Introduction to Non-linear Optics and its Applications
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Lecture - 23
Kleinman's Symmetry,
Neumann's Principle

So, welcome student to the new class of Introduction to Non-linear Optics and its Application. So, in the previous class we have started a very important concept and that is the contraction of the indices of the d matrix. Today we will start from that point and like to know what is the implication of d matrix and how we can contract the d matrix indices and if I do then by applying other symmetries how it is possible to even find out different components of the d matrix.

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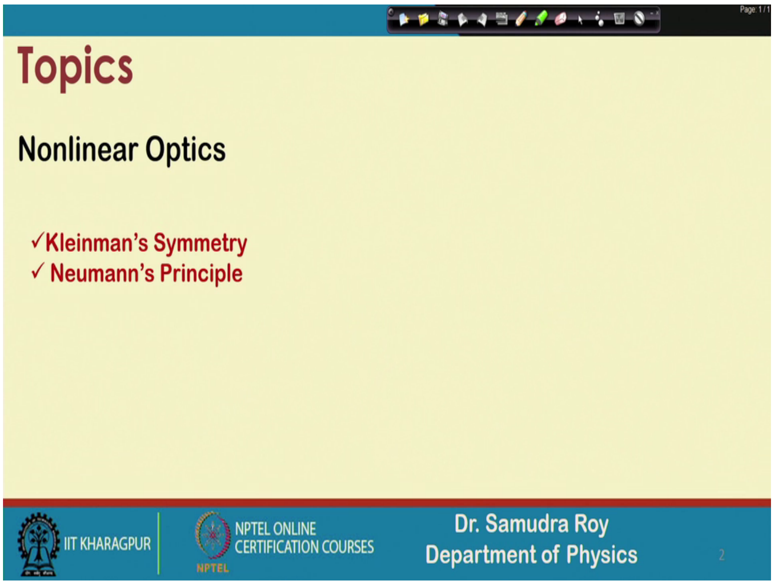

So, let us see what we have in today's class. So, today's main topic will be 2 important concepts; one is the concept of Kleinman's symmetry, which we will going to apply to find out the different relationship in d matrix.

And second is Neumann's principle; so, what is Neumann's principle and using Neumann's principle how it is possible to find out the different component of the d matrix; that we will going to learn in this in this class.

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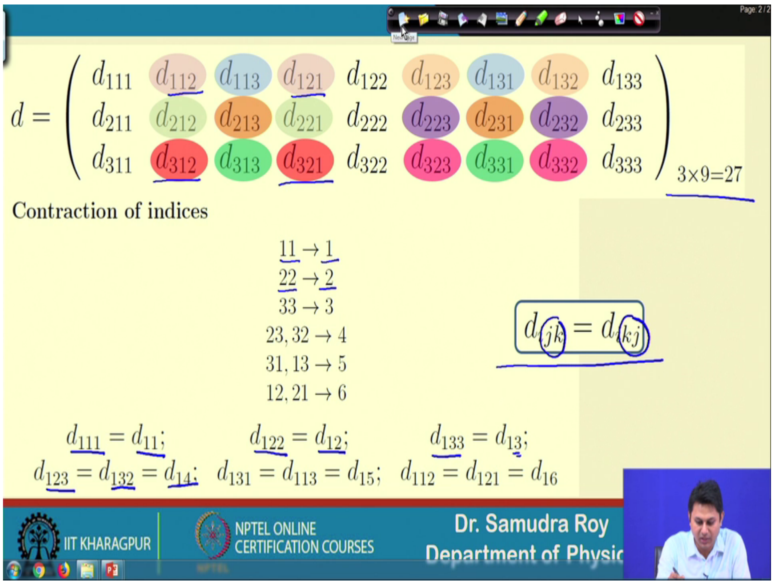

So, let us go back to our previous class; so, this is the d matrix has shown here in this slide. So, in principle it should have 27 different components; so, as you can see that the number of components are 27, but there are few components which are colored or which are shaded by some color. And this particular components, which are colored in a different color with a same shades are in fact the same value; that means, d ijk is equal to djki.

So, here we have written this things that how d ijk and dikj are same; that means, if I change the indices of the second 2 term here; then eventually the d matrix will remain same. So, this is this symmetry because of this symmetry we find that there is several terms in the total matrix, which contain 27 terms and several terms in this d matrix are same. So, 27 terms are eventually reduces to 18 independent terms that is very important because using this permutation symmetry, we can have now only 18 different terms. So, let us see that here d 112 and d 121; these are same and it is indicated by same color.

In the similar way, d 312 for example, and d 321 are the same value the; they have the same value. So, that is why they are indicated with the same color. So, if I now able to write this d matrix in contraction indices under the contraction of indices, then since ij here jk is equal to kj.

So, we will not going to write every time the 3 independent terms like ijk rather we will contract the indices and there is a new way to write this components so that we can now have a reduced form of d matrix. So, iy 11 became 1; 22 became 2, 33 became 3 and so on 23 and 32 which is eventually same became 4 and then 31, 13 which are again the same quantity become 5 and so on.

