Tensor networks for many-body quantum spin models

Learning outcomes

- Understand the degree of quantum entanglement in different models
- Rationalize how and when tensor-networks allow solving quantum many-body Hamiltonians
- Understand how observables in large systems allow probing phase transitions

The quantum many-body problem

Let us go back to a simple many-body problem $$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

And let us imagine that we have L different sites on our system and S=1/2

For example, for L=2 sites the elements of the basis are

$$|\uparrow\uparrow\rangle \quad |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \quad |\downarrow\downarrow\rangle$$

For L=3 sites the elements of the basis are

$$|\uparrow\uparrow\uparrow\rangle \quad |\uparrow\uparrow\downarrow\rangle \quad |\uparrow\downarrow\uparrow\rangle \quad |\uparrow\downarrow\downarrow\rangle$$

$$|\downarrow\uparrow\uparrow\rangle \quad |\downarrow\uparrow\downarrow\rangle \quad |\downarrow\downarrow\uparrow\rangle \quad |\downarrow\downarrow\downarrow\rangle$$

The quantum many-body problem

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For L=4 sites, the elements of the basis are

$$\begin{array}{cccc}
|\uparrow\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\uparrow\downarrow\rangle & |\uparrow\uparrow\downarrow\uparrow\rangle & |\uparrow\uparrow\downarrow\downarrow\rangle \\
|\uparrow\downarrow\uparrow\uparrow\rangle & |\uparrow\downarrow\uparrow\downarrow\rangle & |\uparrow\downarrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\downarrow\rangle \\
|\downarrow\uparrow\uparrow\uparrow\rangle & |\downarrow\uparrow\uparrow\downarrow\rangle & |\downarrow\uparrow\downarrow\uparrow\rangle & |\downarrow\uparrow\downarrow\downarrow\rangle \\
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\end{array}$$

The quantum many-body problem

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$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

And let us imagine that we have L different sites on our system and S=1/2

The dimension of the Hilbert space grows as

$$d = 2^L$$

The quantum many-body problem

Let us go back to a simple many-body problem

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

A typical wavefunction is written as

$$|\Psi\rangle = \sum c_{s_1, s_2, \ldots, s_L} |s_1, s_2, \ldots s_L\rangle$$

We need to determine in total 2^L coefficients

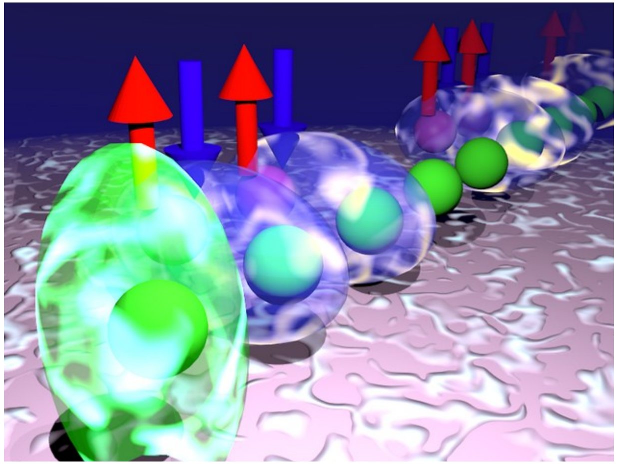
Is there an efficient way of storing so many coefficients?

The fundamental idea of tensor-networks

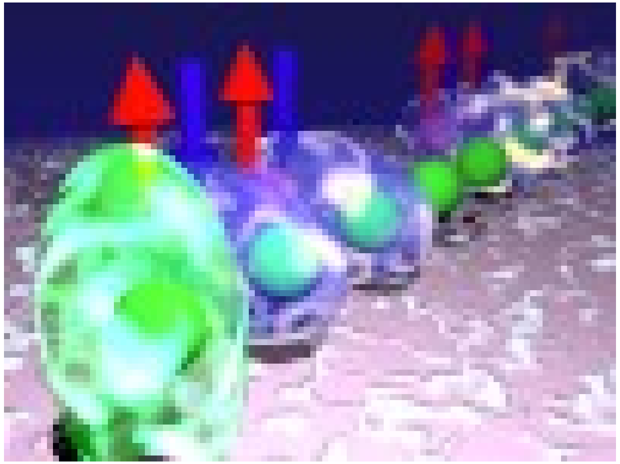
A many-body wavefunction a is a very high dimensional object

$$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L} |s_1, s_2, \ldots s_L\rangle$$

Tensor-networks allow "compressing" all that information in a very efficient way



"True wavefunction"



"Tensor-network wavefunction"

Matrix product states and tensor networks

The matrix-product state ansatz

For this wavefunction $|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L}|s_1, s_2, \ldots s_L\rangle$

Let us imagine to propose a parametrization in this form

$$c_{s_1,s_2,\ldots.,s_L} = M_1^{s_1} M_2^{s_2} \ldots . M_L^{s_3}$$

dimension 2^L

dimension $\sim Lm^2$

(m dimension of the matrix)

Why is this is a good parametrization of a wavefunction?

The matrix-product state ansatz

- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- One-dimensional problems, have ground states that can be captured with this ansatz

$$c_{s_1,s_2,\ldots,s_L} = M_1^{s_1} M_2^{s_2} \ldots M_L^{s_3}$$

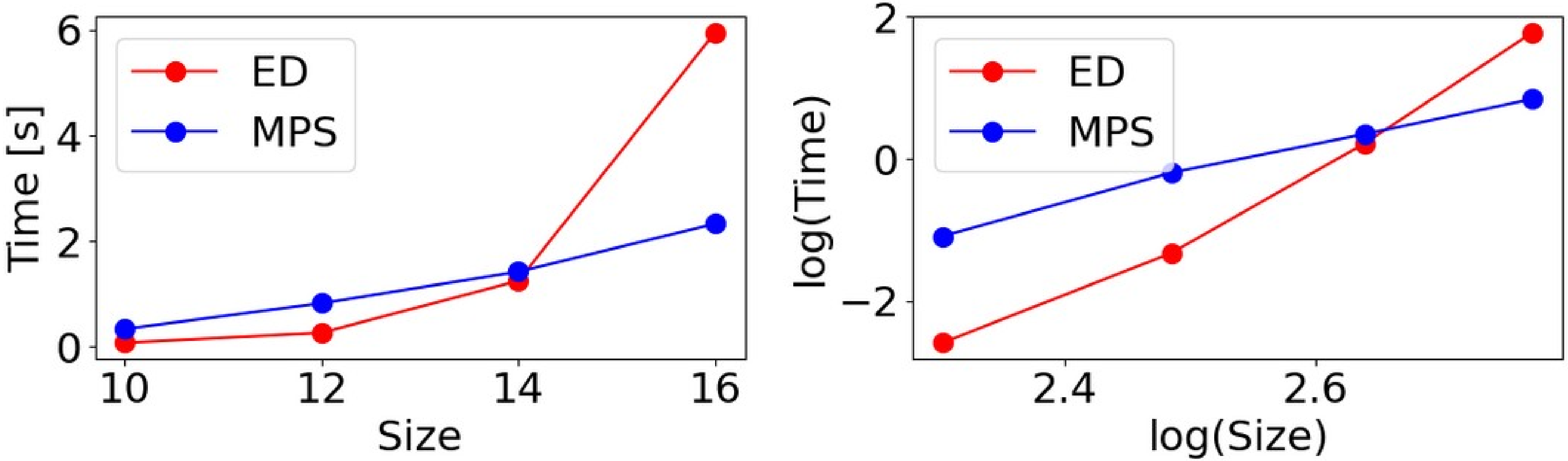
This ansatz can be generalized for time-evolution, excited states, open systems.

