

## Problem Set 3

### Exercise: Single-site DMRG

- Consider the 1D spin-1/2 XY chain with open boundary condition:

$$H_{\text{XY}} = -\frac{1}{2} \sum_{j=1}^{N-1} (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+)$$

- What is the MPO form of the Hamiltonian  $H_{\text{XY}}$ ?



- Calculate the ground-state energy of  $H_{XY}$  with the **single-site DMRG** algorithm. Compare your result with the exact result ( $N$  even):

$$E_{GS} = \frac{1}{2} - \frac{1}{2 \sin \frac{\pi}{2(N+1)}}$$

- Calculate the nearest-neighbor spin correlation function  $\langle \psi | S_j^+ S_{j+1}^- | \psi \rangle$  by **using the MPS obtained from DMRG**. Compare your result with the exact result ( $N$  even):

$$\langle \psi | S_j^+ S_{j+1}^- | \psi \rangle = -\frac{1}{2(N+1)} \left[ \frac{(-1)^j}{\sin \frac{(2j+1)\pi}{2(N+1)}} - \frac{1}{\sin \frac{\pi}{2(N+1)}} \right]$$

SS2021: Tensor Networks

Institut für Theoretische Physik, TU Dresden

Lecturer: Hong-Hao Tu

Tutorial: 20.05.2021



**TECHNISCHE  
UNIVERSITÄT  
DRESDEN**

- (**Bonus**) How would you adapt the single-site DMRG for obtaining an MPS approximation of the **first-excited state**?