So, here we wrote in the some example that d 11 should be written d 11, d 22 written d 12, d 13 written d 13; d 123 or which is equal to d 132 can be represented at d 14 and so on. So, this is very important because we can reduce verily we can reduce by applying this symmetric property of the d matrix; we can reduce the d matrix from the 27 different component to 18 components.

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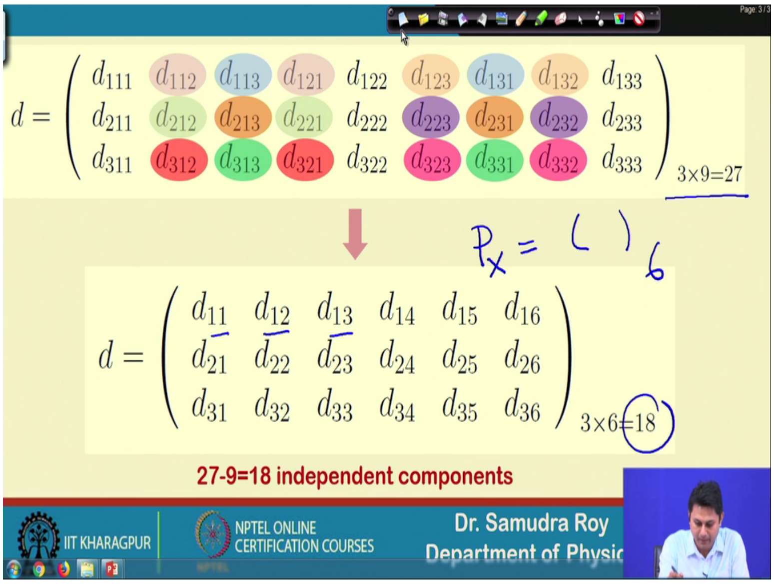

So, last class we discussed this; so again; we are discussing yes. So, this is the compact form of the d matrix.

So, now you can see here we had 27 components and now we have reduced to 8 component. So, now, d 11, d 12, d 13; these are changing, so for every value, for every for one say one; if I want to find out P X; then in the right hand side we have 6 terms that we have shown in the previous class. So, 1 2 3 is nothing, but x y z to understand this thing in a clear way we just use 1 2 3. So, that it is easier for us to understand, but eventually this 1 2 3 is nothing, but x y z components.

Well after having the reduction of this d matrix the next thing is to apply the Kleinman's symmetry.

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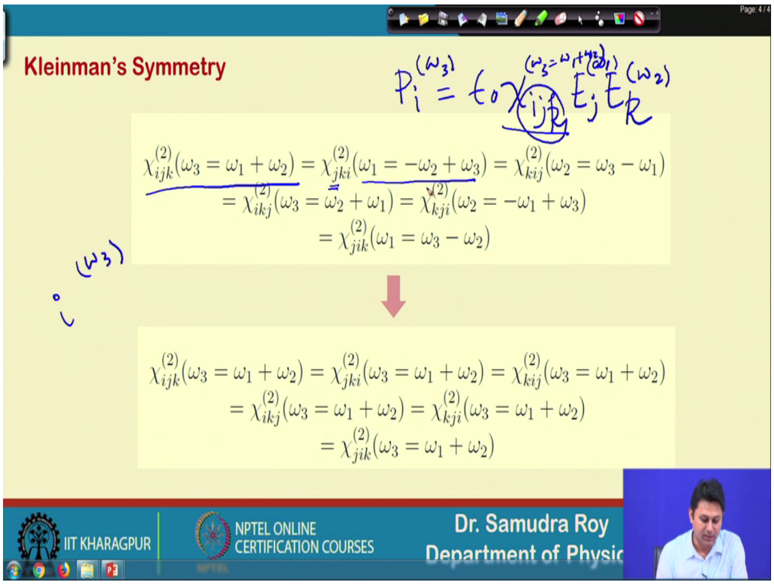

So, Kleinman's symmetry is nothing, but the condition where we assume that the susceptibility is not a function of frequency. Normally what happen that when we find out the susceptibility term this susceptibility term was a function of frequency. So, here if I look this transformation then we can find one interesting thing that when I find susceptibility term ijk, for example, this one where ith components contain omega 3 term which is combined by the jkth term.

If I if you remember that P of i it was epsilon 0 susceptibility ijk and E j E k that was our main equation in terms of non-linear polarization; obviously, P i is non-linear. So, that is why 2 component E j and E k is associated with this term.

But now if we have E j component has some value say omega 1 and E j E k components has some value say omega 2 E j multiplied by E k basically give raise to one frequency which is omega 3. So, my susceptibility is written as omega 3 is equal to omega 1 plus omega 2.

