

Computational Many-Body Physics - Sheet 4

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The full implementation of all exercises can be found under https://github.com/Fhoeddinghaus/cmbp22-exercises/tree/main/sheet_4.

1. Spin-models on a three-site cluster

Consider the following (general) Hamiltonian for a spin-model on a three-site cluster:

$$H = - \sum_{\alpha} \sum_{i < j} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$$

with $i, j = 1, 2, 3$ and $\alpha = x, y, z$.

a).

With the operators

$$\begin{aligned} S_i^{\pm} &= S_i^x \pm i S_i^y, \quad \text{and} \quad S_i^z \\ \rightsquigarrow S_i^x &= \frac{1}{2}(S_i^+ + S_i^-), \\ \rightsquigarrow S_i^y &= \frac{1}{2i}(S_i^+ - S_i^-) \end{aligned}$$

we can rewrite the Hamiltonian to

$$\begin{aligned} \underline{\underline{H}} &= - \sum_{i < j} (J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z) \\ &= - \sum_{i < j} \left(J_{ij}^x \frac{1}{4} (S_i^+ + S_i^-) \cdot (S_j^+ + S_j^-) - J_{ij}^y \frac{1}{4} (S_i^+ - S_i^-) \cdot (S_j^+ - S_j^-) + J_{ij}^z S_i^z S_j^z \right) \\ &= - \sum_{i < j} \left(J_{ij}^x \frac{1}{4} (S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-) - J_{ij}^y \frac{1}{4} (S_i^+ S_j^+ - S_i^+ S_j^- - S_i^- S_j^+ + S_i^- S_j^-) + J_{ij}^z S_i^z S_j^z \right) \end{aligned}$$

b). Hamilton matrix for the Ising model

In the Ising model it is $J_{ij}^{\alpha} = J \delta_{\alpha z}$, therefore the Hamiltonian reduces to

$$H = -J \sum_{i < j} S_i^z S_j^z.$$

We can then construct the Hamilton matrix \bar{H} calculating $\langle n | H | m \rangle$ for $n, m = 000, 100, 010, 110, 001, 101, 011, 111$ (notation: inverse binary numbers $0, \dots, 2^3 - 1$).

For the z -term, we use that $S_i^z |m_i\rangle = \pm \frac{1}{2} |m_i\rangle$ and therefore $S_i^z S_j^z |m\rangle = \text{sgn}_z \frac{1}{4} |m\rangle$ with

$$\text{sgn}_z = \begin{cases} +1 & : m_i = m_j \\ -1 & : m_i \neq m_j \end{cases}.$$

Therefore, we can rewrite the Hamilton-operator as

$$\begin{aligned}
H &= -\frac{J}{4} \sum_{i < j} (\text{sgn}_z(m_i, m_j)) \\
&= -\frac{J}{4} (\text{sgn}_z(m_1, m_2) + \text{sgn}_z(m_1, m_3) + \text{sgn}_z(m_2, m_3)) = -\frac{J}{4} \cdot \begin{cases} 3 & : m = 000, 111 \\ -1 & : \text{else} \end{cases}
\end{aligned}$$

$$\begin{aligned}
H |m\rangle &= -\frac{J}{4} (\text{sgn}_z(m_1, m_2) + \text{sgn}_z(m_1, m_3) + \text{sgn}_z(m_2, m_3)) |m\rangle \\
\rightsquigarrow \langle n | H |m\rangle &= -\frac{J}{4} (\text{sgn}_z(m_1, m_2) + \text{sgn}_z(m_1, m_3) + \text{sgn}_z(m_2, m_3)) \langle n | m\rangle \\
&= -\frac{J}{4} (\text{sgn}_z(m_1, m_2) + \text{sgn}_z(m_1, m_3) + \text{sgn}_z(m_2, m_3)) \delta_{n,m}
\end{aligned}$$

i.e.

