Quantum Mechanics (P304H)
Part 2 – Lecture 16

Dr. Dan Protopopescu, Room 524
dan.protopopescu@glasgow.ac.uk

Angular Momentum Recap

- General QM properties of angular momenta follow purely from commutation relations between the associated operators
- Starting from the classical definition of $\underline{L}$, we have constructed our operator $\hat{L}$
- We've constructed various observables, we have found that $\left[\hat{L}_z,\hat{L}^2\right]=0$ and have chosen $\hat{L}^2$ and $\hat{L}_z$ for our set of compatible observables
- In polar coordinates

$$\hat{L}^2=-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) \quad (1)$$

$$\hat{L}_z=-i\hbar\frac{\partial}{\partial\varphi} \quad (2)$$

- We were looking for the eigenfunctions and eigenvalues of these operators

$$\hat{L}^2Y_{lm}(\theta,\varphi)=l(l+1)\hbar^2Y_{lm}(\theta,\varphi) \quad (3)$$

$$\hat{L}_zY_{lm}(\theta,\varphi)=m\hbar Y_{lm}(\theta,\varphi) \quad (4)$$

where by $Y_{lm}(\theta,\phi)$ we have denoted the wave function (for reasons we will discover later on).

Angular Momentum Recap

- Without implying any properties for the numbers l and m, we have chosen for convenience to write the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ as

$$\lambda' = l(l+1)\hbar^2$$
$$\lambda = m\hbar$$

- We've performed a separation of variables by writing $Y_{lm}(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$
- With (2), we've solved the eigenvalues equation (4) for $\Phi(\varphi)$ and from boundary conditions we've found out that m must be quantised $m=0,\pm1,\pm2,\ ...$
- Using the substitution $F_{lm}(w) = \Theta_{lm}(\theta)$ with $w = \cos\theta \quad (-1 \le w \le 1)$ we have obtained from (1) and (3) the equation

$$\left(\left(1-w^2\right)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2} \right) F_{lm}(w) = 0$$

- This we have identified as Legendre's equation - the solutions of which are known.

Angular Momentum Recap

- For the special case $m=0$

$$\left(\left(1-w^2\right)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) \right) F_{l0}(w) = 0$$

we had the solution (normalised)

$$F_{l0}(w) = \left(\frac{2l+1}{2}\right)^{1/2} P_l(w) \qquad (5)$$

where by $P_l(w)$ we denote the Legendre polynomial or order l, given by the formula:

$$P_l(w) = \frac{1}{2^l l!}\frac{d^l}{dw^l}\left[(w^2-1)^l\right]$$

- We will continue today with the more general case when $m \neq 0$

8. Angular Momentum (cont.)

- The case when $m \neq 0$:

$$\left(\left(1-w^2\right)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2} \right) F_{lm}(w) = 0 \qquad (6)$$

  – Note that this equation is independent of the sign of m; its solutions depend only on l and $|m|$.

- The solutions of this equation are known to be of the form $F_{lm}(w) = P_l^{|m|}(w)$ or more exactly:

Phase factor *Normalisation* *Associated Legendre polynomial*

$$F_{lm}(w) = (-1)^m \left[\frac{(2l+1)(l-m)!}{2(l+m)!} \right]^{1/2} P_l^m(w), \quad m \geq 0$$

$$F_{lm}(w) = (-1)^m F_{l|m|}(w), \qquad m < 0$$

where $P_l^m(w)$ are called associated Legendre functions.

8. Angular Momentum

- The associated Legendre functions are defined as:

$$P_l^{|m|}(w) = \left(1-w^2\right)^{\frac{|m|}{2}} \frac{d^{|m|}}{dw^{|m|}} P_l(w)$$

where $P_l(w)$ is the Legendre polynomial defined in (5).

