Principles and Applications of Electron Paramagnetic Resonance Spectroscopy

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Lecture - 22
Anisotropic Interactions in ERP Spectroscopy

Today, we are going to learn how E P R spectroscopy can enable has to study Anisotropic interactions, that is this today's topic is anisotropic interactions and E P R.

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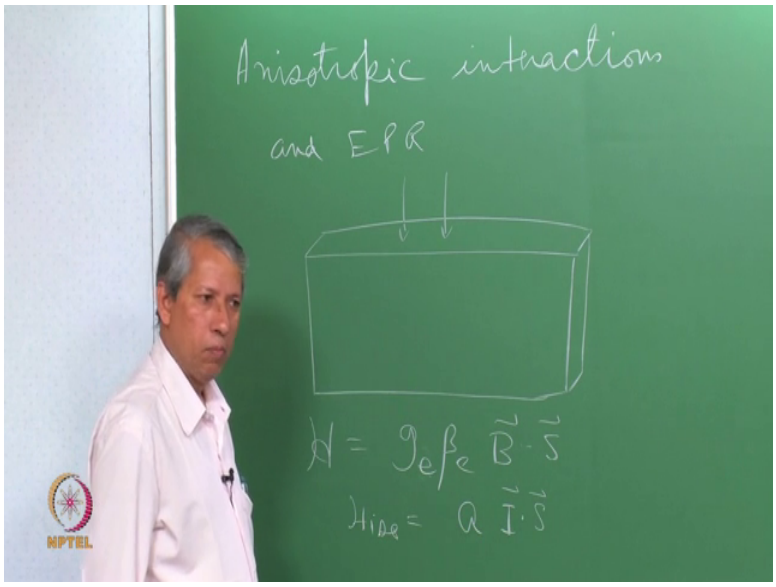

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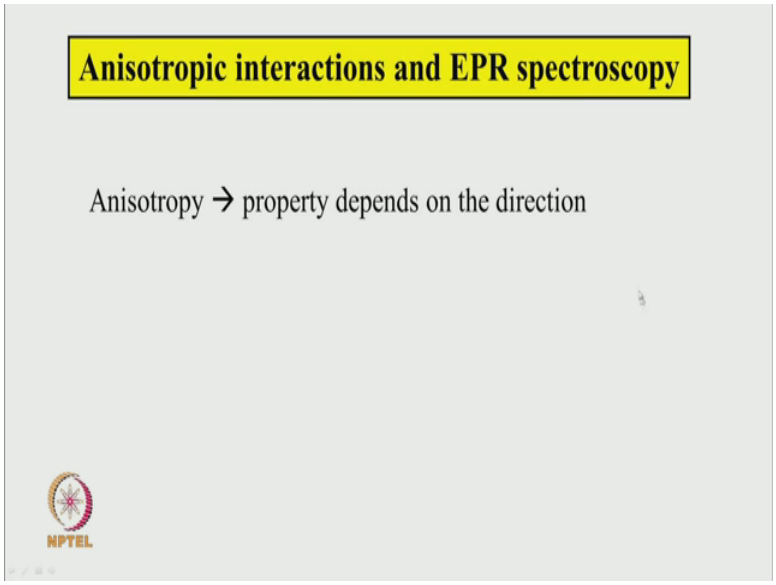

What is Anisotropic interactions? Anisotropic is something which makes that some property depends on the direction, when there many properties that depends on the direction. One very familiar example is, the way some substance behaves to a force that we apply from outside.

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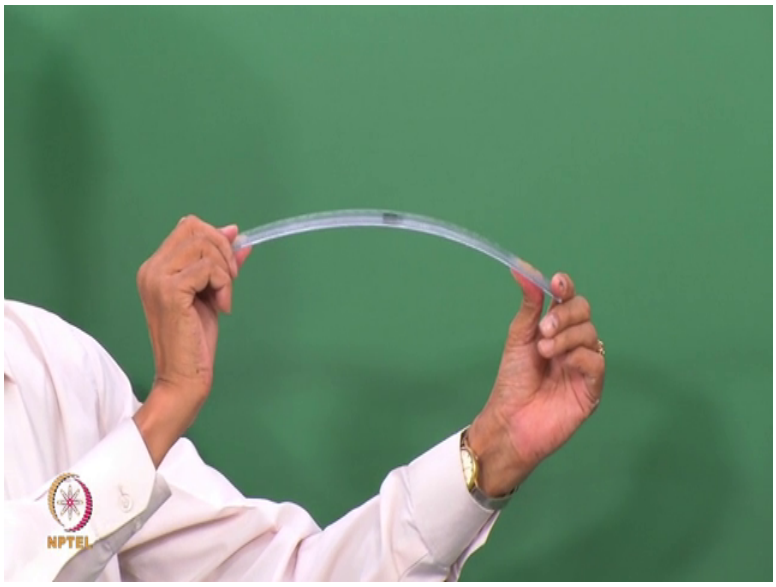

Here is a simple example; we have this ruler, I will apply some force on this and try to bend it.

Now, if I apply force this way, see how easy it is to bend it, but if I try to apply force in this fashion then it is very difficult. See in other words this is an object, the way it response to my force depends on, in which direction I am applying the force. So, this response of this object is an anisotropic in a similar manner, the beams on the sealing is given this set of side. So, that is this side is wider and this side is thinner and the load is carried along this direction.

So, the example that I gave on the ruler is essentially applicable here also. The way this beam response to the stress is not same in all directions, in magnetic resonance many phenomenon or anisotropic, we have not considered them. So far, all we have assumed is that electron Zeeman interaction for example, is isotropic and though wave we wrote is that Hamiltonian was written as g e beta e this fashion. So, this ways consider scalar quantity, we also considered the isotropic hyperfine spitting constant which is written as isotropic is written as.

So, a times, I dot S this is also a pure number, but we did mention that electron nuclear. Dipolar interaction is a directional dependent interaction, which we have neglected. So, far we will see those things here and then how far of this thing can we applicable or needs to be modified at the outside, we should keep in mind that a paramagnetic spices which is underground going. So, the rapid tumbling in a solution, for example, then it is experiences all possible orientations very quickly.

So, what property will measure for this sort of system is an average property. So, all the directional dependencies will not be seen in the experiment except to certain extent the average value of this direction on the dependent property will be seen there. So, 2 acts get the true directional dependent properties we must stop this motion as far as possible. So, 1 into 2 is to steady the solid state system or in powder form where the tumbling motions are almost gone or have a solution, but freeze it to a very low temperature. So, that it is a frozen solution sample and again the tumbling motions are substantially stopped.

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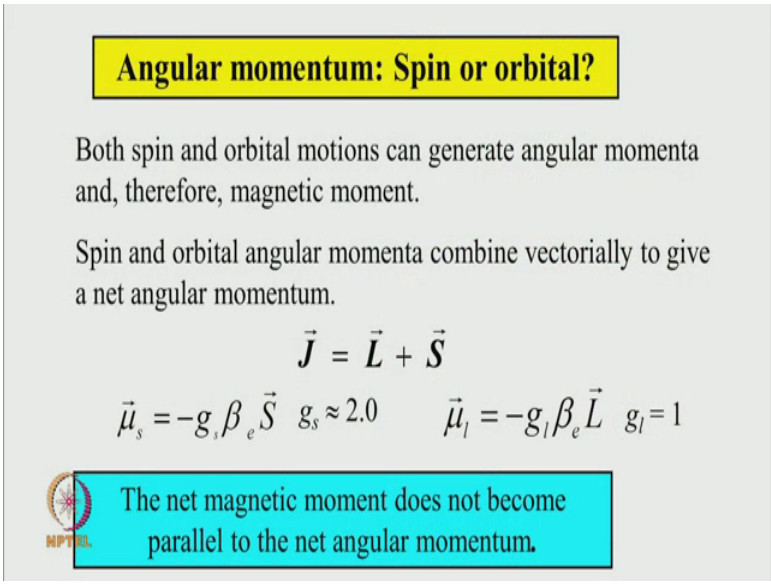

We have seen many times earlier that angular momentum of an electron can come from either spin motion or orbital motion and both orbital motion and spin motion can give raise to the respective magnetic moment in magnetic moment for these 2 motions are written in this fashion.

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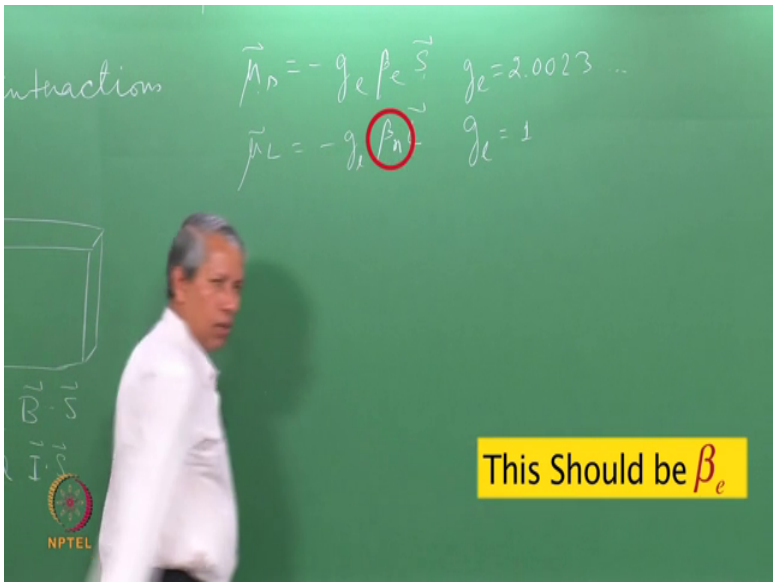

This is the magnetic moment; due to spin motion g e beta e is this spin angular momentum, where g e is really 2.0023 and something like this are similar to orbital motion. This could exactly similar fashion; we write g of l is 1. So, here both the equations says that this vector and this vector are parallel to each other.

Similarly, this and this are also parallel to each other. Now, if paramagnetic species has both this angular momentum.

