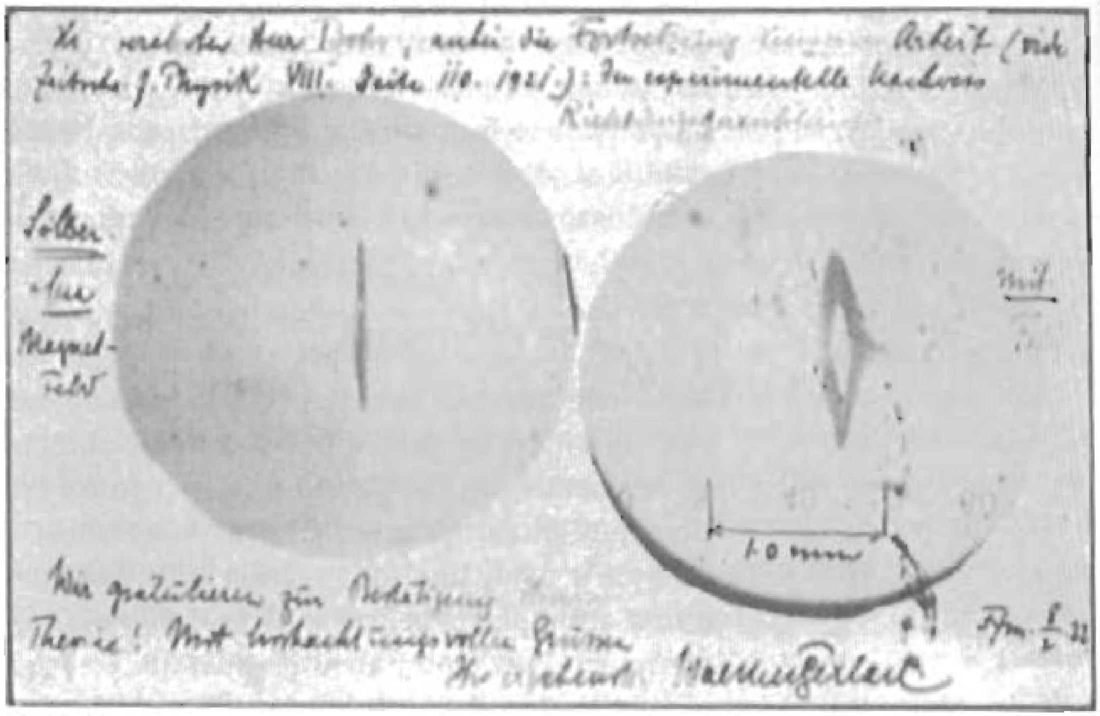
Advanced Quantum Physics

Lecture 3



David Ritchie

www.sp.phy.cam.ac.uk/~dar11/pdf

Section 1 - Review of Quantum Physics

1.1 Postulates of quantum mechanics, operator methods, time dependence.

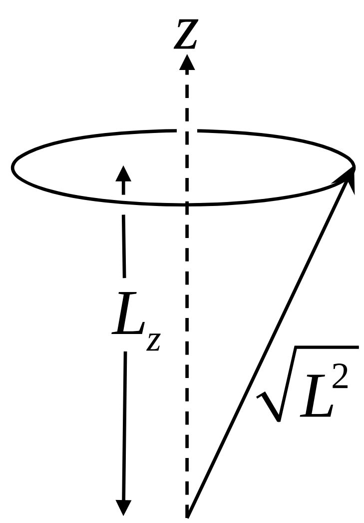
1.2 Solutions of Schrodinger's equation.

1.3 Angular momentum and spin, matrix representation.

1.4 Identical particles.

Angular momentum and spin

- Important properties of Angular momentum can be derived from commutation relations e.g: $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$ etc
- All components of L commute with $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$
- So you can measure $\hat{L}^2$ and one component of L (e.g. $\hat{L}_z$)
- A vector model can represent this situation:



