OPTI 570 LECTURE Th NOV 6

Spinless Hydrogen

CSCO of $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$

(1) $\hat{H} \,|\psi_{n \ell m_\ell}\rangle = E_n |\psi_{n\ell m_\ell}\rangle$

- n, ℓ, m : integers

$E_n = -\frac{E_I}{n^2}$, $n \geq 1$ $\qquad E_I = \frac{1}{2}\alpha^2 \mu c^2$

(2) $\hat{L}^2 |n \ell m_\ell\rangle = \hbar^2 \ell(\ell+1) |n\ell\, m_\ell\rangle$

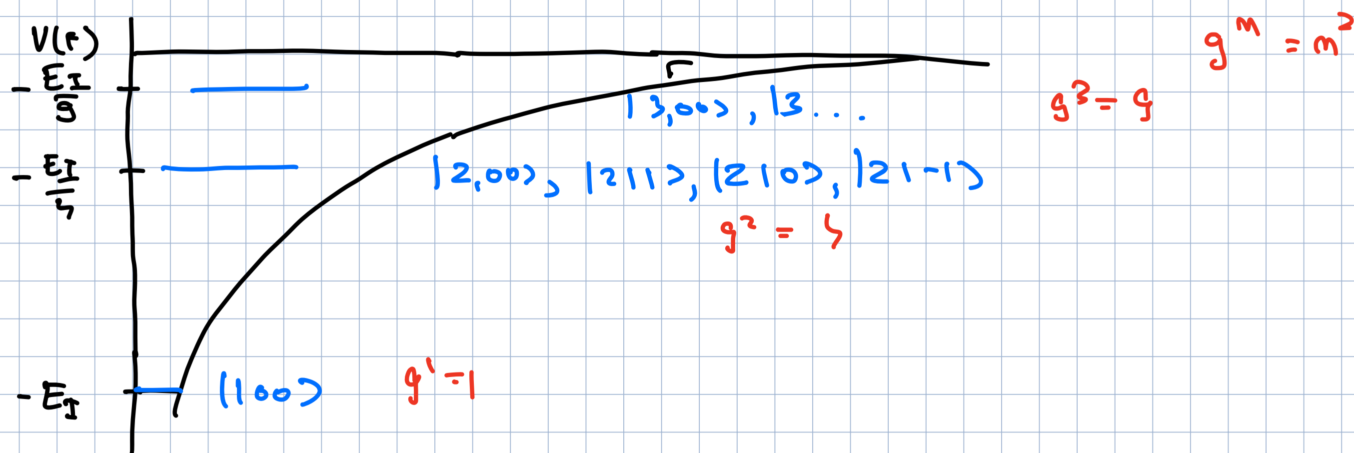
$\hat{L}_z |n\ell\, m_\ell\rangle = \hbar\, m_\ell |n \ell m_\ell\rangle$

