

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

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

$$\begin{aligned}H &= J \sum_{i=1}^N \vec{I}_i \cdot \vec{I}_{i+1} + \sum_{i=1}^N \beta_i I_i^z \\ &= J \sum_{i=1}^N (I_i^x I_{i+1}^x + I_i^y I_{i+1}^y + I_i^z I_{i+1}^z) + \sum_{i=1}^N \beta_i I_i^z\end{aligned}$$

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.  $\beta_i = 0 \quad \forall i$

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

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

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

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

⋮

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

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

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

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

$$|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\downarrow\downarrow\downarrow\rangle$$

$$\Rightarrow H^0 = \frac{J}{2} \begin{pmatrix} 1 & & & & & & & \\ & 0 & & & & & & \\ & & -1 & & & & & \\ & & & 0 & & & & \\ & & & & 0 & & & \\ & & & & & -1 & & \\ & & & & & & 0 & \\ & & & & & & & 1 \end{pmatrix}$$

2. Now with all spin directions:

$$\begin{aligned} H^1 &= J \sum_{i=1}^N \vec{I}_i \cdot \vec{I}_{i+1} = J \sum_{i=1}^N I_i^z I_{i+1}^z + I_i^x I_{i+1}^x + I_i^y I_{i+1}^y \\ &= J \underbrace{\sum_{i=1}^{N-1} I_i^z I_{i+1}^z}_{H^0} + \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \end{aligned}$$

$$H_{ii}^1 = H_{ii}^0$$

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

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

$$S_- |\frac{1}{2}, \frac{1}{2}\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle, \quad S_- |\frac{1}{2}, -\frac{1}{2}\rangle = 0$$

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

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

Integer values:

( $\uparrow=1, \downarrow=0$ )

$$H^1 = \frac{J}{2} \cdot \begin{pmatrix} | \uparrow \uparrow \uparrow \rangle & | \uparrow \uparrow \downarrow \rangle & | \uparrow \downarrow \uparrow \rangle & | \uparrow \downarrow \downarrow \rangle & | \downarrow \uparrow \uparrow \rangle & | \downarrow \uparrow \downarrow \rangle & | \downarrow \downarrow \uparrow \rangle & | \downarrow \downarrow \downarrow \rangle \\ \hline 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

3) Now with magnetization terms:

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

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

Diagonalization:

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

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

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

$$= \sum_i \langle \psi | \varphi_i \rangle \langle \varphi_i | e^{iH\epsilon} \hat{G}_i^z e^{-iH\epsilon} | \varphi_i \rangle \langle \varphi_i | \psi \rangle$$

$$= \sum_i \langle \psi | \varphi_i \rangle \langle \varphi_i | e^{iE_i\epsilon} \hat{G}_i^z e^{-iE_i\epsilon} | \varphi_i \rangle \langle \varphi_i | \psi \rangle$$