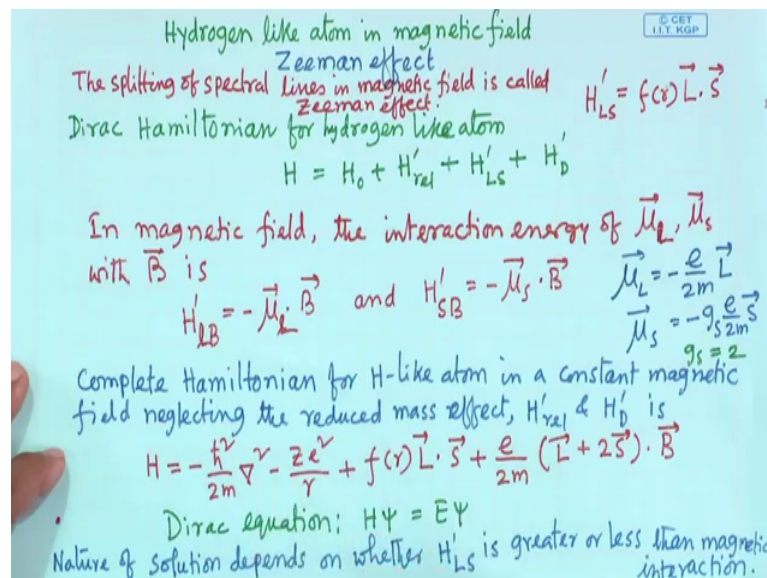


Atomic and Molecular Physics
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Lecture 38
Hydrogen like atom in magnetic field

So, today I will discuss about the Effect of magnetic field on hydrogen like atom.

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So, for that is basically Effect of magnetic field in hydrogen like atom. So, that is basically Zeeman Effect. So, already we have seen earlier, but now what I want to do that using the quantum mechanics, how we can get the how we can explain this Zeeman Effect, ok? So, for so Zeeman Effect in nothing but the splitting of spectral lines in magnetic field and we know this without magic field; what is the Hamiltonian, basically Dirac Hamiltonian for hydrogen like atom so that is, H equal to H 0 that is non-relativistic and spin less Hamiltonian H 0; then relativistic term H relativistic dash. Then LS coupling term plus Darwin terms that we have seen earlier for hydrogen like atom, what is the Dirac Hamiltonian.

So, these LS coupling that H LS that is the function of r L dot S ok. this specially this I have written because this has importance for Zeeman Effect. And when we apply magnetic field then additional interaction energy this called magnetic interaction energy. That is that is basically mu dot B. So, 2 kind of magnetic moment is there for electron in

hydrogen atom, one is this μ_L angular magnetic moment. So, this energy corresponding energy will be $-\mu_L \cdot B$, similarly for spin magnetic moment that will be $-\mu_S \cdot B$. So, this 2 term due to magnetic interaction so these 2 term in Hamiltonian it will be included. So, total Hamiltonian for hydrogen like atom in a constant magnetic field; will be this H_0 this is H_0 plus this LS coupling term it kept it; and then plus this $\frac{e}{2m}$ you know this μ_L equal to $-\frac{e}{2m} L$ and μ_S equal to $-\frac{g}{2} \frac{e}{m} S$ ok. $g = 2$. So, basically this Hamiltonian term that is if I write H_B due to magnetic field H_B that will be $\frac{e}{2m} L + 2 S \cdot B$ because $g = 2$. So, $2 S \cdot B$ so that will be the Hamiltonian term for the magnetic interaction.

Now, here I have excluded the relativistic term and the Darwin term because these terms are small compared to the magnetic interaction term ok. So, that is why in this case we have we have neglected because this magnetic field is it is such that it is not very weak field; it is such that this term this energy term or term in Hamiltonian magnetic interaction term. It is tenth is quite high compare to this relativistic term and Darwin term. So, so that is why we have neglected this term, but when this term magnetic interaction term will be weak, small or it is comparable to $H_{relativistic}$ and H_{Darwin} term then one has to consider this. So, here I assume that this field is not very small. So, this term is appreciable ok. And it is higher than this relativistic and Darwin term ok. So, that is why I have written complete Hamiltonian for this hydrogen like atom in a constant magnetic field. So, this is the H_0 basically this is the LS coupling term and this is the magnetic field interaction term.

So now you have Hamiltonian for your system means hydrogen like atom in a magnetic field; constant magnetic field; so one has to solve basically Dirac equation. So, Dirac equation will be $H \psi = E \psi$ right. So, nature of solution depends on this H_{LS} term. So, we can put condition that whether H_{LS} term is greater or less than magnetic field interaction term ok.

