Mathematics for Chemistry
Prof. M. Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 3

So far, we have seen what we mean by vectors, we have seen vector spaces and we have found we have seen the very useful concept of linear independence. Which lead us to the concepts of basis and dimensionality and on the way we also looked at various ways of defining products of vectors. Now, next thing we will consider general operators and what we mean are operations on a vector.

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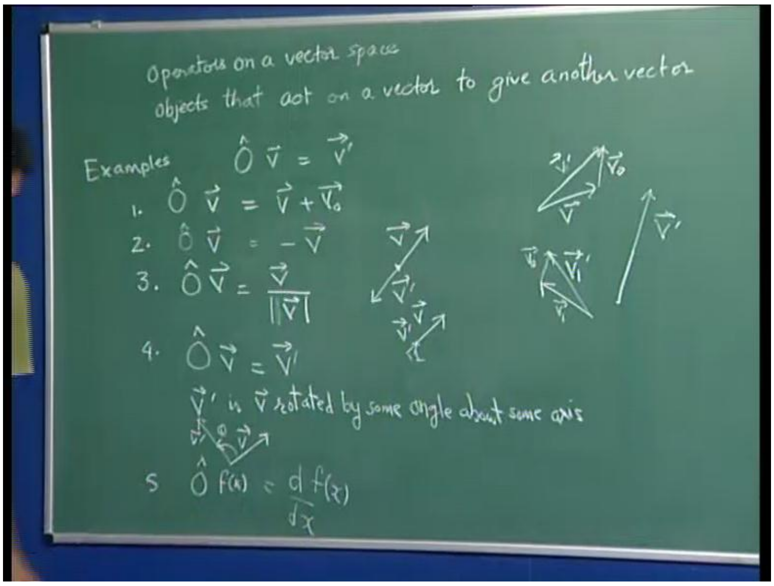

So, we defined something called operators; these are objects, so operators on a vectors vector space see so, these are operators, these are objects that act on a vector to give another vector. So, this is a very general definition of an operator; it is in some cases the term operator is used to referred to operations on scalars that give vectors but, we will use this as the general starting point.

For example, you could an operator that acts on a vector V to give another vector V prank. So, in general you it does something to one vector and it gives you another vector. So, you can think of it as you had V pointing in one direction when you operated by o you get another vector V prime which might point in some other direction might have a different length also. And these can be defined for any vector space, so you can define you operators for the space of functions, you can define operators for vectors in the coordinate space, and there is really no restriction for defining these operators. Let us take some examples of operators, so that the idea of what an operator is it will become clear.

Notice that the operator is not a member of the vector space, the operator is not a vector, operator is some object that is not a member of the vector space but it acts on a member of the vector space to give another member. So, you should be very clear that operator does not belong to the vector space. Now let us look at some examples; let us take the first example; an operator acts on a vector acts on a vector V and you define it as you define this operator in the following way; it takes any vector V and to that vector it adds a constant vector V 0. So, this is an operator it acts on every vector to give a new vector and it is a valid operator.

So, if V was if, so here this is a first example of an operator where it acts on a vector to give you a new vector and that vector is the original vector translated by some vector V 0. So, for example, if V was pointing in this direction and V 0 is a constant vector that might be pointing in this direction then the action of the operator on V gives you a new vector that points in this direction this is V prime. So, operator takes V.

To this new vector V prime pointing in that direction. So, this is the first example of an operator and in fact if you had some other vector pointing in say this direction then if you if you had some let us call this V 1 then the operator this operator will still translated by the same amount. So, you take this vector put it here and you will get this vector V 0 and it will translate it and. So, and. So, it will take V 1 to V 1 prime.

So, this is what this translation operator does it always translates by the same vector. So, the same vector is. So, you add the same vector to the original vector. Second example, let us consider these are examples, let us consider operator acting on V minus V. So, this is sometimes called the inversion operator. So, it takes a vector and gives you vector of the same length and the same magnitude in the opposite direction. So, if you had a if you if you had vector like this if this was your original vector then V prime will be the same vector but, pointing in of the same length but, pointing in the opposite direction. So, it takes any vector and makes it point in the opposite direction.

So, this is sometimes called the inversion operator this operator sometimes referred to as a translation operator because it translates a vector by a fixed vector this is called the inversion operator because it takes a vector and points it in the opposite direction. Another example of an operator is an operation that takes the vector and scales it by it lengths by the length of the vector. So, if you take vector and you divide it by the length of the vector then, you will get a unit vector in that direction.

So, suppose you had your vector pointing this was your V then V prime will point in the same direction but, will have length 1 it will have a length of 1 and this is your V prime. So, this operator takes a vector and shrinks it to a vector of length 1 in the same direction pointing in the same direction. Let us look at some more examples, now this example will not write the explicit form in all these case we wrote the explicit form. In the next example, I will just mention it; I will just state it we will look at the explicit form later in this course when we are when we are dealing with rotations. So, here is an operator that acts on a vector and V prime it gives you a vector V prime where V prime is V rotated by some angle about some axis.

So, if you had a for example, if your V was pointing in this direction if this was your direction of V and let us say you rotate by an angle of by an angle of theta about the about this axis the axis coming out of an axis perpendicular to V. So, you will get a new vector V prime in this direction. So, this is the rotation operation and the rotation operation is a very interesting operation, because it preserves length of the vector length of V and length of V prime are the same. So, if I take a vector rotate it by an angle theta about any axis I will preserve the length of the vector. Similarly, if I the rotation operation has the property that suppose I take two vectors and I rotate them then the angle between them is preserved in the even after the rotation. So, these are things that will be useful when we are dealing with various operations on vectors, and I will just mention them briefly here. So, far we have looked at operations on vectors and though I have not mentioned it explicitly.