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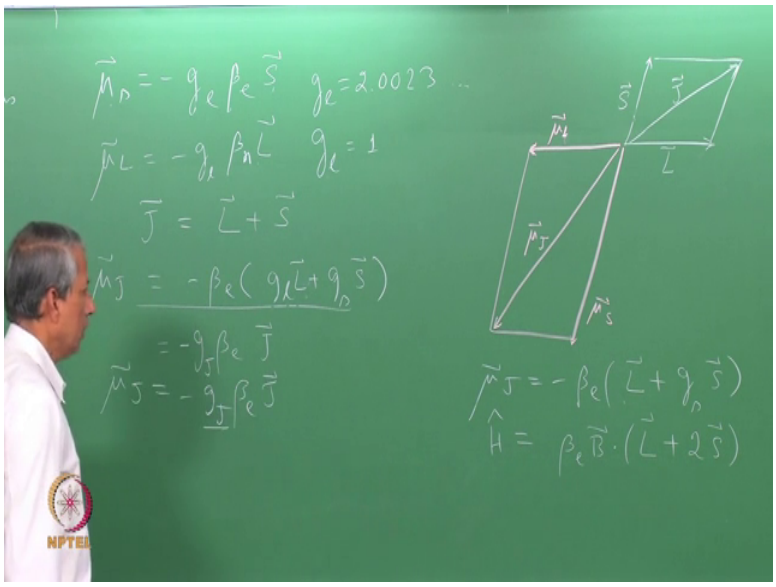

Then they can combine together according to the quantum molecular rules of addition angular momentum. Let us say this J is the total angular momentum made up of this L plus S, then this will also produce sudden net magnetic moment and I can write by adding this, they something like mu of J could be written as. Now here by analogy of these 2 equations, I am tempted to write that something like let us say this angular momentum and some sort of g factor, let us call it g of J and this. This is written strictly on the basis of this similarity, that S gives mu s they are parallel to each other L gives mu L again parallel to each other. So, this equations is fine, it is addition of these 2, but can I write and expression of this kind that mu J, that is magnetic moment arising out of the total angular momentum is something, some constant. Here, this gives the power of the constant between these and the these possible. Now, if this is true of course, then the these and these are going to be parallel and we are going to see a moment that this net magnetic moment does not become parallel to the net angular momentum.

Let us see how that is possible. So, using this one let us say, I have got, this is let us take this one first, that is L vector and this gives the angular momentum of this magnitude and corresponding magnetic moment, which points in opposite direction, because of the negative sign gl is equal to 1. So, let us say, this is my mu of the to L, then I have the spin angular momentum. Let us say, this is the magnitude of that and the direction and this angle is such that these two can be added according to the loss of addition of angular momentum given by quantum magnetics.

Now, the corresponding magnitude moment due to s will be twice the size of this one, because this is value of this is 2. So, this is mu of S, the net of this and this is given by this addition rule of vectors. So, this gives the vector J, similarly the net of these two an magnitude moment is given by this addition, this is the mu of J. Now, it has mu has formed here that, because this is twice, this one, these vector cannot be parallel to this one therefore, I cannot write equation of this kind, there is I cannot have a some g factor, which gives a magnetic moment associated with the net angular momentum. This cannot be a pure number that is not possible. So, what is the remedy? How do I proceed that? This is not possible, we can do it two ways; we can use this total angular momentum expression, the way we have written here and the corresponding magnitude moment. So, now g L is 1. So, let us write to 1. Now, we do not have write that a g of s and with this I

can write the introduction of this magnetic one moment in a magnetic field in this fashion.

Now, this is where in earlier equal to 2, 2.0023. Let us write 2 approve, which is approximately quite acceptable. This is the way one can write them Hamiltonian, which is fine. Another way of doing, it is to say that, because is cannot be parallel to each other, I cannot use the pure number.

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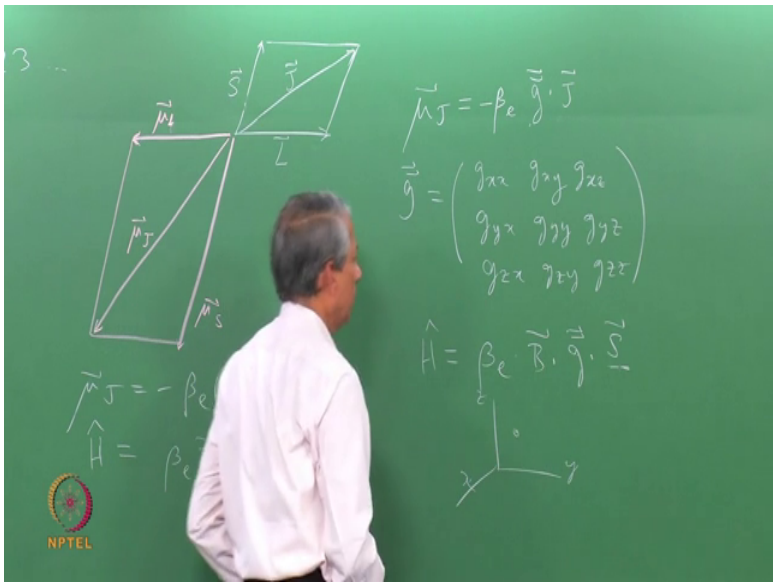

So, how about using a 3 by 3 matrix, here mu of J is something I write in this fashion, where this is 3 by 3 matrix. Let us call it g x x, then this and this need not point to the same direction. So, both are acceptable only the approach is different. Here, the approach is that, we just treat this interaction by assuming that the interaction could be written as using this type of g matrix, this could replaced at this one. So, here we treat this S to be some sort of effective spin angular momentum and the interaction can be written in the same fashion that is we do not express, will be think of the contribution of orbital angular momentum. The effect of this is to make these two non-linear. So, that is taken care of by changing g from a pure scalar number to a 3 by 3 matrix and these therefore, is to considered to be an effective spin angular momentum and that gives a same interaction, which is given by this one. We will take this approach, because it is sort of easy to visualise what is happening, but nevertheless both are equivalent approach there.

So, here when a define this of course, you need to define a coordinate system. So, this could be a some coordinate system to start with where the element paramagnetic which is kept, here we say this is the x y and z. Now, in this product we have to keep in mind how these three items are multiplied.

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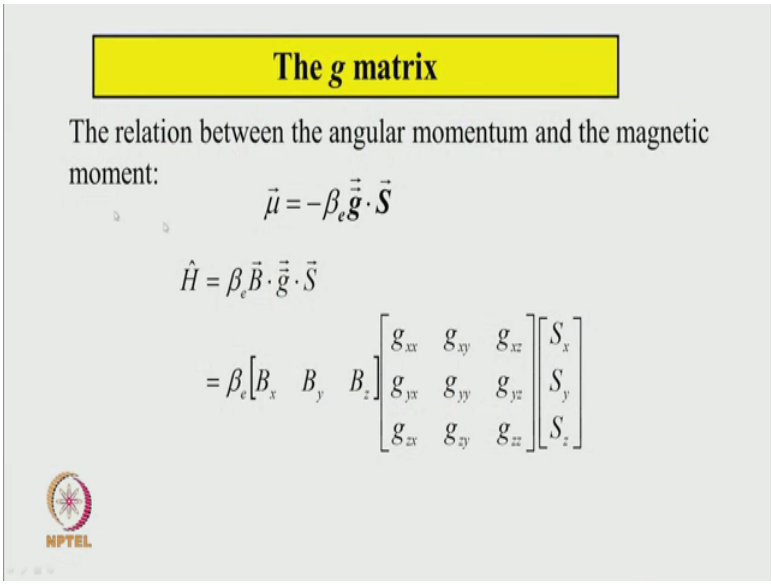

This is shown here. So, I said earlier that mu is written as the product of this 3 by 3 matrix with this effective, a spin angular momentum given raise to this sort of multiplication. So, here B is the magnetic field written as a grow vector, because that is why the multiplication has to be carried out for compatibility of the rules, of compatibility with the rules of matrix multiplication.

Now, with this one a c taken to be the effective spin;, in a magnetic field this will give raise to two energy level E 1 and E 2 .

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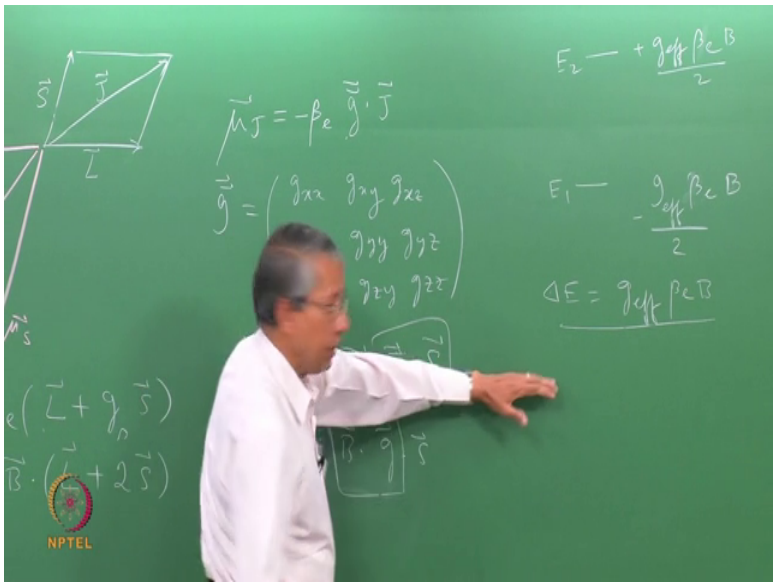

So, this could be written as energy of this will be g of effective and this will be similarly plus g of effective. Total energy delta E is g of effective beta e B. So, what it is g effective now? So, once again if we look at it that these two terms together gave some set of effective magnetic moment, which is interacting with this magnetic field, but we can look at it differently, also that is

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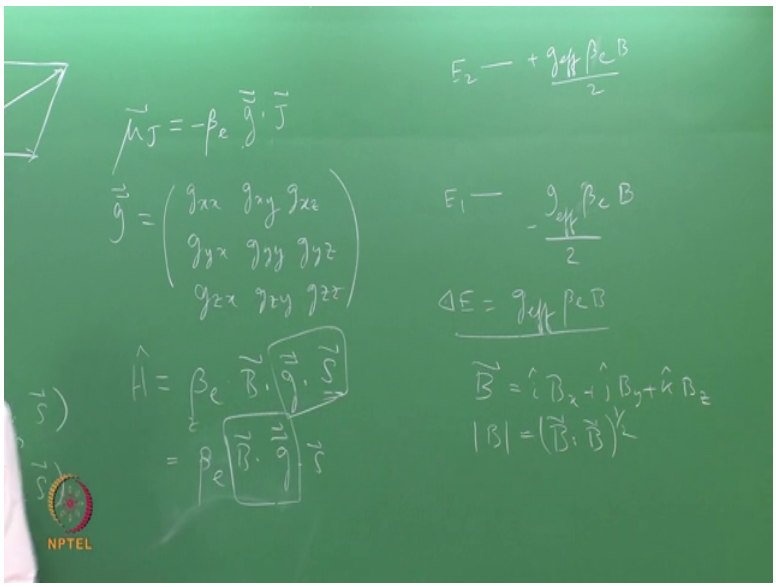

We look at it as, this is an effective magnetic field, which is interacting with the spin angular momentum and that is the way, the energy levels can be thought of that. So,

these gives an effective g value for a given value of the magnetic field B here and the energy level of spirit, both are equivalent, they actually the, how we look at it. So, these give the effective spin there interact together. Magnetic field here or this gives the effective magnetic field, which is interacting with the spin.

Now, with that idea, now if this is the way, it is should be able to get some expression of this, in terms of these things, total energies square; this is a scalar quantity can be written as a scal, scalar product of these with itself.

