

Condensed Matter Physics
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Lecture - 6
Physical Properties of Crystals

In the last few lectures, we have been discussing how the crystal structure of a solid, may be determined using scattering techniques or diffraction techniques. And this gives you the information about the position of atoms and molecules inside the crystal, having d1 that we are now in a position to go on to discussing the physical properties of crystals and the role of symmetry in determining these physical properties. So, this will be the subject of a discussion today.

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Introduction

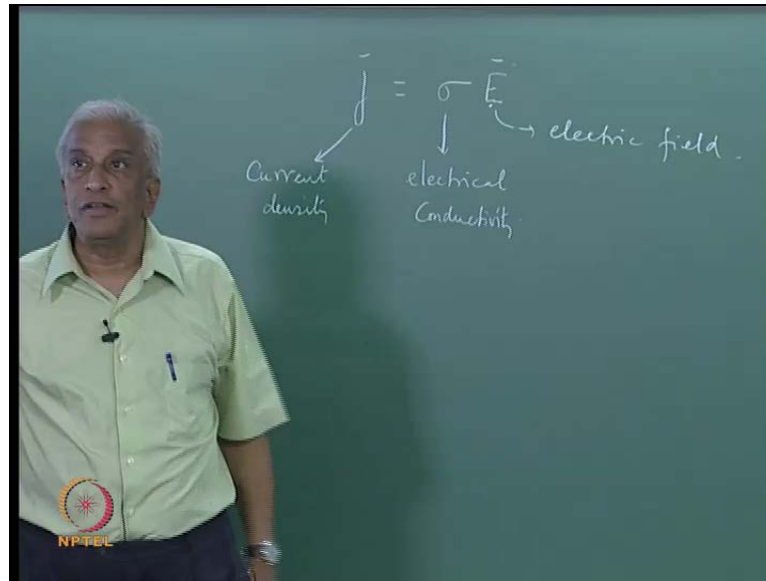
- All crystals, by virtue of their regular periodic arrangement of atoms in three dimensions, are anisotropic with respect to their physical properties, i.e., the physical properties are different in different directions.
- So, while specifying properties of crystals it becomes necessary to include information on the directions.



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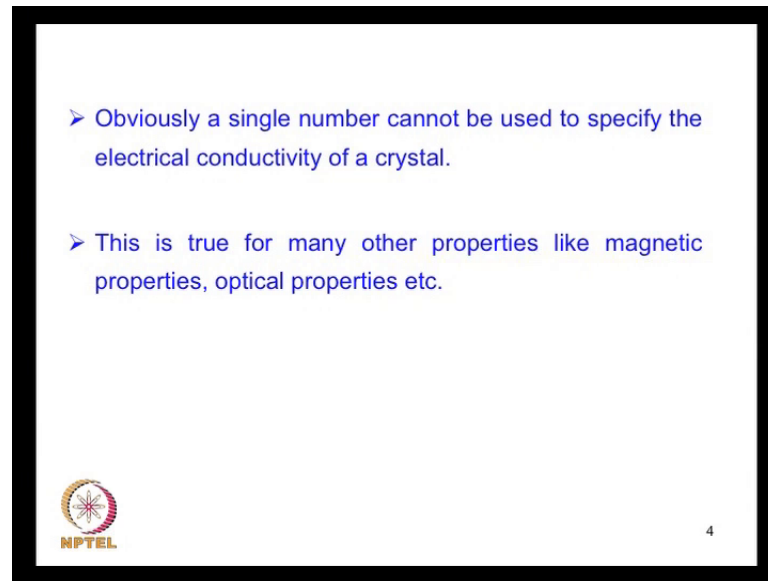
All crystals, by virtual the regular periodic arrangement of atoms in three dimensions, are anisotropic with respect to their physical properties, as we have already mentioned. This means that the physical properties are different in different directions. So, while specifying properties of crystals, it becomes necessary to include information on the directions. For instance, the electrical conductivity for crystal involves two directions.

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Because the electrical conductivity is given by the general relation \vec{j} equals $\sigma \vec{E}$, where this is electrical conductivity which we want to determine, this is the electric field and this is the current density. So, the direction in which the electric field is applied as given by the vector \vec{E} , and the direction in which the current density produce this measure as given by the vector \vec{j} , these are the 2 directions. Both of which have to be specified in order to state, what is the value of the conductivity, and if these directions are changed, the value of the conductivity will be different. So, it is necessary to mention these 2 directions of the 2 vector quantities involved in the measurement while specifying the conductivity.

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➤ Obviously a single number cannot be used to specify the electrical conductivity of a crystal.

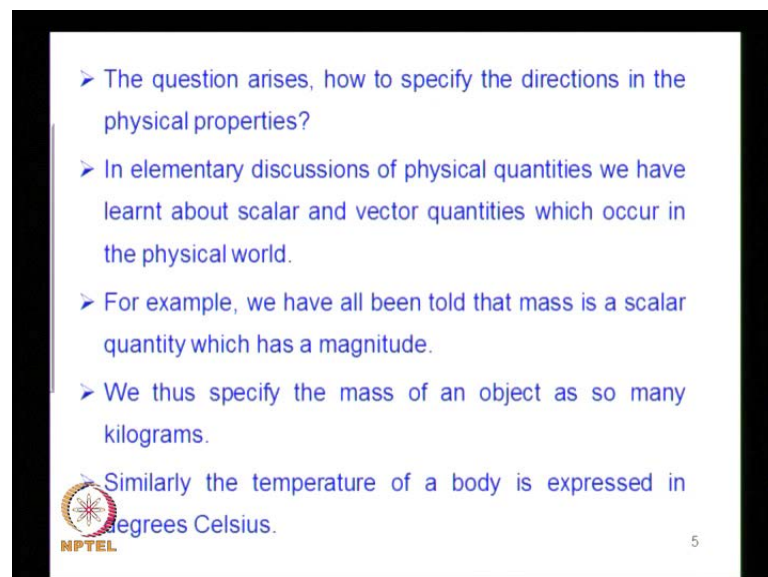
➤ This is true for many other properties like magnetic properties, optical properties etc.