So, omega 3 components are generated by omega 1 plus omega 2; now of I change the entire permutation. So, for example now I try to find out what is jth? So, jth component contain omega 1 frequency; so in susceptibility terms if I look this. So, here we can see that ith component are related to omega 3, jth component is related to omega 1 and kth component is related to omega 2.

So, now, if I make a permutation of this terms; then what happened this frequency distribution will also going to change. So, omega j which is related to omega 1 can be represented as omega 2 minus of omega 2 plus omega 3.

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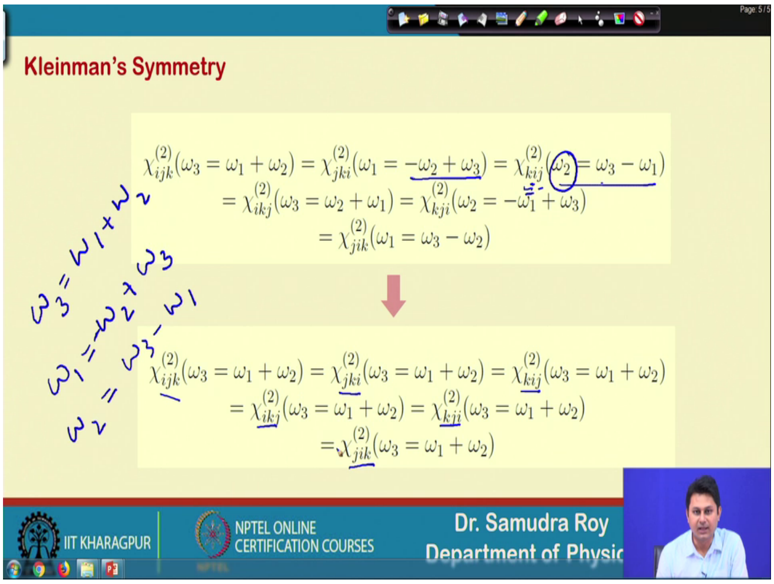

We know that omega 3 can be represented as omega 1 plus omega 2. So, if I wanted to write omega 1 it should be omega 2 minus omega 3; sorry it should be represented as minus of omega 2 plus omega 3, which is this term. In the similar way if I want to write omega 2 in terms of omega 1 and omega 3; it should be simply omega 3 minus of omega 1 which is this.

And now omega 2 is a component related to j we know omega 3 is related to i and omega 1 is related to j. So, all the combinations they are same if I consider susceptibility does not depend on frequency so; that means, there is no dispersion in to the system.

If we assume this that all these ijks components ijk, jik, kij all the permutation of ijk components will be eventually the same value because I am not considering their frequency dependency. So, all the cases I just write omega 3, omega 3, omega 3 which is equal to omega 1 plus omega 2 and so, on. So, they are not depend on the frequency at all. So, when I reduce these things; that means, omega ijk is I change this as a omega jki. So, we have additional permutation combination permutation symmetry.

So, these additional permutation symmetry is nothing, but the Kleinman's symmetry. So, this Kleinman's symmetry basically tells us I can I can make a permutation of entire term according to my choice; if we consider that the susceptibility does not depends on any kind of frequency the; that means, the system is eventually dispersionless.

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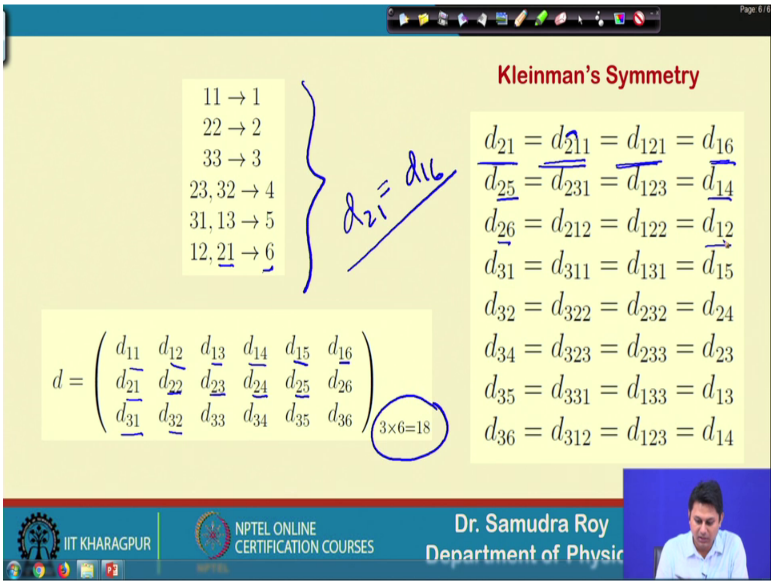

Well if I now look these d terms which were is given here having 18 independent terms; now we can have additional terms which is same by applying the Kleinman's symmetry.

