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Exercise class in HCI J7.

Exercise 1. *Bitwise Operations and the Transverse Field Ising Model*

In this exercise we will get familiar with the way the states in a Fock space can be represented by integers using their decomposition into bits. We will see how we can use this representation to facilitate operations and decompose the Hilbert space into symmetry sectors of a given Hamiltonian. We will use this in the context of the transverse field Ising model. The transverse field Ising chain with open boundary conditions is defined by the following Hamiltonian

$$\hat{H} = \hat{H}_{\text{Ising}} + \hat{H}_{\text{transv}} = J\sum_{i=1}^{N-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z - h^x\sum_{i=1}^{N}\hat{\sigma}_i^x \tag{1}$$

where we replaced the spin operators $\hat{S}_i^\mu = \frac{\hbar}{2}\hat{\sigma}_i^\mu, \mu = x, y, z$ with the Pauli matrices $\hat{\sigma}^\mu$ and set $\hbar = 1$. As the dimension of the Hilbert space grows exponentially in the number of sites on the chain we will only be able to tackle small problems. The symmetries of the Hamiltonian however allow us to simplify the problem: By organizing the basis states so that elements corresponding to the same symmetry sector are grouped together, the Hamiltonian becomes block diagonal. We can then solve the eigenvalue problem for the blocks independent of each other.

Part 1

As a warm up, let us contemplate on the size of the Fock (sub-)spaces for different particles. Suppose a geometry of N sites. What is the size of the Fock space for:

1. Bosons
2. Spinless Fermions
3. Spinful Fermions
4. Spin-$\frac{1}{2}$'s

Assume that we are dealing with spinless fermions, and that $\hat{H}$ commutes with the number operator $\hat{n} = \sum_i \hat{n}_i$, i.e. $[\hat{H}, \hat{n}] = 0$.

5. What are the dimensions of the invariant subspaces, labeled by the filling $n = \frac{1}{N}\sum_i \hat{n}_i$?
6. Same as for 5., but this time we consider spinful fermions, i.e. the number operator on site $i, \hat{n}_i$, becomes $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$. Since we are dealing with spinful fermions, be aware that every site can host one of the following states: $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

Assume that we are dealing with a chain of spin- $\frac{1}{2}$'s, and assume that $\hat{H}$ commutes with the total magnetization $m = \frac{1}{N}\sum_i \hat{\sigma}_i^z$.

7. What are the dimensions of the invariant subspaces, labeled by the magnetization m?

Solution. The dimensions of the Hilbert spaces for the different cases are

1. $D =$ Infinite for bosons. At each site, there can reside an arbitrary number of bosons, since the Pauli exclusion principle only applies to fermions.
2. $D = 2^N$ for spinless fermions, since each site can either be empty or occupied by a fermion.
3. $D = 4^N$ for spinful fermions; the local Hilbert space at each site consists of the four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$, $|\uparrow\downarrow\rangle$.
4. $D = 2^N$ for spin $\frac{1}{2}$'s, since the spin at each site can either point upwards or downwards. Note that, usually, when one discusses a chain of spin $\frac{1}{2}'s$, it is always assumed that one, and exactly one, particle resides at each site that can either have spin up or spin down, as opposed to e.g. the case of spinful fermions, where one usually also allows for the states $|0\rangle$ and $|\uparrow\downarrow\rangle$ to occur.
5. The filling n is commonly defined as $n = \frac{1}{N}\sum_i \hat{n}_i$, where $\hat{n}_i$ is the operator counting the particles at site i. In the case of spinless fermions, each site can either be occupied or empty. If we are at a particular filling n, this means that we have to accomodate nN particles on N sites, leading to $D = \begin{pmatrix} N \\ Nn \end{pmatrix} = \frac{N!}{(N-Nn)!(Nn)!}$.
6. $D = \begin{pmatrix} 2N \\ Nn \end{pmatrix} = \frac{(2N)!}{(2N-Nn)!(Nn)!}$. We still have N sites, but each site can host a fermion with spin up, as well as a fermion with spin down. This means that we have $2N$ available spaces to accommodate Nn fermions.
7. This one is slightly more involved. We know that $m = (n_\uparrow - n_\downarrow)$ as well as $1 = n_\uparrow + n_\downarrow$. This leads to $n_\uparrow = \frac{m+1}{2}$. Accommodating $Nn_\uparrow$ particles on N sites leads to $D = \begin{pmatrix} N \\ N\left(\frac{1+m}{2}\right) \end{pmatrix} = \frac{N!}{(N-N(\frac{1+m}{2}))!(N(\frac{1+m}{2}))!}$.