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Obviously a single number cannot be used to specify the electrical conductivity of a crystal. This is actually true for many other properties like the the magnetic susceptibility, the refractive index etcetera.

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➤ The question arises, how to specify the directions in the physical properties?

➤ In elementary discussions of physical quantities we have learnt about scalar and vector quantities which occur in the physical world.

➤ For example, we have all been told that mass is a scalar quantity which has a magnitude.

➤ We thus specify the mass of an object as so many kilograms.

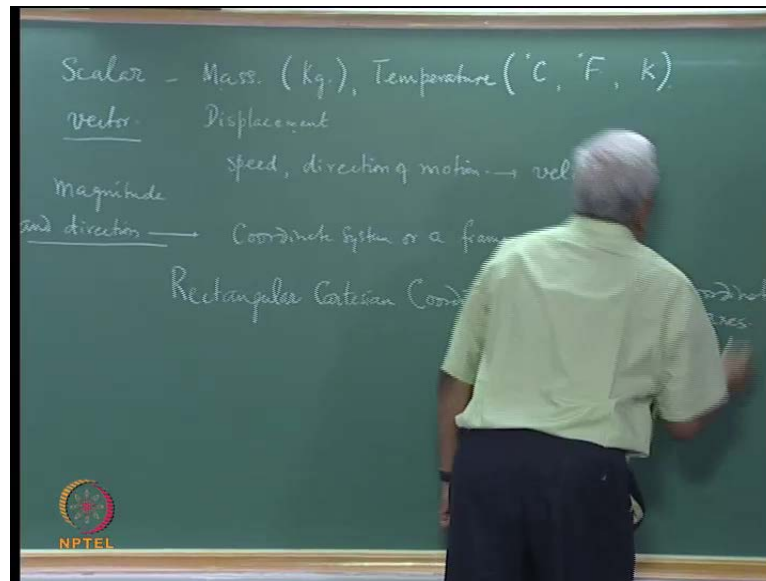
➤ Similarly the temperature of a body is expressed in degrees Celsius.



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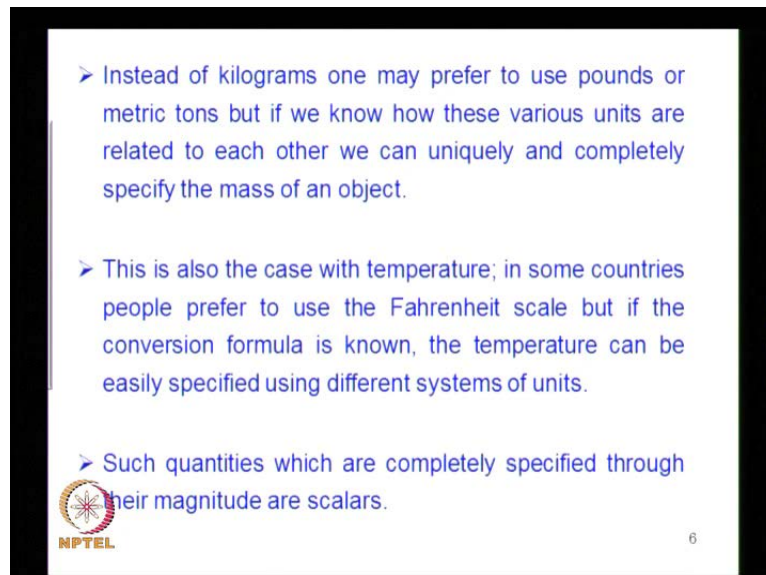
The question then arises, how to specify the directions regarding the physical property measurements and specifications. Now in elementary discussions about physical quantities, we have learnt about scalars and vector quantities, for example, we have all been told that the mass is a scalar.

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We specify the mass of an object as for example, so many kilograms. Another quantity which comes to the mind for a examples of a scalar quantity is the temperature. We specify the temperature of an object in degrees Celsius or degree Fahrenheit or degree Kelvin and so on.

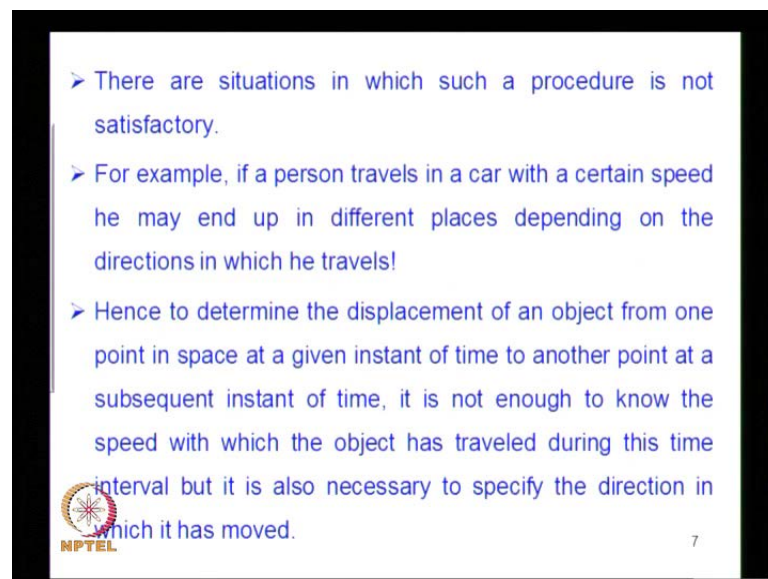
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So, there are different units in which these quantities are specified. If instead of kilograms one prefers to use pounds or metric tons, but then we know how these various units are related to each other. So, we can uniquely and completely specifying the mass

of an object regardless of which system of units we adopt. This is also the case with the temperature, we may specify the temperature in degree Celsius or in Fahrenheit scale or in the thermodynamic absolute Kelvin scale, but as long as we know how these different values are related to each other, there is no ambiguity regarding what a given object, what is the temperature of heat is. So, such quantities like the mass and the temperature are completely specified once their magnitudes are given, such quantities are example of scalar quantities.