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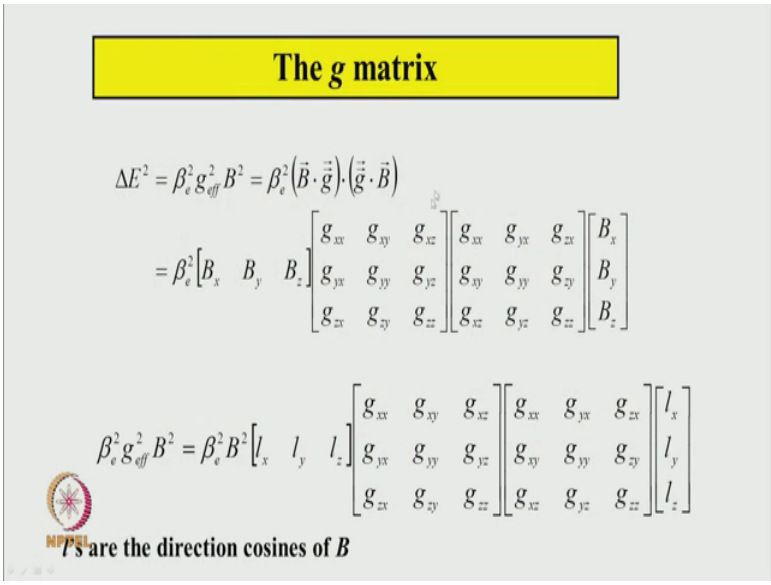

So, that is done here is delta E square is product of these with these of course, here to again the maximums of the multiples and vectors and this matrixes, these have to one has to take the appropriate transpose of the matrix here, there is done here. So, then why simplifying the g effective square, with these two constants gives comes out to be this, here the B x B y B z are the three components of the magnetic field. So, if B is, let us say I, B x is the three components and magnetics of this is given by these, then one can write these three components in terms of the direction, cosines of this B with respect to the external, coordinate system that we had earlier. So, l x l y l z are the direction cosines of B, in the similarly here.

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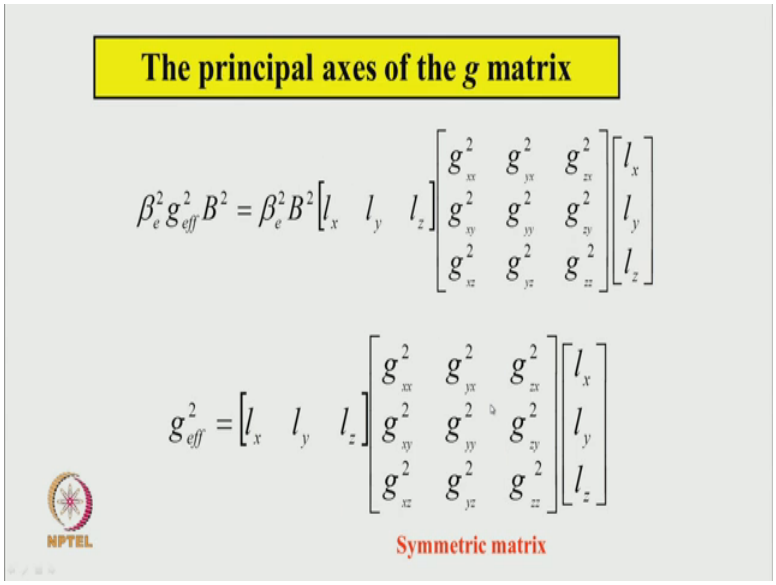

So, then B square comes out then this quantity g eff's effective square is actually, is these, which is written here, g effective square is the direction cosines of the magnetic field and square of this g matrix, this square matrix defined by taking the product of these. Now, if you see these matrix and is the transpose of this matrix. So, no matter whether g is symmetric or not these will always be a symmetric matrix that is very important.

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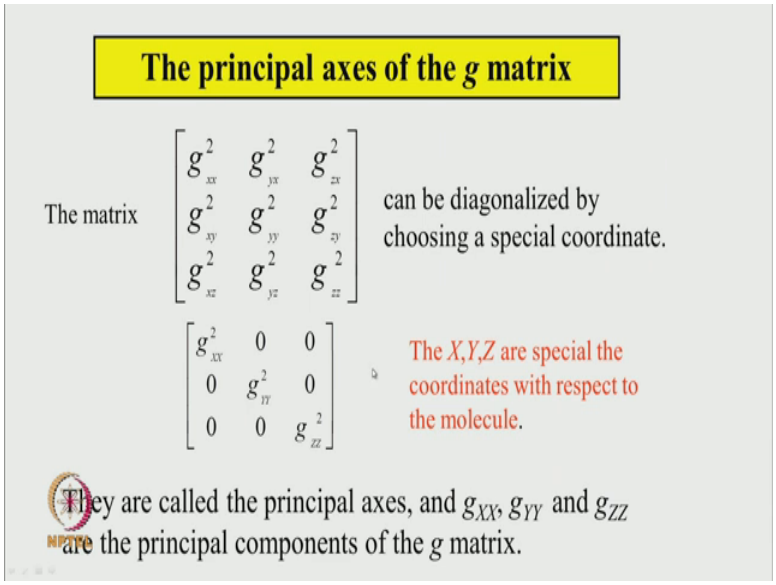

So, then because g square is a symmetric matrix now, we can choose suitable coordinate system. So, initially I have some, I had some coordinate system, whatever it is in the laboratory and the experiments done, and this is a paramagnetic centre sitting here and whether(Refer Time: 19:43) with this x y and z, the g square matrix here was defined. Now, because it is symmetric matrix, I can have a special coordinate by suitably rotating this one. So, that the g square matrix become a diagonal matrix. So, these special coordinate call let us X Y and Z are the special coordinates with respect to the molecule. So, that this becomes diagonal g square matrix diagonal. So, if it is square root of these three, then I get g xx g yy and g zz, these are called the principle components of the g matrix. So, here if the magnetic field is now pointing towards either this, if this special coordinate or the principle access one a X Y and Z.

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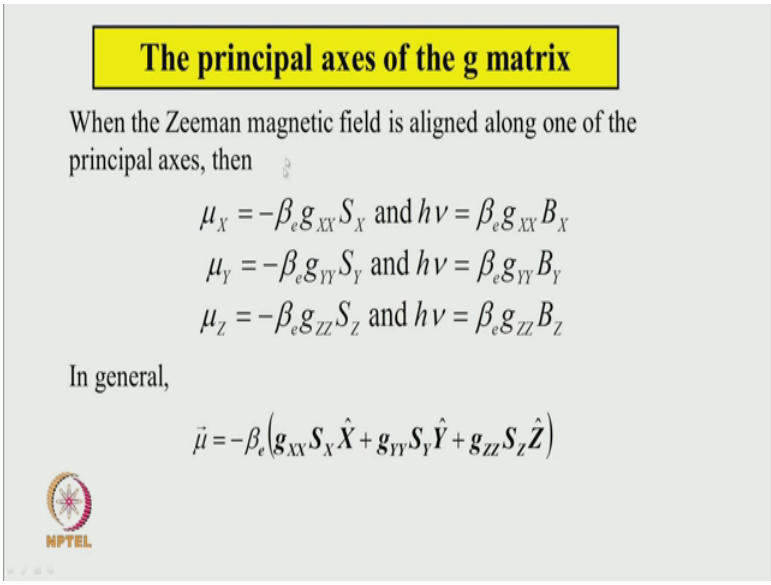

Then you see the equations, because very simple, now with the magnetic moment along that particular direction x, becomes beta e g xx S x, which is what we known always, get that this type of thing, but then this the important thing, is there, here the magnetic fields pointing to one particular direction of the molecule, that is a principle axes.

Similarly, for S y and is S z and if the corresponding energy of transition will be the, if the magnetic field is along the X direction and H nu is beta e g xx B x similar for the others. See in general, the magnetic moment can be written in terms of this principle

component g xx g yy g zz, in this fashion well X Y and Z are the unit vectors which are pointing towards this principle axes, this is shown here.

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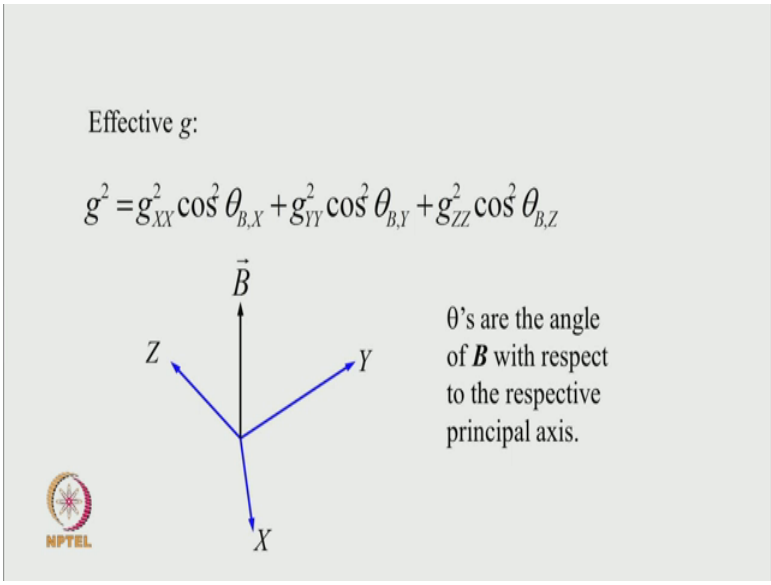

So, these are the cap principle axes. Let us say B is pointing along this, then effective g square which is from this expression, there diagonal element appears to be this. So, at these are the three direction, cosines with of B Y, respect to this principle coordinate. So, this shows that the interaction depends on directions and depending upon the value of this g xx g yy and g zz, one can get complicated E P R spectrum as the angle changes the effective g value changes therefore, the spectrum will also change.

Now, how different these three values are that will tell us about the symmetry.

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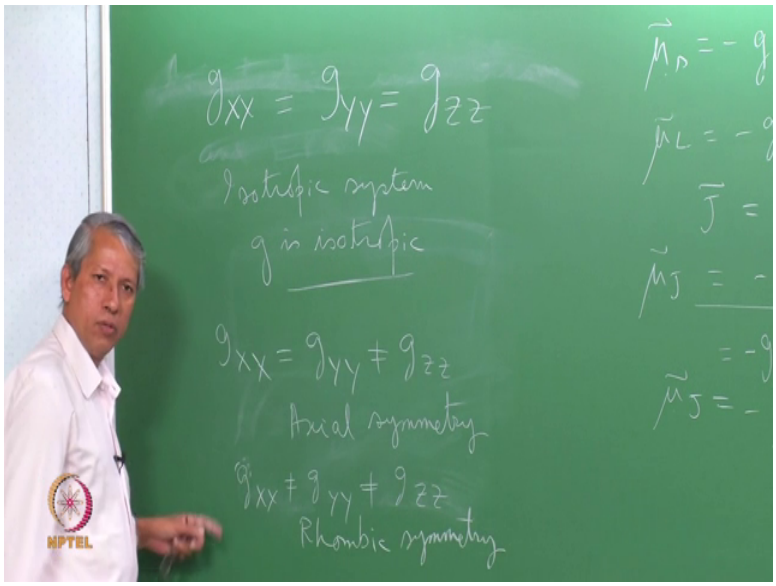

So, we have got three principle component, if all three are same then we call this an Isotropic system or g is Isotropic, this is what we have been using, actually using. So, far in our previous examples g does not depend on the direction, all the possibility let us say, two of them are equal third one is not, then we will call this system to have an Axial symmetry and if all three are different, then we can say this is a Rhombic symmetry, in essence no symmetry. So, far is that g values are concern to if get a interactions of this kind, the molecule has to be kept in a frozen solution or in the crystal.

