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ANGULAR MOMENTUM: revision

In 2nd year course, we learnt about orbital angular momentum, $\hat{L} = \hat{i}\hat{L}_x + \hat{j}\hat{L}_y + \hat{k}\hat{L}_z$

$$\begin{aligned}
\hat{L} &= \hat{R} \times \hat{P}; \quad \hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \\
\hat{L}_x &= y\hat{P}_z - z\hat{P}_y = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\
\hat{L}_y &= z\hat{P}_x - x\hat{P}_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\
\hat{L}_z &= x\hat{P}_y - y\hat{P}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}\right)
\end{aligned}$$

FROM WHENCE *WE PROVED*:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \ + \ \text{CYCLIC PERMUTATIONS OF } x, y, z \text{ ie :}$$

$$[\hat{L}_i, \hat{L}_j] = i\hbar\hat{L}_k \tag{4.1}$$

and also,

$$[\hat{L}_i, \hat{L}^2] = 0 \text{ where } \hat{L}_i = \hat{L}_x, \hat{L}_y, \hat{L}_z \tag{4.2}$$

We conclude that we can know simultaneously the total angular momentum of a quantum particle *and* one component. However, individual components do not commute with each other. We cannot have simultaneous knowledge of L_x, L_y, L_z.

In 2nd/3rd year courses, $\hat{L}_i$ were transformed from cartesian to spherical polars, (θ, ϕ) *eg*,

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

We used this spherical polar coordinate representation to obtain simultaneous eigenfunctions of $\hat{L}^2$ and one component ($\hat{L}_z$) to *derive*:

$$\hat{L}^2 Y_{\ell m}(\theta, \phi) = l(l+1)\hbar^2 Y_{\ell m}(\theta, \phi) \tag{4.2a}$$

$$\hat{L}_z Y_{\ell m}(\theta, \phi) = m\hbar Y_{\ell m}(\theta, \phi) \tag{4.2b}$$

The $Y_{\ell m}(\theta, \phi)$ function are 'spherical harmonics'.

They appeared in our *solution of the hydrogen atom* (year 2, course 2B22) since

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$$

They give the well known shape of the *s, p, d, f atomic orbitals*

We can generalise (4.1) & (4.2) to other types of angular momentum (not necessarily *orbital* angular momentum).

eg spin *s*. The electron is associated with spin with two possible projection on the z-axis, $m_s = \frac{1}{2}$ or $m_s = -\frac{1}{2}$. This spin is associated with a magnetic moment, and this quantisation $m_s = \pm\frac{1}{2}$ was seen in the *Stern-Gerlach* experiment.

Spin of an electron is an abstract concept (the electron has no know internal structure). But we don't need a coordinate representation of the spin eigenfunctions. Much can be derived from commutator algebra. Go to Dirac notation, eg

$$Y_{\ell m}(\theta, \phi) \to |lm\rangle$$

For other types of angular momentum, we define Hermitian operators

$$J^2, \hat{J}_x, \hat{J}_y, \hat{J}_z,$$

where

$$\begin{aligned} [J_x, J_y] &= i\hbar J_z \text{ (+ cyclic permutations)} \\ [J^2, J_i] &= 0 \quad (i \equiv x, y, z) \end{aligned}$$

Then $\hat{J}^2|JM\rangle = J(J+1)\hbar^2|JM\rangle$ etc; we will derive this below from commutator algebra.

Note that in 2B24 (for example) when we analysed *atomic spectra* we considered a *total* angular momentum $J = L + S$

Vector addition, but J is quantised

$$|L - S| \leq J \leq |L + S|$$

eg of $L = 1$, $S = \frac{1}{2}$ then

$$\begin{matrix} \uparrow \\ \uparrow \end{matrix} \; J = \frac{3}{2} \; \begin{matrix} \downarrow \\ \uparrow \end{matrix} \; J = \frac{1}{2}$$

NOTE DIFFERENCE BETWEEN EIGEN VALUE OF $|J| = \sqrt{J(J+1)}\hbar$ AND THE $\hat{J}^2$ QUANTUM NUMBER J.

