Chemistry Atomic Structure and Chemical Bonding
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Lecture – 13
Linear Vector Spaces: Matrix Representations

Welcome to the course on Atomic Structure and Chemical Bonding. My name is Mangala Sunder and I am a Professor of Chemistry in the Department of Chemistry in Indian Institute of Technology Madras, ok. My email id is given to you here.

Now, in this lecture we shall look into the first few lessons of the mathematics of Quantum Mechanics and in doing so, we shall introduce the concept of Linear Vector Spaces.

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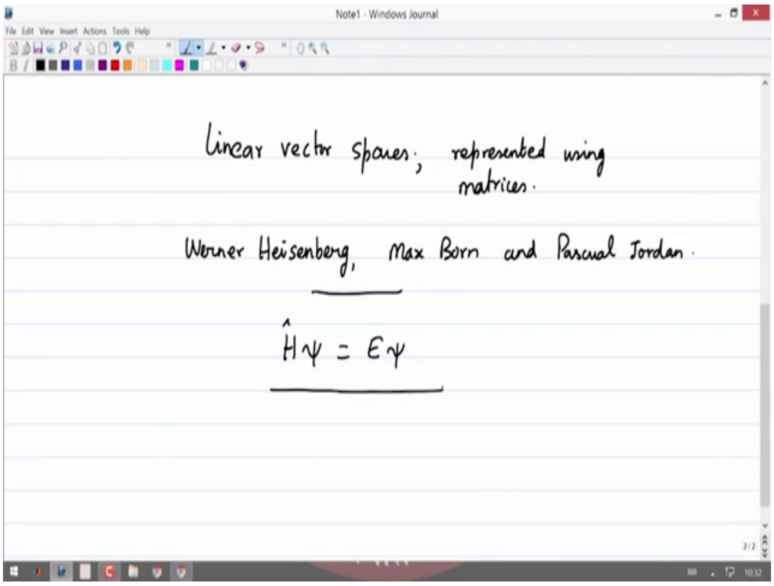

The introduction to this is through vectors, but then vectors represented formally using matrices. As you know through the lectures in the last few that the quantum mechanics proposed by Schrodinger started with differential equation model and we have a, we will be solving a few of the differential equations further in addition to what was already done, but the other form of quantum mechanics, this was done by the use of matrix mechanics and that was proposed by Werner Heisenberg, Max Born and Pascal Jordan, well Werner Heisenberg, Max Born and.

So, in this lecture of course I would give you an elementary introduction. I am not going to give you proofs and the mathematical definitions until the end of this lecture. We will start with some definitions and become comfortable using the column vectors and row vectors and matrices representing important quantities in quantum mechanics, the measurement quantities represented as operators using matrices.

So, we shall do all those things and towards the end of the lecture, I shall give you a formal introduction to the mathematics in the sense of the definition using the axiomatic method of the linear vector spaces, but this whole lecture is still hands on in the sense you should be able to do things as and be operational in the use of matrices. Please understand the Schrodinger equation which is written as H psi is equal to E psi for this course that is a time independent Hamiltonian with the wave function which of course is dependent on time, but its position dependence is what is more important to us. This equation is actually a matrix equation if you represent to the Hamiltonian which is an operator in the form of a matrix and then, you will see that the function psi is known as the Eigen function and the quantity E which is a constant and which has the dimensions of energy, the total energy is known as the Eigen value.

Therefore, whatever we do today and in the next few lectures will be very important in understanding the solutions of the Schrodinger equation using matrix methods and today practical calculations involving large scale programming and computational chemistry programs used in biology, used in medicine, used in the material science, used in physics and chemistry, all use matrix Eigen value problems are solutions. Therefore, this lecture is fundamentally important for us to understand the basics, ok.

