Chemistry Atomic Structure and Chemical Bonding
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Lecture – 34
Spin Angular Momentum and Coupling of 2 Spin-1/2 Angular Momenta

Welcome back, to the lectures in Chemistry and to the Atomic Structure and Chemical Bonding. My name is Mangala Sunder, I am in the Department of Chemistry IIT, Madras and my e-mail addresses are given here, the coordinates are here for you to communicate to me.

The lecture continues from what I left in the previous one, the Properties of Spin Angular Momentum. We saw in the previous lecture the spin half angular momentum and we looked at the Pauli spin matrices, the relation that we have with the Pauli spin matrices, the commutation relation and the anti commutation relations, all those things were explained the bit and in this lecture, we continue with the same. But now with integer angular momenta and higher angular momenta namely not spin half systems, but spin 1, spin 3 halves a little bit of that before we proceed to the understanding of the interactions between 2 spin half systems in this course. Of course, the importance is to the interaction between two electrons or two angular momenta of two spin one half systems.

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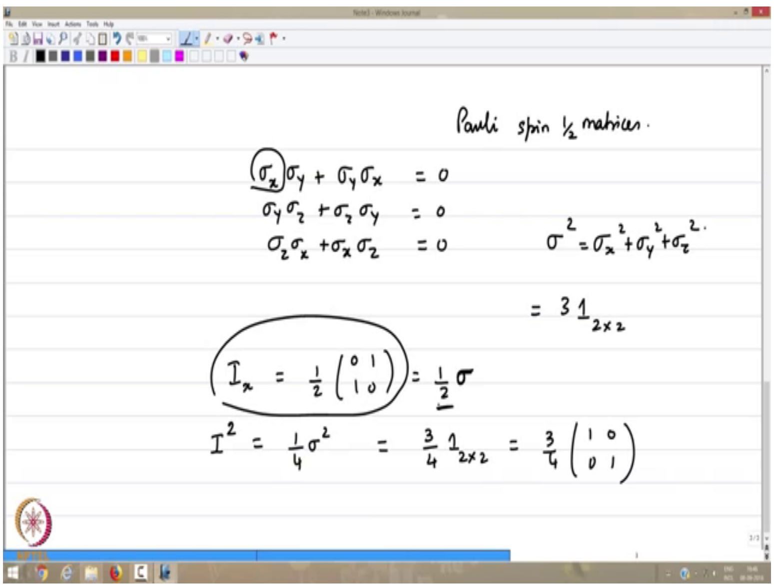

Let me first restate or recall what we wrote down in the last couple of minutes of the last lecture, we did sigma x sigma y plus sigma y sigma x Pauli spin matrices spin one half matrices that is equal to 0 and likewise for sigma y sigma z plus sigma z sigma y and sigma z sigma x plus sigma x sigma z is equal to 0 and then we had sigma square as sigma x square plus sigma y square plus sigma z square. And that is 3 times the identity matrix 2 by 2. But, recall that then we wrote down the spin angular momentum operator I x we had it as 1 by 2, 0 1 1 0 and therefore, this was written as 1 by 2 sigma.

Therefore, if you are looking at I square then essentially it is 1 by 4 sigma squared, therefore, it is 3 by 4 into the identity matrix 2 by 2 namely 1 0 0 1. This is the spin half angular momentum, this is the Pauli representation of the angular momentum spin half in terms of matrices, the relation between the two is given by this numerical factor one half, I think that is important to remember.

