Computational Many-Body Physics - Sheet 4

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May 21th, 2022

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

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

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 $0, \ldots, 2^3 - 1$).
For the z-term, we use that $S_i^z |m_i\rangle = \pm\frac{1}{2} |m_i\rangle$ and therefore $S_i^z S_j^z |m\rangle = \mathrm{sgn_z} \frac{1}{4} |m\rangle$ with

$$\mathrm{sgn_z} = \begin{cases} +1 & : \quad m_i = m_j \\ -1 & : \quad m_i \neq m_j \end{cases} .$$

Therefore, we can rewrite the Hamilton-operator as

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

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

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

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

c). Hamilton matrix for the isotropic Heisenberg model

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

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

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

$$
\mathrm{sgn_y} = \begin{cases} +1 & : \quad m_i \neq m_j \\ -1 & : \quad m_i = m_j \end{cases} .
$$

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

$$
\mathrm{sgn_z} = -\,\mathrm{sgn_y} = \begin{cases} +1 & : \quad m_i = m_j \\ -1 & : \quad m_i \neq m_j \end{cases} .
$$

Therefore, we can rewrite the Hamiltonian as

$$H = -\frac{J}{4}\sum_{i<j}\left(\sigma_i^x\sigma_j^x + \mathrm{sgn_y(m_i,m_j)}\cdot\sigma_i^x\sigma_j^x + \mathrm{sgn_z(m_i,m_j)}\right) = -\frac{J}{4}\sum_{i<j}\left((1+\mathrm{sgn_y(m_i,m_j)})\cdot\sigma_i^x\sigma_j^x + \mathrm{sgn_z(m_i,m_j)}\right)$$

$$= -\frac{J}{4}\left((1+\mathrm{sgn_y(m_1,m_2)})\,\sigma_1^x\sigma_2^x + (1+\mathrm{sgn_y(m_1,m_3)})\,\sigma_1^x\sigma_3^x + (1+\mathrm{sgn_y(m_2,m_3)})\,\sigma_2^x\sigma_3^x\right.$$
$$\left. + \underbrace{\mathrm{sgn_z(m_1,m_2)} + \mathrm{sgn_z(m_1,m_3)} + \mathrm{sgn_z(m_2,m_3)}}_{=\begin{cases} 3 & : \quad m = 000, 111 \\ -1 & : \quad \text{else}\end{cases}}\right)$$

Then it is

$$\begin{aligned}
H\left|m_1m_2m_3\right\rangle &= -\frac{J}{4}((1+\mathrm{sgn_y(m_1,m_2)})\,\sigma_1^x\sigma_2^x\left|m_1m_2m_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_1,m_3)})\,\sigma_1^x\sigma_3^x\left|m_1m_2m_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_2,m_3)})\,\sigma_2^x\sigma_3^x\left|m_1m_2m_3\right\rangle \\
&\quad + (\mathrm{sgn_z(m_1,m_2)} + \mathrm{sgn_z(m_1,m_3)} + \mathrm{sgn_z(m_2,m_3)})\left|m_1m_2m_3\right\rangle) \\
&= -\frac{J}{4}((1+\mathrm{sgn_y(m_1,m_2)})\left|\bar{m}_1\bar{m}_2m_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_1,m_3)})\left|\bar{m}_1m_2\bar{m}_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_2,m_3)})\left|m_1\bar{m}_2\bar{m}_3\right\rangle \\
&\quad + (\mathrm{sgn_z(m_1,m_2)} + \mathrm{sgn_z(m_1,m_3)} + \mathrm{sgn_z(m_2,m_3)})\left|m_1m_2m_3\right\rangle) \\
\rightsquigarrow \left\langle n_1n_2n_3\right| H\left|m_1m_2m_3\right\rangle &= -\frac{J}{4}((1+\mathrm{sgn_y(m_1,m_2)})\left\langle n_1n_2n_3\middle|\bar{m}_1\bar{m}_2m_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_1,m_3)})\left\langle n_1n_2n_3\middle|\bar{m}_1m_2\bar{m}_3\right\rangle \\
&\quad + (1+\mathrm{sgn_y(m_2,m_3)})\left\langle n_1n_2n_3\middle|m_1\bar{m}_2\bar{m}_3\right\rangle \\
&\quad + (\mathrm{sgn_z(m_1,m_2)} + \mathrm{sgn_z(m_1,m_3)} + \mathrm{sgn_z(m_2,m_3)})\left\langle n_1n_2n_3\middle|m_1m_2m_3\right\rangle) \\
&= -\frac{J}{4}((1+\mathrm{sgn_y(m_1,m_2)})\,\delta_{n_1,\bar{m}_1}\delta_{n_2,\bar{m}_2}\delta_{n_3,m_3} \\
&\quad + (1+\mathrm{sgn_y(m_1,m_3)})\,\delta_{n_1,\bar{m}_1}\delta_{n_2,m_2}\delta_{n_3,\bar{m}_3} \\
&\quad + (1+\mathrm{sgn_y(m_2,m_3)})\,\delta_{n_1,m_1}\delta_{n_2,\bar{m}_2}\delta_{n_3,\bar{m}_3} \\
&\quad + (\mathrm{sgn_z(m_1,m_2)} + \mathrm{sgn_z(m_1,m_3)} + \mathrm{sgn_z(m_2,m_3)})\delta_{n,m})
\end{aligned}$$

