November 4, 2008

ADDITION OF ANGULAR MOMENTUM

Interacting quantum particles can form quantum states which are e'functions of *total* angular momentum; eg for spin-$\frac{1}{2}$ particles

$$\hat{S} = S_1 + S_2$$
$$\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z} \quad |SM_s\rangle \text{ is an eigen function of } S^2 \text{ and } S_z$$

$$\hat{S}^2|SM_s\rangle = S(S+1)\hbar^2|SM_s\rangle \tag{4.64a}$$

$$\hat{S}_z|SM_s\rangle = M_s\hbar|SM_s\rangle \tag{4.64b}$$

There are 4 possible combinations of spin up & down $(\alpha_1\ \alpha_2)(\beta_1\ \beta_2)(\alpha_1\ \beta_2)(\beta_1\ \alpha_2)$ with eigenvalues $M_s = 1, -1, 0, 0$ which gives $S = 0, 1$. Shorthand for $|\alpha_1\rangle|\ \alpha_2\rangle$ etc.

For $s = 1,\ M_s = -1, 0, 1$ (Spin Triplet)

$$|SM_s\rangle = \beta_1\beta_2 \quad M_s = -1 \begin{smallmatrix}\downarrow\\\downarrow\end{smallmatrix}$$

$$|SM_s\rangle = \alpha_1\alpha_2 \quad M_s = +1 \begin{smallmatrix}\uparrow\\\uparrow\end{smallmatrix}$$

For the $S = 1$, $M_s = 0$, we form a symmetrized combination (we will show why below)

$$|SM_s\rangle = |1\ 0\rangle = \frac{1}{\sqrt{2}}[\alpha_1\beta_2 + \beta_1\alpha_2] \tag{4.65}$$

and

$$|S = 0\ M_s = 0\rangle = \frac{1}{\sqrt{2}}[\alpha_1\beta_2 - \beta_1\alpha_2] = |00\rangle \tag{4.66}$$

is SPIN SINGLET.

We can show that $|1\ 0\rangle$ is an eigen function of S^2:

$$S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2S_1 \cdot S_2 \tag{4.67}$$

also

$$\begin{aligned} 2\hat{S}_1 \cdot \hat{S}_2 &= 2\hat{S}_{1x}\hat{S}_{2x} + 2\hat{S}_{1y}\hat{S}_{2y} + 2\hat{S}_{1z}\hat{S}_{2z} \\ &= S_{1+}S_{2-} + S_{1-}S_{2+} \end{aligned}$$

Hence,

$$\hat{S}^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S_{1z}}\hat{S_{2z}} + \hat{S}_{1+}\hat{S}_{2-} + \hat{S}_{1-}\hat{S}_{2+} \tag{4.68}$$

Suppose $|\chi\rangle = a\alpha_1\beta_2 + b\beta_1\alpha_2$ is an eigenstate with $M = 0$. We want to adjust a, b so

$$S^2|\chi\rangle = S(S+1)\hbar^2|x\rangle \quad \text{for } S = 1$$

Now, we use (4.68):

$$\begin{aligned} S^2|\chi\rangle &= a\left[\frac{3}{4}\hbar^2\alpha_1\beta_2 + \frac{3}{4}\hbar^2\alpha_1\beta_2\right. \\ &\quad \left. + 2\left(\frac{\hbar}{2}\right)\alpha_1\left(-\frac{\hbar}{2}\right)\beta_2 + \hbar^2\beta_1\alpha_2\right] \quad [S_{1-}S_{2+}\ a\alpha_1\beta_2] \text{ is } \neq 0 \\ &\quad + b\left[\frac{6}{4}\hbar^2\beta_1\alpha_2 + 2\left(-\frac{\hbar}{2}\right)\beta_1\left(\frac{\hbar}{2}\right)\alpha_2 + \hbar^2\alpha_1\beta_2\right] \\ &= \alpha_1\beta_2\left[\frac{3}{2}\hbar^2 a - \frac{\hbar^2}{2}a + \hbar^2 b\right] \\ &\quad + \beta_1\alpha_2\left[\frac{3}{2}\hbar^2 b - \frac{\hbar^2}{2}b + \hbar^2 a\right] \end{aligned}$$

$$S^2|10\rangle = \alpha_1\beta 2\ [a+b]\hbar^2 + \beta_1\alpha_2\ [a+b]\hbar^2 \tag{4.69}$$

