Chemistry Atomic Structure and Chemical Bonding

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Lecture – 33
Spin ½ Angular Momentum

Welcome back to the lectures in Chemistry on the Atomic Structure and Chemical Bonding. My name is Mangala Sunder and I am in the Department of Chemistry, Indian Institute of Technology, Madras. And my email coordinates are given here for you to communicate course related inquiries and things like that ok.

Now, this is a continuation of the last lecture on the introduction to angular momentum. And in this lecture let us look at the properties of the Spin Half System Angular Momentum. The electron spin is the most famous example proton spin the nucleus proton also has an spin angular momentum given by the angular momentum magnitude one half. So, this is the purely quantum mechanical spin property that we were studying.

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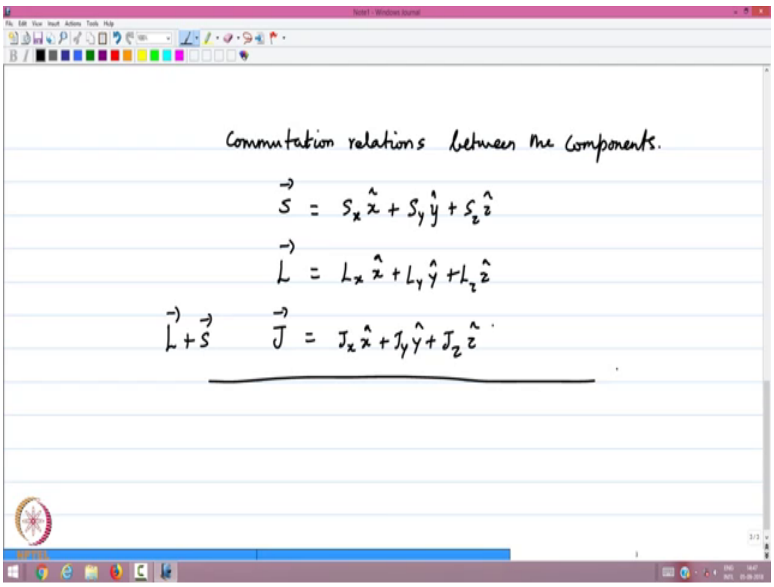

Now, in the last lecture I think I left with the question the on the commutation of the component commutation relations basically relations of the components relations between the components. I think we were looking at angular momenta with the following notation; S as the spin angular momentum and in the coordinate representation given by three components; Sx, Sy and Sz. The orbital angular momentum also given by the three coordinates with the corresponding symbols and the total angular momentum which is the sum of L plus S, L and S the sum of L and S is Jx of x plus the corresponding components in the other directions ok.

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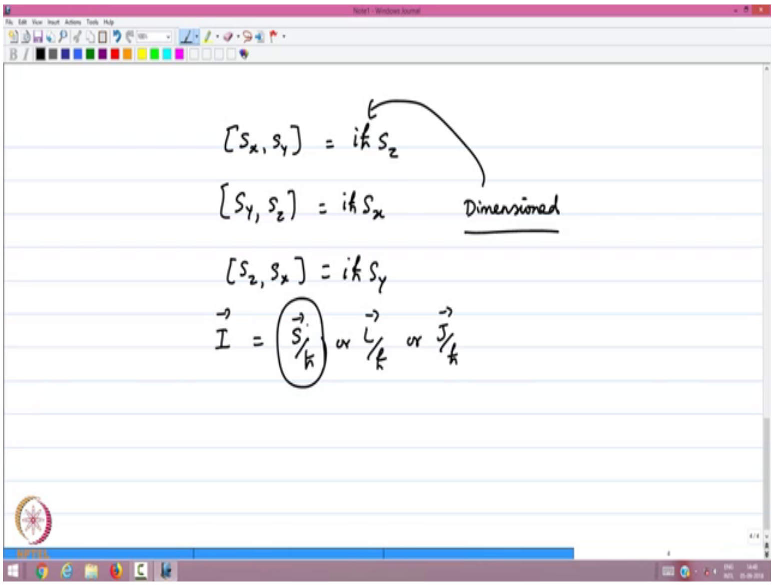

Now, the question that we want to address and also pursue further is the fact that the components Sx, Sy, the commutator between them is given by this relation ih bar S z. And likewise the commutator of Sy and Sz is given by ih bar Sx and Sz, Sx commutator is i h bar Sy ok. These are dimensioned angular momenta, the dimension is there in the h bar that you use. Therefore, for the logical development of some of the algebraic properties of them let us define an angular momentum without the dimension namely I as S by h bar or L by h bar or J by h bar whichever that we want to deal with ok.

