Transport Phenomena in Materials
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Lecture - 03
Coordinate Transformations

So, welcome to the session on Coordinate Transformations. In this session we will be using the subscript notation which we have covered in the last 2 sessions, and we will apply these coordinate transformations to define certain parameters that we will be using in this course transport phenomena. And we will also be using these expressions to derive some of the equation that we will need later on.

This coordinate transformation has 3 components, which is basically relocation of the origin of the coordinate system, and the dilation of the unit cell, which is basically either contraction or expansion, and then rotation of the coordinate axes. We will be taking up only the rotation at this juncture; we will look at the other 2 aspects later on as we will need.

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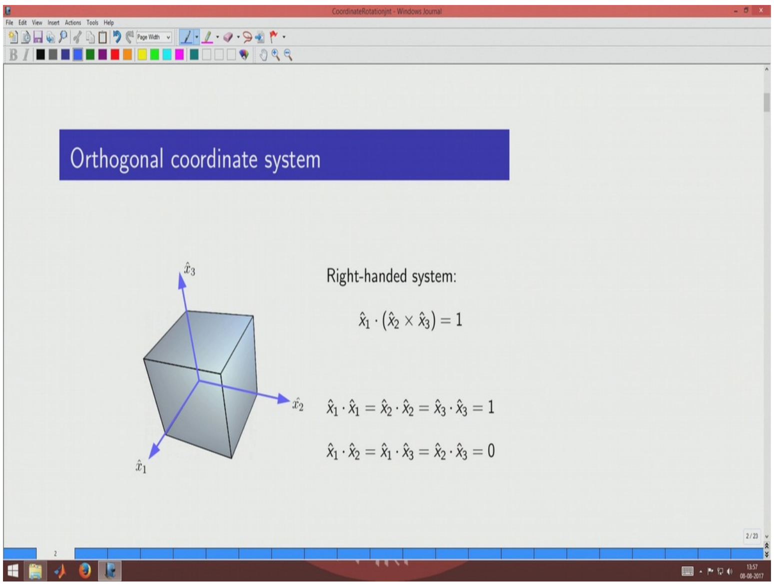

So, we will be looking at what are called Cartesian coordinate system which means basically we are looking at orthogonal coordinate system, and what we mean by orthogonal coordinate system is indicated here. Let us look at for example, here x y z axis defined as x_1, x_2, x_3 with hat symbol showing that they are the 3-unit vectors along the 3 normal directions.

What we mean by the normal directions is that when we take a dot product of any unit vector with itself, then we would see that it should be equal to 1, and then whenever we take the dot product respect to something that is normal to it then we should get a 0. So, this part is defining the orthogonality of the axis. We also have another aspect that is embedded in this particular system namely the so called right handed system. So, we could choose the coordinate system to be either right handed or left handed. So, what we mean by right handed system is that if we take a cross product of x_1 and x_2, and then dot that with x_3, we should get one if we get -1 then it would be a left-handed system and the dimension what we get for the triple product x_1 x_2 x_3.

This gives us whether the unit cell has been normalized with 3-unit vectors being of magnitude 1 or not. So, we can choose these to be different in any other coordinate system, but in Cartesian coordinate system particularly the orthonormal x y z axis that we are very familiar with, then we are going to use the way we are defined here, with the 3-unit vectors normal to each other.

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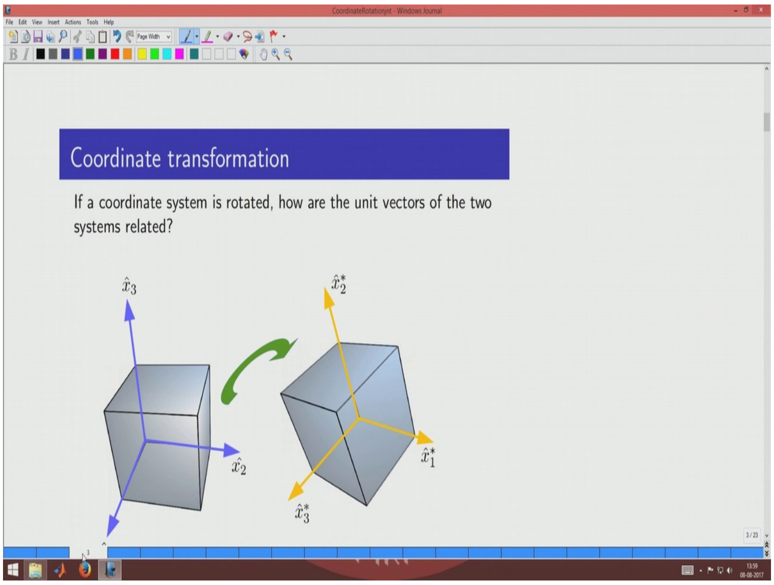

So, by coordinate transformation as I mentioned earlier we are only going to look at the rotation. So, assume that the origin of the coordinate system has not changed, and we have only done the rotation. So, ensure that the way we have describe the 3-axis x_1 x_2 x_3

ensure that the handedness has not changed. Namely the right-handed nature of the coordinate system is preserved.

So, this is what we mean by the rotation of the coordinate system as I have shown in the image the location of the 3-unit vectors has now changed. Now when that changes how do we then represent the new coordinate system in terms of the old coordinate system and vice versa? And then if there are quantity such as vectors then how do we represent the components when the coordinate system has changed. So, this is the task that we have ahead for this session.

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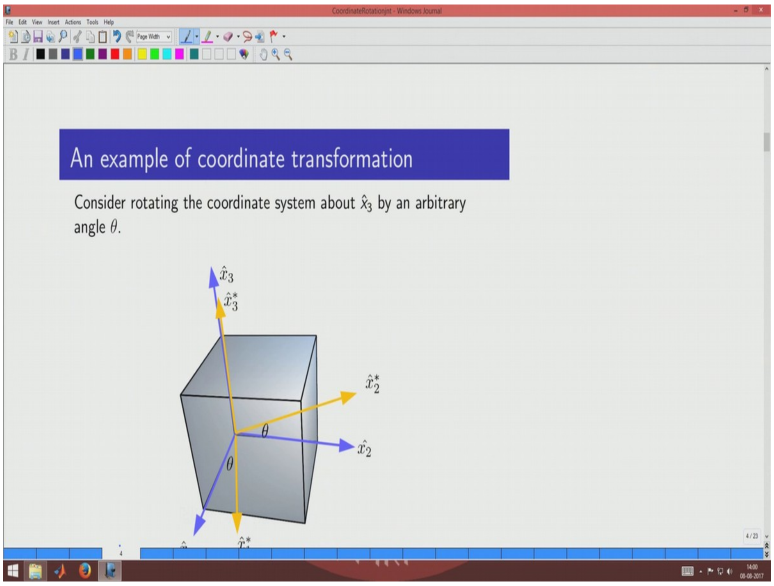

So, the example transformation can be then taken up and we will do a 2D rotation so that we can derive the expression easily. So, what we do is basically we will rotate the coordinate system about the x ray axis, and we rotate by a certain amount which is basically given by θ angle, which I have given here. So, which means that basically the new and the old x_3-unit vector is coinciding, but the x_1 and x_2 are now rotated by certain angle θ, that is given here. So, what we will do is we will derive how we can represent the unit vectors with respect to the older ones and vice versa.

