Deriving the Hamiltonian in Matrix form

$$\langle \hat{G}^z(t)\rangle = \langle \psi | U^\dagger \hat{G}^z U | \psi \rangle \quad \text{with } U = e^{-iHt}$$

$$= \langle \psi | e^{iHt} \hat{G}^z e^{-iHt} | \psi \rangle$$

eigenbasis of G^z : $\left\{ \bigotimes_{i=1}^{N} \{ |\uparrow\rangle, |\downarrow\rangle \} \right\}$

$$H = J \sum_{i=1}^{N} \vec{I}_i \cdot \vec{I}_{i+1} + \sum_{i=1}^{N} B_i I_i^z$$

$$= J \sum_{i=1}^{N} \left(I_i^x I_{i+1}^x + I_i^y I_{i+1}^y + I_i^z I_{i+1}^z \right) + \sum_{i=1}^{N} B_i I_i^z$$

For $N=3$: $\{ |\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle,$
$|\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle \}$

In eigenbasis $|\varphi_i\rangle$ of H: $H|\varphi_i\rangle = E_i |\varphi_i\rangle$

1. Simplifications for starters

I. Only coupling in z-direction

II. $B_i = 0 \quad \forall i$

$$\Rightarrow H^0 = J \sum_{i=1}^{N} I_i^z I_{i+1}^z$$

$$\Rightarrow H_{11}^0 = \langle \uparrow\uparrow\uparrow | J \sum_{i=1}^{3} I_i^z I_{i+1}^z | \uparrow\uparrow\uparrow \rangle = J \cdot \left(\tfrac{1}{4} + \tfrac{1}{4} \right) = J/2$$

$$H_{22}^0 = \langle \uparrow\uparrow\downarrow | H^0 | \uparrow\uparrow\downarrow \rangle = J \cdot \left(\tfrac{1}{4} - \tfrac{1}{4} \right) = 0$$

$$H_{33}^0 = \langle \uparrow\downarrow\uparrow | H^0 | \uparrow\downarrow\uparrow \rangle = J \cdot \left(-\tfrac{1}{4} - \tfrac{1}{4} \right) = -J/2$$

$\vdots$

$$H_{ii}^0 = \langle s_1 s_2 s_3 | H^0 | s_1 s_2 s_3 \rangle = J \cdot \left(s_1 \cdot s_2 + s_2 \cdot s_3 \right)$$

$$= \frac{J}{4} \left(\mathrm{sgn}(s_1 \cdot s_2) + \mathrm{sgn}(s_2 \cdot s_3) \right)$$

$$H^0_{ii'} = \langle s_1 s_2 s_3 | H^0 | s_1' s_2' s_3' \rangle \quad , i \neq i'$$

$$= \frac{J}{4} \left(\mathrm{sgn}(s_1 \cdot s_2) + \mathrm{sgn}(s_2 \cdot s_3) \right) \underbrace{\langle s_1 s_2 s_3 | s_1' s_2' s_3' \rangle}_{=0} = 0$$

$$\Rightarrow H^0 = \frac{J}{2} \begin{array}{c} \begin{matrix} |\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle & |\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\rangle \end{matrix} \\ \begin{pmatrix} 1 & & & & & & & \\ & 0 & & & & 0 & & \\ & & -1 & & & & & \\ & & & 0 & & & & \\ & & & & 0 & & & \\ & 0 & & & & -1 & & \\ & & & & & & 0 & \\ & & & & & & & 1 \end{pmatrix} \end{array}$$

2. Now with all spin directions:

$$H^1 = J \sum_{i=1}^{N} \vec{S}_i \vec{S}_{i+1} = J \sum_{i=1}^{N} S_i^z S_{i+1}^z + S_i^x S_{i+1}^x + S_i^y S_{i+1}^y$$

$$= \underbrace{J \sum_{i=1}^{N} S_i^z S_{i+1}^z}_{H^0} + \frac{1}{2} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right)$$

$$H^1_{ii} = H^0_{ii}$$

$$S_\pm |s, m_s\rangle \overset{\hbar=1}{=} \sqrt{s(s+1) - m_s(m_s \pm 1)}\, |s, m_s \pm 1\rangle$$

