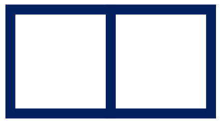
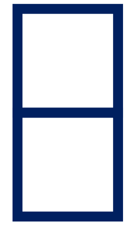
XV. Explicit construction of wave functions for a certain Young diagram

Two identical particles:  $\{2\}$  $\{1,1\}$

$$\hat{P}_{12}\Psi_{\{2\}} = \Psi_{\{2\}} \qquad \hat{P}_{12}\Psi_{\{1,1\}} = -\Psi_{\{1,1\}}$$

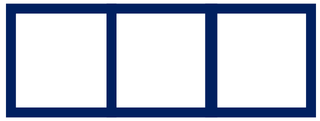
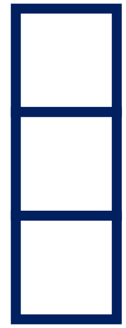
spin j and spin j yield the total spin $J = 0,\ 1,\ 2,\ \ldots\ ,\ 2j$.

$$\hat{P}_{12}|jj;JM\rangle = \hat{P}_{12}\sum_{m_1,m_2} C^{JM}_{jm_1\,jm_2}|jm_1\rangle|jm_2\rangle = \sum_{m_1,m_2} C^{JM}_{jm_2\,jm_1}|jm_1\rangle|jm_2\rangle =$$

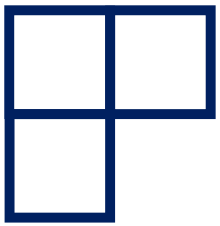
$$= (-1)^{2j-J}\sum_{m_1,m_2} C^{JM}_{jm_1\,jm_2}|jm_1\rangle|jm_2\rangle = (-1)^{2j-J}|jj;JM\rangle$$

$\{2\}$: $J = 2j,\ 2j-2,\ 2j-4,\ \ldots$

$\{1,1\}$: $J = 2j-1,\ 2j-3,\ \ldots$

Three identical particles:  $\{3\}$  $\{1,1,1\}$

$$\hat{P}_{ij}\Psi_{\{3\}} = \Psi_{\{3\}} \qquad \hat{P}_{ij}\Psi_{\{1,1,1\}} = -\Psi_{\{1,1,1\}}$$



$\{2,1\}$, an IR of S_3 with $d = 2$, transformation properties can be derived as follows:

$\psi(\sigma_1)\psi(\sigma_2)\varphi(\sigma_3)$, $\psi(\sigma_3)\psi(\sigma_2)\varphi(\sigma_1)$, $\psi(\sigma_1)\psi(\sigma_3)\varphi(\sigma_2)$ comprise a basis of a reducible representation $\{3\} + \{2,1\}$.

$$\Psi_{\{3\}}(\sigma_1,\sigma_2,\sigma_3) = [\psi(\sigma_1)\psi(\sigma_2)\varphi(\sigma_3)+\psi(\sigma_3)\psi(\sigma_2)\varphi(\sigma_1)+\psi(\sigma_1)\psi(\sigma_3)\varphi(\sigma_2)]/\sqrt{3}$$

Orthogonal states:

$$\Psi_{\{2,1\},a}(\sigma_1,\sigma_2,\sigma_3) = [\psi(\sigma_1)\psi(\sigma_2)\varphi(\sigma_3)+\psi(\sigma_3)\psi(\sigma_2)\varphi(\sigma_1)-2\psi(\sigma_1)\psi(\sigma_3)\varphi(\sigma_2)]/\sqrt{6}$$

$$\Psi_{\{2,1\},b}(\sigma_1,\sigma_2,\sigma_3) = [\psi(\sigma_1)\psi(\sigma_2)\varphi(\sigma_3) - \psi(\sigma_3)\psi(\sigma_2)\varphi(\sigma_1)]/\sqrt{2}$$

$$\hat{P}_{ij} \begin{pmatrix} \Psi_{\{2,1\},a} \\ \Psi_{\{2,1\},b} \end{pmatrix} = \mathcal{P}_{ij} \begin{pmatrix} \Psi_{\{2,1\},a} \\ \Psi_{\{2,1\},b} \end{pmatrix}$$

$$\mathcal{P}_{12} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \mathcal{P}_{13} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \qquad \mathcal{P}_{23} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

Spin j and spin j couple to an intermediate momentum K =0, 1, ... , $2j$.
Then K and j couple to the final total spin $J = |K - j|, \ldots, K + j - 1, K + j$.
Although these 3 particles are identical, we write for the sake of clarity their spins as j_1, j_2, j_3.
The basis functions (those obtained by permutations of 1,2,3 are equivalent) for each K:

$|j_1, j_2 (K); j_3; JM>$.

