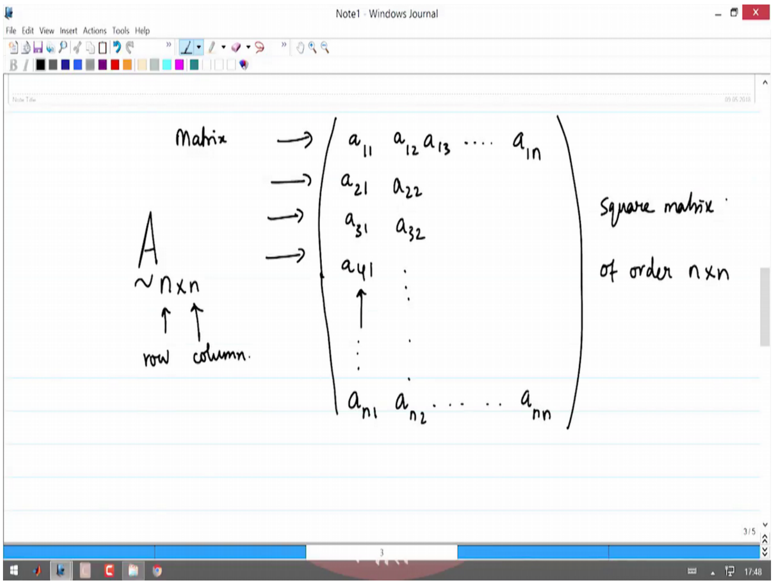

First of all matrix, matrix is an array and you write a matrix, it is essentially an array of quantities which are usually labeled by the row numbers and the column numbers. It consists of rows; row 1, row 2, row 3, row 4, etcetera and the first index of the entries are usually given by the row numbers; a 3 1, a 4 1 so, all these indices the first index. All of these are row numbers and then we have the column numbers a 1, 2, a 1 3 etcetera. So, a matrix is an n by n matrix, if it has n rows; a n 1, a 2 2, a 3 2 it has and n columns.

So, we have a n n, such a matrix is called the square matrix and the entities inside the entries inside can be numbers, can be functions, can be any other quantities with specific properties and so on, but once you write this in the form of a matrix, it has a very special structure. The arrangement and the order is extremely important. This is a square matrix of order n by n, we call it as order n by n. So, if you write this as a matrix a then you simply write this as a n by n to indicate that this is a row and this is the column number. Therefore the matrices can also be rectangular.

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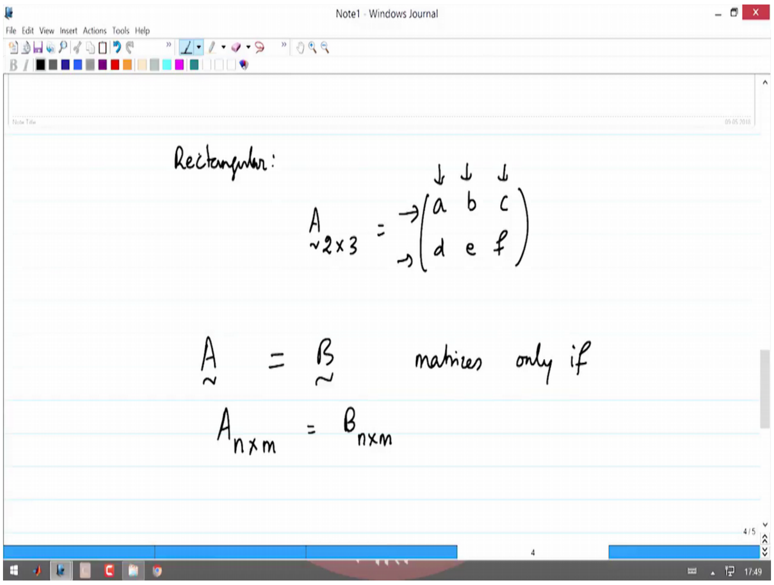

For example; if you write a matrix a as say two by three you can have something like a b c d e f. If you like, these are some entries of the, these are all the entries inside the matrix and so, this has 2 rows and 3 columns. This is a rectangular matrix ok. Now, the simplest property of the matrices is that, if you say your matrix A is equal to a matrix B matrices only, if the order of the matrix is the same. Suppose, this is n by m then B is also n by m. Therefore, if it has n rows and m columns, B should also have n rows and m columns not anything else.