See section 8.2 QP course

Ladder Operators

- Defined by $\hat{L}_+ = \hat{L}_x + i\hat{L}_y, \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y$
- Transform between eigenstates of $\hat{L}_z$.
- Since $\hat{L}_z \left|\psi_m\right\rangle = m\hbar\left|\psi_m\right\rangle$ and $\left[\hat{L}_z, \hat{L}_\pm\right] = \pm\hbar\hat{L}_\pm \Rightarrow \hat{L}_z\hat{L}_\pm = \hat{L}_\pm\hat{L}_z \pm \hbar\hat{L}_\pm$
- then….. $\hat{L}_z\left(\hat{L}_\pm\left|\psi_m\right\rangle\right) = (m\pm 1)\hbar\left(\hat{L}_\pm\left|\psi_m\right\rangle\right)$
- Hence $\hat{L}_\pm\left|\psi_m\right\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\left|\psi_{m\pm 1}\right\rangle$
- Coefficient comes from normalization of wavefunction.
- Values of m are integer spaced, symmetric about zero:
  $-l, -l+1, -l+2 .... l-1, l$ e.g. $-3, -2, -1, 0, 1, 2, 3$
- $2l+1$ possible values of m so l is integer or half integer ≥ 0
- Eigenvalues of $\hat{L}^2$ are $l\left(l+1\right)\hbar^2$.

See section 8.3 QP course

Orbital angular momentum

•Consider explicit form of $\hat{L}^2$ in terms of (θ, ϕ)

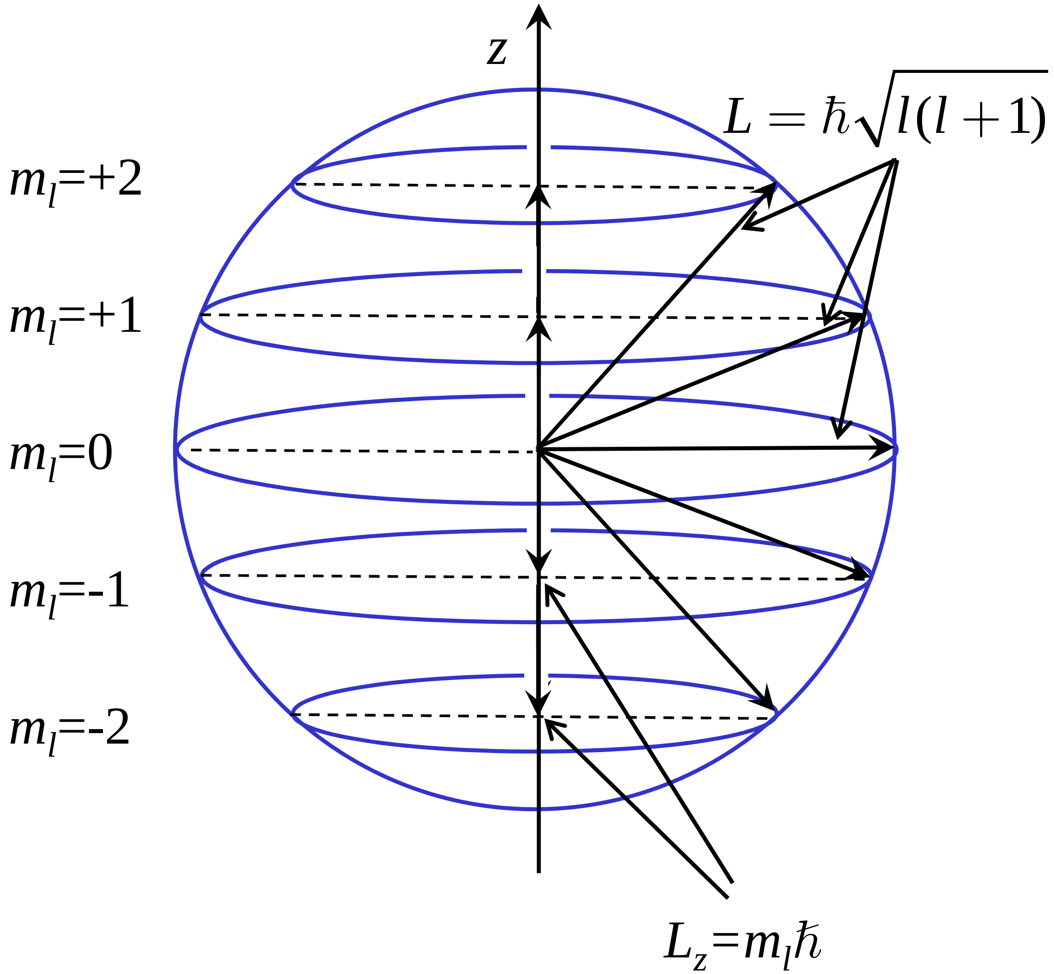
•The eigenfunctions are *Spherical Harmonics:*

$Y_{lm}(\theta,\phi) : l, m$ integers.