Part 2

We will now restrict ourselves to spin- $\frac{1}{2}$'s (meaning that we are only considering strings where exactly 1 spin- $\frac{1}{2}$ resides at each site), and we will represent each basis state as an integer via its bit representation. For instance, working on 4 sites, the state $|\uparrow\uparrow\downarrow\uparrow\rangle$ will be thought of as $|1101\rangle$, which corresponds to the bit representation of the integer 13. Using the bitwise operators in python depicted in Table (1), implement functions to do the following operations on a state:

1. Shift all the spins cyclically to the right
2. Shift all the spins cyclically to the left
3. Count all the upspins in your state
4. Return the spin of a state at site j
5. Flip the spin at site j
6. Flip all the spins in the state
7. We will now use this method the check question 7. of part 1 . Assume a system of spin $-\frac{1}{2}$'s with $N = 10$. Using the the integers $0, 1, \ldots, 1023$ as the basis of the Hilbert space (via their bit representation), divide the Hilbert space into the different magnetization sectors. Check that the sizes of the sectors match the analytical result obtained in part 1.

&	AND
$\|$	OR
ˆ	XOR
>>	Signed right shift
<<	Zero fill left shift
∼	NOT

Table 1: Bitwise operations in python

Solution. Check out the notebook.

Part 3

1. In the transverse field Ising model, the parity symmetry is defined as $\hat{P} = \prod_i \sigma_i^x$. Show that it commutes with the Hamiltonian.

Solution. To show that $\hat{P}$ commutes with the Hamiltonian and is indeed a symmetry of $\hat{H}$, we use the commutation relations of the Pauli matrices:

$$\left[\sigma^a, \sigma^b\right] = 2i\epsilon_{abc}\sigma^c. \tag{2}$$

Considering both terms separately

$$[\hat{H}, \hat{P}] = \left[\hat{H}_{\text{Ising}} + \hat{H}_{\text{transv}}, \hat{P}\right] \tag{3}$$

$$\left[\hat{H}_{\text{Ising}}, \hat{P}\right] = \left[J\sum_{i=1}^{N-1} \hat{\sigma}_i^z\hat{\sigma}_{i+1}^z, \prod_j \sigma_j^x\right] = J\sum_{i=1}^{N-1}\left[\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z, \prod_j^N \sigma_j^x\right] \tag{4}$$

we can see that for every i in the summation, the operators will commute trivially with the product over σ_j^x, except for the case when $j = i, i+1$. Using the composition rules of commutators we only have to consider the term

$$[\sigma_i^z\sigma_{i+1}^z, \sigma_i^x\sigma_{i+1}^x] = \sigma_i^z\underbrace{[\sigma_{i+1}^z, \sigma_i^x]}_{=0}\sigma_{i+1}^x + [\sigma_i^z, \sigma_i^x]\,\sigma_{i+1}^z\sigma_{i+1}^x + \sigma_i^x\sigma_i^z\,[\sigma_{i+1}^z, \sigma_{i+1}^x] + \sigma_i^x\underbrace{[\sigma_i^z, \sigma_{i+1}^x]}_{=0}\sigma_{i+1}^z, \tag{5}$$

where we already used the fact that operators acting on different sites commute. Using eq.(2) and $\sigma_i^x\sigma_i^z = -i\sigma_i^y$, we obtain:

$$[\sigma_i^z\sigma_{i+1}^z, \sigma_i^x\sigma_{i+1}^x] = -2\sigma_i^y\sigma_{i+1}^y + 2\sigma_i^y\sigma_{i+1}^y = 0. \tag{6}$$

Since this is true for every i in the summation, $\left[\hat{H}_{\text{Ising}}, \hat{P}\right] = 0$. Also since σ^x commutes with itself,

$$\left[\hat{H}_{\text{transv}}, \hat{P}\right] = \left[-h^x\sum_{i=1}^{N} \hat{\sigma}_i^x, \prod_j \sigma_j^x\right] = 0 \tag{7}$$

Therefore $[\hat{H}, \hat{P}] = 0$ and the parity defined by $\hat{P}$ is a symmetry of the transverse field Ising Hamiltonian.