Computational complexity of matrix product states

Matrix product states provide a highly favorable scaling with system size

For concreteness for this Hamiltonian $H = \sum \vec{S}_n \cdot \vec{S}_{n+1}$

$$T_{ED} \sim e^L \qquad T_{MPS} \sim L^n$$



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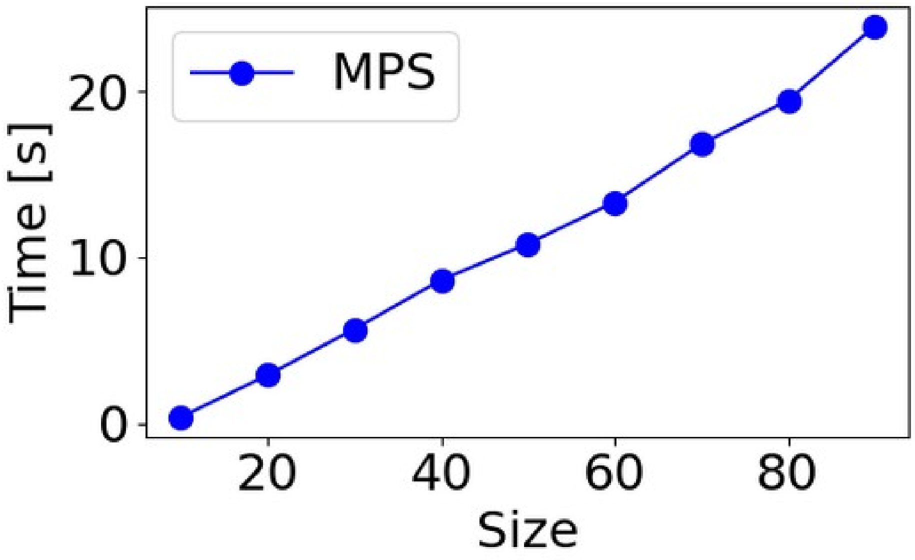
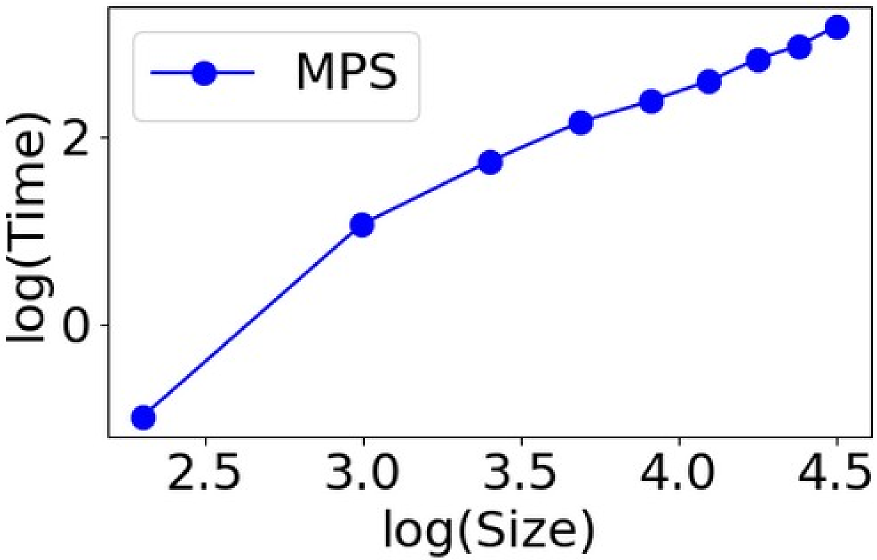
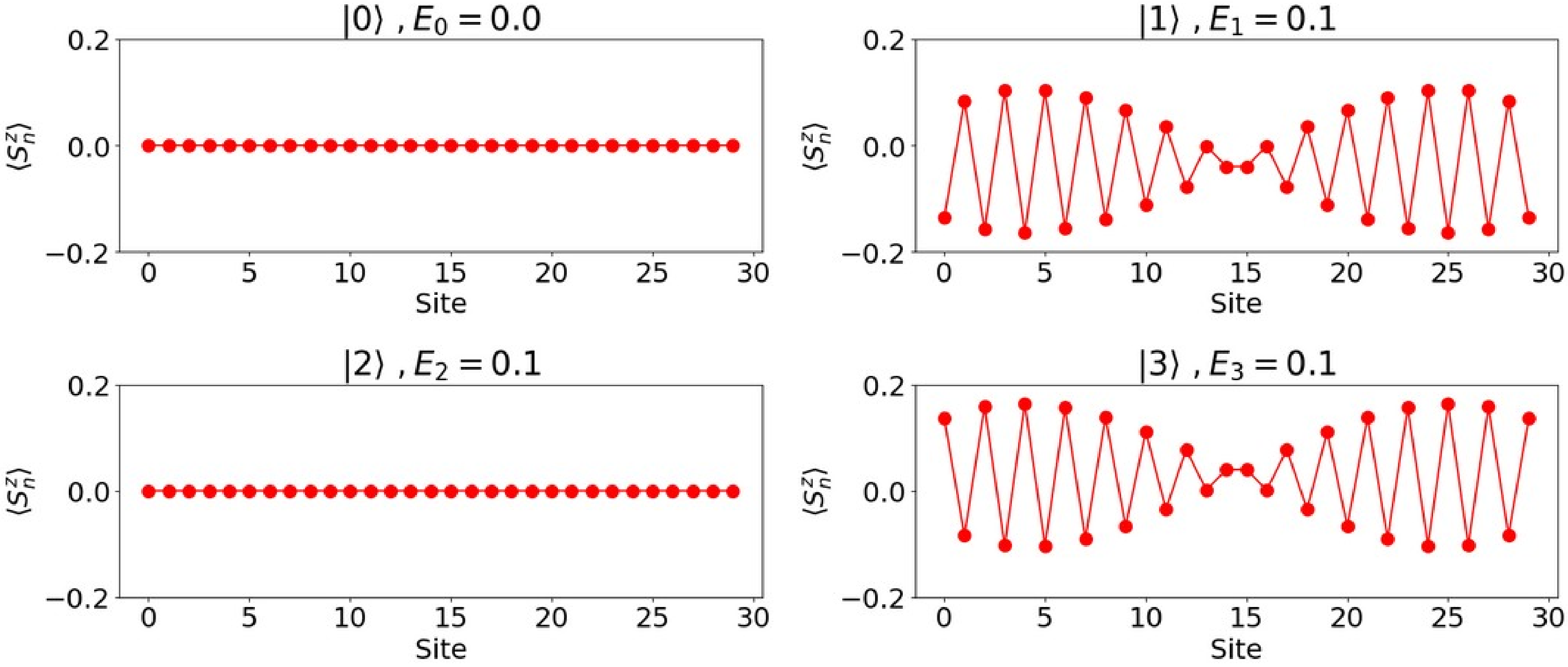




Magnetization in excited states of long chains

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$$

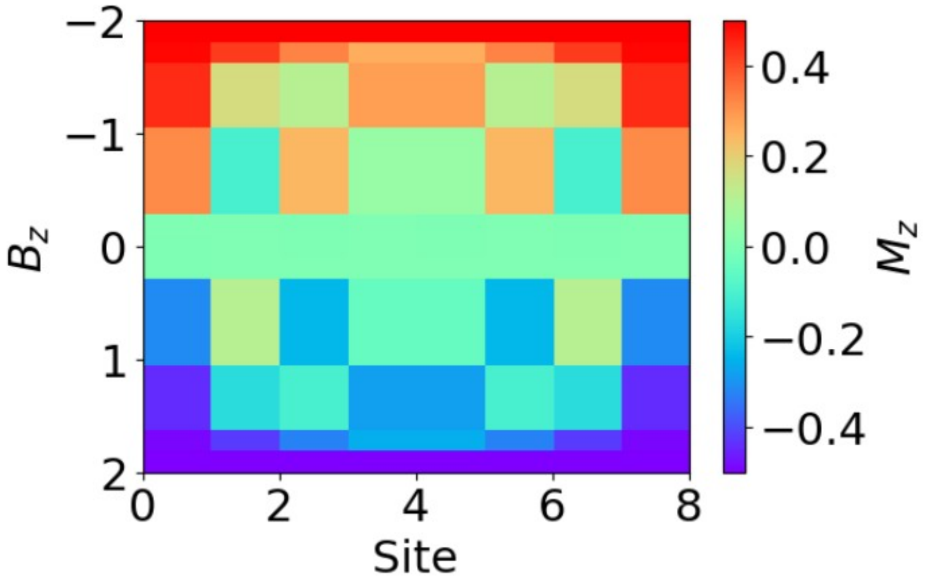


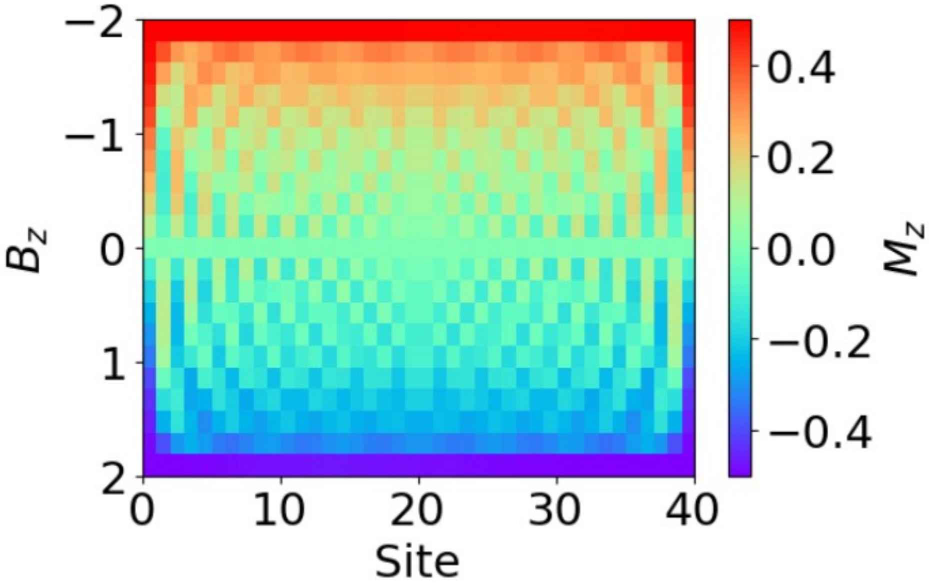
Level crossing with matrix product states