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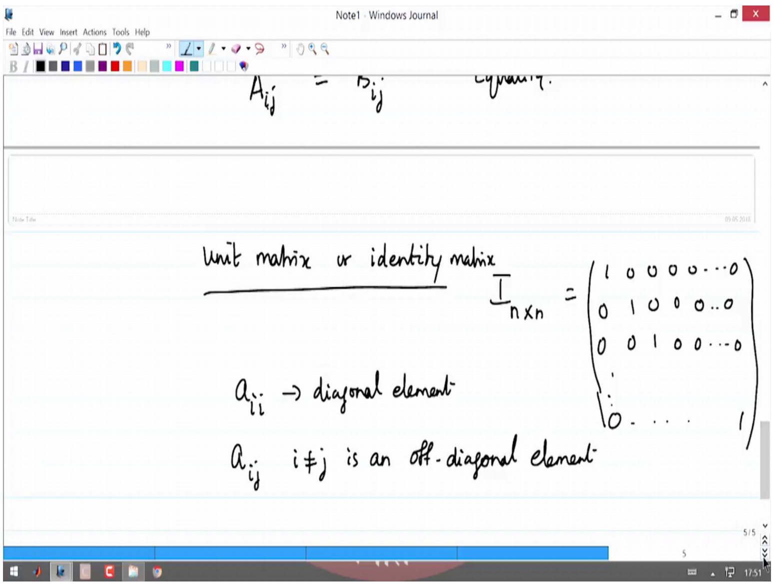

Secondly, every element of the matrix A i j corresponding to the entry in the ith row and the jth column. Every element should be the same as the corresponding element B i j. So, two matrices are equal only if on both sides you have exactly, the same number of rows and columns and each element in a specific row and the column is exactly the same as the, element in the other matrix in the same row and column. So, this is equality, second is an important property called the, unit matrix or identity matrix or identity and we usually write this by i, an unit matrix and identity matrix is square. So, we call this I n by n and all it has is 1 0 0 0 that is the diagonal elements of the matrix, all have entry 1 and last is 1.

So, a i i is the diagonal element a i j i not equal to j is known as the, is an off diagonal element, but this we see that the unit matrix are the identity matrix, as we have it, has once along all the diagonals and 0s along all the other entries along all the off diagonal elements. Now, what is meant by addition of two matrices.

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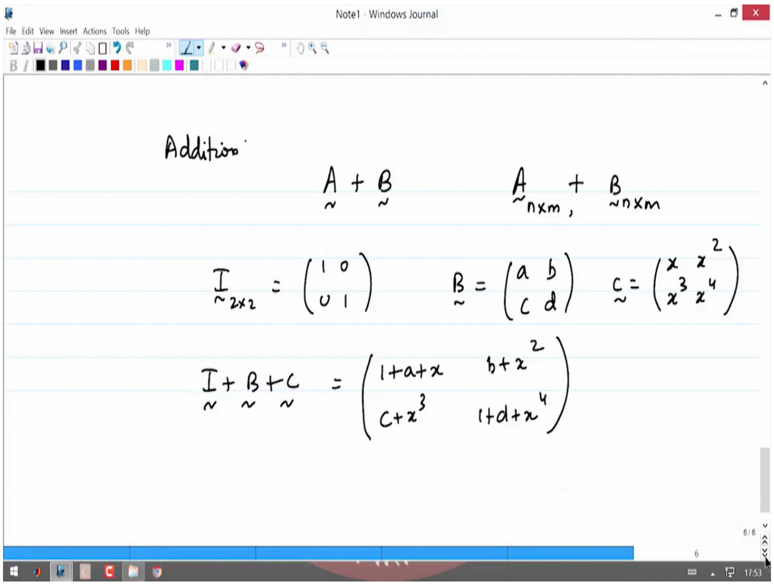