$$\begin{aligned}
\langle 000 | H | 000 \rangle &= -\frac{J}{4} \cdot 3, & \langle 100 | H | 100 \rangle &= -\frac{J}{4} \cdot (-1), \\
\langle 010 | H | 010 \rangle &= -\frac{J}{4} \cdot (-1), & \langle 110 | H | 110 \rangle &= -\frac{J}{4} \cdot (-1), \\
\langle 001 | H | 001 \rangle &= -\frac{J}{4} \cdot (-1), & \langle 101 | H | 101 \rangle &= -\frac{J}{4} \cdot (-1), \\
\langle 011 | H | 011 \rangle &= -\frac{J}{4} \cdot (-1), & \langle 111 | H | 111 \rangle &= -\frac{J}{4} \cdot 3
\end{aligned}$$

are the non-zero elements. The full Hamilton matrix is given by

$$\bar{H} = \begin{array}{c} \begin{matrix} \langle 000 | \\ \langle 100 | \\ \langle 010 | \\ \langle 110 | \\ \langle 001 | \\ \langle 101 | \\ \langle 011 | \\ \langle 111 | \end{matrix} \end{array} \begin{bmatrix} \begin{matrix} |000\rangle & |100\rangle & |010\rangle & |110\rangle & |001\rangle & |101\rangle & |011\rangle & |111\rangle \\ -\frac{3 \cdot J}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{4} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{J}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{J}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{J}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{J}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{J}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3 \cdot J}{4} \end{matrix} \end{bmatrix}$$

c). Hamilton matrix for the isotropic Heisenberg model

In the isotropic Heisenberg model it is $J_{ij}^\alpha = J$, therefore the Hamiltonian is

$$H = -J \sum_{i < j} \left(\frac{1}{4} (S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-) + \frac{1}{4} (-S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ - S_i^- S_j^-) + S_i^z S_j^z \right)$$

For convenience, we can use that only one of the terms $S_i^\beta S_j^\gamma$ ($\beta, \gamma = \pm$) in the sum results in a non-zero result for $H |m\rangle$, and identify that this results in exactly flipped spins i, j of $|m\rangle$.

Therefore, we can rewrite the Hamilton-operator using the X-Pauli-operator σ^x ($\hat{=}$ spin-flip). With this approach, we can first rewrite the x -terms using $\sigma_i^x \sigma_j^x$ (only one non-zero term) and likewise for the y -terms, but with a sign

$$\text{sgn}_y = \begin{cases} +1 & : m_i \neq m_j \\ -1 & : m_i = m_j \end{cases} .$$

For the z -term, we use that $S_i^z |m_i\rangle = \pm \frac{1}{2} |m_i\rangle$ and therefore $S_i^z S_j^z |m\rangle = \text{sgn}_z \frac{1}{4} |m\rangle$ with

$$\text{sgn}_z = -\text{sgn}_y = \begin{cases} +1 & : m_i = m_j \\ -1 & : m_i \neq m_j \end{cases} .$$

Therefore, we can rewrite the Hamiltonian as

$$\begin{aligned}
H &= -\frac{J}{4} \sum_{i < j} (\sigma_i^x \sigma_j^x + \text{sgn}_y(\mathbf{m}_i, \mathbf{m}_j) \cdot \sigma_i^x \sigma_j^x + \text{sgn}_z(\mathbf{m}_i, \mathbf{m}_j)) = -\frac{J}{4} \sum_{i < j} ((1 + \text{sgn}_y(\mathbf{m}_i, \mathbf{m}_j)) \cdot \sigma_i^x \sigma_j^x + \text{sgn}_z(\mathbf{m}_i, \mathbf{m}_j)) \\
&= -\frac{J}{4} ((1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_2)) \sigma_1^x \sigma_2^x + (1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_3)) \sigma_1^x \sigma_3^x + (1 + \text{sgn}_y(\mathbf{m}_2, \mathbf{m}_3)) \sigma_2^x \sigma_3^x \\
&\quad + \underbrace{\text{sgn}_z(\mathbf{m}_1, \mathbf{m}_2) + \text{sgn}_z(\mathbf{m}_1, \mathbf{m}_3) + \text{sgn}_z(\mathbf{m}_2, \mathbf{m}_3)}_{= \begin{cases} 3 & : m = 000, 111 \\ -1 & : \text{else} \end{cases}})
\end{aligned}$$

