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Tutorial 9 (AKLT model[1])

The AKLT state has historically played an important role as analytically tractable, exact ground state in MPS form of a spin-1 model. In this tutorial we will construct this quantum state, which is sometimes deemed as the simplest non-trivial MPS. We start from the following Hamiltonian, which acts on spin-1 particles arranged on a one-dimensional lattice with periodic boundary conditions:

$$H = \sum_{j=1}^{L} P_j, \qquad P_j = \frac{1}{2}\vec{S}_j \cdot \vec{S}_{j+1} + \frac{1}{6}(\vec{S}_j \cdot \vec{S}_{j+1})^2 + \frac{1}{3}I,$$

where $\vec{S} = (S^x, S^y, S^z)$ collects the following "spin-1 operators":

$$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \text{and} \quad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The notation $\vec{S}_j$ means that $\vec{S}$ acts on the j-th particle, and $\vec{S}_j \cdot \vec{S}_{j+1} = S_j^x\, S_{j+1}^x + S_j^y\, S_{j+1}^y + S_j^z\, S_{j+1}^z$. It turns out that P_j is a projector, i.e., it is Hermitian and $P_j^2 = P_j$, and thus has eigenvalues 0 and 1. Since the Hamiltonian is a sum of positive semidefinite terms, its smallest possible eigenvalue is 0. The AKLT state is constructed as eigenstate of H with eigenvalue 0, and is thus a ground state (which turns out to be unique).

The basis states for a spin-1 particle are $|\hat{1}\rangle$, $|\hat{0}\rangle$ and $|-\hat{1}\rangle$. It is possible to combine two qubits to represent a spin-1 particle, via

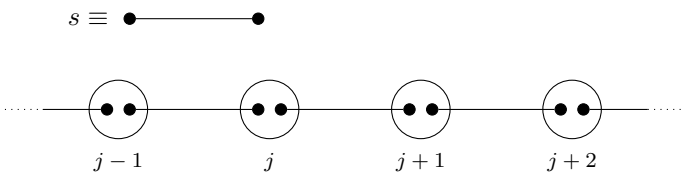
$$|\hat{1}\rangle = |00\rangle\,, \quad |\hat{0}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \quad \text{and} \quad |-\hat{1}\rangle = |11\rangle\,.$$

(a) Write down an operator $\mathcal{P}$ that maps states from this two-qubit subspace to the spin-1 space. Then define the degree-three tensor M such that $\mathcal{P} = \sum_{\sigma\in\{1,0,-1\}} \sum_{a,b\in\{0,1\}} m_{\sigma ab}\, |\hat{\sigma}\rangle\langle ab|$, where $|\hat{\sigma}\rangle\langle ab| \equiv |\hat{\sigma}\rangle \circ |ab\rangle$ denotes the outer product of $|\hat{\sigma}\rangle$ and $|ab\rangle$.

(b) As shown in the diagram below, the AKLT construction puts adjacent qubits of two neighboring sites into a so-called "singlet state":

$$s = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).$$

Assemble the matrix G such that $s = \sum_{a,b} g_{ba}\, |b\rangle\, |a\rangle$. Use it to write an expression for a state ψ with L lattice sites and periodic boundary conditions, where each site is in the state shown in the diagram.



(c) Project the state into the spin-1 subspace, $\hat{\psi} = \prod_{j=1}^{L} \mathcal{P}_j\, \psi$, and find the left-orthonormal MPS tensors A such that

$$\hat{\psi} = \sum_{\sigma\in\{1,0,-1\}^L} \mathrm{tr}\,[A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_L}]\, |\sigma\rangle\,.$$

[1] Original AKLT papers: I. **A**ffleck, T. **K**ennedy, E. H. **L**ieb, H. **T**asaki: *Rigorous results on valence-bond ground states in antiferromagnets*, Phys. Rev. Lett. 59, 799 (1987) and I. **A**ffleck, T. **K**ennedy, E. H. **L**ieb, H. **T**asaki: *Valence bond ground states in isotropic quantum antiferromagnets*, Commun. Math. Phys. 115, 477–528 (1988)

Exercise 9.1 (Commuting matrices and conservation laws)
The *commutator* of two square matrices A and B is defined as

$$[A, B] = AB - BA.$$

We say that the matrices commute if $[A, B] = 0$. An important property of two commuting, normal matrices A and B is that they can be "simultaneously diagonalized", i.e., there exists a common basis of eigenvectors; in other words, we can find a unitary matrix U such that both $U^\dagger AU$ and $U^\dagger BU$ are diagonal. As sketch of the proof, note that the matrices leave eigenspaces invariant: namely, if (λ, v) is an eigenpair of A such that $Av = \lambda v$, then Bv remains in the λ-eigenspace of A, since $A(Bv) = (AB)v = BAv = B(\lambda v) = \lambda(Bv)$. Thus we can first find the eigenspaces of A, and then diagonalize B within each eigenspace (or other way around), which will result in a common eigenbasis.