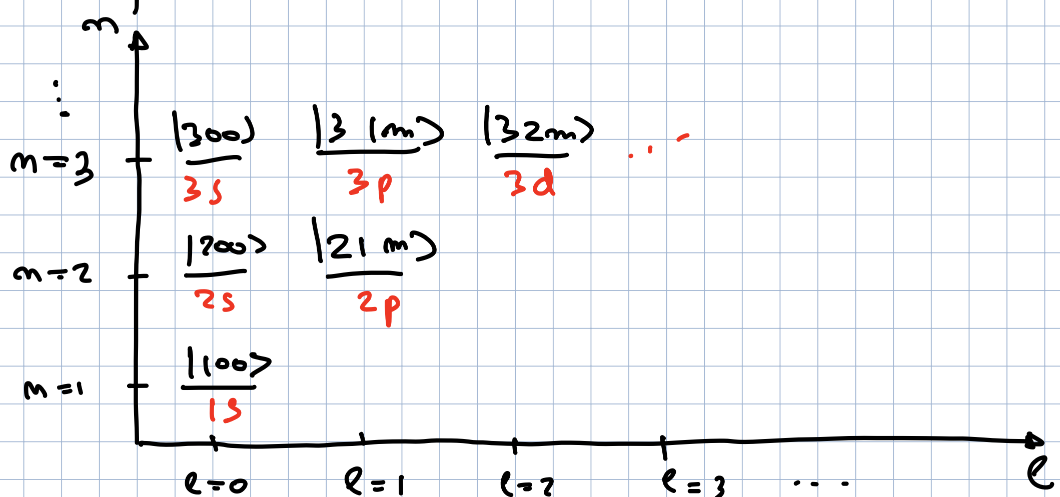
any $\ell \in \{0, 1, 2, \ldots n-1\}$

any $m \in \{\ell, \ell-1, \ell-2, \ldots, -\ell\}$

$\psi_{n\ell m_\ell}(r, \theta, \varphi) = R_{n\ell}(r)\, Y_\ell^{m_\ell}(\theta, \varphi)$

Energy level diagrams





s p d f g. h i . .

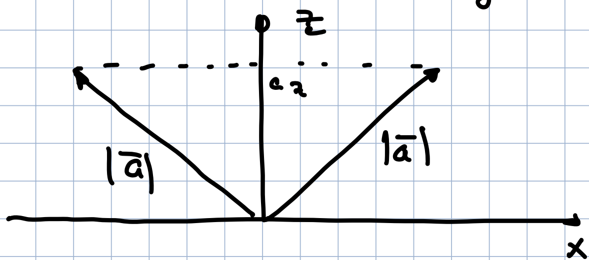
'sharp' 'principal' 'diffuse' 'fundamental'.

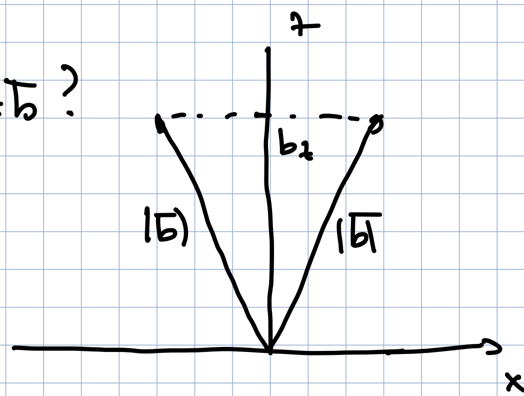
Addition of AM

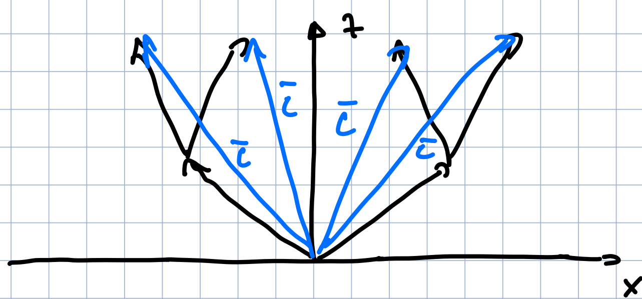
$\bar{a}, \bar{b}$ x − z plane

Given $|\bar{a}|, |\bar{b}|, a_z, b_z$

What can I say about $\bar{c} = \bar{a} + \bar{b}$?





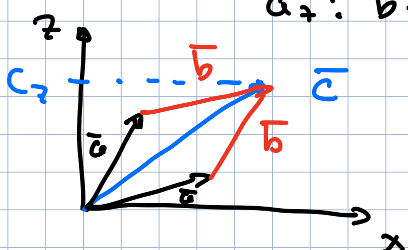


Known: $c_z = a_z + b_z$

- $c = ?$

Given: $|\bar{a}|, |\bar{b}|, |\bar{c}|, c_z$

a_z? b_z?



