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Tutorial 11 (Quantum numbers and conservation laws in tensor networks)
In Exercise 9.1 we have introduced the concept of a symmetry operator, P. In physics one typically denotes the eigenvalues of P as *quantum numbers*, and it is desirable to work with "symmetric" quantum states (i.e., eigenvectors of P). In case a state ψ is represented as tensor network, like a MPS, it can be possible to enforce such a symmetry on the level of the individual tensors.

To better understand how this works, let us interpret the qubit basis state $|0\rangle$ as "empty state" and $|1\rangle$ as "occupied state" with one particle. For a systems of (possible several) qubits, the overall quantum number is the total particle number. This also applies to a superposition like $\frac{1}{\sqrt{2}}(|101\rangle + |011\rangle$, as long as each basis state has the same quantum number, 2 in this case.

We now define an "annihilation operator" a and its adjoint (conjugate transpose) $a^\dagger$ denoted "creation operator", which satisfy

$$\begin{aligned} a^\dagger |0\rangle &= |1\rangle\,, \\ a\,|1\rangle &= |0\rangle\,, \\ a^\dagger a\,|1\rangle &= |1\rangle\,. \end{aligned}$$

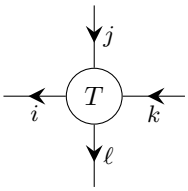
Application to any other basis state not specified here gives zero. Intuitively, $a^\dagger$ "creates" and a "annihilates" a particle, and $a^\dagger a$ counts the particle number.

(a) Write down the matrix representation of a and label the columns and rows. Can you notice any relationship between these indices and the particle number?

Graphically, we keep track of the "inflow" and "outflow" of quantum numbers by augmenting tensor legs with arrows, and associating a quantum number with each possible value of an index:

For example, a non-zero entry a_{12} changes the quantum number by -1, from 1 to 0.

(b) Consider the following tensor T of degree 4. How could one impose particle number conservation?



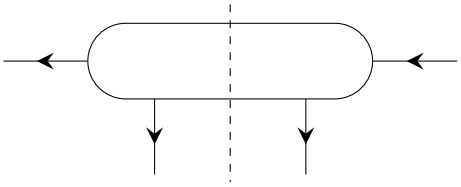
(c) Given a block matrix

$$M = \begin{pmatrix} A & C \\ B & D \end{pmatrix},$$

find a decomposition of M in terms of the SVD of A, B, C and D. Assume now that M is block diagonal and write down the SVD of M.

(d) How could one efficiently compute the SVD of a matrix which is known to conserve a quantum number?

(e) You are given the tensor from the diagram below and are asked to split it via SVD. Knowing that the quantum number represented by the arrows is conserved and making use of part (d), briefly explain an algorithm that is able to do this efficiently.



Exercise 11.1 (Conservation laws for the Ising model)
For this exercise we use an alternative convention for the Ising Hamiltonian (on a one-dimensional lattice with open boundary conditions), namely

$$H_{\text{ising}} = -J \sum_{j=1}^{L-1} X_j X_{j+1} - g \sum_{j=1}^{L} Z_j.$$

(It results from the hitherto version by a conjugation with the unitary matrix $H \otimes \cdots \otimes H$, with H the Hadamard gate. This form simplifies the discussion of quantum numbers.) The corresponding symmetry operator is now

$$P = \prod_{j=1}^{L} Z_j = Z \otimes \cdots \otimes Z.$$

(a) Show that the eigenstates of P are precisely the computational basis states $|a_1\rangle \otimes \cdots \otimes |a_L\rangle \equiv |a_1 \dots a_L\rangle$ with $a_j \in \{0, 1\}$ for all j, with corresponding eigenvalues ± 1. How is the eigenvalue related to the bit string $a_1 \dots a_L$?

In the following, we associate the overall quantum number 0 with eigenvalue 1 of P, and the overall quantum number 1 with eigenvalue -1, such that $\lambda = (-1)^q$, where λ is the eigenvalue and q the quantum number. Addition of quantum numbers is understood modulo 2.

(b) At each lattice site, we likewise attach the (local) quantum number 0 to $|0\rangle$ and 1 to $|1\rangle$. Based on the sparsity pattern of I_2, X and Z, decide which of these matrices leave the quantum number invariant, and which change it (equivalent to incrementing it by 1 modulo 2).

Recall that the Ising Hamiltonian admits a MPO representation, with tensors (for the current convention)

$$A^1 = \begin{pmatrix} -gZ & -JX & I_2 \end{pmatrix}, \quad A^j = \begin{pmatrix} I_2 & 0 & 0 \\ X & 0 & 0 \\ -gZ & -JX & I_2 \end{pmatrix} \ \forall j = 2, \dots, L-1, \quad A^L = \begin{pmatrix} I_2 \\ X \\ -gZ \end{pmatrix}.$$

(c) Assign quantum numbers 0 and 1 to the virtual bonds (the finite automaton "states" a, b, c from the lecture, or equivalently the input and output channels of A^j) such that they are compatible with the behavior of the entries I_2, X and Z of A^j found in (b).

Remark: Since the initial finite automaton state in the MPO form is always a, and the final state always c, one can conclude also from the MPO representation (together with the result of (c)) that the Hamiltonian does not change the overall quantum number, as expected (since it leaves the eigenspaces of P invariant).

Exercise 11.2 (DMRG and TEBD algorithm)
This exercise is concerned with an actual implementation of the two-site DMRG and TEBD algorithms. Please download and familiarize yourself with the Jupyter notebook template from the Moodle page, and then complete the following tasks:

(a) Implement the function `contract_right_block(A, W, R)` for performing a block contraction step.

(b) Complete the implementation of `dmrg_two_site(H, psi, numsweeps, tol)` by calling `split_mps_tensor` at the indicated locations, with appropriate distributing (absorption) of the singular values in the left or right tensor.

(c) Complete the implementation of `tebd_step(psi, U, tol)`.

(d) Finally, run the overall notebook. How many sweeps does DMRG require to converge to the ground state of the Ising model?