

**Fundamentals of Spectroscopy**  
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**Lecture 45**  
**Resonance Spectroscopy - Introduction 1**

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Spin Resonance Spectroscopy  
Magnetic Resonance Spectroscopy  
magnetic field

spin  
fundamental property → elementary particle

spin quantum number  
spin angular momentum ( $\vec{S}$ )  
 $|\vec{S}| = \hbar \sqrt{S(S+1)}$  quantized  
spin quantum number

$S = 1/2$   
magnetic moment ( $\vec{\mu}_s$ ) ←  $\vec{S}$

Hello, welcome to the lecture. In today's lecture, we will start a new module on Resonance spectroscopy. So, it can be Spin Resonance spectroscopy or Magnetic Resonance spectroscopy. This Spectroscopy differs from most other kinds of the Spectroscopy. Here, the light matter interaction involves the magnetic field, so, the matter interacts with the magnetic field of light and not the electric field of light. The magnetic field is used to provide the energy level separations probed by the radiation.

So, both the Spectroscopy involves spin. So, spin is a fundamental property of an elementary particle. So it is a fundamental property of any elementary particle. So, for example electron is an elementary particle and electron has spin. So, this spin has no classical analogue. So, the

introduction of spin quantum number, in quantum mechanics could explain many puzzling features. So, the spin is manifested but the presence of an intrinsic angular momentum.

So, in this case, is the spin angular momentum which is represented by  $S$  and the spin angular momentum is a vector. A convenient formalism is that Spin angular momentum arises from the rotation of electrons around its Axis and the magnitude of this spin angular momentum, which is given by modulus of  $S$  is  $h$  cross root over  $s$  times  $s + 1$ . So here, this small  $s$  represents spin quantum number. This means the angular momentum of the spin angular momentum is quantized.

So for an electron the value of the spin quantum number that is  $S$  equal half. So, Electron being a charge particle it has something known as magnetic moment which is denoted by  $\mu_s$  which is vector and this magnetic moment  $\mu_s$  is associated with the spin angular momentum capital  $S$ .

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**Resonance Spectroscopy**

$|\vec{S}| = h \sqrt{s(s+1)}$   
 $s = \frac{1}{2}$   
 $\vec{\mu}_s = \frac{g_s}{2m_e} \vec{S}$  (charge of  $e^-$ , mass of electron)  
 2.002 →  $g_s$  (electron g-factor)  
 quantized →  $\mu_s = g_s \frac{e \hbar}{2 m_e} \sqrt{s(s+1)} = \left( g_s \frac{e \hbar}{2 m_e} \right) \hbar \sqrt{\frac{1}{2} \left( \frac{1}{2} + 1 \right)}$   
 $\frac{g_s e \hbar}{2 m_e} \rightarrow \gamma$  (gyromagnetic ratio)  
 $\frac{e \hbar}{2 m_e} \rightarrow$  quantum of magnetic moment (Bohr magneton  $\beta$ )  
 $g_s \beta = \gamma \hbar$

And the relation between this  $\mu_s$  and this spin angular momentum is given by  $\mu_s = g_s \frac{e \hbar}{2 m_e} S$  when the screen angular momentum social the  $g_s$  is electron g factor and this small  $e$  is the charge of electron and  $m_e$  is the mass of electron so we can write  $\mu_s$  equals to  $g_s$  by  $2 m_e$  and because  $s = h$  cross root over  $s$  times  $s + 1$  so we can write  $h$  cross root over  $s$  times  $s + 1$  and now  $s$  equals to half. So, we can further write this as  $g_s \frac{e \hbar}{2 m_e} \sqrt{\frac{1}{2} \times \frac{1}{2} + 1}$ . So, we can write now that this equals  $h$  cross root over  $\frac{1}{2} \times \frac{1}{2} + 1$ .

And the value of this electron g factor that is g s is 2.002 so we wrote g s e by 2m e so g s e by 2m e this we wrote as gamma and gamma is known as the shadow magnetic ratio. So, we can see that this Mu s is also quantized and the quantity that e h cross divided by 2m e is known as the Quantum of magnetic moment and it is also known as Bohr Magneton which is denoted by beta. So by comparing the two expressions in which we have beta and gamma we can write g s beta = gamma h cross. So before proceeding further, let us study the general properties of angular momentum.