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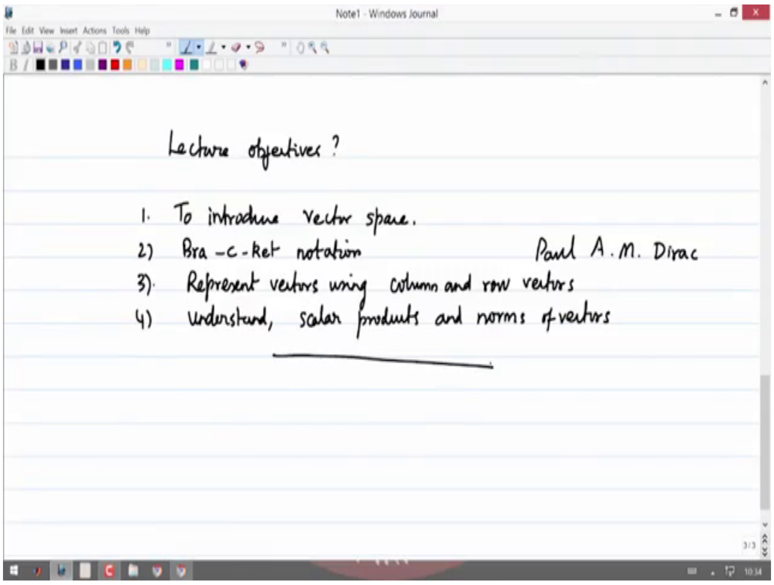

What are the lecture objectives to introduce the vector space? A special notation which has been used by Paul Dirac, Adrienne Morris Dirac known as the Bra-c-ket notation to represent vectors using matrices; basically column and row vectors and row vectors. Understand scalar products scalar products and norms of vectors all using matrices.

The sequence to this lecture will then represent the operators using matrices and we will also give you a representation the operators using what are known as the basis operator matrices and so on. Here in this lecture, we will see the vectors being represented by row vectors and column vectors.

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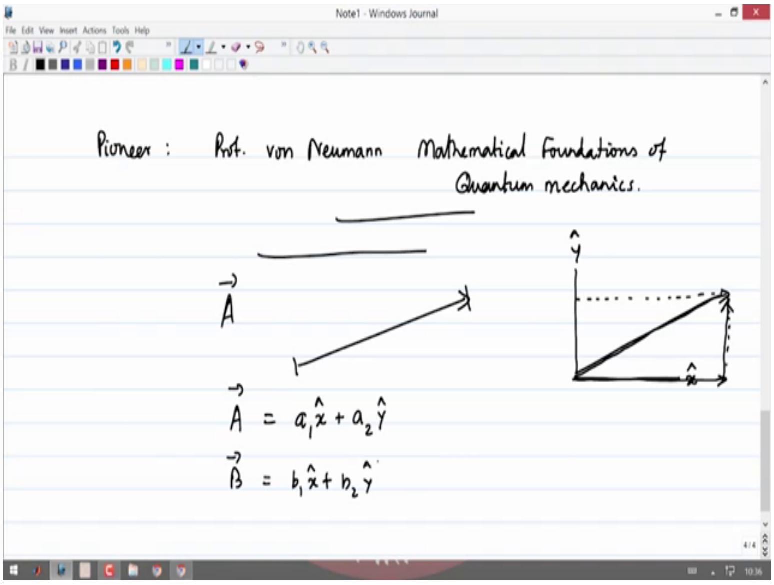

In the beginning was Professor Von Neumann who published a very famous book known as the Mathematical Foundations of Quantum Mechanics. The mathematics in this course and in many other advanced courses in quantum mechanics have all built on the fundamentals and the foundational methods which are first proposed by a Professor Von Neumann.

Now, let us start with very simple vectors in two dimensions. All of you know that if you write any vector A in two dimensions, you normally represent this vector by some arrow and the arrow tells you the direction in which the vector is a pointing to and the length of the arrow giving you the magnitude of the vector. Now, one further step is to associate a coordinate system in two dimensions. It is a planar coordinate system in which the two coordinates x and y are orthogonal to each other and if we represent the vector in the coordinate system, then we write to this vector in terms of its components namely the x component and the y component, ok.

So, this is the unit vector in the x and y direction and therefore, you write the vector A in terms of the component in the unit direction a 1 x and the component in the unit direction y, so that you know that when you have to add this to get this vector, essentially you are adding a times x which is the unit vector and two times y which is the vector in the y direction.

So, this is the point and in a similar way if you write another vector b, it has a different component b 1 x plus b 2 y and so on.