But we know

$$\begin{aligned} S^2|10\rangle &= S(s+1)\hbar^2|10\rangle = 2\hbar^2|10\rangle \\ &= 2\hbar^2(a\ \alpha_1\beta_2 + b\ \alpha_2\beta_1) \end{aligned} \tag{4.70}$$

Comparing (4.69) and (4.70), implies $2a = a + b = 2b \Rightarrow a = b$

Normalising, $|a|^2 + |b|^2 = 1 \quad \Rightarrow a = b = \frac{1}{\sqrt{2}}$

So the spin state $|SM_s\rangle = |10\rangle$

$$|10\rangle = \frac{1}{\sqrt{2}}[\alpha_1\beta_2 + \beta_1\alpha_2] \tag{4.71}$$

If $a = -b$, $\quad S^2|\chi\rangle = 0$, hence this would be the spin singlet; by the same procedure can show

$$|00\rangle = \frac{1}{\sqrt{2}}[\alpha_1\beta_2 - \beta_1\alpha_2] \tag{4.72}$$

is the $S = 0$ eigenstate with $m = 0$.

GENERAL ADDITION OF ANGULAR MOMENTA

Eg could add spin AM and orbital AM

$J = L + S$ and seek eigenfunctions of

$$J^2 = J \cdot J = (L+S)^2 = L^2 + S^2 + 2L \cdot S$$

and, as in (4.68)

$$= L^2 + S^2 + 2L_zS_z + L_+S_- + L_-S_+ \tag{4.73}$$

Also

$$J_Z = Lz + Sz$$

Most generally,

$$\begin{aligned} J &= J_1 + J_2 \\ J^2 &= J_1^2 + J_2^2 + 2J_1 \cdot J_2 \end{aligned} \tag{4.74}$$

$$= J_1^2 + J_2^2 + 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{2+}J_{1-} \tag{4.75}$$

now, J_1 and J_2 are *independent* so $[J_{1k}, J_{2y}] = 0$ all components commute

eg $[J_{1x}, J_{2y}] = 0$. While $[J_{1x}, J_{1y}] = i\hbar J_{1z}$ FROM (4.74),

$$[J^2, J_1^2] = [J^2, J_2^2] = 0 \tag{4.76}$$

We can show $[J_z, J^2] = 0$, FIRST CONSIDER

$$[J_{1z}, J_1 \cdot J_2] = [J_{1z}, (J_{1x}J_{2x} + J_{1y}J_{2y} + J_{1z}J_{2z})]$$

now

$$\begin{aligned} [J_{1z}, J_{1x}J_{2x}] &= J_{1z}J_{1x}J_{2x} - J_{1x}J_{1z}J_{2x} \\ &= J_{1z}J_{1x}J_{2x} - J_{1x}J_{1z}J_{2x} \\ &= [J_{1z}, J_{1x}]J_{2x} = i\hbar J_{1y}J_{2x} \end{aligned}$$

Similarly

$$\begin{aligned} [J_{1z}, J_{1y}J_{2y}] &= -i\hbar J_{1x}J_{2y} \\ [J_{1z}, J_{1z}J_{2z}] &= 0 \end{aligned}$$