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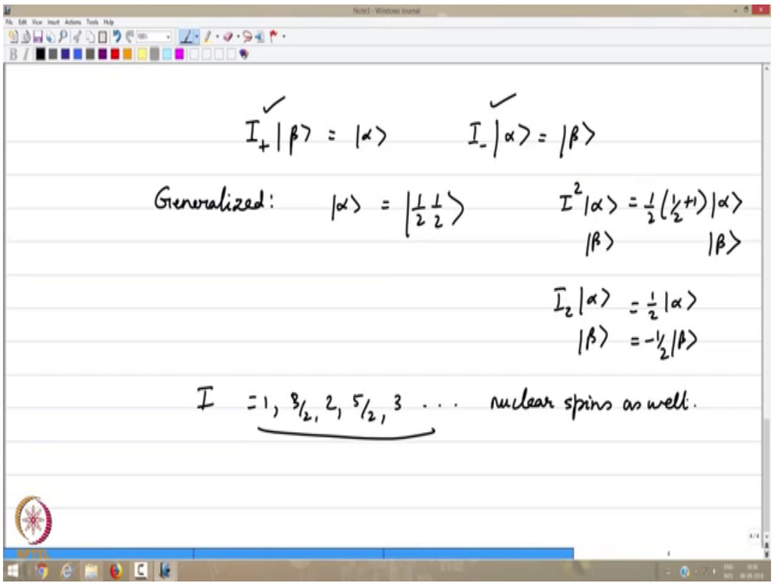

Now, also recall the properties that when we wrote down I plus on beta we had it as alpha and I minus on alpha is equal to beta. These things can be generalized the angular momentum properties of I plus and I minus on any spin angular momentum states can be generalized to the following relations. Recall that when we wrote down alpha as a state it was the quantum numbers half and half corresponding to the I squared on alpha or beta giving you half into half plus 1 which is what was written as 3 by 4 times alpha times beta and I z on alpha and beta.

This is just to recall, so that we continue from here. You remember this was the one half and alpha and this is was a minus one half and beta. Now, the general relations for all these things is I for 1, 3 by 2, 2, 5 by 2, 3 and so on. These are all important in the coupling between the angular momenta as well as nuclear spins when we study at some point of time later the nuclear magnetic resonance spins as well, but the properties of the angular momentum are all the same and they are generalized by the following relations.

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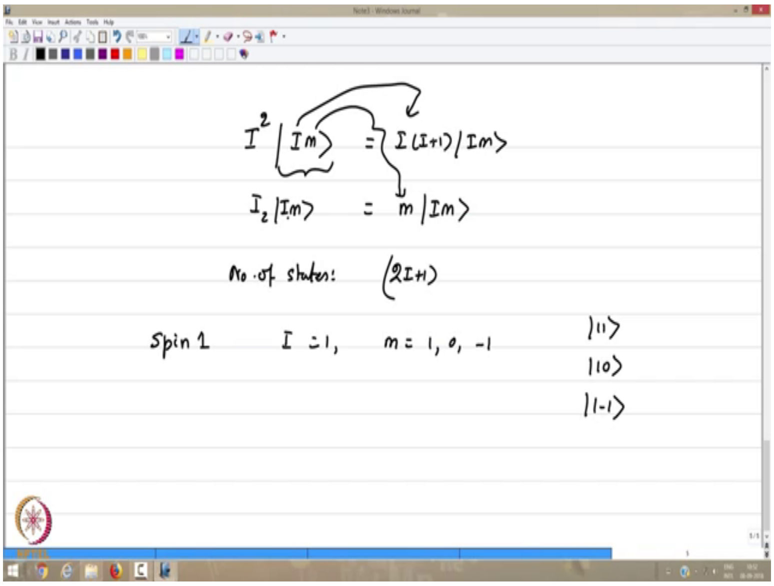

Namely, I z on the spin state I m the 2 values the quantum numbers are given as I m, this is given as I into I plus 1, I m and I z on m again sorry I m is given as m times I m and the number of states I m for any given I is 2 I plus 1. Therefore, if you think about a spin one the I here corresponds to this quantum number the m here corresponds to this quantum number because this is I square I am sorry, this is not I z this is I square the I square and I z being the operators which commute among themselves only two quantum numbers describe the spin state of the single spin and these two quantum numbers basically are used to represent to the state I m. Therefore, for a spin 1 we have I is equal to 1 and m is equal to 1, 0 and minus 1.

So, we have three states 1 1, 1 0 and 1 minus 1 with the corresponding values for the I z operator, where I z on 1 1 gives you one times a 1 I z 1 0 is 0, I z on 1 minus 1 gives you minus 1 and I square gives you 2.