So, let us try to find out which are the terms which are same for example, these are this is the contraction notation that what is my a contraction in terms of 11, 22, 33 which is going to be 1, 2, 3 eventually. And this is the 18 different terms in d matrix d 11, d 12, d 13, d 14, d 15, d 16 all are distinct d 21, d 22, d 23, d 24, d 25, d 31, d32. So, all are distinct terms here 18 distinct terms are there this was our initial d matrix after applying the permutation symmetry.

Now, we are going to apply another symmetry as I mentioned which is Kleinman's symmetry which suggest that if I now write d 211; these components what should I write? It should one is nothing, but 11, so I should write d 211. If I write d 211 then my Kleinman's symmetry suggest if I make a permutation of this term. So, d 211 is nothing, but d 121; if I exchange this 1 and 2, which we can do because it is under Kleinman's symmetry; then it becomes d 121 and d 121 is nothing, but d 211 according to Kleinman's symmetry.

But if I look d 121 it is a different coefficient in terms of these index contractions. So, d 121 should be eventually d 16; so 21 we know that 21 is 6; so, I should write it is d 16. So, one very important thing that I figure out that d 21 coefficient and d 16 coefficient they are same. In the similar way, we can find many other terms which are same for example, d 25, d 26 which are equal to d 14, d 12 and so on.

So, how many terms we find they are same to each other?

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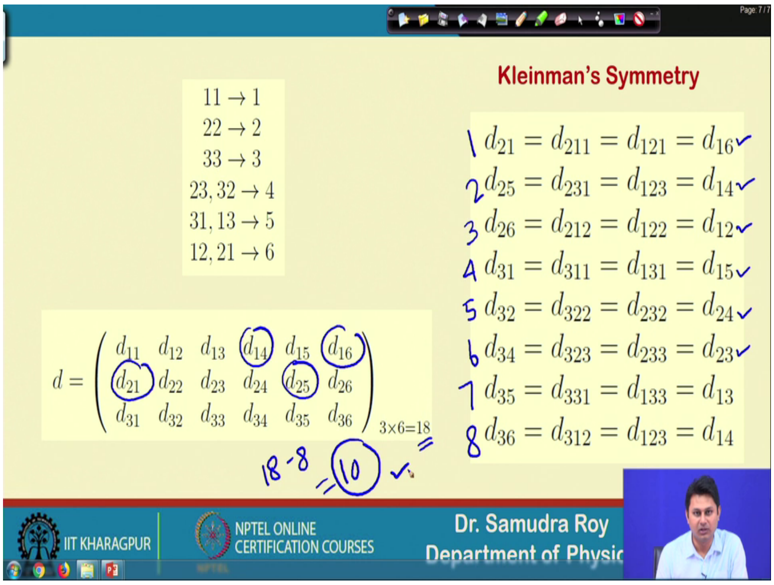

So, if I calculate it is 1, 2, 3, 4, 5, 6, 7, 8; so, 8 different terms are there which are equal to same value of other terms. So; that means, whatever the independent coefficients here d matrix coefficients here are not really independent, but there are some kind of symmetry which we call Kleinman's symmetry under which few of the terms are same.

So, if I now write d 21; so d 16 and d 21 they are same; d 25 and d 4 they are same. So, this 18 coefficient now reduces to if I write if I use this symmetry 18 minus 8 which is 10. So, eventually we come to a point where we find that d matrix which looks very heavy initially. And after contraction of the indices we find there are only 10 components are there which are independent to each other.

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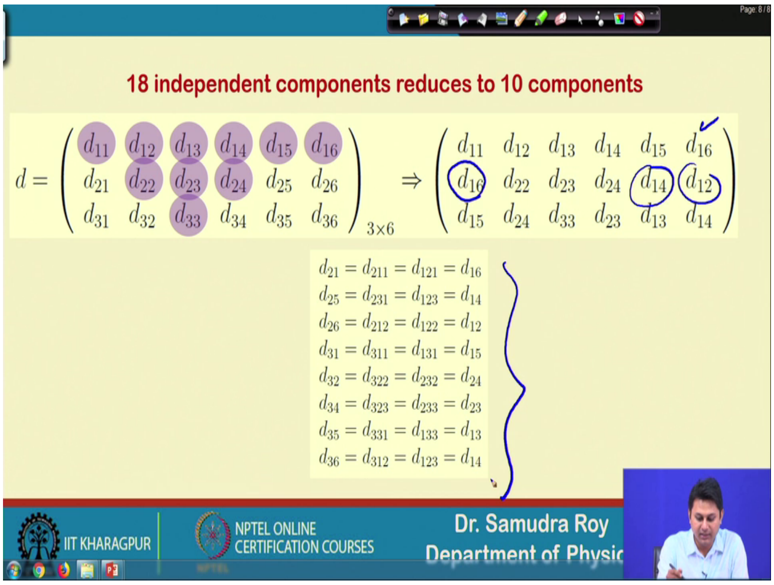

So, if I go to the next slide we can see here what we are telling that d 11, d 12, d 13, d 14, d 15, d 16, d 22, d 23, d 24 and d 33; these are the coefficients which are independent to each other; all other coefficients can be represented in terms if this. So, if I do then we find a new form of d matrix and here we can see that d 11, 12, 13, 14, 15, 16; these are the independence coefficient, but d 21 can be represented in terms of d16.

