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Computational Quantum Physics
Solution Exercise Sheet 2

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Exercise 2. Transverse field Ising model - Part I

In this exercise we will get familiar with the symmetries 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.

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

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

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

   Considering both terms separately

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

   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

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

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

   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 $\left[\hat{H}, \hat{P}\right] = 0$ 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

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

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 $k = 0, ..., N-1$. 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:

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

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

$$|\chi_k\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k}\ T\right)^\nu |\phi\rangle \qquad k = 0, 1, ..., N-1. \tag{8}$$

If the dimension of the cycle does not equal the number of lattice sites N, k is changed according to $k = 0, N/D, ..., (D-1)N/D$ 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 $p_k \in \{0, \pi/2, \pi, 3\pi/2\}$, by constructing the translation cycles for each basis state.*

   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.

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

   If $D = N = 4$ we have a full cycle and k spans from $k = 0, 1, ..., N-1$. If $D < N$, k is changed according to $k = 0, N/D, ..., (D-1)N/D$. 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
$\|\phi_1\rangle = \|\uparrow\uparrow\uparrow\uparrow\rangle$	1	0
$\|\phi_2\rangle = \|\downarrow\uparrow\uparrow\uparrow\rangle$	4	$0,\ \frac{\pi}{2},\ \pi,\ \frac{3\pi}{2}$
$\|\phi_3\rangle = \|\downarrow\downarrow\uparrow\uparrow\rangle$	4	$0,\ \frac{\pi}{2},\ \pi,\ \frac{3\pi}{2}$
$\|\phi_4\rangle = \|\downarrow\uparrow\downarrow\uparrow\rangle$	2	$0,\ \pi$
$\|\phi_5\rangle = \|\downarrow\downarrow\downarrow\uparrow\rangle$	4	$0,\ \frac{\pi}{2},\ \pi,\ \frac{3\pi}{2}$
$\|\phi_6\rangle = \|\downarrow\downarrow\downarrow\downarrow\rangle$	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	$\|\uparrow\uparrow\uparrow\uparrow\rangle,\ \|\downarrow\uparrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\uparrow\uparrow\rangle,\ \|\downarrow\uparrow\downarrow\uparrow\rangle,\ \|\downarrow\downarrow\downarrow\uparrow\rangle,\ \|\downarrow\downarrow\downarrow\downarrow\rangle$
$\frac{\pi}{2}$	$\|\downarrow\uparrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\downarrow\uparrow\rangle$
π	$\|\downarrow\uparrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\uparrow\uparrow\rangle,\ \|\downarrow\uparrow\downarrow\uparrow\rangle,\ \|\downarrow\downarrow\downarrow\uparrow\rangle$
$\frac{3\pi}{2}$	$\|\downarrow\uparrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\uparrow\uparrow\rangle,\ \|\downarrow\downarrow\downarrow\uparrow\rangle$

$$|\chi^{1,..,6}_{k=0}\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_0}\ T\right)^\nu |\phi_{1,..,6}\rangle$$

$$|\chi^{2,3,5}_{k=\pi/2}\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_{\pi/2}}\ T\right)^\nu |\phi_{2,3,5}\rangle$$

$$|\chi^{2,3,4,5}_{k=\pi}\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_\pi}\ T\right)^\nu |\phi_{2,3,4,5}\rangle$$

$$|\chi^{2,3,5}_{k=3\pi/2}\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_{3\pi/2}}\ T\right)^\nu |\phi_{2,3,5}\rangle$$

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.*

   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

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

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

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

   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*

   $$\langle\chi'_{k'}|H_{\text{Ising}}|\chi_k\rangle,$$
   $$\langle\chi'_{k'}|H_{\text{transv}}|\chi_k\rangle.$$

   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 $\hat{H}_{\text{Ising}}$:

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

   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:

   $$\langle\chi^{2,3,5}_{k=0,\pi/2,\pi,3\pi/2}|H_{\text{Ising}}|\chi^{2,3,5}_{k=0,\pi/2,\pi,3\pi/2}\rangle = 0, \tag{13}$$
   $$\langle\chi^{4}_{k=0,\pi}|H_{\text{Ising}}|\chi^{4}_{k=0,\pi}\rangle = -4J, \tag{14}$$
   $$\langle\chi^{1,6}_{k=0}|H_{\text{Ising}}|\chi^{1,6}_{k=0}\rangle = 4J. \tag{15}$$

   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 that we can translate the obtained state $|\phi'\rangle$ back to the reference state of each cycle $|\phi\rangle$.

$$|\phi'\rangle = T^{-\mu}|\phi\rangle \tag{22}$$

We can then use

$$\begin{aligned} H_{\text{transv}}|\chi_k\rangle &= \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k}\ T\right)^{\nu} H_{\text{transv}}|\phi\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k}\ T\right)^{\nu} |\phi'\rangle \\ &= \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} e^{-ip_k\nu}\ T^{\nu-\mu}|\tilde{\phi}\rangle \overset{indexshift}{=} e^{-ip_k\mu} \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} e^{-ip_k\nu}\ T^{\nu}|\tilde{\phi}\rangle = e^{-ip_k\mu}\sqrt{\frac{N_{\tilde{\phi}}}{N_\phi}}|\tilde{\chi}_k\rangle. \end{aligned} \tag{23}$$

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:

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

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

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

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

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

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

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

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

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

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

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

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

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.