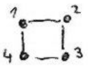
HEISENBERGOV MODEL

lastne funkcije in energije za model štirih spinov →  $\Big\}$ 16 možnih konfiguracij : matrika 16×16 → preveč zamudna diagonalizacija

hamiltonian za izotropni Heisenbergov model : $\boxed{H = J \sum_{i=1}^{4} \vec{S}_i \cdot \vec{S}_{i+1}}$

Poiščemo operatorje, ki komutirajo in delamo s tako bazo. (spomnimo se $[S_{\alpha i}, S_{\beta j}] = i\hbar\, \varepsilon_{\alpha\beta\gamma} S_\gamma \delta_{ij}$)

Operator celotnega spina $\vec{S} = \sum_{i=1}^{4} \vec{S}_i$ komutira z H :

$$[H, \vec{S}]_\alpha = [H, S_\alpha] = \Big[J \sum_{i=1,\beta}^{4} S_{i\beta} S_{i+1,\beta} , \sum_{j=1}^{4} S_{j\alpha} \Big] = J \sum_{i,j,\beta} \Big([S_{i\beta}, S_{j\alpha}] S_{i+1,\beta} + S_{i\beta} [S_{i+1,\beta}, S_{j\alpha}] \Big) =$$
$\alpha = x, y, z$

$$= J \sum_{i,j,\beta,\gamma} i\hbar \Big(\delta_{ij}\, \varepsilon_{\beta\alpha\gamma} S_{i\gamma} S_{i+1,\beta} + S_{i\beta}\, \delta_{i+1,j}\, \varepsilon_{\beta\alpha\gamma} S_{i+1,\gamma} \Big) = i\hbar J \sum_{i,\beta,\gamma} S_{i\gamma} S_{i+1,\beta} \underbrace{\big(\varepsilon_{\beta\alpha\gamma} + \varepsilon_{\gamma\alpha\beta} \big)}_{0} = \underline{\underline{0}}$$

H, S^2, S^z in T (operator translacije) komutirajo med seboj.
↳ premakne spine za eno mesto naprej : $T|\uparrow\uparrow\downarrow\downarrow\uparrow\rangle = |\downarrow\downarrow\uparrow\uparrow\rangle$

Lahko najdemo lastne funkcije, ki so lastne funkcije vseh štirih operatorjev. ☺

$$\boxed{\begin{aligned} \hat{S}_z |\psi\rangle &= S_z |\psi\rangle \\ S^2 |\psi\rangle &= S(S+1) |\psi\rangle \\ T|\psi\rangle &= e^{ika} |\psi\rangle \end{aligned}}$$

$a = 1$
$\hbar = 1$
ψ - lastna funkcija

ker je $T^4|\psi\rangle = e^{4ik}|\psi\rangle = |\psi\rangle$: $k = n\frac{\pi}{2} \in \{0, \frac{\pi}{2}, \pi, -\frac{\pi}{2}\}$

Kvantna števila bodo: $\underline{S, S_z \text{ in } k}$

PRODUKTNA BAZA (ta stanja že imajo dober celoten S_z)

$S_z = 2$: $|\uparrow\uparrow\uparrow\uparrow\rangle$
$S_z = 1$: $|\downarrow\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\uparrow\downarrow\rangle$
$S_z = 0$: $|\downarrow\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle$
$S_z = -1$: $|\uparrow\downarrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\downarrow\rangle, |\downarrow\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\downarrow\uparrow\rangle$
$S_z = -2$: $|\downarrow\downarrow\downarrow\downarrow\rangle$

Stanje $|\uparrow\uparrow\uparrow\uparrow\rangle$ ima tudi dober $S = 2$ (ne more biti manjši od 2, saj je $S_z = 2$, niti večji, saj imamo le 4 spine) in dober $k = 0$ ($T|\uparrow\uparrow\uparrow\uparrow\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle$), torej $\boxed{|\uparrow\uparrow\uparrow\uparrow\rangle = |220\rangle}$

Ostala stanja z $S = 2$ dobim tako, da na $|\uparrow\uparrow\uparrow\uparrow\rangle$ delujem z operatorjem S_- :

$$\boxed{\begin{aligned} &S_\pm = S_x \pm i S_y \\ &S_-|\uparrow\rangle = |\downarrow\rangle \\ &S_-|\downarrow\rangle = \emptyset \end{aligned}}$$

$$S_-|\uparrow\uparrow\uparrow\uparrow\rangle = \sum_{i=1}^{4} S_{i-} |\uparrow\uparrow\uparrow\uparrow\rangle = |\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\rangle = S_-|220\rangle =$$
$$= \sqrt{S(S+1) - S_z(S_z - 1)}\, |210\rangle = 2|210\rangle$$

