2. Beispiel: Heisenberg-Modell, $N=4$ (Fortsetzung)

Hamilton-Matrix für $m_z=0$:

$$H \hat{=} -J \begin{array}{c} \begin{array}{cccccc} \uparrow\downarrow\uparrow\downarrow & \downarrow\uparrow\downarrow\uparrow & \uparrow\uparrow\downarrow\downarrow & \downarrow\uparrow\uparrow\downarrow & \downarrow\downarrow\uparrow\uparrow & \uparrow\downarrow\downarrow\uparrow \end{array} \\ \left(\begin{array}{cccccc} -4 & 0 & 2 & 2 & 2 & 2 \\ 0 & -4 & 2 & 2 & 2 & 2 \\ 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 & 0 \end{array}\right) \end{array} \begin{array}{c} \\ \uparrow\downarrow\uparrow\downarrow \\ \downarrow\uparrow\downarrow\uparrow \\ \uparrow\uparrow\downarrow\downarrow \\ \downarrow\uparrow\uparrow\downarrow \\ \downarrow\downarrow\uparrow\uparrow \\ \uparrow\downarrow\downarrow\uparrow \end{array}$$

Impuls $p=0$:

$$\Rightarrow \quad H\,|0,1\rangle = -J\frac{1}{\sqrt{2}}\begin{pmatrix}-4\\-4\\4\\4\\4\\4\end{pmatrix} = 4J\,|0,1\rangle - 4\sqrt{2}\,J\,|0,3\rangle$$

$$H\,|0,3\rangle = -\frac{J}{2}\begin{pmatrix}8\\8\\0\\0\\0\\0\end{pmatrix} = -4\sqrt{2}\,J\,|0,1\rangle$$

$$\Rightarrow \quad H \hat{=} J \begin{array}{c} \begin{array}{cc} |0,1\rangle & |0,3\rangle \end{array} \\ \begin{pmatrix} 4 & -4\sqrt{2} \\ -4\sqrt{2} & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ |0,1\rangle \\ |0,3\rangle \end{array}$$

$$p(\lambda) = (\lambda-4)\lambda - 32 = \lambda^2 - 4\lambda - 32$$

$$\lambda_\pm = 2 \pm \sqrt{36} = 2 \pm 6 = \begin{cases} 8 \\ -4 \end{cases}$$

$$\text{EW 8:} \begin{pmatrix} 4 & 4\sqrt{2} \\ 4\sqrt{2} & 8 \end{pmatrix}\vec{x} = 0 \Rightarrow \vec{x} = \frac{1}{\sqrt{3}}\begin{pmatrix}\sqrt{2}\\-1\end{pmatrix}$$

$\Rightarrow$ $\sqrt{\frac{2}{3}}\,|0,1\rangle - \frac{1}{\sqrt{3}}\,|0,3\rangle$ ist EV zum EW $8J$.

$EW\ -4: \quad \begin{pmatrix} -8 & 4\sqrt{2} \\ 4\sqrt{2} & -4 \end{pmatrix} \vec{x} = 0 \Rightarrow \vec{x} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix}$

$\Rightarrow \frac{1}{\sqrt{3}} |0,1\rangle + \sqrt{\frac{2}{3}} |0,3\rangle$ ist EV zum $EW\ -4J$

$p=\pi$:

$H|0,2\rangle = -\frac{J}{\sqrt{2}} \begin{pmatrix} -4 \\ 4 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 4J\,|0,2\rangle$ EV

$H|0,6\rangle = -\frac{J}{2} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0J\,|0,6\rangle$ EV

$p=\frac{\pi}{2}, \frac{3\pi}{2}$: $\quad H|0,4\rangle = -\frac{J}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0J\,|0,4\rangle$ EV

$H|0,5\rangle = -\frac{J}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0J\,|0,5\rangle$ EV

$$\begin{array}{cccccc} p=0 & p=0 & p=\pi & p=\pi & p=\frac{\pi}{2},\frac{3\pi}{2} & \\ E=8J & E=-4J & E=4J & E=0J & E=0J & E=0J \end{array}$$

$\Rightarrow EVs: \frac{1}{2\sqrt{3}} \begin{pmatrix} 2 \\ 2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}$

$m_z = 4$: $\quad p=0 \quad \uparrow\uparrow\uparrow\uparrow = |4,1\rangle; \quad H|4,1\rangle = -4|4,1\rangle$