In general, we write

$$\hat{J}^2|jm\rangle = \alpha|jm\rangle \tag{4.3a}$$

$$\hat{J}_z|jm\rangle = \beta|jm\rangle \tag{4.3b}$$

we will prove

$$\begin{aligned} \hat{J}^2|jm\rangle &= j(j+1)\hbar^2|jm\rangle \\ \hat{J}_z|jm\rangle &= m\hbar|jm\rangle \end{aligned}$$

with no reference to a coordinate representation.

We begin by defining *raising and lowering* operators:

$$\begin{aligned} \hat{J}_+ &= \hat{J}_x + i\hat{J}_y \\ \hat{J}_- &= \hat{J}_x - i\hat{J}_y \end{aligned} \tag{4.4a}$$

$\hat{J}_\pm$ are not HERMITIAN.

Now

$$[\hat{J}^2, \hat{J}_\pm] = [\hat{J}^2, \hat{J}_x] \pm i[\hat{J}^2, \hat{J}_y] = 0 \tag{4.4b}$$

and

$$\begin{aligned} \hat{J}_+\ \hat{J}_- &= \hat{J}_x^2 + \hat{J}_y^2 - i[\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x] \\ &= \hat{J}^2 - \hat{J}_z^2 + \hbar\hat{J}_z \end{aligned} \tag{4.4c}$$

(Try $\hat{J}_-\hat{J}_+$ too)

hence

$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z \tag{4.5}$$

and

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm \tag{4.6}$$

Now, to obtain α and β. J^2, J_z are Hermitian. So α, β are *real*.

Operate on 4.3b with $\hat{J}_+$

$$\hat{J}_+\hat{J}_z|jm\rangle = \beta\hat{J}_+|jm\rangle \tag{4.7}$$

Form (4.6)

$$\hat{J}_z\hat{J}_+ - \hat{J}_+\hat{J}_z = \hbar\hat{J}_+$$

so

$$(\hat{J}_z\hat{J}_+ - \hbar\hat{J}_+)|jm\rangle = \beta\hat{J}_+|jm\rangle \tag{4.8}$$

$$\Rightarrow \hat{J}_z(\hat{J}_+|jm\rangle) = (\beta + \hbar)(\hat{J}_+|jm\rangle) \tag{4.9}$$

Operating again on (4.3b), but now with $\hat{J}_- J_z|jm\rangle$

we can show

$$\hat{J}_z(\hat{J}_-|jm\rangle) = (\beta - \hbar)(\hat{J}_-|jm\rangle) \tag{4.10}$$

Hence, $(J_+|jm\rangle)$ is still an eigenfunction of $\hat{j}_z$, but with eigenvalue $|\beta+\hbar\rangle$ and $(J_-|jm\rangle)$ is still an eigenfunction of $\hat{j}_z$, but with eigenvalue $|\beta-\hbar\rangle$.

Also, from (4.4b) we know, ie $[\hat{J}^2, \hat{J}_\pm] = 0$:

$$\hat{J}_\pm \hat{J}^2 |jm\rangle = \hat{J}^2 \hat{J}_\pm |jm\rangle \tag{4.11}$$

$$= \alpha\ (\hat{J}_\pm |jm\rangle) = \hat{J}^2 (\hat{J}_\pm |jm\rangle) \tag{4.12}$$

ie $\hat{J}_\pm|jm\rangle$ are also eigenfunction of $\hat{J}^2$, with eigenvalue still $= \alpha$.

From (4.9) by repeatedly operating $J_+|jm\rangle$, a sequence of eigenfunction of $\hat{J}_z$, with eigenvalues $\beta,\ \beta+\hbar,\ \beta+2\hbar\ldots\beta+n\hbar$ can be built up.

Similarly, $(\hat{J}_-)^n|jm\rangle$ yields functions with eigenvalue of $\hat{J}_z$:

$$= \beta, \beta-\hbar, \beta-2\hbar\ldots\beta-n\hbar$$

However, both series must terminate; β is the z component of the angular momentum, which cannot exceed the total L. We infer that $\alpha \overline{>} \beta^2 \quad (\alpha \equiv e'\text{val of } \hat{L}^2)$ so there is a maximum $|\beta \pm n\hbar|$.