Then d 22 independent, d 23 independent, d 24 independent have shown here by shaded terms; this shaded terms are independent terms and how many shaded terms are there 1, 2, 3, 4, 5, 6, 7, 8, 9, 10. So, 10 independent components are here; other components if I replace it will look like this. So, d 16 and d 16 they are same in the similar way d 25; I can write as d 14, d 26, I can d 12; all this things are written here that which term is change in to 1. So, the important thing here is that we can reduce the number of terms significantly, if we apply some kind of symmetry in d matrix.

So, after having the knowledge of d matrix next it is time to find out that what should be the value of the d matrix?

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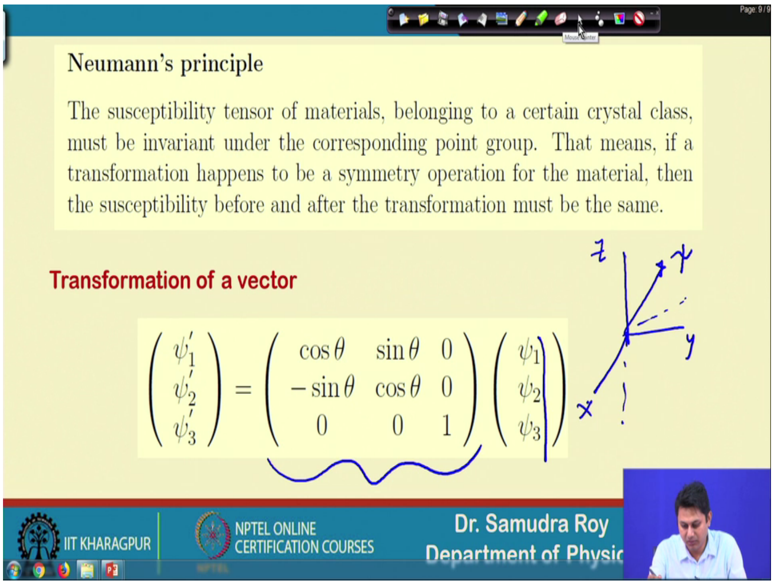

Now how to find out the values; independent values of this or the coefficient of d matrix; in order to understand that we need to know about Neumann's principle; before going to Neumann's principle let me give you the make you a remainder that in the birefringence process, where we try to generate the second harmonic this birefringence things are happening inside crystals.

So, crystals are there where we can have the birefringence for which we are getting the phase matching. And this crystal should have some sort of symmetry so; that means, if I apply some kind of symmetry operation; so the crystal will remain same.

So, applying this condition we can have Neumann's principle. So, now let us try to find out what Neumann's principle suggest, but before that we should understand that since we are using crystal; there are different kind of symmetry in the crystals we called the point group symmetries. So, this point groups though some kind of symmetry operation we can make over on the crystal. And if I do that then what happen? That the crystal the orientation of the crystal will change, but not the property.

So, using that thing we can say in the Neumann's principle that the susceptibility tensor of a material belonging to a certain crystal class must be invariant under corresponding point group; that means, if I put some kind of operation over that then there will be no change on the crystal. So, if we make a transformation symmetry operation over this material then the susceptibility before and the susceptibility after the transmission must be same.

So, if I change the, if I put some kind of operation because of that if the susceptibility tensor changes; then the new susceptibility tensor and the old susceptibility tensor which was before the operation. Suppose to be the same thing if my operation is a symmetry operation, well before going to apply this kind of transformation over a tensor or matrix; let us find out how the vector is transform over some kind of operation.

So, here very simple example is given where you can identify that this is you can identify that this is a rotation matrix, this is a rotation matrix around axis z if the theta amount of rotation is there. So, we have an axis like this and if I make a rotation sometime new axis is dotted one and it is something like this. So, then what happened if I have a vector in my previous say this is X, Y, Z if I write.

So, if I have a vector here psi which has a component psi 1, psi 2, psi 3 after rotation of the axis what happened? We have a new component psi 1 prime, psi 2 prime and psi 3 prime; how psi 1 prime, psi 2 prime and psi 3 psi 3 prime is related to the previous components; the original component psi 1, psi 2, psi 3 can be represented by this operation which is quite straight forward and I believe most of the students are aware of this kind of things.

So, now the question is what happened when we going to apply this on a tensor this kind of operation on a tensor.

