Chemistry: Atomic Structure and Chemical Bonding Prof. K. Mangala Sunder Department of Chemistry Indian Institute of Technology, Madras

Lecture – 32 Introduction to Angular Momentum

Welcome, to the lectures in Chemistry and the topic of Atomic Structure and Chemical Bonding.

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My name is Mangala Sunder and I am in the Department of Chemistry as a professor and also in the Indian Institute of Technology, Madras. My email coordinates are given here for you to contact.

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The topic today is the beginning of a series of lectures on angular momentum at the introductory level and in quantum mechanics. Angular momentum in quantum mechanics is not a visualizable quantity. Like the way we visualize rotational motion or we visualize the tops that we play with, those are all visual representations for classical objects.

In quantum mechanics angular momentum is a property is a fundamental property of the system and it was first discovered in the spectra of hydrogen atom when the spectral lines split into doublets in the presence of a magnetic field for the hydrogen atom. The theory of angular momentum was of course, put forward by the famous physicist Wolfgang Pauli and the experiments for the basis of the theory were given by Uhlenbeck and Goudsmit around 1925 - 27. The same time quantum mechanics was being formulated by several scientists.

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Now, let us not get to the history of it we will do that later, but get to the operational principles of angular momentum for the purpose of the atomic structure and chemical bonding for the electron spin angular momentum is a fundamental property and it is usually written as by the symbol spin angular momentum by S. The orbital angular momentum which probably was introduced in a cursory way earlier in hydrogen atom for the electron is often denoted by the symbol L.

And, then the total angular momentum of the electron which is the sum of the two vectors L and the S is denoted by the symbol J. These are conventions in textbooks and in the usage in the literature. Now, this lecture will start with the definition of angular momentum and in the next lecture what we would do is to describe the commutation relations in detail for various angular momentum operators.

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The experimental evidence that angular momentum is quantized, quantization that came from the famous experiments of Stern and Gerlach. A brief summary is that if beam of silver atoms when pass through a magnetic field which is inhomogeneous, the field at various points between the two magnets are different for different points, inhomogeneous.

When a beam of silver atoms is passed through the inhomogeneous magnetic field H, the beam splits into two parts and you can see two intensity patterns and this was the first indication that the angular momentum of the electron is quantized and the spin could be calculated to be h bar into root 3 by 2 the magnitude and it was also found out that these two would have a component of the magnetic mode the angular momentum as h bar by 2 minus h bar by 2 that is plus or minus half in units of h bar.

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Classically all of you know that the angular momentum is given by L, is given by the cross product of the position vector and the momentum vector of a particle, going around some point the position vector is at any point is given by r and the momentum is of course, tangential to the point of motion and the cross product of the two is represented in classical mechanics as angular momentum. And, the direction of the angular momentum is if in the plane perpendicular to the plane of r and p, because any way you remember the cross product of two vectors is in the direction perpendicular to the plane containing the two vectors and we use the right handed coordinate system to actually describe the directions.

Now, for if the system is moving this way around the point and this is r cross p then you see it is this and this. The cross product of the two when you go this will be pointing up. This is a classical definition, in quantum mechanics we use this definition to characterize angular momentum components, but with the additional restriction that not all components of angular momentum can be measured simultaneously. L for example, as a vector in classical mechanics is given by the three components in a 3-dimensional coordinate system L x, L y and L z in some axis system x y z. The square of the angular momentum is L dot L and that is given by L x square plus L y square plus L z square.

And, the precise direction of the angular momentum can be visualized, is known and you will have complete knowledge of the components of angular momentum L x, L y, L z all of this is true in classical mechanics or classical systems which behave classically.



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However, the quantum mechanical angular momentum or the electron angular momentum is not a classical quantity obviously, and it is not possible for us to write the spin angular momentum S x, S y and S z components simultaneously. They cannot be simultaneously measured exactly. What can be measured experiments tell us that we can determine the S square and one component; S square is the square of the magnitude of the angular momentum of S and one component of S which is usually written as the z component by saying that the direction of the angular momentum is chosen and the component of the angular momentum in that direction. Usually it is done by associating a magnetic field or an electric field to the system.