Definition of 6j-symbols:

$$\langle j_1 j_2 (j_{12}) j_3 j m \mid j_1, j_2 j_3 (j_{23}) j' m' \rangle = \delta_{jj'} \delta_{mm'} U(j_1 j_2 j j_3;\ j_{12} j_{23}) =$$

$$= \delta_{jj'} \delta_{mm'} (-1)^{j_1+j_2+j_3+j} \sqrt{(2j_{12}+1)(2j_{23}+1)} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix}.$$

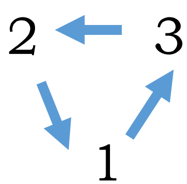
therefore

$$\langle j_1 j_2 (j_{12}) j_3 j m \mid j_1 j_3 (j_{13}) j_2 j' m' \rangle = \delta_{jj'} \delta_{mm'} (-1)^{j+j_1-j_{12}-j_{13}} U(j_2 j_1 j j_3;\ j_{12} j_{13}) =$$

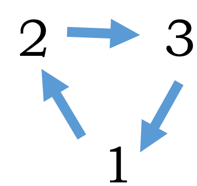
$$= \delta_{jj'} \delta_{mm'} (-1)^{j_2+j_3+j_{12}+j_{13}} \sqrt{(2j_{12}+1)(2j_{13}+1)} \begin{Bmatrix} j_2 & j_1 & j_{12} \\ j_3 & j & j_{13} \end{Bmatrix},$$

Cyclic permutations of 1, 2, 3:

$\hat{C}$



$\hat{C}^{-1}$



$$\hat{P}_{23} = \hat{P}_{12} \hat{C}, \qquad \hat{P}_{13} = \hat{P}_{12} \hat{C}^{-1}$$

$$\hat{P}_{12}|j_1, j_2(K); j_3; JM\rangle = (-1)^{2j-K}|j_1, j_2(K); j_3; JM\rangle$$

$$\hat{P}_{23}|j_1, j_2(K); j_3; JM\rangle = \hat{P}_{12}|j_2, j_3(K); j_1; JM\rangle =$$

$$= (-1)^{3j+J}\hat{P}_{12}\sum_{Q=0}^{2j}\sqrt{(2K+1)(2Q+1)}\left\{\begin{array}{ccc} j & j & Q \\ j & J & K \end{array}\right\}|j_1.j_2(Q); j_3; JM\rangle =$$

$$= \sum_{Q=0}^{2j}(-1)^{j+J-Q}\sqrt{(2K+1)(2Q+1)}\left\{\begin{array}{ccc} j & j & Q \\ j & J & K \end{array}\right\}|j_1.j_2(Q); j_3; JM\rangle$$

$$\hat{P}_{13}|j_1.j_2(K); j_3; JM\rangle =$$

$$= \sum_{Q=0}^{2j}(-1)^{2j+K+Q}\sqrt{(2K+1)(2Q+1)}\left\{\begin{array}{ccc} j & j & Q \\ j & J & K \end{array}\right\}|j_1.j_2(Q); j_3; JM\rangle$$

Then we construct linear superpositions of $| j,j\,(K); j; JM >$ that are transformed under permutations according to IR $\{\lambda\}$.

Ammonia molecule NH_3

Total-spin states of 3 hydrogene atoms

j	J	K	$\{\lambda\}$
0	0	0	$\{3\}$
$\frac{1}{2}$	$\frac{3}{2}$	1	$\{3\}$
$\frac{1}{2}$	$\frac{1}{2}$	1	$\{2, 1\}$
$\frac{1}{2}$	$\frac{1}{2}$	0	$\{2, 1\}$

Fully deuterated ammonia ND_3

Total-spin states of 3 deuterium atoms

j	J	$\Sigma\, \alpha_K \lvert(K)\rangle$	$\{\lambda\}$
1	3	$\lvert(2)\rangle$	$\{3\}$
1	2	$\lvert(2)\rangle$	$\{2, 1\}$
1	2	$\lvert(1)\rangle$	$\{2, 1\}$
1	1	$\frac{\sqrt{5}}{3}\lvert(0)\rangle + \frac{2}{3}\lvert(2)\rangle$	$\{3\}$
1	1	$\frac{2}{3}\lvert(0)\rangle - \frac{\sqrt{5}}{3}\lvert(2)\rangle$	$\{2, 1\}$
1	1	$\lvert(1)\rangle$	$\{2, 1\}$
1	0	$\lvert(1)\rangle$	$\{1, 1, 1\}$