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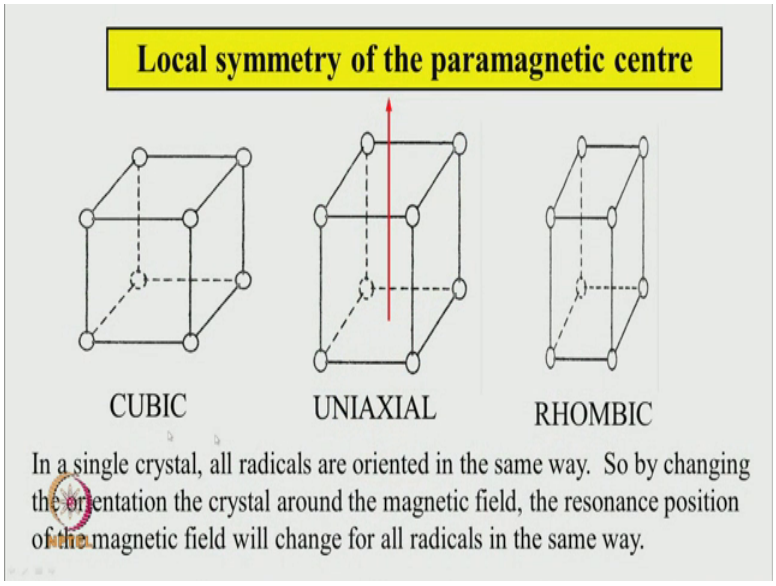

So, write now let us consider the situation in crystals. So, crystals have certain symmetries see the paramagnetic centre is sitting in this crystal. They will express the local symmetry, in local symmetry could be cubic symmetry here or it could be Uniaxial, where there is a axis, one axis of symmetry. So, there is, if it rotate in this fashion, it will be at least three fold axis of symmetries, will be their or Rhombic symmetry. Now, symmetric axis higher than c 2 here. So, when I said a Rhombic between symmetric is no symmetric that is not quite correct. This is the crystal, can have c 2 symmetry, but there is no symmetry axis higher then c 2, if there is higher than c 2, then c 3 or c 4, then it will be either here or here, probably here this one as c 4 axis of symmetry this as c 4 no doubt.

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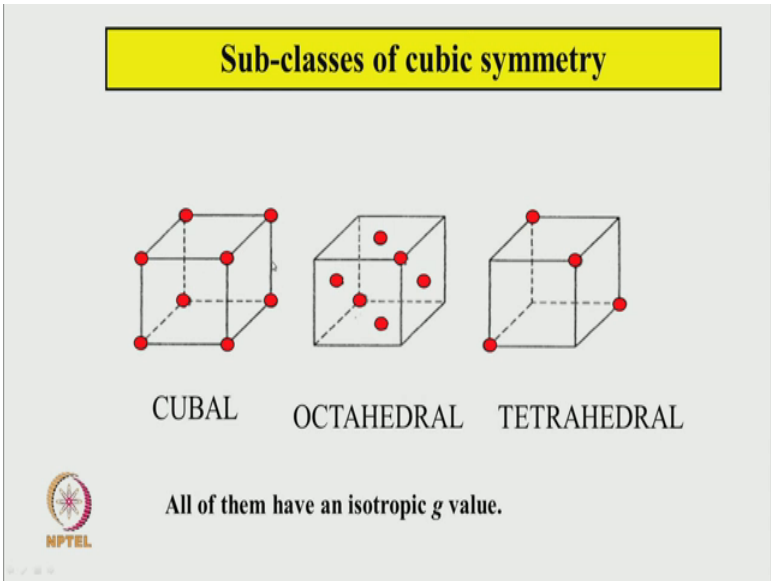

Now, it will also diagonal, if it, now it will have c 3 axis of symmetry. Now, a Cubic symmetry; a cubic symmetry is essentially, will give raise to this Isotropic g value, these a various subclasses of, Cubic symmetry is a cube, Cubal when you say ended a cube, all this a lengths are same, there the way the atoms are placed or it could be Octahedral or it could be Tetrahedral. These are all subclasses of cubic symmetry and all of them have an Isotropic g value.

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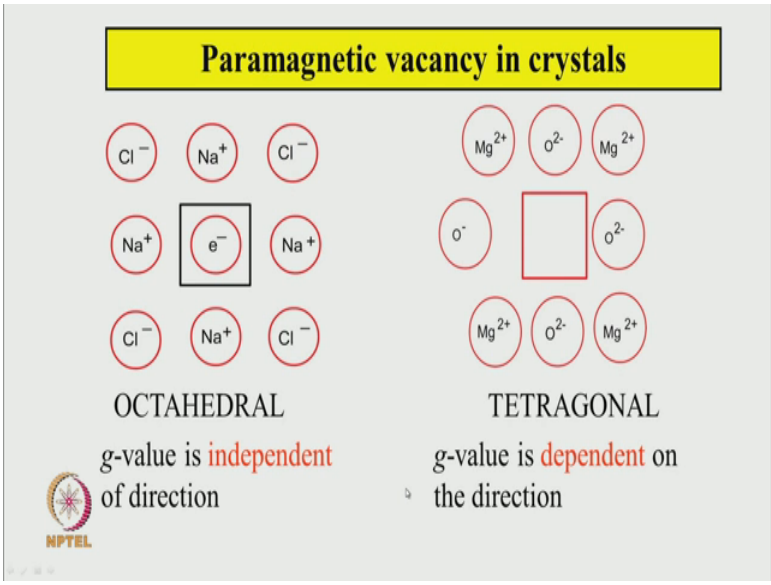

Now, we take some examples of E P R and C in crystals, in a single crystal all radicals are oriented in the same way. So, by changing the orientation and the resonance position of the magnetic field will change for all radicals in the same way, which as you rotate the crystal all the radical, which are inside, will explain the same magnetic field. Now, here is an example of a paramagnetic centre trap inside a sodium chloride crystal lattice. Here, this block or the square is the place, where a chloride atom should have been there, but that has disappeared to make a vacancy and instead a single electron is residing here.

So, these are some called defect centres or color centres type of names given to this. So, this is the centre of paramagnetism. So, here this belongs to this Octahedral symmetry. You can see the four nitrogen and sodium atom. They own on the top or the bottom. So, here this is purely Octahedral. So, that belongs to this a 3 values to be same and. So, g value will be isotropic what is the experimental observation that if I take this crystal this is a crystal and do the E P R experiment as a function of magnetic field.

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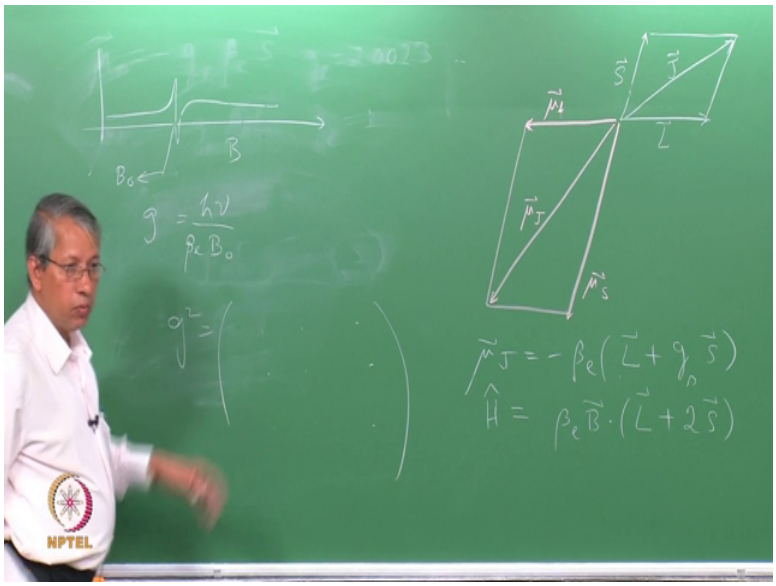

So, this will give us spectrum somewhere, let us say here and you keep rotating the crystal around certain axis. This will not move, will be preside the same place that is same thing, what I have been to trying to say that g values Isotropic and it does not depend on the orientation of the crystal with respect to the magnetic field. So, this remains constant. So, this is the place which gives me the value of B 0, then the g value will be correspond to this one and this is not going to change.

No matter which direction the magnetic field is applied. In contrast, there is another such vacancy centre, here magnesium oxide crystal. Again this defective created where a magnesium atom a disappeared, it was done by (Refer Time: 27:55) this crystal with x ray now. So, that is magnesium ion, is disappeared and the same time this O 2 minus oxides were there from one of those, this one electron was knocked out. So, this O 2 minus because O minus, now in the process the position of this thing is got slightly moved from the normal usual position. Here, usual position is the very similar to this Octahedral symmetry, but because these has gone and such therefore, the little repulsion between this and this. So, that repulsion push this away from that. So, this therefore, is no more a cubic symmetry. So, it has a symmetry axis along this direction now.

Now, for these the g values dependent on the direction that is if you do that same experiment here and rotate the crystal the position is going to change in certain way and

wherever you changes, I get a effective g at that particular way understand and that magnetic field.

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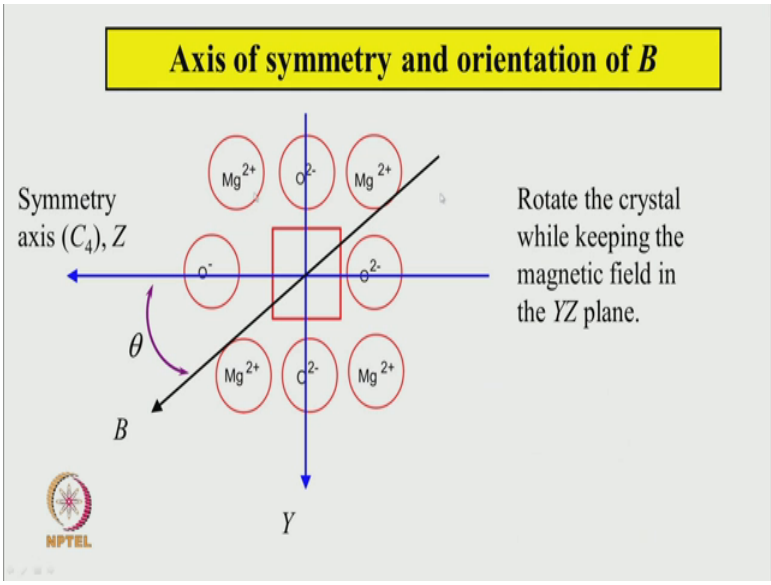

So, once again this is the symmetry axis C 4 axis is here and let us say B is magnetic field, is applied along this direction, which makes an angle theta and this is the perpendicular of direction. So, here if the crystal is rotated around this C 4 axis then, because is symmetry axis the interaction is not going to change. So, this will be staying right here, wherever it is on, does not here the interaction depends on the angle. So, if these angle is varied in the Y Z plane then the effective g is going to change, that will be seen as the change of the line position.