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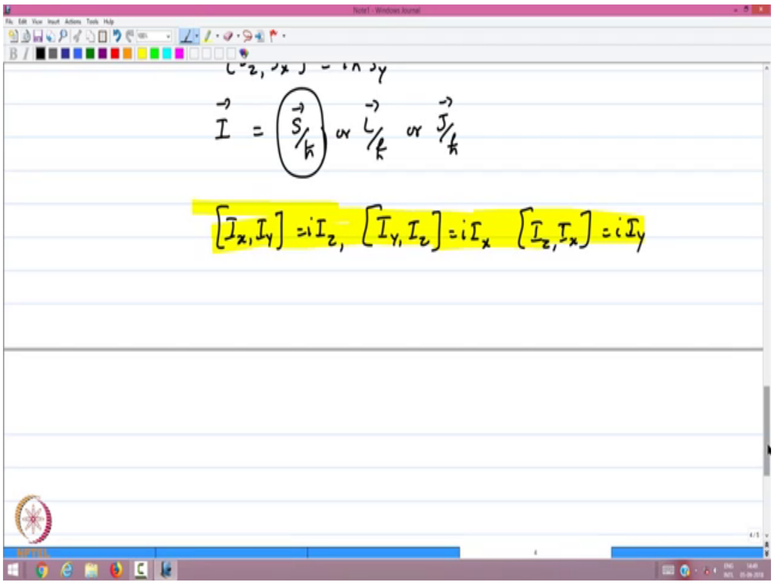

We are going to deal with the spin angular momentum and let us define I in such a way that if I is defined without the h bar then it is immediate that the commutator Ix, Iy is i Iz Iy Iz commutator is i Ix and Iz Ix commutator is i Iy ok. We shall use these as the starting point for all the algebraic properties that we study in this lecture ok, now h bar here.

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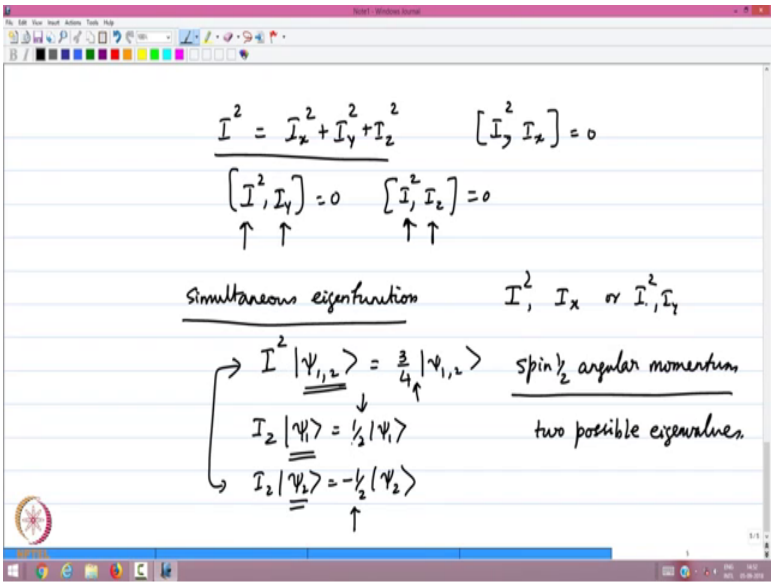

It is important to note that I square which is given as the sum of the squares of the components Ix and Iy and Iz. I square commutes with all the three components; I square comma Ix commutator is 0, I square comma Iy commutator is 0 and I square Iz commutator is also 0 ok. Therefore because these are operators angular momentum operators and because they commute, it is possible to have simultaneous eigenfunction for the pairs, but only one of the pairs I square Ix or I square Iy or I square Iz.