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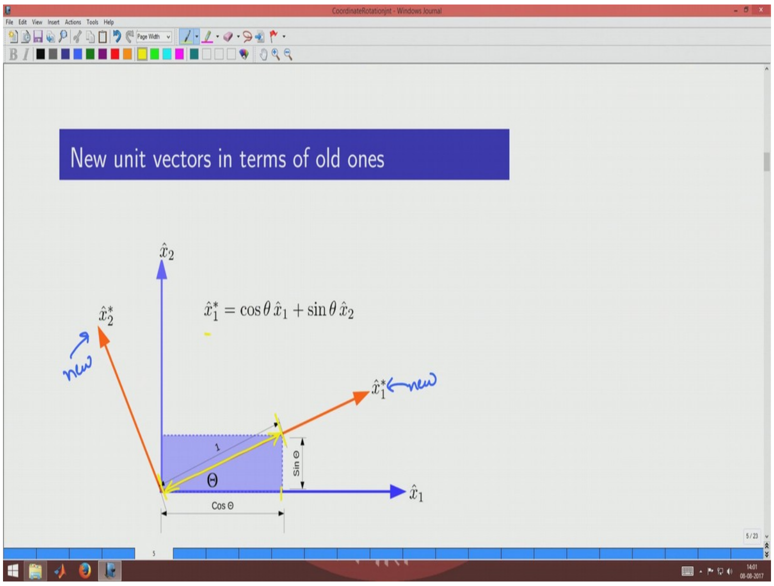

So, what for that what we do is basically, we draw a line of unit length about the unit vector which we want to express. And so, what we want to do first is, write the new unit vectors in terms of the old ones. So, what we do is that let us first write x_1 in terms of the older coordinate systems.

So, $x_1^{¿}$is the new one. So, this is the new one. So, we take a unit vector here we have shown it here. So, this length is 1. So, if this length is one and the angle it makes with respect to the old x_1 axis is θ, then we can see that the components along the x_1 and x_2 are then given by $\cos\theta \sin\theta$ respectively which means that we can express $x_1^{¿}$in terms of x_1 and x_2 as given here. So, similarly we can also express the $x_2^{¿}$, and for that what we do the same way we take up a unit vector along the $x_2^{¿}$.

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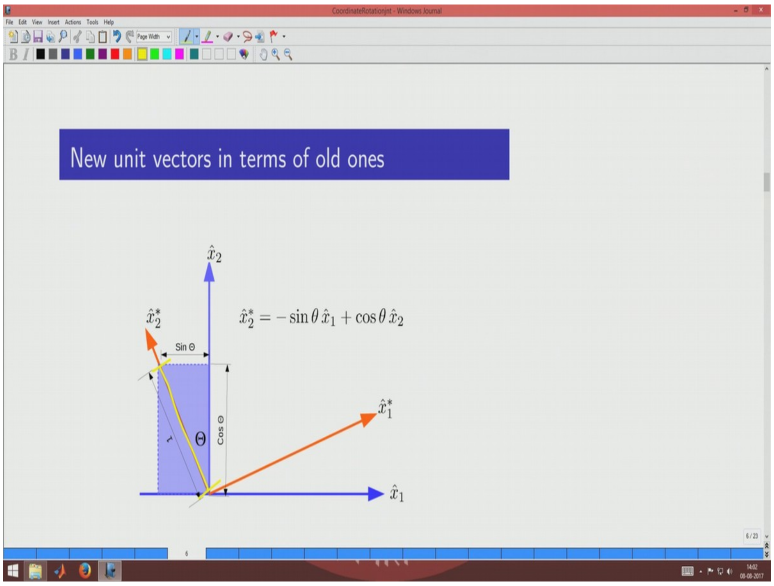

and then take it is components along x_1 and x_2 the old coordinate system, and then we see that when we express that in terms of the old coordinate system we get this relationship $x_2^{¿}=-\sin\theta\,\hat{x}_1$ + $\cos\theta\,\hat{x}_2$. We can see that the sine theta and cos theta have change their position and then there is a minus sign coming, that is going to be of use later on to see what will happen to the transpose of certain matrices that will be talking about. So, at this junction we can just write this, and do we need to write $x_3^{¿}$in terms of anything else. So, we see that we do not need to worry, because we know that $x_3^{¿}$is a same as x_3, because the rotation is about the x_3 axis. So, x_3 axis has not changed it is orientation at all. So, we can just leave it like that.

So, we now have basically the 3 new unit vectors in terms of the 3 old unit vectors. So, we can then connect them and see how those expressions look like.

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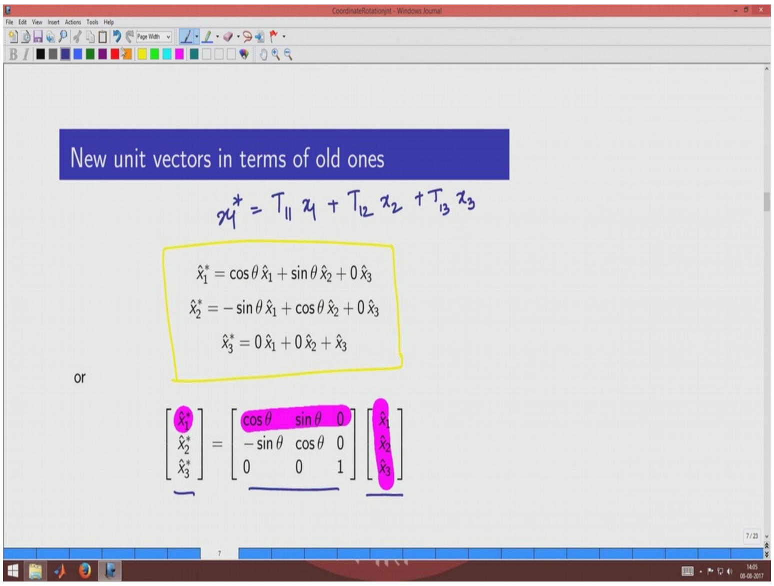

So, that is then given in this form here. So, you could see that these 3 are the equations that we have now come up with. So, $x_1^{¿}$ in terms of x_1 x_2 x_3 $x_2^{¿}$in terms of x_1 x_2 x_3 and then $x_3^{¿}$in terms of x_1 x_2 x_3. So, we can now represent these 3 equations linear equations in matrix forms the reason why we are going to do it in matrix form is because we could then give symbols to those matrices. And then use a subscript notation to make the same expression in a very brief manner. So, what we do is that we write it in the form of matrix multiplication.