Addition of AM

CT X

subsystem 1

j_1

$\mathcal{E}_{j_1}$

$\{|j_1\, m_1\rangle\}$

$\vec{J}_1$

$\hat{J}_1^2 |j_1 m_1\rangle = \hbar^2 j_1(j_1+1)|j_1 m_1\rangle$

$J_{1z}|j_1 m_1\rangle = m_1 \hbar\, |j_1 m_1\rangle$

subsystem 2

j_2

$\mathcal{E}_{j_2}$

$\{|j_2\, m_2\rangle\}$

$\vec{J}_2$

$\hat{J}_2^2 |j_2 m_2\rangle = \hbar^2 j_2(j_2+1)|j_2 m_2\rangle$

$J_{2z}|j_2 m_2\rangle = m_2 \hbar\, |j_2 m_2\rangle$

Now $\quad \mathcal{E} = \mathcal{E}_{j_1} \otimes \mathcal{E}_{j_2}$

TP basis $\{\, |j_1 m_1\rangle |j_2 m_2\rangle \}$

$\{\, |j_1\, j_2\, m_1\, m_2\rangle \}$

$\bar{J} = \bar{J}_1 + \bar{J}_2$

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

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

New basis: total AM (TAM) basis $\{|jm\rangle\}$

Questions:

- given j_1, j_2, what are the possible values of j?
- how do I write $\{|jm\rangle\}$ w.respect to $\{|j_1\, j_2\, m_1\, m_2\rangle\}$ basis

So: $|j_1\, j_2\, m_1\, m_2\rangle = \sum_{j,m} \underbrace{c_{jm}}\, |j m\rangle$

$|j\, m\rangle = \sum_{m_1, m_2} \underbrace{c_{j_1 j_2 m_1 m_2}}\, |j_1\, j_2\, m_1\, m_2\rangle$

Solutions:

$\bar{J} = \bar{J}_1 + \bar{J}_2$

$\bar{J} = (\hat{J}_x, \hat{J}_y, \hat{J}_z) = (\hat{J}_{1x} + \hat{J}_{2x}, \hat{J}_{1y} + \hat{J}_{2y}, \hat{J}_{1z} + \hat{J}_{2z})$

$$[\hat{J}_x, \hat{J}_y] = [J_{1x} + J_{2x}, J_{1y} + J_{2y}] =$$
$$= i\hbar J_{1z} + i\hbar J_{2z} =$$
$$= i\hbar J_z$$

. . .

- $J^2 = J_x^2 + J_y^2 + J_z^2$
- J is AM operator

$$J^2 = (\bar{J}_1 + \bar{J}_2)(\bar{J}_1 + \bar{J}_2) =$$
$$= J_1^2 + J_2^2 + 2 J_1 J_2 =$$
$$= J_1^2 + J_2^2 + 2(J_{1x} J_{2x} + J_{1y} J_{2y} + J_{1z} J_{2z})$$

<u>so:</u> $[J^2, J_{1z}] \neq 0$

$[J^2, J_{2z}] \neq 0$

<u>also:</u> $J^2 = J_1^2 + J_2^2 + 2 J_{1z} J_{2z} + \underbrace{J_{1+} J_{2-}} + \underbrace{J_{1-} J_{2+}}$

ladder operators

- tensor product states are not eigenstates of J^2

<u>also:</u> $\underbrace{\bar{J}_1 \cdot \bar{J}_2 = \frac{1}{2}(\hat{J}^2 - \hat{J}_1^2 - \hat{J}_2^2)}$

<u>What do we know</u> ?

<u>know:</u> j_1, j_2, m_1, m_2

<u>conclusions so far:</u> <u>1.</u> Not sufficient to exactly determine j

$$\hat{J}_z |j_1 j_2 m_1 m_2\rangle = \hat{J}_{1z} |j_1 j_2 m_1 m_2\rangle + \hat{J}_{2z} |j_1 j_2 m_1 m_2\rangle =$$
$$= \hbar (m_1 + m_2) |j_1 j_2 m_1 m_2\rangle$$

<u>2.</u> $\hat{J}_z$ associated eigenvalue is precisely known

$$m = m_1 + m_2$$

Q: j_1, j_2, what are the largest poss value of m_1, m_2?

- j_1, j_2

Q: Largest poss. value of $m_1 + m_2 = m$?

- $j_1 + j_2$

Q: Largest poss. value of j?