For a system with periodic boundary conditions we can also exploit translational symmetries. Such a translation is represented by the operator T or a multiple of it. T is thereby defined as

$$T\,|s_1, s_2, \ldots, s_N\rangle = |s_N, s_1, \ldots, s_{N-1}\rangle$$

The eigenvalues of the translation operator are the N-th roots of unity $z_k = \exp\left(i\frac{2\pi k}{N}\right)$ with $k = 0, \ldots, N-1$. The shift operator commutes with the Hamiltonian. It can therefore be decomposed into different $p_k = 2\pi k/N$ momentum subspaces. This means constructing cycles of states which are connected by T :

$$|\psi_n\rangle = T^n|\phi\rangle \quad n \in \{1, 2, \ldots, N-1\}.$$

This cycle is spanned by the eigenstates of T with momentum p_k :

$$|\chi_k\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k}T\right)^\nu |\phi\rangle \quad k = 0, 1, \ldots, N-1$$

If the dimension of the cycle does not equal the number of lattice sites N, k is changed according to $k = 0, N/D, \ldots, (D-1)N/D$ with D being the dimension of the cycle.

2. Consider a system with N = 4 lattice sites. Find the momentum states $|\chi_k\rangle$ with momenta $p_k \in \{0, \pi/2, \pi, 3\pi/2, 2\pi\}$, by constructing the translation cycles for each basis state.

Solution. To find the momenta p_k corresponding to the basis states, we have to consider the smallest number of allowed translations D with a given basis state, until we recover the initial state.

$$|\phi\rangle = T^D|\phi\rangle \quad D \in \{1, 2, \ldots, N\} \tag{9}$$

If $D = N = 4$ we have a full cycle and k spans from $k = 0, 1, \ldots, N-1$. If $D < N$, k is changed according to $k = 0, N/D, \ldots, (D-1)N/D$. Since all the states in a cycle are connected by translations, it is sufficient to keep only one state as a representative.

Representative state	D	p_k
$\vert\phi_1\rangle = \vert\uparrow\uparrow\uparrow\uparrow\rangle$	1	0
$\vert\phi_2\rangle = \vert\downarrow\uparrow\uparrow\uparrow\rangle$	4	$0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$
$\vert\phi_3\rangle = \vert\downarrow\downarrow\uparrow\uparrow\rangle$	4	$0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$
$\vert\phi_4\rangle = \vert\downarrow\uparrow\downarrow\uparrow\rangle$	2	$0, \pi$
$\vert\phi_5\rangle = \vert\downarrow\downarrow\downarrow\uparrow\rangle$	4	$0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$
$\vert\phi_6\rangle = \vert\downarrow\downarrow\downarrow\downarrow\rangle$	1	0

We can now group the states according to their momenta p_k and construct the momentum eigenstates $|\chi_k\rangle$.

p_k	States
0	$\vert\uparrow\uparrow\uparrow\uparrow\rangle, \vert\downarrow\uparrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\uparrow\uparrow\rangle, \vert\downarrow\uparrow\downarrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\downarrow\rangle$
$\frac{\pi}{2}$	$\vert\downarrow\uparrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\uparrow\rangle$
π	$\vert\downarrow\uparrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\uparrow\uparrow\rangle, \vert\downarrow\uparrow\downarrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\uparrow\rangle$
$\frac{3\pi}{2}$	$\vert\downarrow\uparrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\uparrow\uparrow\rangle, \vert\downarrow\downarrow\downarrow\uparrow\rangle$

$$
\begin{aligned}
|\chi_{k=0}^{1,\dots,6}\rangle &= \frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}(e^{-ip_0}T)^\nu\,|\phi_{1,..,6}\rangle \\
|\chi_{k=\pi/2}^{2,3,5}\rangle &= \frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}(e^{-ip_{\pi/2}}T)^\nu\,|\phi_{2,3,5}\rangle \\
|\chi_{k=\pi}^{2,3,4,5}\rangle &= \frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}(e^{-ip_\pi}T)^\nu\,|\phi_{2,3,4,5}\rangle \\
|\chi_{k=3\pi/2}^{2,3,5}\rangle &= \frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}(e^{-ip_{3\pi/2}}T)^\nu\,|\phi_{2,3,5}\rangle
\end{aligned}
$$

3. How should we choose the normalization constant N_ϕ of the states $|\chi_k\rangle$? If it helps, consider explicitly the case of $N = 4$ lattice sites.