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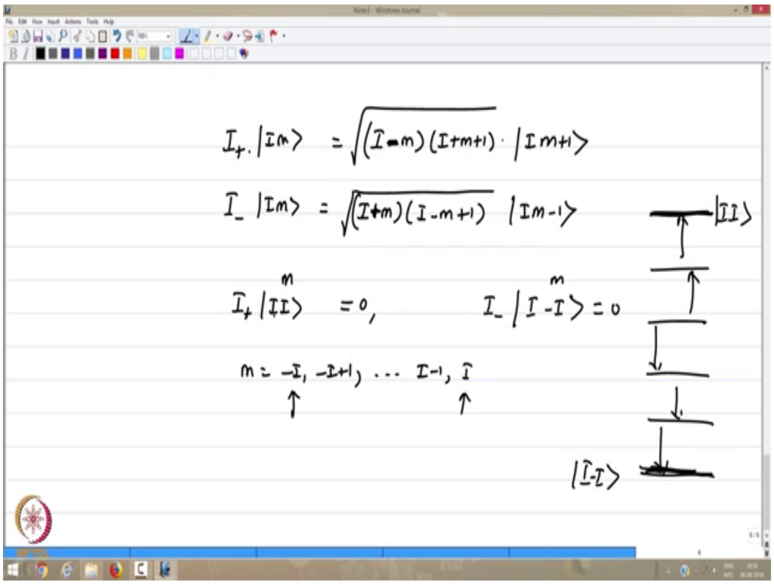

Now, what about the I plus on I m? This can be obtained in general and I am going to give you the relation namely, it is I minus m into I plus m plus 1 square root I m plus 1 and likewise I minus on I m is square root of I plus m and I minus m plus 1 I m minus 1. One way to remember this combination whether it is a plus or minus in the first term is to recall the fact that I plus on I I the highest state is 1 and I minus on the lowest state I minus I is 0 this is the m value, these are the m value.

So, m takes the value minus I, minus I plus 1, I minus 1, I this is what you had for a spin the half it was very easy this was a minus half and this was a plus half there were only two states because minus I plus one stopped with I. Therefore, for a spin half system the I plus on I was essentially I plus on half that was 0, and you can see that right away that I minus m ensures that m never exceeds I, m never exceeds I. Therefore, if you were to arrange the states in some ladder form then in the ladder the lowest is I minus I and the highest is I I and the I plus operator takes it up and the I minus operator takes it down, but there is nothing below the lowest and there is nothing above the highest.

So, it is easy to remember that the moment you remember I minus m you can immediately recall that it is I plus m plus 1 so, some way of numeric form to recall and remember important relations.

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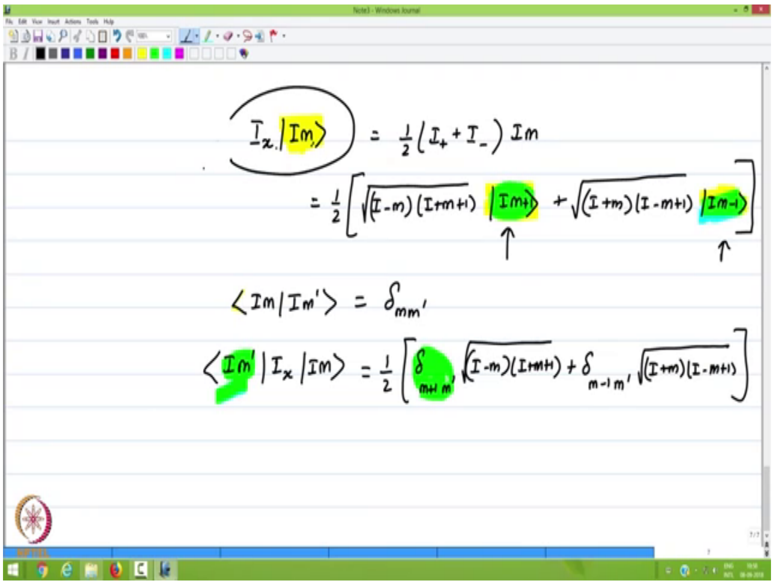

Therefore, if you were to write on I x the action of I x on I m it is 1 by 2 of I plus plus I minus on I m. Thus the answer would be 1 by 2 square root of I minus m times I plus m plus 1 with the state I m plus 1 and I minus giving you plus square root of I plus m I minus m plus 1 on the state I m minus 1. That is the matrix, that is the action of the operator on the state I m. Therefore, the state I m is not an Eigen function of the operator I x the same way like the Pauli spin matrix that is the I x was not giving you the Eigen value for the alpha state or the beta state it gives you I m plus 1 or I m minus 1.