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- There are situations in which such a procedure is not satisfactory.
- For example, if a person travels in a car with a certain speed he may end up in different places depending on the directions in which he travels!
- Hence to determine the displacement of an object from one point in space at a given instant of time to another point at a subsequent instant of time, it is not enough to know the speed with which the object has traveled during this time interval but it is also necessary to specify the direction in which it has moved.

In contrast to this, there are other situations in which such a procedure will not be satisfactory. For example, suppose we think of a person who travels in a car with a certain speed, he will end up in different places depending on the direction in which he travels. So, in order to determine the displacement of an object from one point in space to at a given instant of time to another point in space at a subsequent instant of time, it is not just enough to know the speed with which the object as travel during this interval. But it is also necessary to specify in which direction it is moving, then only we will have the complete information required to determine the displacement.


The displacement in order to specify the displacement, it is not enough if we just specify the speed of the object, but also it is necessary to specify the direction of motion. We may specify this speed along with the information about the direction of motion, we refer to this as the velocity. So, the velocity as a magnitude given by this speed under direction

such a quantity is known as the vector. So, in dynamic, we come across several such quantities such as the displacement, velocity, acceleration, force, linear momentum etcetera. So, these are all vector quantities which have not only a magnitude, but also a direction. So, this is something that we are all familiar with.

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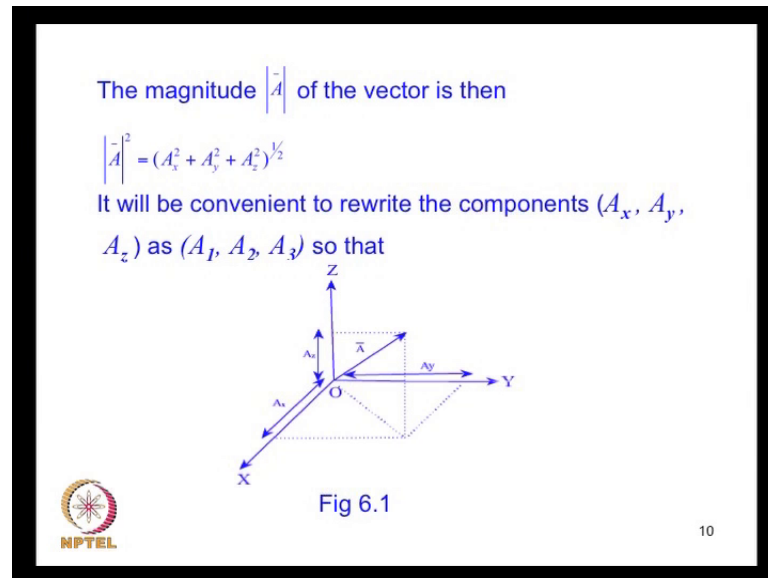
Frames of Reference

- The direction of a vector is specified with reference to a set of coordinate axes (X, Y, Z) which form a rectangular Cartesian coordinate system or a reference frame whose origin is at O .
- A vector \vec{A} may then be resolved into its components A_x, A_y, A_z along the X, Y, Z axes respectively.
- We choose unit vectors $\hat{e}_x, \hat{e}_y, \hat{e}_z$ along these directions so that we may write: $\vec{A} = \hat{e}_x A_x + \hat{e}_y A_y + \hat{e}_z A_z$

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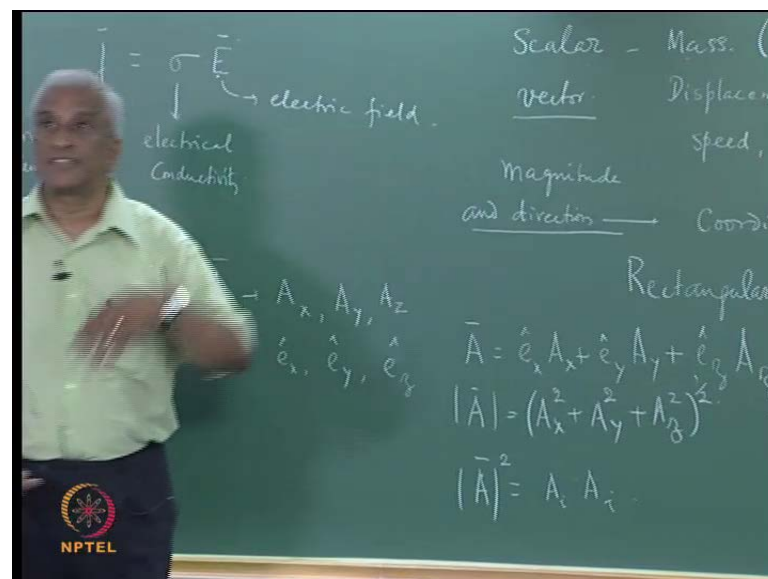
In order to proceed further, in order to be able to talk about quantities like the electrical conductivity, it is necessary for us to know, how to specify this direction with respect to a certain fixed coordinate system or a frame of reference. So, the direction yesterday specified with respect to such a coordinate system. Suppose, we have a rectangular Cartesian coordinates, which with we all are familiar which is specified by a certain origin and then X, Y, Z ; and origin - O and X, Y, Z are the axis - coordinate axis.

