$|S_1, S_2, S, m_S\rangle = |S, m_S\rangle$ because S_1, S_2 fixed.

HW ① With $H = k\vec{S}_1 \cdot \vec{S}_2$ for two spin-$\frac{1}{2}$ electrons, check states $|S_1, S_2, S, m_S\rangle$ defined in lecture note are eigen states, and find relevant eigenenergies. (here k is a constant).

Mr. Zhang tutorial of Quiz II, Sat. 3pm.

coupled density matrix not going to appear in later quiz or exams

- coupled spin-$\frac{1}{2}$ system (or general cases)

suppose we have an electron orbiting around an nuclei

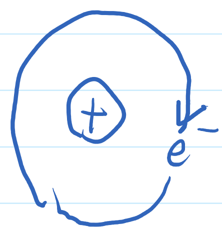
we only consider the spin of an electron

ignore nuclear spin for now.

in the electron's fram

the positive charge orbits around e^- and creates a magnetic field

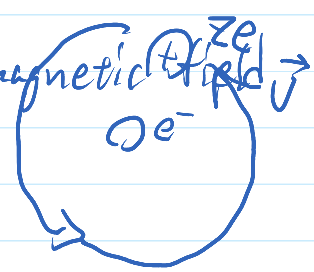
$B \propto \vec{L}$



similar to $\vec{\mu} \cdot \vec{B}$ spin under of a magnetic field

here we have $H \propto \vec{S} \cdot \vec{L}$

$\vec{L} \Rightarrow$



$\vec{S} \cdot \vec{L}$

spin of e^- orbital angular momentum

classically how much is $\vec{B}$?

classically how much is $\vec{B}$?

* not in exam, we apply Biot-Savart law

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{Ze}{r^3}\underline{(-\vec{v})\times\vec{r}} \qquad \underline{\vec{L} = \vec{r}\times\vec{p} = \vec{r}\times m_e\vec{v}}$$

$$= \frac{\mu_0}{4\pi}\frac{Ze}{m_e r^3}\vec{L}$$

托马斯进动

not quite the truth, $\frac{1}{2}$ off — Thomas precession relativistic effect.

$$\vec{B} \propto \vec{L}$$

$$\boxed{H \propto \vec{S}\cdot\vec{L}}$$

$\Leftarrow$ classically if the spin is aligned with orbital angular momentum, it has a negative sign compare to anti-align.

generalize to Quantum.

$$H = \Omega\hat{\vec{S}}\cdot\hat{\vec{L}} = \Omega(\hat{S}_x\otimes\hat{L}_x + \hat{S}_y\otimes\hat{L}_y + \hat{S}_z\otimes\hat{L}_z)$$

① recap on angular momentum.

total spin $\vec{S}$, projection along z to be S_z.

we can define eigenstate $|s, m_s\rangle$

$$\begin{cases} \vec{S}^2 |s,m_s\rangle = \hbar^2 s(s+1)|s,m_s\rangle \\ S_z|s,m_s\rangle = \hbar m_s |s,m_s\rangle \end{cases}$$

orbital $\vec{L}$, L_z

$$\begin{cases} \vec{L}^2 |l,m_l\rangle = \hbar^2 l(l+1)|l,m_l\rangle \\ L_z|l,m_l\rangle = \hbar m_l |l,m_l\rangle \end{cases}$$

state for this combined system is defined as

$$|\psi\rangle = \sum_{m_s}\sum_{m_l} C_{m_s,m_l}\underline{|s,m_s\rangle\otimes|l,m_l\rangle}$$

$|\psi\rangle = \sum_{m_s}\sum_{m_l} C_{m_s,m_l} \underline{|s,m_s\rangle \otimes |l,m_l\rangle}$

spin-orbit coupling, which is useful in atomic physics

we can also define the total angular momentum

$\vec{J} = \vec{S} + \vec{L}$ ← classical.

in quantum, $\hat{\vec{J}} = \vec{S} \otimes \underset{\uparrow}{\mathbb{1}_L} + \mathbb{1}_S \otimes \vec{L}$ ← quantum.