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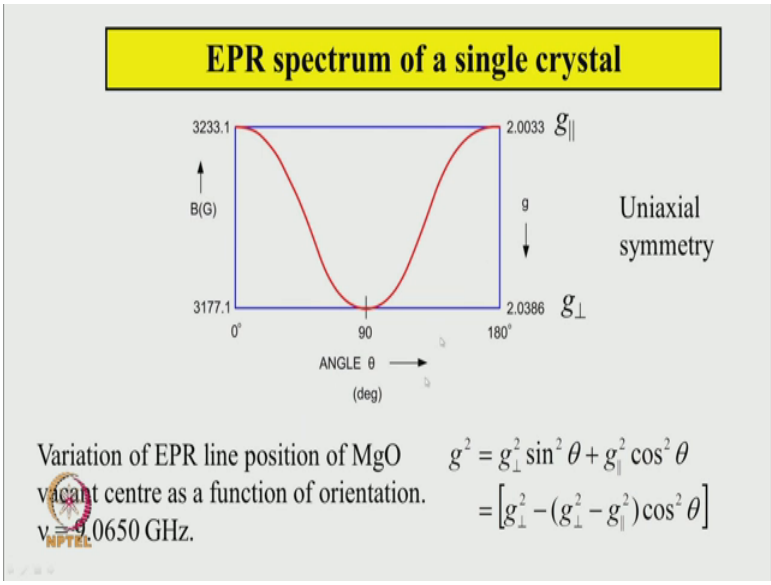

This is the result here. So, you see that angle is varied from 0 to 100 degree they this is the position of the E P R signal in the magnetic field unit we starts with 3 2 3 3.1 gauss and as an angle is change this becomes smaller and smaller and somewhere at 90, it reaches minimum, again it goes back here.

So, far. So, starts from here go is down down down, again goes back. So, for each orientation one can, that determine the g value and this is shown here as the angle is varied, g changes from 2. 0033 to 2.0386 Now, this is 01180 degree is nothing, but the magnetic field is pointing along the direction of the symmetry axis. So, we call the g value to g parallel value an 90 degree, is this direction so that it the g perpendicular value. So, this expression can be feted to an expression of this kind g parallels and g perpendicular expression and angle is theta. So, that is for axial symmetry.

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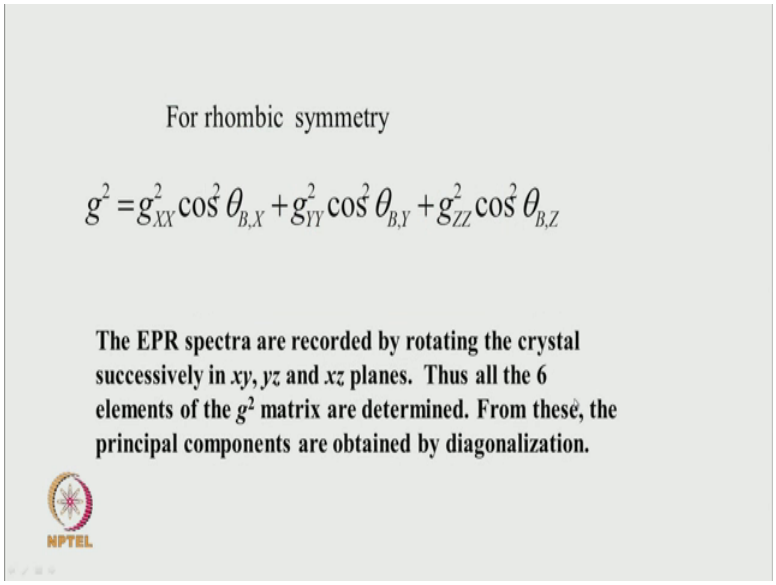

Now, for Rhombic symmetry, where all 3 are different, the expression for effective g is given here, depends on all the three principle component of g and also the angle that the magnetic field makes with respect to the principle axis. Now, to determine these E P R spectra are recorded by rotating the crystal successively in X Y Y Z and X Z planes then for this measurement each of them will give curve of this kind, then the corresponding elements of this g square matrix, I have got this elements, could be determined from this measurement and then one can know diagonalize it to get the principle component of the g matrix, at then outside the angle of the principle component of the g matrix that gives raise to, we have an Isotropic interaction.

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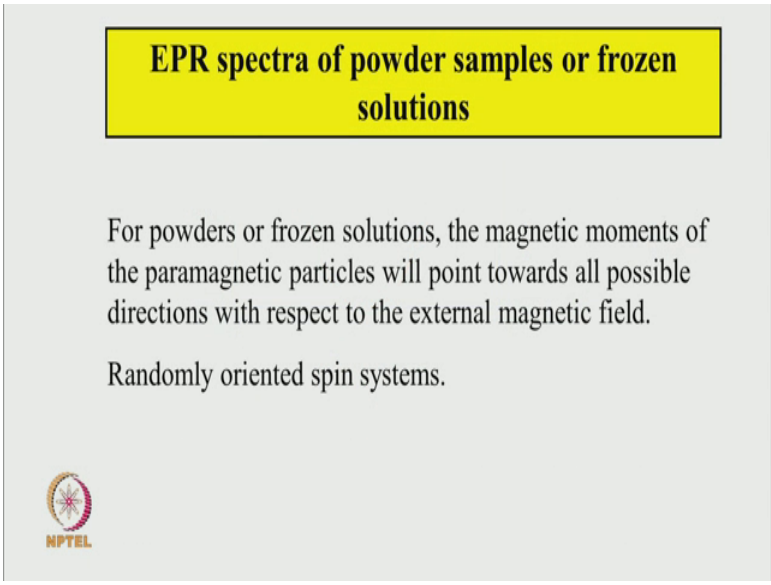

Now, that is the way one can study the single crystal and find out the corresponding an Isotropic interactions, but is not always easy to form single crystal. So, these experiments are difficult in that sense. So, what one does is that one can frees a liquid solution if paramagnetic sample and then try to see if one can get similar results from studying the E P R spectrum of a frozen solution or powder for example, if a crystal is not form, one can do E P R on powder samples, but then main problem is that if powder and frozen solution can magnetic moment of paramagnetic particles, will point to all possible directions with respect to the external magnetic field. So, we have randomly oriented spin system.

So, here we need to find out that how the random orientations are reflected in the spectrum of the E P R signal when recorded in case a powder for crystal.

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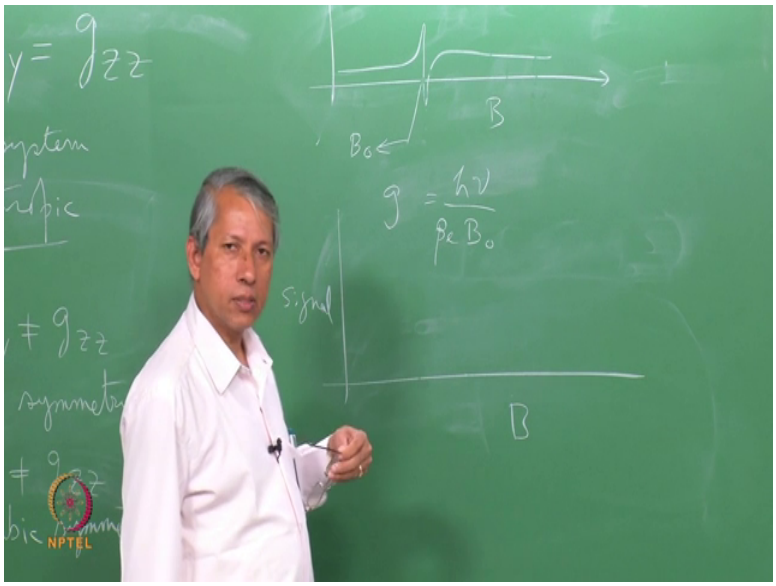

For example; as the orientation changes these magnetic field goes on change for powder or frozen solution similar, there will be magnetic field direction this is the signal. So, as the different orientations are available in case of powder. So, this will also certain range of allowed magnetic field as we have to find out whether all such magnetic field positions are equally likely or there are some selectivity.

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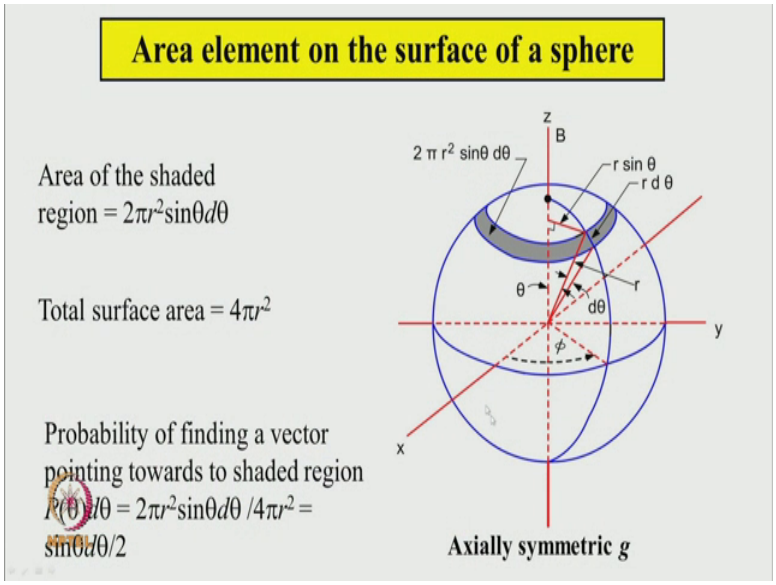

It is very obvious there all orientations equally likely. So, where we are going to see that is within all over orientations equally, likely this all magnetic field position all not equally likely.

So, first let us find out therefore, that how many were magnetic moment will point to sudden direction here for a, let us say the case of axial symmetric g. So, these are here to find out how many molecules will point to a this direction given by r theta and phi and r givens constant, theta changes from theta to d theta here and says the axial symmetric the g does not depend on the phi. So, for all values of phi so that happens to be this particular band here. Let us, easy to see that area of this band is 2 pi r square sin theta d theta, the total surface area as 4 pi r square therefore, the probability of finding a vector, pointing towards the shaded region, is given by these divided by these which is sin theta d theta by 2.

Now, So, will. So, when, these vector which a pointing in this direction will give the same in the neighbourhood of same magnetic field in the E P R spectrum. So, where are they going to appear? May be they will appear somewhere here. Let us, now if, now this, if a theta is change now the resonance position is going to change somewhere here. So, when we cover all the possible orientations, how this distributions are going to be appearing a different magnetic field region?