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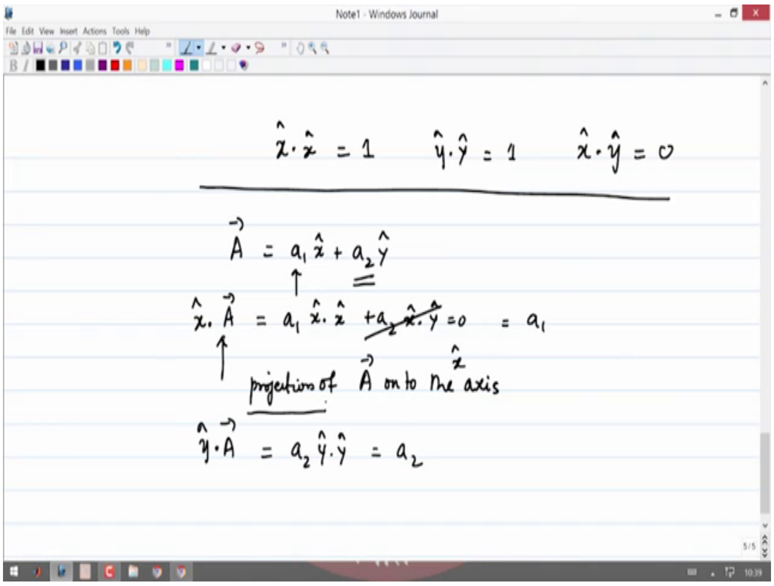

What do we mean by that? We mean by that the vector x dotted with x is unity. It is scalar 1 the vector y dotted with y, the unit vector is 1 and the scalar product between the two vectors x and y. If you recall the dimensions, the scalar product definition it is a magnitude of x and magnitude of y multiplied by the cosine theta, where theta is the angle between x and y and you know that theta is 90 degrees. Therefore, this is 0, ok.

So, this is meant as the orthogonal and normalization representation of the unit vectors. Therefore, when you write the vector A as a 1 of x plus a 2 of y, you know that the component a 1 is nothing, but the projection of the vector A onto x axis and that you know immediately it gives you a 1 x dotted with x plus a 2 x dotted with y which is 0 and therefore, and this is 1. Therefore, you have a 1. So, you know when you say component a 1 and a 2, it is a projection of the vector in that particular coordinate system projection of a onto the x axis and likewise for x axis onto the x axis and likewise for the component a 2, it is the projection of a onto the y axis which will give you a 2 times y dotted with y and that gives you a 2.

Therefore, these are projections and the word projection is important also in a later context. Therefore, keep this in mind.

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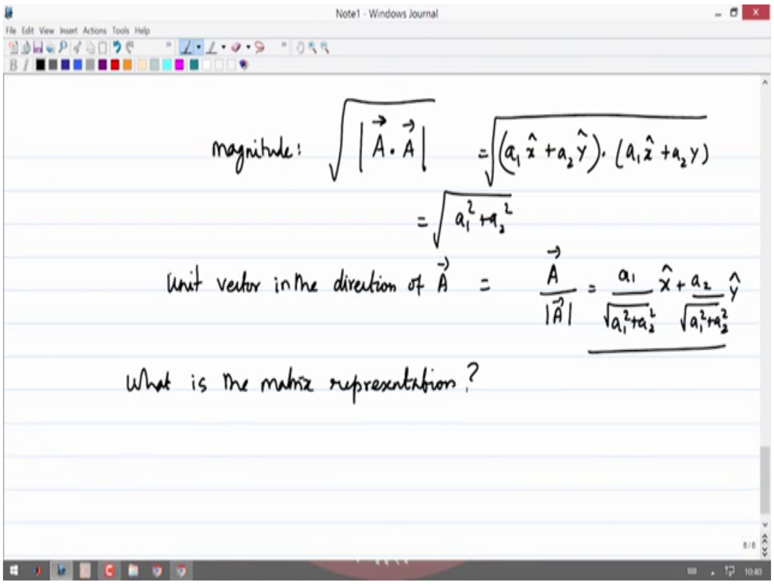

Now, when we say that a vector A has a magnitude, the vector A magnitude is actually calculated as the magnitude of a dot a. The magnitude and it is a square root, ok. A dot a gives you the square of the vector A and therefore, the magnitude of the vector A is the square root of a square and that is also very easy to write down because you write this as a 1 x plus a 2 y dotted with a 1 x plus a 2 y and it is a square root of it and therefore, that gives you a 1 square plus a 2 square and gives you the square root, ok.