Let us take a quantum magnet in the presence of an external magnetic field

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S^z_n$$

Matrix product states allows computing level crossings for large systems

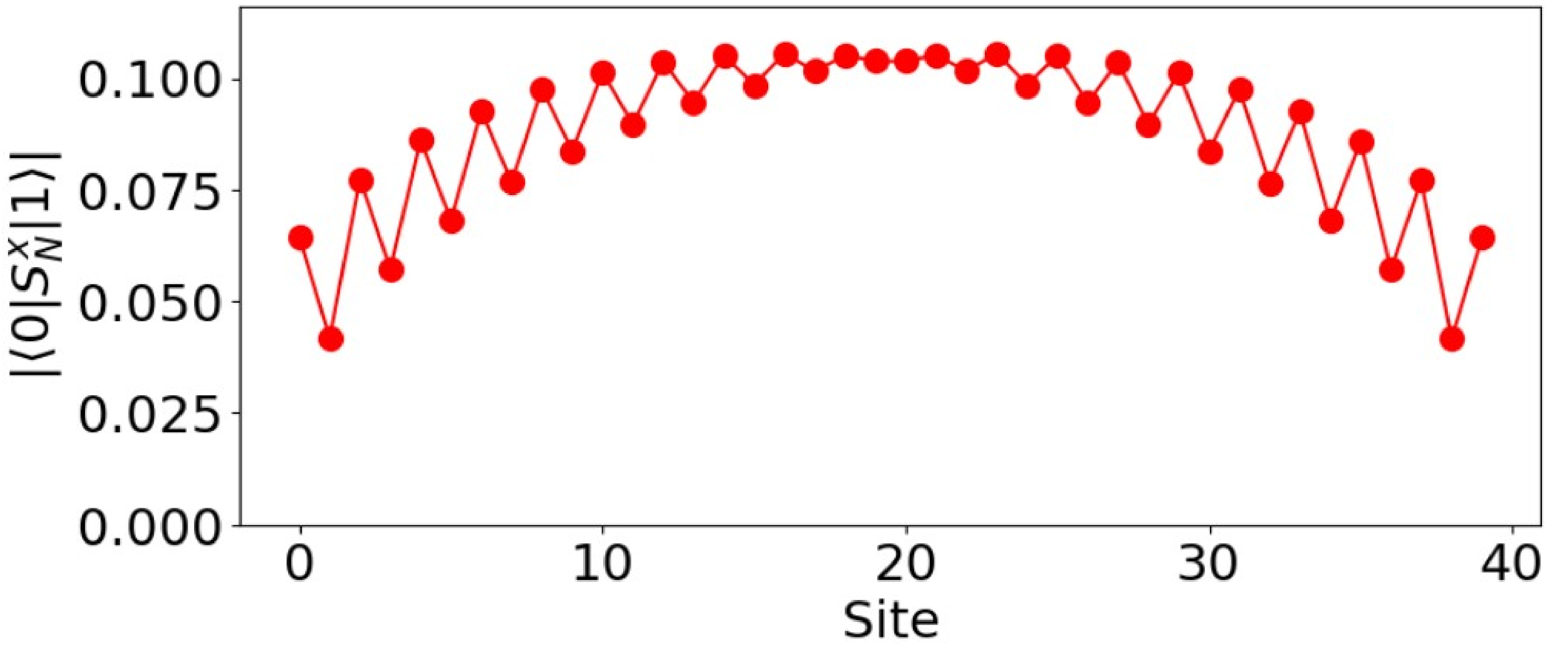




Matrix elements between ground state and excited states

We can compute matrix elements between the ground state and excited states

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z \qquad M_{0\to 1} = |\langle 1 | S_n^x | 0 \rangle|$$



Matrix elements between ground state and excited states

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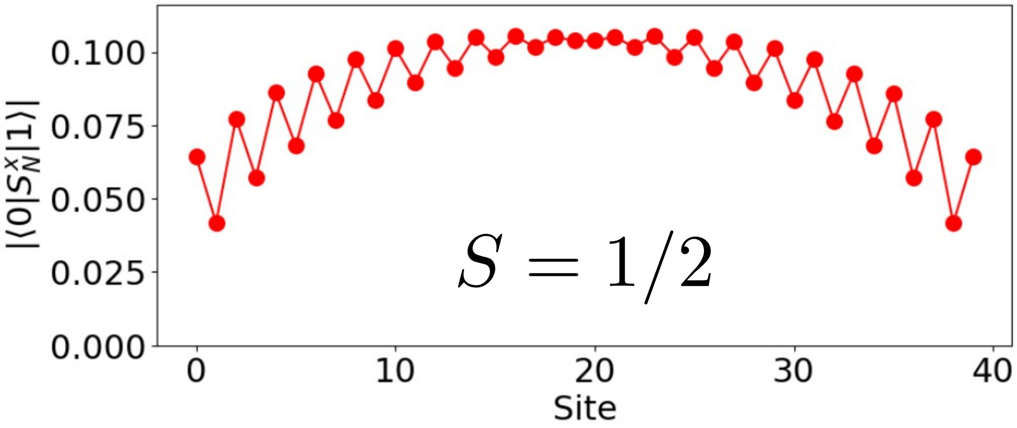
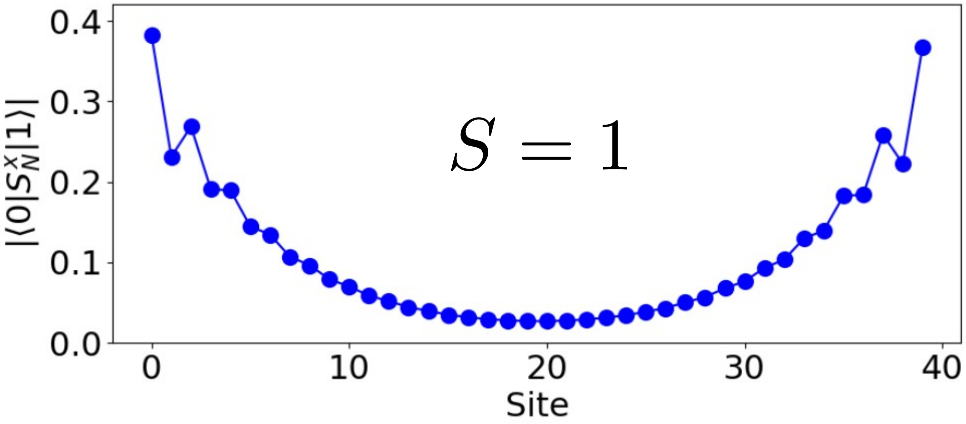
Bulk excitation