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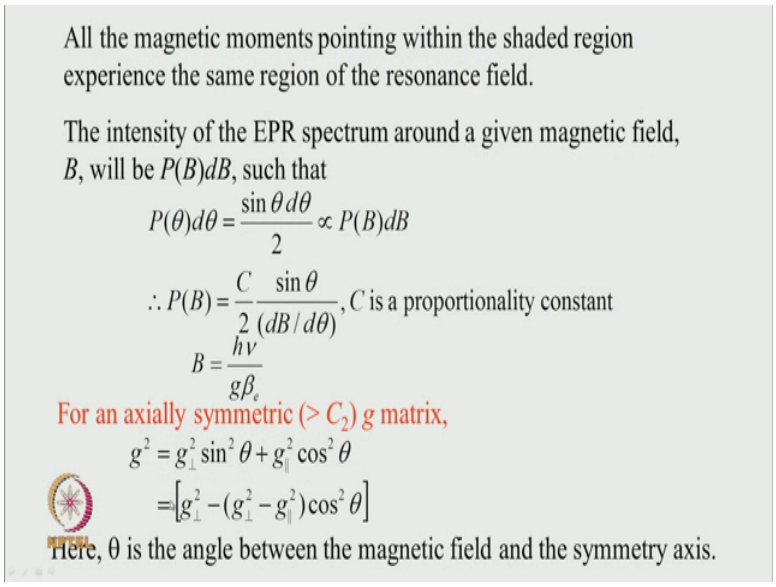

So, that is P theta d theta, which is already found out to be this proportional to some distribution of intensity as a function of magnetic field B to d B. So, P B is just a, these divided by this one. So, we have to find out this relationship B is equal to H nu by g beta e

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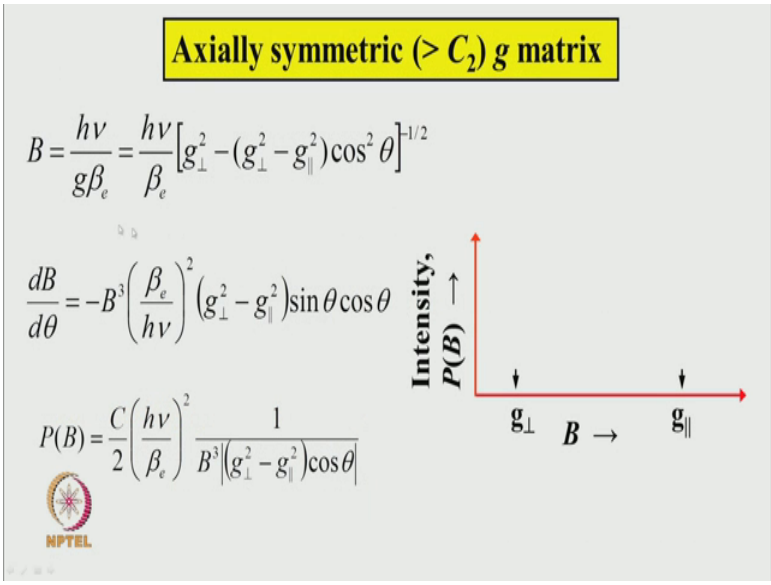

Now, we have seen that for axially symmetric g this is the relationship. So, we just do the algebra that necessary to simplify these. So, B is given by this relation and that, but g itself is given by this. So, if we, the differentiation the B P happens to be in this fashion. So, this let us take a closer look at that; that means, all values of magnetic field orientations are not allowed. Here, it can range from that is a g paramagnetic value to the g parallel value. This is the range of allowed B and as the cos theta changes from 0 to 90 degree and for each angle the B is given by this relationship. So, for that angle theta I find B, that B is a put here and here to, for find out the value of the probability here see the moment cos theta becomes 0, this would sub.

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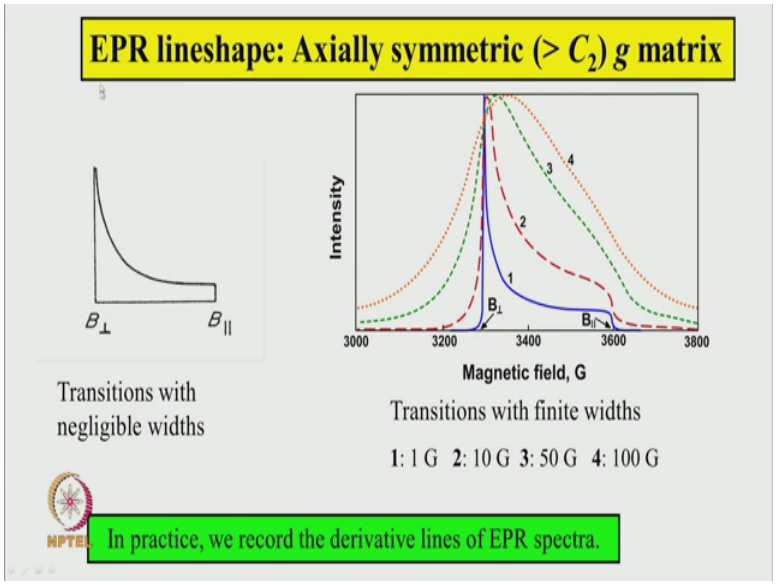

So, this goes to very large value for otherwise is smoothly comes, to comes maximum upto B parallel see of course, this is here, this is going to if it is not very serious these. So, because this transitions width we have supposed to be 0 for once we have a finite width then they all. So, the broaden seven these sharp edges are gone. So, this is given here, the blue has a very small width of transit one gauss, then has width goes bigger and bigger, say how they become less (Refer Time: 37:15). Now, here the g perpendicular value is here correspond to this magnetic field, an G parallely be correspond this magnetic field. So, we can get the corresponding values from this powder spectrum, as well when practice we do not get the associative spectrum. We get the derivatives spectrum. So, we have, can derivative of this one and that is the way this looks like.

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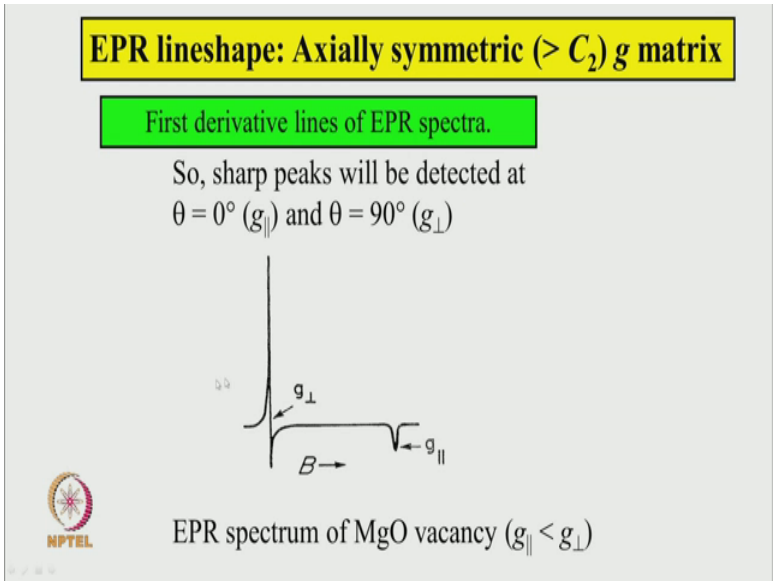

So, here, if you take a derivative of this this, let me go up and come down and here again that is going to be.

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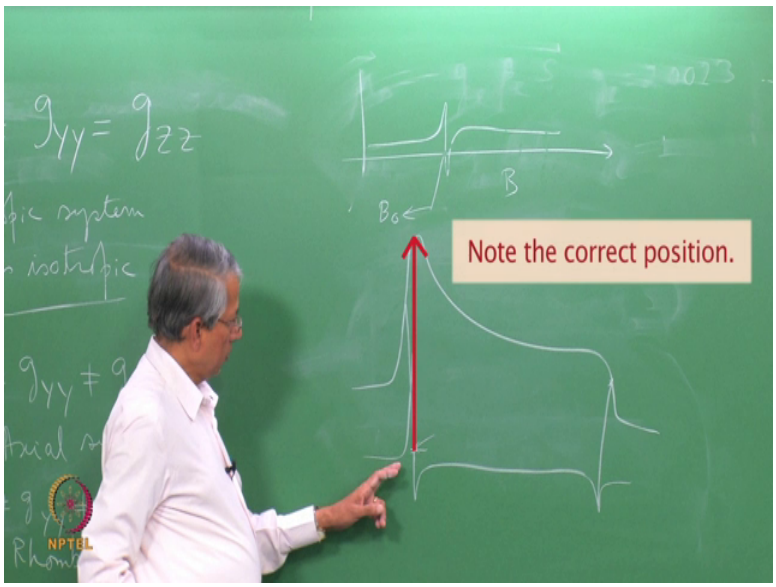

So, this point is corresponding to with. Here, this point corresponds to this one. So, g val perpendicular will be corresponding to this magnetic field position and g parallel correspond to this magnetic field position. So, that is the way it is going to be. So, these are the example for the magnesium oxide vacancy and g perpendicular is here, g parallel here.

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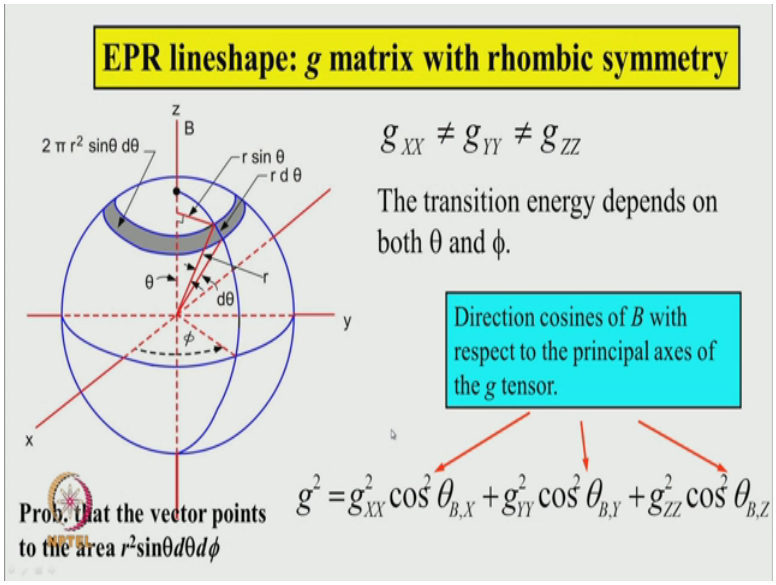

Now, for Rhombic symmetry, we have to do the same calculation, but little bit more complicate instead of shaded area. Now, here we have to see the probability, the vector points to certain, only small region here that r square sin theta d theta d phi shown here and then as theta and phi valid. How this similar distribution; we going to change with the condition that g square is given by this relationship.