So, in this case we have been looking at vectors which are of the form that you seen before which is basically vectors in 3 dimensional Cartesian space. But, you can define similar operations even for vectors which are not of the 3 dimensional Cartesian space. So, you can define an operator. So, suppose you had the vector space where which consisted of functions of a single variable. So, then you can define operator acting on f of x and it will give you some other function g of x and one example of this is it could be d f by d x d f of x by d x. So, an operator acts on a function f of x to give you another function d f of x by d x or it could be or you could have an operator that acts on a function to give you a new function which is a square of this function.

So, you can define many such operations and what I want to show you is that it is not just for vectors in 3 dimensional space operators can be defined for all kinds vectors in all kinds of spaces. So, we have looked at various examples of operators.

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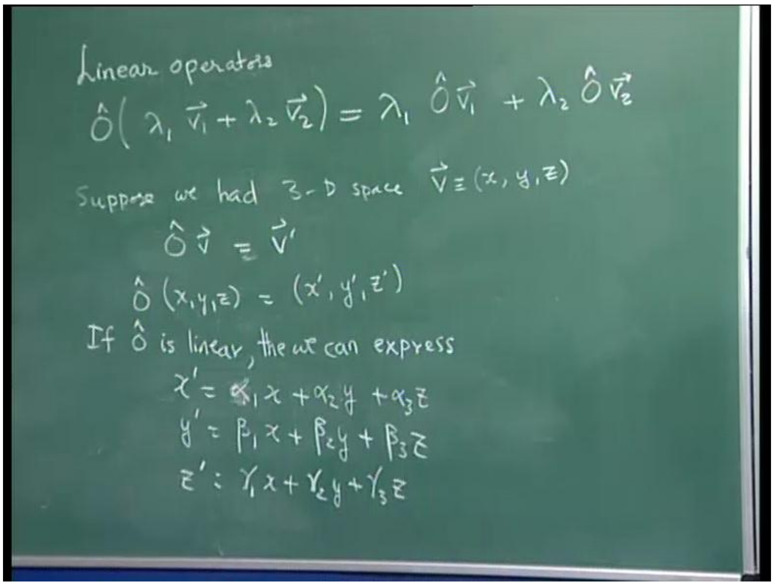

And now, we will just mention briefly that there are certain kinds of operators that have a special place in linear algebra and these are called the linear operators and linear operator is an operator that satisfies a property, that if you have the operator acting on a linear combination of two vectors. So, when this operator acts in a linear combination of two vectors.

So, lambda 1 and lambda 2 are scalars V 1 and V 2 are vectors then. So, since V 1 and V 2 are vectors this sum is also a vector and this whole thing is a vector and when this operator acts on this vector the result is the same as lambda 1 times operator acting on V 1 plus lambda 2 times operator acting on V 2. So, this it is a linear operator in the sense it preserve the additive property and it is linear operator in the sense it preserves the scalar multiplication. So, operator acted on lambda 1 V 1 is just lambda 1 times operator acting on V 1.

Similarly, operator acted on lambda 2 V 2 is just lambda 2 times operator acted on V 2 and operator acted on a sum of two vectors is just the sum of the operator acted on each of the vectors. So, this such operators are called linear operators and these have a special place in linear algebra and we will again this will become more clear when we look at other examples of operators. So, I will just mention again just to give you an example of how these linear operators appear in linear operator suppose we had 3 D space and where a vector is a sum of is denoted by 3 components.

So, now this operator acts on this vector V to give some other vector to give a new vector V prime and. So, if you say that V has coordinates x y z then this has coordinates x prime y prime z prime. So, in general what this operator does is it takes the 3 coordinates and gives you some new coordinates. So, it takes 3 coordinates x y z and gives you a set of new coordinates x prime y prime and z prime then.

Now, this is what any operator does. So, what is special about a linear operator linear operator has to satisfy this relation and if you work it out you can show that, this implies that what the linear operator does is essentially take linear combinations of these of x y and z and give you x prime y prime and z prime. So, in other words if you have a if this operator is linear then we can express x prime as a linear combination of and say alpha 1 and 1 x 1 plus alpha 2 x 2 alpha 3 x 3 similarly, you can write y prime as may be beta 1 x 1plus beta 2 x 2 i meant to say x y and z. So, it is not x 1 x 2 x 3 it is x y z. So, it is alpha 1 x plus alpha 2 y plus alpha 3z.

Similarly, y prime is written as beta 1 x plus beta 2 y plus beta 3 z and z prime can be written as another linear combination. So, gamma 1 x gamma 2 y plus gamma 3 z where all the alpha 1 alpha 2 alpha 3 beta 1 beta 2 beta 3 gamma 1 gamma 2 gamma 3 are all scalars. So, all the alphas all the betas and all the gammas are scalars. So, if the operator is linear then you can show that all these x prime y prime, and z prime can be written in this form And you can also show the converse that suppose I can write x prime y prime and z prime in this form you can show that the operator is a linear operator and that is that is again not very difficult to show. So, the point is this, I mean, this will be a trailer to what we will do in matrices.

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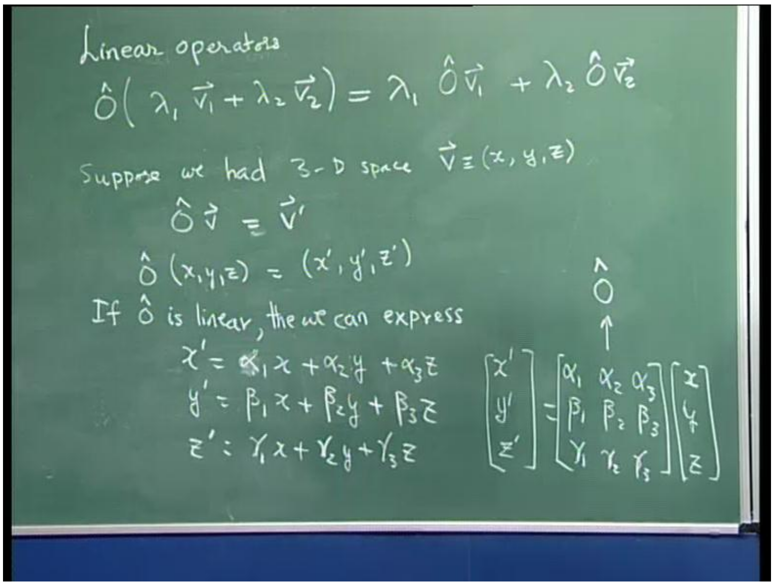