By convention we normally choose the pair of operators for which the eigenfunctions are defined simultaneously as I square and I z. The spin a half angular momentum corresponds to the following property. I square acting on this function it is been a half angular momentum corresponds to two possible Eigen values of the Iz operator ok. I z acting on psi 1 gives you half psi 1 and Iz acting on the other eigenfunction psi 2 gives you minus half psi 2.

So, these are the two discrete values for the z component of the spin half angular momentum. And I think we discussed this in Stern Gerlach experiment that was done in the last class last lecture. What about I square? I square on psi 1 and 2 whichever it is ok, gives you the same result namely I into I plus 1. And I in this case this 1 half therefore, it gives you 3 by 4 on psi 1 or 2, it is a same value ok. So, we have a wave function psi 1, 2 psi which is defined by the same Eigen value of I into I plus 1 for the operator I square, but different Eigen values half and minus half for the Iz operator.

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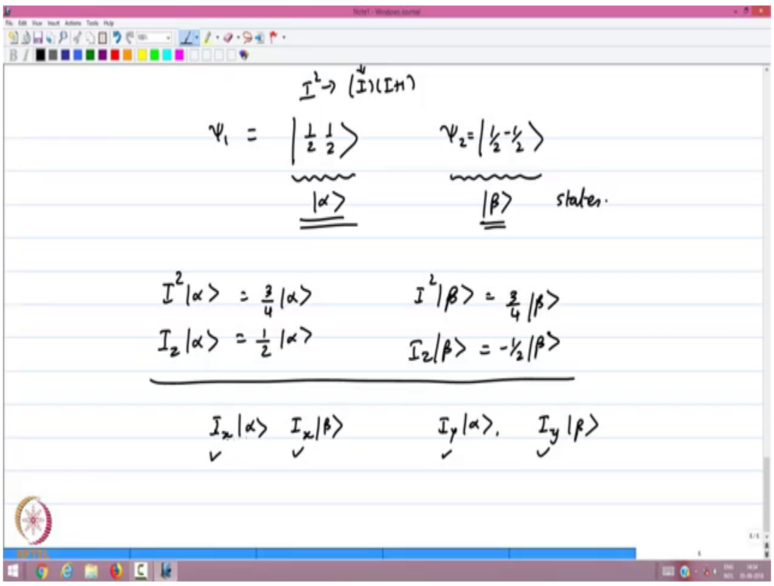

The usual convention is to write psi 1 with these Eigen values as the descriptors namely the half for the Iz square sorry I square the half for the operator I square where I into I plus 1 this one. So, this is half and then the other half is the Eigen value of the Iz operator. So, psi 2 will be 1 half and minus 1 half. And the convention in text books and in the literature physics literature and also in the chemistry in the NMR and all these subjects, the convention is to write to this as alpha and beta states, spin half states. These are spin half eigenfunctions with the specific properties as I have given here, I square on alpha or I square on beta gives you 3 by 4 alpha or beta I z or alpha gives you half alpha and I z on beta gives you minus half beta.

Now, while this is clear what about the action of I x on alpha, Ix on beta, I y on alpha, I y on beta? Because these are the other two spin angular momentum components. And even though they are not simultaneously Eigen I mean alpha and beta are not simultaneously eigenfunctions of Ix and Iy we must know what happens when Ix operates on alpha or Ix operates on beta and likewise Iy on alpha or beta.

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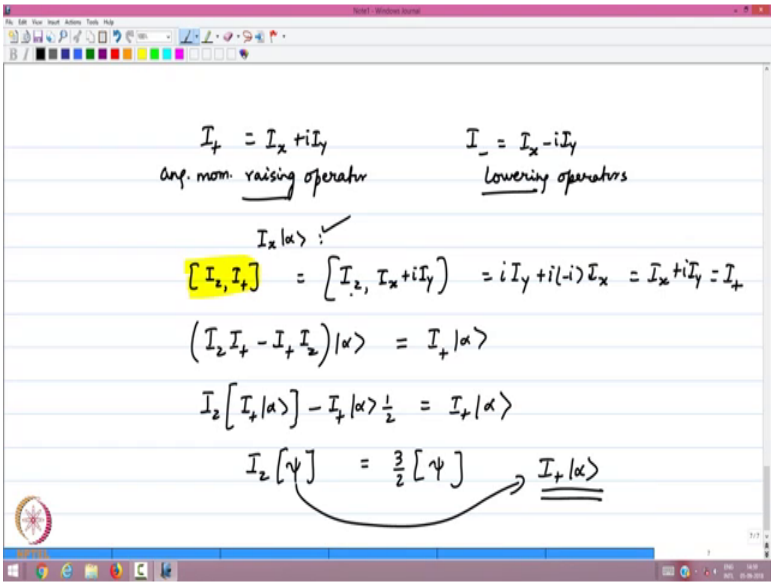