Edge excitation

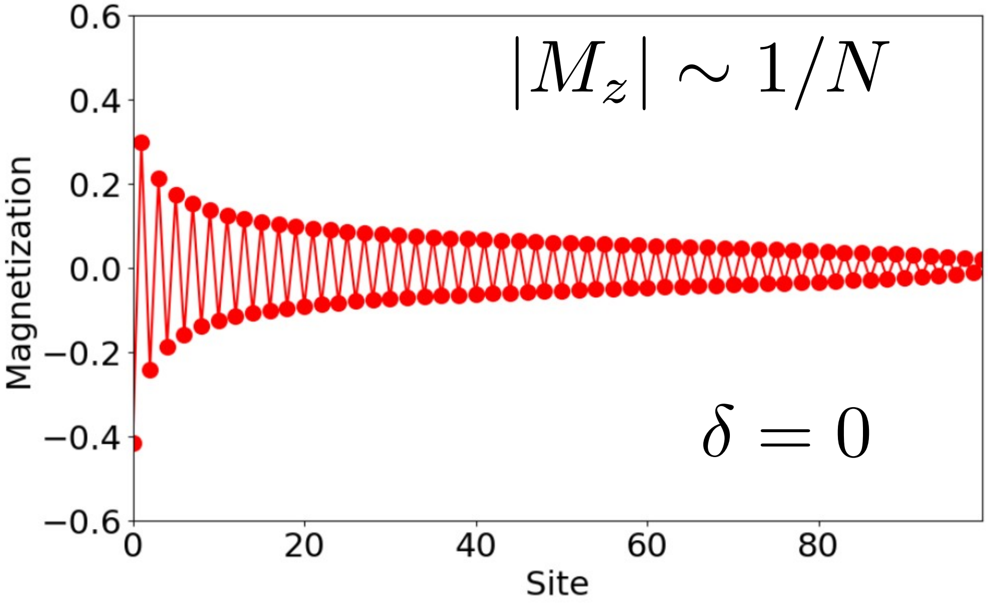


Response of a large quantum magnet to a magnetic impurity

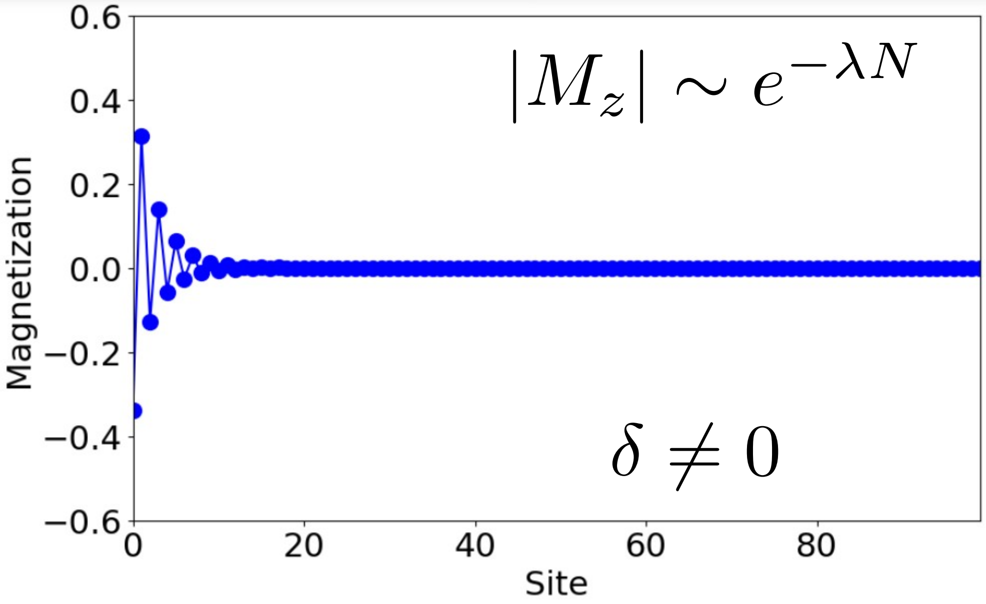
Quantum chain with a local field

$$H = \sum_n (1+\delta(-1)^n)\vec{S}_n \cdot \vec{S}_{n+1} + B_z S_0^z$$

Uniform chain

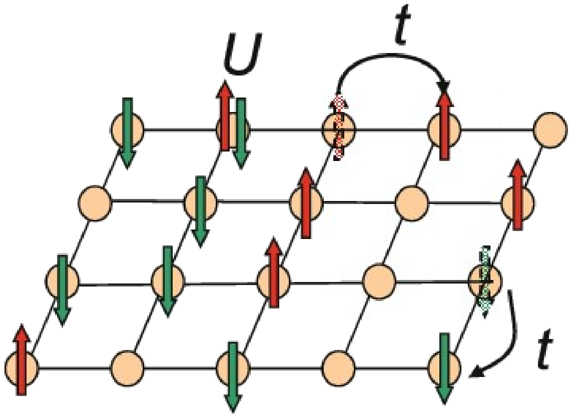


Dimerized chain



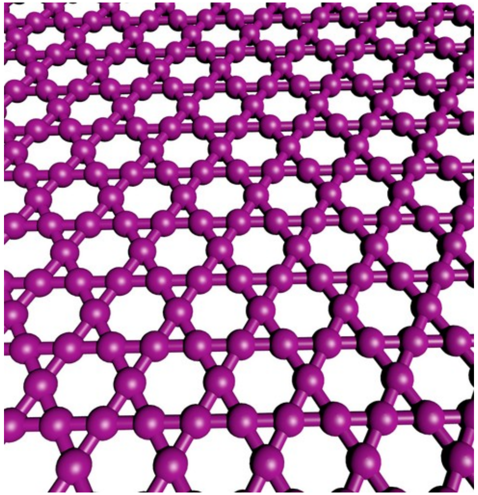
Some paradigmatic quantum materials tackled with tensor networks

Solving the 2D Hubbard model at finite doping



$$H = \sum_{ij,s} t_{ij} c^{\dagger}_{is} c_{js} + \sum_{i} U c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$$

Solving the 2D Heisenberg model in frustrated lattices



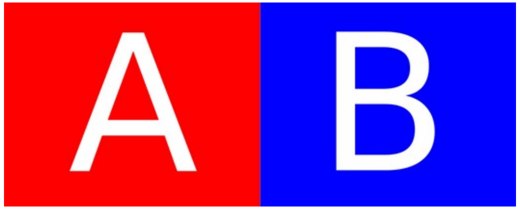
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

The entanglement entropy and the bond dimension

Entanglement in a many-body wavefunction

If a state can be written as

$$|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$$



Then we say that it is not entangled

For example the following states are not entangled

$$|\Psi\rangle = |\uparrow\downarrow\rangle \qquad |\Psi\rangle = (|\uparrow\rangle_1 + |\downarrow\rangle_1) \otimes (|\uparrow\rangle_2 + |\downarrow\rangle_2)$$

But this state is entangled $$|\Psi\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]$$

How can we know, and quantify, how entangled an state is?

The entanglement entropy

We can quantify the entanglement in a system through the entanglement entropy

Define the density matrix $$\rho = |\Psi\rangle \langle\Psi|$$

Trace over one subsystem (reduced density matrix) $$\rho_A = \mathrm{Tr}_B(\rho)$$

Defining the entropy of the state $$S_A = -\mathrm{Tr}(\rho_A \log \rho_A)$$

For a product state $$|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$$

the entanglement entropy is identically zero

The transverse field Ising model

Let us look at the transverse field Ising model

$$H = -\sum_n S_n^z S_{n+1}^z + B_x \sum_n S_n^x$$

It has two different ground states

Out -of plane ferromagnet

$$|B_x| \ll 1$$

$$|GS\rangle \approx |\uparrow\uparrow\uparrow\uparrow\rangle$$

Phase transition at

$$B_x = 1/2$$

In-plane ferromagnet

$$|B_x| \gg 1$$

$$|GS\rangle \approx |\rightarrow\rightarrow\rightarrow\rightarrow\rangle$$

For intermediate values of the field, a quantum phase transition takes place

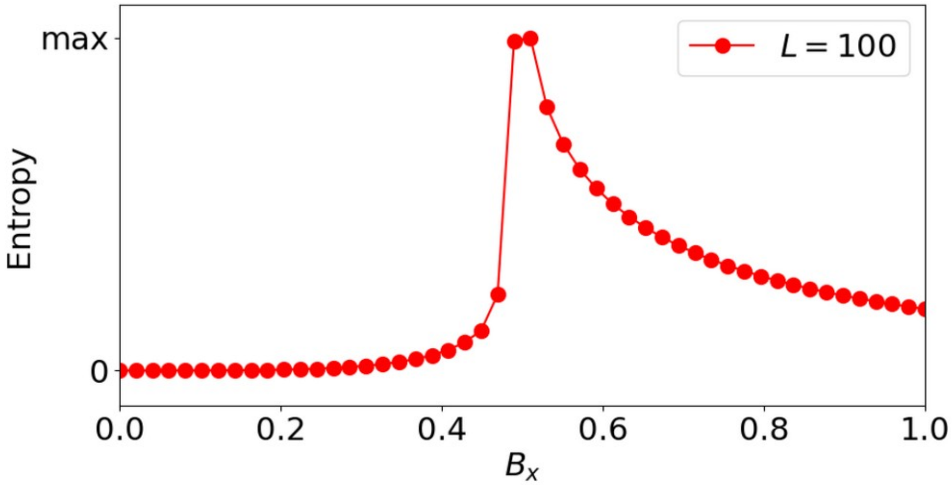
Can such a phase transition be observed from the entanglement entropy?