Two matrices can be added A plus B if and only if A is n by m and B is also n by m otherwise, matrices cannot be added. There is a special edition which we will consider later, when we study group theory called a director edition, but in this course, we will not need that. So, direct edition essentially means that putting these added elements along a super matrix for this course. Addition essentially means that two matrices can be added only if they have the same number of rows and the same number of columns.

So, an example that we have is if you write I 2 by 2. Let us write that as 1 0 0 1 and let us write another matrix B as a b c d and a third matrix C as some quantity x x squared x cubed and x raised to 4, then what is meant by A plus B plus C, these are all matrices. So, I will keep the underscore to indicate that they are sort of operators. We will see that later A B C is clearly the addition; when each element in a particular row in the column is added to the element of the other matrix in the same row, in the column. So, the first row in the first column, the element will be 1 plus a plus x.

The first row and the second column will be 0 plus b plus x square and the second row, first column it is c plus x cube and the second row, second column is 1 plus d plus x raise to 4 ok. This is what is meant by addition. Now, subtraction is addition with a minus sign therefore, if you say A plus B minus C; obviously, all the elements of C will be minus. Now, let me do that.

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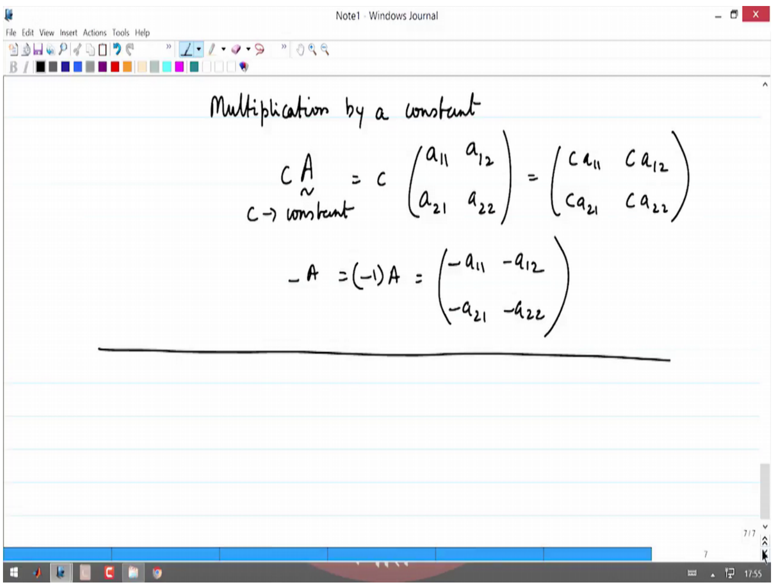

Therefore, multiplication of a matrix by a constant is to be introduced multiplication by a constant. So, if we write c times a and we write the c is a constant and a; for example, let us write this using the notation. The first row element, first column, first row, second column, second row, first column, second row, second column.

This means that every element is multiplied by the constant c a 1 1, c a 1 2, c a 2 1, c a 2 2. This is what is meant by multiplication of a matrix, using a constant therefore, minus a is minus 1 times a, which means minus a 1 1 minus a 1 2 minus a 2 1 minus a 2 2 therefore, now for the same A B C matrix that we have.