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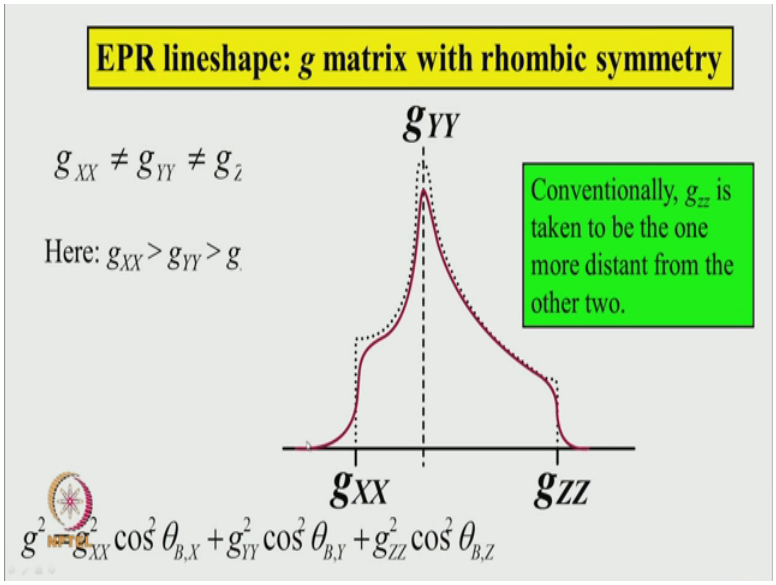

So, here the (Refer Time: 38:39) profile looks like this, the given by the dotted line with a, where the transition has no width, but we, the finite width, this coloured line is the appearance of the spectrum.

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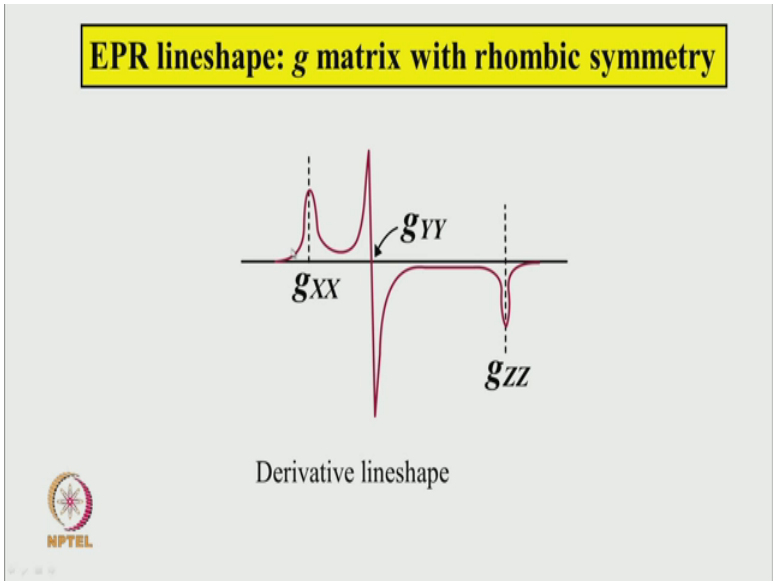

Now, again if you do that I derivative then the signal way look like something like this this is the g X X g Y Y and g Z Z. This is g Z Z the one is second to be the one, which is for this from the other two. So, here the g Z Z and g Y Y is the intermediate values.

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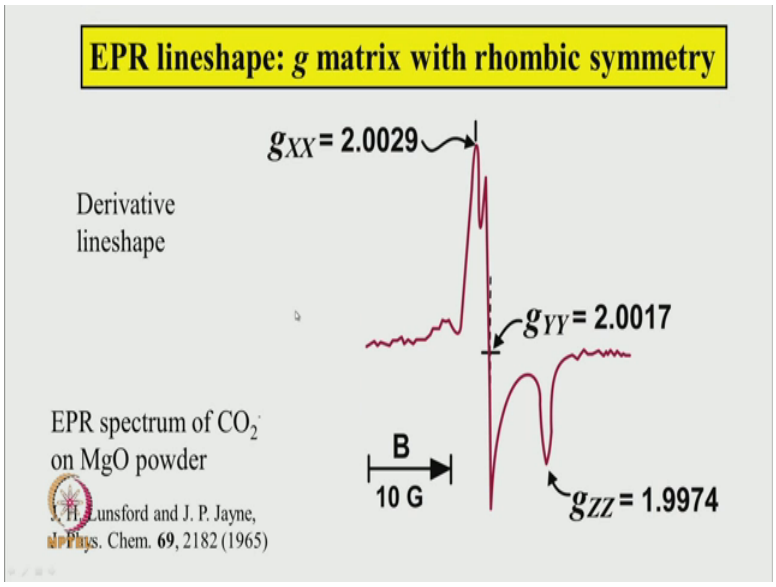

And here then example that this C O 2 dot. This is one radical, which a trapped in the magnesium oxide powder. This is the a g X X somewhere here, g Y Y and g Z Z.

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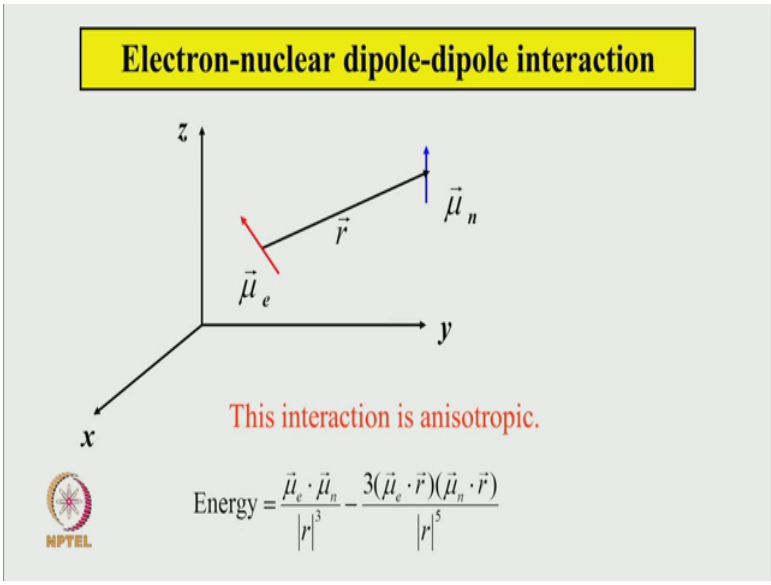

So, this now we take the next item, which is electron nuclear dipolar interaction. We have seen, this is the interaction which is highly direction on depended.

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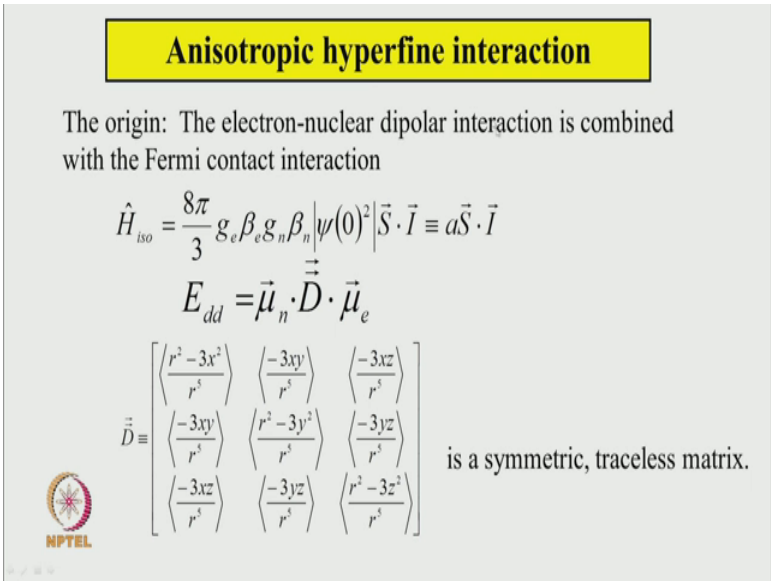

On the other isotropic part is given by this sort of expression dipole interaction is this. So, both of them have this type of S dot, I type of interaction here.

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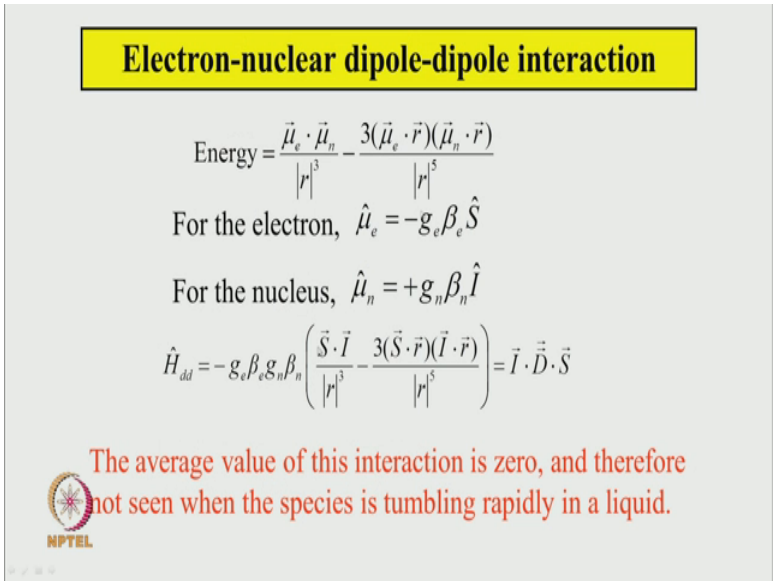

This also is equal to S dot I. So, we can as well add this isotropic interaction dipole-dipole interaction to get a single expression which looks like this.

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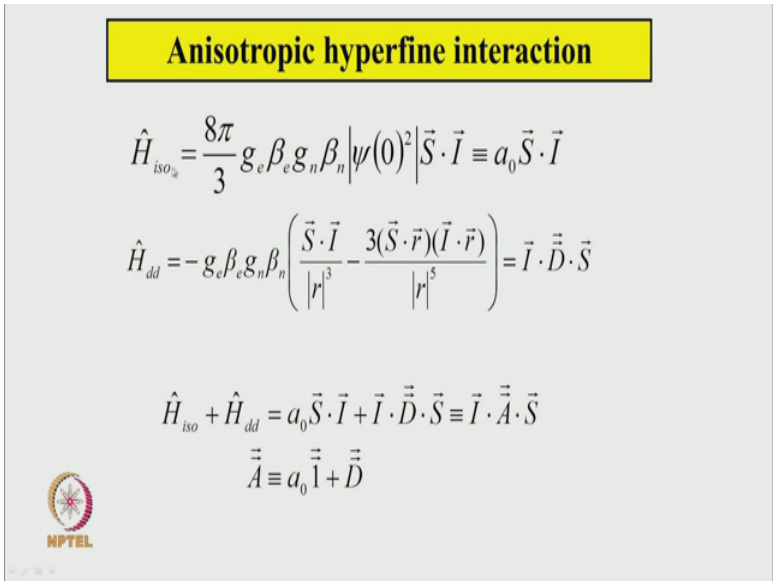

I is the nuclear spin, a is now a matrix 3 matrix and S is the spin angular momentum and a here now, we automatically a symmetric, because of the way this d is defined, but here if it is average of this diagonal element, these terms out to be 0, that is average dipole, interaction is 0, that is again into tumbling motion is fast. In solution one does not see this, but in original true influence solution or in crystals.

