

“Atoms” summary

$$\hat{H} = \hat{T} + \hat{V} \quad \hat{T} = -\frac{\hbar^2}{2m} \nabla^2 \quad \hat{p} = -i\hbar \nabla \quad \hat{\ell} = \hat{r} \times \hat{p}$$

Schrödinger Equation:

$$\hat{H}\mathbf{y} = E\mathbf{y} \quad \Leftrightarrow \quad \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \mathbf{y} = E\mathbf{y}$$

“central potential”

Rearranging:  $\nabla^2 \mathbf{y} - \frac{2m}{\hbar^2} (E - V) \mathbf{y} = 0$

Potential due to orbital angular momentum:

$$V_\ell = \frac{\ell(\ell+1)\hbar^2}{2mr^2}$$

Thus, the effective potential is a combination of that due to orb.ang.mom and the coulomb potential:

$$V_{eff} = V_\ell - \frac{e^2}{4\pi\epsilon_0 r}$$

The minimum potential occurs at:

$$\frac{d}{dr} V_{eff} = 0$$

Hence, the corresponding radius is:

$$r_{\min} = \ell(\ell+1)a_0$$

Where:

$$a_0 \equiv \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad \text{“Bohr Radius”}$$

Now:

$$V_{eff}(r_{\min}) = -\frac{E_R}{\ell(\ell+1)}$$

$$n_r = n - \ell - 1$$

number of radial nodes

$$R_{n,\ell} = N L_{n,\ell}(r) r^\ell e^{-r/na_0}$$

radial wavefunction form

“Atoms” summary

$$P(r)dr = r^2 R^2(r)dr$$

$$E_n = -\frac{E_R}{n^2} \quad n = 1, 2, 3, \dots$$

$$\ell = 0, 1, 2, \dots, n-1$$

$$|m| \leq \ell$$

All quantum states with the same value of  $n$  have the same energy. Thus degeneracy  
Notation:

$\ell =$	0	1	2	3	...
	s	p	d	f	...

*Franck-Hertz experiment:*

Electrons are accelerated by a voltage towards a positive grid. On the other side of the grid is a small negative plate.

The values of accelerating voltage where current drops gives the energy needed to put an electron in an excited state.

The current drop is due to inelastic scattering of electrons in the mercury vapour surrounding the experiment.

The energy difference between adjacent peaks gives energy.

$\ell(\ell + 1)\hbar^2$  are eigenvalues of orbital angular momentum

$|\ell| = \hbar\sqrt{\ell(\ell + 1)}$  is the magnitude of orb.ang.mom

Magnetic dipole moment:

$$\underline{m} = IA = -\frac{ev}{2\pi r} \cdot \pi r^2 = -\frac{evr}{2}$$

The modulus of angular momentum is given by  $|\ell| = rmv \Rightarrow v = \frac{|\ell|}{rm}$

Hence:

$$\underline{m} = -\frac{er}{2} \frac{|\ell|}{rm} = -\frac{e|\ell|}{2m}$$

Thus:

$$\underline{m} = -\frac{e}{2m} \underline{\ell} \quad \text{“dipole moment”}$$

Now, the potential of a magnetic field:

$$V_{mag} = -\underline{m} \cdot \underline{B} = -g_\ell \frac{e}{2m} \underline{\ell} \cdot \underline{B}$$

“Atoms” summary

Define the “magneton” as:

$$\mathbf{m}_M \equiv \frac{e\hbar}{2m} \quad \text{for “bohr magneton” use mass of electron}$$

Thus:

$$\underline{\mathbf{m}} = g_\ell \frac{\mathbf{m}_M \underline{\ell}}{\hbar}$$

The “precession frequency” is:

$$\omega_L = \frac{\mathbf{m}\mathbf{B}}{\hbar} = g_\ell \frac{\mathbf{m}_B \mathbf{B}}{\hbar}$$

*Stern-Gerlach experiment:*

“quantisation of magnetic moments of electrons due to spin”

- a beam of electrons is passed through an inhomogeneous magnetic field. The electrons are deflected by the mag.field according to their spin. Two spots are seen on a screen. A discrete pattern. i.e. not continuous.