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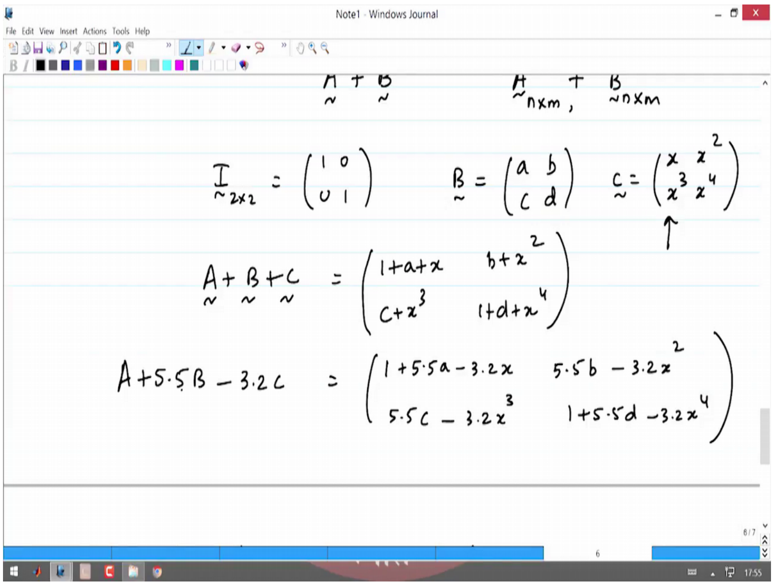

Suppose, I want to write A plus 5.5 B minus 3.2 C. Suppose I have to write that then you have to multiply each of the matrix by the corresponding constant and in this case B is 5.5 and A is 1. So, you have 1 plus 5.5 a minus 3.2 x c multiplied by 3.2 minus 3.2 and likewise 5.5 b minus 3.2 x square and c is also 5.5 c minus 3.2 x cube and the last one is, there is 1 here for this a. So, 1 then we have plus 5.5 d minus 3.2 x to the 4.

So, this is what is meant by addition of matrices and multiplication by a constant. So, there are quite lot of simple exercises that you can do, but let us get very quickly, this is a refresher. Therefore, let us, very quickly move to what is called the matrix multiplication ok, multiplication of two matrices ok.

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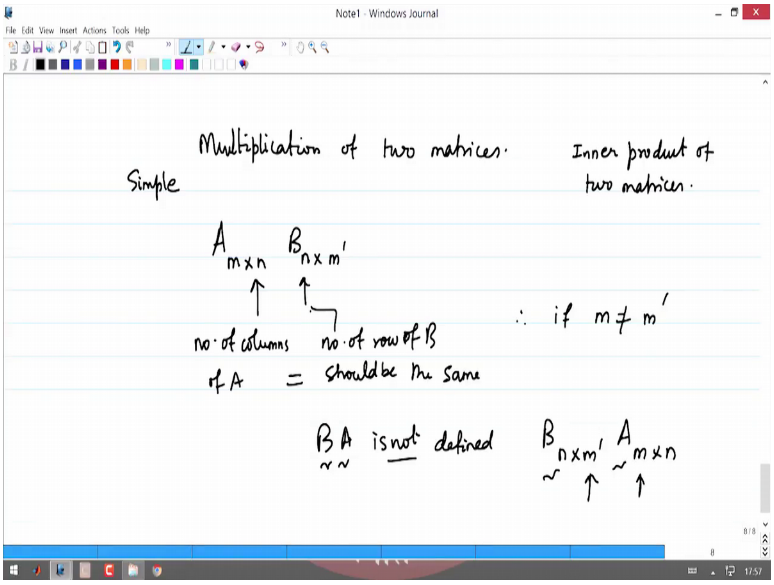

So multiplication for two matrices simple multiplication are called the inner product of matrices. It is also called the inner product of two matrices, it can be done if only A is for example, order m by n then B has to have n rows and any number of columns. So, the number of columns of A and the number of rows of B should be the same should be the same rows of B.

Therefore, if m is not equal to m prime then B A is not defined. It is not defined, why? Because B is n m prime and A is m n, if these two are different then this multiplication is not defined. So, in multiplying two matrices, it is important to have the number of columns of the left hand matrix to be the same as the number of rows of the right hand matrix, that is all. On the other hand, if you have say for example, two rectangular matrices.