- They satisfy the orthogonality relation:

$$\int_{-1}^{1} P_l^{|m|}(w) P_{l'}^{|m|}(w)\, dw = \frac{2}{2l+1} \frac{(l+|m|)!}{(l-|m|)!} \delta_{ll'}$$

- There are $2l+1$ allowed values for m:

$$|m| \leq l \quad \Rightarrow \quad -l, -l+1, \ldots, 0, \ldots, l-1, l$$

Proof: $$\left\langle \hat{L}^2 \right\rangle = \left\langle \hat{L}_x^2 \right\rangle + \left\langle \hat{L}_y^2 \right\rangle + \left\langle \hat{L}_z^2 \right\rangle \geq \left\langle \hat{L}_z^2 \right\rangle \quad \Rightarrow \quad l(l+1) \geq m^2$$

and therefore:

$$\begin{aligned} l &= 0 \quad \Rightarrow \quad m = 0 \\ l &= 1 \quad \Rightarrow \quad m = -1, 0, 1 \\ l &= 2 \quad \Rightarrow \quad m = -2, -1, 0, 1, 2 \\ &\vdots \qquad\qquad\quad \vdots \end{aligned}$$

8. Angular Momentum

- The associated Legendre functions also satisfy the recurrence relations:

$$(2l+1)wP_l^m = (l+1-m)P_{l+1}^m + (l+m)P_{l-1}^m$$

$$(2l+1)\sqrt{1-w^2}\,P_l^{m-1} = P_{l+1}^m - P_{l-1}^m$$

- The first few associated Legendre functions are:

$$P_1^1(w) = \left(1-w^2\right)^{1/2}$$

$$P_1^2(w) = 3\left(1-w^2\right)^{1/2} w$$

$$P_2^2(w) = 3\left(1-w^2\right)$$

$$P_3^1(w) = \frac{3}{2}\left(1-w^2\right)^{1/2}\left(5w^2-1\right)$$

$$P_3^2(w) = 15w\left(1-w^2\right)$$

$$P_3^3(w) = 15\left(1-w^2\right)^{3/2}$$

8. Angular Momentum

- Remember that the full solution for the wave function was

$$Y_{lm}(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi) \qquad \text{where} \qquad \Theta(\theta) = F_{lm}(w), \quad w = \cos\theta$$

- Hence, the <u>normalised</u> eigenfunctions $Y_{lm}(\theta,\varphi)$ common to the operators L^2 and L_z are:

$$Y_{lm}(\theta,\varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\varphi}, \qquad m \geq 0$$

$$Y_{lm}(\theta,\varphi) = (-1)^m\, Y_{l|m|}^*(\theta,\varphi), \qquad m < 0$$

- These functions are called spherical harmonics. They are orthonormal:

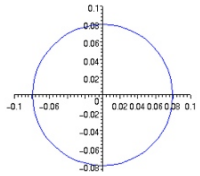
$$\int_{-1}^{1} Y_{l'm'}^*(\theta,\varphi) Y_{lm}(\theta,\varphi)\, d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta\, Y_{l'm'}^*(\theta,\varphi) Y_{lm}(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$$

Prove this

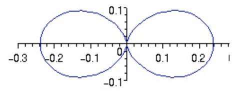
8. Angular Momentum

- The expressions and 3D-graphs of some spherical harmonics:

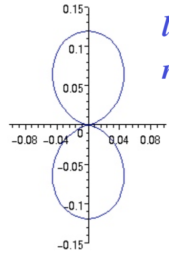
$Y_0^0 = \sqrt{\frac{1}{4\pi}}$	$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos(\theta)$	$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
	$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$	$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$
	$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$	$Y_2^{-1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{-i\phi}$
		$Y_2^2 = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{2i\phi}$
		$Y_2^{-2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{-2i\phi}$