So, let me highlight and show you how this looks like. So, if $\hat{x}_1$ is then given by this multiplied by this that is $\hat{x}_1$cosθ+ $\hat{x}_2$ sinθ+ (0* $\hat{x}_3$). So, that is how we are doing. So, this is the typical way matrix multiplication is done in the engineering mathematics courses. So, this must be familiar to us. So, what we now want to do is that we want to then write these expressions with some symbols. So, that using the subscript we know the positions. So, that is what we are going to do now. So, we want to call each of those terms as the elements of a matrix T. So, $T_{11}T_{12}T_{13}$ are then nothing but cosθ sinθ and 0 respectively.

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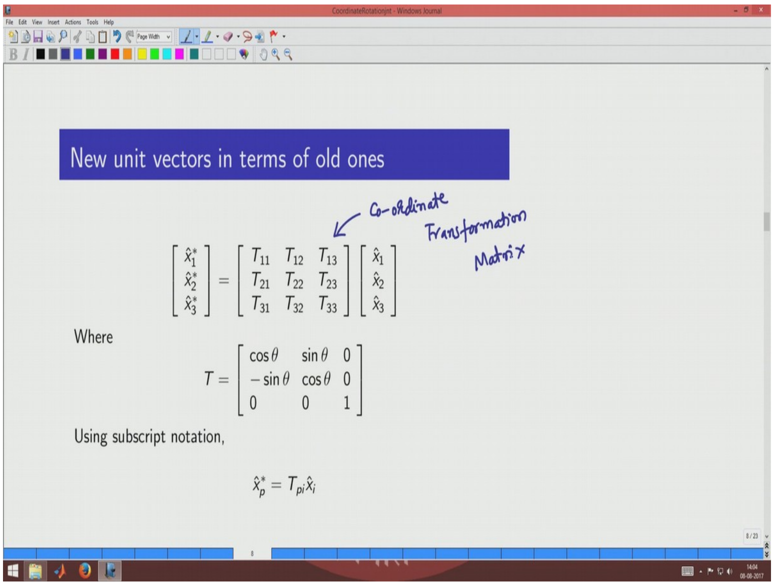

So, we could then write this expression. So, we are now using the short form T. So, that we represent that as a matrix. So, this matrix is nothing but the transformation matrix. So this, this has a specific name. So, that is basically coordinate transformation matrix. So, this is unique to the kind of rotation that we have done. So, when the rotation angle changes then the elements of this matrix also will change. And the matrix itself is expanded here.

So, when we look at the expression here; so if you notice the expression; so here in this expression if you notice here. So, let us just write $x_1^{¿}$. And we write this as $T_{11}x_1 + T_{12}x_2 + T_{13}x_3$. So, you could see that there is a summation that is being taking place, and that is about the second index here. So, we could then use the subscript notation to indicate. So, when we have a dummy index in the second position of T, then we can see that we get the summation implied by the subscript notation itself. So, that is what we are going to do here.

So, here basically what we have written here is that we have use the second index as a dummy index matching with that of x. So, that it is implying that it is summed up over the i index from 1 - 3, and the first index corresponds to what is the new unit vector that is being expanded. So, in a very brief manner we are able to write the transformation of the unit vectors from old to new using this expression. So, we could also do the reverse.

So, when we do the reverse we have very interesting observation to make. So, let us go through that exercise now.

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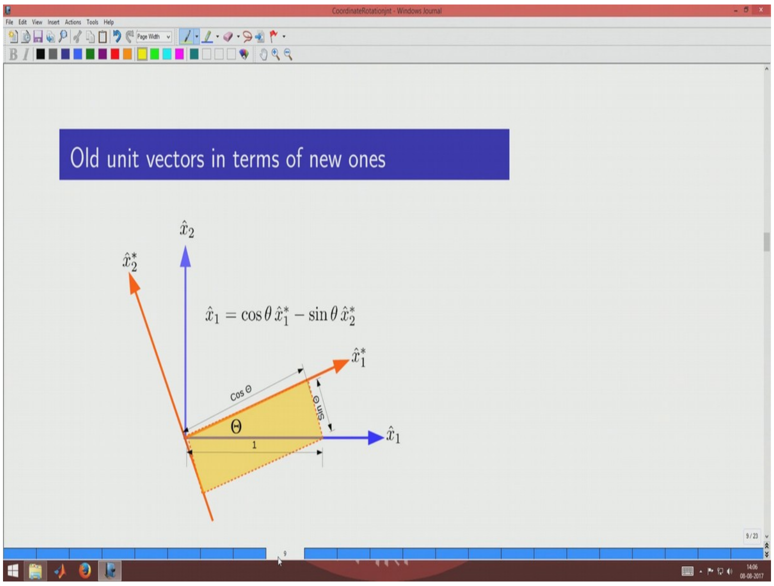

So, the reverse is as follows we have to now write the old unit vectors in terms of the new ones. So, what we do is same as what we have done earlier. So, here we have seen that there is a unit vector which we want to expand in terms of the components along the new axis. So, the unit vector is along the x_1 the old one and it is components are given by cosθ and sinθ and we could also see that the expression comes like this. So, x_1 in terms of $x_1^{¿}$and $x_2^{¿}$are written here. So, we could again expand the x_2 in terms of the 2 components.

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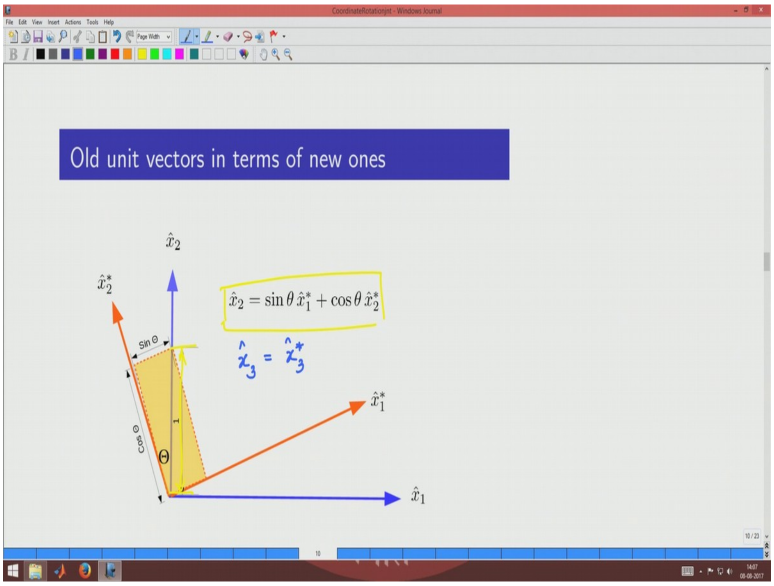

So, we do the same thing here. So, we take up the unit vector along x_2, and then take it is components along $x_1^{¿}$and $x_2^{¿}$and then we obtain this equation. And the equation for x_3 is of course, known to us because we have not changed it is orientation at all. So, you would write this way. So, we have now also the old unit vectors in terms of the new one. So, we could again express these 3 relationships as set of 3 equations and with a matrix form. So, that is what it done here.