What we will do when we are doing matrices is that we will say that this x prime y prime and z prime are elements of a vector and of a vector in matrix prorogation is denoted by a column matrix. And then, this set of equations can be written a in matrix form as alpha 1 alpha 2 alpha 3 beta 1 beta 2 3 and gamma 1 gamma 2 gamma 3 times x y z and now what we here this representation we identified this as a matrix and. So, this operator your operator o can be represented like a matrix. So, the most general linear operator.

So, any linear operator can be expressed as a matrix the dimensionality of the matrix depends on the dimensionality of the vector space you are considering. So, since you consider 3 dimensional space the dimensionality of the matrix is 3 by 3. So, the point is any operator can be represented as a matrix any liner operator and this is something that we will use repeatedly whenever we are studying various kinds of operators. So, there is now I had briefly mentioned the operation where you rotate one vector to get a new vector.

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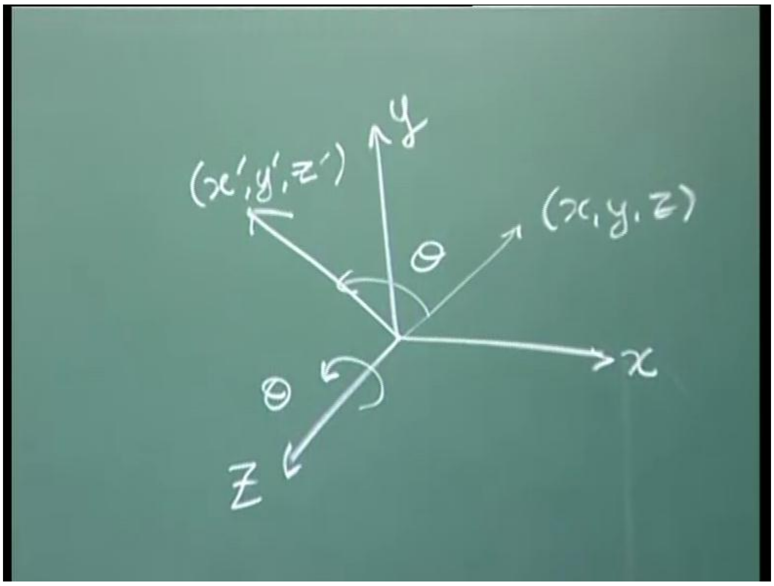

So, you take a vector and rotate about some coordinate and to get a new vector. So, for example, if you have 3 dimensional space where you have x y and z coordinates now, if I had a vector that had coordinates x y z I can operate, I can consider an operation where I rotate about the rotate about the z axis by angle theta. So, what I will get is I will get a new vector the coordinates of that vector x prime y prime z prime. So, and you are rotating by angle theta and if you have this operator then good exercise would be to try to calculate what are the matrix elements of this rotation matrix.

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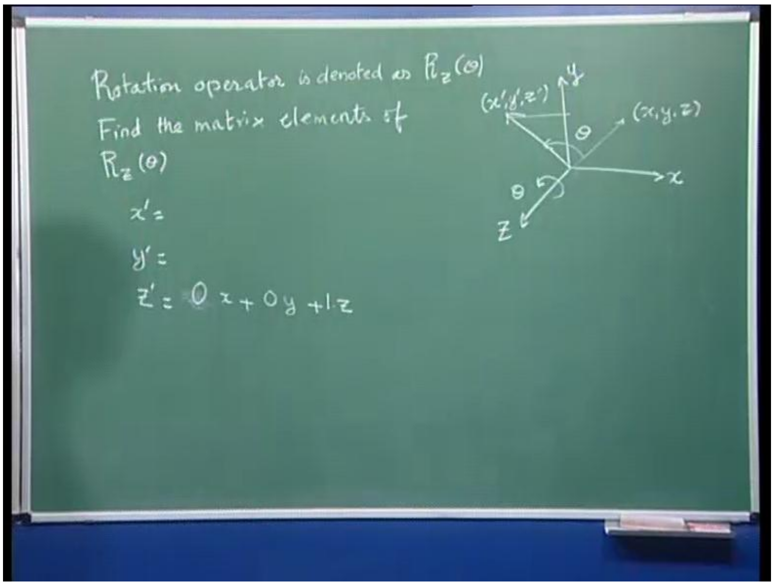

So, the rotation operator is denoted as r z theta. So, we are rotating about the z axis by an angle theta therefore, I am using the symbol r z theta. And the point is you want to find the matrix elements of r z theta. So, find the matrix elements. So, what we need to do is we need to find x prime, y prime, and z prime in terms of the original x y and z in terms of the original x y and z. We need to find out what is x prime? What is y prime? And what is z prime? Now, in order to do this we need some basic coordinate geometry and we need to know how to calculate how to calculate this vector where you rotated about the z axis by angle theta. So, we need to find the x and y components of this vector.

Now, first thing you will say is that if I rotate about the z axis the z component will not change and this is something that is intuitively obvious since z component is nothing but, the length along the z axis now since you are keeping the z axis the same and you are just rotating the vector about the z axis. So, the projection on to the z axis will not change and therefore, z prime will just be equal to z. So, in other words you can write this as zero times x plus zero times y plus z one times z. So, this is something that is that you will it is always true whenever you rotate about one axis that coordinate is not changed.

