

We have the following Hamiltonian in XXX-Heisenberg model in one dimension with periodic boundary conditions.

$$\hat{H} = -J \sum_{j=1}^N (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z)$$

if we compute the commutator of \hat{H} and spin vector operator $\vec{S} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$, this is

$$\begin{aligned} [\hat{H}, \vec{S}] &= \left[-J \sum_{j=1}^N (\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z), (\hat{S}^x, \hat{S}^y, \hat{S}^z) \right] = -J \sum_{j=1}^N [\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z, (\hat{S}^x, \hat{S}^y, \hat{S}^z)] \\ &= -J \sum_{j=1}^N ([\hat{S}_j^y \hat{S}_{j+1}^y + \hat{S}_j^z \hat{S}_{j+1}^z, \hat{S}^x], [\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^z \hat{S}_{j+1}^z, \hat{S}^y], [\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y, \hat{S}^z]) = \vec{0} \end{aligned}$$

so we can use eigenvectors of any component of \vec{S} .

For preference let use S_z then the we can use the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. Indeed the number of N_\uparrow and N_\downarrow is fixed. Also the total number $N = N_\uparrow + N_\downarrow$ is fixed.

In this sense it's useful to express $\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y$ in terms of operators \hat{S}_+^j and \hat{S}_-^j defined by

$$\begin{aligned} \hat{S}^+ &= \hat{S}^x + i\hat{S}^y \\ \hat{S}^- &= \hat{S}^x - i\hat{S}^y \end{aligned}$$

and the operators \hat{S}^x and \hat{S}^y expressed in terms of these operators

$$\begin{aligned} \hat{S}^x &= \frac{1}{2}(\hat{S}^+ + \hat{S}^-) \\ \hat{S}^y &= \frac{i}{2}(\hat{S}^- - \hat{S}^+) \end{aligned}$$

then

$$\begin{aligned} \hat{S}_j^x \hat{S}_{j+1}^x &= \left(\frac{1}{2}(\hat{S}_j^+ + \hat{S}_j^-) \right) \left(\frac{1}{2}(\hat{S}_{j+1}^+ + \hat{S}_{j+1}^-) \right) = \frac{1}{4}(\hat{S}_j^+ \hat{S}_{j+1}^+ + \hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ + \hat{S}_j^- \hat{S}_{j+1}^-) \\ \hat{S}_j^y \hat{S}_{j+1}^y &= \left(\frac{i}{2}(\hat{S}_j^- - \hat{S}_j^+) \right) \left(\frac{i}{2}(\hat{S}_{j+1}^- - \hat{S}_{j+1}^+) \right) = -\frac{1}{4}(\hat{S}_j^- \hat{S}_{j+1}^- - \hat{S}_j^- \hat{S}_{j+1}^+ - \hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^+ \hat{S}_{j+1}^+) \end{aligned}$$

so

$$\hat{S}_j^x \hat{S}_{j+1}^x + \hat{S}_j^y \hat{S}_{j+1}^y = \frac{1}{2}(\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+)$$

and the hamiltonian now is

$$\hat{H} = -\frac{J}{2} \sum_{j=1}^N (\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ + 2\hat{S}_j^z \hat{S}_{j+1}^z)$$

we know that

$$\hat{S}^+|\uparrow\rangle = 0 \quad \hat{S}^+|\downarrow\rangle = |\uparrow\rangle \quad \hat{S}^-|\uparrow\rangle = |\downarrow\rangle \quad \hat{S}^-|\downarrow\rangle = 0 \quad \hat{S}^z|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle \quad \hat{S}^z|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle$$

Construction of the basis

Now we will explore that N_{\uparrow} and N_{\downarrow} are constants. Also we explore translational invariance and periodic boundary conditions.

So we will have a set of representative states $|r_k\rangle = \hat{P}_k \frac{|r\rangle}{\sqrt{\langle r|\hat{P}_k|r\rangle}}$. And we will apply \hat{H} to these states