•Note dependence of $Y_{\ell m} \propto e^{im\phi}$ - so we have eigenstates of

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

with eigenvalues: $m_l \hbar$

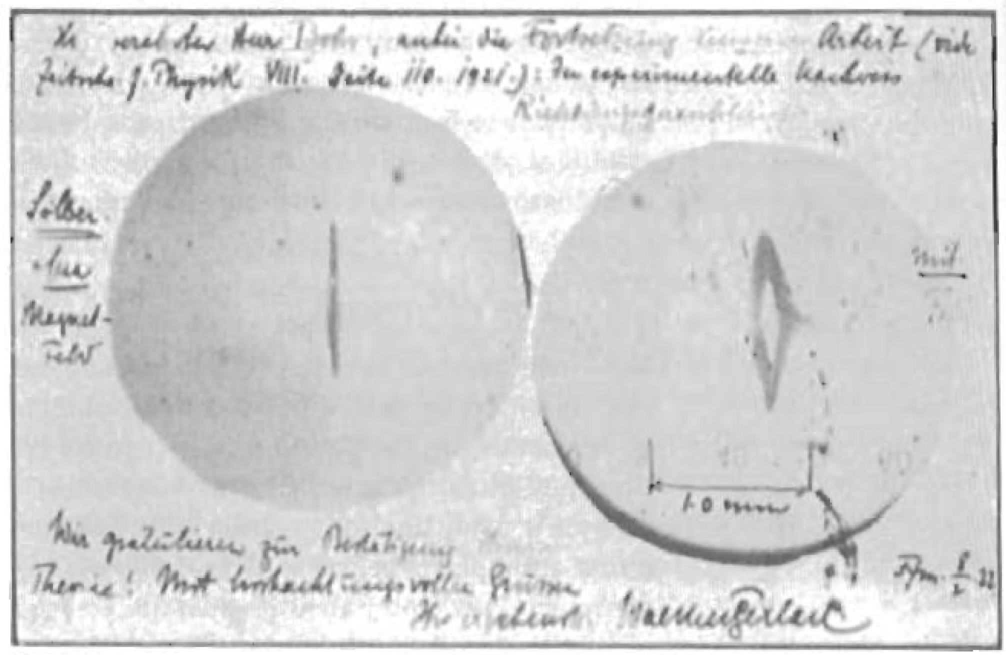


L is quantised so that $L = \hbar\sqrt{l(l+1)}$ and $L_z = m_l\hbar$. L_x and L_y are indeterminate. In this case $l=2$, $m_l = 0, \pm 1, \pm 2$.(fig. 8.1 QP course)

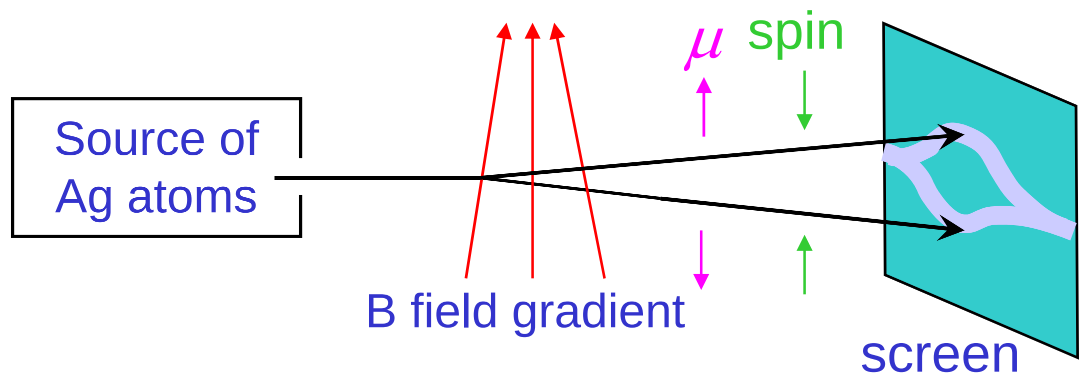
Stern-Gerlach effect - spin

- Half integer values of l are allowed by commutation relations but are not solutions of $\hat{L}^2$.
- Experimentally many particles (electron, proton, neutron….) have half integer *"spin".*
- Example: To explain the many lines observed in atomic spectra, $S=1/2$ for an electron was required.
- Example: Silver atoms split into 2 beams by Stern-Gerlach experiment.

from "The new quantum universe" Hey and Walters



A postcard sent by Gerlach to Neils Bohr announcing their discovery in 1921.



See section 9.1 QP course

Spin

•Dirac Equation – relativistic quantum mechanical wave equation needed – will be discussed later in this course.