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So, we have something like this, we have this given in figure four 1 you have O X, O Y, O Z are orthogonal directions along the three mutually perpendicular standard directions. In three-dimensional base and a specify the coordinates of an object by specifying a vector for example can then a vector a maybe specify by giving its components A x, A y, A z along these three coordinate axis.

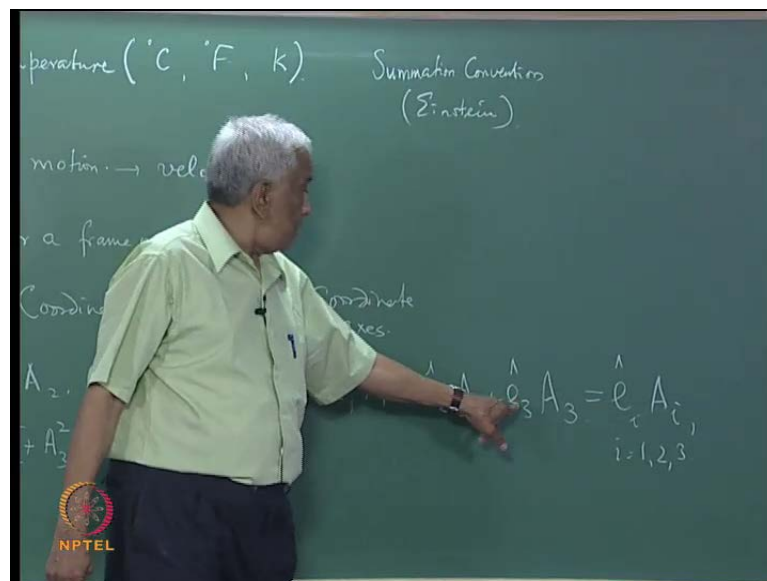
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So, that and the unit vector along these are given as e x, e y, e z with respect to e then the vector a may be written as e x A x e y A y plus e z A z. It is fairly well-known, it

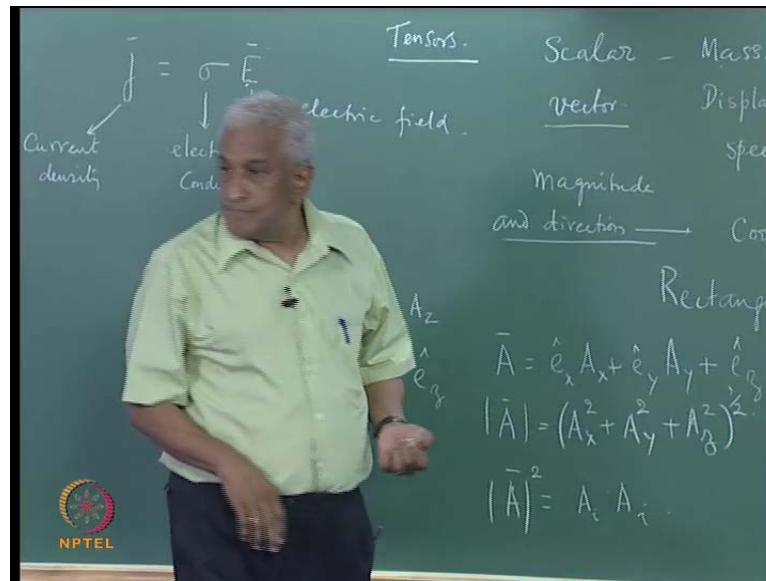
straightforward to know that the magnitude of this vector is just the square root of the sum of the squares of these components $\sqrt{a_x^2 + a_y^2 + a_z^2}$ half the magnitude. So, in general, far more general representations, it is more convenient to drop these x , y and z and replaced them by a_1 , a_2 , a_3 by which we understand that a symbol subscripted 1, 2, 3 stands for the x , y and z components. So, that I can write the same relation as $a_1^2 + a_2^2 + a_3^2$ to the power half and this 1 we can write this relation as $e_1 A_1 + e_2 A_2 + e_3 A_3$. The advantages of this notation will become obvious when we introduced.

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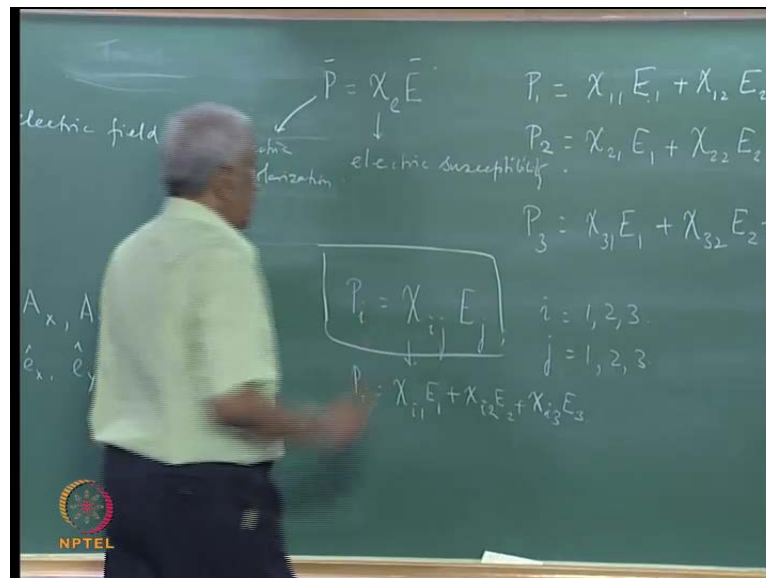
What is known as the summation convention, which was introduced by Einstein according to this convention whenever a particular subscript is repeated it implies a summation over that subscript. For example, we can write this using the summation convention as $e_i A_i$, where i is 1, 2, 3 since i is repeated this means that there is a summation. So, $e_1 A_1 + e_2 A_2 + e_3 A_3$; i ranges over 1, 2, 3. And similarly, the magnitude square is $a_i a_i$ again, since i is repeated this means that there is a summation over this induces. So, I have $A_1^2 + A_2^2 + A_3^2$ which is $A_1^2 + A_2^2 + A_3^2$ giving us the same expression, but we have arrived at a much more compact notation in both cases.