So, let me just highlight that alone. So, the state I m when it is acted on by I x gives you I m plus 1 or I m minus 1. Therefore, recalling that the states I m and I m prime or orthogonal delta m m prime it is immediately possible for us to write that if I write I m prime I x on I m I will get the result namely delta m m prime square root of I minus m I plus m plus 1, And here the m prime is what? The m here is m plus 1 m plus 1 m prime because the m prime has to be equal to this in order for I x on I m which gives you I m plus 1 to be nonzero. Therefore, m prime so, this I m prime will recover this I m plus 1 on the action of I x 1 I m provided this m prime is equal to m plus 1, that is what this is the part.

Now, what about this term? This term tells you that if m prime; let me use a different label, if m prime were equal to m minus 1, then m minus 1 will be recovered. So, the second term that you will get is delta m minus 1 m prime square root of I plus m I minus m plus 1.

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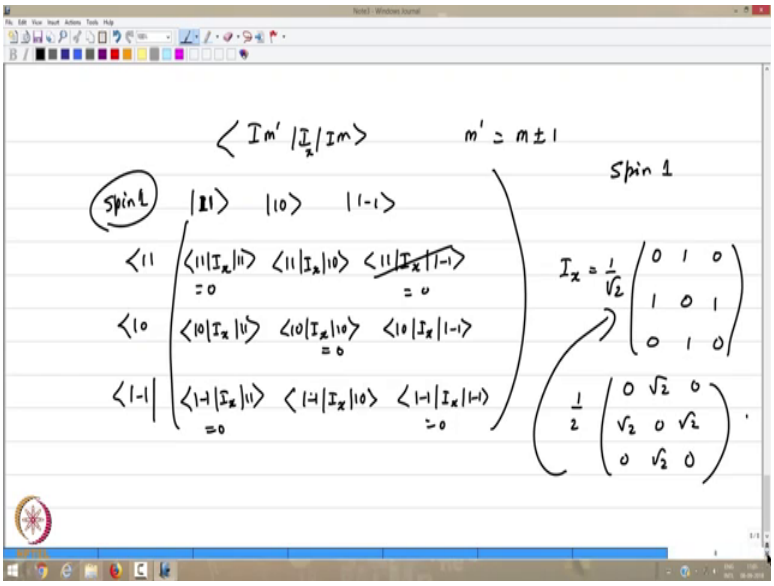

So, the matrix elements of this quantity I x, if I have to write the general operator I m prime I x I m the matrix elements of this operator I x or nonzero provided m prime is equal to m plus or minus 1, those are the only two possibilities. If m prime is equal to m plus 1, this is the matrix element. If m prime is equal to m minus 1, this is the matrix element. Therefore, if you write this in the matrix notation generally I for example, let us write this for spin 1.

If we write this for spin 1, the I m will be 1 1, 1 0, 1 minus 1 and the prostates are 1 0 1 minus 1. Now, this element is 1 1 I x 1 1, this is 0 because the two states are identical. This element is 1 1 I x 1 0. This is not 0 because m prime is equal to m minus 1 because there is a plus component of this which will raise 0 to 1 and therefore, this element is nonzero. But, on the other hand this will be 0 because here m prime this minus 1 is not m plus minus 1, but it is actually 2 off. So, this is 0, this is nonzero and likewise you have 1 0 I x 1 1 this is nonzero 1 0 I x 1 0, this is 0, 1 0 I x 1 minus 1, this is nonzero and likewise 1 minus 1 I x 1 1 this is 0, 0 this is nonzero 1 minus 1 I x 1 0 and then the diagonal element 1 minus 1 I x 1 minus 1 this is 0.