- the dipoles are deflected by inhomogeneous mag.field

$$F_z = -\frac{\partial}{\partial z} V_{mag} = \mathbf{m}_z \frac{\partial B_z}{\partial z}$$

Thus, if two spots seen:  $s = \frac{1}{2}$

$$|\underline{s}|^2 = \hbar^2 s(s+1)$$

$$[\hat{s}^2, \hat{s}_z] = 0$$

$$\underline{\mathbf{m}}_s = -g_s \frac{e}{2m} \underline{s} = -g_s \mathbf{m}_B \frac{\underline{s}}{\hbar}$$

Total angular momentum:

$$\underline{j} = \underline{\ell} + \underline{s} \quad |\underline{j}| = \hbar \sqrt{j(j+1)} \quad j \leq |\ell \pm s|$$

$$j = \begin{cases} \ell + s \\ \ell + s - 1 \\ \dots \\ \ell - s \end{cases}$$

Note:  $j^2 = (\underline{\ell} + \underline{s})(\underline{\ell} + \underline{s}) = \ell^2 + s^2 + 2\underline{\ell}\underline{s}$

And  $\ell^2 = \hbar^2 \ell(\ell+1) \dots$

Now, states with same  $j$  have the same energy... thus degeneracy.

“Atoms” summary

Notation:

$$\begin{array}{lll} n^{2s+1} \ell_j & n^{2S+1} L_J & \\ \text{Single} & \text{multi} & \dots \text{ electron atoms} \end{array}$$

*Fine structure* ... spin-orbit ang.mom coupling of electron

*Hyperfine structure* ... coupling of spin of proton/nucleus & ang.mom of electrons  
 - HFS gives 21cm line in hydrogen

*Lamb Shift* – QED – lifts  $j$ -degeneracy – virtual particles

Transitions between energy levels governed by absorption/emission of photons.

Photons: spin  $1\hbar$

*Zeeman Effect*

Applying external magnetic field splits  $m_j$  's – because of precession

frequency of electrons:  $\omega_L = \frac{g_\ell \mathbf{m}_B B}{\hbar}$

If spin = 0 → ordinary Zeeman Effect

$$g_\ell = 1 \Rightarrow \omega_L = \frac{\mathbf{m}_B B}{\hbar}$$

$\omega = \omega_0 \pm \omega_L$  get three lines: **s p s**

Only 3 lines, as  $|\Delta m_j| \leq 1 \dots \Delta m_j = -1, 0, 1$

Now, when viewed in  $z$ -direction,  $\Delta m_j = 0$  line does not exist.

Hence: photons:  $\Delta m_j = \pm 1$  massless

A better derivation is:

$$V_B = -\underline{\mathbf{m}}_j \cdot \underline{\mathbf{B}} = g_j \mathbf{m}_B B_z m_j$$

$$\therefore V_B = \Delta E = \mathbf{m}_B B_z \quad \begin{array}{l} m_j = 1 \\ g_j = 1 \end{array}$$

$$E = \hbar \omega \Rightarrow \Delta \omega = \frac{\Delta E}{\hbar} = \frac{\mathbf{m}_B B_z}{\hbar} = \frac{e B_z}{2m}$$

$$\Delta \omega = \frac{e B_z}{2m} \quad \text{“constant splitting in energy levels”}$$

*Anomalous Zeeman effect:*

Spin non-zero. Thus  $g_j \neq 1$

$$g_j = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \quad \Delta E = g_j \mathbf{m}_B B_z$$

*Helium:*

Parahelium – singlet -  $\uparrow\downarrow$   
 Orthohelium – triplet -  $\uparrow\uparrow$  no ground state due to Pauli

“Atoms” summary

Electrons “prefer” to be parallel... thus, triplet has lower energy than singlet.

*X-rays:*

Produced by firing electrons from a hot plate, onto a sheet. The incident electrons excite the electrons on sheet, which then emit a X-ray photon whilst falling back down.

	K	L	M	N
n =	1	2	3	4

$K_a$  ... from n = 2 into n = 1     $L_a$  ... from n = 3 into n = 2

$K_b$  ... from n = 3 into n = 1     $L_b$  ... from n = 4 into n = 2

$K_g$  ... from n = 4 into n = 1    ...

X-rays produced in two ways:

“Characteristic radiation” - discrete

$$E = E_R (Z - s)^2 \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad s \text{ some “shielding factor”}$$

“Bremsstrahlung” - continuous

- comes from deceleration of incident electrons in atomic field

*Moseley’s Law:*

Notice that  $E \propto Z^2 \Rightarrow Z \propto \sqrt{E} \propto \sqrt{n}$   
 $s \propto \sqrt{n}$