Solution. If all translated states are distinct and $D = N$, the normalization constant is just $N_\phi = N$. As we saw explicitly in the last exercise, there are however cycles with periodicity less than N, which changes the norm of the state. The periodicity of a state is the smallest integer D such that

$$|\phi\rangle = T^D|\phi\rangle \quad D \in \{1, 2, \dots, N\}$$

If $D < N$, the momentum state as defined in eq. (8) contains a sum over multiple copies of the same state. These add up to

$$\sum_{\nu=0}^{N/D-1} e^{-ip_k D\nu} = \frac{N}{D} \tag{10}$$

since k is chosen as $k = 0, N/D, \dots, (D-1)N/D$, to ensure that the phase factor remains a multiple of 2π. The normalization is therefore given as

$$N_\phi = \langle \chi_k \mid \chi_k\rangle = D\left|\frac{N}{D}\right|^2 = \frac{N^2}{D} \tag{11}$$

Note: Another possibility would be to adapt the summation in eq. (8).

4. Express the Hamiltonian of the transverse field Ising model in this new basis, i.e. calculate

$$
\begin{aligned}
&\left\langle \chi'_{k'}\,\right| H_{\text{Ising}} \left|\,\chi_k\right\rangle, \\
&\left\langle \chi'_{k'}\,\right| H_{\text{transv}} \left|\,\chi_k\right\rangle.
\end{aligned}
$$

Solution. Since the Hamiltonian does commute with the translation operator, we only have to consider matrix elements between momentum states of the same momentum k. This causes the Hamiltonian to be block diagonal and simplifies the calculation of eigenvalues. First we consider the Ising Hamiltonian $\hat{H}_{\text{Ising}}$:

$$H_{\text{Ising}}\;|\chi_k\rangle = J\sum_{i=1}^{N-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z\frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}\left(e^{-ip_k}T\right)^\nu|\phi\rangle = \frac{1}{\sqrt{N_\phi}}\sum_{\nu=0}^{N-1}\left(e^{-ip_k}T\right)^\nu J\sum_{i=1}^{N-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z|\phi\rangle, \tag{12}$$

where in the last step we used the fact that the Hamiltonian commutes with the translation operator. This means we only have to calculate the action of H_{Ising} on the representative states $|\phi\rangle$. Since H_{Ising} is a diagonal operator it holds:

$$\left\langle \chi^{2,3,5}_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{Ising}} \left| \chi^{2,3,5}_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = 0, \tag{13}$$

$$\left\langle \chi^{4}_{k=0,\pi} \right| H_{\text{Ising}} \left| \chi^{4}_{k=0,\pi} \right\rangle = -4J, \tag{14}$$

$$\left\langle \chi^{1,6}_{k=0} \right| H_{\text{Ising}} \left| \chi^{1,6}_{k=0} \right\rangle = 4J. \tag{15}$$

Similarly, we compute the action of H_{transv}. Since it commutes with the translation operator, too, we can again directly consider its action on the representative states $|\phi\rangle$.

$$H_{\text{transv}}\ |\phi_1\rangle = -h^x \underbrace{|\downarrow\uparrow\uparrow\uparrow\rangle}_{|\phi_2\rangle} - h^x \underbrace{|\uparrow\downarrow\uparrow\uparrow\rangle}_{T^{-3}|\phi_2\rangle} - h^x \underbrace{|\uparrow\uparrow\downarrow\uparrow\rangle}_{T^{-2}|\phi_2\rangle} - h^x \underbrace{|\uparrow\uparrow\uparrow\downarrow\rangle}_{T^{-1}|\phi_2\rangle} \tag{16}$$

$$H_{\text{transv}}\ |\phi_2\rangle = -h^x \underbrace{|\uparrow\uparrow\uparrow\uparrow\rangle}_{|\phi_1\rangle} - h^x \underbrace{|\downarrow\downarrow\uparrow\uparrow\rangle}_{|\phi_3\rangle} - h^x \underbrace{|\downarrow\uparrow\downarrow\uparrow\rangle}_{|\phi_4\rangle} - h^x \underbrace{|\downarrow\uparrow\uparrow\downarrow\rangle}_{T^{-1}|\phi_3\rangle} \tag{17}$$