remember $\mathbb{1}|\phi\rangle = |\phi\rangle$ not changed. L-space

more about $\hat{\vec{J}} = (J_x, J_y, J_z)$

$$\begin{cases} J_x = S_x \otimes \mathbb{1} + \mathbb{1} \otimes L_x \\ J_y = S_y \otimes \mathbb{1} + \mathbb{1} \otimes L_y \\ J_z = S_z \otimes \mathbb{1} + \mathbb{1} \otimes L_z. \end{cases}$$

later on we will see with $\vec{J} = \vec{S} + \vec{L}$ ← still quantum but use a shorthand (简写)

with atomic physics, we know

$|l-s| \le \underset{\uparrow}{j} \le s+l$

the quantum number of $\vec{J}$

the possible choice of j is
$|l-s|,\ |l-s|+1,\ |l-s|+2,\ \dots,\ s+l-1,\ s+l$

<u>example</u>: the ground orbital of H-atom

$l=0,\ s=\frac{1}{2}$ ← electron, ignore nuclei for now

$j=\frac{1}{2},\ m_j:\ -\frac{1}{2}$ or $\frac{1}{2}$.

- we have j_z the projection along z.

with a given j, $-j \le j_z \le j$

choice is $-j, -j+1, \dots, j-1, j$.

another example. H-atom, first excited orbital $l=1$

e^- : $s=\frac{1}{2}$

j : $\frac{1}{2}$ or $\frac{3}{2}$ ← three halfs.

- termsymbol $\quad {}^{2S+1}L_J$

for example

${}^2S_{\frac{1}{2}}$ atomic state $\Rightarrow$ $s=\frac{1}{2}$, $j=\frac{1}{2}$, $l=0$

$$L = \begin{matrix} 0, & 1, & 2, & 3, & 4, & 5 \\ S, & P & D & F & G & H \end{matrix}$$

another example

${}^2P_{\frac{3}{2}}$: $\quad s = \underline{\frac{1}{2}}$, $j = \underline{\frac{3}{2}}$, $l = \underline{1}$.

- formal theory of coupled angular momentum.

we have two spins $\vec{S}$, $\vec{L}$, $\vec{L}$ may not be orbital angular.

l = integer

= also half integer 半整数.

$$\begin{cases} \vec{J} = \vec{S} + \vec{L} \\ \quad = \vec{S} \otimes \mathbb{1}_s + \mathbb{1}_L \otimes \vec{L} \\ \text{we have commuters} \\ \quad [S_k, S_l] = i\hbar\, \varepsilon_{klm} S_m \end{cases}$$

$\rightarrow \begin{cases} [S_z, S_y] = -i\hbar S_x \\ [S_x, S_y] = i\hbar S_z \end{cases}$

$$[L_k, L_l] = i\hbar\, \varepsilon_{klm} L_m.$$

$$\varepsilon_{klm} = \begin{cases} +1 & \text{if } k\text{-}l\text{-}m \text{ in order} \\ -1 & \text{if not.} \end{cases}$$

$\Rightarrow \quad J_i = S_i \otimes \mathbb{1} + \mathbb{1} \otimes L_i$, $i = x, y, z$

$\Rightarrow \quad J_i = S_i \otimes \mathbb{1} + \mathbb{1} \otimes L_i \, , \quad i = x, y, z$

$[J_k, J_l] = i\hbar \, \varepsilon_{klm} J_m$. ← can be proved from definition.

$J_i^2 = (S_i \otimes \mathbb{1} + \mathbb{1} \otimes L_i)^2$

$= S_i^2 \otimes \mathbb{1} + 2 S_i \otimes L_i + \mathbb{1} \otimes L_i^2 \, ; \quad i = x, y, z$

$\Rightarrow \quad \vec{J}^2 = J_x^2 + J_y^2 + J_z^2$

$= \vec{S}^2 + 2 \vec{S} \cdot \vec{L} + \vec{L}^2$

$(\vec{S}^2 \otimes \mathbb{1} + 2 (S_x \otimes L_x + S_y \otimes L_y + S_z \otimes L_z) + \mathbb{1} \otimes \vec{L}^2$

if we have $H = \Omega \vec{S} \cdot \vec{L}$

$= \frac{\Omega}{2} (\vec{J}^2 - \vec{S}^2 - \vec{L}^2)$

lets try to find eigenstates for $\vec{J}^2$, J_z.

we define $|j, m_j\rangle$, $\begin{cases} \vec{J}^2 |j, m_j\rangle = \hbar^2 j(j+1) |j, m_j\rangle \\ J_z |j, m_j\rangle = \hbar m_j |j, m_j\rangle . \end{cases}$

we need to find out relation between j, m_j and l, m_l, s, m_s.