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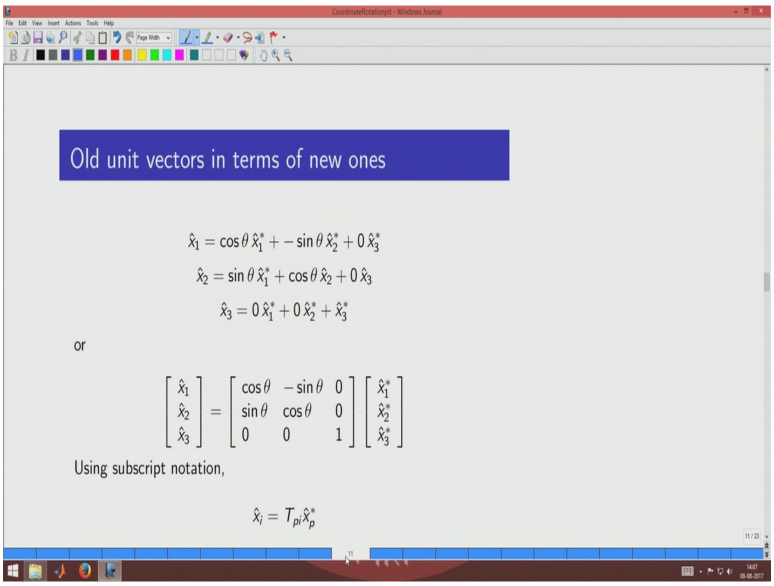

So, they are expressed here as 3 equations, and then they are then converted into a matrix form here and this is a transformation matrix here. So, this is a transformation from the new one to the old one. And we can see that there is one difference with respect to the previous matrix and that comes at these terms. So, you could see that the minus is now appearing on the first row. Earlier when we are expressing the new unit vectors in terms of the old ones the minus was appearing here. And in terms of the old unit vectors here we have getting this. So, this is the only difference that we are getting otherwise the elements are same. We also notice that it is a transpose of the other matrix.

And then we want to expand this in terms of the subscript notation, we write it here in this manner. And you could see that we are able to use the same symbol T_{pi} same as earlier the reason being that the summation is now over the first index of T. Whereas, in the earlier case it was over the second index of T. So, by changing the index we are then able to retain the same transformation matrix T. So, I want to just alert you here about this particular difference, because it is it is very important that we do not lose out on this particular difference.

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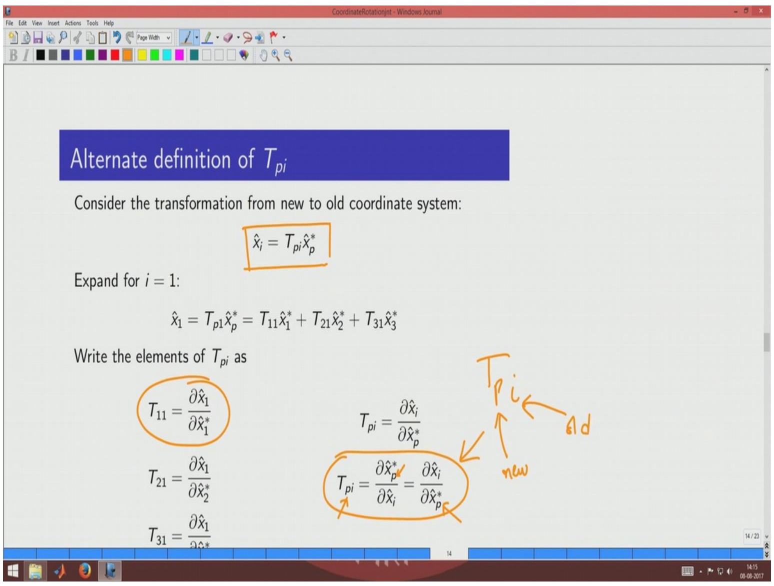

So, I want to highlight here you see that when we are expressing the new unit vectors in terms of the old ones or old ones in terms of the new ones, the transformation matrix will come as T_{pi} only. And then the index p is meant for the new coordinate system, the index I is meant for the old coordinate system. However, the way these 2 are different is evident because the summation is over the second 2 indices here, but here it is over the first and the index of x^* .

So, you could see that the way we multiply the 2 matrices is different. The way we multiply the first one is this way, and the second one is this way. So, you could see that that is a difference why we are able to write the same expression, but just swap the indices over which summation is happening and then retain the meaning. So, this is also coming up because of one particular property of the transformation matrix. Namely for the transformation matrix, we realize that its inverse is the same as the transpose. So, this property is what allows us to write this.

And the reason why this property comes up is because the determinant of the transformation matrix T is unity it is one because of that this particular property comes up. And therefore, then we are able to write. So, what we now need to remember is only one expression here. So, whether it is new in terms of the old or old in terms of the new, we have to remember that x^* is T times x and the indices should be such that you keep one index. On the left side one index on the right side and then put them side by side here below, and then the expression would work for you. And the rest of it basically is subscript notation because you know how to expand this ones you know the subscript notation the dummy index is i.

So, you sum up over the i index. So, that is how you can get the new unit vectors in terms of the old ones or vice versa. So, there are other ways of defining the transformation matrix T. And I would like to then cover them because different text books may adopt different ways of defining them. So, the idea is how do we get the elements of transformation matrix T for any given arbitrary rotation of the coordinate system. So, the way to derive is being illustrated here. So, when it is only one θ about x_3 axis we already know how to do that, but any general case we can just do that here.

So, let us look at the transformation which is given in terms of the expression here. And when we expand it we are getting this expression. So, we take p value to be 1. So, we are looking at the first unit vector of the new coordinate system and expanding it in terms of the 3-unit vectors of the old system. Now you see I want to get T_{11}, and that is what I want to now check. So, I want to get this now we can see that if we were to pretend x_1 x_2 x_3, the old ones as well as the new ones were to be like variables. Then differentiating this expression with respect to this variable will get me only this term out. So, that is what is being done. Here a partial differentiation is going to get me that term. So, you could then look at the entire expression, in this form which is very, very brief it just shows you that by looking at the differentiation, you could get the elements of the transformation matrix in this form.