$$\Rightarrow S_+ |\tfrac{1}{2}, \tfrac{1}{2}\rangle = 0 , \quad S_+ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle$$

$$S_- |\tfrac{1}{2}, \tfrac{1}{2}\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \qquad S_- |\tfrac{1}{2}, -\tfrac{1}{2}\rangle = 0$$

$$H^1_{ii'} = \langle s_1 s_2 s_3 | H^1 | s_1' s_2' s_3' \rangle$$

$$= \frac{1}{2}\left(\delta_{s_1\, s_1'+1}\, \delta_{s_2\, s_2'-1} + \delta_{s_1\, s_1'-1}\, \delta_{s_2\, s_2'+1} + \delta_{s_2\, s_2'+1}\, \delta_{s_3\, s_3'-1} + \delta_{s_2\, s_2'-1}\, \delta_{s_2\, s_2'+1} \right)$$

Integer values:
($\uparrow = 1, \downarrow = 0$)

$$H^1 = \frac{J}{2} \cdot \begin{array}{cccccccc} 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \\ |\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle & |\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\rangle \end{array}$$
$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

3) Now with magnetization terms:

$$H^2 = J \sum_{i=1}^{N} \vec{I}_i \vec{I}_{i+1} + \sum_{i=1}^{N} B_i I_i^z = H^1 + \underbrace{\sum_{i=1}^{N} B_i I_i^z}_{H^M}$$

$$H^M = \mathrm{diag}(B_1 \cdot s_1 + B_2 \cdot s_2 + B_3 \cdot s_3)$$

Diagonalization:

With eigenstates of H: $|\varphi_i\rangle$

$$H|\varphi_i\rangle = E_i|\varphi_i\rangle$$

$$\Rightarrow \langle\psi| e^{iHt} \hat{G}^z e^{-iHt} |\psi\rangle$$

$$= \sum_{i,j} \langle\psi|\varphi_i\rangle\langle\varphi_i| e^{iHt} \hat{G}^z_k e^{-iHt} |\varphi_j\rangle\langle\varphi_j|\psi\rangle$$

$$= \sum_{i,j} \langle\psi|\varphi_i\rangle\langle\varphi_i| e^{iE_it} \hat{G}^z_k \underbrace{e^{-iE_jt} |\varphi_j\rangle\langle\varphi_j|\psi\rangle}_{|\psi(t)\rangle}$$

$$\langle\psi_0| e^{iHt} \hat{G}^z e^{-iHt} |\psi_0\rangle$$

$$= \langle\psi_0| U^+ e^{iDt} U \hat{G}^z \underbrace{U^+ e^{-iDt} U |\psi_0\rangle}_{|\psi(t)\rangle}$$

Derivation of G^z:

$|\psi(t)\rangle \equiv (\psi_1(t), \psi_2(t) \dots \psi_D(t))^T$ with $D = 2^N$

For $N=3$

$$\hat{G}^z = \sum_i \psi_i(t) \cdot (\hat{S}_{i,1} \;\; \hat{S}_{i,2} \;\; \hat{S}_{i,3}) \equiv \underline{S} \cdot |\psi\rangle$$

$(3\times D)\,(D\times 1) \to (3\times 1)$

$$(\hat{G}^z_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_3)\, |\varphi_1\rangle$$

eigenstate of $\hat{G}^z_1$

Explicitly for N=3:

$$\begin{array}{ccc} 0 & 1 & 2 \\ |\downarrow\downarrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle \end{array}$$

$$\hat{G}^z = \psi_0 \cdot \left(-\tfrac{1}{2} - \tfrac{1}{2} - \tfrac{1}{2}\right) + \psi_1 \left(-\tfrac{1}{2} - \tfrac{1}{2} + \tfrac{1}{2}\right) + \dots$$

$$0 \qquad + \psi_1 (0 \;\; 0 \;\; 1) + \dots$$

Time evo vectorized:

for one specific t_0 (not vectorized):

$$|\psi(t_0)\rangle = U^\dagger \quad e^{iDt_0} \quad U \quad |\psi(t=0)\rangle$$

as matrices: $(d\times d)$ $(d\times d)$ $(d\times d)$ $(d\times 1)$

with $\dim(H) = \dim(D) = \dim(U) \equiv d$

$$\Rightarrow (d\times 1)$$

with vectorized t with array of size t_N:

goal: $|\psi(t)\rangle : (d \times t_N)$

$$\underbrace{\underbrace{\big(\underbrace{\underset{(d\times d)}{U^\dagger} \quad \underset{(t_N\times d\times d)}{e^{iDt}}}_{(t_N\times d\times d)^T}\big)^T \quad \underset{(d\times d)}{U}}_{(t_N\times d\times d)} \quad \underset{(d\times 1)}{\psi_0}}_{(t_N\times d\times 1) \,=\, (t_N \times d)}$$