•Spin arises naturally from this equation and has no classical analogue.

•Dirac equation predicts S=1/2 for electron (and existence of the positron).

•Spin operator $\hat{S}$ - an intrinsic angular momentum - similar to $\hat{L}$ - the orbital angular momentum operator.

•Spin operators satisfy same commutation relations as $\hat{L}$ e.g. $\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$

• $\hat{S}$ doesn't act on spatial coordinates but on internal "spin" coordinate.

•Spin raising and lowering operators $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$.

•Spin ½ particle – two spin states (eigenstates of $\hat{S}_z$):

$$m_s = +\tfrac{1}{2} \text{ or } \chi_+ \text{ or } \uparrow$$

$$m_s = -\tfrac{1}{2} \text{ or } \chi_- \text{ or } \downarrow$$

•Intrinsic spin can also be an integer - for $W^\pm, Z^0$ particles S=1.

Spin – matrix represention

- Operators can be represented by "Pauli spin matrices"

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- These satisfy commutation relations e.g. $\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z$ – check!

- Represent states by

$$\left.\begin{array}{l} m_s = +\tfrac{1}{2} \Rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ m_s = -\tfrac{1}{2} \Rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{array}\right\}$$

Eigenvectors of $\hat{S}_z$!

- Similarly

$$\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \hat{S}^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

have the expected properties – but are not a unique representation.

See section 9.4 QP course

Matrix representation (1)

- Take a complete set of orthonormal basis states such as:

$$\psi_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \; ; \; \psi_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

A general state: $\Phi = \sum_n c_n \psi_n = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$

- To find eigenvalues α and eigenvectors ϕ of operator $\hat{A}$ (where $\hat{A}\phi = \alpha\phi$)

we can expand ϕ in the chosen basis $\phi = \sum_n c_n \psi_n$

so that operating with $\hat{A}$ we have $\hat{A}\phi = \sum_n c_n \hat{A}\psi_n = \alpha \sum_n c_n \psi_n$.

- Multiplying by ψ_j^* and integrating gives $\sum_n c_n A_{jn} = \alpha c_j$ where

the *matrix element* A_{jn} is defined by $A_{jn} \equiv \int \psi_j^* \hat{A} \psi_n d\tau \equiv \left\langle \psi_j \,|\, \hat{A} \,|\, \psi_n \right\rangle$.

See section 9.4 QP course

Matrix representation (2)

- On the last slide we saw that $\sum_n c_n A_{jn} = \alpha c_j$

- This can also be written:

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix} = \alpha \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

- This is a standard eigenvalue problem for a Hermitian[1] Matrix.

- The solution is given by:

$$\begin{vmatrix} A_{11}-\alpha & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22}-\alpha & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33}-\alpha & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{vmatrix} = 0$$

[1] If $\hat{A}$ is Hermitian then it has real eigenvalues and $A_{jn} = A_{nj}^{\;*}$

Matrix representation (3)

- If we choose as a basis the eigenstates of $\hat{A}$; ϕ such that $\hat{A}\phi_n = \alpha_n \phi_n$ then the matrix representation is diagonal with eigenvalues along the diagonal:

$$\begin{pmatrix} \alpha_1 & 0 & 0 & \cdots \\ 0 & \alpha_2 & 0 & \cdots \\ 0 & 0 & \alpha_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- The matrix elements A_{jn} contain all the information we need about $\hat{A}$.
- For example: they tell us how $\hat{A}$ operates on an arbitrary function Φ .
- If we expand $\Phi = \sum_n c_n \psi_n \Rightarrow \hat{A}\Phi = \sum_n c_n \hat{A}\psi_n$

and we know that $\hat{A}\psi_n = \sum_j A_{jn}\psi_j$ so $\hat{A}\Phi = \sum_{n,j} c_n A_{jn} \psi_j$.

- This is convenient for computational work if the number of basis states is finite.

Matrix representation (4)

The following list of various matrix properties will be of use

Matrix	Definition	Matrix elements
Symmetric	$A=A^T$	$A_{jn}=A_{nj}$
Antisymmetric	$A=-A^T$	$A_{jn}=-A_{nj}$
Orthogonal	$A=(A^T)^{-1}$	$(A^TA)_{jn}=\delta_{jn}$
Real	$A=A^*$	$A_{jn}= A^*_{jn}$
Pure Imaginary	$A=-A^*$	$A_{jn}= -A^*_{jn}$
Hermitian	$A=A^\dagger$	$A_{jn}= A^*_{nj}$
Anti-Hermitian	$A=-A^\dagger$	$A_{jn}= -A^*_{nj}$
Unitary	$A=(A^\dagger)^{-1}$	$(A^\dagger A)_{jn}= \delta_{jn}$
Singular	$\|A\|=0$	

^{T} denotes the transpose $|A|$ the determinant of a matrix and * the complex conjugate.