Then it is

$$\begin{aligned}
H |m_1 m_2 m_3\rangle &= -\frac{J}{4} ((1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_2)) \sigma_1^x \sigma_2^x |m_1 m_2 m_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_3)) \sigma_1^x \sigma_3^x |m_1 m_2 m_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_2, \mathbf{m}_3)) \sigma_2^x \sigma_3^x |m_1 m_2 m_3\rangle \\
&\quad + (\text{sgn}_z(\mathbf{m}_1, \mathbf{m}_2) + \text{sgn}_z(\mathbf{m}_1, \mathbf{m}_3) + \text{sgn}_z(\mathbf{m}_2, \mathbf{m}_3)) |m_1 m_2 m_3\rangle) \\
&= -\frac{J}{4} ((1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_2)) |\bar{m}_1 \bar{m}_2 m_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_3)) |\bar{m}_1 m_2 \bar{m}_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_2, \mathbf{m}_3)) |m_1 \bar{m}_2 \bar{m}_3\rangle \\
&\quad + (\text{sgn}_z(\mathbf{m}_1, \mathbf{m}_2) + \text{sgn}_z(\mathbf{m}_1, \mathbf{m}_3) + \text{sgn}_z(\mathbf{m}_2, \mathbf{m}_3)) |m_1 m_2 m_3\rangle) \\
\rightsquigarrow \langle n_1 n_2 n_3 | H |m_1 m_2 m_3\rangle &= -\frac{J}{4} ((1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_2)) \langle n_1 n_2 n_3 | \bar{m}_1 \bar{m}_2 m_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_3)) \langle n_1 n_2 n_3 | \bar{m}_1 m_2 \bar{m}_3\rangle \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_2, \mathbf{m}_3)) \langle n_1 n_2 n_3 | m_1 \bar{m}_2 \bar{m}_3\rangle \\
&\quad + (\text{sgn}_z(\mathbf{m}_1, \mathbf{m}_2) + \text{sgn}_z(\mathbf{m}_1, \mathbf{m}_3) + \text{sgn}_z(\mathbf{m}_2, \mathbf{m}_3)) \langle n_1 n_2 n_3 | m_1 m_2 m_3\rangle) \\
&= -\frac{J}{4} ((1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_2)) \delta_{n_1, \bar{m}_1} \delta_{n_2, \bar{m}_2} \delta_{n_3, m_3} \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_1, \mathbf{m}_3)) \delta_{n_1, \bar{m}_1} \delta_{n_2, m_2} \delta_{n_3, \bar{m}_3} \\
&\quad + (1 + \text{sgn}_y(\mathbf{m}_2, \mathbf{m}_3)) \delta_{n_1, m_1} \delta_{n_2, \bar{m}_2} \delta_{n_3, \bar{m}_3} \\
&\quad + (\text{sgn}_z(\mathbf{m}_1, \mathbf{m}_2) + \text{sgn}_z(\mathbf{m}_1, \mathbf{m}_3) + \text{sgn}_z(\mathbf{m}_2, \mathbf{m}_3)) \delta_{n, m})
\end{aligned}$$

Using this, the non-zero elements are

$$\begin{aligned}
\langle n|H|n\rangle &= -\frac{J}{4}(\text{sgn}_z(n_1, n_2) + \text{sgn}_z(n_1, n_3) + \text{sgn}_z(n_2, n_3)) = -\frac{J}{4} \begin{cases} 3 & : [n]_2 = 000, 111 \\ -1 & : \text{else} \end{cases} \\
&\rightsquigarrow \langle 000|H|000\rangle = \langle 111|H|111\rangle = -\frac{3J}{4} \\
&\rightsquigarrow \langle 100|H|100\rangle = \langle 010|H|010\rangle = \langle 110|H|110\rangle \\
&= \langle 001|H|001\rangle = \langle 101|H|101\rangle = \langle 011|H|011\rangle = +\frac{J}{4} \\
\langle n_1 n_2 n_3|H|\bar{n}_1 \bar{n}_2 \bar{n}_3\rangle &= -\frac{J}{4}(1 + \text{sgn}_y(\bar{n}_1, \bar{n}_2)) = \begin{cases} -\frac{J}{2} & : n_1 \neq n_2, \\ 0 & : n_1 = n_2 \end{cases} \\
&\rightsquigarrow \langle 100|H|010\rangle = \langle 010|H|100\rangle = \langle 101|H|011\rangle = \langle 011|H|101\rangle = -\frac{J}{2} \\
\langle n_1 n_2 n_3|H|\bar{n}_1 n_2 \bar{n}_3\rangle &= -\frac{J}{4}(1 + \text{sgn}_y(\bar{n}_1, \bar{n}_3)) = \begin{cases} -\frac{J}{2} & : n_1 \neq n_3, \\ 0 & : n_1 = n_3 \end{cases} \\
&\rightsquigarrow \langle 100|H|001\rangle = \langle 001|H|100\rangle = \langle 110|H|011\rangle = \langle 011|H|110\rangle = -\frac{J}{2} \\
\langle n_1 n_2 n_3|H|n_1 \bar{n}_2 \bar{n}_3\rangle &= -\frac{J}{4}(1 + \text{sgn}_y(\bar{n}_2, \bar{n}_3)) = \begin{cases} -\frac{J}{2} & : n_2 \neq n_3, \\ 0 & : n_2 = n_3 \end{cases} \\
&\rightsquigarrow \langle 010|H|001\rangle = \langle 001|H|010\rangle = \langle 110|H|101\rangle = \langle 101|H|110\rangle = -\frac{J}{2}
\end{aligned}$$

