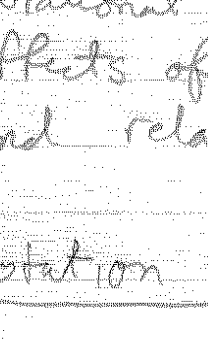
Physics 531 - Lecture 2

Review: Angular Momentum in Quantum Mechanics

Angular momentum plays a central role in the description of atomic and molecular structure because of rotational symmetry of central forces and the effects of intrinsic spin on exchange symmetry and relativistic corrections.

Rotation Symmetry

Angular momentum is the generator of rotations. Given axis $\vec{e}_n$ and rotation angle θ



$$V'_i = \sum_i \underset{\uparrow\ \text{rotation matrix}}{R_{ij}}\, V_j$$

Operators: $\{\hat{V}_i\}$ ← Vector operator

$$\hat{V}'_i = \hat{D}^{\dagger}(\vec{e}_n,\theta)\ \hat{V}_i\ \hat{D}(\vec{e}_n,\theta) = \sum_j R_{ij}\hat{V}_j$$

Rotation operator: $\hat{D}(\vec{e}_n,\theta) = e^{-\frac{i}{\hbar}\theta\, \vec{e}_n\cdot\hat{\vec{J}}}$

$\hat{\vec{J}}$ = Angular momentum operator

In order to generate rotations, the components of $\vec{J}$ must satisfy commutation relation

$$\boxed{[\hat{J}_i, \hat{J}_j] = i\hbar\, \epsilon_{ijk} \hat{J}_k}$$

Examples: • Orbital angular momentum

$$\hat{\vec{J}} = \hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$$

(follows from $[x_i, p_j] = i\hbar\, \delta_{ij}$

• Spin angular momentum: Intrinsic property of elementary particles, like charge

From now on, we will measure $\vec{J}$ in units of $\hbar$, so it becomes dimensionless

Other commutation relations:

$$[\hat{J}^2, \hat{J}_i] = 0$$

where $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ = magnitude squared

$\Rightarrow$ Can specify magnitude and any one component

Also define $\hat{J}_\pm = \hat{J}_x \pm i \hat{J}_y$

$$\Rightarrow [\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \qquad [\hat{J}_z, \hat{J}_\pm] = \pm \hat{J}_\pm$$

Eigenvalue problem:

Complete set of commuting ops: $\hat{J}^2$ and $\hat{J}_i$ for $i = 1, 2,$ or 3. Typically choose $i = 3 \Rightarrow \hat{J}_z$
$\Rightarrow$ "Quantization axis"

Eigenstates $\{ |j, m\rangle \mid \underbrace{m = -j, -j+1, \ldots, j-1, j}_{2j+1 \text{ values}} \}$

$j =$ whole (orbital or spin = boson) or half-integer (only for spin ang. mom.) = fermion

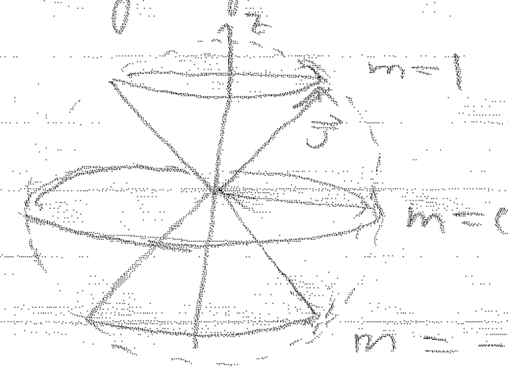
$$\hat{J}^2 |j, m\rangle = j(j+1) |j, m\rangle$$

$$\hat{J}_z |j, m\rangle = m |j, m\rangle$$

$$\hat{J}_\pm |j, m\rangle = \sqrt{j(j+1) \mp m(m\pm 1)}\; |j, m\pm 1\rangle$$

raising/lowering operators

Vector picture e.g. $j = 1$



Three different projections on z-axis. Note J_x, J_y are uncertain

Spherical harmonics

For orbital angular momentum, we can look at position representation

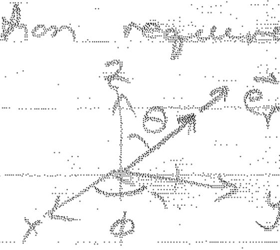
e.g. $\hat{L}_z = -i \frac{\partial}{\partial \phi}$