Entanglement entropy and phase transitions

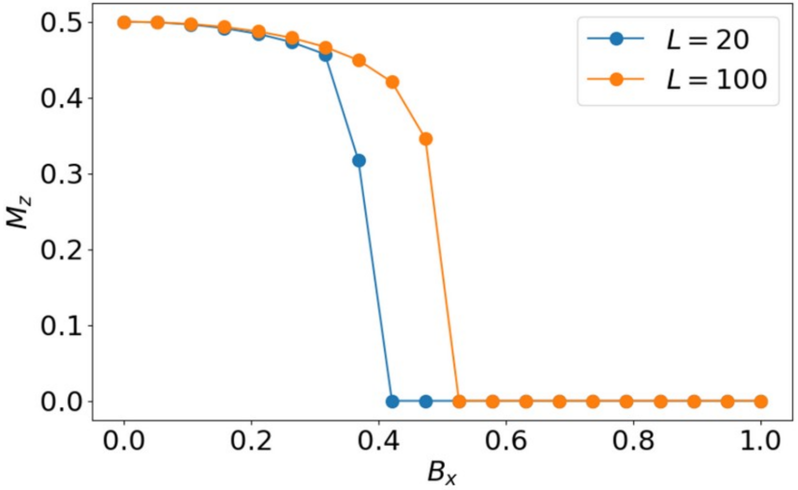
Let us look at the transverse field Ising model