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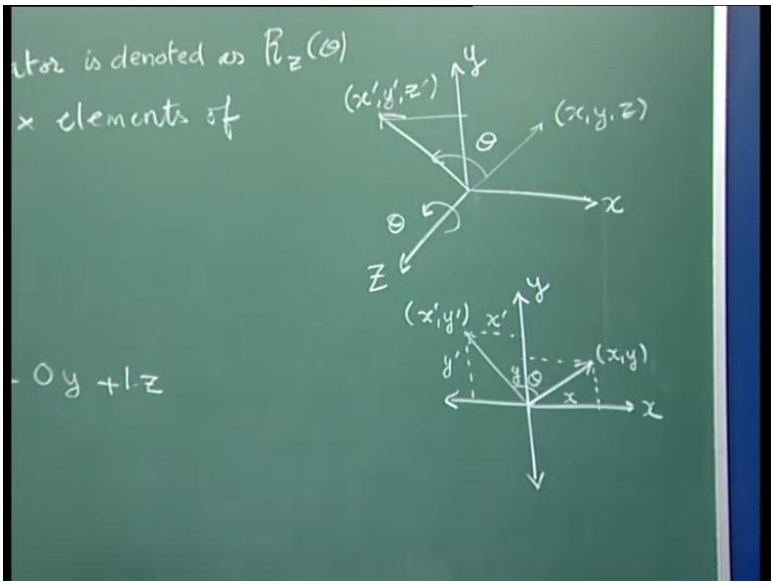

So, the next thing is to find out x prime and y prime in terms of x and y. So, in order to do that lets look at the let us just look at a two dimensional vector. So, if you have the x axis the y axis and you have a two dimensional vector. So, this is this vector has two components this is the x component this is the y component this is the vector x y. Now rotate it by an angle theta. So, if you rotate it by an angle theta then what you get this is your x prime component this is your y prime. So, you get a new vector x prime y prime.

Now, we need to calculate what x prime and y prime are in terms of x and y and I will leave this as an exercise to you but, you can do some fairly simple coordinate geometry to get these lengths and what you will get is x prime is x cost theta plus y sin theta plus 0 times z.

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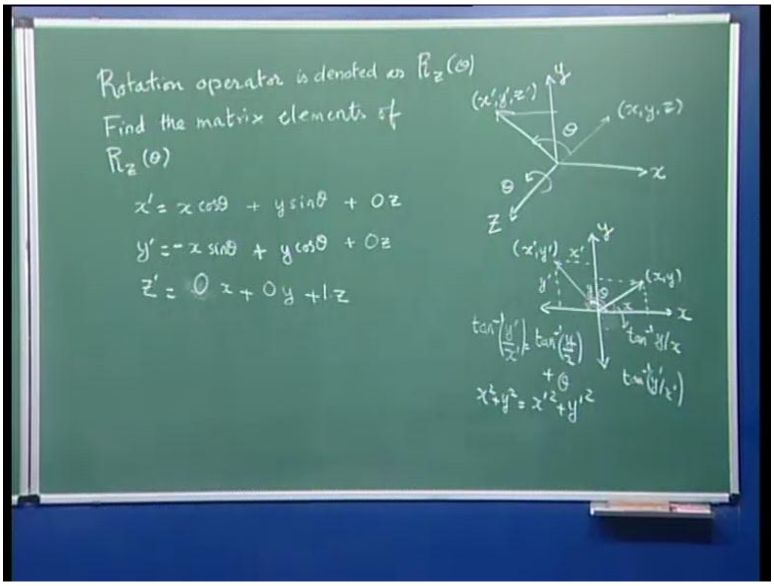

So, the 0 z should be something that is that will always work out. So, since x prime and y prime are independent of the z component since the z component is not changing and the z component is not affecting the values of x prime and y prime and this. So, the way the way you will work out is you need to find out this length and in order to find out that length, what will you do will you take this as this is the original angle and this is this angle is tan inverse y by x and what you will say is that this whole angle tan inverse y prime by x prime y prime by x prime which is this angle and that is that i can call it theta prime.

So, this angle is tan inverse y prime by x prime and you can immediately that tan inverse y prime by x prime is tan inverse y by x plus theta. So, you immediately notice plus theta and second equation that we need is that is that x square plus y square is equal to x prime square plus y prime square since the since when you rotate this vector the length does not change. So, x square plus y square is equal to x prime square plus y prime square and if you use these two relations and you work out the details you can show that this works out to be theta cos theta it will be the other way round minus x sin theta plus y cos theta.

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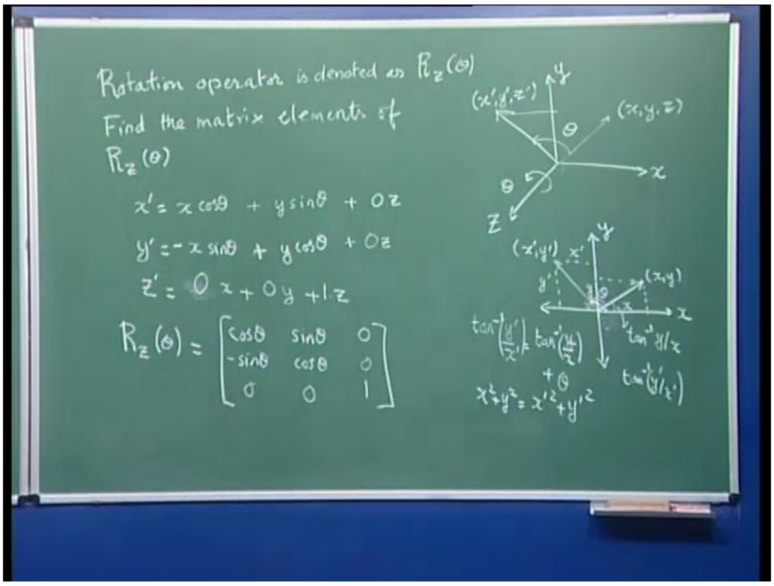

So, now you can define you can see that your r z as a function of theta is given by a matrix cos theta sin theta 0 minus sin theta cos theta 0 and 0 one. So, we expressed this operator which is rotation about z axis by an angle theta in terms of a matrix ok. So, there are many other operators that you will encounter in the remaining part of this course.