But, there is a specific directional axis about which the angular momentum has component S z and the magnitude of the S which is given by the square root of the dot product S dot S the same thing for L orbital angular momentum, L square and one component of angular momentum can be known simultaneously. And this is generalized by, you can do it in two ways this is generalized using a Cartesian representation for the angular momentum in spherical polar coordinates, but that the representation is limited to integer angular momentum.

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Integer values for angular momentum whereas, such a Cartesian representation the polar angle representation cannot be given for the spin angular momentum which is a purely quantum mechanical quantity and the basis set for spin angular momentum is known as a spinner. These have theta phi integer values of angular momentum they all can be the Eigenfunctions of the operator angular momentum square operator can be given theta phi representation namely polar coordinate representation this is for the L, but not necessarily for the J not necessarily for the S. The Eigenfunctions of S are known as spinners.

Therefore, we have a limitation in the visualization. If this is not sufficient you have the next additional property that the S z itself does not have arbitrary values, but only two possible values for a spin a half system. S z for a spin one half system has only two possible values plus or minus h bar by 2 and the S square for the spin a half system has a value 3 h bar by 4. You see therefore, the square root of it is root three h bar square root 3 by 2 h bar and the magnitude of the angular momentum therefore, is not equal to the component of the angular momentum, but it is greater.

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The magnitude of the angular momentum is greater than the largest value of the component of the angular momentum which means that angular momentum does not point in the direction of the z; is not in the direction of z axis or whatever the component of S z. So, this defines an axis the angular momentum does not point in the axis. So, the representation is done, if this is the z axis and if you write to the magnitude of the angular momentum as S, which is the length of this vector this is root 3 by 2 h bar and the maximum value of the component of the angular momentum this one is h bar by 2.

Therefore, you see that there is an angle theta such that cos theta is 1 by root 3 or 3 cos square theta minus 1 is equal to 0. The other possibility minus h bar by 2 corresponds to an angular momentum vector orientation of this form, giving you the minus if this is the 0, this is minus h bar by 2. But, even writing the vector this way is not a correct thing because the vector does not point in this direction, but it is anywhere in the plane perpendicular to that, if you take the projection of the this S into the plane then the angular momentum vector pointing in this direction is also half h bar.

Therefore, what you see is that you cannot simultaneously give the S z values as half h bar and then the S axis is either this or S y is that the average. This is going to be later studied as a precessional characteristics of angular momentum in a magnetic field of S in a magnetic field. All of this is to only if S is in a certain chosen field, if the field is not there then the angular momentum can point in any arbitrary direction and in a beam of

silver atoms one would expect that different atoms have the angular momentum pointing in different directions and therefore, when you pass it through a magnetic field which has radians the magnetic field gradient introduces what is known as a torque and the torque results in the deflection of the magnetic moment in various directions.

Therefore, if the magnetic moment points in all the directions the torque will be such that the reflections the deflection happens in all the directions and therefore, you would see a beam with intensities on the entire detector all the entire range of the detector, but you do not see it, what you see here is exactly two beams as was first drawn. So, this was the first indication that angular momentum is quantized with respect to a chosen field and the quantization the angular momentum also means that there are only finite number of components which we will later call as the eigenvalues for the angular momentum operator in that direction and, the finite number is such that for a spin angular momentum you have two components.

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And, for orbital angular momentum you have, for any L if we write for orbital angular momentum we have the L and the L z. L z and the L square such that L z can have the maximum value of 1 h bar, 1 minus 1 h bar which is with these are all the possible values of the z component of the orbital angular momentum or any integer angular momentum with L equal to 0 or 1 or 2 or 3 whatever and then you have up to minus 1 h bar

and minus 1 h bar. So, there are 2 l plus 1 L z values for any and the L square, the magnitude of the L square is l into l plus 1 h bar square.

So, this is the introductory remark on the angular momentum that one it is quantized and two the angular momentum components do not or do not commute among themselves and therefore, they cannot be simultaneously measured and let me close this part and continue the actual mathematics in the next part. The components of the angular momentum L x, L y the commutator is not 0, L x, L z the commutator is not 0 and L y, L z. And, the same thing can be written for S x and S y S x and S z, S y and S z they are not 0, but what is 0?

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What is 0 is the square of the angular momentum S square commutes with all the components the square S y and S square S z all are 0. Let us see these relations in more detail and then evaluate the properties of the spin angular momentum in the next part until then.

Thank you very much.