

# Spin-spin interactions

Two possible bases:

Individual spins  $s=1/2$   
 $|1\rangle = |\uparrow\uparrow\rangle$     $|2\rangle = |\uparrow\downarrow\rangle$   
 $|3\rangle = |\downarrow\uparrow\rangle$     $|4\rangle = |\downarrow\downarrow\rangle$   
 operators  $\rightarrow$   $4 \times 4$  matrix

Total spin (of  $S^2$  and  $S_z$ ) eigenstates  
 $|S, m\rangle$     $S=0, 1$     $m=0$   
 $S=1$ ,    $m=0, \pm 1$   
 operators  $\rightarrow$   $4 \times 4$  matrix (different!)

$$|1, \pm\rangle = |\uparrow\uparrow\rangle, |1, -\rangle = |\downarrow\downarrow\rangle$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|0, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Which basis to use? Either one will work to find the hamiltonian eigenstates, but sometimes one is more convenient

1. Non-interacting spins    $\hat{H} = \omega_0 \hat{S}_{1z} + \omega_0 \hat{S}_{2z} = \omega_0 \hat{S}_z$

2. Interacting spins    $\hat{H}_{int} = \frac{2A}{\hbar} \hat{S}_1 \cdot \hat{S}_2$

Individual spins:    $\hat{H}_{int} = \frac{2A}{\hbar^2} (\hat{S}_{1x} \hat{S}_{2x} + \hat{S}_{1y} \hat{S}_{2y} + \hat{S}_{1z} \hat{S}_{2z}) =$   
 $= \frac{2A}{\hbar^2} (\frac{1}{2} \hat{S}_{1+} \hat{S}_{2-} + \frac{1}{2} \hat{S}_{1-} \hat{S}_{2+} + \hat{S}_{1z} \hat{S}_{2z})$

Using these expressions we can find matrix elements of  $\hat{H}_{int}$  in  $|1\rangle, |2\rangle, |3\rangle, |4\rangle$  basis

$$\hat{H}|1\rangle = \frac{A}{2}|1\rangle \quad \hat{H}|4\rangle = \frac{A}{2}|4\rangle \quad \hat{H}|2\rangle = +\frac{A}{2}|3\rangle + \frac{A}{2}|2\rangle$$

$$\hat{H}|3\rangle = +A|2\rangle - \frac{A}{2}|3\rangle$$

$$\hat{H} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ A/2 & 0 & 0 & 0 \\ 0 & -A/2 & A & 0 \\ 0 & A & -A/2 & 0 \\ 0 & 0 & 0 & A/2 \end{pmatrix} \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \end{matrix}$$

$$H_{11} = \langle 1|\hat{H}|1\rangle = H_{44} = \langle 4|\hat{H}|4\rangle = \frac{A}{2}$$

$$H_{22} = H_{33} = -\frac{A}{2}$$

$$H_{23} = H_{32} = A$$

Clearly, states  $|1\rangle$  &  $|4\rangle$  are the eigenstates of  $\hat{H}$   $\hat{H}|1\rangle = \frac{A}{2}|1\rangle$   $\hat{H}|4\rangle = \frac{A}{2}|4\rangle$

The states  $|2\rangle$  &  $|3\rangle$  are mixed!

Note that the central part of the Hamiltonian reminds us of the one we used for the flipping ammonia molecule!

$$\hat{H}_{\text{int}} = \begin{pmatrix} -A/2 & A \\ A & -A/2 \end{pmatrix}$$

$$\lambda_{\pm} = A/2, -3A/2$$

$$|\lambda_{+}=A/2\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |3\rangle)$$

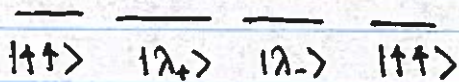
$$|\lambda_{-}=-3A/2\rangle = \frac{1}{\sqrt{2}}(|2\rangle - |3\rangle)$$

$$\hat{H}_{\text{amm}} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

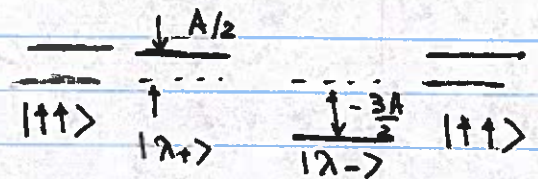
eigenvalues  $\lambda_{\pm} = E_0 \pm A$

$$|\lambda_{\pm}\rangle = \frac{1}{\sqrt{2}}(|1\rangle \mp |2\rangle)$$

Non-interacting spins  
all states have same energy (degenerate)



Interacting spin  
- degeneracy partially lifted



## Alternative solution

$$\hat{S} = (\hat{S}_1 + \hat{S}_2) \quad \hat{S}^2 = (\hat{S}_1 + \hat{S}_2)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2 \cdot \hat{S}_1 \cdot \hat{S}_2$$

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2} [\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2]$$

Recall that  $\hat{S}_i^2 = \frac{3\hbar^2}{4} \hat{1}$  acting on any wavefunction of a spin  $1/2$  particle doesn't change it

$$\hat{S}_1^2 |s, m\rangle = \frac{3\hbar^2}{4} |s, m\rangle \quad \hat{S}_2^2 |s, m\rangle = \frac{3\hbar^2}{4} |s, m\rangle$$

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

$$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2} \left[ \hbar^2 s(s+1) \hat{1} - \frac{3\hbar^2}{4} \hat{1} - \frac{3\hbar^2}{4} \hat{1} \right] = \frac{\hbar^2}{2} \left[ s(s+1) - \frac{3}{2} \right]$$

$$\hat{H} |s=1, m\rangle = \frac{2A}{\hbar^2} \cdot \frac{\hbar^2}{2} \left[ 2 - \frac{3}{2} \right] = \frac{A}{2}$$

$$\hat{H} |s=0, m=0\rangle = \frac{2A}{\hbar^2} \cdot \frac{\hbar^2}{2} \left( -\frac{3}{2} \right) = -\frac{3A}{2}$$

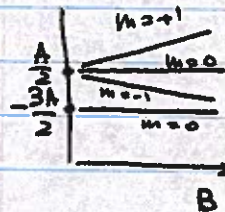
### 3. Interacting spins in the magnetic field

$$\hat{H} = \omega_0 \hat{S}_{1z} + \omega_0 \hat{S}_{2z} + \frac{2A}{\hbar^2} \hat{S}_1 \cdot \hat{S}_2 = \omega_0 \hat{S}_z + \frac{A}{\hbar^2} \left[ \hat{S}^2 - \frac{3\hbar^2}{2} \hat{1} \right]$$

still convenient to use  $|s, m\rangle$  basis

since these are still eigen states.

$$\hat{H} |s=1, m\rangle = \hbar\omega_0 m + A/2, \quad \hat{H} |s=0, m=0\rangle = -3A/2$$



### 4. Positronium atom



$$\hat{H} = \omega_0 \hat{S}_{1z} - \omega_0 \hat{S}_{2z} + \frac{2A}{\hbar^2} \hat{S}_1 \cdot \hat{S}_2$$

diagonal in  $|1z\rangle \dots |1z\rangle$  basis

diagonal in  $|s, m\rangle$  basis

← neither is ideal

Need to choose what basis, and honestly calculate matrix elements, and find eigenvalues.