$m_z = 2$:

$$\begin{array}{llcccccl} & & & \downarrow\uparrow\uparrow\uparrow & \uparrow\downarrow\uparrow\uparrow & \uparrow\uparrow\downarrow\uparrow & \uparrow\uparrow\uparrow\downarrow & \\ & p=0: & \frac{1}{2} & (1 & 1 & 1 & 1) & |2,1\rangle \\ \cos & p=\frac{\pi}{2}: & \frac{1}{\sqrt{2}} & (1 & 0 & -1 & 0) & |2,2\rangle \\ \sin & & 1/\sqrt{2} & (0 & 1 & 0 & -1) & |2,3\rangle \\ & p=\pi: & \frac{1}{2} & (1 & -1 & 1 & -1) & |2,4\rangle \end{array}$$

$p=0$ $\quad H|2,1\rangle = -\frac{J}{2}\begin{pmatrix} 0 & 2 & 0 & 2 \\ 2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \\ 2 & 0 & 2 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = -\frac{J}{2}\begin{pmatrix} 4 \\ 4 \\ 4 \\ 4 \end{pmatrix} = -4J\,|2,1\rangle$

$p=\frac{\pi}{2},\frac{3\pi}{2}$ $\quad H|2,2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0J|2,2\rangle \qquad H|2,3\rangle = 0J|2,3\rangle$

$p=\pi$ $\quad H|2,4\rangle = -\frac{J}{2}\begin{pmatrix} -4 \\ 4 \\ -4 \\ 4 \end{pmatrix} = 4J|2,4\rangle$

Damit haben wir das 4Spin-Heisenberg-Modell mit periodischen Randbedingungen vollständig analytisch gelöst – durch Ausnutzen der Symmetrien!

3. Beispiel: Heisenberg-Modell, $N=4$, offene Randbed.

keine Translationsinvarianz!

$N=4,\ s_z=4$: $\quad |4,1\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle\,; \quad H|4,1\rangle = -3J\,|4,1\rangle$

$s_z=2$:

		$\downarrow\uparrow\uparrow\uparrow$	$\uparrow\downarrow\uparrow\uparrow$	$\uparrow\uparrow\downarrow\uparrow$	$\uparrow\uparrow\uparrow\downarrow$
symm	$\|2,1\rangle = \frac{1}{\sqrt{2}}($	1	0	0	1)
	$\|2,2\rangle = \frac{1}{\sqrt{2}}($	0	1	1	0)
asymm	$\|2,3\rangle = \frac{1}{\sqrt{2}}($	1	0	0	−1)
	$\|2,4\rangle = \frac{1}{\sqrt{2}}($	0	1	−1	0)

$$\hat{H} = -J\begin{array}{c} \begin{array}{cccc} \downarrow\uparrow\uparrow\uparrow & \uparrow\downarrow\uparrow\uparrow & \uparrow\uparrow\downarrow\uparrow & \uparrow\uparrow\uparrow\downarrow \end{array} \\ \begin{pmatrix} 1 & 2 & 0 & 0 \\ 2 & -1 & 2 & 0 \\ 0 & 2 & -1 & 2 \\ 0 & 0 & 2 & 1 \end{pmatrix} \end{array} \begin{array}{c} \downarrow\uparrow\uparrow\uparrow \\ \uparrow\downarrow\uparrow\uparrow \\ \uparrow\uparrow\downarrow\uparrow \\ \uparrow\uparrow\uparrow\downarrow \end{array}$$

symm:

$$H\,|2,1\rangle = \frac{-J}{\sqrt{2}}\begin{pmatrix}1\\2\\2\\1\end{pmatrix} = -J\,|2,1\rangle - 2J\,|2,2\rangle$$

$$H\,|2,2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}2\\1\\1\\2\end{pmatrix} = 2J\,|2,1\rangle - J\,|2,2\rangle$$

$$H \hat{=} J\begin{pmatrix}-1 & -2\\ -2 & -1\end{pmatrix}; \quad p(\lambda) = (\lambda+1)(\lambda+1) - 4$$

$$= \lambda^2 + 2\lambda - 3$$

$$\Rightarrow \lambda_\pm = -1 \pm \sqrt{4} = \{1, -3\}$$

asymm:

$$H\,|2,3\rangle = \frac{-J}{\sqrt{2}}\begin{pmatrix}1\\2\\-2\\-1\end{pmatrix} = -J\,|2,3\rangle - 2J\,|2,4\rangle$$

$$H\,|2,4\rangle = \frac{-J}{\sqrt{2}}\begin{pmatrix}2\\-3\\3\\-2\end{pmatrix} = -2J\,|2,3\rangle + 3J\,|2,4\rangle$$

$$H \hat{=} J\begin{pmatrix}-1 & -2\\ -2 & 3\end{pmatrix}; \quad p(\lambda) = (\lambda+1)(\lambda-3) - 4$$

$$= \lambda^2 - 2\lambda - 7$$

$$\Rightarrow \lambda = 1 \pm 2\sqrt{2}$$

$S_z = 0$ (Basis abweichend von Vorlesung!)

		↑↑↓↓	↓↓↑↑	↑↓↓↑	↓↑↑↓	↑↓↑↓	↓↑↓↑
symm	$\|0,1\rangle = \frac{1}{\sqrt{2}}$	1	1				
	$\|0,2\rangle = \frac{1}{\sqrt{2}}$			1	1		
	$\|0,3\rangle = \frac{1}{\sqrt{2}}$					1	1
as	$\|0,4\rangle = \frac{1}{\sqrt{2}}$	1	−1				
	$\|0,5\rangle = \frac{1}{\sqrt{2}}$			1	−1		
	$\|0,6\rangle = \frac{1}{\sqrt{2}}$					1	−1

$$
\begin{array}{cc}
 & \begin{array}{cccccc} \uparrow\uparrow\downarrow\downarrow & \downarrow\downarrow\uparrow\uparrow & \uparrow\downarrow\downarrow\uparrow & \downarrow\uparrow\uparrow\downarrow & \uparrow\downarrow\uparrow\downarrow & \downarrow\uparrow\downarrow\uparrow \end{array} \\
H \mathrel{\hat{=}} -J & \begin{pmatrix} 1 & 0 & 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & -1 & 0 & 2 & 2 \\ 0 & 0 & 0 & -1 & 2 & 2 \\ 2 & 0 & 2 & 2 & -3 & 0 \\ 0 & 2 & 2 & 2 & 0 & -3 \end{pmatrix} \begin{array}{c} \uparrow\uparrow\downarrow\downarrow \\ \downarrow\downarrow\uparrow\uparrow \\ \uparrow\downarrow\downarrow\uparrow \\ \downarrow\uparrow\uparrow\downarrow \\ \uparrow\downarrow\uparrow\downarrow \\ \downarrow\uparrow\downarrow\uparrow \end{array}
\end{array}
$$

symm

$$H|0,1\rangle = \frac{-J}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 2 \\ 2 \end{pmatrix} = -J\left(1\,|0,1\rangle + 2\,|0,3\rangle\right)$$

$$H|0,2\rangle = \frac{-J}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ -1 \\ -1 \\ 4 \\ 4 \end{pmatrix} = -J\left(-1\,|0,2\rangle + 4\,|0,3\rangle\right)$$

$$H|0,3\rangle = \frac{-J}{\sqrt{2}} \begin{pmatrix} 2 \\ 2 \\ 4 \\ 4 \\ -3 \\ -3 \end{pmatrix} = -J\left(2\,|0,1\rangle + 4\,|0,2\rangle - 3\,|0,3\rangle\right)$$

$$H \mathrel{\hat{=}} J \begin{pmatrix} -1 & 0 & -2 \\ 0 & 1 & -4 \\ -2 & -4 & 3 \end{pmatrix}$$

$$\begin{vmatrix} \lambda+1 & 0 & 2 \\ 0 & \lambda-1 & 4 \\ 2 & 4 & \lambda-3 \end{vmatrix}$$

$$
\begin{aligned}
p(\lambda) &= (\lambda^2-1)(\lambda-3) - 4(\lambda-1) - 16(\lambda+1) \\
&= \lambda^3 - 3\lambda^2 - \lambda + 3 - 4\lambda + 4 - 16\lambda - 16 \\
&= \lambda^3 - 3\lambda^2 - 21\lambda - 9
\end{aligned}
$$