$$H = -\sum_n S_n^z S_{n+1}^z + B_x \sum_n S_n^x$$

Phase transition from entropy

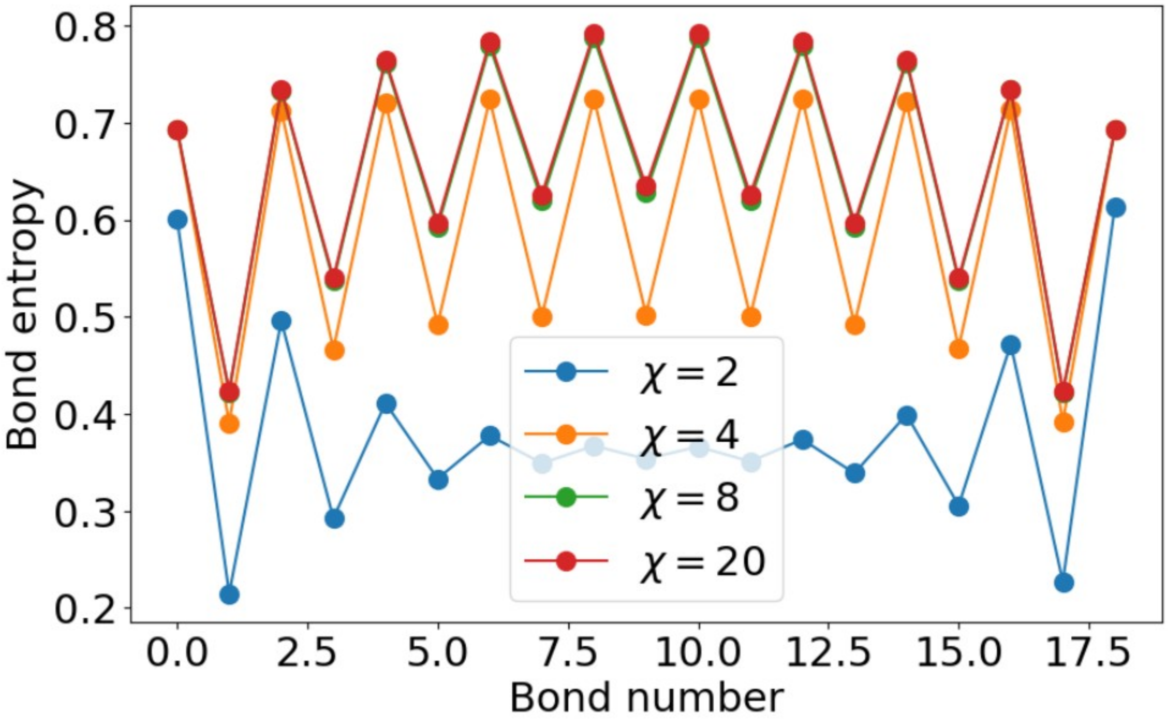


Phase transition from order parameter



Entanglement entropy in space and the bond dimension

The bond dimension determines the maximal entanglement entropy



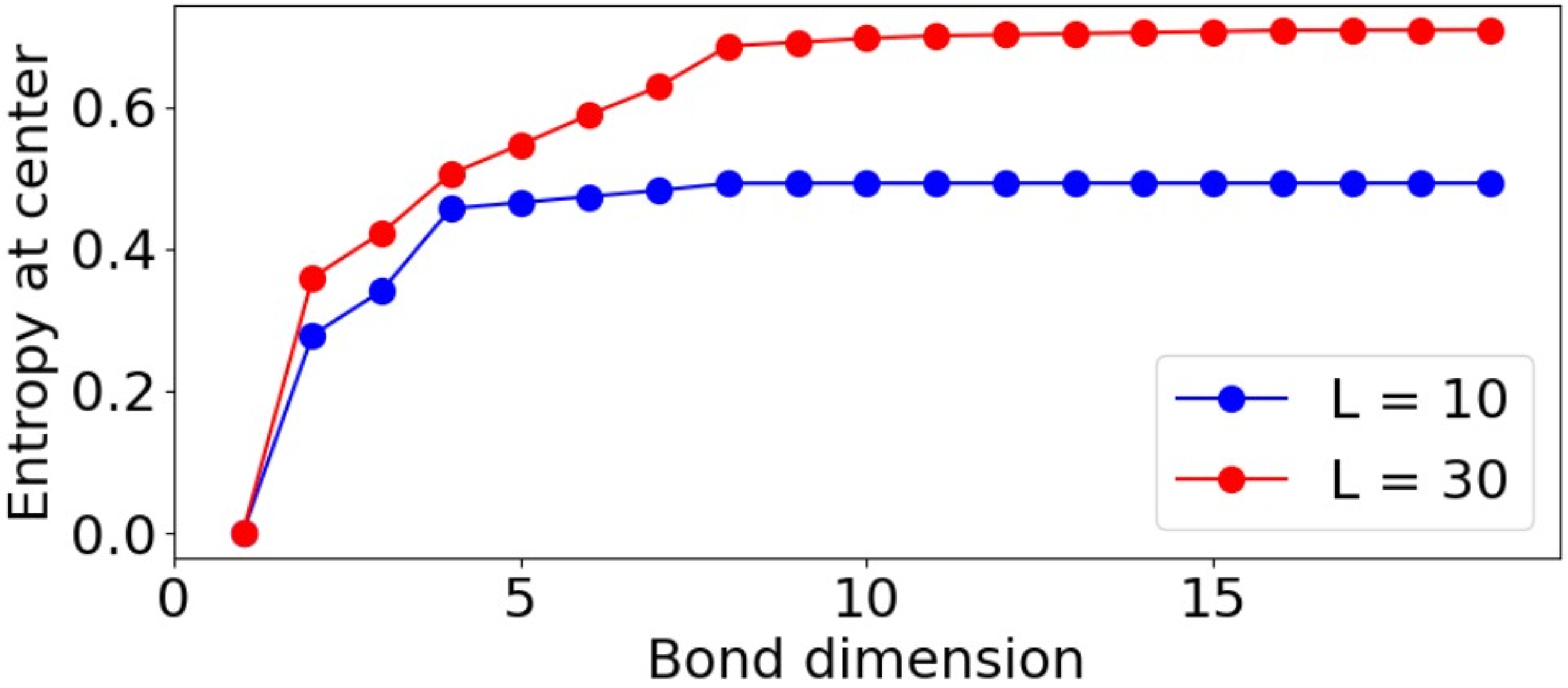
Heisenberg model

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

Entanglement entropy and the bond dimension

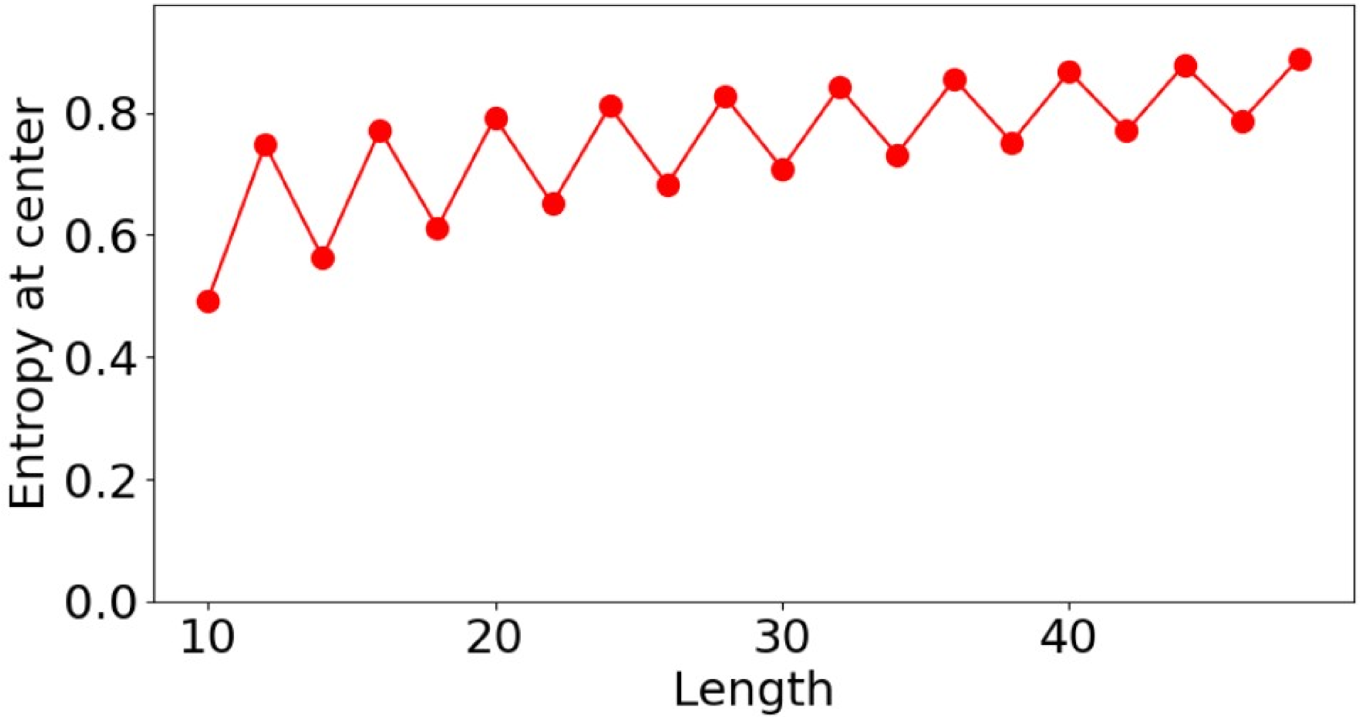
The entanglement of the MPS saturates with the bond dimension

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$



Entanglement entropy and the area law

For one dimensional systems, the entanglement entropy is (almost) system size independent



Heisenberg model

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

The entanglement entropy of a gaped 1d model

Take a dimerized Heisenberg model of the form $$H = \sum_n J\vec{S}_{2n} \cdot \vec{S}_{2n+1}$$

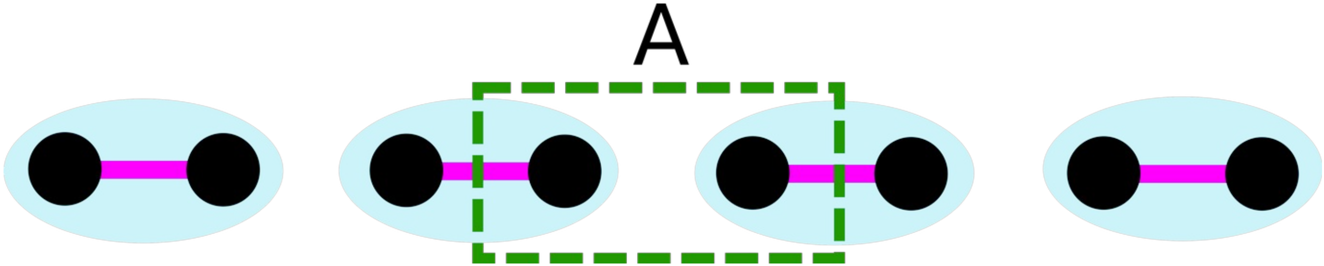
The many-body wavefunction is just a product of singlet between dimers

$$|\Psi\rangle \sim \prod_{\otimes n} \left(|\uparrow_{2n}\downarrow_{2n+1}\rangle - |\downarrow_{2n}\uparrow_{2n+1}\rangle\right)$$

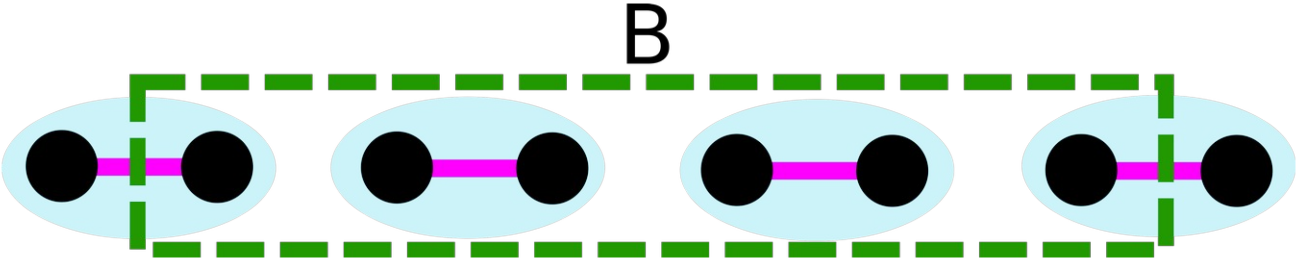
What is the entanglement entropy when making a bipartition?

The entanglement entropy of a gaped 1d model

Let us first take a small partition A, and compute the entanglement entropy



The entanglement entropy stems from the number of singlets that are cut
If the bipartition is bigger, the number of singlets that are cut remains the same

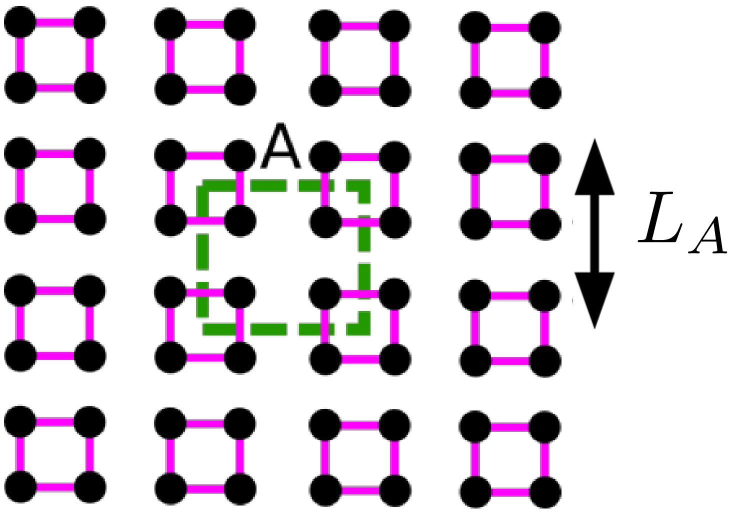


The entanglement entropy does not depend on the size of the partition $S_A \sim S_B \sim 2\log(2)$

The entanglement entropy of a gaped 2d model

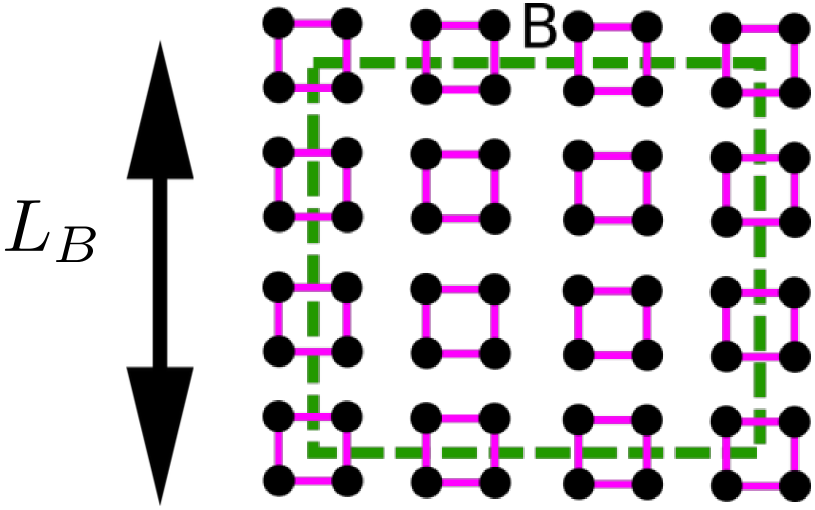
Let us consider the analogous Heisenberg model dimerized in 2D $H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Partition A