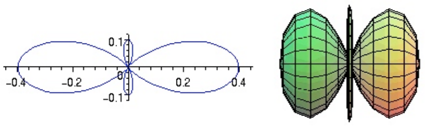
l=0; m=0



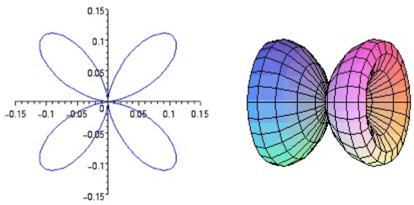
l=1; m=0



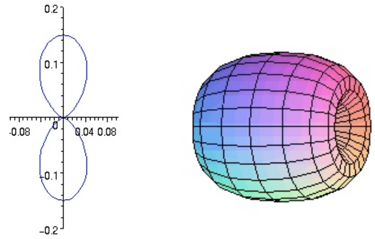
l=1; m=+1



l=2; m=0



l=2; m=+1



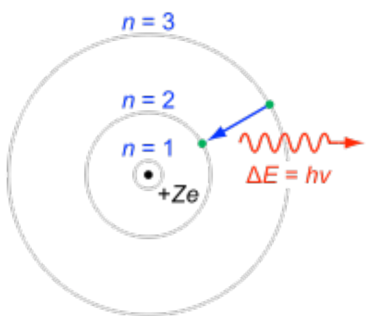
l=2; m=+2

8. Angular Momentum

- We have written the eigenvalues of $\hat{L}^2$ and $\hat{L}_z$ as $l(l+1)\hbar^2$ and $m\hbar$.
- The possible values of the angular momentum are

$$L = \sqrt{l(l+1)}\hbar$$

rather that the values $L = l\hbar$ suggested by the Bohr model.



$$L = n\hbar \qquad \text{with} \qquad n = 0,1,2,\ldots$$

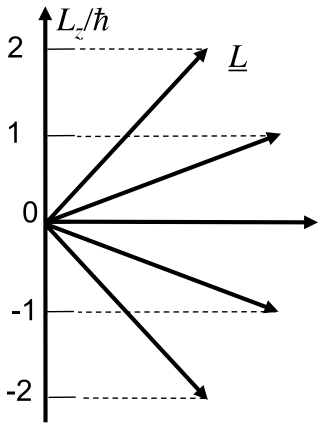
$(n = \textit{principal quantum number})$

For the n^{th} orbit: $m_e v r_n = n\hbar$

$$r_n = \frac{n^2\hbar^2}{Ze^2 k_e m_e} \qquad E_n = -\frac{Ze^2 k_e}{2r_n}$$

8. Angular Momentum

- The vector interpretation of angular momentum:



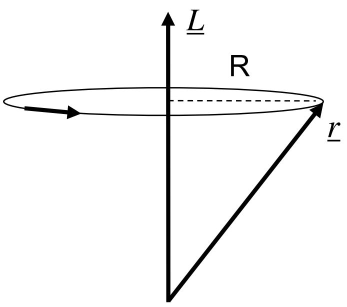
The angular momentum vector $\underline{L}$ can only have a fixed number of orientations with respect to the z axis (the L_z component). For example when $l=2$, there is no state where the angular momentum is parallel to the z axis and the possible values of L_z will be:

$$-2\hbar,\ -\hbar,\ 0,\ \hbar,\ 2\hbar$$

- Angular momentum is measured experimentally by observing the effect of magnetic fields on the motion of particles.

8. Angular Momentum

- Experimental measurement of angular momentum:
  – Classical electron moving with angular velocity ω on an orbit of radius R:



$$L = m_e \omega\, R^2 \Rightarrow \quad \text{Magnetic moment: } \underline{\mu} = -\frac{e}{2m_e}\underline{L}$$

– This in QM corresponds to $\hat{\underline{\mu}} = -\dfrac{e}{2m_e}\hat{\underline{L}}$

– If a component of the magnetic moment is measured along z one measures angular momentum L_z

– Inside a magnetic field, the energy of the interaction is:

$$\Delta\hat{H} = \hat{\underline{\mu}}\cdot\hat{\underline{B}} = \frac{eB}{2m_e}\hat{L}_z$$

– If the system is in an eigenstate of L_z with eigenvalue $m\hbar$, a measurement of the interaction energy will give:

$$\Delta E = \mu_z B = m\mu_B B \quad \text{where} \quad \mu_B = \frac{e\hbar}{2m_e} \quad \text{is the Bohr magneton}$$