- $j_1 + j_2$

Q: Guess: min. poss value of j?

$\cancel{j_1 - j_2}$, $j_2 > j_1$

$|j_1 - j_2|$

Summary of solutions

j_1, j_2 $\quad \mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$

TP Basis

$\{ |j_1 j_2 m_1 m_2\rangle \}$

Eigenstates of

$\hat{J}_1^2, \hat{J}_2^2$

$\hat{J}_{1z}, \hat{J}_{2z}$

also J_z

TAM basis

$\{ |\underline{j_1 j_2} \, j \, m\rangle \}$

$|j \, m\rangle$ - simple notation.

Eigenstates of $\hat{J}_1^2, \hat{J}_2^2$,

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

- $j \in \{ j_1 + j_2, j_1 + j_2 - 1, \dots \; |j_1 - j_2| \}$
- $m \in \{ j, j-1, \dots \; -j+1, -j \}$ for each j

Bases:

TP: $\{ |j_1 j_2 m_1 m_2\rangle \} \Rightarrow \mathbb{1} = \sum_{m_1 = -j_1}^{j_1} \sum_{m_2 = -j_2}^{j_2} |j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2|$

TAM: $\{ |j \, m\rangle \} \Rightarrow \mathbb{1} = \sum_{j = |j_1 - j_2|}^{j_1 + j_2} \sum_{m = -j}^{j} |j \, m\rangle\langle j \, m|$

Given $|\psi\rangle \in \mathcal{E}$

- write $|\psi\rangle$ in TP or TAM representation?
- convert from one to other?

Example

- subspace that is hydrogen w/ $2p \Rightarrow \ell = 1$
- add spin of e^- — $s = \frac{1}{2}$ ignore the p^+ spin

$$\mathcal{E}_{2p} = \mathcal{E}_{\ell=1} \otimes \mathcal{E}_{s=\frac{1}{2}}$$

$$\bar{J} = \bar{L} + \bar{S}$$

qu #: $j \quad \ell \quad s$

$m_j \quad m_\ell \quad m_s$

TP basis $\{|j_1\, j_2\, m_1\, m_2\rangle\} \Rightarrow \{|\ell=1\;\; s=\frac{1}{2}\;\; m_\ell\;\; m_s\rangle\}$

$\{|1\;\; \frac{1}{2}\;\; m_\ell\;\; m_s\rangle\}$

$L^2,\ L_z,\ S^2,\ S_z$

$$L^2 |1\; \tfrac{1}{2}\; m_\ell\; m_s\rangle = 2\hbar^2 |1\; \tfrac{1}{2}\; m_\ell\; m_s\rangle$$

Dimension of $\mathcal{E}_{2p}$? $= (2\ell+1)(2s+1) =$

$= 3 \cdot 2 = 6$

Standard basis ordering.

- largest $m_1 + m_2$ and decrease
- for each $m_1 + m_2$, start with largest m_1 and decrease:

TP basis

$\{|1\;\frac{1}{2}\;\; 1,\frac{1}{2}\rangle,\ |1\;\frac{1}{2}\;\; 1\; -\frac{1}{2}\rangle,\ |1\;\frac{1}{2},\, 0\;\frac{1}{2}\rangle,\ |1\;\frac{1}{2}\;\; 0\; -\frac{1}{2}\rangle,$

$|1\;\frac{1}{2}\;\; -1\;\; \frac{1}{2}\rangle,\ |1\;\; \frac{1}{2}\;\; -1\;\; -\frac{1}{2}\rangle\}$

$$\begin{pmatrix}1\\0\\0\\0\\0\\0\end{pmatrix} \qquad\qquad \longrightarrow \qquad\qquad \begin{pmatrix}0\\0\\0\\0\\0\\1\end{pmatrix}$$

