TPSA Workshop Solutions

Derivation of Heisenberg Hamiltonian

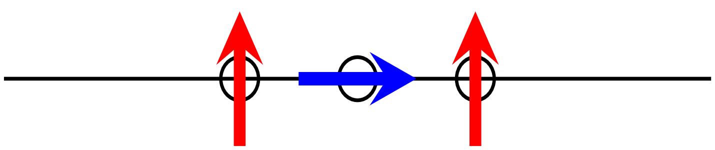
$$H = J\sum_{i<j}\vec{S}_i\cdot\vec{S}_j + B\sum_{k=0}^{2}S_{k,z} \tag{1}$$

$$\vec{S}_i = I\otimes\cdots\otimes\vec{S}\otimes I\cdots\otimes I \tag{2}$$

$$\vec{S} = \frac{1}{2}\vec{\sigma} \tag{3}$$

$$\vec{\sigma} = (X, Y, Z) \tag{4}$$

The operator $\vec{S}_i$ means the operator $\vec{S}$ acts on spin site i. Also note generally $\vec{S}$ has a factor of $\hbar$ but here $\hbar = 1$.
For the chain with 3 spins considered here, consider the first term of H.



$$\sum_{i<j}\vec{S}_i\cdot\vec{S}_j = \vec{S}_0\cdot\vec{S}_1 + \vec{S}_1\cdot\vec{S}_2 \tag{5}$$

First take the dot product as normal

$$\vec{S}_0\cdot\vec{S}_1 = S_{0,x}S_{1,x} + S_{0,y}S_{1,y} + S_{0,z}S_{1,z} \tag{6}$$

Then sub in the expressions for $S_{i,k}$ in their tensor product decomposed form

$$\vec{S}_0\cdot\vec{S}_1 = (X\otimes I\otimes I)(I\otimes X\otimes I) + (Y\otimes I\otimes I)(I\otimes Y\otimes I) + (Z\otimes I\otimes I)(I\otimes Z\otimes I) \tag{7}$$

The component of the spin vector corresponds to the Pauli matrix acting on the given site. Multiplication including tensor products acts on each site.

$$\vec{S}_0\cdot\vec{S}_1 = X\otimes X\otimes I + Y\otimes Y\otimes I + Z\otimes Z\otimes I \tag{8}$$

By repeating the same process for $\vec{S}_1\cdot\vec{S}_2$ we get

$$\vec{S}_1\cdot\vec{S}_2 = I\otimes X\otimes X + I\otimes Y\otimes Y + I\otimes Z\otimes Z \tag{9}$$

Notice that the results for the terms are a sum over the directions of the spin vector, with the Pauli matrices acting on the sites under consideration in the dot product.
We then get

$$H = \frac{J}{4}(X \otimes X \otimes I + Y \otimes Y \otimes I + Z \otimes Z \otimes I) + \frac{B}{2}(Z \otimes I \otimes I + I \otimes Z \otimes I + I \otimes I \otimes Z) \tag{10}$$

Constructing the Initial State

For a spin chain of length 3, the dimension of the Hilbert space is $2^3 = 8$. We therefore have to construct a statevector of length 8.
For example, initialising the chain in the state $|\psi_0\rangle = |0\rangle \otimes |+\rangle \otimes |0\rangle = \frac{|000\rangle+|010\rangle}{\sqrt{2}}$

$$|\psi_0\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{11}$$

The basis vectors in an 8-dimensional Hilbert space are ordered as follows, $|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle$. This is just counting but in binary.