① $J_z = S_z + L_z$. $\quad \langle \psi | \hat{J}_z - \hat{S}_z - L_z | \phi \rangle = \langle \psi | \hat{0} | \phi \rangle = 0$

$\hat{J}_z - \hat{S}_z - \hat{L}_z = 0$

$0 = (\langle s, m_s | \otimes \langle l, m_l |) \cdot (\hat{J}_z - S_z - L_z) \cdot | j, m_j \rangle$

$= (\hbar m_j - \hbar m_s - \hbar m_l) (\langle s, m_s | \otimes \langle l, m_l |) \cdot | j, m_j \rangle .$

{for $|j, m_j\rangle$ overlap (交叠) with $|s, m_s\rangle \otimes |l, m_l\rangle$
i.e. $(\langle s, m_s| \otimes \langle l, m_l|) \cdot |j, m_j\rangle \neq 0$

to be true we have $m_j - m_s - m_l = 0$ or

$\boxed{m_j = m_s + m_l}$ ☆ $\rightarrow$ $C_{m_l, m_s} \neq 0$ if and only if $m_l + m_s = m_j$.

$$|j, m_j\rangle = \sum_{m_l, m_s} \underline{C_{m_l m_s}} |s, m_s\rangle \otimes |l, m_l\rangle$$

↖ Clebsch-Gordan coefficient.

example, $s = \frac{1}{2}$, $l = \frac{1}{2}$ ⟵ 2 spin-$\frac{1}{2}$ system.

choices are

$|s, m_s\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$ or $|\frac{1}{2}, -\frac{1}{2}\rangle$

$|\uparrow\rangle$ $|\downarrow\rangle$

$|l, m_l\rangle = |\uparrow\rangle'$ or $|\downarrow\rangle'$

four choices of state

$|\uparrow\uparrow'\rangle$, $|\uparrow\downarrow'\rangle$, $|\downarrow\uparrow'\rangle$, $|\downarrow\downarrow'\rangle$.

forms a basis for the coupled system.

* get into the choice for j.

$|l - s| \leq j \leq l + s$.

let $l > s$, we know $-j \leq m_j \leq j$

$-j \leq m_l + m_s \leq j$

for the space defined by $|s, m_s\rangle \otimes |l, m_l\rangle$
how many possible state in this basis $\underline{(2s+1) \times (2l+1)}$
for a given s, l. ↑ times.

by choosing $|j, m_j\rangle$ as a basis instead, it won't change the dimension of Hilbert space.

for all the possible choices of $|j, m_j\rangle$ there are $(2s+1)\cdot(2l+1)$ states.

let $l > s$

$2l+1$ choices.

m_s+m_l	$m_l = l$	$m_l = l-1$	---	$m_l=-l+1$	$m_l=-l$
$m_s = s$	$s+l$	$s+l-1$			
$m_s = s-1$	$s+l-1$	$s+l-2$			
$\vdots$					
$m_s = -s+1$					
$m_s = -s$					$-s-l$

$2s+1$ choices

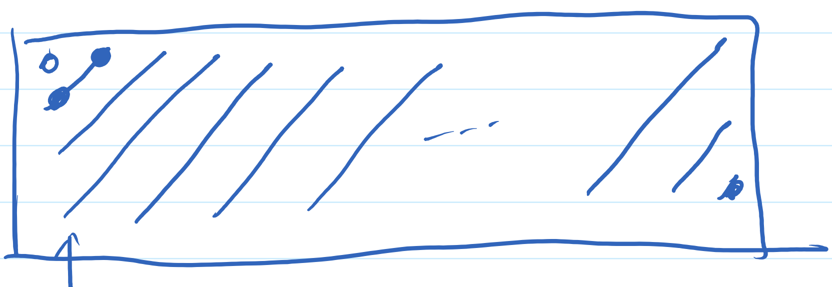
we have the maximum choice of $m_j = j = s+l$

second biggest choice of $m_j = s+l-1$.