Combination of Angular Momentum (1)

- Addition of angular momenta arises in many physical situations e.g. atoms may have contributions from electron orbital angular momenta, and spin as well as nuclear spin…….
- Addition of angular momenta is non-trivial:- they are vectors, and quantum mechanics quantises components and restricts orientation.
- Consider electron of orbital angular momentum l ,spin s .
- Operator for total angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ i.e. $\hat{J}_z = \hat{L}_z + \hat{S}_z$
- Commutation relations for $\hat{\mathbf{J}}$ are of same form as for $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$:

$$\begin{aligned}\left[\hat{J}_x, \hat{J}_y\right] &= \left[\hat{L}_x + \hat{S}_x, \hat{L}_y + \hat{S}_y\right] \\ &= \left[\hat{L}_x, \hat{L}_y\right] + \left[\hat{L}_x, \hat{S}_y\right] + \left[\hat{S}_x, \hat{L}_y\right] + \left[\hat{S}_x, \hat{S}_y\right] \\ &= i\hbar\hat{L}_z + 0 + 0 + i\hbar\hat{S}_z\end{aligned}$$

- So $\left[\hat{J}_x, \hat{J}_y\right] = i\hbar\hat{J}_z$.

See section 9.6 QP course

Combination of Angular Momentum (2)

- So we can characterize eigenstates of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ by quantum numbers j and m_j
- j is an integer or half integer and m_j takes values $-j, -j+1, \ldots. j-1, j$
- Ladder operators are defined in the usual way: $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y = \hat{L}_\pm + \hat{S}_\pm$
- The allowed values of j are $j = l+s, l+s-1, \cdots |l-s|$
- To show this: $\hat{J}_z = \hat{L}_z + \hat{S}_z \Rightarrow m_j = m_l + m_s$
- So maximum possible value of $j = l + s$
- And we must have states with $m_j = l+s, l+s-1, \cdots -l-s$
- There are two ways to make $m_j = l+s-1$ $\begin{cases} m_l = l, m_s = s-1 \\ m_l = l-1, m_s = s \end{cases}$
- And one linear combination of these two states will correspond to $j = l + s$ and the other to $j = l+s-1$.

Combination of Angular Momentum (3)

• Similarly there are three ways to make $m_j = l + s - 2$

$$\left| m_\ell , m_s \right\rangle = \left| l, s-2 \right\rangle \text{ or } \left| l-2, s \right\rangle \text{ or } \left| l-1, s-1 \right\rangle$$

• Argument continues until either m_l reaches $-l$ or m_s reaches $-s$ when you have proved that $j = \left| l - s \right|$ exists

• In general we didn't specify which particular combination of m_l and m_s corresponded to each value of j. In general it will be a mixture because

$$\left[\hat{J}^2, \hat{L}^2 \right] = 0, \quad \left[\hat{J}^2, \hat{S}^2 \right] = 0, \quad \left[\hat{J}^2, \hat{J}_z \right] = 0$$

but $$\left[\hat{J}^2, \hat{L}_z \right] \neq 0, \quad \left[\hat{J}^2, \hat{S}_z \right] \neq 0$$

so we can't define $\hat{L}_z$ or $\hat{S}_z$ at the same time as $\hat{J}^2$.

Combination of Angular Momentum (4)

- To show this : $\hat{J}^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{L}\cdot\hat{S} = \hat{L}^2 + \hat{S}^2 + 2\left[\hat{L}_x\hat{S}_x + \hat{L}_y\hat{S}_y + \hat{L}_z\hat{S}_z\right]$
- $\hat{L}_z$ commutes with $\hat{L}^2$,and with all $\hat{S}$ operators. The term $2\left[\hat{L}_x\hat{S}_x + \hat{L}_y\hat{S}_y + \hat{L}_z\hat{S}_z\right]$ commutes with $\hat{L}^2$ but not with $\hat{L}_z$ because

$$2\left[\hat{S}_x\left[\hat{L}_x,\hat{L}_z\right] + \hat{S}_y\left[\hat{L}_y,\hat{L}_z\right] + \hat{S}_z\left[\hat{L}_z,\hat{L}_z\right]\right] = 2i\hbar\left(-\hat{S}_x\hat{L}_y + \hat{S}_y\hat{L}_x\right) \neq 0$$

- Hence $\left[\hat{J}^2,\hat{L}_z\right] \neq 0, \quad \left[\hat{J}^2,\hat{S}_z\right] \neq 0$.