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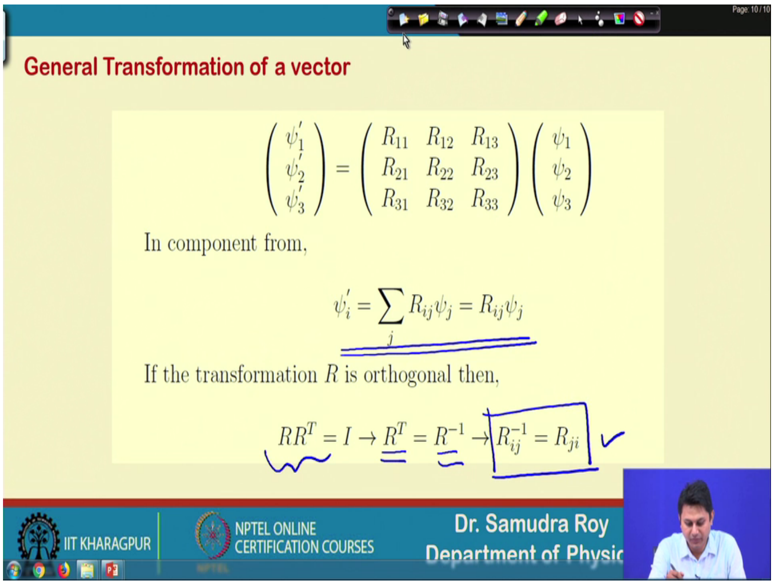

But before that we generalize the transformation of vector. So, if R 1, R 2, R 3 is a generalized operation matrix. So, I can write these in index notation like this; so ith component is represented by if I write this psi 1 prime; it is represented by R at 11, R 12 and R 13; so, it is eventually R ij j.

So, now, if my transformation whatever the transformation I am talking about in terms of R is octagonal in nature; then we have a relationship between them for orthogonal matrix that is R R transpose is equal to identity matrix that we know; that means, R transpose is nothing, but R inverse.

So, if my operation is orthogonal in nature then what happened? We have a relationship between R and R transpose and R transpose is nothing, but the inverse of the R; where R is the operation matrix; so every operation can be represented in matrix; so that we are doing, so we have an expression like this for orthogonal transformation; why the orthogonal transformation is important here?

Because whatever the operation we are talking about are essentially the orthogonal transformation and orthogonal transformation what happened that we should have a change of vector, the coefficients of the vector change. But since the orthogonal transformation is there, so there is a additional relationship between the different coefficient of the operation matrix R ij in general ok

So, once we have the information of this R matrix.

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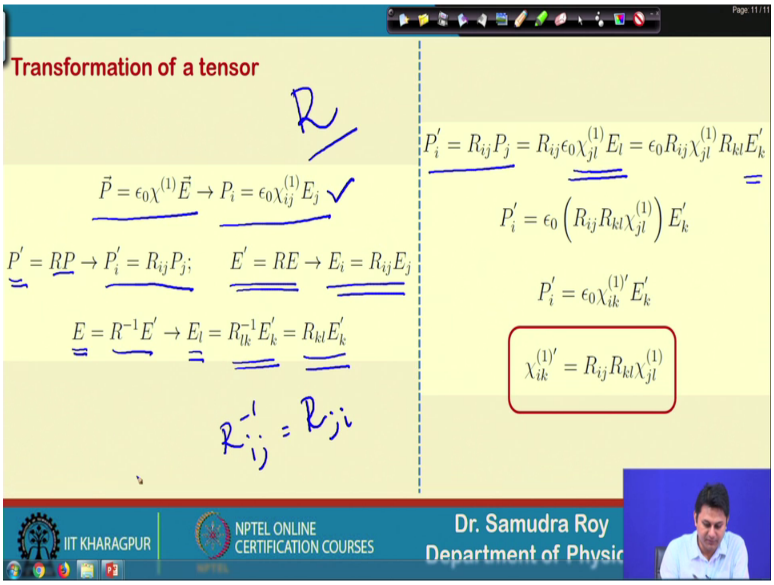

Next we try to apply this things over a tensor. So, before doing that let us try to apply this in our old equation polarization and electric field equation and that is this it will be easier for you to understand. So, this is the P vector which is related to E vector like P is equal to epsilon 0 Xi 1 e which is straight forward.

Now if I write it in component form it should be P i is equal to epsilon 0 susceptibility ij and E j. Now what we try to do? We try to write this P vector in different coordinate system, where this coordinate system is represented by or some operation is there for which the coordinate system is changed and this operation is represented by the matrix R.

So; that means, if I operate R over P; then I will have P prime. So, in component notation P i prime is R ij, P j which is before as before we have shown in terms of psi we have same expression, but here in place of psi we consider that P is there so; that means, polarization term is there. Next what the electric field E is also going to change and electric filed is a vector. So, the components of the vector will change in a similar notation.

So, E can be represented in terms of R inverse like R inverse E prime because if I make the inverse both the side then this will be the case. Then E l is component can be represented in terms of E k component like this. So, just I use a similar principle; here I just reproduce the P i th prime component in terms of P j. Here I am doing non prime component to prime component that is a relation and I will eventually have this.