The full Hamilton matrix is then given by

$$\bar{H} = \begin{bmatrix} -\frac{3J}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{J}{4} & -\frac{J}{2} & 0 & -\frac{J}{2} & 0 & 0 & 0 \\ 0 & -\frac{J}{2} & \frac{J}{4} & 0 & -\frac{J}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{J}{4} & 0 & -\frac{J}{2} & -\frac{J}{2} & 0 \\ 0 & -\frac{J}{2} & -\frac{J}{2} & 0 & \frac{J}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{J}{2} & 0 & \frac{J}{4} & -\frac{J}{2} & 0 \\ 0 & 0 & 0 & -\frac{J}{2} & 0 & -\frac{J}{2} & \frac{J}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3J}{4} \end{bmatrix}$$

d).

Let a model have $J_{12}^x = J_{23}^y = J_{13}^z = J$ and all other $J_{ij}^\alpha = 0$, therefore the Hamiltonian reduces to

$$\begin{aligned}
H &= - \left(J_{12}^x \frac{1}{4} \underbrace{(S_1^+ S_2^+ + S_1^+ S_2^- + S_1^- S_2^+ + S_1^- S_2^-)}_{=\sigma_1^x \sigma_2^x} + J_{23}^y \frac{1}{4} \underbrace{(-S_2^+ S_3^+ + S_2^+ S_3^- + S_2^- S_3^+ - S_2^- S_3^-)}_{=\text{sgn}_y(m_2, m_3) \sigma_2^x \sigma_3^x} + J_{31}^z \underbrace{S_3^z S_1^z}_{=\text{sgn}_z(m_1, m_3) \frac{1}{4}} \right) \\
&= -\frac{J}{4} (\sigma_1^x \sigma_2^x + \text{sgn}_y(m_2, m_3) \sigma_2^x \sigma_3^x + \text{sgn}_z(m_1, m_3))
\end{aligned}$$

Then it is

$$\begin{aligned}
H |m_1 m_2 m_3\rangle &= -\frac{J}{4} (\sigma_1^x \sigma_2^x |m_1 m_2 m_3\rangle + \text{sgn}_y(m_2, m_3) \sigma_2^x \sigma_3^x |m_1 m_2 m_3\rangle + \text{sgn}_z(m_1, m_3) |m_1 m_2 m_3\rangle) \\
&= -\frac{J}{4} (|\bar{m}_1 \bar{m}_2 m_3\rangle + \text{sgn}_y(m_2, m_3) |m_1 \bar{m}_2 \bar{m}_3\rangle + \text{sgn}_z(m_1, m_3) |m_1 m_2 m_3\rangle) \\
\rightsquigarrow \langle n_1 n_2 n_3|H|m_1 m_2 m_3\rangle &= -\frac{J}{4} (\langle n_1 n_2 n_3|\bar{m}_1 \bar{m}_2 m_3\rangle + \text{sgn}_y(m_2, m_3) \langle n_1 n_2 n_3|m_1 \bar{m}_2 \bar{m}_3\rangle \\
&\quad + \text{sgn}_z(m_1, m_3) \langle n_1 n_2 n_3|m_1 m_2 m_3\rangle) \\
&= -\frac{J}{4} (\delta_{n_1, \bar{m}_1} \delta_{n_2, \bar{m}_2} \delta_{n_3, m_3} + \text{sgn}_y(m_2, m_3) \delta_{n_1, m_1} \delta_{n_2, \bar{m}_2} \delta_{n_3, \bar{m}_3} + \text{sgn}_z(m_1, m_3) \delta_{n, m})
\end{aligned}$$