- This suggests that eigenstates of $\hat{J}^2, \hat{J}_z$ are not in general eigenstates of $\hat{L}_z, \hat{S}_z$.
- There are two commuting sets of operators:

$$\hat{L}^2 \quad \hat{S}^2 \quad \hat{L}_z \quad \hat{S}_z \qquad\qquad \hat{J}^2 \quad \hat{L}^2 \quad \hat{S}^2 \quad \hat{J}_z$$

- Which set to use depends on the problem – usually the one which more nearly commutes with $\hat{H}$.

Example- the Hydrogen atom (1)

- This has one electron with orbital angular momentum l spin $\frac{1}{2}$
- Now: $$j = l+s, l+s-1, \cdots |l-s| \quad \Rightarrow \begin{cases} j = l \pm \frac{1}{2} & if \quad l \geq 1 \\ j = \frac{1}{2} & if \quad l = 0 \end{cases}$$
- Therefore all states other than $l = 0$ can have two different values of total angular momentum j .
- In fact these states have slightly different energies due to the spin-orbit interaction – discussed later.
- The simplest non-trivial example is the ground state of the hydrogen atom.
- $l = 0$, but both electron and proton have $s = \frac{1}{2}$ so total spin $= 0,1$

$$S = 1 \quad m_s = 1 \qquad \psi_{11} = \uparrow_e \uparrow_p$$

$$S = 1 \quad m_s = -1 \qquad \psi_{1-1} = \downarrow_e \downarrow_p$$

$$S = 1 \quad m_s = 0 \qquad \psi_{10} = ???$$

The Hydrogen atom (2)

•For the combination $S=1, m_s=0$ we construct the state ψ_{10} using $\hat{S}_-$

$$\hat{S}_- \uparrow_e \uparrow_p = \left(\hat{S}_-^e + \hat{S}_-^p\right) \uparrow_e \uparrow_p = \hbar\sqrt{\tfrac{1}{2}\cdot\tfrac{3}{2}+\tfrac{1}{2}\cdot\tfrac{1}{2}}\left(\downarrow_e \uparrow_p + \uparrow_e \downarrow_p\right)$$

•Hence three values of m_s - called a *triplet* state, the $m_s=0$ state has been normalised by the factor of $\frac{1}{\sqrt{2}}$.

$$S=1, m_s=1 \qquad \psi_{11} = \uparrow_e \uparrow_p$$

$$S=1, m_s=0 \qquad \psi_{10} = \frac{1}{\sqrt{2}}\left(\downarrow_e \uparrow_p + \uparrow_e \downarrow_p\right)$$

$$S=1, m_s=-1 \qquad \psi_{1-1} = \downarrow_e \downarrow_p$$

•The $S=0, m_s=0$ state must be orthogonal to the $S=1, m_s=0$ state.

•So we have a *singlet* state: $S=0, m_s=0 \qquad \psi_{00} = \frac{1}{\sqrt{2}}\left(\downarrow_e \uparrow_p - \uparrow_e \downarrow_p\right)$

> The $S=0,1$ states of H actually have different energies - the electron and protons have magnetic moments associated with their spins - transitions at RF $\lambda \approx 21\text{cm}$

Clebsch-Gordan Coefficients

- The coefficients ($\pm\frac{1}{\sqrt{2}}$) in the wavefunctions on the last slide are called Clebsch-Gordan Coefficients
- The method adopted can be generalised to compute them:

1) Start with largest $j = l + s, m_j = l + s$ state.
2) Use $\hat{J}_-$ to generate other $j = l + s$ states.
3) Use orthogonality to find the state $j = l + s - 1, m_j = l + s - 1$.
4) Use $\hat{J}_-$ on the $j = l + s - 1$ states.
5) And so on…..

Lecture 3 - Summary

Angular momentum and spin:

- Ladder operators.
- Orbital angular momentum.
- Stern-Gerlach effect.
- Spin.
- Matrix representation.
- Combination of orbital angular momentum and spin.
- Example – the hydrogen atom.

Lecture 3

The End!!

(www.sp.phy.cam.ac.uk/~dar11/pdf)