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So, this rotation enables us generalize this considerations to more complex physical quantities which are in general known as tensors in order to know what these stencils means letters go back to these two vector quantities which are related to each other just to make life more interesting.

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Let us take a different a similar, but different relation which relates the electric polarization p which is a vector to the applied electric field e and the relation these 2 quantities polarization and the electric field are related by a so called electric

susceptibility. This is the electric polarization this is very similar to this relation, but I am just for interest sake I am taking a different example. So, in general p and e which are vector will not have the same direction therefore, it is necessary to specify their directions.

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Hence we have

$$P_1 = x_{11}E_1 + x_{12}E_2 + x_{13}E_3$$

where

$$x_{11}, x_{12}, x_{13}$$


are constants of proportionality which define the response of the dielectric medium to the field components E_1, E_2, E_3 .

The summation here is due to the principle of superposition. We have similar relationships

$$P_2 = x_{21}E_1 + x_{22}E_2 + x_{23}E_3$$

and

$$P_3 = x_{31}E_1 + x_{32}E_2 + x_{33}E_3$$

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So, then I will have P_1 equals $x_{11}E_1$ let me write this relation then explain. So, the electric field is applied in a general election such that it as component E_1, E_2 and E_3 along the three coordinate axis in a chosen reference frame. So, the component p_1 of the polarization vector which is along the x direction is given is due to not only E_1 , but also E_2 and E_3 . Therefore, we have to write this general relationship between p and e in terms of a sum, which includes the contribution due to the polarization produced by the component E_1 and the contribution from E_2 and the contribution from e three using the principle of superposition. So, the contribution sum E_1 to 1 is known as the component x_{11} and the contribution which means that this is the contribution due to the electric field component E_1 for the polarization component P_1 .

Similarly the contribution from the component E_2 the polarization component p_1 is x_{12} . So, there are two subscripts now for each of these quantities 1 subscript indicating which component of the polarization it contributes to and the other component subscript indicating due to which component or the electric field it arises. Similarly, I will have other relations like $p_2 = x_{21}E_1 + x_{22}E_2 + x_{23}E_3$ and $P_3 = x_{31}E_1 + x_{32}E_2 + x_{33}E_3$

$\vec{P} = \epsilon_0 \chi \vec{E}$. These are the that gives you all the three components of the polarization vector which arrives from contribution from three components E_1, E_2, E_3 of the electric field. So, this vector quantities $x_{11}, x_{12}, x_{13}, x_{21}, x_{22}, x_{23}, x_{31}, x_{32}, x_{33}$. This entire set of quantities together determine the total response to the electric field the polarization produced by the electric field this looks very complicated, but I can use summation convention and write this as a very compact relationship in this way where i runs over 1, 2, 3; j also runs over 1, 2, 3. So, I use since I have $x_{ij} E_j$ is subscript j there is a repetition. So, there is a summation over a subscript j . So, this really mean as I substitute this is going to give me this is really the following $P_i = x_{i1} E_1 + x_{i2} E_2 + x_{i3} E_3$ and if I give the values i for i from 1, 2, 3. I will get back all these three relationships. So, this compact relationship is really a very compact way to represent this complex relationship.

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➤ The equation $\vec{P} = \epsilon_0 \chi \vec{E}$ then is given in component form by the above three equations.


➤ Alternatively we may use matrix notation and write

$$\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$$

which leads to the above three equations according to the rule of matrix multiplication.

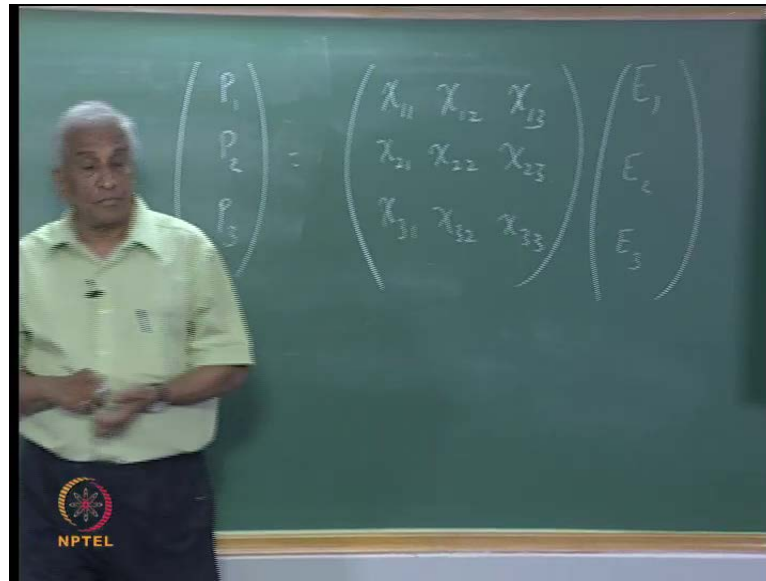
➤ The column matrix $\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix}$ thus represents the vector \vec{P} .

while the column matrix $\begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$ represents the vector \vec{E} .