Using this, the non-zero elements are

$$\begin{aligned}
\langle n|H|n\rangle &= -\frac{J}{4} \text{sgn}_z(n_1, n_3) = \begin{cases} -\frac{J}{4} & : n_1 = n_3 \\ +\frac{J}{4} & : n_1 \neq n_3 \end{cases} \\
&\rightsquigarrow \langle 000|H|000\rangle = \langle 010|H|010\rangle = \langle 101|H|101\rangle = \langle 111|H|111\rangle = -\frac{J}{4} \\
&\rightsquigarrow \langle 100|H|100\rangle = \langle 110|H|110\rangle = \langle 001|H|001\rangle = \langle 011|H|011\rangle = +\frac{J}{4} \\
\langle n_1 n_2 n_3|H|\bar{n}_1 \bar{n}_2 \bar{n}_3\rangle &= -\frac{J}{4} \\
&\rightsquigarrow \langle 000|H|110\rangle = \langle 100|H|010\rangle = \langle 010|H|100\rangle = \langle 110|H|000\rangle \\
&= \langle 001|H|111\rangle = \langle 101|H|011\rangle = \langle 011|H|101\rangle = \langle 111|H|001\rangle = -\frac{J}{4} \\
\langle n_1 n_2 n_3|H|n_1 \bar{n}_2 \bar{n}_3\rangle &= -\frac{J}{4} \cdot \text{sgn}_y(\bar{n}_2 \bar{n}_3) = \begin{cases} -\frac{J}{4} & : n_2 \neq n_3 \\ +\frac{J}{4} & : n_2 = n_3 \end{cases} \\
&\rightsquigarrow \langle 010|H|001\rangle = \langle 110|H|101\rangle = \langle 001|H|010\rangle = \langle 101|H|110\rangle = -\frac{J}{4} \\
&\rightsquigarrow \langle 000|H|011\rangle = \langle 100|H|111\rangle = \langle 011|H|000\rangle = \langle 111|H|100\rangle = +\frac{J}{4}
\end{aligned}$$

The full Hamilton matrix is then given by

$$\bar{H} = \begin{bmatrix} -\frac{J}{4} & 0 & 0 & -\frac{J}{4} & 0 & 0 & \frac{J}{4} & 0 \\ 0 & \frac{J}{4} & -\frac{J}{4} & 0 & 0 & 0 & 0 & \frac{J}{4} \\ 0 & -\frac{J}{4} & -\frac{J}{4} & 0 & -\frac{J}{4} & 0 & 0 & 0 \\ -\frac{J}{4} & 0 & 0 & \frac{J}{4} & 0 & -\frac{J}{4} & 0 & 0 \\ 0 & 0 & -\frac{J}{4} & 0 & \frac{J}{4} & 0 & 0 & -\frac{J}{4} \\ 0 & 0 & 0 & -\frac{J}{4} & 0 & -\frac{J}{4} & -\frac{J}{4} & 0 \\ \frac{J}{4} & 0 & 0 & 0 & 0 & -\frac{J}{4} & \frac{J}{4} & 0 \\ 0 & \frac{J}{4} & 0 & 0 & -\frac{J}{4} & 0 & 0 & -\frac{J}{4} \end{bmatrix}$$

2. Hamilton matrices for spin models

Consider a spin model of the form

$$H = - \sum_{ij\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha}$$

with $i, j = 1, \dots, N$ and $\alpha = x, y, z$.

a). Implementation

First, we need a way to store the Hamilton matrix and the couplings J_{ij}^{α} efficiently. This can be done using so called SparseArrays¹, which only store the non-zero elements.