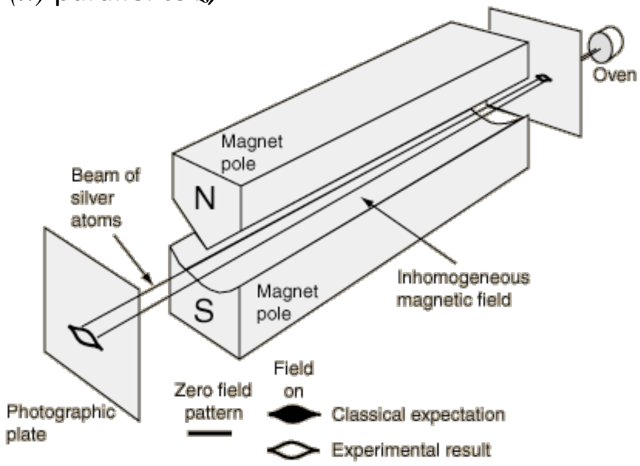
– The dependence on m will therefore introduce a split of the energy levels.

8. Angular Momentum

- The Stern-Gerlach experiment:
  - Experiment performed in 1922 by Otto Stern and Walter Gerlach to test the Bohr–Sommerfeld hypothesis that the direction of the angular momentum of a silver atom is quantised.
  - Neutral atoms do not get deflected in a uniform magnetic field
  - However, if an atom with a magnetic moment μ_z is in an inhomogeneous magnetic field $B(x)$ parallel to z, then a force emerges:

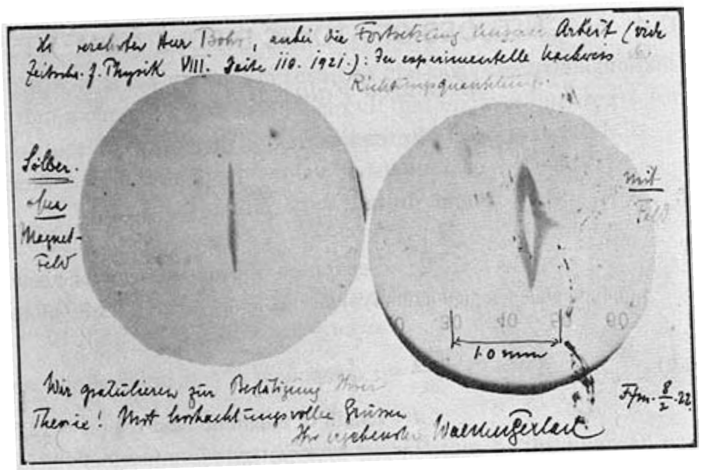
$$F = \mu_z \frac{\partial B(x)}{\partial x}$$

  - Stern and Gerlach used a beam of Ag atoms that was passing through a non-uniform magnetic field before falling onto a collection plate



8. Angular Momentum

- The Stern-Gerlach experiment continued:
  - Classically, if the atom is in the ground state (l=0) then the deflection should be random and the image on the collection plate should be symmetrical about the centre
  - Quantum Mechanics predicts that the beam will split into $2l+1$ parts
  - However, Stern and Gerlach observed two lines
  - This fits with neither the classical case nor with any possible $2l+1$ multiplicity



Collection plates from the original Stern-Gerlach experiment

8. Angular Momentum

- The Stern-Gerlach experiment (cont.):
  - The two lines observed implied that

$$2l+1=2 \quad \Rightarrow \quad l=\frac{1}{2}$$

  - An explanation was given in 1926 by Uhlenbeck and Goudsmit who introduced a quantised intrinsic angular momentum named spin

$$s=\frac{1}{2}, \quad m_s=\pm\frac{1}{2}$$

  - The electron spin must be considered to be a purely quantum mechanical concept, without any classical analogy
  - The electron is not a spinning charged sphere!

Plaque at the Frankfurt FFM institute commemorating the experiment