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**Resonance Spectroscopy** Angular momentum ( $J$ )

1.  $J = |J| = h \sqrt{j(j+1)}$   
 $\hookrightarrow$  quantum number
2. space quantization  
 $J_z = J \cos \theta = m_j h$   
 $\hookrightarrow$  quantum number  
 $m_j = \sqrt{j(j+1)} \cos \theta$   
 $m_j = j, (j-1), (j-2), \dots, 0, \dots, -j$  (2j+1) values

So, show the angular momentum is in general denoted by J. So let us study the general properties of angular momentum in quantum mechanics. So, the first property is and we saw this during our discussion on this spin angular momentum just like couple of days back, the angular momentum vector that is the vector J has a magnitude which is given by so, the magnitude of is given by h cross Root over j times j+1 where the small j is a Quantum number which is the angular momentum quantum number.

That means it is a quantum number characterizing angular momentum. So, secondly, there are only certain possible orientations of the vector that is affected j with respect to Z axis. This is known as Space Quantization. So, let us say, if the vector J this is our Z-axis let us say vector J makes an angle theta with the z-axis. So this is our vector J and the magnitude of J equals h cross

root over j times j+1. So, the possible values of theta will be such that the Z component of J, Z component of J which we can denote by this link.

That is the projection of J on the Z axis which we can call J<sub>Z</sub> will also be quantized. So, we can write J<sub>Z</sub> equals J cos theta and because it is quantized it is m<sub>j</sub> h cross. So, this m<sub>j</sub> is the Quantum number. So, we can write that m<sub>j</sub> = Root over j times j+1 quantized. So, we have seen this during a discussion on angular momentum in rotational Spectroscopy. So, from this relation, it follows that that m<sub>j</sub> quantum number can have the following values.

It can have values of like m<sub>j</sub> can be the can take the values of j, j-1, j-2 dot dot dot dot 0 is another value and it will go up to -j. So, in total there can be 2j + 1 value of m<sub>j</sub> particle with angular momentum of j and magnetic moment m<sub>j</sub>.

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**Resonance Spectroscopy**

$\vec{J} = \hat{i}J_x + \hat{j}J_y + \hat{k}J_z$   
 $\vec{B} = \hat{k}B \quad (B_x=0, B_y=0, B_z=B)$

$\vec{\mu}_j = \gamma \vec{J}$   
 $\frac{d\vec{J}}{dt} = \vec{\mu}_j \times \vec{B} = \gamma \vec{J} \times \vec{B} = \gamma (\vec{J} \times \vec{B})$

$\vec{J} \times \vec{B} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ J_x & J_y & J_z \\ 0 & 0 & B \end{vmatrix} = \begin{bmatrix} \hat{i}J_y B - \hat{j}J_x B \\ 0 \\ 0 \end{bmatrix}$

$\frac{dJ_x}{dt} = \gamma [\hat{j}J_y B - \hat{k}J_z B]$   
 $\frac{dJ_y}{dt} = \gamma [\hat{k}J_z B - \hat{i}J_x B]$   
 $\frac{dJ_z}{dt} = 0$

$a \times b = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \hat{i} \begin{vmatrix} a_2 & a_3 \\ b_2 & b_3 \end{vmatrix} - \hat{j} \begin{vmatrix} a_1 & a_3 \\ b_1 & b_3 \end{vmatrix} + \hat{k} \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix}$

So, the particle has angular momentum of J and magnetic moment  $\mu_j$ , so  $\mu_j$  is given by Gama diamagnetic ratio x j. So, when this particle is placed in a magnetic field applied in the Z direction, then, for an orientation of J, so let us say this is my Z direction and the magnetic field is applied in the Z direction. And our J is in this direction. So, then, for an orientation of j which is this export x on the magnet which is given by dJ by dt which is given by  $\mu_j$  cross B and because  $\mu_j$  is given by gamma J, we can write this gamma J cross B or gamma J cross B.

So, the vector  $\mathbf{J}$  written in terms of its Cartesian coordinates. So, we can write, vector  $\mathbf{J}$  written as  $i \hat{J}_x + j \hat{J}_y + k \hat{J}_z$ . So, this  $i, j$  and  $k$ , this  $i, j$  and  $k$  are the 3 unit vectors along  $X, Y$  and  $Z$ . And for the magnetic field because  $\mathbf{B}$  is applied along the  $Z$  Axis we have we can write  $\mathbf{B} = k \hat{B}$ . This is because it is only along the  $Z$  axis So  $B_x = 0, B_y = 0$  and  $B_z = B$ . So now let us look into what do you mean by cross products. Let us say we have two vectors: one is  $\mathbf{a}$  and vector  $\mathbf{a}$  is given by  $i \hat{a}_1 + j \hat{a}_2 + k \hat{a}_3$  and you have another vector that is  $\mathbf{b}$  which is given by  $i \hat{b}_1 + j \hat{b}_2 + k \hat{b}_3$ .