Using this, we initialize the couplings Js as a three-component vector consisting of empty $N \times N$ sparse matrices:

```
1 function reset_Js(N)
2     Js = [sparse(zeros(N,N)) for α in 1:3]; # 3 NxN matrices (α = x, y, z)
3     return Js
4 end
```

Listing 1: Function to set-up the storage for the couplings J_{ij}^{α} .

This corresponds to $J_{ij}^{\alpha} = 0 \forall i, j, \alpha$. The non-zero values have to be set later for specific models before calculating the Hamilton matrix.

Now, we introduce a few smaller helper functions, that will make the implementation² of the algorithm later easier.

- `n_dual()`: convert $[n]_{10}$ to $[n]_2$ (in reversed³ order of notation, that is also used for $|n\rangle$)

```
1 n_dual(n) = digits(n, base=2, pad=N)
```

- `l()`: calculating $l(n)$ for the action of $S_i^{\alpha} S_j^{\alpha}$ for $\alpha = x, y$, defined as

$$l = n + (1 - 2z_i)2^{i-1} + (1 - 2z_j)2^{j-1}$$

for $n = [z_1 z_2 \dots z_N]$.

```
1 l(n,i,j) = n + (1 - 2 * n_dual(n)[i]) * 2^(i-1) + (1 - 2 * n_dual(n)[j]) * 2^(j-1)
```

¹Concretely, we use the matrix-type SparseMatrixCSC from the package SparseArrays.jl.

²The full code for this exercise can be found in 2_hamilton_matrices_for_spin_models.ipynb

³Normally, we would write a binary number n as $[z_{N-1} z_{N-2} \dots z_1 z_0]_2$, but in this lecture we write it as $[z_1 z_2 \dots z_N]$ (reversed order and shifted index)

- the three prefactors for the different terms of $\alpha = x, y, z$:

```

1  # prefactor  $\lambda^x$  for the x-component of the interaction of spins i and j of  $|n\rangle$ 
2  #  $-J^x_{ij} S^x_i S^x_j |n\rangle \mapsto \lambda^x |l\rangle$ 
3  function x_link_prefactor(Js, n, i, j)
4       $\alpha = 1$  #  $x \hat{=} 1$ 
5      return  $-1/4 * Js[\alpha][i, j]$ 
6  end
7
8  # prefactor  $\lambda^y$  for the y-component of the interaction of spins i and j of  $|n\rangle$ 
9  #  $-J^y_{ij} S^y_i S^y_j |n\rangle \mapsto \lambda^y |l\rangle$ 
10 function y_link_prefactor(Js, n, i, j)
11      $\alpha = 2$  #  $y \hat{=} 2$ 
12     # calculate the sign, +1 for  $n_i \neq n_j$ , -1 for  $n_i = n_j$ 
13     s = - (2 * n_dual(n)[i] - 1) * (2 * n_dual(n)[j] - 1)
14     return  $-1/4 * s * Js[\alpha][i, j]$ 
15 end
16
17 # prefactor  $\lambda^z$  for the z-component of the interaction of spins i and j of  $|n\rangle$ 
18 #  $-J^z_{ij} S^z_i S^z_j |n\rangle \mapsto \lambda^z |l\rangle$ 
19 function z_link_prefactor(Js, n, i, j)
20      $\alpha = 3$  #  $z \hat{=} 3$ 
21     # calculate the sign, +1 for  $n_i = n_j$ , -1 for  $n_i \neq n_j$ 
22     s = (2 * n_dual(n)[i] - 1) * (2 * n_dual(n)[j] - 1)
23     return  $-1/4 * s * Js[\alpha][i, j]$ 
24 end

```

Listing 2: Functions to calculate the x -, y - and z -link terms separately.