$$\begin{aligned}\langle r_q|\hat{H}|r_k\rangle &= \frac{\langle r_q|\hat{H}\hat{P}_k|r\rangle}{\sqrt{\langle r|\hat{P}_k|r\rangle}} = \frac{\langle r_q|\hat{P}_k\hat{H}|r\rangle}{\sqrt{\langle r|\hat{P}_k|r\rangle}} = \langle r_q|\hat{P}_k \left(-\frac{J}{2} \sum_{j=1}^N (\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ + 2\hat{S}_j^z \hat{S}_{j+1}^z) \right) \hat{c}_{N,\sigma}^\dagger \cdots \hat{c}_{j,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger \frac{|0\rangle}{\sqrt{\langle r|\hat{P}_k|r\rangle}} \\ &= -\frac{J}{2} \sum_{j=1}^N \frac{\langle r_q|\hat{P}_k (\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ + 2\hat{S}_j^z \hat{S}_{j+1}^z) \hat{c}_{N,\sigma}^\dagger \cdots \hat{c}_{j,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle}{\sqrt{\langle r|\hat{P}_k|r\rangle}}\end{aligned}$$

Since we know that

$$\begin{aligned}[\hat{S}_l^z, \hat{c}_{m,\sigma}^\dagger] &= \frac{1}{2} \delta_{lm} \hat{c}_{m,\sigma}^\dagger \\ [\hat{S}_l^+, \hat{c}_{m,\sigma}^\dagger] &= \frac{1}{2} \delta_{lm} \hat{c}_{m,\sigma}^\dagger \delta_{\sigma,\uparrow} \\ [\hat{S}_l^-, \hat{c}_{m,\sigma}^\dagger] &= \frac{1}{2} \delta_{lm} \hat{c}_{m,\sigma}^\dagger \delta_{\sigma,\downarrow}\end{aligned}$$

so for each term in the hamiltonian we will have

$$\begin{aligned}\hat{S}_j^z \hat{S}_{j+1}^z |r\rangle &= \hat{c}_{N,\sigma}^\dagger \cdots \hat{S}_j^z \hat{S}_{j+1}^z \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle = \hat{c}_{N,\sigma}^\dagger \cdots \hat{S}_j^z \hat{c}_{j,\sigma}^\dagger \hat{S}_{j+1}^z \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle \\ &= \hat{c}_{N,\sigma}^\dagger \cdots \left(\frac{1}{2} \hat{c}_{j,\sigma}^\dagger + \hat{c}_{j,\sigma}^\dagger \hat{S}_j^z \right) \left(\frac{1}{2} \hat{c}_{j+1,\sigma}^\dagger + \hat{c}_{j+1,\sigma}^\dagger \hat{S}_{j+1}^z \right) \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle = \hat{c}_{N,\sigma}^\dagger \cdots \left(\frac{1}{2} \hat{c}_{j,\sigma}^\dagger + \hat{c}_{j,\sigma}^\dagger \hat{S}_j^z \right) \left(\frac{1}{2} \hat{c}_{j+1,\sigma}^\dagger \right) \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle \\ &= \frac{1}{4} \hat{c}_{N,\sigma}^\dagger \cdots \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle = \frac{1}{4} |r\rangle \\ \hat{S}_j^+ \hat{S}_{j+1}^- |r\rangle &= \hat{c}_{N,\sigma}^\dagger \cdots \hat{S}_j^+ \hat{S}_{j+1}^- \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle = \hat{c}_{N,\sigma}^\dagger \cdots \hat{S}_j^+ \hat{c}_{j,\sigma}^\dagger \hat{S}_{j+1}^- \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle \\ &= \hat{c}_{N,\sigma}^\dagger \cdots \left(\frac{1}{2} \hat{c}_{j,\sigma}^\dagger \delta_{\sigma,\uparrow} + \hat{c}_{j,\sigma}^\dagger \hat{S}_j^+ \right) \left(\frac{1}{2} \hat{c}_{j+1,\sigma}^\dagger \delta_{\sigma,\downarrow} + \hat{c}_{j+1,\sigma}^\dagger \hat{S}_{j+1}^- \right) \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle = \hat{c}_{N,\sigma}^\dagger \cdots \left(\frac{1}{2} \hat{c}_{j,\sigma}^\dagger \delta_{\sigma,\uparrow} + \hat{c}_{j,\sigma}^\dagger \hat{S}_j^+ \right) \left(\frac{1}{2} \hat{c}_{j+1,\sigma}^\dagger \delta_{\sigma,\downarrow} \right) \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle \\ &= \frac{1}{4} \delta_{\sigma_{j+1},\downarrow} \delta_{\sigma_j,\uparrow} \hat{c}_{N,\sigma}^\dagger \cdots \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma}^\dagger \cdots \hat{c}_{1,\sigma}^\dagger |0\rangle\end{aligned}$$