Hence

$$[J_{1z}, J_1 \cdot J_2] = i\hbar[J_{1y}J_{2x} - J_{1x}J_{2y}] \neq 0 \tag{4.77}$$

we can also show that

$$[J_{2z}, J_1 \cdot J_2] = i\hbar[J_{2y}J_{1x} - J_{1y}J_{2x}] \neq 0 \tag{4.78}$$

$$[J_{1z}+J_{2z}, J_1\cdot J_2] = [J_z, J_1\cdot J_2] = 0 \tag{4.79}$$

So

$$\begin{aligned}[J_z, J^2] &= [J_{1z}+J_{2z}, \quad J_1^2+J_2^2+2J_1\cdot J_2] \\ &= [J_{1z}+J_{2z}, 2J_1\cdot J_2] = 0\end{aligned}$$

ie

$$[J_z, J^2] = 0 \tag{4.80}$$

But

$$\begin{aligned}[J^2, J_{1z}] \neq 0 \\ [J^2, J_{2z}] \neq 0\end{aligned}$$

Now (4.76) and (4.80) mean that we can construct states $|j_1j_2JM\rangle$ which are simultaneous eigenfunction of J^2, J_z, J_1^2, J_2^2. But are superpositions of $|j_1m_1\rangle\ |j_2m_2\rangle$

We write these superpositions as

$$|j_1j_2JM\rangle = \sum_{\substack{m_1\\m_2}} C(j_1j_2m_1m_2;\ JM)|j_1m_1\rangle|j_2m_2\rangle \tag{4.81}$$

The probability amplitudes $C(\ldots;\ JM)$ are known as Clebsch-Gordan coefficients. If you know $|j_1j_2JM\rangle$ they can be obtained from the scalar product with the

$$|j_1m_1\rangle|j_2m_2\rangle \equiv |j_1m_1j_2m_2\rangle$$

ie

$$C(j_1j_2m_1m_2; JM) = \langle j_1m_1j_2m_2|j_1j_2JM\rangle \tag{4.82}$$

alternative notation, see tables.

The sum in (4.81) ranges from

$$-j_1 \leq m_1 \leq j_1, \quad -j_2 \leq m_2 \leq j_2$$

But is constrained by $M = m_1 + m_2$. ie

$$\begin{aligned}J_z|j_1m_1\rangle|j_2m_2\rangle &= (J_{1z}+J_{2z})|j_1m_1\rangle|j_2m_2\rangle \\ &= \underbrace{(m_1+m_2)}_{M}\hbar|j_1m_1\rangle|j_2m_2\rangle\end{aligned}$$

Hence, sum in (4.81) is actually over one index only.

$$\sum_{\substack{m_1=-j_1\\m_2=M-m_1}}^{+j_1} \quad \text{or} \quad \sum_{\substack{m_2=-j_2\\m_1=M-m_2}}^{j_2} \tag{4.83}$$

EXAMPLE

Construct the state $|j_1, j_2JM\rangle = \left|\frac{3}{2}|\frac{1}{2}\frac{1}{2}\right\rangle$ using e'states $|j_1m_1\rangle|j_2m_2\rangle$, using the tables.

$$A: \quad \frac{1}{\sqrt{2}}\left|\frac{3}{2}\frac{3}{2}\right\rangle|1-1\rangle - \frac{1}{\sqrt{3}}\left|\frac{3}{2}\frac{1}{2}\right\rangle|10\rangle + \sqrt{\frac{1}{6}}\left|\frac{3}{2}\frac{-1}{2}\right\rangle|11\rangle$$

Table 1: Clebsch–Gordan Coefficients $\langle j_1 j_2 m_1 m_2 | j_1 j_2 j_m \rangle$. $\langle j_1 j_2 m_1 m_2 | j_1 j_2 j_m \rangle = (-1)^{j_1+j_2-j} \langle j_2 j_1 m_2 m_1 | j_2 j_1 j_m \rangle$