Operators - matrices with 6x6

$$S_z = \hbar \begin{pmatrix} \frac{1}{2} & & & & & \\ & -\frac{1}{2} & & & 0 & \\ & & \frac{1}{2} & & & \\ & & & -\frac{1}{2} & & \\ & 0 & & & \frac{1}{2} & \\ & & & & & -\frac{1}{2} \end{pmatrix}$$

$$= \frac{\hbar}{2} \begin{pmatrix} 1 & & & & & \\ & -1 & & & 0 & \\ & & 1 & & & \\ & 0 & & -1 & & \\ & & & & 1 & \\ & & & & & -1 \end{pmatrix}$$

TAM basis

$\max j = l + s = \frac{3}{2}$

$\min j = \frac{1}{2}$

$j = \frac{3}{2}$, $m_j = \left\{ \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \right\}$

$j = \frac{1}{2}$, $m_j = \left\{ \frac{1}{2}, -\frac{1}{2} \right\}$

standard ordering:
- largest to smallest m
- for each m_j start w/ largest to smallest j

TAM basis: $\{ |j\, m_j\rangle \}$

$\left\{ \left|\frac{3}{2}\, \frac{3}{2}\right\rangle, \left|\frac{3}{2}, \frac{1}{2}\right\rangle, \left|\frac{1}{2}, \frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{1}{2}\right\rangle, \left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{3}{2}\right\rangle \right\}$

TP	$m_j = m_1 + m_2$	TAM
$\lvert 1 \; \tfrac{1}{2} \; 1 \; \tfrac{1}{2} \rangle$	$3/2$	$\lvert \tfrac{3}{2} \; \tfrac{3}{2} \rangle$
$\lvert 1 \; \tfrac{1}{2} \; 1 \; -\tfrac{1}{2} \rangle$	$\tfrac{1}{2}$	$\lvert \tfrac{3}{2} \; \tfrac{1}{2} \rangle$
$\lvert 1 \; \tfrac{1}{2} \; 0 \; \tfrac{1}{2} \rangle$		$\lvert \tfrac{1}{2} \; \tfrac{1}{2} \rangle$
$\lvert 1 \; \tfrac{1}{2} \; 0 \; -\tfrac{1}{2} \rangle$	$-\tfrac{1}{2}$	$\lvert \tfrac{3}{2} \; -\tfrac{1}{2} \rangle$
$\lvert 1 \; \tfrac{1}{2} \; -1 \; \tfrac{1}{2} \rangle$		$\lvert \tfrac{1}{2} \; -\tfrac{1}{2} \rangle$
$\lvert 1 \; \tfrac{1}{2} \; -1 \; -\tfrac{1}{2} \rangle$	$-3/2$	$\lvert \tfrac{3}{2}, -\tfrac{3}{2} \rangle$

Example:

$$\left| \tfrac{3}{2}, \tfrac{1}{2} \right\rangle = \underbrace{\sqrt{\tfrac{1}{3}}}\, \left| 1 \; \tfrac{1}{2} \; 1 \; -\tfrac{1}{2} \right\rangle + \underbrace{\sqrt{\tfrac{2}{3}}}\, \left| 1 \; \tfrac{1}{2} \; 0 \; \tfrac{1}{2} \right\rangle$$

- 2p state $\left| \tfrac{3}{2}, \tfrac{1}{2} \right\rangle$

  what is the probability of measuring the electron spin to be down along z?

$$P = \frac{1}{3}$$

General rule:

$$|j_1\, j_2\, m_1\, m_2\rangle = \underbrace{\sum_{j=|j_1-j_2|}^{j_1+j_2} \sum_{m_j=-j}^{j} |j\, m\rangle\langle j\, m|}\, \underbrace{j_1\, j_2\, m_1\, m_2\rangle}$$

$$= \sum \sum \underbrace{\langle j\, m | j_1\, j_2\, m_1\, m_2\rangle}_{\text{coefficients}}\; |j\, m\rangle$$

$$|j\, m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \underbrace{\langle j_1\, j_2\, m_1\, m_2 | j\, m\rangle}_{\text{Clebsch-Gordan coefficients}}\; |j_1\, j_2\, m_1\, m_2\rangle$$

- real # $\Rightarrow$

FG: p118-121