$$H_{\text{transv}}\ |\phi_3\rangle = -h^x \underbrace{|\uparrow\downarrow\uparrow\uparrow\rangle}_{T^{1}|\phi_2\rangle} - h^x \underbrace{|\downarrow\uparrow\uparrow\uparrow\rangle}_{|\phi_2\rangle} - h^x \underbrace{|\downarrow\downarrow\downarrow\uparrow\rangle}_{|\phi_5\rangle} - h^x \underbrace{|\downarrow\downarrow\uparrow\downarrow\rangle}_{T^{-1}|\phi_5\rangle} \tag{18}$$

$$H_{\text{transv}}\ |\phi_4\rangle = -h^x \underbrace{|\uparrow\uparrow\downarrow\uparrow\rangle}_{T^{-2}|\phi_2\rangle} - h^x \underbrace{|\downarrow\downarrow\downarrow\uparrow\rangle}_{|\phi_5\rangle} - h^x \underbrace{|\downarrow\uparrow\uparrow\uparrow\rangle}_{|\phi_2\rangle} - h^x \underbrace{|\downarrow\uparrow\downarrow\downarrow\rangle}_{T^{-2}|\phi_5\rangle} \tag{19}$$

$$H_{\text{transv}}\ |\phi_5\rangle = -h^x \underbrace{|\uparrow\downarrow\downarrow\uparrow\rangle}_{T^{1}|\phi_3\rangle} - h^x \underbrace{|\downarrow\uparrow\downarrow\uparrow\rangle}_{|\phi_4\rangle} - h^x \underbrace{|\downarrow\downarrow\uparrow\uparrow\rangle}_{|\phi_3\rangle} - h^x \underbrace{|\downarrow\downarrow\downarrow\downarrow\rangle}_{|\phi_6\rangle} \tag{20}$$

$$H_{\text{transv}}\ |\phi_6\rangle = -h^x \underbrace{|\uparrow\downarrow\downarrow\downarrow\rangle}_{T^{-3}|\phi_5\rangle} - h^x \underbrace{|\downarrow\uparrow\downarrow\downarrow\rangle}_{T^{-2}|\phi_5\rangle} - h^x \underbrace{|\downarrow\downarrow\uparrow\downarrow\rangle}_{T^{-1}|\phi_5\rangle} - h^x \underbrace{|\downarrow\downarrow\downarrow\uparrow\rangle}_{|\phi_5\rangle} \tag{21}$$

Where we used the fact that we can translate each obtained state $\left|\phi^{(i)}\right\rangle$ on the right-hand side of the expressions for $H_{transv}\,|\phi\rangle$ back to the reference state of each cycle $|\phi\rangle$.

$$\left|\phi^{(i)}\right\rangle = T^{-\mu_i}|\phi\rangle \tag{22}$$

We can then use

$$\begin{aligned} H_{\text{transv}}\ |\chi_k\rangle &= \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k} T\right)^\nu H_{\text{transv}}\ |\phi\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k} T\right)^\nu (-h^x) \sum_{i=1}^{N} \left|\phi^{(i)}\right\rangle \\ &= (-h^x) \sum_{i=1}^{N} \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} e^{-ip_k\nu} T^{\nu-\mu_i} |\tilde{\phi}^{(i)}\rangle \overset{\text{indexshift}}{=} (-h^x) \sum_{i=1}^{N} e^{-ip_k\mu_i} \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} e^{-ip_k\nu} T^{\nu} |\tilde{\phi}^{(i)}\rangle \\ &= (-h^x) \sum_{i=1}^{N} e^{-ip_k\mu_i} \sqrt{\frac{N_{\tilde{\phi}^{(i)}}}{N_\phi}} \left|\tilde{\chi}_k^{(i)}\right\rangle . \end{aligned} \tag{23}$$

In some cases we have to account for the fact that the reference state $|\tilde{\phi}\rangle$ has changed, with a new normalization constant. The corresponding non-zero matrix elements are:

$$\left\langle \chi^2_{k=0} \right| H_{\text{transv}} \left| \chi^1_{k=0} \right\rangle = -4h^x \sqrt{\frac{N_{\phi_2}}{N_{\phi_1}}}, \tag{24}$$

$$\left\langle \chi^1_{k=0} \right| H_{\text{transv}} \left| \chi^2_{k=0} \right\rangle = -h^x \sqrt{\frac{N_{\phi_1}}{N_{\phi_2}}} = -4h^x \sqrt{\frac{N_{\phi_2}}{N_{\phi_1}}}, \tag{25}$$