And also, you will see the rotation operation appear multiple times but, what I would like to do next is to look at functions in involving vectors. So, we define vectors as objects that are in a vector space. Now, the question is can you have a function of a vector just as your function of x or function of y can you a function of a vector.

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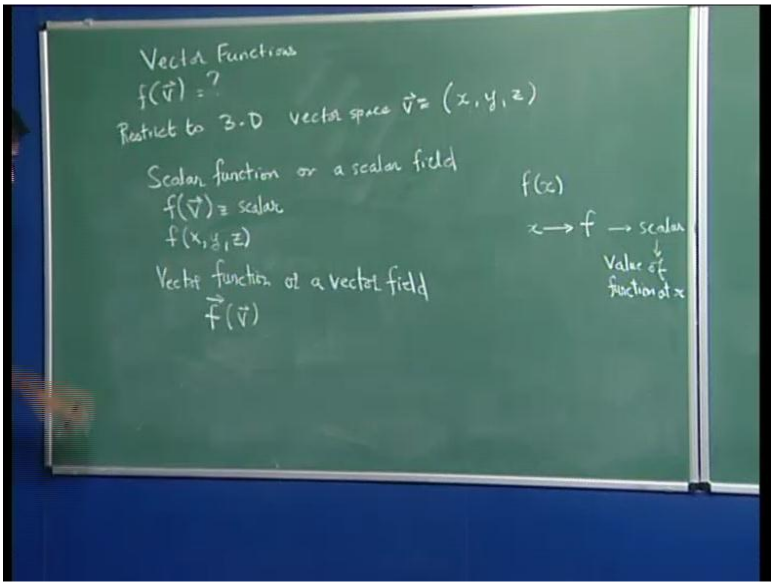

So, that will be next part of this of this lecture. So, the next topic we are going to discuss is vector functions now can you have a function of a vector. So, can we have a function of a vector now there are many ways to look at this and I will restrict for now, restrict to 3 dimensional vector space. So, that is represented by a vector has 3 components x y and z. So, V is has these 3 components.

So, we will restrict the discussion in the class to 3 dimensional vectors but, you can extend this concept to arbitrary vectors. So, what would be a function of a vector now there are two kinds of functions you can consider one is called scalar function or a scalar field and the other is called a vector function or a vector field. So, the idea is a following now when you consider when you consider normal functions of a single variable x. So, when you say f of x.

Then, our idea is that you have you give a value of x to f and out you will get a scalar. So, f of x will be some scalar some value and this is the value of this function. So, it is the value of the function at x. So, that is the idea now here instead of feeding a scalar you are going to feed a vector and. So, when you feed a function to a vector there are two kinds of functions those functions that will give you a scalar and those functions that will give you a vector the function that give you a scalar are called scalar fields. So, scalar field takes a vector and gives me a scalar whereas, vector field will take a vector and give me another vector. So, it is a function of a vector which itself is a vector.

So, now there are two questions that remained what do you mean by a function of a vector, what do you mean by a function of a vector and to answer this you just look at this representation of the vector. So, vector is just 3 components x y z. So, a function of a vector is just thought of as a function of x y and z.

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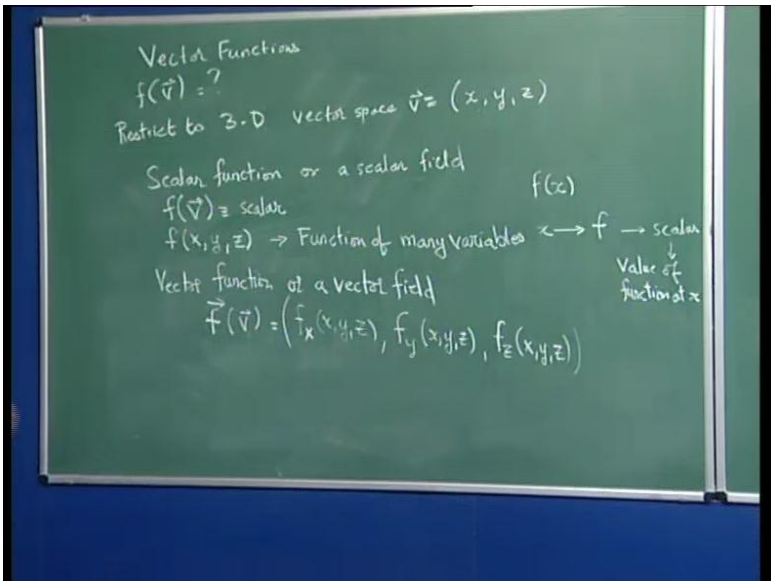

So, any function of x y and z that is a scalar function is a scalar field. So, this is just a function of many variables. So, any function of many variables you can call it as scalar field. So, scalar field is just a function of many variables and these variables corresponds to the components of the vector and now the definition of vector function should also be obvious.

So, vector function is the function of a vector. So, that means it is a function of x y z it is a function of x y z but, instead of getting a scalar what you get is a vector. So, the function itself has 3 components. So, the function has 3 components you can write the x component it has on a y component and it has a z component. So, both the argument of the function and the functions has 3 components. So, it takes a vector and gives you another vector and this vector is a function of that vector. So, these are the two kinds of functions that we will look at now let us look at some examples of scalar fields and vector fields.