$$\boxed{|210\rangle = \frac{1}{2}\big(|\downarrow\uparrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\uparrow\downarrow\rangle \big)}$$

$$S_-|210\rangle = \sqrt{2(2+1) - 1(1-1)}\, |200\rangle = \sqrt{6}\, |200\rangle = \frac{1}{2} \begin{pmatrix} |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + \\ + |\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + \\ + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle \end{pmatrix}$$

$$\boxed{|200\rangle = \frac{1}{\sqrt{6}} \big(|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle \big)}$$

$$\boxed{|2\,{-1}\,0\rangle = \frac{1}{2} \big(|\uparrow\downarrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\downarrow\uparrow\rangle \big)}$$

$$\boxed{|2\,{-2}\,0\rangle = |\downarrow\downarrow\downarrow\downarrow\rangle}$$

$\Big\}$ preostali dve lahko kar že zapišem

Zdaj imam že 5 stanj, še 11!

Matrični elementi med stanji, ki se razlikujejo v vsaj enem kvantnem številu, so nič! ②

primer: $\langle S S_z k | [H, S_z] | S' S_z' k' \rangle = \langle S S_z k | H S_z | S' S_z' k' \rangle - \langle S S_z k | S_z H | S' S_z' k' \rangle =$

$= (S_z' - S_z) \langle S S_z k | H | S' S_z' k' \rangle = 0$ komutator je nič

Če $S_z' \neq S_z$, potem je matrični element nič (in podobno za S^2 in T)

Pokažemo lahko, da sta energiji stanj $|S S_z k\rangle$ in $S_- |S S_z k\rangle$ enaki (isto velja za S^2 in k, $S_-|S S_z k\rangle$ ima isti S in k kot $|S S_z k\rangle$. To sledi iz $[T, S_-] = 0$ in $[S^2, S_-] = 0$)

$$[H, S_-] = [H, S_x - i S_y] = 0$$

$$[H, S_-] |S S_z k\rangle = 0 = H S_- |S S_z k\rangle - S_- H |S S_z k\rangle = \underbrace{H(S_-|S S_z k\rangle) - E(S S_z k)(S_- |S S_z k\rangle)}_{\text{Schrödingerjeva enačba } H|\psi\rangle = E|\psi\rangle}$$

Vidimo, da so taka stanja degenerirana, torej bo izračun $H|\uparrow\uparrow\uparrow\uparrow\rangle$ zadostoval za vse ostale.

$$H|\uparrow\uparrow\uparrow\uparrow\rangle = J \sum_{i=1}^{4} \left[S_i^z S_{i+1}^z + \frac{1}{2} \cancel{(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)} \right] |\uparrow\uparrow\uparrow\uparrow\rangle = J \sum_{i=1}^{4} \frac{1}{2} \cdot \frac{1}{2} |\uparrow\uparrow\uparrow\uparrow\rangle = \frac{1}{4} J \cdot 4 |\uparrow\uparrow\uparrow\uparrow\rangle =$$
$$= \underline{\underline{J |\uparrow\uparrow\uparrow\uparrow\rangle}}$$

Iz produktnih stanj z $S_z = 1$ tvorimo stanja z dobrim k:

$$|\psi\rangle = \frac{1}{2} \left(|\downarrow\uparrow\uparrow\uparrow\rangle + e^{ik} |\uparrow\downarrow\uparrow\uparrow\rangle + e^{2ik} |\uparrow\uparrow\downarrow\uparrow\rangle + e^{3ik} |\uparrow\uparrow\uparrow\downarrow\rangle \right) \longrightarrow \text{Blochova stanja}$$

$$T|\psi\rangle = e^{ik} |\psi\rangle$$

$$\boxed{\begin{aligned} |1\,1\,-\tfrac{\pi}{2}\rangle &= \tfrac{1}{2} \left(|\downarrow\uparrow\uparrow\uparrow\rangle - i |\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle + i |\uparrow\uparrow\uparrow\downarrow\rangle \right) \\ |1\,1\,\tfrac{\pi}{2}\rangle &= \tfrac{1}{2} \left(|\downarrow\uparrow\uparrow\uparrow\rangle + i |\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - i |\uparrow\uparrow\uparrow\downarrow\rangle \right) \\ |1\,1\,\pi\rangle &= \tfrac{1}{2} \left(|\downarrow\uparrow\uparrow\uparrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\uparrow\uparrow\downarrow\rangle \right) \end{aligned}}$$

funkcija z $k = 0$ pa je že zapisana $|2\,1\,0\rangle$

Stanja z nižjim S_z spet dobim tako, da delujem z S_-:

$$S_-|1\,1\,k\rangle = \sqrt{2}\,|1\,0\,k\rangle = \frac{1}{2} \begin{pmatrix} |\downarrow\downarrow\uparrow\uparrow\rangle + e^{ik} |\downarrow\downarrow\uparrow\uparrow\rangle + e^{2ik} |\downarrow\uparrow\downarrow\uparrow\rangle + e^{3ik} |\downarrow\uparrow\uparrow\downarrow\rangle + \\ + |\downarrow\uparrow\downarrow\uparrow\rangle + e^{ik} |\uparrow\downarrow\downarrow\uparrow\rangle + e^{2ik} |\uparrow\downarrow\downarrow\uparrow\rangle + e^{3ik} |\uparrow\downarrow\uparrow\downarrow\rangle + \\ + |\downarrow\uparrow\uparrow\downarrow\rangle + e^{ik} |\uparrow\downarrow\uparrow\downarrow\rangle + e^{2ik} |\uparrow\uparrow\downarrow\downarrow\rangle + e^{3ik} |\uparrow\uparrow\downarrow\downarrow\rangle \end{pmatrix} =$$

$$= \frac{1}{2} \left[(1 + e^{ik}) \left(|\downarrow\downarrow\uparrow\uparrow\rangle + e^{ik} |\uparrow\downarrow\downarrow\uparrow\rangle + e^{2ik} |\uparrow\uparrow\downarrow\downarrow\rangle + e^{3ik} |\downarrow\uparrow\uparrow\downarrow\rangle \right) + (1 + e^{2ik}) \left(|\downarrow\uparrow\downarrow\uparrow\rangle + e^{ik} |\uparrow\downarrow\uparrow\downarrow\rangle \right) \right]$$

$$\boxed{\begin{aligned} |1\,0\,-\tfrac{\pi}{2}\rangle &= \tfrac{1}{2} \left(|\downarrow\downarrow\uparrow\uparrow\rangle - i |\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle + i |\downarrow\uparrow\uparrow\downarrow\rangle \right) \\ |1\,0\,\tfrac{\pi}{2}\rangle &= \tfrac{1}{2} \left(|\downarrow\downarrow\uparrow\uparrow\rangle + i |\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - i |\downarrow\uparrow\uparrow\downarrow\rangle \right) \\ |1\,0\,\pi\rangle &= \tfrac{1}{\sqrt{2}} \left(|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\downarrow\rangle \right) \end{aligned}}$$

Poznamo tudi stanja $|1\,{-1}\,{-\tfrac{\pi}{2}}\rangle$, $|1\,{-1}\,\tfrac{\pi}{2}\rangle$ in $|1\,{-1}\,\pi\rangle$ (lahko delujemo z S_- na $|1\,0\,k\rangle$ ali pa zamenjamo $\uparrow$ in $\downarrow$ v $|1\,1\,k\rangle$.

Zdaj imam že 5+9 stanj, še 2!

Stanja z $S_z = -1, 0, 1$ imajo enako energijo - **enomagnonska vzbujena stanja FM**:

$$E(S{=}1, S_z, k) = E(S{=}2, S_z, 0) - J \sin^2\frac{k}{2} = J\left(1 - \sin^2\frac{k}{2}\right) \xrightarrow{k = \pi} 0 \qquad \xrightarrow{k = \pm\frac{\pi}{2}} J/2$$

Preostali 2 stanji imata $S_z=0$ (imamo že $|200\rangle$, $|10{-}\tfrac{\pi}{2}\rangle$, $|10\tfrac{\pi}{2}\rangle$, $|10\pi\rangle$). Iz šestih produktnih stanj z $S_z=0$ lahko tvorim šest stanj z dobrim k:

$$|a\rangle = \frac{1}{2}\left(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \right) \quad k=0$$

$$|b\rangle = \frac{1}{2}\left(|\downarrow\downarrow\uparrow\uparrow\rangle + i|\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - i|\downarrow\uparrow\uparrow\downarrow\rangle \right) \quad k=\frac{\pi}{2} \longrightarrow |10\tfrac{\pi}{2}\rangle$$

$$|c\rangle = \frac{1}{2}\left(|\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle \right) \quad k=\pi \longrightarrow |00\pi\rangle$$

$$|d\rangle = \frac{1}{2}\left(|\downarrow\downarrow\uparrow\uparrow\rangle - i|\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle + i|\downarrow\uparrow\uparrow\downarrow\rangle \right) \quad k=-\frac{\pi}{2} \longrightarrow |10{-}\tfrac{\pi}{2}\rangle$$

$$\begin{matrix}\uparrow & \uparrow\\ \downarrow & \downarrow\end{matrix}$$

$$|e\rangle = \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle \right) \quad k=0$$

$$|f\rangle = \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\downarrow\uparrow\downarrow\rangle \right) \quad k=\pi \longrightarrow |10\pi\rangle$$

$$\begin{matrix}\uparrow & \downarrow\\ \downarrow & \uparrow\end{matrix}$$

Iz stanj $|a\rangle$ in $|e\rangle$ tvorim $|200\rangle$: $\quad |200\rangle = \dfrac{2|a\rangle + \sqrt{2}|e\rangle}{\sqrt{6}}$

ortogonalno stanje je $|000\rangle$: $\quad |000\rangle = \dfrac{\sqrt{2}|a\rangle - 2|e\rangle}{\sqrt{6}}$