To calculate this there is a very standard method namely to first look up to the commutator, first define a pair of operators called I plus spin angular momentum raising operators; we will see why it is angular momentum raising operator. And the other one I minus as I x minus i I y as the lowering operator, you see in a few minutes why this names raising and lowering come in. To calculate the effect of Ix on alpha, let us start with the commutator I z comma I plus and then act on the state alpha, but first let us look at the commutator. That is easy to write down because it is Iz comma I x plus i Iy and the commutator of z with the x gives you Iy it gives you i Iy and the commutator of z with Iy gives you with y gives you minus Ix and for with plus i into minus i I x, the answer is Ix plus i Iy is equal to I plus ok.

Therefore, the action of I z I plus minus I plus Iz on the state alpha is the same as the action of I plus on alpha. And you can write this down immediately as I z acting on the state obtained by the action of I plus 1 alpha minus I plus on the state obtained by I z on acting on alpha and that is of course, 1 by 2 alpha is 1 by 2 and that is equal to I plus on alpha. Therefore, I z acting on this state is equal to 3 by 2 acting on the same state. What is the state? The state is the state obtained by the action of I plus 1 alpha. Therefore, I z has an Eigen function psi which is this which has an Eigen value 3 by 2 on psi.

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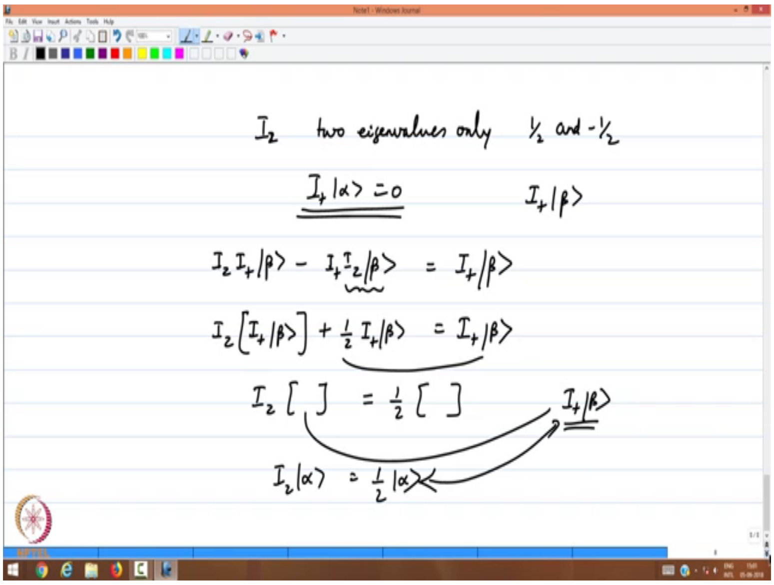

That is not possible because we have started with the requirement with the properties that I plus Iz has only 2 Eigen values plus and minus half; plus a half and minus a half. Therefore, the state Iz acting on that state giving you 3 by 2 the state is not a possible state for the operator Iz, which means I plus on alpha has to be 0, it does not exist ok. So, this is property 1. What about the same thing I plus on beta? You can do the same commutator namely Iz I plus acting on beta minus I plus Iz acting on beta.