Therefore, A unit vector in the direction of a, yes a divided by the magnitude of a. So, what you will have is, therefore a 1 by square root of a 1 square plus a 2 square on x plus a 2 divided by square root of a 1 square plus a 2 square on y. So, this is what is called the unit vector in the direction of a unit vector in the direction of x is of course, x hat and likewise y hat. Now, all of this is very familiar to you. Now, what is the matrix representation for all these things?

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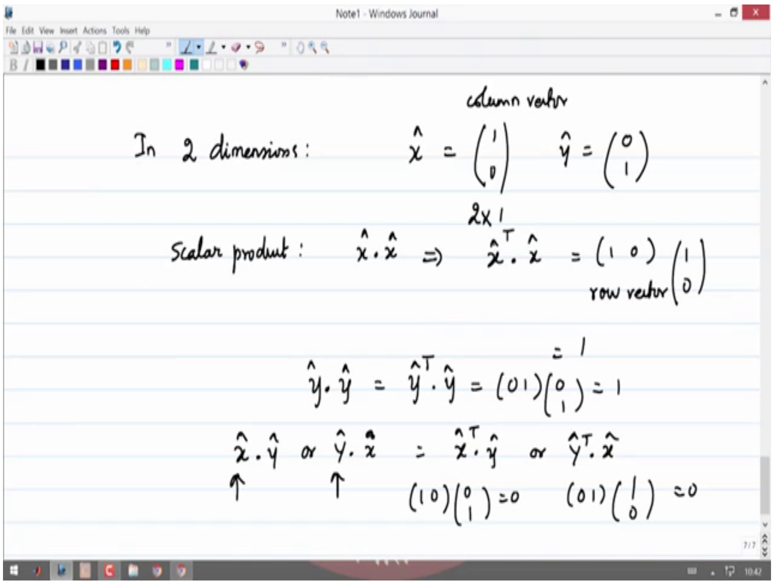

In 2 dimensions, one represents the unit vector x by a column vector 1 0. It is 2 by 1 column that is it is A matrix with the two rows and one column. That is what is 2 by 1 mean. The unit vector y is represented as 0 1 and in matrix, the scalar product between these vectors if you want to write x dotted x, then the scalar product is actually x of t, the transpose of this unit this column multiplying the vector itself.

So, the transpose of 1 0 is the transpose which is a row vector, this is a column vector and a row vector multiplied by the column vectors 1 0 gives you 1. Likewise when you write y dot y in the matrix notation, it is the transpose of the column y representing the vector y multiplying the vector y itself which is 0 1 multiplying 0 1 giving you 1 and in this notation, it is also very clear when you write x dot y or y dot x. You know both of which are 0. Essentially what it means is the left hand vector is written as transpose x T dotted y or as y T dotted x and you can see right away that if you do this x T is 1 0 and y is 0 1 which is 0 and likewise y T is 0 1 multiplying 1 0 and that is also 0.

So, this is the translation of the idea of vectors in simple physical dimension in a geometric space into a linear vector space involving abstract quantities, such as the matrices column vectors and row vectors and so on. So, this translation is important. This representation is important in understanding how to carry on this process for vectors generally in n dimension and then, the scalar products of them, then manipulating those vectors with the solutions of the Schrodinger equation and all those things etcetera.