There will be a maximal e'val/e function such that

$$\hat{J}_+|jm\rangle_T = 0 \tag{4.13}$$

$$\hat{J}_z|jm\rangle_T = \beta_T|jm\rangle_T \tag{4.14}$$

Similarly, there is a minimum:

$$\hat{J}_-|jm\rangle_B = 0; \quad \hat{J}_z|jm\rangle_B = \beta_B|jm\rangle_B \tag{4.15a}$$

$$\beta_T - \beta_B = n\hbar \tag{4.15b}$$

since $J_\pm$ raise β by integer multiples where $n = 0, 1, 2\ldots$ of $\hbar$.

From (4.13)

$$J_- J_+ |jm\rangle_T = 0$$

From (4.4c):

$$\Rightarrow (J^2 - J_z^2 - \hbar J_z)|jm\rangle_T = 0$$

using e'vals:

$$\Rightarrow (\alpha - \beta_T^2 - \hbar\beta_T) = 0 \tag{4.16}$$

From (4.15), we can use similar precess to deduce:

$$\alpha - \beta_B^2 + \beta_B\hbar = 0$$

$$\alpha = \beta_B(\beta_B - \hbar) \tag{4.17a}$$

and

$$\alpha = \beta_T(\beta_T + \hbar). \tag{4.17b}$$

equating, (4.17a) and (4.17b):

$$\begin{aligned}\beta_B(\beta_B - \hbar) &= \beta_T(\beta_T + \hbar)\\ \beta_B^2 - \beta_B\hbar &= \beta_T^2 + \beta_T\hbar\\ \Rightarrow \beta_T &= -\beta_B\end{aligned}$$

or

$$\beta_T = \beta_B - \hbar;$$

this case implies $\beta_B > \beta_T$ which is not acceptable, from(4.15b) thus

$$\beta_T = -\beta_B$$

hence, From (4.15b) ($\beta_T - \beta_B = n\hbar$):

$$\beta_T = \frac{n}{2}\hbar \quad n = 0, 1, 2 \ldots$$

let $n = 2j$ (j is integer or $\frac{1}{2}$ integer)

so

$$\beta_T = j\hbar = -\beta_B.$$

From (4.16):

$$\begin{aligned}\alpha &= \beta_T^2 + \beta_T\hbar\\ \alpha &= j(j+1)\hbar^2; \quad \beta = m\hbar\\ \frac{\beta}{\hbar} &= j, j-1 \ldots . -(j+1), -j = m\end{aligned}$$

with j integer or half-integer.

Finally

$$\begin{aligned}J^2|jm\rangle &= j(j+1)\hbar^2|jm\rangle\\ \hat{J}_z|jm\rangle &= m\hbar|jm\rangle\end{aligned}$$

Which is what we set out to show.

Effect of Raising-Lowering operators

In (4.9) and (4.10) we showed that $\hat{J}_\pm|jm\rangle = \phi_\pm$ are still eigenfunctions of $\hat{J}^2$ and $\hat{J}_z$ but, with eigenvalues $j(j+1)\hbar^2$ and $(m \pm 1)\hbar$.

So we deduce that $\phi_\pm$ are proportional to $|jm \pm 1\rangle$.

Let

$$\begin{aligned}\phi_+ = (J_+|jm\rangle) = C_+|jm+1\rangle\\ \phi_- = (J_-|jm\rangle) = C_-|jm-1\rangle\end{aligned} \tag{4.18}$$

Now, J_+, J_- are adjoint operators, so:
From I.2.1

$$\langle\phi|J_+\psi\rangle = \langle J_-\phi|\psi\rangle$$
$$\langle\phi|J_+\psi\rangle = \langle\psi|J_-\phi\rangle^* \tag{4.19}$$

Hence

$$\begin{aligned}
\langle jm+1|J_+jm\rangle &= \langle jm|J_-jm+1\rangle^* \\
\langle jm|J_-|jm+1\rangle &= \langle jm+1\ J_+jm\rangle^* \\
&= C_+^*\langle jm+1|jm+1\rangle^* \\
&= C_+^* \qquad (4.20)
\end{aligned}$$

now

$$\langle jm|J_-J_+|jm\rangle = C_+\langle jm|J_-|jm+1\rangle \tag{4.21}$$

Comparing (4.20) and (4.21) we have

$$\langle jm|J_-J_+|jm\rangle = C_+C_+^* = \langle J_-J_+\rangle \tag{4.22}$$

From (4.4c) (etc)

$$\begin{aligned}
J_-J_+ &= J^2 - J_z^2 - \hbar J_z \qquad (4.23)\\
\langle J_-J_+\rangle &= [j(j+1) - m(m+1)]\hbar^2 = |C_+|^2
\end{aligned}$$