With these functions and using the function `findnz()`, which enables us to iterate only over the non-zero elements of J_s , we can implement the algorithm to calculate the Hamilton matrix for a given N and $\{J_{ij}^\alpha\}$:

```

1  function calculate_hamilton_matrix(Js, N)
2       $\tilde{H}$  = sparse(zeros(2^N, 2^N)) # empty  $2^N \times 2^N$  matrix
3      for n in 0:(2^N-1)
4          # for each  $|n\rangle$  set the non-zero matrix elements
5
6          # 1. loop over all components  $\alpha = x, y, z$ 
7          for  $\alpha$  in [1, 2, 3]
8              # 2. loop over only non-zero links in Js
9              # iterate over non-zero elements by using findnz()
10             for (i, j, J) in zip(findnz(Js[ $\alpha$ ])...)
11
12                 if  $\alpha == 1$  #  $\alpha \hat{=} x$ 
13                     m = l(n, i, j) # calculate  $|l\rangle$  from  $|n\rangle$  for i, j
14                     # add to the matrix element  $\langle l | H | n \rangle$  the x-link-term
15                      $\tilde{H}[m+1, n+1] += x\_link\_prefactor(Js, n, i, j)$ 
16                 elseif  $\alpha == 2$  #  $\alpha \hat{=} y$ 
17                     m = l(n, i, j) # calculate  $|l\rangle$  from  $|n\rangle$  for i, j
18                     # add to the matrix element  $\langle l | H | n \rangle$  the y-link-term
19                      $\tilde{H}[m+1, n+1] += y\_link\_prefactor(Js, n, i, j)$ 
20                 else
21                     #  $\alpha \hat{=} z$ , diagonal element
22                      $\tilde{H}[n+1, n+1] += z\_link\_prefactor(Js, n, i, j)$ 
23                 end
24             end
25         end
26     end
27     return  $\tilde{H}$ 
28 end

```

Listing 3: Function to calculate a Hamilton matrix from a given set of couplings $\{J_{ij}^\alpha\}$ for a general N -site spin-model.

b). Three-site clusters

We can now verify the results from the first exercise by calculating the Hamilton matrices using the code from above. After that, we can calculate the eigenenergies of each model just by using `eigvals()` from `LinearAlgebra.jl`.

An important note is, that in exercise 1 the Hamiltonians had the restriction of $i < j$. This has to be considered while setting up the matrices representing $\{J_{ij}^\alpha\}$ (or by introducing a factor $\frac{1}{2}$, if symmetric J s are used).

Furthermore, we used the packages `SymPy` and `Latexify` for easier comparison with the results from above⁴.

b).1. Ising model

We recall: $J_{ij}^\alpha = J\delta_{\alpha,z}$ and $i < j$.

The couplings are set-up like this:

```

1  N = 3
2
3  # Ising
4  Js_ising = reset_Js(N)
5  # 1 (J) for all i<j for  $\alpha \hat{=} z$ , 0 for  $\alpha \neq z$ 
6  Js_ising[3] = [
7      0 1 1
8      0 0 1
9      0 0 0
10 ]

```

leading to $J_{ij}^{x,y} = 0 \forall i, j$ and

$$J^z = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

The resulting Hamilton matrix from `H_ising = calculate_hamilton_matrix(Js_ising, N)` is then analogous to exercise 1⁵:

$$\bar{H}_{Ising} = \begin{bmatrix} -\frac{3J}{4} & & & & & & \\ & \frac{J}{4} & & & & & \\ & & \frac{J}{4} & & & & \\ & & & \frac{J}{4} & & & \\ & & & & \frac{J}{4} & & \\ & & & & & \frac{J}{4} & \\ & & & & & & -\frac{3J}{4} \end{bmatrix}$$

The eigenenergies are with

```

1  E_ising = eigvals(Matrix(rationalize.(H_ising)) * sympify("J"))

```

given by

$$E_{n=0,7} = -\frac{3J}{4} \qquad E_{n=1,\dots,6} = \frac{J}{4}.$$

In this case, the eigenstates correspond to $|n\rangle$.

⁴We can output our results with the symbol "J" instead of leaving $J = 1$

⁵`latexify(Matrix(rationalize.(H_ising)) * sympify("J"))` used for conversion to LaTeX

b).2. Isotropic Heisenberg model

We recall: $J_{ij}^\alpha = J$ and $i < j$.