Um das allgemeine Verfahren zur Lösung von Polynomen 3. Grades zu umgehen, raten wir, dass eine schon gefundene ganzzahlige Nullstelle wieder auftritt:

$$p(\lambda) = (\lambda+3)(\lambda^2 - 6\lambda - 3)$$

$$\Rightarrow \quad \lambda_1 = -3$$

$$\lambda_{2,3} = 3 \pm 2\sqrt{3}$$

asymm: $H|0,5\rangle = J|0,5\rangle$

$$H|0,4\rangle = \frac{-J}{\sqrt{2}}\begin{pmatrix}1\\-1\\0\\0\\2\\-2\end{pmatrix} = -J|0,4\rangle - 2J|0,6\rangle$$

$$H|0,6\rangle = -\frac{J}{\sqrt{2}}\begin{pmatrix}2\\-2\\0\\0\\-3\\3\end{pmatrix} = -2J|0,4\rangle + 3J|0,6\rangle$$

$$H \hat{=} J\begin{pmatrix}-1 & -2\\-2 & 3\end{pmatrix} \qquad p(\lambda) = (\lambda+1)(\lambda-3) - 4$$

$$= \lambda^2 - 2\lambda - 7$$

$$\lambda_\pm = 1 \pm 2\sqrt{2}$$

Damit ist auch das 4-Spin-Modell mit offenen Randbedingungen exakt gelöst.

↓ nicht in Vorlesung

4. Beispiel: Heisenberg-Modell, $N=3$ (periodisch):

$m_z = 3$: $|3,1\rangle = \uparrow\uparrow\uparrow$; $H|3,1\rangle = -3\,H|3,1\rangle$

$m_z = 1$: Zustände $\downarrow\uparrow\uparrow,\ \uparrow\downarrow\uparrow,\ \uparrow\uparrow\downarrow$ antisymm Kombination muss EV sein

symm

muss EV sein	$q=0$ $\frac{1}{\sqrt{3}}$	1	1	1	$|1,1\rangle$
	$q=\frac{2\pi}{3}$ $\sqrt{\frac{2}{3}}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	$|1,2\rangle$
	$\frac{1}{\sqrt{2}}$	0	1	-1	$|1,3\rangle$

$$H \hat{=} -J\begin{pmatrix}-1 & 2 & 2\\2 & -1 & 2\\2 & 2 & -1\end{pmatrix}$$

$$H\,|1,1\rangle = -\frac{J}{\sqrt{3}}\begin{pmatrix}3\\3\\3\end{pmatrix} = -3J\,|1,1\rangle$$

$$H\,|1,2\rangle = -\sqrt{\tfrac{2}{3}}\,J\begin{pmatrix}-3\\ \frac{3}{2}\\ \frac{3}{2}\end{pmatrix} = -3J\,|1,2\rangle$$

$$H\,|1,3\rangle = -\frac{J}{\sqrt{2}}\begin{pmatrix}0\\-3\\3\end{pmatrix} = 3J\,|1,3\rangle$$

Vergleich mit allg. vollst. verbundenem Modell

$$H = -J\sum_{i\neq j}\vec{\sigma}_i\cdot\vec{\sigma}_j = -4J\sum_{i\neq j}\vec{S}_i\vec{S}_j = -2J\left(\vec{S}_{ges}^{\,2} - \sum_i \vec{S}_i^{\,2}\right)$$

$$\overset{\hbar=1}{=} -2J\left(\vec{S}_{ges}^{\,2} - \tfrac{3}{4}N\right); \quad \vec{S}_{ges}^{\,2} = S_{ges}(S_{ges}+1);$$

$S_{ges} \in \{0, 1, \ldots, \frac{N}{2}\}$ für N gerade

$S_{ges} \in \{\frac{1}{2}, \frac{3}{2}, \ldots, \frac{N}{2}\}$ " N ungerade

N	S_{ges}	$\vec{S}_{ges}^{\,2}$	$\frac{3}{4}N$	E/J
1	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{3}{4}$	0
2	0, 1	0, 2	$\frac{3}{2}$	3, −1
3	$\frac{1}{2}, \frac{3}{2}$	$\frac{3}{4}, \frac{15}{4}$	$\frac{9}{4}$	3, −3
4	0, 1, 2	0, 2, 6	3	6, 2, −6
5	$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$	$\frac{3}{4}, \frac{15}{4}, \frac{35}{4}$	$\frac{15}{4}$	6, 0, −10

nicht-ww.

$N=2$ offene Randb.

$N=3$ periodische "

$N=4$ " + NNN-WW