So, for a spin one if you calculate these things using the formula you must get the operator representation the matrix representation of the operator will turn out to be 1 by root 2, 0 1 0, 1 0 1, 0 1 0. This 1 by root 2 is basically 1 by 2 and the matrix elements that you calculate will all be root 2 0 2 0 root 2. So, I have cancelled the root 2 to give you this. This is what you will get, this is what you will get from this calculation. So, this is what I x, what about I y?

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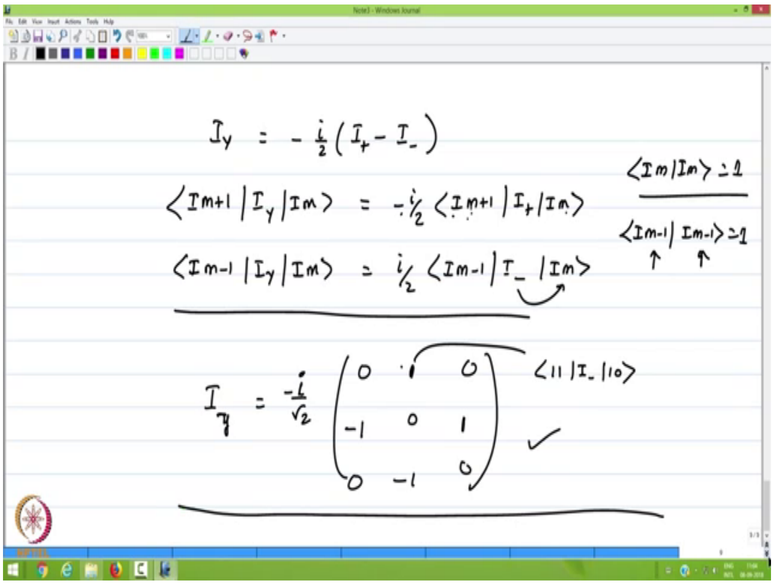

I y is minus I by 2 I plus minus I minus. Therefore, you can see that I m plus 1 let me write because we know it is going to be only one not the other I y I m will be minus I by 2 I m plus 1 I plus on I m, the minus will bring it down to m minus 1. Therefore, they are orthogonal to each other and I m minus 1 on I y I m will be there is a minus sign here. So, it will be plus I by 2, I m minus 1 I minus on I m, I minus on I m lowers it to one value down and therefore, the normalization property of the states I m I m is one that takes care of and therefore, you can write the same thing as I m minus 1 I m minus 1 that is also what any value of m which is the same on both the (Refer Time: 17:11)

So, given this if we can write the I minus, the I y operator as 1 by or minus I by root 2. Now, let us see this is the first element is 0, because it is diagonal you can write all these things of 0 and to the two of diagonal they are also 0. Therefore, what you have is this element is this element is 1 1 I plus 1 0. So, that corresponds to this type of matrix element 1 1, when m is 0 then you have that and therefore, the corresponding value will be there is a minus I by 2 2 is already taken therefore, this is 1 this would be 1 this will be minus 1 this would be minus 1.

So, this is the representation where you can calculate it based on this formula. There will be some tutorial examples for you to do that, but try to follow this formula namely the first very first one, this formula keep this in mind. These are the properties of spin one operators.

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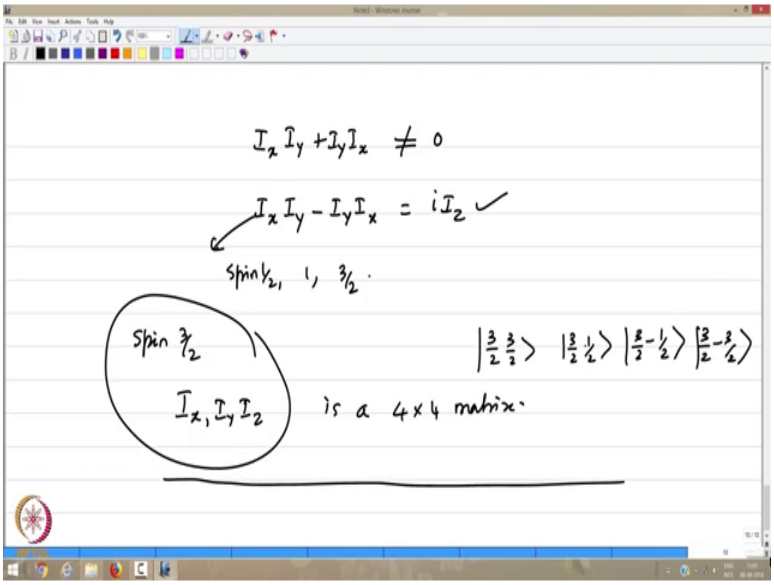