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Case I. Strong field ($B > Z^4$ Tesla): Normal Zeeman effect

H'_{LS} is negligible

$$H = H_0 + H'_B = H_0 + \frac{e}{2m} (\vec{L} + 2\vec{S}) \cdot \vec{B}$$

$\vec{B} \parallel \hat{z}$ $H = H_0 + \frac{eB}{2m} (L_z + 2S_z)$

Since spin-orbit interaction is negligible, so $\Psi_{nlm_l m_s}$ can be taken as an eigen wavefunction

$$H_0 \Psi_{nlm_l m_s} = E_n \Psi_{nlm_l m_s}$$

$$L_z \Psi_{nlm_l m_s} = m_l \hbar \Psi_{nlm_l m_s}$$

$$S_z \Psi_{nlm_l m_s} = m_s \hbar \Psi_{nlm_l m_s}$$

$$H \Psi_{nlm_l m_s} = E \Psi_{nlm_l m_s}$$

$$E_n + \frac{eB}{2m} (m_l + 2m_s) \hbar = E$$

$$E = E_n + \mu_B B (m_l + 2m_s)$$

$$\Delta E = (E_{n'} - E_n) + \mu_B B [(m_{l'} - m_l) + 2(m_{s'} - m_s)]$$

where $\Delta m_l = 0, +1, -1$ $\Delta m_s = 0$

As per Selection rule $= \pm 1, 0$

Now, let us consider the case; however, this magnetic field is very strong where this magnetic field is very strong ok. So; that means, strong field, how strong it is? Now generally we tell this B should be greater than Z to the power 4 Tesla. So, if B magnetic field is very strong then we basically see the Zeeman Effect that is called Normal Zeeman Effect. So, this H B dash term; means magnetic interaction term that is now that is very very strong. So, for so compare to this H B term this LS term is very, very small so one can neglect this one, in case of very strong field. So, LS term also one can neglect ok. So, ultimate Hamiltonian will be H 0 plus H B dash.

So, H 0 is have as I told that this is the basically Schrodinger Hamiltonian for it is the non-relativistic and spinless Hamiltonian. So, so if you consider that magnetic field is applied along Z direction. So, magnetic field is parallel to Z directions; then we can take basically Z component of L and S. So, we have written e B by 2 m, B is along the Z direction and then L dot B means we have taken component along the Z direction. So, L Z and then plus 2 S Z, so under the circumstance under the condition, now ultimate Hamiltonian for hydrogen like atom in a very strong field so this the Hamiltonian.

So, this to get the solution for this Hamiltonian; so, we will use really will use perturbation in case of perturbation generally; we have to consider unperturbed term and then the correction term perturbed term ok. So, here one can consider H 0 is unperturbed term and this interaction term can be perturbed term ok. So, already we know the solution of this H 0. So, H 0 for that is if we apply on this wave function. So, energy will be E_n where E_n , you know this minus $\mu_B Z^2 e^2$ to the power 4 divide by $n^2 n$

square h cross square ok. So, for H_0 we know the energy also we know the wave function ok. So, that already we have solved and this is known to us.

Now, this wave function, now will be used for calculating this correction term perturbed term ok. So, how to calculate that is already know. So, if you see that this in this term whatever if it commutes this operator it commutes with the with the H_0 then this $\psi_{n l m}$ will be simultaneous wave function and we will get the Eigen value for this operator L_z and S_z . And it is true that L_z and S_z is commutes with the H_0 . So, this $\psi_{n l m}$, this basically wave function of L_z and S_z also. So, if we apply L_z on this wave function. So, you will get the Eigen value that is $m_l h$ cross and for S_z it will $m_s h$ cross ok. So, if you basically apply this Hamiltonian on this wave function. So, that equal to so that equal to basically will get the energy value E ; and that energy value E will be E_n plus $e B$ by $2 m_l$ plus $2 m_s$ h cross.

So now, final energy level whatever initially it was n due to magnetic field. Now energy level so there so energy level will change ok. So, how much it will change that will depend on this term; basically, in this term $m_l m_s$ is there. So, value of m_l and m_s will control the change of energy level due to magnetic field ok. So, so for now for this spectral lines is basically the transaction between 2 energy levels right? So, energy of the spectral lines will be ΔE , ΔE equal to say $E_{n'} - E_n$ plus $\mu_B B m_l - m_s$ ok.