Central spin Hamiltonian

$$H_{CS} = \frac{A}{N} \sum_{i=1}^{N} \hat{\vec{S}}_c \cdot \hat{\vec{S}}_i$$

Chain length

central spin

spin in Chain

$$= \frac{A}{k} \left(\sum_{i=1}^{N} S_c^z S_i^z + S_c^x S_i^x + S_c^y S_i^y \right)$$

$$S^+ = S^x + i S^y \qquad S^- = S^x - i S^y \quad \longleftrightarrow \quad S^x = \frac{1}{2}(S^+ + S^-) \qquad S^y = \frac{1}{2i}(S^+ - S^-)$$

$$S_c^x S_i^x + S_c^y S_i^y = \frac{1}{4}\left[(S_c^+ + S_c^-)(S_i^+ + S_i^-) - (S_c^+ - S_c^-)(S_i^+ - S_i^-) \right]$$

$$= \frac{1}{4}\left[\cancel{S_c^+ S_i^+} + \underline{S_c^+ S_i^-} + \underline{S_c^- S_i^+} + \cancel{S_c^- S_i^-} - \left(\cancel{S_c^+ S_i^+} - \underline{S_c^+ S_i^-} - \underline{S_c^- S_i^+} + \cancel{S_c^- S_i^-} \right) \right]$$

$$= \frac{1}{2}\left(S_c^+ S_i^- + S_c^- S_i^+ \right)$$

$$= \frac{A}{k} \left(\sum_{i=1}^{N} S_c^z S_i^z + \frac{1}{2}\left(S_c^+ S_i^- + S_c^- S_i^+ \right) \right)$$

Corresponding Matrix for $N = 3$:

$$\dim = 2^{N+1} = 16$$

Only Coupling term (all values $\cdot \frac{J}{2}$):

↑ = central spin

↑ = chain spins

		0 ↓↓↓ ↓	1 ↑↓↓ ↓	2 ↓↑↓ ↓	3 ↑↑↓ ↓	4 ↓↓↑ ↓	5 ↑↓↑ ↓	6 ↓↑↑ ↓	7 ↑↑↑ ↓	8 ↓↓↓ ↑	9 ↑↓↓ ↑	10 ↓↑↓ ↑	11 ↑↑↓ ↑	12 ↓↓↑ ↑	13 ↑↓↑ ↑	14 ↓↑↑ ↑	15 ↑↑↑ ↑
0	↓↓↓ ↓	$\frac{3}{2}$															
1	↑↓↓ ↓		$\frac{1}{2}$							1							
2	↓↑↓ ↓			$\frac{1}{2}$						1							
3	↑↑↓ ↓				$-\frac{1}{2}$						1	1					
4	↓↓↑ ↓					$\frac{1}{2}$				1							
5	↑↓↑ ↓						$-\frac{1}{2}$				1			1			
6	↓↑↑ ↓							$-\frac{1}{2}$				1		1			
7	↑↑↑ ↓								$-\frac{3}{2}$				1		1	1	
8	↓↓↓ ↑		1	1		1				$-\frac{3}{2}$							
9	↑↓↓ ↑				1		1				$-\frac{1}{2}$						
10	↓↑↓ ↑				1			1				$-\frac{1}{2}$					
11	↑↑↓ ↑								1				$\frac{1}{2}$				
12	↓↓↑ ↑						1	1						$-\frac{1}{2}$			
13	↑↓↑ ↑								1						$\frac{1}{2}$		
14	↓↑↑ ↑								1							$\frac{1}{2}$	
15	↑↑↑ ↑																$\frac{3}{2}$