So, the convention is that first index goes to the numerator, and the second index goes to the denominator, and p corresponds to that of the index of the new coordinate system, i correspond to the systems of the old coordinate system. So, if you stick to this kind of a connotation then we will not make a mistake. So, you could you could arrive at the elements of the transformation matrix by looking at the differentiation and this is particularly useful when the transformation is given as a functional form, then we could use this kind of an expression.

We are now taking up the reverse transformation the old in terms of the new ones, and here you can see from the previous slide we can see that here we have got star on the left-hand side which means that the new ones, in terms of the old ones and here I am writing the old ones in terms of the new ones. So, whichever way we write we are seeing that we are getting the same expression. So, we can get the same expression, which is very interesting. So, it just shows you that when you want to express the elements of transformation matrix, you take partial differentiation of the old and the new, and the order is not important the reason why it is happen is of the same principle basically the inverse of T is same as the transpose.

So, here you can see that the index positions are changed and what it implies is that we are taking the transpose, when we are doing the second way of differentiating and therefore, the inverse transformation is giving you the same T_{pi}. So, it does not matter now how to remember the expression of T. You just differentiate old in terms of the new coordinate system or the vice versa and as long as you are able to remember the position of the indices the first position T_{pi} we write.

So, we remember the first index corresponds to that of the new, second index corresponds to that the old coordinate system, then the expression is going to be correct. So, if we make a swap here then we will have a transpose of those matrices coming out.

So, we should watch out for that; so an alternate way of defining the elements of T when the unit vectors are given in vectorial form is shown here.

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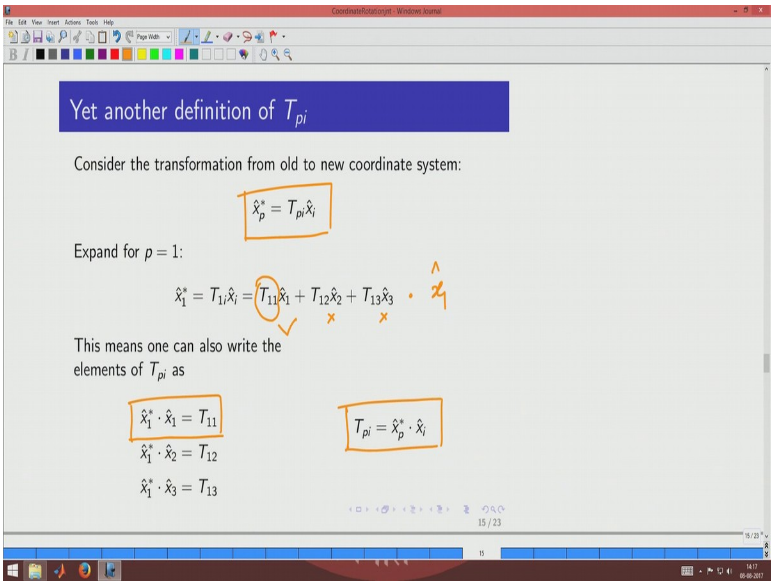

So, here what we do is that instead of looking at partial differentiation, we basically look at as a dot products. So, we do the same exercise. And we see that we want to get T_{11} out. So, what we do is basically we realize that from the orthogonality property of the coordinate system. If we were to dot this with something that will leave behind only this term and not have these 2 terms which means that if I were to dot that with x_1 then what happens is the first term will remain the second because it is x_2 dot x_1 it will drop of third one x_3 dot x_1 it will drop of. So, I could then imagine that. T_{11} is nothing but a dot product of $x_1^{¿}$and x_1 similarly the other terms.

So, you could also imagine the elements of the transformation matrix as dot products of the new and the old coordinate system. So, which means that in case the new coordinate system axis are given as a vectorial form of the old coordinate system then we can just do the dot product and we can get all the 9 elements of the transformation matrix directly using this kind of relationship. So, either way we need to get the matrix T so that we can define the transformation completely.

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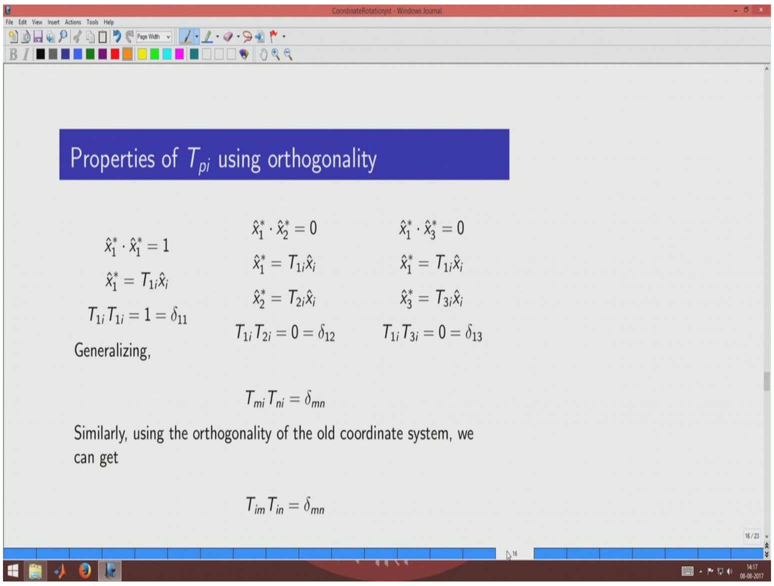

So, there are certain properties of the transformation matrix which are derived from the nature of the coordinate system that is being used here which is basically the orthogonal coordinate system. So, these properties of transformation matrix are then used to reduce some of the expressions as we derived various quantities later on. So, we know that both the new and old coordinate systems are orthogonal.

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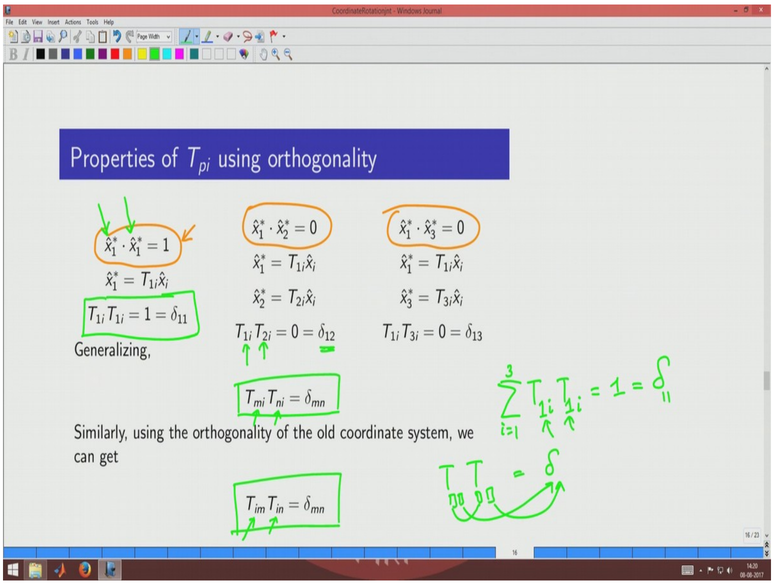

And which means that when we dot the new unit vectors we should get one, and this is true also for the old ones. So, each of these the way we proceed as follows. So, we know this form the orthogonality. What we do is that we take up each of these vectors, and express them in terms of the old vectors. And then when we express them in terms of old and then do the dot, we see that we get an expression which involves transformation matrix being multiplied twice. And then we will see whether the value is unity or 0. So, using the first expression that is express $x_1^{¿}$ in terms of x_1 x_2 x_3 and then dot it with itself then we will see that this expression, which is basically if I want to expand a T_{1i} T_{1i} i=1-3 is equal to 1. So, this comes up because we are actually what we are doing is $T_{11}T_{11}$ + T_{12} T_{12} + T_{13} T_{13} .