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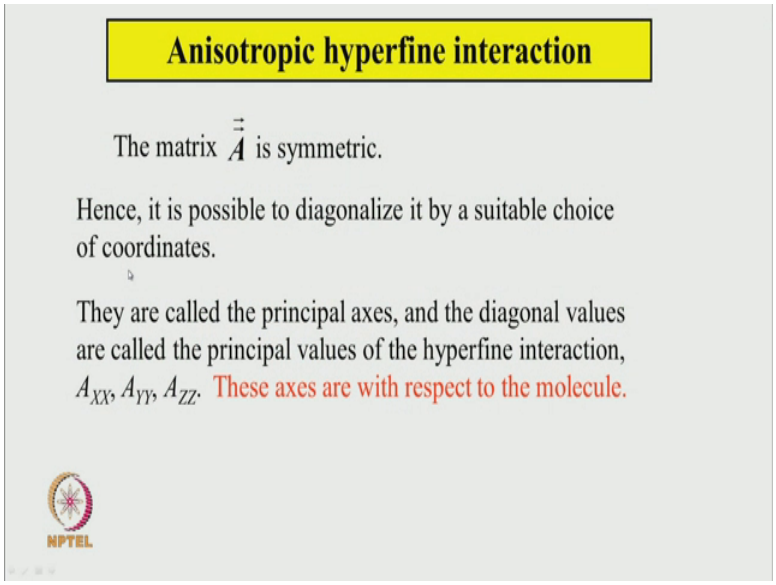

So, matrix a is symmetric. Hence it is again in a similar to this. We should be able to diagonalize the matrix by choosing suitable axis. These are called the principle axis of the hyperfine matrix.

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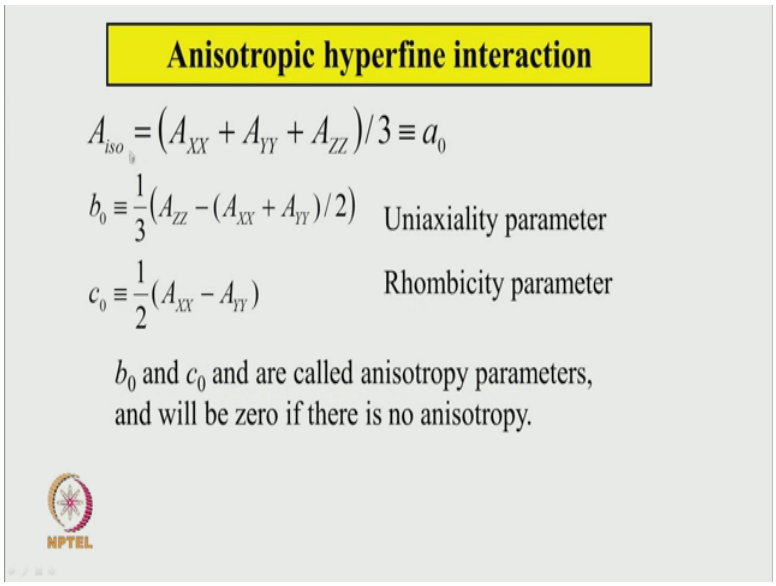

Now, average of this three principle component will be nothing, but a 0; obviously, because that is why these are added, then we add this constant isotropic value. So, that is the average value, is the sum of all this an isotropic. Values are now given by these two parameters, these are gives how for the z is different from the other two, and c is how

this other two x and y different from each other. So, b 0 and c 0 are called the an isotropic parameters, and particular b 0 is called Uniaxiality parameter and c 0 is called the Rhombicity parameter.

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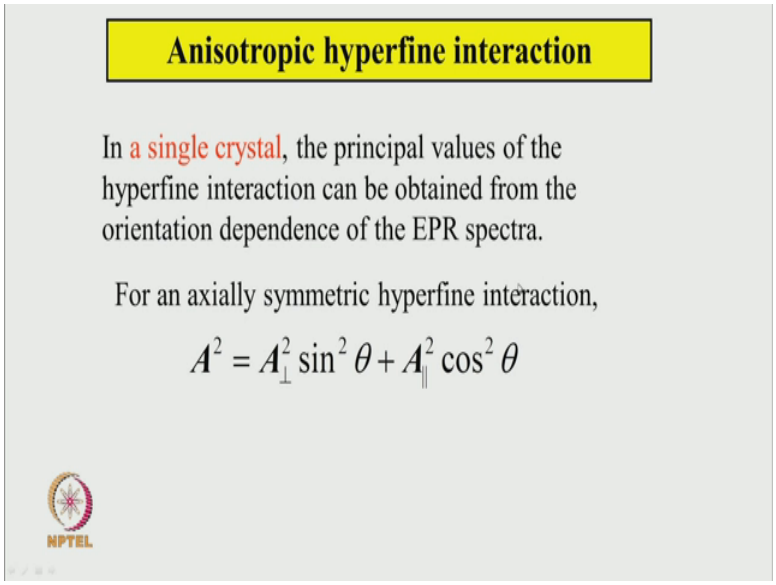

Now, is a single crystal in principle one, can find out the orientation dependence of the E P R spectrum, an axial symmetric is this equation looks very similar to g an isotropic, and in frozen solution, again the same type of relationship can be derived as we did for g an isotropic.

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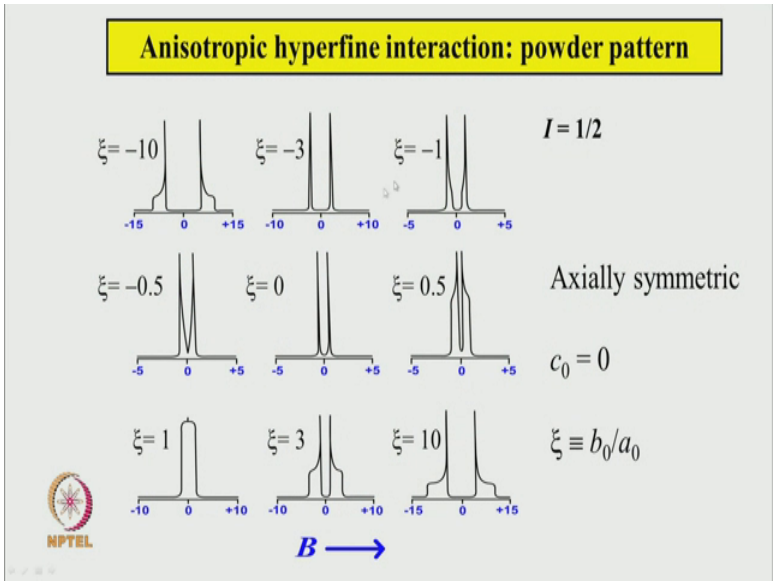

Now, here is a type of patterns we can get an axial symmetric I is half if c 0 that axial symmetry. Now b 0 defines how far it is deviating here, uniaxiality parameter here. So, you see b is 0, means is really isotropic

So, you will get two double lines. Now as b is 0 changes, we changes the xi, get various types of patterns, and these two patterns, particular you can recognize, they are very similar to axially symmetric g type of thing. So, each of the hyperfine transition, I get similar pattern as they xi, because smaller, they come closer and closer and closer, and they give all sorts of pattern of this kind.

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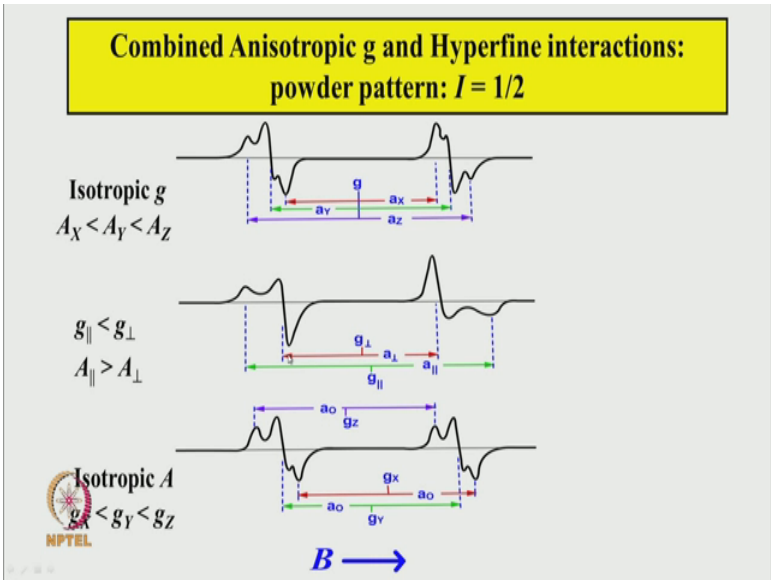

It is also possible that g matrix and a matrix are both present, the isotropic g an isotropic a. So, they can have this type of appearance, then here isotropic g that is all three transition. Here the pair of transition corresponding to A x A y A z as this centre value of all three of them are same. So, these g is isotropic, and the other hand g is axially symmetric, then I can get these two centre of these, and this corresponding to a perpendicular centre of these and this. The distance between these and this is a parallel and centre of this is g parallel. So, these and this a different, this are different, therefore, but values also different, but here in another place isotropic a, where a 0 is same for all of them. There is the gap between the corresponding lines are same, but the g is not isotropic. So, these are three different values of g.

So, that way one can get various type of combination and identify the, an anisotropic contribution, and the parameters of g and A from this powder pattern as well. So, we have seen how the E P R studies on single crystals powder or in frozen solution; one can determine all the, an isotropic interactions arising from g and A.

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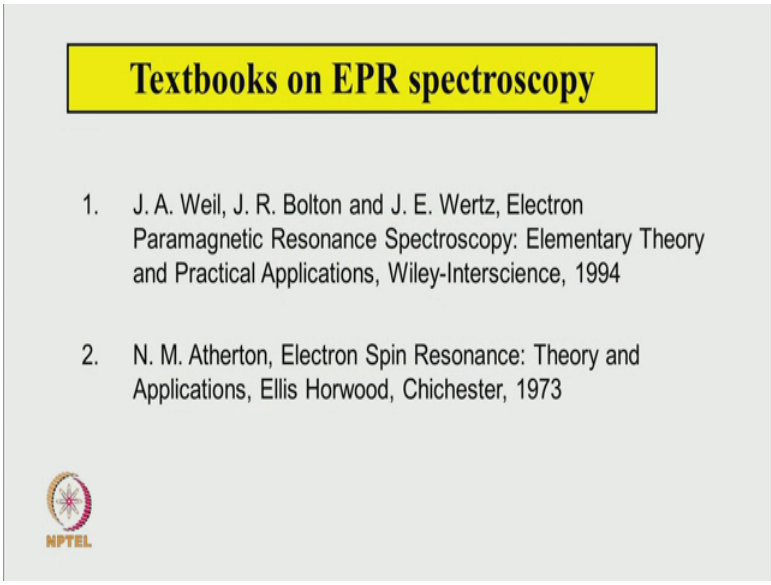

This slide shows in the two textbooks from which we have taken match of our material in this lecture.