It is the same as the I plus on beta and you can see immediately that this gives you a minus half. And therefore, you will get I z on the state I plus on beta plus 1 by 2, I plus on beta you have this size z on beta has already given you, 1 by 2 times beta for what is left over is this and a plus on beta on the right hand side which tells you that the two together gives you Iz acting on a state gives the result of one-half on that state. What is the state? The state is a plus operator acting on beta. Now, remember the eigenfunction of Iz with the Eigen value half is alpha. Therefore, I plus on beta is equal to this or its proportional to this.

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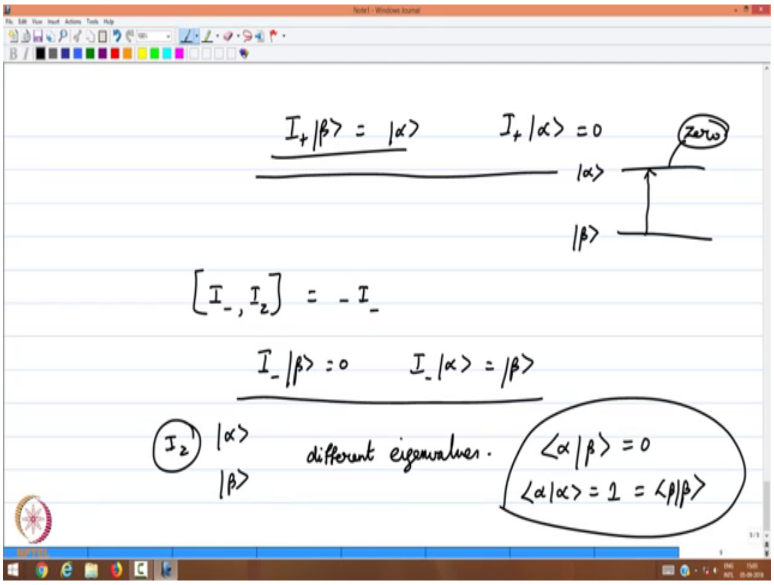

Linear algebraic calculation tell us that the action of I plus on beta is alpha, ok. The action of I plus on alpha is 0. So, if you think of alpha and beta are two states you call this as alpha and you call this as beta. Then you see I plus acting on the state takes it up and I plus acting on the state takes in to 0; no further states ok. This is the action of the raising and lowering raising operator on the alpha and beta. The action of the lowering operator be exactly the same argument is obtained by calculating the commutator I minus on I z and I will leave it to you to verify that this is the same as I minus.

And therefore, you will get the relations I minus on beta is 0 I minus on alpha is equal to beta so you have that. Now, also remember that alpha and beta are 2 Eigen states of the Iz operator with different Eigen values. Therefore, the states are orthogonal to each other alpha on beta is equal to 0. The states are normalizable and therefore, we will use only those normalized states namely alpha alpha is 1 and that is equal to beta beta. So, this is the orthogonality property of the Eigen functions of the Iz operator. And the states are such that the action of I plus and minus operators on alpha or beta or what you have already seen.

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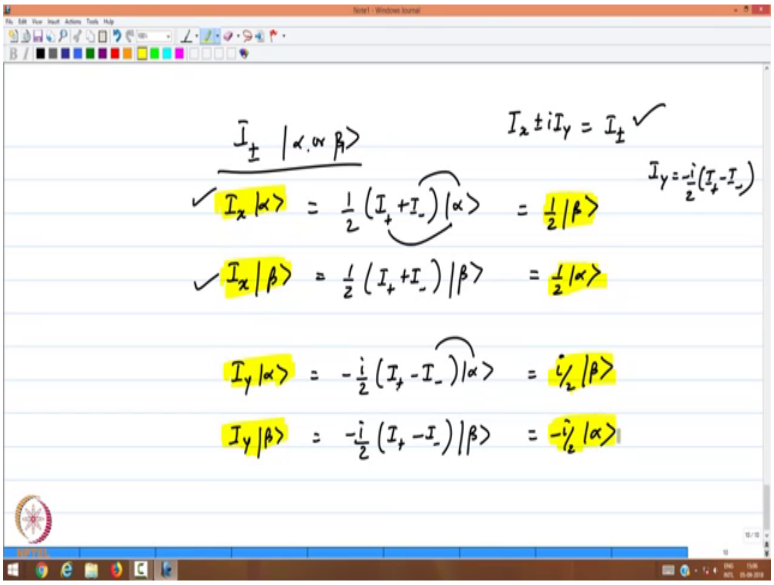