So, this expression is going to be 1, because of the orthogonality of the new coordinate system. And this one I want now imagine as if it were to be coming from 2 indices of a δ , and I want to take those 2 indices to be what are here. And we know the property of δ. So, we just write it as one. So, the reason why we write this because we see a very general form that is evolving here when we take the orthogonality, relationship were $x_1^{¿}$ and $x_2^{¿}$we get a 0. So, here again we choose those 2 indices here, and realize that the expression is actually valid.

So, we can then generalize saying that if the index is such that it is m and n then we can write the expression using δ_{mn} whenever there is a summation of i the other 2 indices can be used for the indices of δ. And this is basically nothing but statement of orthogonality of the coordinate systems both new and old. So, when we write the orthogonality of the new coordinate system express in terms of the old coordinate system we get this expression. Where the second index is being used as dummy index, but if we do the reverse that is we express the old coordinate system orthogonality and express the old coordinate system unit vectors in terms of the new ones and do the same analysis. Then we see that the dummy x index is actually in the first position of T.

So, we can see that either way we are getting the δ, on the right-hand side. So, is essentially what it implies is that whenever there are 2 t's coming up together then inspect there are 2 indices. And let us say the first index is matching. Then put the other 2 indices here. So, that is how we can write the expression using the subscript notation. And there is no deeper meaning in this expression, than the orthogonality of the 2 coordinate systems.

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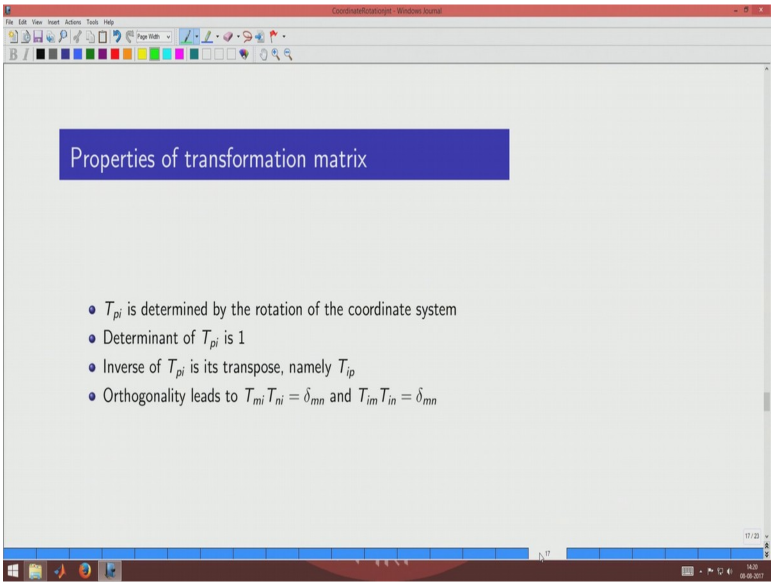

Now, there are some more properties of the transformation matrix that we can use we can say that transformation matrix is completely determined by the rotation of the coordinate systems. So, whenever we know the rotations by what axis by what amount then we can then determine the elements of T completely. Determinant of T is 1. The reason why this is so because, we are talking about a pure rotation, we do not want to consider situations where the new unit vectors when you look at the triple product it is not different from 1, the unit cell is not expanding or contracting the unit cell is of the same volume we are only rotating the coordinate axis.

So, because of that the determinant of T will be 1, and inverse is the same as it is transpose we have come across that already and orthogonality, leads to these 2 relationships. So, these are the 4 aspects of the transformation matrix to summarize, what we have done till now. So now, we are going to use these to make some more analysis.

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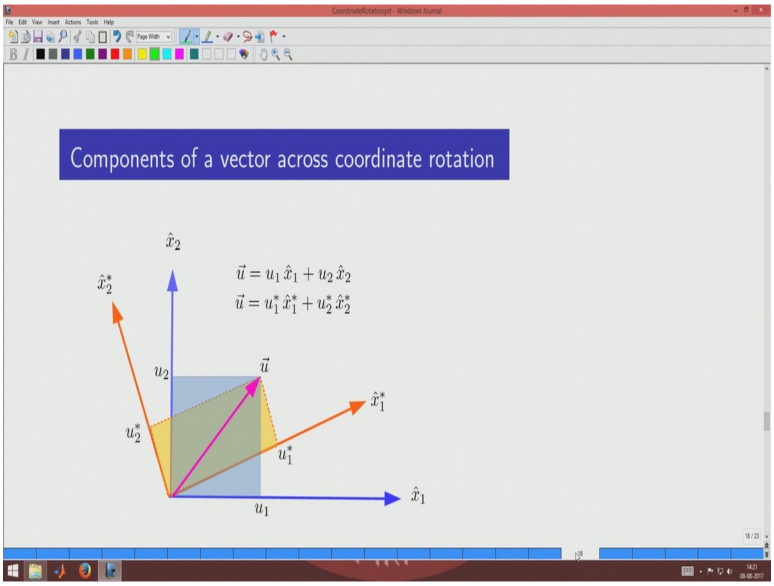

So, why do we do all this? The whole idea is as follows.

So, there are certain quantities which we want to represent irrespective of how the coordinate system is raid out. In other words, if take the example of a $\vec{u}$. So, the $\vec{u}$, if you look at it is components in the old coordinate system the components are u_1 and u_2, and in the new coordinate system the components are $u_1^{¿}$and $u_2^{¿}$.

Now if this $\vec{u}$ were to be for example, a velocity vector or a gradient etcetera, then we know that it sense of the magnitude and direction does not change whichever way we chose the coordinate axis to be, which means that. When we rotate the coordinate system from x_1 x_2 to $x_1^{¿}$and $x_2^{¿}$ then the elements u_1 and u_2 should change over to $u_1^{¿}$and $u_2^{¿}$, and maintain the direction and magnitude of the vector. So, the sense of the vector should be preserved when we rotate the coordinate system, and only those quantities whose elements are following this sense being preserved will be actually called as vectors, otherwise it just becomes a bunch of numbers which change randomly when we change the coordinate system. So, this is the principle behind writing this expression. And let us just go through the small algebra that is behind; so identical to what we done with the unit vector.