The couplings are set-up like this:

```

1 N = 3
2
3 # Isotropic Heisenberg
4 Js_Heisenberg = reset Js(N)
5 # 1 (J) for all i<j for  $\alpha \hat{=} z$ , 0 for  $\alpha \neq z$ 
6 Js_Heisenberg[1] = [
7     0 1 1
8     0 0 1
9     0 0 0
10 ]
11 Js_Heisenberg[2] = Js_Heisenberg[1]
12 Js_Heisenberg[3] = Js_Heisenberg[1]

```

leading to

$$J^x = J^y = J^z = \begin{bmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

The resulting Hamilton matrix from $\bar{H}_{\text{Heisenberg}} = \text{calculate_hamilton_matrix}(\text{Js_Heisenberg}, N)$ is then analogous to exercise 1 ($\hat{=} 0$ for visual clarity):

$$\bar{H}_{\text{Heisenberg}} = \begin{bmatrix} -\frac{3J}{4} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{J}{4} & -\frac{J}{2} & \cdot & -\frac{J}{2} & \cdot & \cdot & \cdot \\ \cdot & -\frac{J}{2} & \frac{J}{4} & \cdot & -\frac{J}{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \frac{J}{4} & \cdot & -\frac{J}{2} & -\frac{J}{2} & \cdot \\ \cdot & -\frac{J}{2} & -\frac{J}{2} & \cdot & \frac{J}{4} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\frac{J}{2} & \cdot & \frac{J}{4} & -\frac{J}{2} & \cdot \\ \cdot & \cdot & \cdot & -\frac{J}{2} & \cdot & -\frac{J}{2} & \frac{J}{4} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{3J}{4} \end{bmatrix}$$

The eigenenergies are with

```

1 E_Heisenberg = eigvals(Matrix(rationalize.(\bar{H}_Heisenberg)) * sympify("J"))

```

given by

$$E = -\frac{3J}{4} \qquad E' = \frac{3J}{4},$$

each with 4 (mostly non-trivial) eigenstates.

b).3.

We recall the model from (1d): $J_{12}^x = J_{23}^y = J_{13}^z = J$ and all other $J_{ij}^\alpha = 0$ and $i < j$.

The couplings are set-up like this:

```

1 N = 3
2
3 # Isotropic Heisenberg
4 Js_1d = reset Js(N)
5 # 1 (J) for all (1,2,x), (2,3,y), (1,3,z)
6 Js_1d[1][1,2] = 1
7 Js_1d[2][2,3] = 1
8 Js_1d[3][1,3] = 1

```

leading to

$$J^x = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad J^y = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}, \qquad J^z = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

The resulting Hamilton matrix from `H_1d = calculate_hamilton_matrix(Js_1d, N)` is then analogous to exercise 1 ($\cdot \hat{=} 0$ for visual clarity):

$$\bar{H}_{Heisenberg} = \begin{bmatrix} -\frac{J}{4} & \cdot & \cdot & -\frac{J}{4} & \cdot & \cdot & \frac{J}{4} & \cdot \\ \cdot & \frac{J}{4} & -\frac{J}{4} & \cdot & \cdot & \cdot & \cdot & \frac{J}{4} \\ \cdot & -\frac{J}{4} & -\frac{J}{4} & \cdot & -\frac{J}{4} & \cdot & \cdot & \cdot \\ -\frac{J}{4} & \cdot & \cdot & \frac{J}{4} & \cdot & -\frac{J}{4} & \cdot & \cdot \\ \cdot & \cdot & -\frac{J}{4} & \cdot & \frac{J}{4} & \cdot & \cdot & -\frac{J}{4} \\ \cdot & \cdot & \cdot & -\frac{J}{4} & \cdot & -\frac{J}{4} & -\frac{J}{4} & \cdot \\ \frac{J}{4} & \cdot & \cdot & \cdot & \cdot & -\frac{J}{4} & \frac{J}{4} & \cdot \\ \cdot & \frac{J}{4} & \cdot & \cdot & -\frac{J}{4} & \cdot & \cdot & -\frac{J}{4} \end{bmatrix}$$

The eigenenergies are with

```
1 E_1d = eigvals(Matrix(rationalize.(H_1d)) * sympify("J"))
```

given by

$$E = -\frac{\sqrt{3}J}{4} \qquad E' = \frac{\sqrt{3}J}{4},$$

each with 4 (non-trivial⁶) eigenstates.

⁶superpositions of different $|n\rangle$