So now, if we apply selection rule so you know this selection rule Δm_s equal to 0 and Δm_l equal to plus minus 1 and 0. So, Δm_s so transition only possible when Δm_s equal to 0. So, we can now this term will not contribute $m_s - m_s$ ok. So only transition possible when Δm_s equal to 0 ok. So, this term is basically we can put 0. So, ultimately our term will be ΔE equal to this $E_{n'} - E_n$ plus $\mu_B B \Delta m_l$, where Δm_l equal to 0 plus 1 minus 1.

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In terms of ~~Lorentz~~ Larmor frequency

$$h\nu_L = \frac{e\hbar B}{2m} \neq \frac{e\hbar}{2m} \frac{1}{\hbar} \cdot B \rightarrow \mu_B B$$

$$\nu_L = \frac{e\hbar B}{2m\hbar}$$

$$\Delta E = (E_{n'} - E_n) + \mu_B B \Delta m_l$$

ΔE corresponds to the energy of spectral lines. So frequency

$$\nu (\Delta E = h\nu) = \nu_0 + \nu_L \Delta m_l$$

So spectral lines $n \rightarrow n'$ split into three components

- one is original line ($\Delta m_l = 0$) called π -line.
- Two splitted lines ($\Delta m_l = \pm 1$) called σ -lines

Three lines are said to form Lorentz triplet.

This splitting is called Normal Zeeman effect.

Apart from the case of very strong field, Lorentz triplet can be observed in many electron systems for which the total L or total S is zero. That means, the L-S coupling is vanished.

As for example, Ne, Hg shows normal Zeeman effect.

So, so in terms of frequency, larmor frequency because when you apply magnetic field, when we apply magnetic field; now this your L and S it basically it will precession around this it will precess around the magnetic field ok.

So, this precess and frequency of this precession (Refer time: 14:40) is called Larmor frequency ok. If Larmor frequency if it is $\mu_B B$. So, energy will be $h\nu_L$. So, this $h\nu_L$ equal to $e\hbar B / 2m$. So, this yes, yes, so this is coming from as I as if we have seen earlier. So, this is the Larmor frequency and corresponding energy, so ν_L will be equal to $e\hbar B / 2m\hbar$ ok. So, this h we have taken down. So, this in terms of frequency of the spectral lines one can tell one can tell yes. So, so basically yes, yes. So, that ΔE equal to $h\nu$. So, in our case ΔE equal to this. So, this is the before applying magnetic field so original, original spectral lines one can see tell. So, so that we can write as a original frequency ν_0 plus $\nu_L \Delta m_l$.

So, this $\mu_B B$, $\mu_B B$ is nothing but $e\hbar B / 2m$ ok. So, so this so this $\mu_B B$ and then B is there this nothing but ν_L so $h\nu_L$ ok. So, I think this $h\nu_L$ so that h will go when will express in terms of energy, and that is why we have written here $\mu_B B$. So, this so this is giving in terms of frequency that ν_0 plus $\nu_L \Delta m_l$. So, this in term of frequency or in terms of energy one can one can tell about the about the spectral lines in presence of magnetic field so; obviously, you can see that Δm_l is 0 plus 1 minus 1.

So, when it is 0 so; that means, this the original line ν_0 before applying magnetic field whatever the spectral line. So, that is that will be there. Now plus minus 1 this one then ν_0 plus minus ν_L . So; that means, another 2 lines will get which will have higher frequency by ν_L and lower frequency by ν_L ok. So, basically we will get we will get 3 lines originally it was one line having frequency ν_0 . Now without applying magnetic field, so after applying magnetic field we will get basically this one line will be split into 3 lines and out of this 3 lines one is original line and other is 2 more lines.

So, so this condition basically for $\Delta m = 0$. So, what about this line will get. So, that is called the pi lines and for $\Delta m = \pm 1$, so that line is called sigma lines. So, in terms of basically polarization is pi and sigma. So, here we can see this any line, basically it will be split into 3 lines in strong magnetic field; and that is why these 3 lines basically is it is tell the Lorentz triplet. So, this type of spitting is called Normal Zeeman Effect. Now question is to see the Normal Zeeman Effect. So, magnetic field we has to be very strong how strong it is B has to be greater than Z to the power 4. Now in case of hydrogen atom so Z is 1 right. So, in case of hydrogen atom Z is one so; that means, minimum you need 1 Tesla field Z to the power 4 means one. So, you need one Tesla field ok.