(Zakaj $S=0$? $|a\rangle$ in $|e\rangle$ imata k in $S_z=0$, za $S=1$ pa bi dobili 3 stanja (ne potrebujemo toliko, zato je edina možnost $S=0$)

$$\boxed{|000\rangle = \frac{1}{\sqrt{12}}\left(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \right) - \frac{1}{\sqrt{3}}\left(|\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle \right)}$$

Stanje $|c\rangle$ se ne meša z $|000\rangle$ ali $|200\rangle$, saj ima drugačen k ($|c\rangle = |00\pi\rangle$) ($S=0$ iz istega razloga kot zgoraj)

$$\boxed{|00\pi\rangle = \frac{1}{2}\left(|\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle \right)}$$

Izračunajmo energiji $|a\rangle$ in $|e\rangle$: energije $|c\rangle$ ne računamo, saj za nas ni zanimiva

$$H|\downarrow\downarrow\uparrow\uparrow\rangle = J\cdot\left(\cancel{\tfrac{1}{4}-\tfrac{1}{4}+\tfrac{1}{4}-\tfrac{1}{4}}\right)|\downarrow\downarrow\uparrow\uparrow\rangle + \overbrace{\frac{1}{2}J\left(|\downarrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle \right)}^{\frac{J}{2}\sum (S_i^+S_{i+1}^- + S_i^-S_{i+1}^+)}$$

in enako za $H|\uparrow\downarrow\downarrow\uparrow\rangle$, $H|\uparrow\uparrow\downarrow\downarrow\rangle$, $H|\downarrow\uparrow\uparrow\downarrow\rangle$

$$H|\uparrow\downarrow\uparrow\downarrow\rangle = J\cdot\overbrace{\left(-\tfrac{1}{4}-\tfrac{1}{4}-\tfrac{1}{4}-\tfrac{1}{4}\right)}^{-1}|\uparrow\downarrow\uparrow\downarrow\rangle + \frac{1}{2}J\left(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \right)$$

in enako za $H|\downarrow\uparrow\downarrow\uparrow\rangle$

torej: $H|a\rangle = \sqrt{2}J|e\rangle \qquad \left(H\cdot 2|a\rangle = \tfrac{1}{2}J\cdot 4\cdot\sqrt{2}|e\rangle \right)$

$H|e\rangle = -J|e\rangle + \sqrt{2}J|a\rangle \qquad \left(H\sqrt{2}|e\rangle = -J\cdot\sqrt{2}|e\rangle + \tfrac{1}{2}J\cdot 4|a\rangle \right)$

$$\begin{pmatrix} \langle a|H|a\rangle & \langle a|H|e\rangle \\ \langle e|H|a\rangle & \langle e|H|e\rangle \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{2}J \\ \sqrt{2}J & -J \end{pmatrix} \longrightarrow \text{lastne vrednosti: } E^2 + JE - 2J^2 = 0$$

$$E = \frac{-J \pm 3J}{2} = \{J, -2J\}$$

lastni vektor $\begin{pmatrix} 2 \\ \sqrt{2} \end{pmatrix}$ lastni vektor $\begin{pmatrix} \sqrt{2} \\ -2 \end{pmatrix}$

Stanje $|200\rangle$ ima energijo J, stanje $|000\rangle$ pa energijo $-2J$.

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za $J<0$ (FM): osnovno stanje ima $E=J$ in je $|\psi\rangle = |\uparrow\uparrow\uparrow\uparrow\rangle = |220\rangle$ (petkrat degenerirano)

za $J>0$ (AFM): osnovno stanje ima $E=-2J$ in je $|\psi\rangle = \frac{1}{\sqrt{12}}\left(|\downarrow\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \right) - \frac{1}{\sqrt{3}}\left(|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle \right) = |000\rangle$

Vidimo, da osnovno stanje antiferomagneta nima le kombinacije $|\uparrow\downarrow\uparrow\downarrow\rangle$ in $|\downarrow\uparrow\downarrow\uparrow\rangle$, temveč tudi ostale člene, ki jih ne bi ravno pripisali antiferomagnetu.