From (4.18) we write

$$\begin{aligned}
J_+|jm\rangle &= C_+|jm+1\rangle \\
&= \sqrt{[j(j+1) - m(m+1)]}\hbar|jm+1\rangle \qquad (4.24)
\end{aligned}$$

Similarly, start from (4.18–4.20) to show.

$$J_-|jm\rangle = \sqrt{[j(j+1) - m(m-1)]}\hbar|jm-1\rangle \tag{4.25}$$

(Homework 4).

SPIN$-\frac{1}{2}$ PARTICLES: eg electrons, protons. [4.1]

In this case, the only possible projection along any axis has magnitude $+\frac{\hbar}{2}$ (SPIN UP) or $-\frac{\hbar}{2}$ (SPIN DOWN).

By analogy to spherical harmonics we write:

$$\begin{aligned}
\hat{S}^2|Sm_s\rangle &= S(S+1)\hbar^2|Sm_s\rangle \qquad (4.26)\\
&= \frac{3}{4}\hbar^2|Sm_s\rangle \quad \text{for } S = \frac{1}{2}
\end{aligned}$$

and

$$\hat{S}_z|Sm_s\rangle = m_s\hbar|Sm_s\rangle \tag{4.27}$$

$S \rightarrow$ 'spin quantum number'

NB (remember 'hat' on operator $\hat{S}$ to differentiate from quantum number S)

$$\begin{aligned} m_s &= +\frac{1}{2} \Rightarrow \text{ SPIN UP STATE } \left|\frac{1}{2}\frac{1}{2}\right\rangle \equiv |\alpha\rangle \\ m_s &= -\frac{1}{2} \Rightarrow \text{ SPIN DOWN STATE } \left|\frac{1}{2} - \frac{1}{2}\right\rangle \equiv |\beta\rangle \end{aligned}$$

Spin states orthonormal:

$$\langle\alpha|\alpha\rangle = \langle\beta|\beta\rangle = 1 \tag{4.28}$$

$$\langle\alpha|\beta\rangle = 0 \tag{4.29}$$

Commutation rules similar to $\hat{L}$:

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_y \text{ (+ cyclic permutations)} \tag{4.30}$$

Whence we find similar relations for $\hat{S}_{\pm}$:

$$\hat{S}_{\pm}|Sm\rangle = [S(S+1) - m(m \pm 1)]^{\frac{1}{2}}\hbar|Sm \pm 1\rangle \tag{4.31}$$

Then

$$\begin{aligned} S_+|\alpha\rangle = 0; \quad S_-|\beta\rangle = 0 \\ S_+|\beta\rangle = \hbar|\alpha\rangle; \quad S_-|\alpha\rangle = \hbar|\beta\rangle \end{aligned} \tag{4.32}$$

Since

$$\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-) \quad and \quad \hat{S}_y = \frac{1}{2i}(\hat{S}_+ - \hat{S}_-) \tag{4.33}$$

Then

$$S_x|\alpha\rangle = \frac{\hbar}{2}|\beta\rangle \tag{4.34a}$$

$$S_x|\beta\rangle = \frac{\hbar}{2}|\alpha\rangle \tag{4.34b}$$

$$\hat{S}_y|\alpha\rangle = i\frac{\hbar}{2}|\beta\rangle \tag{4.34c}$$

$$\hat{S}_y|\beta\rangle = -i\frac{\hbar}{2}|\alpha\rangle \tag{4.34d}$$

$$\hat{S}_z|\alpha\rangle = \frac{\hbar}{2}|\alpha\rangle \tag{4.34e}$$

$$\hat{S}_z|\beta\rangle = -\frac{\hbar}{2}|\beta\rangle \tag{4.34f}$$

Only these are 'e'value equations.