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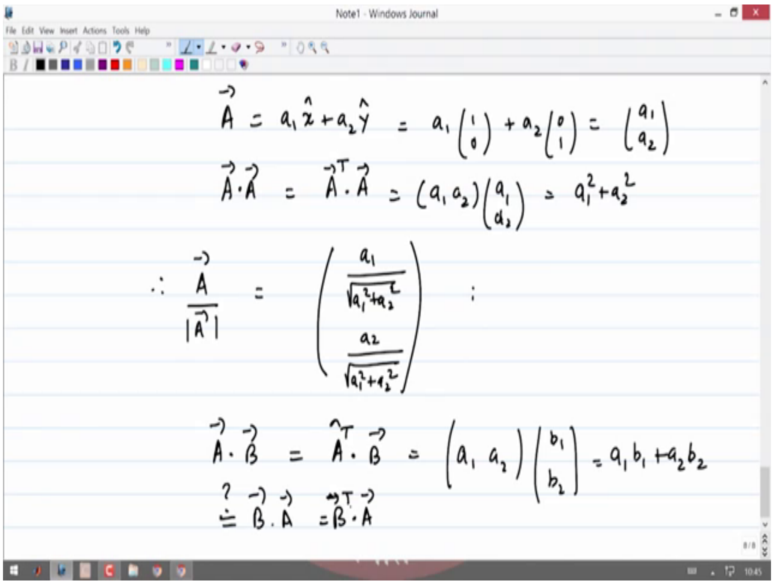

So, now given that if we write an arbitrary vector A, then you know we have written this earlier as a 1 of x and a 2 of y and that obviously now written in terms of columns. It is a 1 times 1 0 plus a 2 times 0 1 and doing the matrix addition you see that this is nothing, but the column a 1 a 2 and therefore, when you write the scalar product of a with itself what it means is it is A T dotted with A. So, what you have is a 1 a 2 a 1 a 2 and you can see right away that this gives you a 1 square plus a 2 square.

Therefore, what is the unit vector a in terms of matrices? It is the vector divided by its magnitude. You can see immediately the column is written as a 1 by square root of a 1 square plus a 2 square and the other is a 2 by square root of a 1 square plus a 2 square,. So, what is a scalar product between two vectors? It is A and B. Again the left hand vector is to be written as a transpose which is a row vector and the right hand vector remains as this. So, you can see that this is a 1 a 2 and b 1 b 2 which gives you a 1 b 1 plus a 2 b 2.

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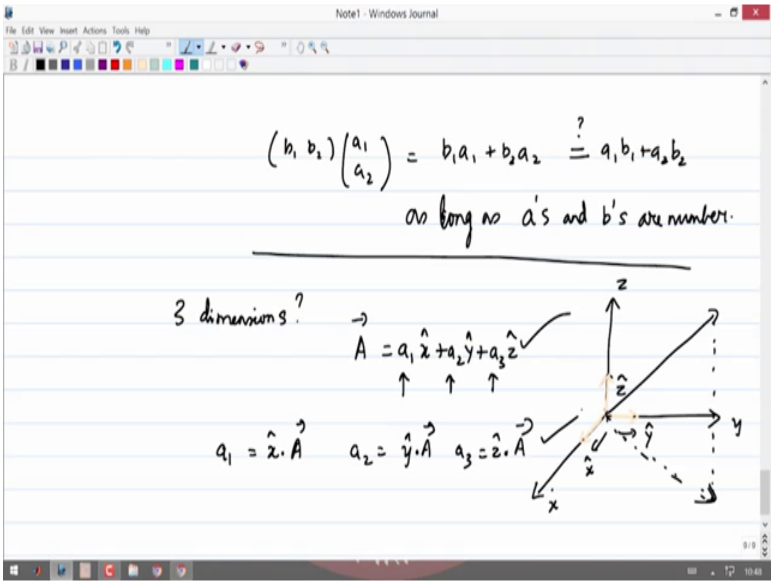

Now, is a dot b the same as b dot a it appears because if you write b T doted a the vectors, then you can see that this is nothing other than b 1 b 2 multiplying a 1 a 2 and so, you have b 1 a 1 plus b 2 a 2 which is equal to a 1 b 1 plus a 2 b 2 as long as a and b are numbers a's and b's are numbers.

This is important. We know that matrices in general do not commute when we take the product of two matrices a b and then, we compute the matrix product b a. It is not necessary that a b will give you b a. In fact, in general it won't give you that. Therefore, the matrices the order in which you multiply the matrices are important, but if we are dealing with numbers, we do not have an issue, ok. So, this is all elementary ideas. So, this is how we represent to the vectors and this is how we represent to the scalar products in two dimensions.