$\Rightarrow$ Eigenfunction $\hat{L}_z \Psi = m \Psi$

$$\Rightarrow \Psi(\phi) = A e^{im\phi}$$

(Note single valued wave function requires m integer)

Given position $\vec{x} = r \vec{e}_r$



$\langle \vec{e}_r | l, m \rangle = Y_{l,m}(\theta, \phi)$ Spherical harmonic

$$= (-1)^m \left[\frac{(2l+1)(l-m)!}{4\pi (l+m)!} \right] \underbrace{P_l^m(\cos\theta)}_{\text{associate Legendre}} e^{im\phi}$$

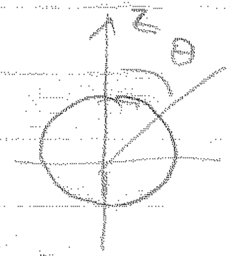
Properties: $Y^*_{l,m}(\theta, \phi) = (-1)^m Y_{l,-m}(\theta, \phi)$

Parity $\vec{x} \Rightarrow -\vec{x}$

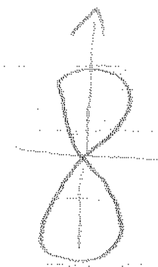
$$Y_{l,m}(\theta, \phi) \Rightarrow (-1)^l Y_{l,m}(\theta, \phi)$$

eigenstate of parity

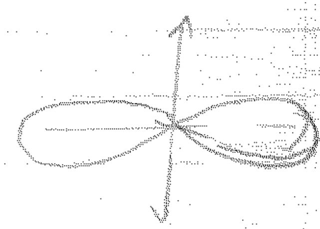
Polar Plots $|Y_{\ell,m}(\theta,\phi)|^2 = N\,|P_\ell^m(\cos\theta)|^2$



$\ell=0, m=0$
s-state

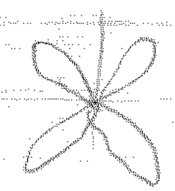


$\ell=1$ $m=0$

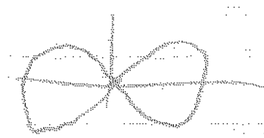


$m=\pm1$
p-state

$\ell=2$ $m=0$



$m=\pm1$



$m=\pm2$

d-state

Real form: $x \pm iy = r\sin\theta\, e^{\pm i\phi}$

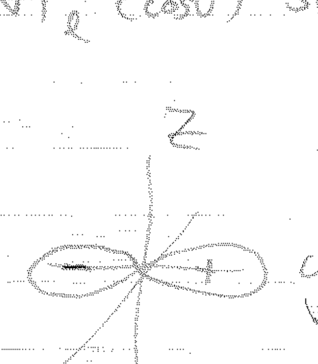
$$Y_{\ell,\cos}(\theta,\phi) = N P_\ell^{|m|}(\cos\theta)\cos|m|\phi = \frac{1}{\sqrt{2}}\left(Y_{\ell,|m|} + Y^*_{\ell,|m|}\right)$$

$$Y_{\ell,\sin}(\theta,\phi) = N P_\ell^{|m|}(\cos\theta)\sin|m|\phi = \frac{1}{i\sqrt{2}}\left(Y_{\ell,|m|} - Y^*_{\ell,|m|}\right)$$

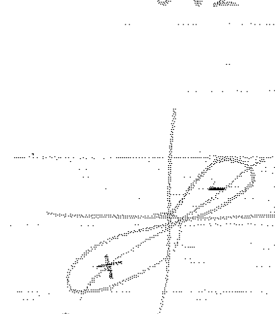
p-states

phase of wave function

P_z



P_y



P_x

Addition of angular momentum

A critical part of the description of atomic and molecular structure is the addition of angular momentum. This is important, e.g., for coupling of spin and orbital angular momentum and for description of identical particles.

Classically, add as vectors $\vec{L} = \vec{L}_1 + \vec{L}_2$

Quantum mechanically, must be careful to consider mutually commuting operators

Two descriptions:

- Uncoupled representation

Complete set of commuting operators $\{\hat{J}_1^2, \hat{J}_{1z}, \hat{J}_2^2, \hat{J}_{2z}\}$

States: $|j_1, m_1\rangle \otimes |j_2, m_2\rangle = |j_1 m_1, j_2 m_2\rangle$

- Coupled representation

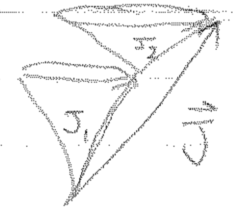
CSCO: $\{\hat{J}^2, \hat{J}_z, \hat{J}_1^2, \hat{J}_2^2\}$