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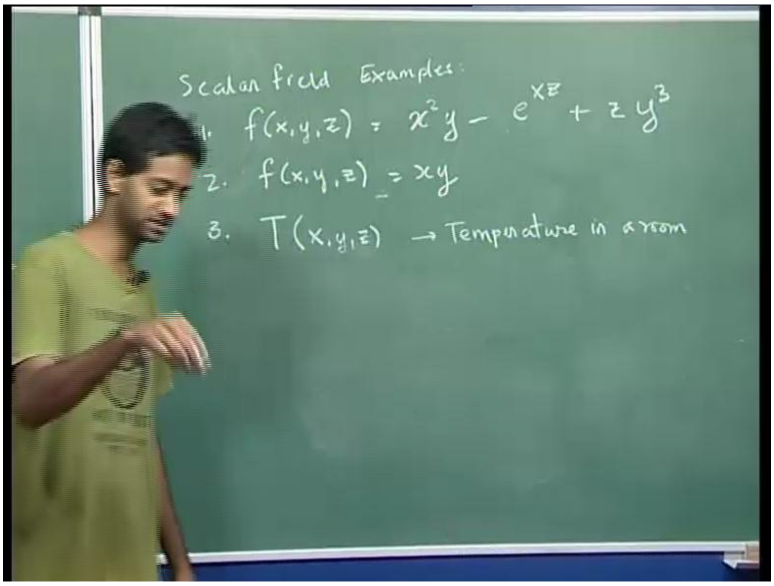

So, scalar field examples I will first, I will just take a mathematical example and then, and then will try to give some physically motivated examples. So, a mathematical example of a scalar field would be is equal to x square y minus e to the x z plus z y cube any function it can be any function of x y z. So, that is the example of a scalar field. Now, you can also consider examples of scalar fields like this. So, second example x y. So, this is also function of x y z but, it is independent of z. So, this is also a general function of x y z but, this is independent of z. So, it need not have all the 3 components appear on the right hand side but, still it can be a function of x y z.

Similarly, you can have only x or you can or you can just have a constant even a constant is also a scalar field. So, here you can have any arbitrary functions of x y and z and that will be a valid scalar field. So, now let us think of physical example of a scalar field. So, a physical example of a scalar field would be you have to think of some property that changes as you change the coordinate. So, as you change x y and z this property changes.

So, let us take a simple example if he if we consider your space as this room then, you have the x and let me call this the x coordinate this is the y coordinate and this is the z coordinate. So, you have the space here and at any point here any point corresponds to some coordinates x y z. So, you have a point here you have a point here you have a point here all these correspond to different values of x y z now you can ask a question what is the what is the temperature at any point the temperature here will be different and the temperature here may be different in general.

So, you can ask a question what is the temperature at each point and in general it may be different it may be the same if you are if your room has a constant temperature everywhere then it may be the same but, however because of various objects like this lights, and other and air conditioner, you will in general have different temperatures in different parts of the room. So, the temperature is a function of where you are in the room.

If you are here you will have a different temperature or at somewhere else you will have a different temperature. So, this is an example this is a physical example of a scalar field. So, temperature in a room you can you can easily construct many more examples I mean I do not need to consider this room I can just consider a container a container of water and I can look at the temperature in different parts of the container that would also be an example of a scalar field you can look at other objects you can ask what is the density? What is the density of air at different parts in the room and in general?

They will be in general they may be different because there is some circulations due to the air conditioners the fans and the other objects and. So, the density in different parts may be slightly different and that is example of a scalar field. So, the important thing is that what you have is a scalar. So, temperature is a scalar and. So, and. So, if you ask what is the temperature in different regions you will get a scalar field. Next, we consider examples of vector field.

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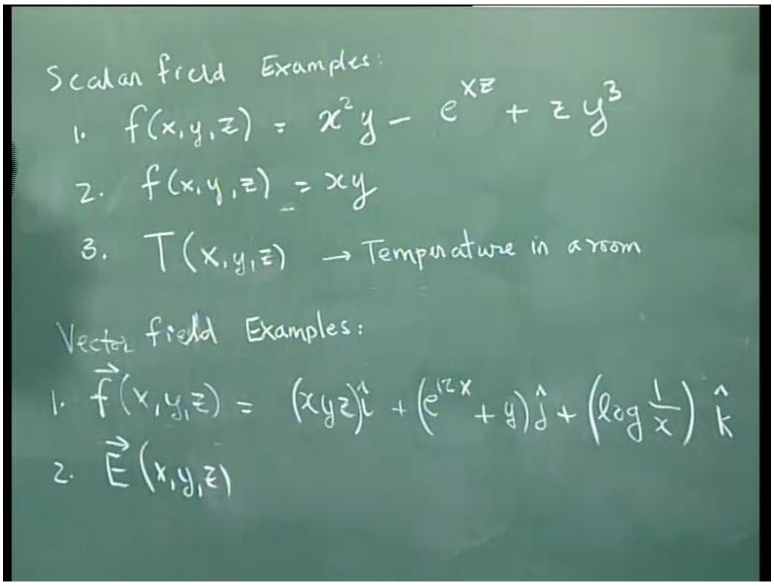

So, examples of vector field now the. So, let us write a mathematical example first. So, will say f vector which is a function of x y z has 3 components and the 3 components might be x y z i plus e to the e to the 12 x plus y times j plus let us say log 1 over x k now notice and I will put this in bracket notice that each of the components is a function of x y z and. So, each of the components is a function of x y z and that is an example of a scalar field. So, this is a mathematical example of a scalar field now the physical of a vector field, I am sorry. So, this is the mathematical example of a vector field, the physical example of a vector field would be seen the electric field. So, you can ask in this room what is the electric field at every point and electric field is a vector. So, it will point in some direction. So, may be if you are close to the light the electric field will point in one direction if you are somewhere else the electric field might point in some other direction it has both the direction and a magnitude.