Now, how do we extend this to three dimensions? It is again very simple. You recall that an arbitrary vector a in three dimensions if you have to represent it geometrically, you remembered now there are 3 coordinate systems, 3 basic coordinates namely the x coordinate and there is a unit vector along the x direction, there is a unit vector along the y coordinate known as the y unit vector and there is a unit vector along the z coordinate which is called to be z. So, if I have to write this in some colors maybe you can see that this is the unit vector z and this is the unit vector x and this is the unit vector y and therefore, any arbitrary vector if you do that, any arbitrary vector is basically if you project that vector on to the xy plane and suppose it the projection looks like that, then you see that it is nothing, but the projection of xy onto this plane plus the vector along the z axis.

Therefore, a can be written as 3 components; a 1 times x plus a 2 times y plus a 3 times z. Therefore, now you have in 3 dimensions 3 independent components and these are nothing other than the projection of the vector A onto the respective axis in the unit, I mean the unit vectors in the direction of the axis. So, a 1 is x dotted A, a 2 is y dotted A and a 3 is z dotted A, ok.

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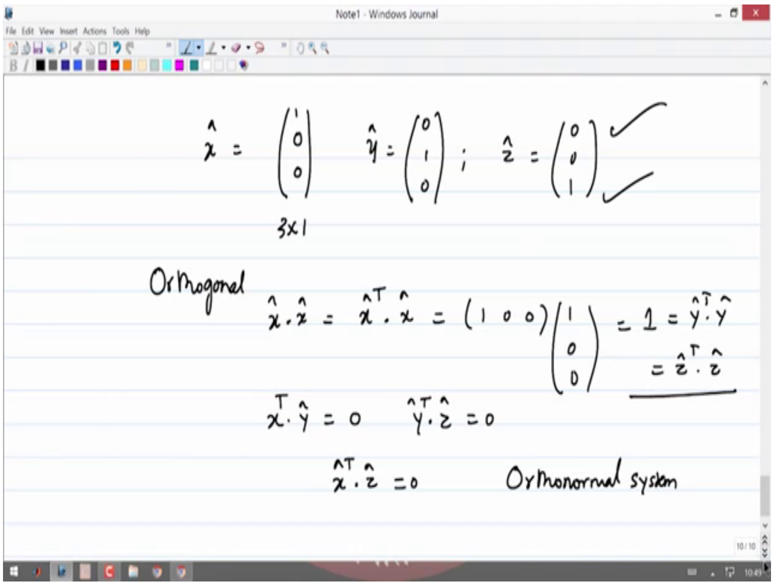

So, this is something you are familiar with; therefore, how do we represent this in terms of matrices; very simple. You write to this in terms of a matrix with a 3 row and one column with the first row being 1, second and third rows being 0 and likewise for y 0 1 0 and for z you have 0 0 1.

This is orthogonal coordinate system meaning that 3 coordinates or 3 directions are mutually perpendicular to each other. Therefore, again it is possible for us to imagine that the unit vectors along these independent 3 mutually perpendicular directions will be orthogonal to each other pair wise. So, x dot y is 0, x dot z is 0, y dot z is 0 and likewise the other way around y dot x is 0 and so on, and x dot x is 1, y dot y is 1, z dot z is 1, all these things are now replicated by these columns.

For example, if you write x dot x is nothing other than the transpose of the matrix x with itself and therefore, you have 1 0 0 multiplying 1 0 0 and that is the number 1 scalar 1 and likewise you can show this to be y T dot y as well as z T dot z, and in the same way you have x dotted with y is 0 and y dotted with z is 0 and x dotted with a z is also 0. So, again this is an orthonormal system.