$j_1 = \frac{3}{2}$	$j_2 = 1$	$j = \frac{5}{2}$						$j = \frac{3}{2}$				$j = \frac{1}{2}$	
m_1	m_2	$m = \frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = -\frac{5}{2}$	$m = \frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$	$m = -\frac{3}{2}$	$m = \frac{1}{2}$	$m = -\frac{1}{2}$
$3/2$	1	1											
$3/2$	0		$\sqrt{2/5}$					$\sqrt{3/5}$					
$3/2$	-1			$\sqrt{1/10}$					$\sqrt{2/5}$			$\sqrt{1/2}$	
$1/2$	1		$\sqrt{3/5}$					$-\sqrt{2/5}$					
$1/2$	0			$\sqrt{3/5}$					$\sqrt{1/15}$			$-\sqrt{1/3}$	
$1/2$	-1				$\sqrt{3/10}$					$\sqrt{8/15}$			$\sqrt{1/6}$
$-1/2$	1			$\sqrt{3/10}$					$-\sqrt{8/15}$			$\sqrt{1/6}$	
$-1/2$	0				$\sqrt{3/5}$					$-\sqrt{1/15}$			$-\sqrt{1/3}$
$-1/2$	-1					$\sqrt{3/5}$					$\sqrt{2/5}$		
$-3/2$	1				$\sqrt{1/10}$					$-\sqrt{2/5}$			$\sqrt{1/2}$
$-3/2$	0					$\sqrt{2/5}$					$-\sqrt{3/5}$		
$-3/1$	-1							1					

Continued

Clebsch-Gordan coefficients

$j_1 = 2$	$j_2 = 1$	$j = 3$							$j = 2$					$j = 1$		
m_1	m_2	$m = 3$	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = -3$	$m = 2$	$m = 1$	$m = 0$	$m = -1$	$m = -2$	$m = 1$	$m = 0$	$m =$
2	1	1														
2	0		$\sqrt{1/3}$						$\sqrt{2/3}$							
2	−1			$\sqrt{1/15}$						$\sqrt{1/3}$				$\sqrt{3/5}$		
1	1		$\sqrt{2/3}$						$-\sqrt{1/3}$							
1	0			$\sqrt{8/15}$						$\sqrt{1/6}$				$-\sqrt{3/10}$		
1	−1				$\sqrt{1/5}$						$\sqrt{1/2}$				$\sqrt{3/10}$	
0	1			$\sqrt{6/15}$						$-\sqrt{1/2}$				$\sqrt{1/10}$		
0	0				$\sqrt{3/5}$						0				$-\sqrt{2/5}$	
0	−1					$\sqrt{6/15}$						$\sqrt{1/2}$				√
−1	1				$\sqrt{1/5}$						$-\sqrt{1/2}$				$\sqrt{3/10}$	
−1	0					$\sqrt{8/15}$						$-\sqrt{1/6}$				−√
−1	−1						$\sqrt{2/3}$						$\sqrt{1/3}$			
−2	1					$\sqrt{1/15}$						$-\sqrt{1/3}$				√
−2	0						$\sqrt{1/3}$						$-\sqrt{2/3}$			
−2	−1							1								

Consider an ensemble of N systems, (in M available quantum states) n_i of which are in state $\psi_i \quad (i = 1, 2, 3 \ldots M)$

We define a density operator:

$$\hat{\rho} = \sum_{i=1}^{\mathrm{M}} \mathrm{P}_i |\psi_i\rangle\langle\psi_i| \tag{4.84}$$

P_i is the probability of a system being in state $|\psi_i\rangle$.

$$P_i = n_i/N \tag{4.85}$$

A state is *pure* of $P_i = 1$ for a single state $j \Rightarrow P_i = \delta_{ij}$

ie

$$\hat{\rho} = |\psi_j\rangle\langle\psi_j| \tag{4.86}$$

If more than one p_i is non-zero ie the general form (4.84), the state is *mixed* clearly $\sum_i p_i = 1$.

Consider an operator $\hat{\mathrm{A}}$, with eigenvalues λ_n ie

$$\hat{\mathrm{A}}|n\rangle = \lambda_n|n\rangle$$

What is $\langle\hat{\mathrm{A}}\rangle$ for the ensemble of systems represented by $\hat{e}$?