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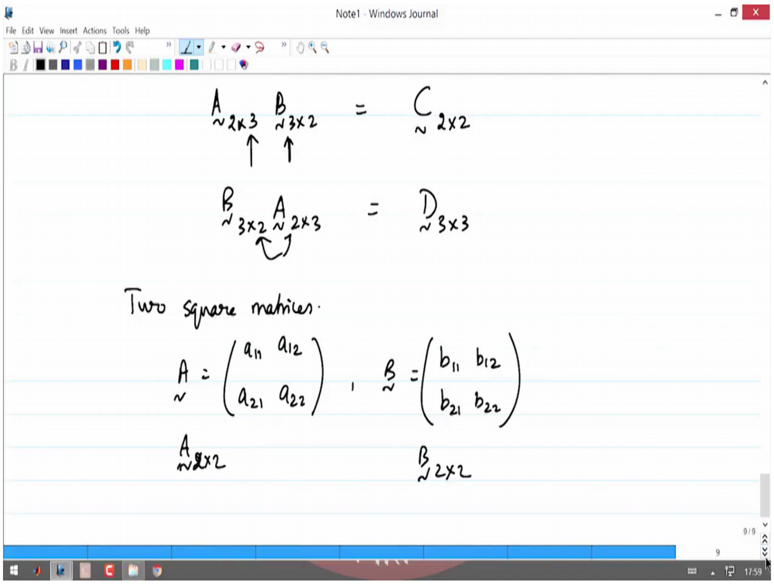

A 2 by 3 and you multiply B with another matrix, which is probably another rectangular matrix 3 by 2. This is defined, because the rows are the columns and the rows are equal, the product is a matrix C, which is A 2 by 2.

However, if you do this product B 3 by 2 and you multiply A 2 by 3 then you see the rows and the columns and rows are still equal, but the product is something else. It is another matrix D 3 by 3 and the C and D are not equal, because they do not match in terms of the rows and columns ok. So, matrix multiplication is something that you have to do. Let us do that very quickly, what is meant by the individual elements in the products. So, let me write two square matrices. So, they have two matrices; A 2 by 2 and B 2 by 2 therefore, the product of this is also A 2 by 2 matrix, what is the product?

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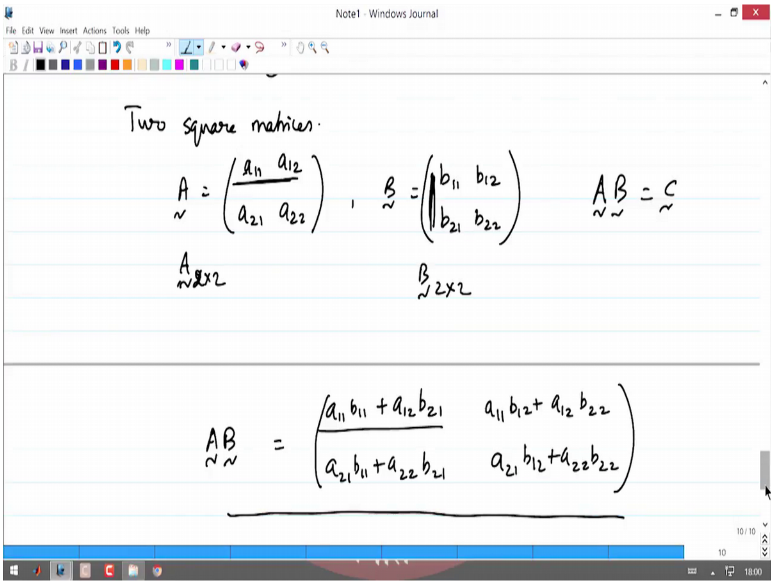

The, the row of the first matrix containing two columns is multiplied element by element with the first column of the second matrix to give the first row, first column element of A B. So, if you define A B to be C then A B is first one is a 1 1 b 1 1 plus a 1 2 b 1 2 b 2 1 a 1 2 b 2 1. This is the first row, first column element of the product obtained by multiplying the row of A with the column of B.