Now, therefore, what is Ix on alpha? Ix on alpha is I plus plus I minus by 2. Remember Ix plus or minus Iy is I plus or minus. Therefore, if you add these two you get this I plus plus I minus is equal to 1 by 2 and therefore, the action of the state on the state alpha by Ix is the same as that. And you know I plus on alpha is 0 and I minus 1 alpha gives you beta; therefore, the answer is 1 by 2 beta ok. And Ix in a similar way acting on beta gives you 1 by 2 I plus plus I minus on beta and I minus on beta is 0 I plus 1 beta gives you alpha, therefore, it gives you 1 by 2 alpha.

So, the action of Ix on both the states are known, therefore, the algebraic details are becoming more and more complete, the only other thing that we need to know is the action of Iy on alpha and beta ok. Iy on alpha and beta I can also be obtained in a similar way because you already know the action of plus and minus on alpha. Remember this gives you that Iy is minus i by 2, I plus minus I minus. If you subtract the one equation from the other this is what you will get. Therefore, Iy acting on alpha is equal to minus i by 2, I plus minus I minus acting on alpha; I plus 1 alpha is 0 I minus 1 alpha gives you beta.

And there is a minus and minus therefore, it is a plus i by 2 beta. And Iy on beta is again minus i by 2 I plus minus I minus on beta and I plus one beta gives you alpha and it gives you minus i by 2 alpha ok. Therefore, summarize these and immediately we can write to the matrices for these operators in no time here ok. I x on alpha is half beta, Ix on beta is half alpha, Iy on alpha is i by 2 beta and Iy beta is minus i by 2 alpha.

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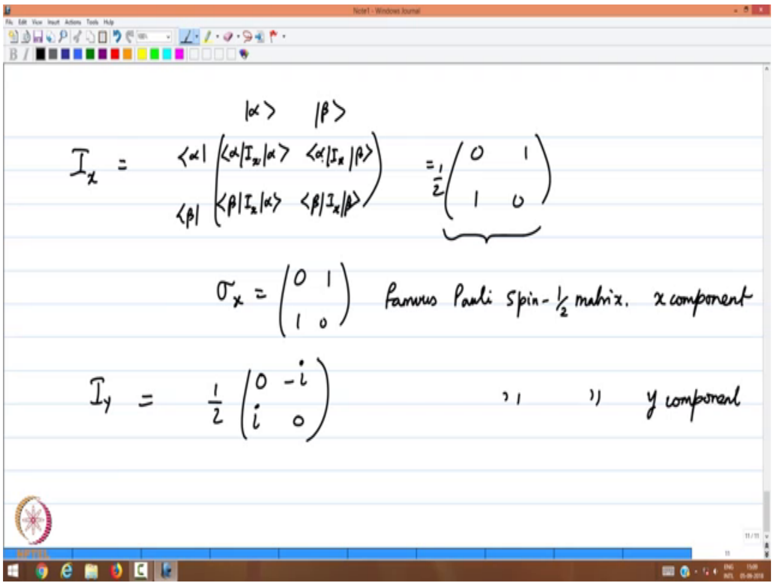

Therefore, in this representation of alpha and beta; what is the matrix representation for the operators Ix Iy? If you recall the vector algebra and the linear operator space that we did earlier it is alpha Ix alpha this is for the Ix operator and then it is alpha Ix beta and this is beta Ix alpha and this one is beta Ix beta. And you can see right way that alpha Ix on beta is given by this ok. Because this will give you sorry this is for Iy and we have to look at this alpha Ix beta is this one.

So, if you write alpha Ix on beta or this then you do the same thing here 1 by 2 alpha on alpha and this is 1; so the answer is 1 by 2 right. This is 0, Ix on alpha gives you beta therefore, alpha beta is orthogonal. So, you have 0 keeping 1 by 2 outside, you have 110. This matrix sigma x as it is denoted 0110 is the famous Pauli spin matrix spin one-half matrix x component ok.