For a *mixed* state

$$\langle\hat{\mathrm{A}}\rangle = \sum_i P_i \langle i\hat{\mathrm{A}}i\rangle \tag{4.87}$$

Now

$$|i\rangle = \sum_n \mathrm{C}_n^i \; |n\rangle \tag{4.88}$$

Note the difference between C_n^i, a (possibly) complex probability *amplitude*, associated with a probability $|\mathrm{C}_n^i|^2$, and p_i which is already a probability $1 \geqq p_i \geqq 0$. We may obtain wave-interference effects between the components of the superposition (4.88), but not between components of the *mixture* in (4.84).

In (6.4) we have a *quantum average*

$$\langle i\hat{\mathrm{A}}i\rangle = \sum_{m,n} \; \mathrm{C}_m^{*(i)}\mathrm{C}_n^{(i)}\langle m\hat{\mathrm{A}}n\rangle \tag{4.89}$$

$$= \sum_n \; \lambda_n|\mathrm{C}_n^{(i)}|^2 \tag{4.90a}$$

And *then* a *classical* average over the mixture:

$$\langle\hat{\mathrm{A}}\rangle = \sum_i p_i \sum_n \lambda_n|\mathrm{C}_n^{(i)}|^2 \tag{4.90b}$$

For a pure state, clearly, we just have the quantum average in (4.90a).

The density operator can be represented as a *matrix*. Choosing any complete bases, the elements of the matrix are

$$\hat{\rho}_{mn} = \langle m \; \hat{\rho} \; n\rangle. \tag{4.91}$$

For the *pure* state, for example, in (4.86)

$$\begin{aligned} \hat{\rho}_{mn}^{(j)} &= \langle m|\psi_j\rangle\langle\psi_j|n\rangle \\ &= C_m^{(j)}C_n^{(j)*}. \end{aligned} \tag{4.92}$$

PROPERTIES OF THE DENSITY MATRIX

1) $\rho = \rho^+$ (HERMITIAN).

2) $T_R(\hat{\rho}) = 1$ eg from (4.92), $\sum_{m=1}|C_m^{(j)}|^2 = 1 \; Tr \Rightarrow$ trace of the matrix $\hat{\rho}$.

3) $\hat{\rho}^2 = \hat{\rho}$ for a pure state.

4) $T_r \quad \rho^2 \leqq 1$; for a pure state of course, $T_r\hat{\rho}^2 = 1$.

5) $\hat{\rho} = \frac{1}{\mathrm{M}}\mathrm{I}$ for an ensemble uniformly distributed over M states.

$$\langle \hat{A} \rangle = Tr\ (\rho \hat{A}) \tag{4.93}$$

FOR AN OBSERVABLE $\hat{x}$ $\quad$ ($\Rightarrow \hat{x}$ is Hermitian operator)

$$Tr\hat{x} = \sum_n \langle n\ \hat{x} n\rangle$$

if $\hat{x}$ is in a matrix representation, $Tr \equiv$ trace of the matrix.

So, take a pure state:

$$\begin{aligned} \hat{x} = (\hat{\rho}\ \hat{\text{A}}) &= |\psi\rangle\ \langle\psi|\hat{\text{A}} \\ Tr\ \hat{\rho}\ \hat{\text{A}} &= \sum_n \langle n|\psi\rangle\ \langle\psi|\text{A}|n\rangle \end{aligned}$$

Since

$$\begin{aligned} |\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle &= \sum_n C_n\ |n\rangle \\ Tr(\hat{\rho}\hat{\text{A}}) &= \sum_n \langle\psi|\text{A}\ |n\rangle C_n \\ &= \langle\psi \text{A} \psi\rangle. \end{aligned}$$

Can also prove that the trace is independent of the basis $|n\rangle$ provided it is a complete orthonormal set.