Therefore, you see why the number of columns of A and the number of rows of A should match. Now, the second element; the first row, second column element is the multiplication of the first row with the second column. So, this is a 1 1 b 1 2 plus a 1 2 b 2 2 and likewise the others a 2 1 b 1 1 plus a 2 2 b 2 1 and a 2 1 b 1 2 plus a 2 2 b 2 2 ok. There is a nice little flash animation that I would like to play and sort of a childhood toy, I should say, but it is still good to see this.

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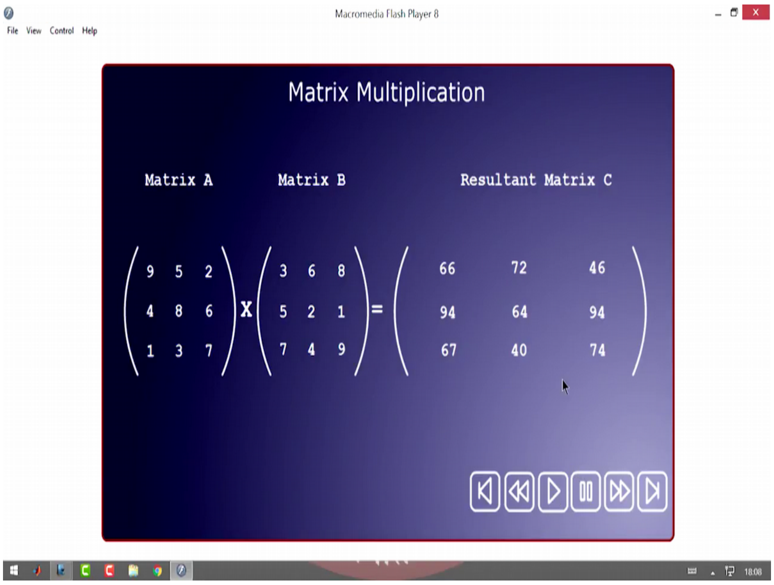

So, I will play a simple 3 by 3 matrix multiplication, through the flash movie. This is matrix A and matrix B. So, you can see that the first row, first column multiplication element by element and addition gives you the first row, first column element 1 1 of the resultant matrix, first row and second column of matrix A and matrix B gives you 1 2 element of matrix C.

This is how simple matrix multiplication is defined and is also known as the inner product of matrices ok. So, pretty good idea. How to do multiply matrices, complex or no complex, you can still do that ok. Now, the same thing holds good for rectangular matrices as well.

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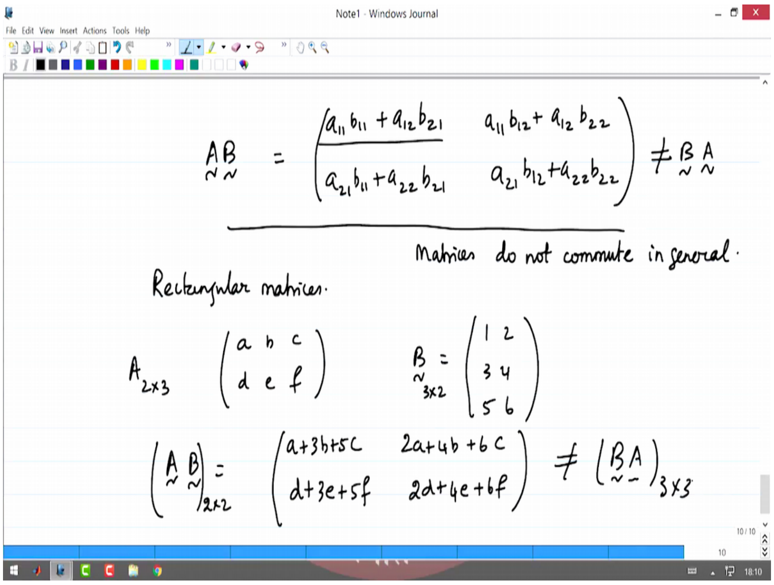

Anyway, before I forget, this is not equal to the matrix B A. If all these elements are non-zero. You see that B A will have a different set of elements and therefore, the matrices do not generally, commute. In general, you cannot move them around a b c. On the other hand, let us take a simple rectangular matrix before we move to more complex multiplication. Let us take a 2 by 3 matrix something like a b c d e f. Let us call this as A 2 by 3 and let us have another matrix B, which is A 3 by 2. So, let us call this as 1 2 3 4 5 6.