So, that is an example of a vector similarly, the magnetic field is another example of a vector field and in general there are many more examples that you can construct of scalar fields and vector fields and these are objects that you see in everyday life and these are not these are not simply obstruct objects you actually see them and you end up using them a lot also. So, far we have studied about vector fields and scalar fields and i have been saying that you know that mostly we focus on this 3-D 3 dimensional vector space and we have been using the coordinate system which is the Cartesian coordinate system but, you may be familiar that with other coordinate systems that we can use to define the same space.

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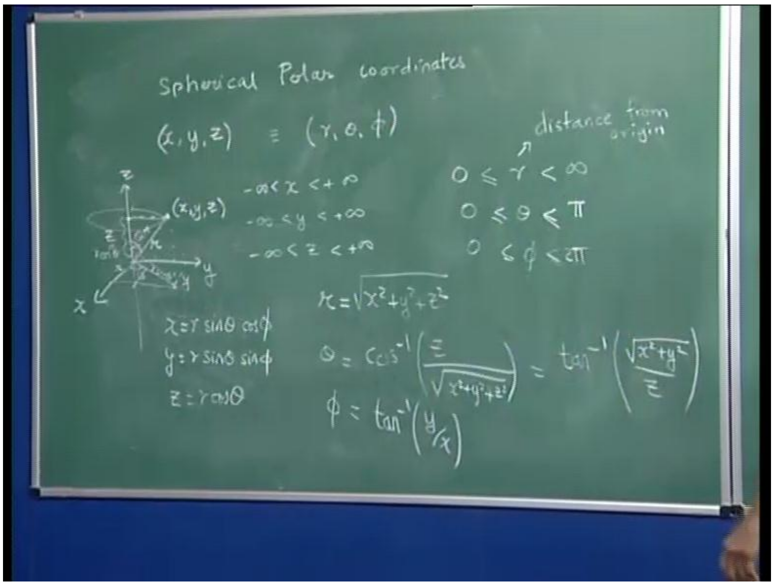

So, the same three dimensional space can be expressed in other coordinates and we will look at two coordinates one is spherical polar coordinates and the other is called cylindrical polar coordinates. And both these coordinates are very widely used.

And so, what I will do here is I will just give you the definitions of both these coordinate systems and just give you a hint on how you work out examples in these coordinate systems. So, the idea is instead of having instead of describing your vector in terms of these 3 coordinates x y z you define your vector 3 other coordinates r theta pi and you can either think of it as describing vectors or you can think of it as describing points in your space. So, if you have this as the x component y component z component and you have an arbitrary point here which corresponds to x y z, you can use this coordinate system. Where, x is the length from the x axis, y is the length from the y axis, z is the length from the z axis you can use this coordinate system or you can use another coordinate system called the spherical polar coordinates. So, in spherical polar coordinates any point is described by 3 by 3 scalars r theta and pi. So, what is r what is theta and what is pi. So, in this in this coordinate system r is r is this length. So, r is the length of this vector it is a scalar which is equal to the length of this vector theta is the angle with the z with the z axis and pi is the angle of the projection of this vector on to the x y plane with the x axis. So, this angle is pi. So, you take the vector you project it on to the x y plane and then you look at the angle with the x axis that is your pi angle now in this case you said that x y and z if you want the entire space they can go from minus infinity to plus infinity. So, then what are the limits for r theta and pi.

So, we say minus infinity is less than x less than plus infinity similarly, for y similarly, for z now what about r theta pi what are the what are the limits for r theta and pi now r is a distance. So, wherever the point is the distance will always be a positive number. So, your distance can be any positive number 0 less than equal to r less than infinity where if your point is at the origin then the distance from the origin is 0.

So, r is the distance from the origin and. So, it has to be a positive quantity but, you can go as far as you want if you want to cover the entire space you have to go to all distances and. So, r can be anywhere between 0 and infinity next question is what about theta now theta is the angle with the z with the z axis now the way theta is defined is that if you had a vector like this then you define this as the angle with the z axis. Now, suppose I take the same vector and I imagine I rotated along this cone. So, when I keep this point this fixed and i rotate it in a chronicle fashion now at these wherever you are here the angle with the z axis will be the angle inside the cone.

So, it is angle of a side of the cone with the line passing right through the middle of the cone and this angle will be theta wherever you are on this cone. So, theta is defined in this way and. So, the limits of theta can be theta can be of when you have a vector that is very close to the z axis then theta will become zero. So, theta can go from 0 but, theta can only go when you go all the way to this end. So, the vector with respect to the z axis it can be all the way aligned this way or it can be aligned all the way in this direction.

So, theta is always between 0 and pi. So, that is the limit of theta now what about pi is an angle in a plane. So, pi is basically this projection now this projection as this vector turns this projection will go all around and. So, it actually goes around the entire plane it goes around an angle of 2 pi. So, 0 less equal to pi or you can say less than because 2 pi is same as zero. So, in this case it will just be less than. So, these are the limits of limits of r theta and pi notice that theta is only between 0 and pi. So, even though it is an angle it is only between it is only defined between 0 and pi it can never be it can never be greater than pi.

So, this defines a system called the spherical polar coordinate now we need to know how to convert from x y z to r theta pi and I will just give the equations that help you convert from one to the other. So, you say that r. So, first what we will do is we will we will express r theta and pi in terms of x y z. So, in terms of x y z r is x square plus y square plus z square under root of that because this is just the length of this vector length of this vector is just x square plus y square plus z square under root. Now, theta to in order to determine theta we see that we see that if this angle is theta then z is just r cos theta z is r cos theta. So, then theta can be written as cos inverse z divided by r and r is just square root of then similarly, pi we can immediately see that pi is this length is r sin theta.