$S_B > S_A$

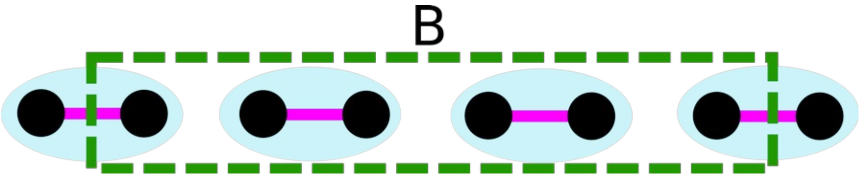
Partition B



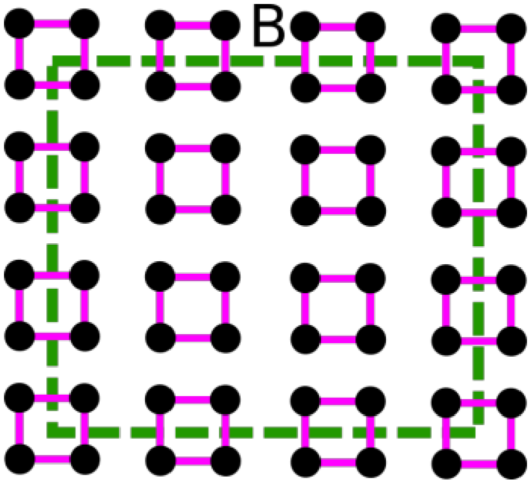
$$S_A \sim L_A \sim \partial A$$
$$S_B \sim L_B \sim \partial B$$

Entanglement entropy and the area law

The ground state of gapped systems follows the area law, meaning that the entanglement entropy of a subsystem depends of the length of the boundary



In 1D, the entropy is independent of the system size

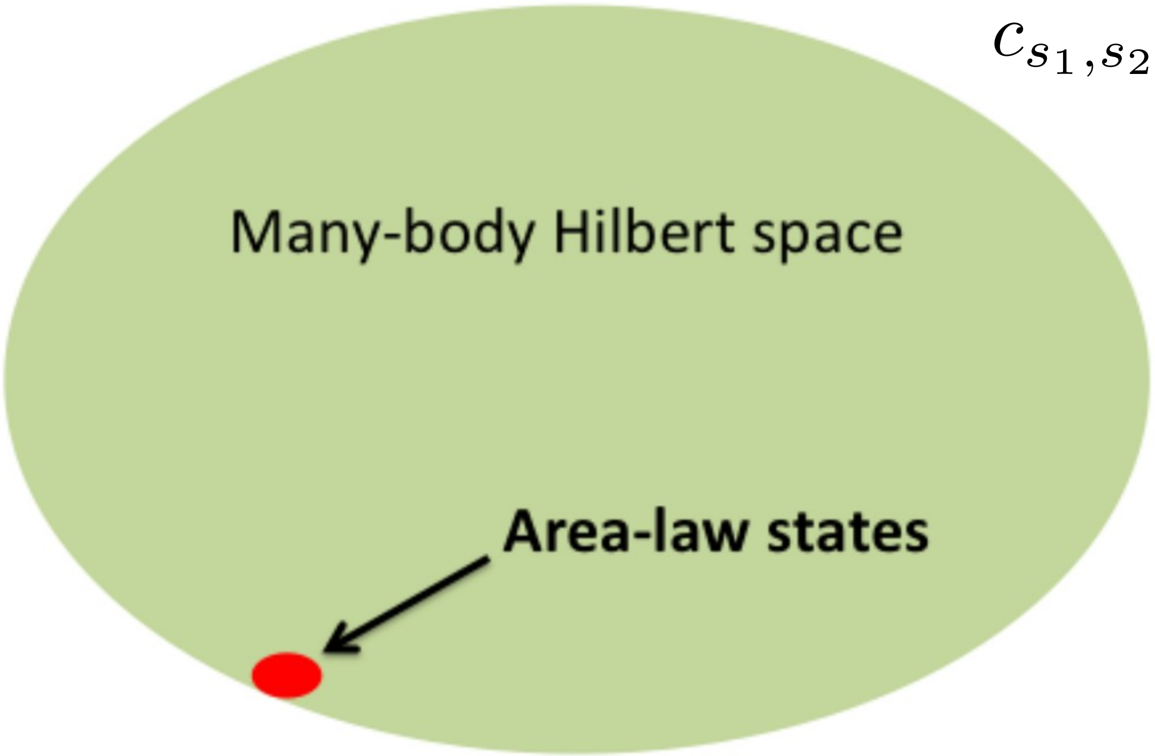


In 2D, it grows linearly with the size of the subsystem

Matrix product states have an entanglement entropy controlled by the size of the matrices

$$c_{s_1,s_2,\ldots,s_L} = M_1^{s_1} M_2^{s_2} \ldots M_L^{s_3}$$

Matrix product states and area law states



$$c_{s_1,s_2,\ldots,s_L} = M_1^{s_1} M_2^{s_2} \ldots M_L^{s_3}$$

$$M \sim m \times m \text{ matrix}$$

Entanglement entropy of an MPS

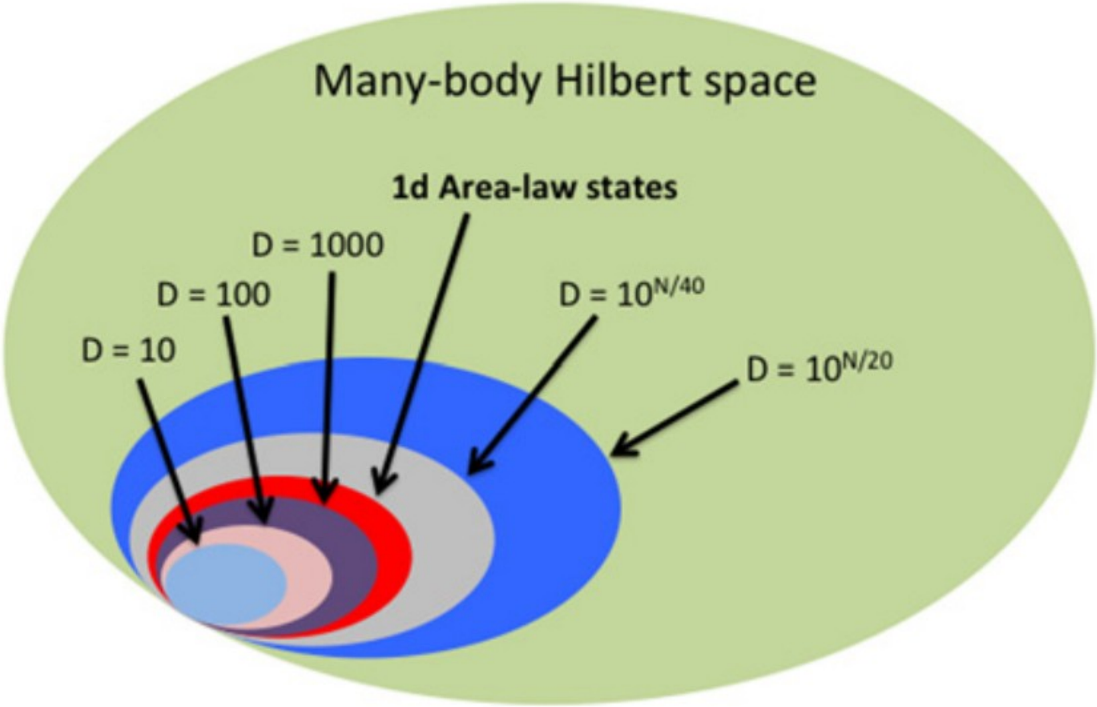
$$S_A \sim \log(m)$$

When do matrix product states fail?

- This ansatz enforces a maximum amount of entanglement entropy in the state $S \sim \log m$
- If the states have too much entanglement, MPS does not capture the state properly
  - Time-evolution to long times
  - Many-body problems above 1D
  - Highly excited states
  - Far from equilibrium states

When do matrix product states fail?