So, let us look at the elements. So, these are the 2 expressions we have taken we have taken a 2D situation, and we have taken this angle θ exactly like what we did in the previous exercise. So, to know how the elements u_1 u_2 are written in terms of $u_1^{¿}$and $u_2^{¿}$.

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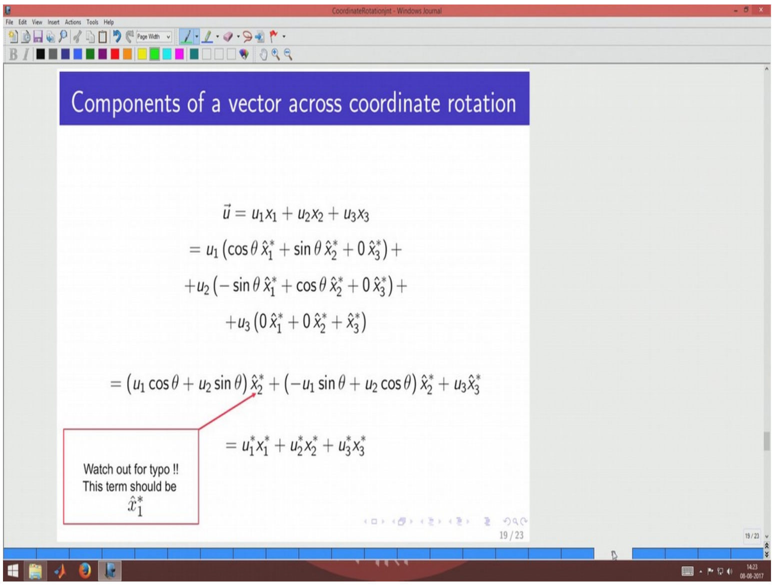

What we do is as follows.

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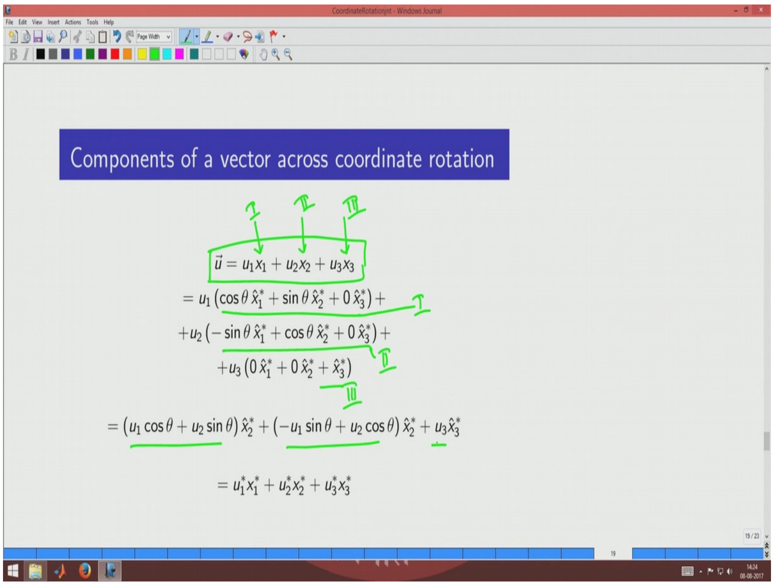

We first write the u in terms of it is components. And then what we do is that each of these unit vectors, which are old unit vectors, which we write in terms of the new ones. And we already have those new ones. So, this is the first one, and this is the first one, and this is the second one, this is the second one, and the third one of course, is unchanged because we are rotating about the x ray axis.

So, we have those expressions coming in. So, once we write the old coordinate system unit vectors in terms of the new one, then we collate all the terms for $x_1^{¿}$and $x_2^{¿}$and $x_3^{¿}$, and then when we collate we get those things here. Then once we write then we now have expression here u is equal to this way. Now you can see that $u_1^{¿}$is now expressed in terms of u_1 and u_2 ,$u_2^{¿}$ is expressed in terms of u_1 and u_2 ,u_3 also expressed in terms of u_3 which we can then write in the form of a matrix.

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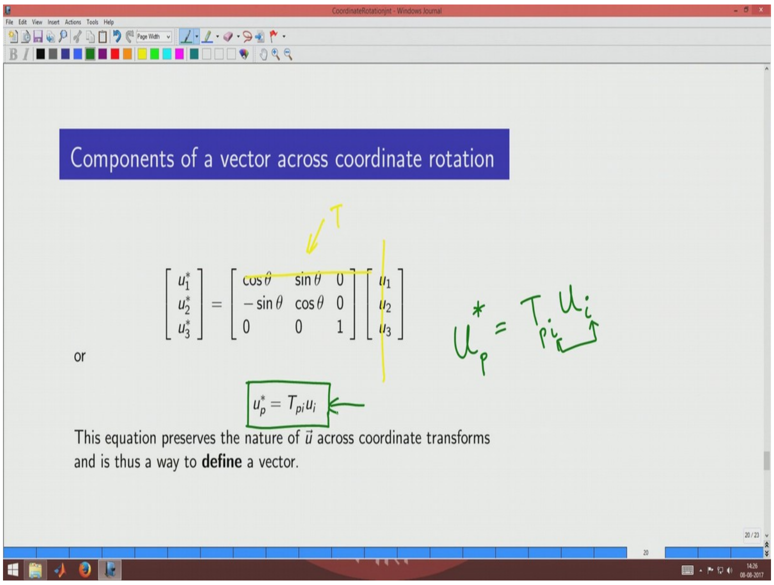

So, that is what we do here and the way we are multiplying is the same as what we have done here. So, this is the way. So, $u_1^{¿}$is u_1 cosθ + u_2 sinθ + (0 * u_3) , $u_2^{¿}$is - u_1 sinθ + u_2 cosθ + (0 * u_3), $u_3^{¿}$is (0 * u_1)+ (0 * u_2) + (1 * u_3) .

So, we have got this expression. And it is actually not surprising that the matrix that is coming in here is nothing but the transformation matrix T. Reason is that we have actually use the unit vectors to arrive at this particular expression. So, the way unit vectors are transforming is given by the transformation matrix. So, we should get the same matrix here. So, we now have that expression here. And so, the way the elements of a vector transform when the coordinate system is rotated is given by the same expression as we have done earlier namely $u_p^{¿}=T_{pi}U_i$. So, let us look at this expression carefully. So, where the new coordinate system indicated by the star the index chosen is p, and then for the old coordinate system you do not have a star and the index chosen is i.