For example now, what is A times B? It is going to be a b c multiplying 1 3 5 and you can see that the resultant number of rows and columns will be 2 by 2 2 and 2. So, this will be the first element being a plus 3 b plus 5 c, the second element is 2 a that is the first row, second column 2 a plus 4 b plus 6 c. And the next one is d plus 3 e plus 5 f and likewise, the last 1 2 d plus 4 e plus 6 f and you know clearly, this is not equal to b a, which is a 3 by 3 matrix and I will leave it to you 3 by 3 matrix, which I will leave it to you as an exercise to calculate. The four matrices do not commute but how about this?

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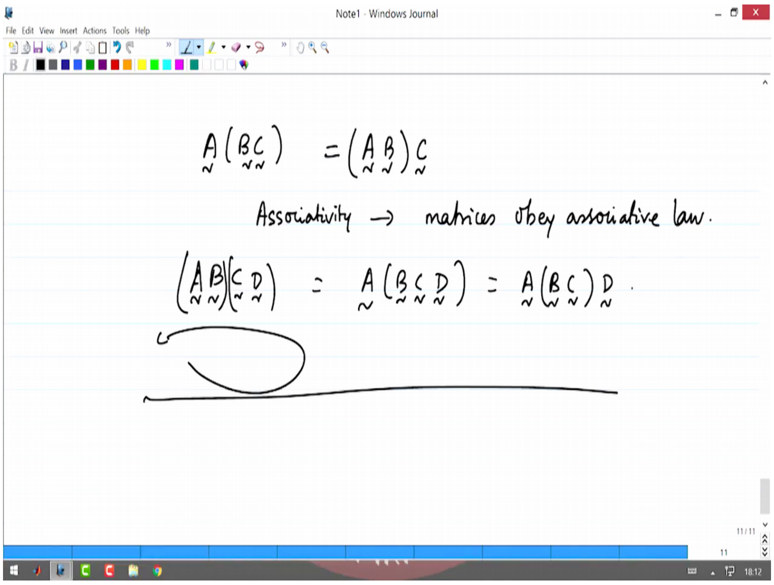

Suppose, I take the product of two matrices B and C and then I take it on the left with the multiplication by A you will always see that this is equal to having the product of A and B first and then multiplying C on the right side, this is called associativity. Matrices obey associative law therefore, if you have A B C D and you do the products first, then you want to do this way, it is the same thing as B C D and this is the same thing as A B C D and so on as long as you do not commute, the matrices around left right. This is, matrices obey that.

Now, let us look at a quick example of A matrix multiplication, it is slightly more difficult I mean somewhat involved, but I would leave the answers to you and, we will give you the answer, but you can work it out.

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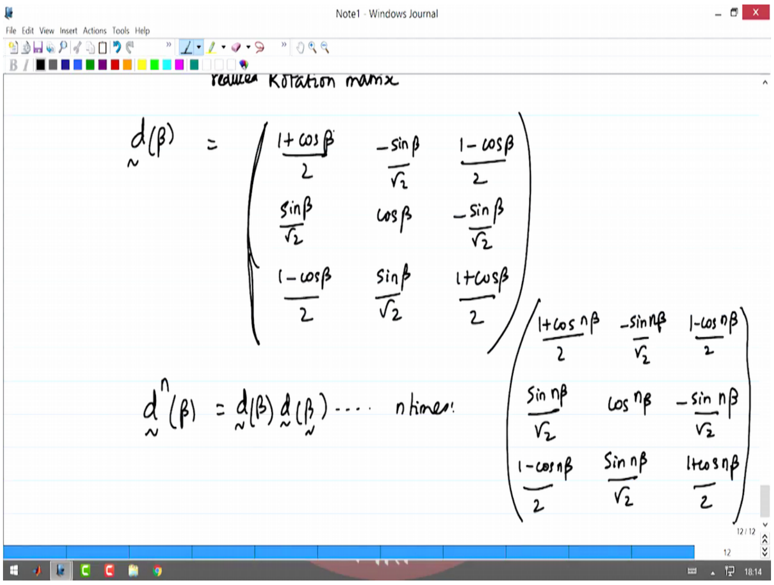