And the entire array of x_{ij} together all the nine quantities they form the components of a tensor known as the electric susceptibility tensor similarly the electrical conductivity is also a tensor we could use for example, instead of the algebraic notation

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This immediately suggests the possibility to write this in matrix form using the method of matrix multiplication we get back the same relationship. So, the column matrix P_1, P_2, P_3 that gives you the component of column vector p while the column matrix here E_1, E_2, E_3 gives us the components of vector E . And this three by three matrix consisting of the array of numbers x_{i1}, x_{i2}, x_{i3} etcetera up to x_{i33} that gives you a three by three matrix which represents the electric susceptibility tensor.

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The (3×3) matrix $\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}$

➤ thus represents the 9 components of the electric susceptibility tensor x_{ij} .

In index notation, we may write the above relation as:

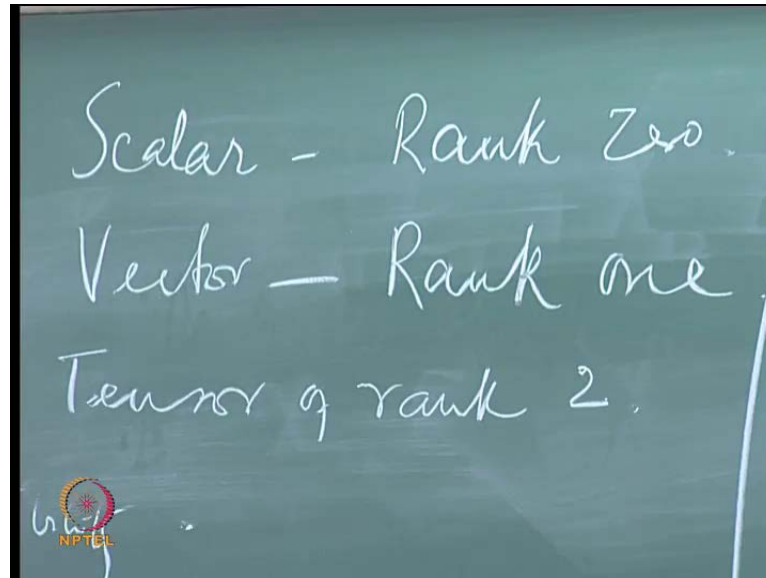
$$P_i = x_{ij} E_j \quad i, j = 1, 2, 3.$$

x_{ij} is then said to be a tensor of rank two.

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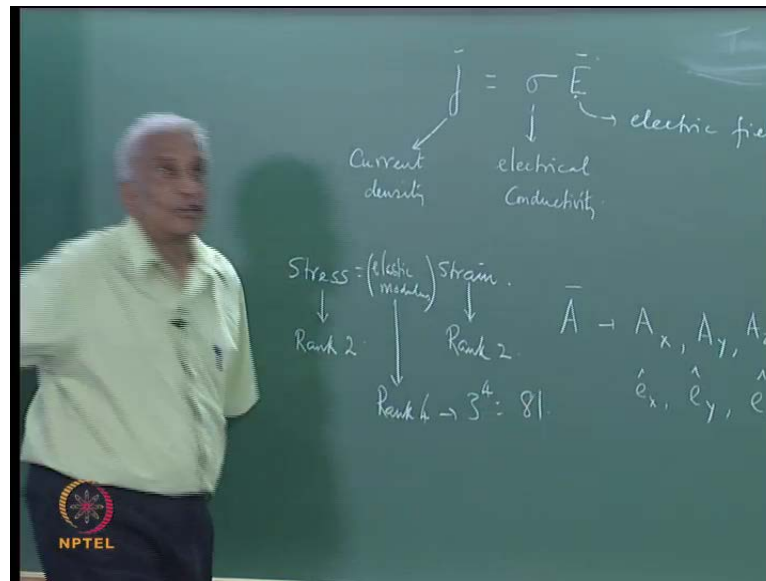
So, that is the general way to represent quantities of this kind. So, you can see already it is not just a tensor it is a tensor of rank two a vector is a tensor of rank 1 a scalar is a tensor of rank zero.

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What does it mean, this means in three-dimensional space. If you raise this to the power 3 to the power zero which is 1 scalar as just one component. It is one quantity, if you specify the magnitude of the tensor scalar you have everything about this scalar whereas, this one has three to the power 1 which is pretty component a vector quantity as the components under tensor of rank two three square nine components has shown here for example. So, it is clear that we can have depending on what are the quantities involved in this relationship you can even have tensor of rank three rank four and so on higher order tensors.

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For example, elastic modulus elastic modulus every1 know s is given by a relation connecting this a stress of the strain. So, the relation connecting the stress is a tensor of rank two a strain is also a tensor of rank two. So, the elastic modulus is a tensor of rank four which means that it as three to the power four in general equal to eighty 1 compounds

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Consider a second rank tensor, say, electrical conductivity (σ), which relates the two vectors electric field (\vec{E}) and (\vec{J}) current density :

$$J_i = \sigma_{ij} E_j \quad (6.1)$$

and each takes values 1, 2 and 3 independently.
Equation (2) actually represents the following three equations:

$$\begin{aligned} J_1 &= \sigma_{11} E_1 + \sigma_{12} E_2 + \sigma_{13} E_3 \\ J_2 &= \sigma_{21} E_1 + \sigma_{22} E_2 + \sigma_{23} E_3 \\ J_3 &= \sigma_{31} E_1 + \sigma_{32} E_2 + \sigma_{33} E_3 \end{aligned} \quad (6.2)$$


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Let us get back to the conductivity tensor specified by this relationship and we know that if we have these conductivity density and then suppose i apply the electric field along a

particular coordinate axis. So, then only that component will be non-zero for example, E_1 is non-zero, but E_2 and E_3 are zero in which case we will simply have J_1, J_2, J_3 . So, this will have only three components which are non-zero, but if the electric field is applied along in arbitrary direction then all the nine components will be non-zero these nine components are written for example, likewise in the more compact notation J_i equal to $\sum_j J_j e_j$. Where i and j run over 1, 2 and 3 the summation convention enables us to skip the summation symbol.