Likewise for Iy all I need to do is to replace the operator Ix with I y in all 4 places. And Iy on alpha gives you here, you have seen that gives you beta therefore, this is 0. Iy on beta gives you alpha and therefore, there is you can see that Iy on beta gives you minus Iy 2 times alpha. Therefore, this matrix Iy turns out to be 1 by 2 0 minus i, i 0 ok. And this is again famous Pauli spin matrix half matrix y component ok.

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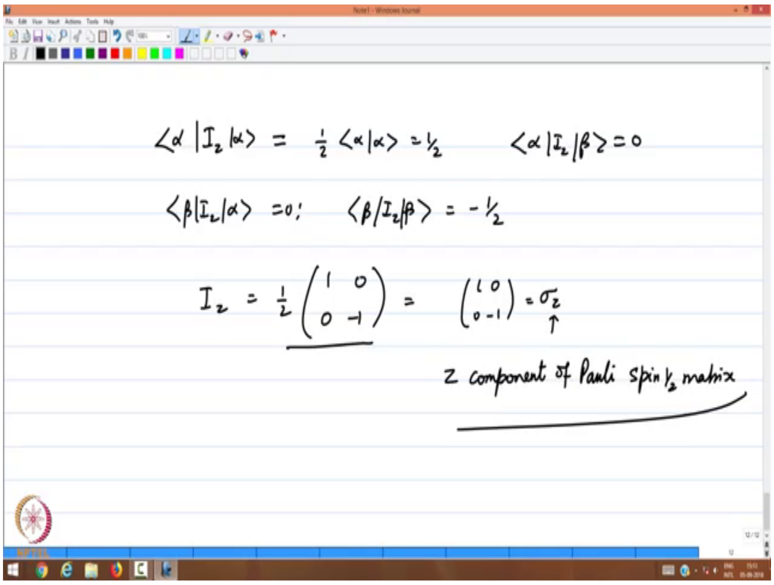

What is a z component? That is easy because Iz on alpha gives you half alpha. Therefore, this element is 1 by 2 alpha alpha and it is 1 by 2. And again alpha on Iz on beta is therefore, 0 because this gives you beta back and orthogonality makes this result equal to 0. And beta Iz on alpha is also 0, beta I z on beta is minus one half.

So, the matrix representation for Iz is 1 by 2 0 sorry 1 by 2 1 1 0 0 minus 1. This is the sigma z 1 0 0 minus 1 is equal to sigma z, the z component of the Pauli spin matrix, one-half matrix ok. So, these are the properties of the angular momentum operators for a spin half system. Since we know all the spatial components Ix Iy Iz acting on alpha or beta the 2 Eigen states for the problem what they give we have complete knowledge of spin half system with respect to the algebraic details ok.

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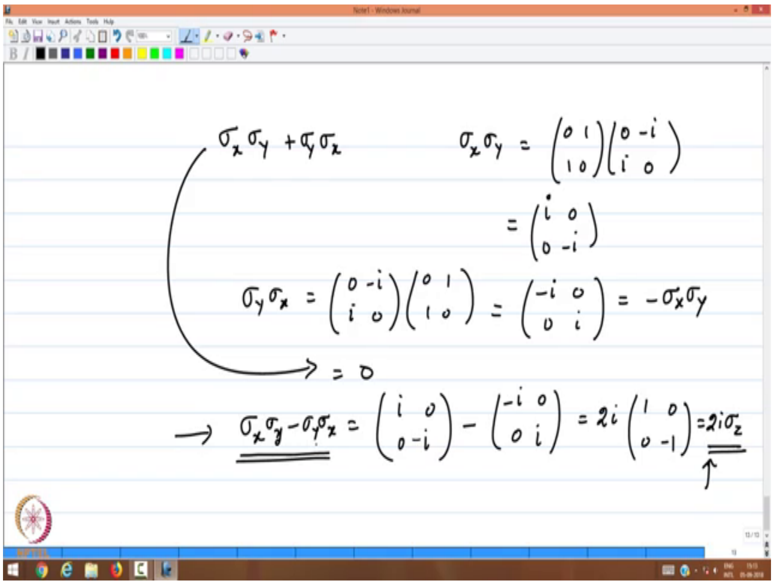