Let me write a matrix in terms of in a symbol d B is this usually called a rotation matrix in angular momentum theory ok. It is a reduced rotation matrix, what we will not concern with those properties, but we will write this as a matrix. You know 1 plus cos beta by 2 minus sin beta by root 2 1 minus cos beta by 2 sin beta by root 2 cos beta minus sin beta by root 2 1 minus cos beta by 2 sin beta by root 2 and 1 plus cos beta by 2.

Now, do the multiplication n times any number n, you can choose as 2 3 4 5 whatever it is do n time d n beta is d of beta ok, multiplied by d of beta, n times. It is a beautiful matrix and it has a very simple result that d n beta is given by 1 plus cos n beta by 2 minus sin n beta by root 2 1 minus cos n beta by 2 sin n beta by root 2 cos n beta minus sin n beta by root 2, 1 minus cos n beta by 2 sin n beta by root 2 1 plus cos n beta by 2.

It is a rotation matrix it is a very special matrix, the used in angular momentum theory and also in rotations and microwave spectroscopy in many other places, beta is the rotation angle about an axis that the system is rotated to and you can see that such matrices have very special properties. A very simple example I made instead of this.

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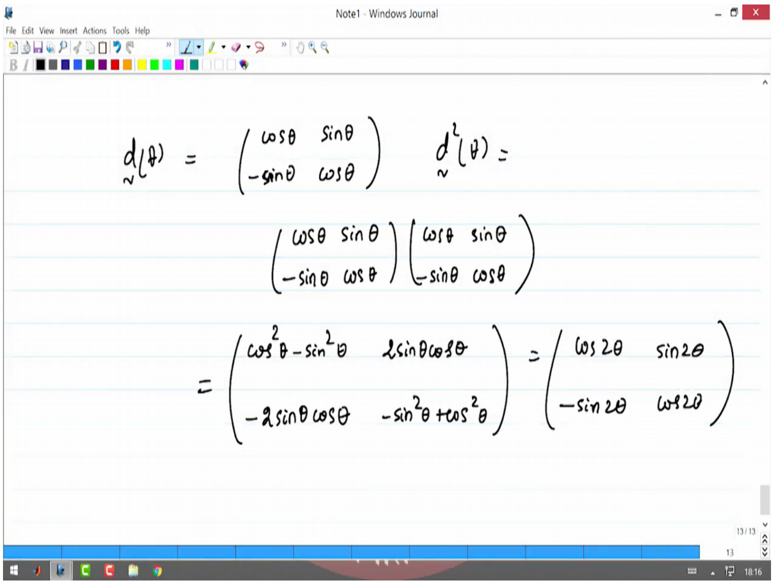

If you do a cos theta, a sin theta, a minus sin theta cos theta, if you call this as a d of theta, then what is d square of theta it is so easy to do that you see all you need to do is to multiply this with itself and you can see that immediately. It gives you cos square theta minus sin squared theta 2 sin theta cos theta minus 2 sin theta cos theta and you have minus sin squared theta plus cos square theta.

So, you see the angle formula right away that this is cos 2 theta is a sin 2 theta. This is minus sin 2 theta and this is cos 2 theta, you see that and I only generalized it to a 3 dimensional system, in the previous example and likewise, you can do many.

Pointless matrix multiplications are some things that you should be absolutely thorough with. So, let us pause for a break and we will continue this in the next session.