As I already told you, it is very important to specify the directions. These directions are specified with respect to a fixed reference frame or coordinate system, but very often in real life we may frequently go from one type of coordinate system to another. For example, we may want to know how a given object is moving inside an elevator as compared to the motion relative to the fixed *pari firmata*. So, we would like to know how these two are related the elevator provides one set of coordinates while the fixed there is outside gives you another coordinate system or a reference frame and it is very necessary.

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- This involves the study of phenomena in different coordinate systems which are in relative motion with respect to each other.
- This in turn requires a knowledge of how different physical quantities transform when there is a change of reference frame.

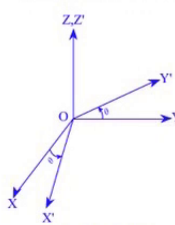

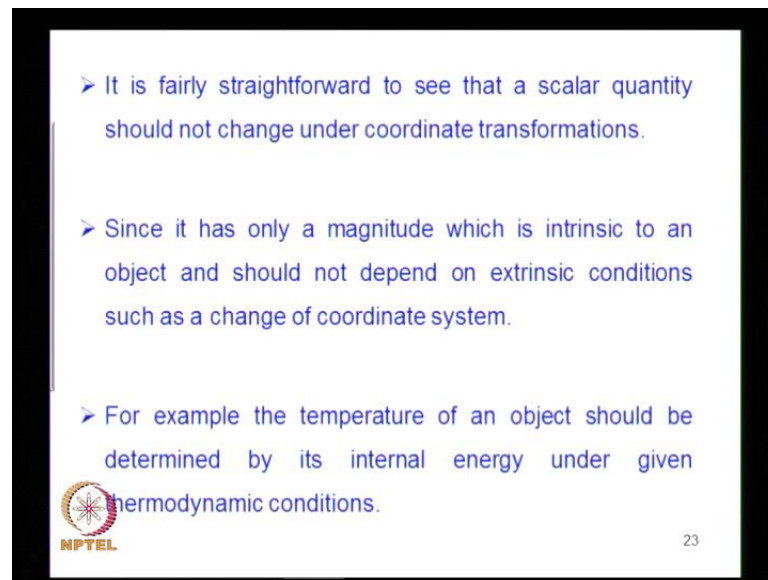


Fig 6.2(a)


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For us to know how the different quantities are transformed when we go from one set of coordinates to another this requires a knowledge of how different physical quantities transform when there is an exchange in the reference frame in this figure shows a simple change effected by a simple rotation about this Z axis by an amount θ .

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➤ It is fairly straightforward to see that a scalar quantity should not change under coordinate transformations.

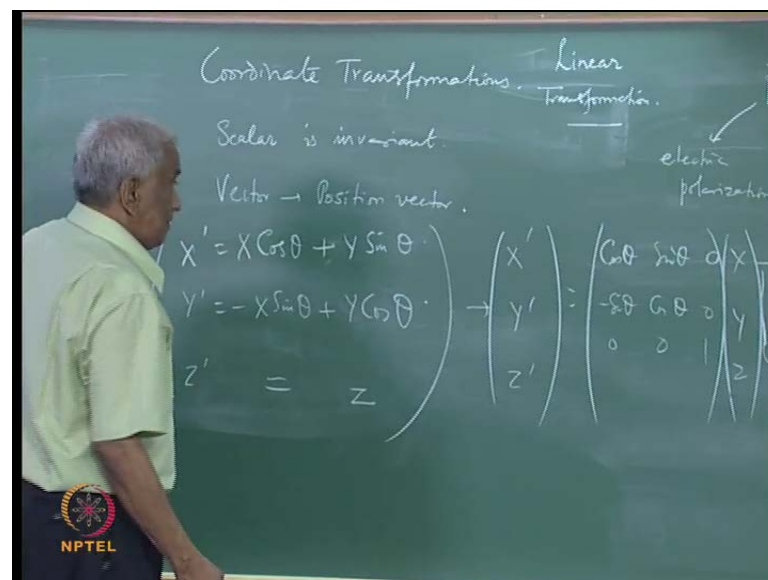
➤ Since it has only a magnitude which is intrinsic to an object and should not depend on extrinsic conditions such as a change of coordinate system.

➤ For example the temperature of an object should be determined by its internal energy under given thermodynamic conditions.

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So, it is fairly straightforward to see that if you have way scalar quantity since it is only a magnitude the magnitude should not change under coordinate transformation. So, a scalar quantity is one which remains invariant under coordinate transformations.

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Coordinate Transformations - Linear Transformation.

Scalar is invariant.

Vector → Position vector.

$X' = X \cos \theta + Y \sin \theta$

$Y' = -X \sin \theta + Y \cos \theta$

$Z' = Z$


$\begin{pmatrix} X' \\ Y' \\ Z' \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}$

elective polarization

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So, we are talking about coordinate transformation now and we are seen that a scalar quantity easy invariant with respect to a changing the reference frame. For example, the mass of an object or the temperature of an object are not determined by what coordinate system we use the specified this.

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- As long as the body is kept isolated from other objects its temperature should not change simply because it has been taken inside a moving train or a lift.
- Thus scalar quantities are invariant w.r.t. coordinate transformations.
- Next we consider what happens to a vector quantity when there is a coordinate transformation.

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So, that is what we mean by saying that the scalar quantity easy invariant under coordinate transformations, but this is not a case for vector and as the tensor quantities a vector changes in magnitude.