The full Hamilton matrix is given by

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

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

$$H = -\left(J_{12}^x\frac{1}{4}\underbrace{(S_1^+S_2^+ + S_1^+S_2^- + S_1^-S_2^+ + S_1^-S_2^-)}_{=\sigma_1^x\sigma_2^x} + J_{23}^y\frac{1}{4}\underbrace{(-S_2^+S_3^+ + S_2^+S_3^- + S_2^-S_3^+ - S_2^-S_3^-)}_{=\mathrm{sgn_y}(m_2,m_3)\sigma_2^x\sigma_3^x} + J_{31}^z\underbrace{S_3^zS_1^z}_{\mathrm{sgn_z}(m_1,m_3)\frac{1}{4}}\right)$$
$$= -\frac{J}{4}\left(\sigma_1^x\sigma_2^x + \mathrm{sgn_y}(m_2,m_3)\sigma_2^x\sigma_3^x + \mathrm{sgn_z}(m_1,m_3)\right)$$

Then it is

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

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 `SparseArrays`[1], 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:

```
function reset_Js(N)
    Js = [sparse(zeros(N,N)) for α in 1:3]; # 3 N×N matrices (α = x,y,z)
    return Js
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 implementation[2] of the algorithm later easier.

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

  ```
  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 $n = [z_1 z_2 \dots z_n]$.

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

[1] Concretely, we use the matrix-type `SparseMatrixCSC` from the package `SparseArrays.jl`.
[2] The full code for this exercise can be found in `2_hamilton_matrices_for_spin_models.ipynb`

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

```
# prefactor λ^x for the x-component of the interaction of spins i and j of |n⟩
#     -J^x_ij S^x_i S^x_j |n⟩      λ^y |l⟩
function x_link_prefactor(Js, n, i, j)
    α = 1 # x =    1
    return -1//4 * Js[α][i,j]
end

# prefactor λ^y for the y-component of the interaction of spins i and j of |n⟩
#     -J^y_ij S^y_i S^y_j |n⟩      λ^y |l⟩
function y_link_prefactor(Js, n, i, j)
    α = 2 # y =    2
    # calculate the sign, +1 for n_i != n_j, -1 for n_i == n_j
    s = - (2 * n_dual(n)[i] - 1) * (2 * n_dual(n)[j] - 1)
    return - 1//4 * s * Js[α][i,j]
end

# prefactor λ^z for the z-component of the interaction of spins i and j of |n⟩
#     -J^z_ij S^z_i S^z_j |n⟩      λ^z |l⟩
function z_link_prefactor(Js, n, i, j)
    α = 3 # z =    3
    # calculate the sign, +1 for n_i == n_j, -1 for n_i != n_j
    s = (2 * n_dual(n)[i] - 1) * (2 * n_dual(n)[j] - 1)
    return -1//4 * s * Js[α][i,j]
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 Js, we can implement the algorithm to calculate the Hamilton matrix for a given N and $\{J_{ij}^{\alpha}\}$:

```
function calculate_hamilton_matrix(Js, N)
    Ĥ = sparse(zeros(2^N, 2^N)) # empty 2^N x 2^N matrix
    for n in 0:(2^N-1)
        # for each |n⟩ set the non-zero matrix elements

        # 1. loop over all components α = x,y,z
        for α in [1,2,3]
            # 2. loop over only non-zero links in Js
            # iterate over non-zero elements by using findnz()
            for (i, j, J) in zip(findnz(Js[α])...)

                if α == 1 # α =    x
                    m = l(n, i, j) # calculate |l⟩ from |n⟩ for i,j
                    # add to the matrix element ⟨l|H|n⟩ the x-link-term
                    Ĥ[m+1,n+1] += x_link_prefactor(Js, n, i, j)
                elseif α == 2 # α =    y
                    m = l(n, i, j) # calculate |l⟩ from |n⟩ for i,j
                    # add to the matrix element ⟨l|H|n⟩ the y-link-term
                    Ĥ[m+1,n+1] += y_link_prefactor(Js, n, i, j)
                else
                    # α =    z, diagonal element
                    Ĥ[n+1,n+1] += z_link_prefactor(Js, n, i, j)
                end
            end
        end
    end
    return Ĥ
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 `Js` are used).

Furthermore, we used the packages `SymPy` and `Latexify` for easier comparison with the results from above[3].

b).1. Ising model

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

The couplings are set-up like this:

```
N = 3

# Ising
Js_ising = reset_Js(N)
# 1 (J) for all i<j for α =   z, 0 for α ≠ z
Js_ising[3] = [
    0 1 1
    0 0 1
    0 0 0
]
```

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 `H̄_ising = calculate_hamilton_matrix(Js_ising, N)` is then analogous to exercise 1[4]:

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

The eigenenergies are with

```
E_ising = eigvals(Matrix(rationalize.(H̄_ising)) * sympify("J"))
```

given by

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

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

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

[4] `latexify(Matrix(rationalize.(H̄_ising)) * sympify("J"))` used for conversion to LaTeX

b).2. Isotropic Heisenberg model

We recall: $J^\alpha_{ij} = J$ and $i < j$.
The couplings are set-up like this:

```
N = 3

# Isotropic Heisenberg
Js_Heisenberg = reset_Js(N)
# 1 (J) for all i<j for α =   z, 0 for α ≠ z
Js_Heisenberg[1] = [
    0 1 1
    0 0 1
    0 0 0
]
Js_Heisenberg[2] = Js_Heisenberg[1]
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 `H̄_Heisenberg = calculate_hamilton_matrix(Js_Heisenberg,N)` is then analogous to exercise 1($\cdot \hat{=} 0$ for visual clarity):

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

The eigenenergies are with

```
E_Heisenberg = eigvals(Matrix(rationalize.(H̄_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): $J^x_{12} = J^y_{23} = J^z_{13} = J$ and all other $J^\alpha_{ij} = 0$ and $i < j$.
The couplings are set-up like this:

```
N = 3

# Isotropic Heisenberg
Js_1d = reset_Js(N)
# 1 (J) for all (1,2,x), (2,3,y), (1,3,z)
Js_1d[1][1,2] = 1
Js_1d[2][2,3] = 1
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 `H̄_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

```
E_1d = eigvals(Matrix(rationalize.(H̄_1d)) * sympify("J"))
```

given by

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

each with 4 (non-trivial[5]) eigenstates.

[5]superpositions of different $|n\rangle$