And the sequence of writing the indices for T is the first on the left second one on the right. So, we should always remember that this is how it is written. And the i is for the old which is coming on the right hand side. And this way if you write then when you swap the quantities then this sense does not change. so in fact, later on we will see that it is this expression that will be used to define what can be called as a vector at all. So, vector is one which transforms in such a way that the elements the components of the vector will change in this manner whenever the coordinate system changes. So, we use that as a definition of vector.

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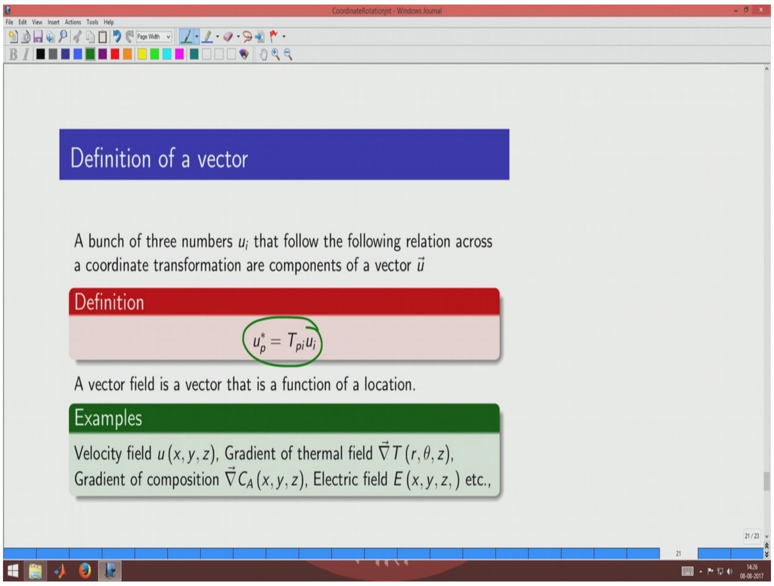

So, this is how we are defining here.

So, we say that any bunch of 3 numbers cannot be a vector. Only those bunches of 3 numbers which follow this relationship can be called as components of a vector. And which can be proven you know there are some quantities which are known to be vector. So, we can go ahead and proof whether they are vectors or not, according to this relationship we will be doing that in a later session. And are there any quantities that we already know are to be vectors we have for example, velocity. So, velocity vector is here and we can look at gradient of temperature gradient of composition, electric of field and so on polarization and so on.

So, these are all various quantities that we know which are part of describing a physical process, where the vectors are involved. Now there is a small terminology I am introducing at this juncture, which is basically field. So, the idea of field is basically the quantity the parameter we are talking about is having a particular value at a particular location, but if you change the location the value could change. So, think of temperature field where the temperature at any given value given location is fixed, but as you change the location the temperature could change. So, such a such a quantity which changes as a function of the location is called a field.

So, what we mean by a vector field is nothing but a vector that is a function of the location. So, velocity field when we use the word velocity field, what we mean is this? A velocity which has 3 components, but those 3 components are functions of the location. And the location is specified in various means sometimes, we specify the location using x y z sometimes we specify the location using r θ z. Sometimes we may specifying r θ ϕ in spherical coordinate system. So, the choice of the coordinate system is up to us, but once a location is specified, and if the value of any vector is at that location specified then it can be called as a field.

And examples for vector examples of velocity fields vector fields are such that you know you can see velocity field gradient of a thermal field gradient of composition field electrical field. So, these are all things that will come across in this subject again and again. So, the word field should immediately indicate to us that there is a location dependency that is coming up. So now, we have defined how the elements of vector should change such that you can call it as a vector. So, we have given this. So, what would be then a scalar should be?

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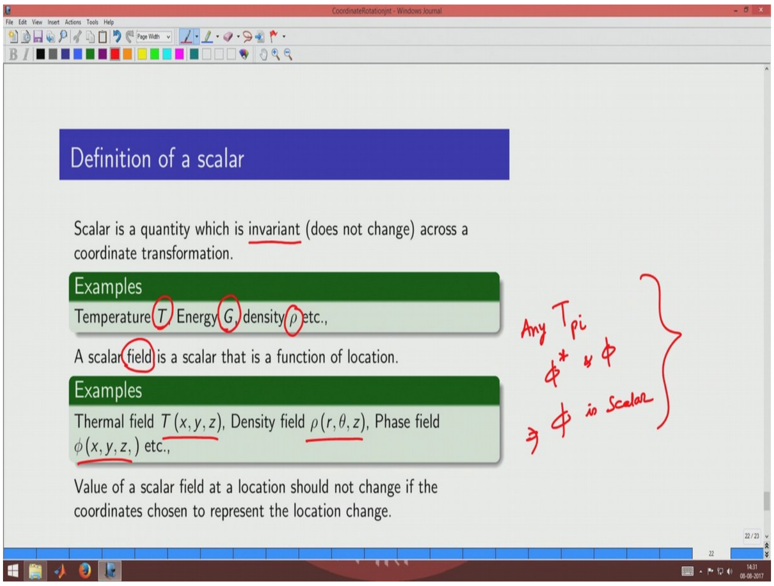

Defined by a fact that the numbers do not change when the coordinate system is changed. So, basically, we use the word invariant. So, a scalar is one which is invariant across a coordinate transformation. So, it does not change when the coordinate system has changed examples are of course, temperature. So, we know that whichever way the x y z coordinate system is oriented, once we specify a location the temperature of that location is fixed it does not matter which way the x and y directions are pointing at. So, such quantities are called scalars and very important note that energies are all scalars.

So, because later on when we define energies in terms of various quantities we realize that because energy is a scalar then whatever quantities we are using should be such that they must be having a functional form which does not change when the coordinate axis are rotated density is also one more example where which is a scalar field. So now, scalar field is something that we are introducing now it is a same sense what we have said for vector field a scalar field is basically a scalar which changes it is value as a function of the location, but not when the coordinate system is rotated. So, we have temperature field we have density field we have phase field and so on. So, these are all various quantities that will be coming up as a part of this course later on.

So, we will be using the word scalar field and in multiple ways and whenever we indicate that what we mean is that whenever the coordinate system changes, then the value does not change and the value is a function of the location. Now the invariance is something that one can be proven. So, that is if there is a quantity which when we rotate the coordinate system has not changed at all for any for any transformation matrix T. Then for any T_{pi} ϕ¿and ϕ are the same which means that a ϕ is scalar. So, this is the idea that we are going to use later on to define what is this scalar and what is not. So, it is not as if any quantity which has just one number at a particular location can be called as a scalar is very important that, that particular number should not change when the coordinate system is rotated by any arbitrary transformation matrix T.

So, this is the essence of it. So, we will practice these with some assignments. So, we can go back to the course website and look at some practice assignments to practice with the coordinate rotations, and arriving at various values of the elements of T, and then using orthogonality arriving at various kinds of derivations that we will be practicing, and look up the course principle for the details.