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- To describe this we consider the position vector of a point in three dimensional space. For simplicity let us consider two coordinate systems $X Y Z$ and $X' Y' Z'$ which are related to each other through an anticlockwise rotation by an angle θ about the Z axis.
- Since the rotation is about OZ , the direction OZ' is the same as OZ , since it coincides with the axis of rotation.
- Hence OX' and OY' are changed and are obtained through an anticlockwise rotation by θ from OX and OY respectively as shown in figure 6.2(a).

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And direction for example, one of the simplest examples is the position vector.

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The coordinates X' and Y' are then given by

$$X' = X \cos \theta + Y \sin \theta$$

$$Y' = -X \sin \theta + Y \cos \theta$$

The Z coordinate remains unchanged.
Therefore $Z' = Z$.

The above three equations which describe the coordinate transformation from $OXYZ$ to $O'X'Y'Z'$ may be rewritten using matrix notation as:

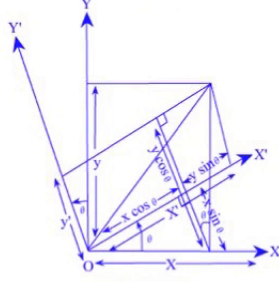



Fig 6.2(b)



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So, be sure the position vector under a coordinate transformation and we specify the position vector in terms of its components x prime y prime and x y in the 2 reference frames which are located by a rotation about this z axis since the rotation is about the z axis the z coordinate remains the same. So, we do not specify the z coordinate it is this same. So, we can simply write z prime equal to z whereas, the x prime and y prime are; obviously, related by things like this equation of this form these are the transformation equations which described it transformation and components x prime y prime and z prime under a coordinate transformation namely rotation by an angle θ about the z axis. So, this can also be straightaway written in matrix form.

So, we can use this basic idea of a coordinate transformation from a basis x, y, z to another basis x prime y prime z prime by a general rotation of what is known as a linear transformation. So, these equation this equation describe such a linear transformation which can in general be written even in a more general form as $a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{23}, a_{31}, a_{32}, a_{33}; x, y, z$. Where the a_{ij} constitute an array of nine number which specify the direction cosines of the new coordinate axis with respect to old coordinate a_{ij} is or in our compact.

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Here the a_{ij} 's are the direction cosines of the various primed coordinate axes OX'_i w.r.t. the unprimed initial coordinate axes OX_j .

Thus a_{11} is the direction cosine of OX'_1 w.r.t. OX_1 .


Thus a_{12} is the direction cosine of OX'_1 w.r.t. OX_2 .

.....

Thus a_{2j} is the direction cosine of OX'_2 w.r.t. OX_j and so on.

We can rewrite this using the compact index notation as:


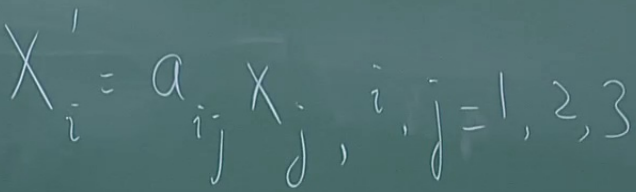
$X'_i = a_{ij} X_j, \quad i, j = 1, 2, 3.$



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In summation notation appear subscript notation i can write $a_{ij} x_j$.

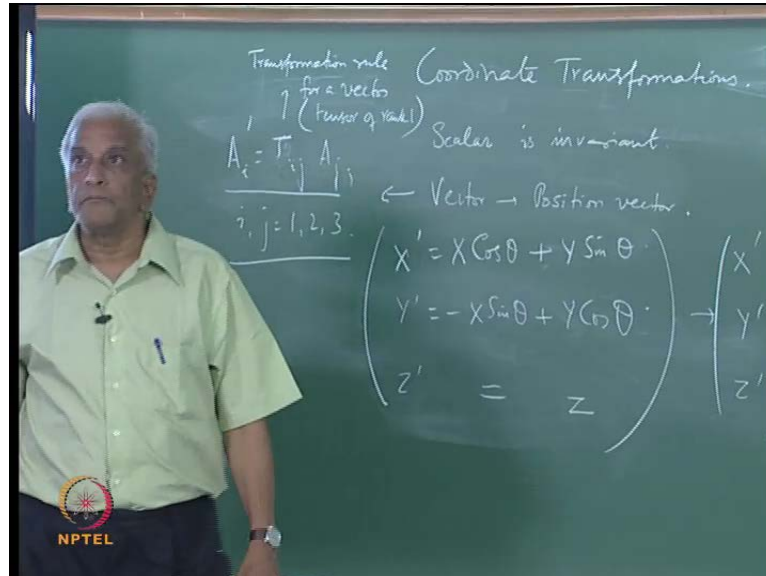
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That is a linear transformation from the coordinate bases x_j to the bases x_i prime where the a_{ij} constitute coefficient of the transformation which give you the connection between the x_j and x_i prime. Again the repeated summation reputation of subscript j implies summation as can be seen here from this from this one. So, this can be used even though we are written it for the components of the position vector this can be

straightaway taken over the specified the components of any arbitrary vector or tensor of rank one.

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And we can say that the components of any vector A_i prime T_{ij} to keep the distinction between the direction cosines of a position vector, but these are these are the components these are the coefficients which relate the components a_{ij} and a_i prime involved in the transformation. So, this defines the transformation rule for a vector a components of a vector which is a tensor of rank 1 . So, now, we can generalize to the case of the transformation rule governing the any higher order tensor. So, we can here itself for example, t_{ij} as we already saw since it connects the 2 vector quantities k_{ij} should be a second rank tensor. So, we can now generalize and find out what happens to the component t_{ij} of this second rank tensor under a linear transformation of this kind using the same principles we will do this in the next time.