As application to quantum physics with a given Hamiltonian H, one often searches for another Hermitian matrix P which commutes with H. P is then denoted "symmetry operator". This allows to partition the eigenvectors of H into symmetry subspaces, i.e., eigenspaces of P.

(a) Different Pauli matrices do not commute, but "anti-commute" instead: one can verify by an explicit calculation that

$$XY = -YX, \quad YZ = -ZY, \quad ZX = -XZ.$$

Nevertheless, it turns out that $X \otimes X$, $Y \otimes Y$ and $Z \otimes Z$ pairwise commute. Prove this statement.

Hint: You can work directly with matrix representations, or combine the general identity $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$ with the anti-commuting property.

(b) A symmetry operator for the Ising model (see below) is

$$P = \prod_{j=1}^{L} X_j = X \otimes \cdots \otimes X,$$

where L denotes the number of lattice sites. Show that $[H, P] = 0$.

Exercise 9.2 (Exact diagonalization of the Ising model)
The transverse-field Ising model Hamiltonian is defined as

$$H = -J \sum_{\langle j,k \rangle} Z_j Z_k - g \sum_j X_j,$$

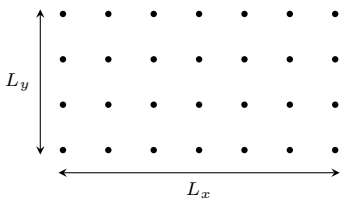
where $J, g \in \mathbb{R}$ are parameters, the first sum runs over nearest neighbor sites of the underlying lattice, the second sum over all lattice sites, and the notations X_j and Z_j mean Pauli-X and Z applied to the j-th lattice site, respectively. The overall goal of this exercise is to construct the Hamiltonian as sparse matrix[2], and investigate its physical properties. Please use the Jupyter notebook template from the Moodle page for the following tasks:

(a) Before assembling the actual Hamiltonian, we construct the *adjacency matrix* of various lattices. The adjacency matrix $A \in \mathbb{Z}^{L \times L}$ (with L the number of lattice sites) has entries (for lattice site indices j, k)

$$a_{jk} = \begin{cases} 1 & \text{if } j, k \text{ are nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Implement the function `adjacency_1D_lattice(L, pbc=True)`, which should return the adjacency matrix of a 1D lattice with L sites as NumPy array. The optional parameter `pbc` specifies whether periodic boundary conditions should be assumed (i.e., sites 0 and $L-1$ regarded as nearest neighbors).

Analogously, implement `adjacency_square_lattice(Lx, Ly, pbc=True)` for a 2D square lattice. `pbc=True` means periodic boundary conditions both in x- and y-direction. We follow the convention of enumerating lattice sites as $(0,0), \ldots, (0, L_y - 1), (1, 0), \ldots, (L_x - 1, L_y - 1)$.



Voluntary challenge: construct the adjacency matrix for a hexagonal or Kagome lattice.

[2] https://docs.scipy.org/doc/scipy/reference/sparse.html contains the documentation for the SciPy sparse matrix package.

(b) To construct Z_j (and similarly X_j) as sparse matrix (with j a zero-based lattice index), we can use that Kronecker products of identity matrices are again identity matrices:

$$Z_j = \underbrace{I_2 \otimes \cdots \otimes I_2}_{j \text{ terms}} \otimes Z \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{L-j-1 \text{ terms}} = I_{2^j} \otimes Z \otimes I_{2^{L-j-1}},$$

where L is the number of lattice sites and I_n denotes the $n \times n$ identity matrix. With that representation and the following pseudocode, you can now implement `construct_ising_hamiltonian(J, g, adj)`, where `adj` is the adjacency matrix of the underlying lattice.

```
H = sparse 2^L × 2^L zero matrix
for j = 0,...,L-1:
    for k = j+1,...,L-1:
        if adj[j,k] > 0:
            H -= J Z_j Z_k
    H -= g X_j
```

Hint: Consult `scipy.sparse.eye` and `scipy.sparse.kron`. `scipy.sparse.csr_matrix((n, n), dtype=float)` generates a sparse $n \times n$ zero matrix with floating-point entries.

(c) Read the documentation of `scipy.sparse.linalg.eigsh`, which implements a variant of the Lanczos algorithm, and use this function to compute the 5 *algebraically smallest* eigenvalues and -vectors of the exemplary Hamiltonian from the notebook.

(d) We can fix the parameter $J = 1$ w.l.o.g., which can be interpreted as unit of energy. It turns out that the Ising model exhibits a so-called *phase transition* at $g = 1$ on an "infinite" 1D lattice (i.e., when taking the limit $L \to \infty$). One can observe this effect by plotting the spin-spin correlation function $\langle \psi_0, Z_0 Z_{L/2} \, \psi_0 \rangle$ as function of g, where ψ_0 denotes the corresponding ground state (lowest energy eigenstate) of H. Complete the notebook template to compute and visualize this quantity for a parameter sweep of $g \in [0, 2]$ and lattice sizes $L \in \{6, 8, 10, 12\}$.

(e) Finally, complete the section on the *excitation energies* (energy difference to ground state energy) for the first two excited states, and run the overall notebook.