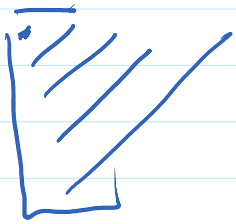
If we have $j = s+l-1$, we have $m_{j,max} = s+l-1$.

$j = s+l$ $\qquad m_j = j-1 = s+l-1$.

$l > s$ above table is in this shape



the first line hits bottom.



$\Rightarrow$ $2s+1$ states. $\Rightarrow$ $j_{min} = l+s-(2s+1)+1 = l-s$.

$|l-s|$

$2s+1$ states.

the completeness with $j_{max} = l+s$

$j_{min} = |l-s|$.

j_{max} the choice of m_j $\quad 2(l+s)+1$

$j_{max}-1$ $\quad$ " $\quad m_j$ $\quad 2(l+s-1)+1$

$\vdots$

j_{min} $\quad$ " $\quad m_j$ $\quad 2|l-s|+1$.

one can show the number of all the state

$$\sum_{i=|l-s|}^{l+s} 2i+1 = (2l+1)\times(2s+1)$$

simple proof $l \geq s$

$$\sum_{i=l-s}^{l+s} 2i+\underline{1} = 2s+1 + \sum_{i=l-s}^{l+s} \underline{2}i$$

$$= 2s+1 + \underline{2} \times \frac{(2s+1)\cdot 2l}{2} = (2s+1)(2l+1)$$

final example two electrons or two spin-$\frac{1}{2}$ system.

$s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$, $\vec{j} = \vec{s}_1 + \vec{s}_2$

what are the choice of $j = 0$ or 1.

we have $|j, m_j\rangle$

$j=0$, $\quad m_j = \underline{0} \quad \Rightarrow |j=0, m_j=0\rangle$

$j=1$, $\quad m_j = -1, 0, 1 \Rightarrow |j=1, m_j=1\rangle$

$|j=1, m_j=0\rangle$

$|j=1, m_j=-1\rangle$.

$$|j=1, m_j=1\rangle = \sum_{m_{s_1}, m_{s_2}} C_{s_1,s_2} |s_1 m_{s_1}\rangle \otimes |s_2, m_{s_2}\rangle$$

$$= \underbrace{|s_1=\tfrac{1}{2}, m_{s_1}=\tfrac{1}{2}\rangle}_{} \otimes |s_2=\tfrac{1}{2}, m_{s_2}=\tfrac{1}{2}\rangle$$

in terms $|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle$. is only state

$m_j = 1 = m_{s_1} + m_{s_2}$.

$$|j=1, m_j=-1\rangle = |s_1=\tfrac{1}{2}, m_{s_1}=-\tfrac{1}{2}\rangle \otimes |s_2=\tfrac{1}{2}, m_s=-\tfrac{1}{2}\rangle$$

$$|j=1, m_j=0\rangle = \frac{1}{\sqrt{2}}\left(|s_1, \tfrac{1}{2}\rangle |s_2, -\tfrac{1}{2}\rangle + |s_1, -\tfrac{1}{2}\rangle |s_2, \tfrac{1}{2}\rangle\right)$$

symmetric 对称

$$|j=0, m_j=0\rangle = \frac{1}{\sqrt{2}}\left(|s_1, \tfrac{1}{2}\rangle |s_2, -\tfrac{1}{2}\rangle - |s_1, -\tfrac{1}{2}\rangle |s_2, \tfrac{1}{2}\rangle\right)$$

anti-symmetric 反对称

$|j=1, m_j=\pm 1, 0\rangle \longrightarrow$ symmetric triplet 三态.

$|j=0, m_j=0\rangle \longrightarrow$ anti-sym singlet 单态.