So now in case of helium Z is 2; that means, you need Z^2 to the power 4 means 16 Tesla; for next one for lithium 3 means 81 not 27, 64 Tesla. So, so for so these are very high magnetic field and it is impossible to get this very high field in laboratory, because generally from electro magnet we get field around maximum field we get around 2 to 3 Tesla. So, if you want to get more than 3 Tesla in lab. So, we use that is superconducting magnet. And superconducting magnet also it has it generally we get field less than less than 50 Tesla ok. More than 50 Tesla I think it is I do not know, generally it is 30 to 50 Tesla maximum magnetic field we can get from super conductor superconducting magnet. So, so for so; that means, that to see the Normal Zeeman Effect in laboratory, it is it is practically impossible for atoms of higher atomic number, even it is it is very difficult to see for lithium atom Z equal to 3. So, for helium atom also it is it is also difficult because you need 16 Tesla.

So, only for hydrogen atom one can see; still you need more than one Tesla magnetic field one Tesla field also quite high so, but if you so if you see in laboratory we see the we demonstrate the Normal Zeeman Effect. using the normal magnetic field less than

one Tesla magnetic field. And for that generally we use mercury neon ok. So, so Z is very high; so, how we see the see the Normal Zeeman Effect.

So, in this case Normal Zeeman Effect you see because here we have to we have to so, yeah we remember that; when we consider this Hamiltonian, then I told this in very high magnetic field this H_B dash term magnetic interaction term is very, very high compared to the LS coupling term H_{LS} dash so; that means, $L S H L S$ that term is very, very small so is negligible compared to H_B term. So, it is so we have not considered the LS coupling; that means, LS coupling if LS coupling is vanished in a in a atom so; that means, LS coupling that term is 0 or very, very small; then only one can see the Normal Zeeman Effect and in that case field has to be this that H_B term has to be higher than the H_{LS} term ok.

So now if H_{LS} term is itself is 0 is vanished; means if LS coupling is not there then that we will show the Normal Zeeman Effect ok. So, that is the ultimate consideration for Normal Zeeman Effect. And if ah] so if I find some atom, where this total L or lot total S is 0 one of them are both are 0 ok. So, in that case that so LS coupling will not be there. So, that atom will show the Normal Zeeman Effect; and that is why this in case of neon, in case of mercury here I have written, in case of neon in case of mercury, yes generally we used in lab to demonstrate the Normal Zeeman Effect for this neon mercury you can check that there L or S or both are 0 ok. So, that is why this atom shows the Normal Zeeman Effect so basically next I can show you that yes.

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Case II. Intermediate field: Paschen-Back effect

H'_{LS} is appreciable, but small compared to the magnetic field interaction term $\frac{eB}{2m} (L_z + 2S_z)$

$$H = H_0 + H'_B + H'_{LS}$$

unperturbed term perturbed term

Normal Zeeman effect term: $E = E_n + (m_l + 2m_s)\mu_B B$
 $\Psi = \Psi_{n l m_l m_s}$

Dirac Solution: $\langle H'_{LS} \rangle = -E_n \frac{Z^2 \alpha^2}{2n l (l + \frac{1}{2})(l + 1)}$
 valid for $l \neq 0$
 $\times \quad l = l + \frac{1}{2}$
 $\quad \quad -l - 1 \quad j = l - \frac{1}{2}$

additional term: $E = E_n + (m_l + 2m_s)\mu_B B + \lambda_{nl} m_l m_s$
 $\Psi = \Psi_{n l m_l m_s}$
 added with normal Zeeman effect

So, next we can choose the intermediate field, it is not very strong it is not very weak, so, then what will happen? So, then we see whatever we see this Effect of magnetic field again this is Zeeman Effect is not called Zeeman Effect, it is a discovered by Paschen back, so it is called Paschen back Effect ok.

So, in this case H is the magnetic field is intermediate field and H LS dash is appreciable, but it is still small compared to this magnetic interaction term; that means, LS coupling term I cannot neglect, but it is small compared to this magnetic interaction term. So, this field is intermediate field and it is not very strong field it is not very weak field. So, it is a intermediate field and for that this interaction term is higher, but it is it is it is higher than this LS coupling term. So, so, but LS coupling term that we cannot neglect, because it is close to that this magnetic interaction term ok. If it is the condition then our Hamiltonian will be H equal to H 0 plus H B magnetic field interactions H B dash plus H LS term ok.

Now, here 3 terms are there, so again during perturbation we have to solve it. So, during perturbation we have to find we have to choose unperturbed term and then perturbed term. So, this is the unperturbed term we can take this one (Refer Time: 26:11) unperturbed term we take if we choosing such a way that the solution of this unperturbed term is known. And that solution that wave function and it is energy will be used for calculating the perturbed term ok. So, here unperturbed term, we have taken H 0 plus H B dash because already for Normal Zeeman Effect this solution of this one is known to us and wave function energy is known to us. So, what was the energy for that? So, it was

E equal to E_n plus m_L plus $2m_S$ then $\mu_B B$ and wave function was ψ equal to $\psi_{n l m l m S}$ ok. So, an unperturbed term this is perturbed term H_{LS} . So, that from Dirac Hamiltonian for Dirac and that using that Hamiltonian that from Dirac solution, this we know this term if we calculate this perturbed term. So, this it is we have seen from Dirac solution we have seen from Dirac.