States $|JM, j_1 j_2\rangle$

$$\hat{J}^2 |JM, j_1 j_2\rangle = J(J+1)|JM, j_1 j_2\rangle$$
$$\hat{J}_z |JM, j_1 j_2\rangle = M|JM, j_1 j_2\rangle$$

Vector picture:

<u>Uncoupled</u>



Total $\hat{J}^2$ uncertain

<u>Coupled</u>

$\hat{J}_{1z}$ and $\hat{J}_{2z}$ uncertain

Note: $[\hat{J}^2, \hat{J}_{1z}] \neq 0$ $\quad [\hat{J}^2, \hat{J}_{2z}] \neq 0$

<u>Triangle rule:</u>

Suppose we consider two angular momenta described by magnitudes j_1 and j_2.
In the uncoupled representation there are

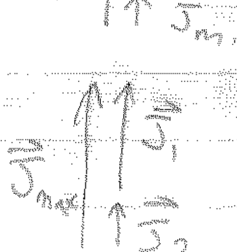
$$(2j_1 + 1)(2j_2 + 1) \text{ different states.}$$

To describe this in the coupled representation we must determine possible values of total J

Solution $J_{min} \leq J \leq J_{max}$ in integer steps

$$J_{min} = |j_1 - j_2|$$

$$J_{max} = j_1 + j_2$$



Can show, total # of states

$$N = \sum_{J=|j_1-j_2|}^{j_1+j_2} \sum_{M=-J}^{J} (2J+1) = (2j_1+1)(2j_2+1)$$

<u>Clebsch-Gordan Coefficients</u> (vector addition coef)
The coupled and uncoupled representations define two different bases for describing two angular momenta. For fixed j_1 j_2 we have a $(2j_1+1)(2j_2+1)$ dimensional space.

Change of basis:

$$|JM, j_1 j_2\rangle = \sum_{m_1, m_2} |j_1 m_1 j_2 m_2\rangle \underbrace{\langle j_1 m_1 j_2 m_2 | J M j_1 j_2\rangle}_{\text{Clebsch-Gordan coeff}}$$

Since j_1 and j_2 are common to both reps usually write

$$|JM\rangle = \sum_{m_1, m_2} |j_1 m_1 j_2 m_2\rangle\langle j_1 m_1 j_2 m_2 | JM\rangle$$

Also

$$|j_1 m_1 j_2 m_2\rangle = \sum_{J=|j_1-j_2|}^{j_1+j_2} \sum_{M=-J}^{J} |JM\rangle\langle JM | j_1 m_1 j_2 m_2\rangle$$

Properties of the C-G coefficients

(1) Real $\Rightarrow$ $\langle JM | j_1 m_1 j_2 m_2 \rangle = \langle j_1 m_1 j_2 m_2 | JM \rangle$

(2) "Selection rules": CG vanishes <u>unless</u>

- $M = m_1 + m_2$ since $\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$
- $|j_1 - j_2| \le J \le |j_1 + j_2|$ (triangle rule)

$$\Rightarrow |JM\rangle = \sum_{m_1 = -j_1}^{j_1} |JM\rangle \langle JM | j_1 m_1 ; j_2 , M - m_1 \rangle$$

(3) Phase convention

- $\langle JM | j_2 m_2 ; j_1 m_1 \rangle = (-1)^{j_1 + j_2 - J} \langle JM | j_1 m_1 \, j_2 m_2 \rangle$
- $\langle J -M | j_1 -m_1 ; j_2 -m_2 \rangle = (-1)^{j_1 + j_2 - J} \langle JM | j_1 m_1 , j_2 m_2 \rangle$
- $\langle j_2 -m_2 | j_1 m_1 ; J \underset{\substack{\uparrow \\ -m_1 - m_2}}{-M} \rangle = (-1)^{j_1 - m_1} \sqrt{\dfrac{2j_2+1}{2J+1}} \langle JM | j_1 m_1 , j_2 m_2 \rangle$

More symmetrical for: <u>Wigner 3J Symbol</u>

$$\boxed{\begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & M \end{pmatrix} = \frac{(-1)^{j_1 + j_2 + m}}{\sqrt{2j+1}} \langle J -M | j_1 m_1 , j_2 m_2 \rangle}$$

Symmetric w.r.t. cyclic permutation