Why? You can see that R inverse of i j was R of ji because they are orthogonal. So, these are the relationship they should hold; well after having this now go back to our old equation that ith component is now going to change; now I put all these things together. So, P j is nothing, but susceptibility j l and E l which is this equation. So, I am writing this equation once again I operate these things over P j; so, P j in terms of E is this.

Now, E l again I can write in terms of E prime; so, this is my prime form which is already I have derived in this place here that how E l is represented in terms of E k prime.

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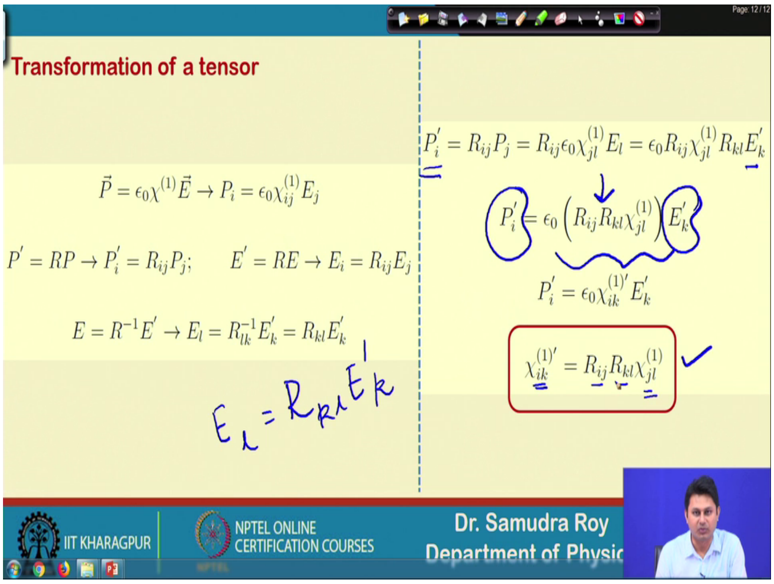

So in prime frame; I just write it; so P prime which is in the left side and E prime which is the right side if I now write it all together. So, I have a term here which suggest that this is nothing, but this is you can see the left hand side P is in P prime frame or the prime frame E k is prime frame; so this has to be in prime frame. So, if I write this into the prime frame the susceptibility which is essentially tensor can be transformed like this.

So, this is the rule of transformation of the susceptibility tensor. So, susceptibility tensor ij component in prime frame can be represented in terms of susceptibility tensor in non prime frame jl and it is related to ij and kl with this notation.

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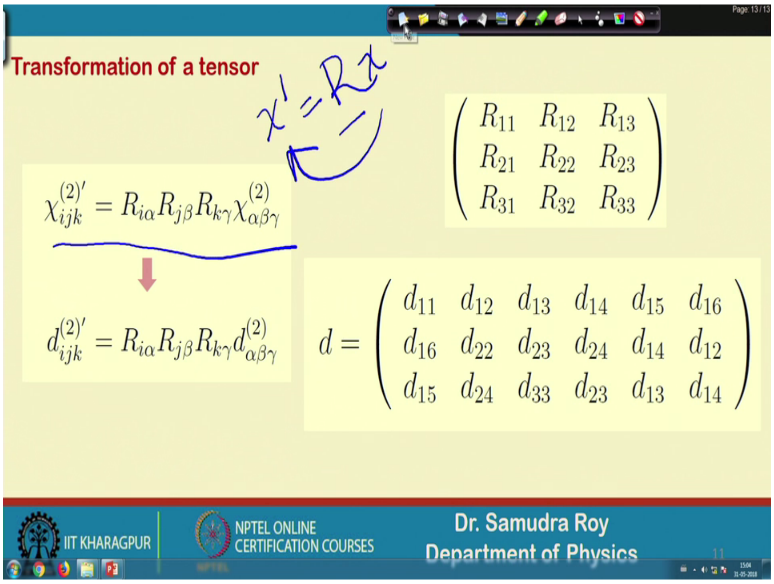

Well after having this general notation what we can do? That we can use this thing here; so, after the rotation or whatever the operation it is not necessarily rotation operation is there; there may be several kind of operation we have a general expression here.

So, the general expression suggest that we have some kind of; so, I have a susceptibility tensor here. In prime frame the susceptibility tensor I can write susceptibility prime and if some operation was there; so, this is the operation that is operated over psi and I am getting this.

So, this is the rule that I am applying some kind of operation on vector I am getting different vector component. In the similar way if I apply the same operation over a tensor then the tensor will going to change in the prime frame.