$$\left\langle \chi^3_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^2_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \left(1 + e^{-ip_k}\right), \tag{26}$$

$$\left\langle \chi^4_{k=0,\pi} \right| H_{\text{transv}} \left| \chi^2_{k=0,\pi} \right\rangle = -h^x \sqrt{\frac{N_{\phi_4}}{N_{\phi_2}}}, \tag{27}$$

$$\left\langle \chi^5_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^3_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \left(1 + e^{-ip_k}\right), \tag{28}$$

$$\left\langle \chi^2_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^3_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \left(1 + e^{ip_k}\right), \tag{29}$$

$$\left\langle \chi^2_{k=0,\pi} \right| H_{\text{transv}} \left| \chi^4_{k=0,\pi} \right\rangle = -h^x \left(1 + e^{-2ip_k}\right) \sqrt{\frac{N_{\phi_2}}{N_{\phi_4}}} \overset{p_k=0,\pi}{=} -h^x \sqrt{\frac{N_{\phi_4}}{N_{\phi_2}}}, \tag{30}$$

$$\left\langle \chi^5_{k=0,\pi} \right| H_{\text{transv}} \left| \chi^4_{k=0,\pi} \right\rangle = -h^x \left(1 + e^{-2ip_k}\right) \sqrt{\frac{N_{\phi_5}}{N_{\phi_4}}} \overset{p_k=0,\pi}{=} -h^x \sqrt{\frac{N_{\phi_4}}{N_{\phi_5}}}, \tag{31}$$

$$\left\langle \chi^3_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^5_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \left(1 + e^{ip_k}\right), \tag{32}$$

$$\left\langle \chi^4_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^5_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \sqrt{\frac{N_{\phi_4}}{N_{\phi_5}}}, \tag{33}$$

$$\left\langle \chi^6_{k=0,\pi/2,\pi,3\pi/2} \right| H_{\text{transv}} \left| \chi^5_{k=0,\pi/2,\pi,3\pi/2} \right\rangle = -h^x \sqrt{\frac{N_{\phi_6}}{N_{\phi_5}}}, \tag{34}$$

$$\left\langle \chi^5_{k=0} \right| H_{\text{transv}} \left| \chi^6_{k=0} \right\rangle = -4h^x \sqrt{\frac{N_{\phi_5}}{N_{\phi_6}}} = -h^x \sqrt{\frac{N_{\phi_6}}{N_{\phi_5}}}. \tag{35}$$

Hereby we used the normalization factors $N_{\phi_1}, N_{\phi_6} = 16, N_{\phi_2}, N_{\phi_3}, N_{\phi_5} = 4$ and $N_{\phi_4} = 8$ as derived in the previous exercise. The correct normalization factors are crucial in order to obtain a hermitian matrix.

We've now done some analytical work on the TFI that will facilitate the task of exact diagonalization. Let us do some numerical preparatory work to exactly diagonalize the model by using what was introduced in part 2 of the exercise. Let's consider again the translation operator $\hat{T}$ which commutes with $\hat{H}$. For every state (bitstring) $|s\rangle$, define its orbits $O(|s\rangle) = \text{set } \hat{T}^n|s\rangle$, e.g. as the set of all possible bitstrings that can be constructed out of $|s\rangle$ by applying $\hat{T}$ arbitrarily many times. This defines an equivalence relation: all the bitstrings split into non-interseting orbits (equivalence classes) $O_1, O_2, \ldots, O_m$. To each orbit, one can assign a representative, which in principle can be any state of the orbit. Note that the momentum states $|\chi_k\rangle$ as constructed above only contain states from the same orbit.

5. Implement a function that creates as an output an array containing exactly one representative of each orbit. Choose as the representative of each orbit the state corresponding to the lowest integer (via the bitstring representation).

6. Lastly, create a function that takes the output of the function created in (5.) and checks which orbits are compatible with the creation of a momentum eigenstate with momentum P_n. Remember that e.g. the orbit created by the state $|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\rangle$ is only compatible with the momenta $P_0 = \frac{2\pi}{8}0 = 0$ and $P_4 = \frac{2\pi}{8}4 = \pi$, because translating the state twice must bring it back to itself, meaning that $\exp(-iP_n 2)$ must be equal to 1 .

Solution. Check out the notebook.