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$H = H_0 + H_1 + H_2 + H_3 \quad H \Psi_{n j m_j} = E_{n j} \Psi_{n j m_j}$
 $E_{n j} = E_n + \Delta E_1 + \Delta E_2 + \Delta E_3$
 $= E_n \left[1 + \frac{Z^2 \alpha^2}{n^2} \left(\frac{n}{j + 1/2} - \frac{3}{4} \right) \right]$
 where $E_n = -\frac{m c^2 Z^2}{2 n^2 \hbar^2}$
 $\Delta E_1 =$ relativistic correction
 $\Delta E_2 =$ spin-orbit interaction
 $\Delta E_3 =$ Darwin correction
 $\Delta E_1 = E_n \frac{Z^2 \alpha^2}{n^2} \left(\frac{n}{l + 1/2} - \frac{3}{4} \right)$
 $\Delta E_2 = -E_n \frac{Z^2 \alpha^2}{2 n l (l + 1/2) (l + 1)}$
 (for $l > 0$) $\times +l$ for $j = l + 1/2$
 (for $l = 0$) $-l - 1$ for $j = l - 1/2$
 $\Delta E_3 = -E_n \frac{Z^2 \alpha^2}{n}$ for $l = 0$
 $\Delta E_3 = 0$ for $l \neq 0$

Solution that is basically from Dirac equation Hamiltonian you know then we found this E_n and this other 3 correction energy and total energy was this. So, other correction energy this one is ΔE_1 was for relativistic, ΔE_2 power for the LS coupling term and ΔE_3 it was for the Darwin term. So, what is the ΔE_2 so ΔE_2 is basically minus $E_n Z^2 \alpha^2$ by $2 n l l + 1/2 + 1$ into plus l for j equal to $l + 1/2$ and are multiplied into minus $l - 1$ for j equal to $l - 1/2$ ok.

So, so basically ΔE_3 term ΔE_2 term this is the solution this is the solution so that we can use here ok. So, and this is valid for only valid for L equal to l is not equal to 0 ok. L equal to 0 this, this, this, this vanish. So, these terms so this solution is this type of solution ah. So, considering this solution so, but this is this solution was not was for this for hydrogen like atom without magnetic field ok.

So now this we have included here so here this term, we have to consider as a unperturbed term and it is wave function we have to consider for to calculate this perturbed term. So, in this case this wave function is $\psi_{n l m l m S}$. So, considering this one so

this energy this energy for un perturbed term plus; from here you can you can just here this we can take as a $\lambda n L$ because it depends on n and l . So, we have written $\lambda n l$ plus into $m l m S$ term ok.

So, this will term when this is because as I mentioned that this is for this is the Hamiltonian and this is, so here we have considered we have considering for in presence of magnetic field that is applied along the along the Z direction ok. So, l is there now if you consider the direction along the Z . So, basically that quantum number along the z . So, that that in case of l so that gives $n l$. In case of S that gives $m S$ ok. So, from here, basically directly we are not in the. So, this we are here from this Dirac Hamiltonian their whatever the solution we have got, now that solution that type of considering the similarity this solution here also solve solution will be similar, but not exactly same because here magnetic field and we have to consider since it is along the Z direction we have to considered the Z component so, that Z component quantized along the fixed directions in case of L and S .

So, that is that in terms of $m l$ and $m S$ we have to write. So, that is why this term will be basically some constant term and this $m l m s$. So, this $\lambda n l$ is nothing but this term ok. So, except this $l l$ minus $1 I$ think, this term we have defined $\lambda n l$ this considering this similarity it will be this term ok. So, from here you can tell $\lambda n l$ it depends on n value and l value. So, in depend it is independent is not independent of l . So, earlier here whatever energy will got; so, that there I will discuss.

So, that basically gives 3 spitting, 3 lines one line gives 3 lines here due to this terms. So, here some what is called symmetry was there. So, that is why we get all the type 3 lines although 6 transition, 9 transition is possible 9 lines would be possible, but due to the symmetrical splitting. So, these 6 lines or 9 lines is basically energy of some lines are same; so that is why this lines are not different line same line so, but when this degeneracy will removed ah. So, then we could get more number of lines and that is what happening here in this case, the degeneracy will be removed due to this term and we will get more number of splitting. So, I will stop here I will discuss in next class.

Thank you.