EXAMPLES

1) We have particles with spin $= \frac{1}{2}$, prepared in a pure state:

$$|\psi\rangle = C_\alpha|\alpha\rangle + C_\beta|\beta\rangle$$

then

$$i = \begin{bmatrix} |C_\alpha|^2 & C_\alpha C_\beta^* \\ C_\beta C_\alpha^* & |C_\beta|^2 \end{bmatrix} \quad \text{if } S_z = \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Check that $\langle S_z\rangle = Tr(\hat{\rho}\hat{S}_z) = |C_\alpha|^2 - |C_\beta|^2$ (as in eq. 4.37).

Suppose we had the superposition $|\psi\rangle = \frac{1}{\sqrt{2}}[|\alpha\rangle + |\beta\rangle]$ then

$$\hat{\rho} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

can easily show $Tr\hat{\rho} = Tr\hat{\rho}^z = 1$. This is a pure state.

On the Other hand, suppose we have a 50:50 mix of atoms in $|\alpha\rangle$ and atoms in state $|\beta\rangle$

The density operator

$$\hat{\rho} = \frac{1}{2}|\alpha\rangle\langle\alpha| + \frac{1}{2}|\beta\rangle\langle\beta| = \sum_i p_i|\psi_i\rangle\langle\psi_i|$$

The density matrix

$$\rho = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$Tr\hat{\rho} = 1$, but $Tr\hat{\rho}^2 = \frac{1}{2}$ as this is a *mixed state.*

Suppose we have two particles. As in our $2-D$ examples (with Floquet theory), we write

$$\psi(1,2) = \sum_{n,m} C_{mn} \quad |1n\rangle|2m\rangle \tag{4.94}$$

If $C_{nm} = b_n \text{d}_m$ and $\sum_n |b_n|^2 = 1$, $\quad \sum_m |d_m|^2 = 1$

Then this is a 'product state'

$$\psi(1,2) = \left(\sum_n b_n|1n\rangle\right)\left(\sum_m d_m|2m\rangle\right) \tag{4.95}$$

ie not an 'entangled' state.

Then

$$\rho(1,2) = \sum_{n,m}\sum_{n'm'} C_{nm}C^*_{n'm'}\ |1n\rangle|2m\rangle\langle 1n'|\langle 2m'| \tag{4.96}$$

$$\langle n\ m\ \rho(1,2) n' m' \rangle = C_{nm}\ C^{*}_{n'm'} \tag{4.97}$$

Suppose that systems (1) and (2) were two particles which were separated so we could only observe particle 1. Operator $\hat{A}$ under investigation only act on particle (1) eg S_1^2 or S_{1z} or $\hat{L}_{1z}$.

If we estimate $\langle \hat{\mathrm{A}} \rangle$ from many measurements, we are automatically average over the corresponding (unknown) state of particle 2.

To get the correct $\langle \hat{\mathrm{A}} \rangle$ from observing particle (1) we evaluate

$$\langle \hat{\mathrm{A}} \rangle = Tr(\tilde{\rho}, \hat{\mathrm{A}})$$

$\tilde{\rho}$ is a reduced density operator obtained by 'tracing out' (averaging over) particle 2. From (4.96)

$$\tilde{\rho}_1 = \sum_k \langle 2k\rho\,(1,2)\,2k\rangle$$

$$\tilde{\rho}_1 = \sum_{n,n'} \sum_k C_{nk} C^{*}_{n'k} |1n\rangle\ \langle 1n'|$$

This is a matrix with elements

$$\langle 1n\ \rho_1 | n' \rangle = \sum_k C_{nk} C^{*}_{n'k} \tag{4.98}$$

It can be shown that unless we started with a product state, as in (4.95), then $\tilde{\rho}_1 \neq \tilde{\rho}_1^2$, so the reduced matrix corresponds to that of a *mixed state*, although *we know* the joint state is a pure state. (4.98) is sometimes termed an 'improper mixture'.