Now, to close this lecture you recall in one of the earlier problems we were looking at sigma x, sigma y plus sigma y, sigma x. And you can see right away that sigma x, sigma y, gives you 1 by 4 sorry there is no 1 by 4 this sigma x is just a matrix ok. It gives you 0 1 1 0 and it gives you 0 minus i i 0. The product of which is i 0 0 and minus i and the product sigma y sigma x is 0 minus i i 0 times 0 1 1 0 and that is equal to minus i 0 0 plus i. Therefore, this is equal to minus sigma x sigma y; therefore, this sum is equal to 0. And it is also easy to see therefore, that sigma x, sigma y minus sigma y sigma x is goings to take the difference between these two operators namely i 0 0 minus i minus minus i 0 0 i.

So, it gives you 2i times 1 0 0 minus 1; so it gives you 2i sigma z. So, the Pauli spin matrices have a numerical coefficient of two in front of an otherwise a spin angular momentum x or y or z component. So, this is a very famous relation called the Pauli's this famous statement that we have that the Pauli spin operators anti commute, meaning that if you take the plus combination they go to 0 that is the negative of the commutator therefore, it is called and take computation and it is not just x and y or z its cyclical.

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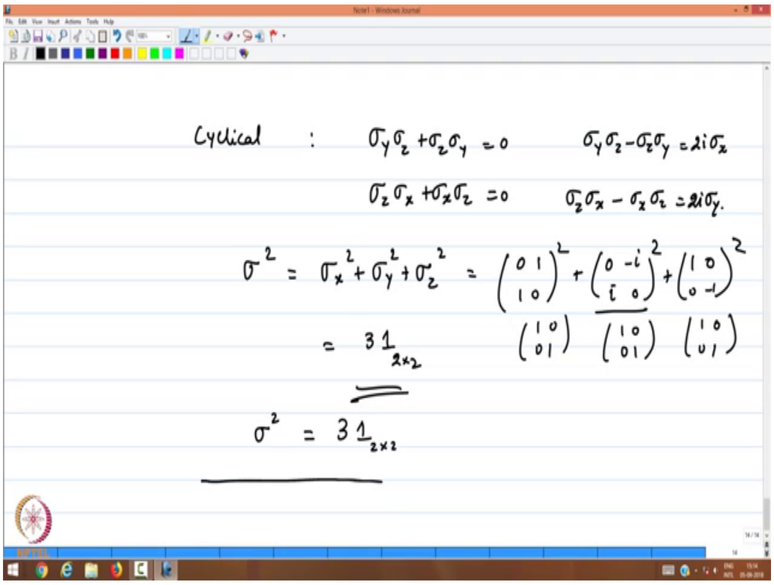

Therefore, the similar relations that you can verify are sigma y, sigma z plus sigma z, sigma y that is 0, sigma z, sigma x plus sigma x, sigma z is 0 and sigma y sigma z minus sigma z sigma y is 2 i sigma x and likewise sigma z sigma x minus sigma x sigma z is 2 i sigma y ok. One last thing namely sigma square is sigma x square plus sigma y squared plus sigma z squared and this you know is 0 1 1 0 squared plus 0 minus i i 0 square plus 1 0 0 minus 1 squared, the answer is 2 times here, this will give you 1 this will give you 1, the answer is 3 times the identity matrix 2 by 2 plus this will give you 1 0 0 1. This will give you 1 0 0 1 this would also give you 1 0 0 1. So, it is 3 times the identity matrix.

Therefore, sigma squared is equal to the operator 3 with the identity right. So, these are angular momentum properties that we need to know for us for the half system. And in the next lecture we will see the angular momentum for two such electrons or two such spin half systems, how do we define them, when the two spins interact with each other strongly or when the two spin systems interact with each other weakly. And this is extremely important in establishing what is known as the anti symmetric state for two identical the spin systems of spin half, namely, the electrons as an example or 2 protons.

And this will also just give you some input insights into the famous principle that Pauli came up with namely the Principle for the Anti Symmetry and the principle of what is called Exclusion, mutual exclusion which is important in the study of atomic structure ok. We will do more of this with the two spins in the next lecture until then.

Thank you very much.