So, this z is r cos theta this length is r sin theta. So, then you can see that x is just r sin theta cos pi and y is r sin theta sin pi. So, then pi is just tan inverse y by x if you want you can also write this as you can write this as tan inverse tan inverse square root of x square plus y square divided by z. So, r sin theta is x square plus y square root of x, square plus y square, and r cos theta is z. So, tan inverse of x square plus y square by z is the same as cos inverse of z divided by square root of x square plus y square plus z square. So, now what we have done is we have written r theta and pi in terms of x y z you can you can write the other way also you can write x is equal to r sin theta cos pi y is equal to r sin theta sin pi and z equal to r cos theta. So, here I have expressed I have expressed x y z in terms of r theta pi here I have expressed r theta pi in terms of x y z. So, these equations will help you convert from one coordinate system to another.

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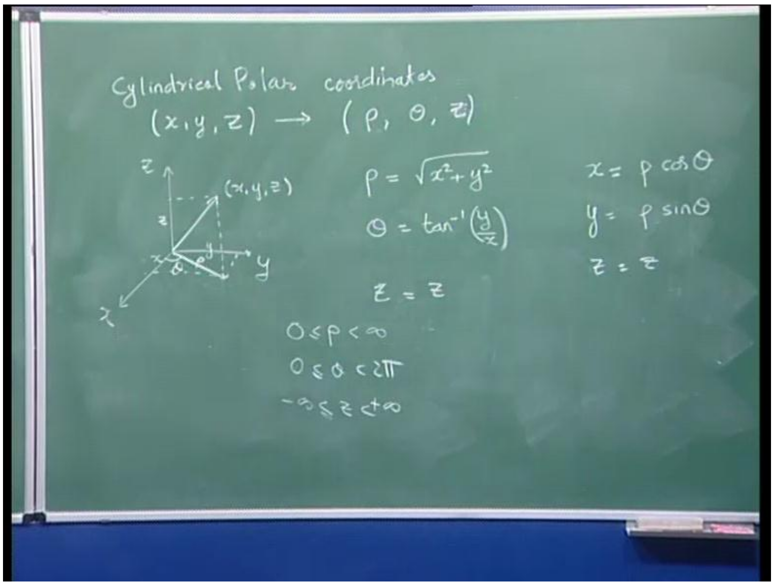

Now, the next example, is something called the cylindrical polar coordinates and here you go from x y z to use a symbol rho theta z, I am deliberately using the symbol rho to differentiate it from this r. However, it is also something sometimes you also call this r. So, the idea of cylindrical coordinate system is a following if you had a point z and you had this so, then we will use 3 coordinates we will use the z coordinate as it is and then, we will take the projection on to the x y plane. So, this is your x coordinate this is your y coordinate.

So, what is done is instead of using x and y you use this length which is rho and this angle which is called theta. So, you call this angle of the projection on to the x y plane with the x axis as theta and the length of this projection as rho and if you use if you do this you can easily show that that this cylindrical polar coordinates are defined in the following way. So, rho is equal to square root of x square plus y square. So, rho is a square root of x square plus y square then theta equal to tan inverse y by x and z is equal to z. So, you leave the z coordinate as it is you just play with the x y coordinates and that is what is called the cylindrical polar coordinates.

So, and then you can also convert it in the other way you can write x is equal to rho cos theta y is equal to rho sin theta and z equal to z. So, these are two of the most common coordinate systems used and if you ask what is the limits you will immediately see that 0 less than equal to rho less than infinity and as far as far as theta goes theta will be vary between 0 less than equal to 0 less than 2 pi and as far as z goes z still has a same limits minus infinity less than z less than infinity plus infinity. So, this completes the specification of the coordinate system and this both these coordinate systems are very widely used in all aspects of chemistry.

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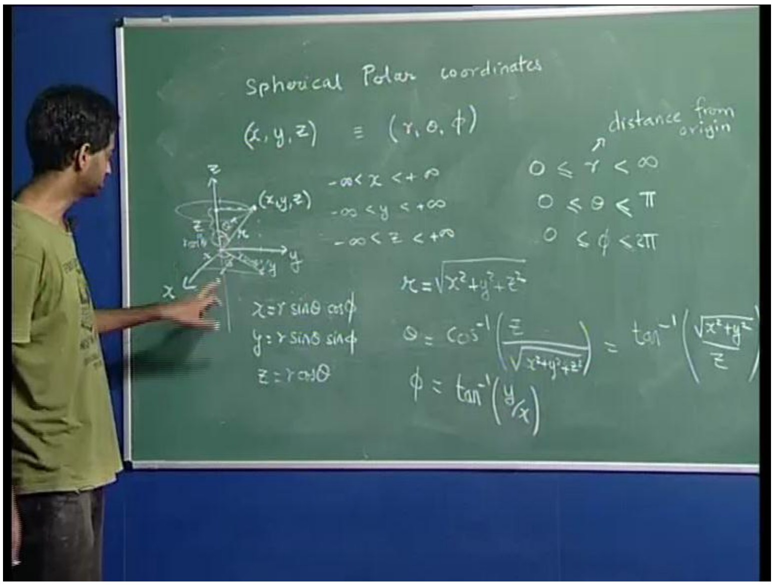

In fact, it is found that when you want to solve the quantum mechanical the time independent equation for the hydrogen atom. It is found that this coordinate system is the most useful whenever you are dealing with angular momentum in 3 dimensions it is this coordinate system that is most useful to solve that.

So, however if you are looking at diatomic molecules sometimes this coordinate system turns out to be fairly useful. So, these are two different coordinate systems and you can immediately see that if I look at a function of x y z I can alternatively write it as a function of r theta pi or I can write it as a function of rho theta z. So, functions of x y z will map on to functions of r theta pi or rho theta z. So, in the next class what I want to do is to look at what is called as differentiation operators on vectors. So, we will start that and the in the next class where we where we try to take various scalar fields and vector fields and try to differentiate them with respect to a vector. So, that will be the topic of the next class.