Direct product

The direct product of two matrices is given by:

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \otimes \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}\mathbf{B} & A_{12}\mathbf{B} \\ A_{21}\mathbf{B} & A_{22}\mathbf{B} \end{bmatrix}$$

$$= \begin{bmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{bmatrix}$$

The direct product is used in all multi-spin treatments.

Spin-spin coupling

The direct product can be used to formally describe products of two spins.

$$I_{\eta}^{(2\,\mathrm{spin})} = I_{\eta}^{(1\,\mathrm{spin})} \otimes \mathbf{E}$$

$$S_{\eta}^{(2\,\mathrm{spin})} = \mathbf{E} \otimes S_{\eta}^{(1\,\mathrm{spin})}$$

where η = x, y or z. Therefore, the linear combination of the two 4x4 matrices gives the correct description:

$$I_{\eta}^{(2\,\mathrm{spin})} + S_{\eta}^{(2\,\mathrm{spin})} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

A closer look at the matrices

- $\mathrm{I}_\eta^{(2\ \mathrm{spin})} = \mathrm{I}_\eta^{(1\ \mathrm{spin})} \otimes \mathbf{E}$

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

- $\mathrm{S}_\eta^{(2\ \mathrm{spin})} = \mathbf{E} \otimes \mathrm{S}_\eta^{(1\ \mathrm{spin})}$

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

Treatment of scalar coupling

The fundamental rule in a two-spin system is

$$\mathbf{AB}|\mathrm{ij}> \equiv (\mathbf{A} \otimes \mathbf{B})(|\mathrm{i}> \otimes |\mathrm{j}>) = \mathbf{A}|\mathrm{i}> \otimes \mathbf{B}|\mathrm{j}>$$

A is an operator that acts in the i spin and B is an operator that acts on the j spin.

Scalar coupling Hamiltonian

$$\mathcal{H}_0 = \mathcal{H}_z + \mathcal{H}_J = \sum_{i=1}^{N} \omega_i I_{iz} + 2\pi \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} J_{ij} \boldsymbol{I_i} \cdot \boldsymbol{I_j}$$

For the two spin, IS, system we have

$$\mathcal{H} = \omega_I I_z + \omega_S S_z + 2\pi J_{IS} \boldsymbol{I} \cdot \boldsymbol{S}$$