So now if you need to compute, it is a cross  $\mathbf{a} \times \mathbf{b}$ . So that  $\mathbf{a} \times \mathbf{b}$  this  $\mathbf{a} \times \mathbf{b}$  so that we have to write as  $i, j, k$  then  $a_1, a_2, a_3, b_1, b_2, b_3$ . So, this is a cross  $\mathbf{a} \times \mathbf{b}$  will be I have to write  $i$  then,  $a_2 b_3 - a_3 b_2 - j a_1 a_3 b_1 b_3 + k a_1 a_2 b_1 b_2$ . So, now we have to compute  $\mathbf{a} \times \mathbf{b}$ . And this is vector  $\mathbf{J}$  and this is vector  $\mathbf{V}$ . So, if you compute this  $\mathbf{J} \times \mathbf{b}$  what we get is so we can write  $i, j, k$  this is  $j_x j_y j_z$  but for  $\mathbf{b}$  this  $i$  and  $j$  component is 0. We only have  $b$  here. So, this will be equal to what we will get this  $i$  times  $J_y B - J$  times  $J_x B$ .

So, we can write that  $i$  because  $j$  equals  $i J_x + i J_y + i J_z$  so this  $d\mathbf{J}/dt$  we can write as  $i dJ_x/dt + j dJ_y/dt + k dJ_z/dt$  and it will be the same thing that have computed but only multiplied by  $b$ , so we can write this as  $\gamma - j$  times  $\mathbf{J} \times \mathbf{B} + i$  times  $\mathbf{J} \times \mathbf{B}$ .

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Resonance Spectroscopy

$$i \frac{dJ_x}{dt} + j \frac{dJ_y}{dt} + k \frac{dJ_z}{dt} = \gamma [-j J_x B + i J_y B]$$

$$\frac{dJ_x}{dt} = \gamma J_y B$$

$$\frac{dJ_y}{dt} = -\gamma J_x B$$


$$\frac{dJ_z}{dt} = 0 \quad J_z \rightarrow \text{constant}$$

$$J_x \frac{dJ_x}{dt} + J_y \frac{dJ_y}{dt} = \gamma J_x J_y B - \gamma J_x J_y B = 0$$

$$\frac{1}{2} \frac{d(J_x^2)}{dt} + \frac{1}{2} \frac{d(J_y^2)}{dt} = 0$$

$$\frac{d(J_x^2 + J_y^2)}{dt} = 0$$

$$J^2 = J_x^2 + J_y^2 + J_z^2 \rightarrow \text{constant}$$



So we have this expression  $I \frac{dJ_x}{dt} + J \frac{dJ_y}{dt} + K \frac{dJ_z}{dt}$  equals  $\gamma - j J_x B + i J_y B$ . So, if you compare the expression we get  $\frac{dJ_x}{dt} = \gamma J_y B$  and  $\frac{dJ_y}{dt} = -\gamma J_x B$  and also we can see that  $\frac{dJ_z}{dt} = 0$ . So this that is  $\frac{dJ_z}{dt} = 0$ , indicates that  $J_z$  is a constant. That means  $J_z$  is concerned but  $J_x$  and  $J_y$  depends on  $i$ ? So, using these two expressions we can write that  $J_x \frac{dJ_x}{dt} + J_y \frac{dJ_y}{dt}$  so  $\frac{dJ}{dt}$  will be  $\gamma J_x J_y B - \gamma J_x J_y B$  so that will be equal to 0. So, because  $J_x \frac{dJ_x}{dt} + J_y \frac{dJ_y}{dt}$  is 0, we can further write as  $\frac{1}{2} \frac{d}{dt} (J_x^2 + J_y^2)$ .

Because if we have  $x^2$  then take the derivative is  $2x$  now we are divided by half so we can write this term as  $\frac{1}{2} \frac{dJ_x^2}{dt}$  and this as  $+\frac{1}{2} \frac{dJ_y^2}{dt} = 0$ . Or in other words what we get is,  $\frac{d}{dt} (J_x^2 + J_y^2) = 0$ . So this expression  $\frac{d}{dt} (J_x^2 + J_y^2) = 0$  tells us that  $J_x^2 + J_y^2$  is a constant. Hence because we have  $J_z^2$  which is a constant and  $x^2 + y^2$  is also a constant.

So, we can write  $J^2$  which is nothing but  $J_x^2 + J_y^2 + J_z^2$  so this is a constant. That is when in an external magnetic field the  $J^2$  and  $J_z$  are constants of motion but  $J_x$  and  $J_y$  can change with time. So, we will end this lecture here. In the next lecture, we will discuss the consequences of what we have learnt today because of this  $J^2$  and  $J_z$  constant.