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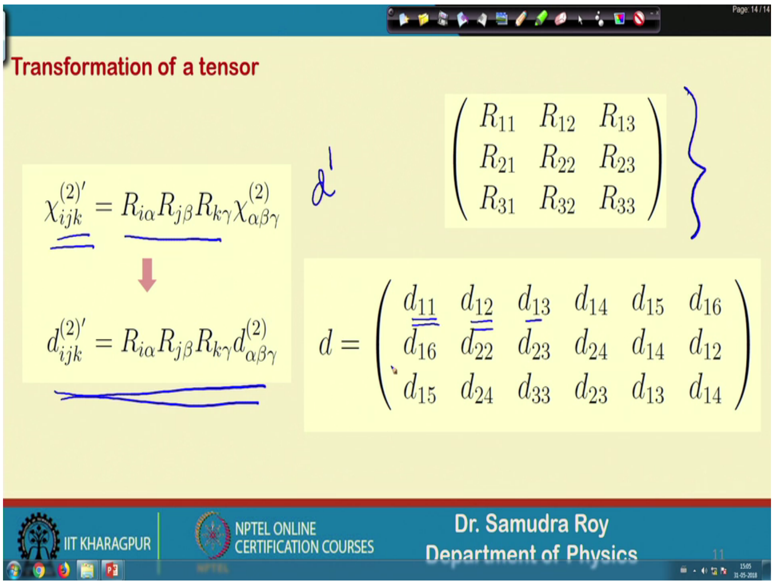

And when the tensor is going to change in the prime frame this is the rule that we have; this is the rule that we have that ijkth component in prime frame can be represented as R i alpha, R j beta, R k alpha; beta gamma. So, this is the rule of change of a tensor under some kind of symmetry operation where R is the operation matrix.

So, if ijk of susceptibility sensor ijk is change in this way; so these tensor in the similar way can be changed in this fashion. So, R 1, R 2, R 3 these are the vector components these are the matrix operation, these are the coefficient and when we have the this coefficient; we can have also the coefficient of d 123 and all the things. So, now, if I want to find out d prime under some kind of rotation then I will going to use these things and operate over that and then individual component can be find out in this way ok.

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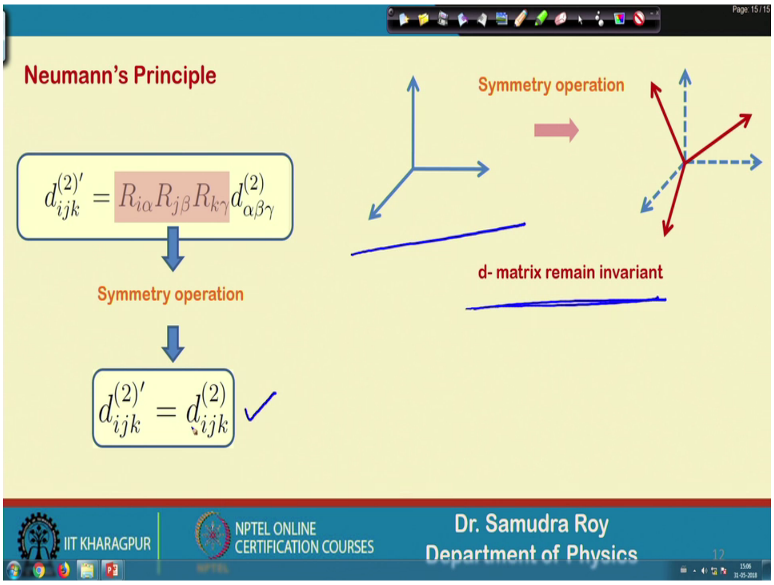

So, let us see what we have; so, let us try to understand once again what is Neumann's principle may be today's class we will not going to complete that in the next class again we will start.

But the important thing we should note once again see this important. So, we are going to apply some kind of symmetry operation; so, this is suppose a system we have a coordinate system we have. So, some kind of symmetry operation we are making so that my operation system is changing. So, d matrix will remain invariant under this operation that is the principle this is the Neumann's principle. So; that means, dijk prime after making the symmetry operation over d alpha beta gamma; then what happen after the operation whatever the value we have that should have the same value that of the previous one.

So, ijk and ijk it should be same value after doing this operation. So, this is essentially the Neumann's principle once again let me state that in Neumann's principle; if I apply some kind of symmetry operation over d matrix, d matrix components will be changed. And this changing d matrix component will be exactly the same d matrix component before the operation.

And from that we can have a relationship between different d matrix components and we find in the next class that we will start using some example that how the d matrix components will be calculated and most of the cases we find that d matrix components will going to be vanished or they are same to each other. And then the number of independent coefficient again reduce significantly and eventually we have 2 to 3 or to 4 different components of d matrix that can form a independent terms and through which we can form the d matrix.

So, well let me conclude here; so today we learned a very important concept of this Kleinman's symmetry and Neumann's principle. So, both are applied over the d matrix and because of that what we find that the number of independent coefficient reduce significantly. Initially we started with 27 different component of d matrix, which is very tedious to handle.

Then we find that after applying this kind of symmetries, we can reduce this d matrix upto 10 independent components and further we will going to see applying the Neumann's principle we can reduce if more and eventually we have only 2 to 3 different d matrix components; which are independent to each other. And we will deal with this things in the previous classes; so, with that note let me conclude here.

Thank you for your attention and see you in the next class.