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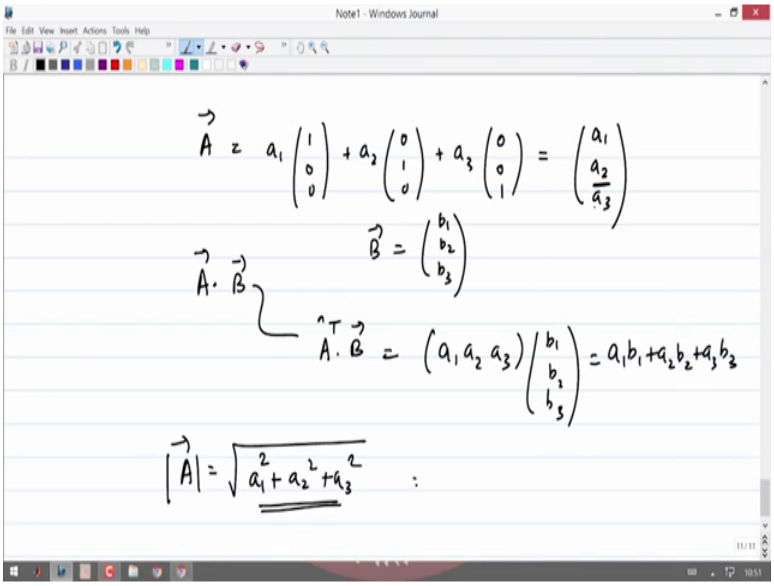

So, immediately you can see that any vector arbitrary which is written as a 1 times x which is 1 0 0 plus a2 times y which is 0 1 0 plus a 3 times z which is 0 0 1 is obviously the column vector a 1 a 2 a 3 and therefore, the scalar product between two vectors a and b if you have to write and if b is the column vector given as b 1 b 2 b 3 as the 3 components of the vector b in this in these directions, then the scalar product is a T dotted with that gives you a 1 a 2 a 3, the row multiplying the column b 1 b 2 b 3 and the answer is a 1 b 1 plus a 2 b 2 plus a 3 b 3 and in a similar way, the unit vectors of A are also very simple that the magnitude of a is now the sum of the 3 squares; a 1 square plus a 2 square plus a 3 square root.

Therefore, the vector A is obviously a 1 divided by the magnitude that is a unit vector in the direction of a, a 1 divided by this magnitude, a 2 divided by this magnitude, a 3 divided by this magnitude.

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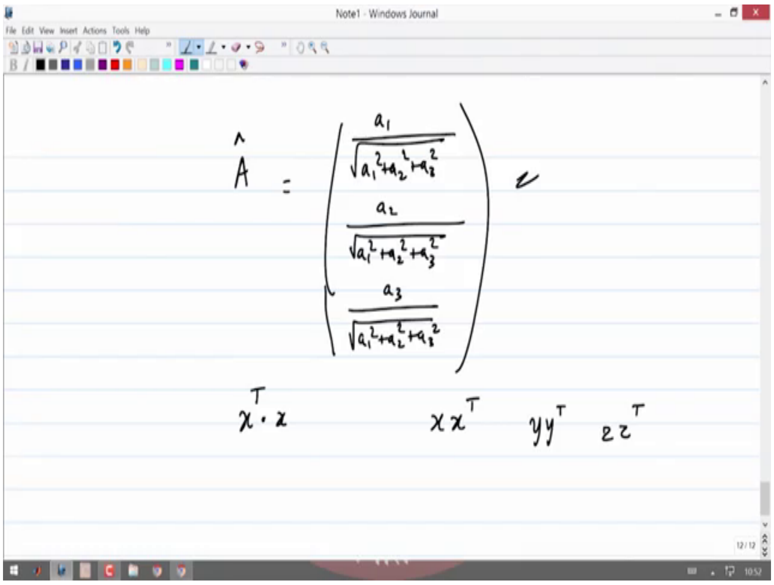

So, unit vector A if you write, so that is the vector, unit vector with the magnitude 1 in the direction of a, ok. Now, we have been careful enough to write x T T dot x. What about x x T, what about y y T or z z T?

In three dimensions or in two dimensions, this if you just do the other way around now that is going to give you not a number. It is going to give you a matrix and such things will become norm as operators and they will be fundamental in representing the quantum mechanical measurement quantities known as the operators and therefore, in the next part of this lecture or the next lecture we will continue with the definition of the operators. I hope this was cleared enough for you to understand the connection between a simple vector representation in geometry and an algebraic representation of the vector using matrices, using column and columns and rows and taking the product. We will continue this in the next lecture to represent the operators until then,

Thank you very much.