However, for spin one or any higher spin angular momentum we cannot write I x I y plus I y I x it is not 0, and for any spin including half the relation is I x I y minus I y I x is always i I z always, no matter whether the I corresponds to spin half or spin 1 or 3 halves and so on.

If the system is a spin three half system chlorine nucleus store in 35 nucleus has a nuclear magnetic moment that corresponds to a spin three half system for spin three halves we will have 4 basis functions I m will be 3 by 2 3 by 2 I minus 1 will be 1 by 2 then you will have 3 by 2 minus 1 by 2 and 3 by 2 minus 3 by 2. So, there are four stage and so, the spin three half representation, the matrix representation for I x I y and I z for a spin three half system is a 4 by 4 matrix, and likewise for any spin I it is a 2 I plus 1 by 2 I plus 1 matrix. So, these are properties of these spin half system spin arbitrary spin I systems.

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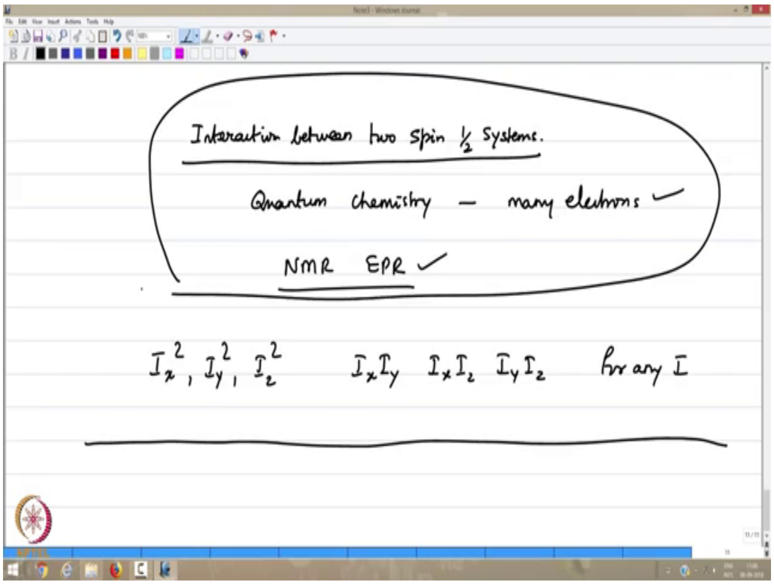

Now, we will get into an extremely important problem in both spectroscopy and in quantum chemistry namely the interaction between 2 spin half systems. The interaction between 2 spin half systems in quantum chemistry is of course, extremely important because of we deal with electrons, many electron systems. And in nuclei we deal with the nuclear magnetic resonance, electron paramagnetic resonance, NMR spectroscopy, EPR spectroscopy and anywhere where the orbital angular momentum of sorry, anywhere 2 spin half systems interact orbital angular momentum is an integer angular momentum we are only talking about 2 spin half systems.

So, these are all areas where we interactions have to be studied, and since the whole concept requires what is called the spin state representation for a 2 spin system it is like what we was introduced earlier in one of the mathematics lecture notes as the direct product of 2 single component systems and let me do that in the next lecture.

We will stop here in concluding that it is possible for us to write matrix representation for all the operators I x, I y, I z and a host of others namely, I x square, I y square, I z square, I x I y, I y, I x I z, I y I z all these operators for any I. So, we will stop here as the component for single spin systems and in the next lecture let me start looking at to the interaction between the 2 spin half systems from the background of what is meant by a true spin half states, what is meant by the operator representation for those for the 2 spin half states and so on.

So, until then thank you very much.