An arbitrary quantum state $|\chi\rangle$,

$$|\chi\rangle = a|\alpha\rangle + b|\beta\rangle \tag{4.35}$$

Is a superposition of SPIN-UP and SPIN-DOWN a, b are complex numbers. As in Appendix I.1 are given by overlap ('scalar product) with $|\chi\rangle$

$$a = \langle\alpha|\chi\rangle$$
$$b = \langle\beta|\chi\rangle$$

Total Spin

$$\hat{S}^2|\chi\rangle = a\hat{S}^2|\alpha\rangle + b\hat{S}^2|\beta\rangle = \frac{3}{4}\hbar^2|\chi\rangle \tag{4.36a}$$

z-Component

$$\hat{S}_z|\chi\rangle = a\frac{\hbar}{2}|\alpha\rangle - b\frac{\hbar}{2}|\beta\rangle \tag{4.36b}$$

So, $|\chi\rangle$ is not an eigenstate of $\hat{S}_z$, but we can still calculate an expectation value average over many measurements of $\hat{S}_z$ on many identically prepared states:

$$\langle\chi\,\hat{S}_z\,\chi\rangle = \frac{\hbar}{2}(|a|^2 - |b|^2) \tag{4.37}$$

S_x^2 and S_y^2

$$\hat{S}_x^2|\alpha\rangle = \hat{S}_x \cdot (\hat{S}_x|\alpha\rangle) = \hat{S}_x\frac{\hbar}{2}|\beta\rangle$$
$$\Rightarrow S_x^2|\alpha\rangle = \frac{\hbar^2}{4}|\alpha\rangle \tag{4.38}$$

also

$$S_x^2|\beta\rangle = \frac{\hbar^2}{4}|\beta\rangle \tag{4.39}$$

hence

$$\begin{aligned} S_x^2|\chi\rangle &= \frac{\hbar^2}{4}(a|\alpha\rangle + b|\beta\rangle) \\ &= \frac{\hbar^2}{4}|\chi\rangle \end{aligned} \tag{4.40}$$

can also show

$$S_y^2|\chi\rangle = \frac{\hbar^2}{4}|\chi\rangle \tag{4.41}$$

$$S_+^2|\alpha\rangle = S_+^2|\beta\rangle = S_+^2|\chi\rangle = 0$$

$$\begin{aligned} S_+^2 &= (S_x + iS_y)(S_x + iS_y) \\ &= \underbrace{S_x^2 - S_y^2}_{\frac{1}{4}\hbar^2 - \frac{1}{4}\hbar^2} + i\underbrace{[S_xS_y + S_yS_x]}_{\text{must}=0} \end{aligned} \tag{4.42}$$

hence

$$\begin{aligned} \{\hat{S}_x, \hat{S}_y\} &= S_xS_y + S_yS_x = 0 \\ &= \text{"anti-commutator"} \end{aligned} \tag{4.43}$$

we can show all components 'anti-commuator', ie

$$\{\hat{S}_x, \hat{S}_y\} = \{\hat{S}_y, \hat{S}_z\} = \{\hat{S}_z, \hat{S}_x\} = 0 \tag{4.44}$$

(order obviously doesn't matter)

Can combine

$$S_xS_y + S_yS_x = 0$$

with normal commutator

$$S_xS_y - S_yS_x = i\hbar S_z \tag{4.45}$$

to get

$$\hat{S}_x\hat{S}_y = \frac{i\hbar}{2}\hat{S}_z \tag{4.46}$$

or, in general,

$$\hat{S}_i\hat{S}_j = i\frac{\hbar}{2}\hat{S}_k \ [i, j, k \text{ are cyclic permutations of } x, y, z] \tag{4.47}$$

Hence, any arbitrary operator formed from products of $\hat{S}_i$.

$$\hat{A} = \sum_{n=x,y,z} C_{nm}\hat{S}_n\hat{S}_m \quad \text{can be reduced} \tag{4.48}$$

to the from

$$\hat{A} = \hat{S}^2 + A_1S_x + A_2S_y + A_3S_z \tag{4.49}$$

$$= A_0 + A \cdot S \tag{4.50}$$

where

$$A = A_1\hat{i} + A_2\hat{j} + A_3\hat{k} \tag{4.51}$$