Sketch of the space parametrized with bond dimension D



The energy fluctuation

Let us imagine that we have an approximate ground state

$$E_\Omega = \langle \Omega | H | \Omega \rangle \qquad\qquad H|n\rangle = E_n |n\rangle$$

How do we know the quality of the ground state?

$$|\Omega\rangle = |0\rangle + \epsilon^2 |1\rangle \qquad\qquad \epsilon \ll 1$$

$$\Delta E_\Omega = \sqrt{\langle \Omega | H^2 | \Omega \rangle - \left(\langle \Omega | H | \Omega \rangle\right)^2}$$

$$\Delta E_\Omega \sim \epsilon (E_1 - E_0)$$

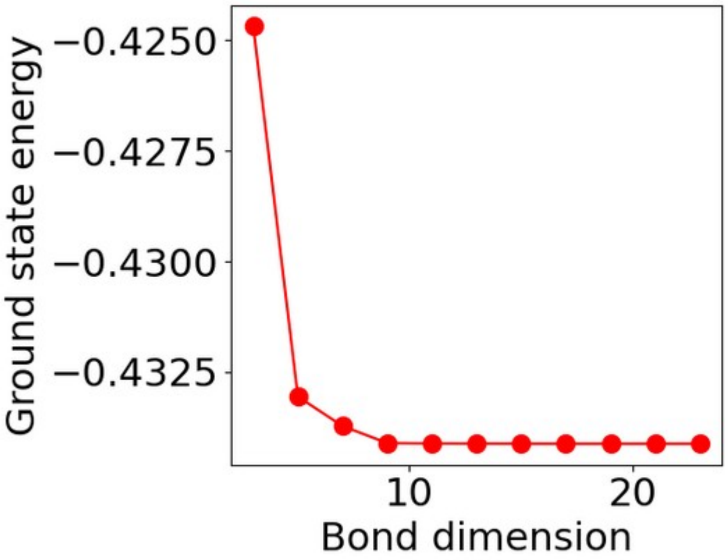
A non-zero fluctuation means that the variational state has some mixing with an excited state

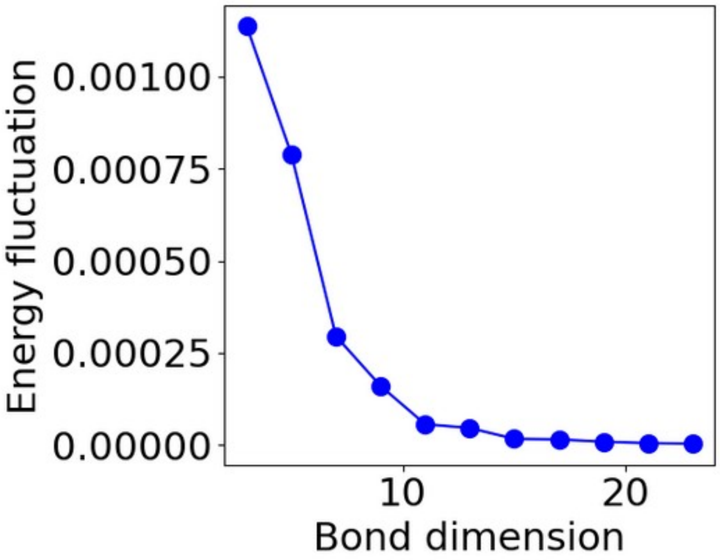
The importance of the bond dimension, ground state

Let us take a Heisenberg model $$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

And compute both the energy per site and energy fluctuation for different bond dimensions

$$H|\Omega\rangle \approx E_0|\Omega\rangle \qquad \sqrt{\langle\Omega|H^2|\Omega\rangle - (\langle\Omega|H|\Omega\rangle)^2}$$





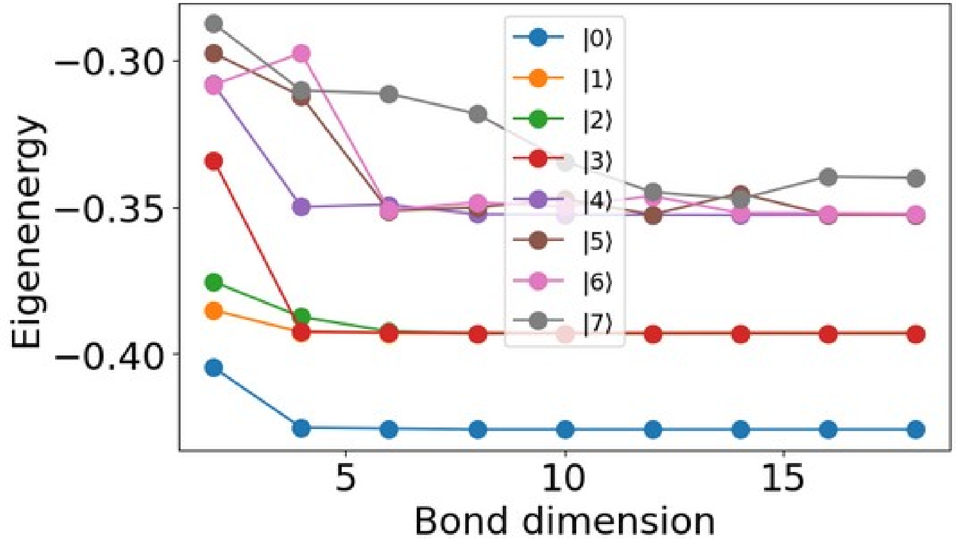
The importance of the bond dimension, excited states

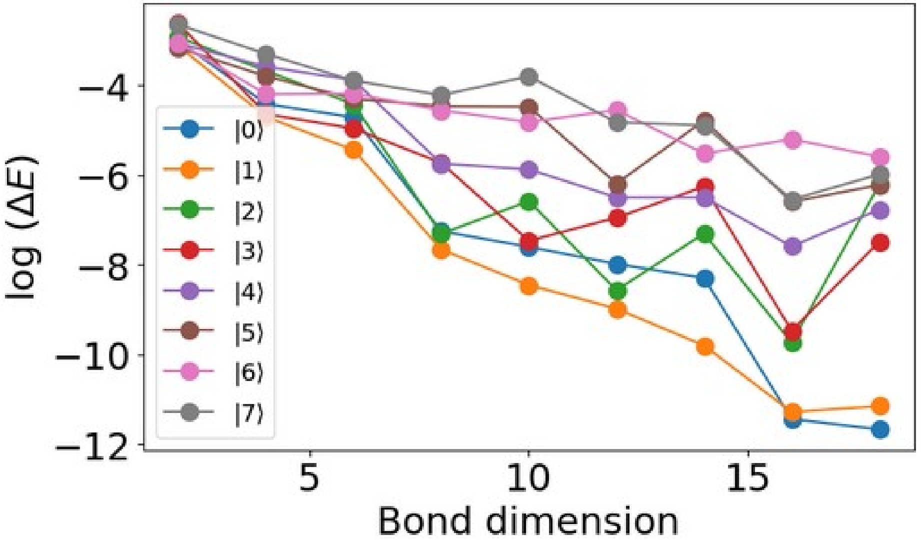
We will now look at excited states $$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

And compute both the energy per site and energy fluctuation for different bond dimensions

$$H|n\rangle \approx E_n|n\rangle$$

$$\sqrt{\langle n|H^2|n\rangle - (\langle n|H|n\rangle)^2}$$

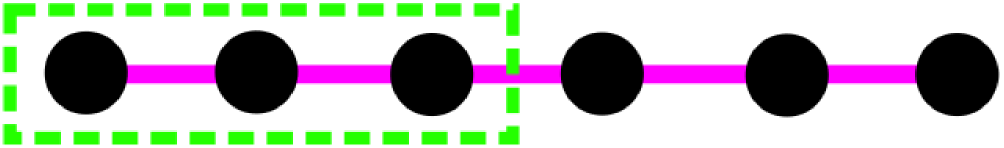




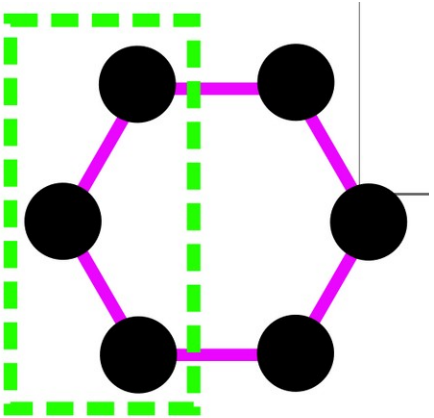
The importance of the boundary conditions in the entropy

When we consider a 1D Hamiltonian we can choose open or closed boundary conditions

Open boundary conditions



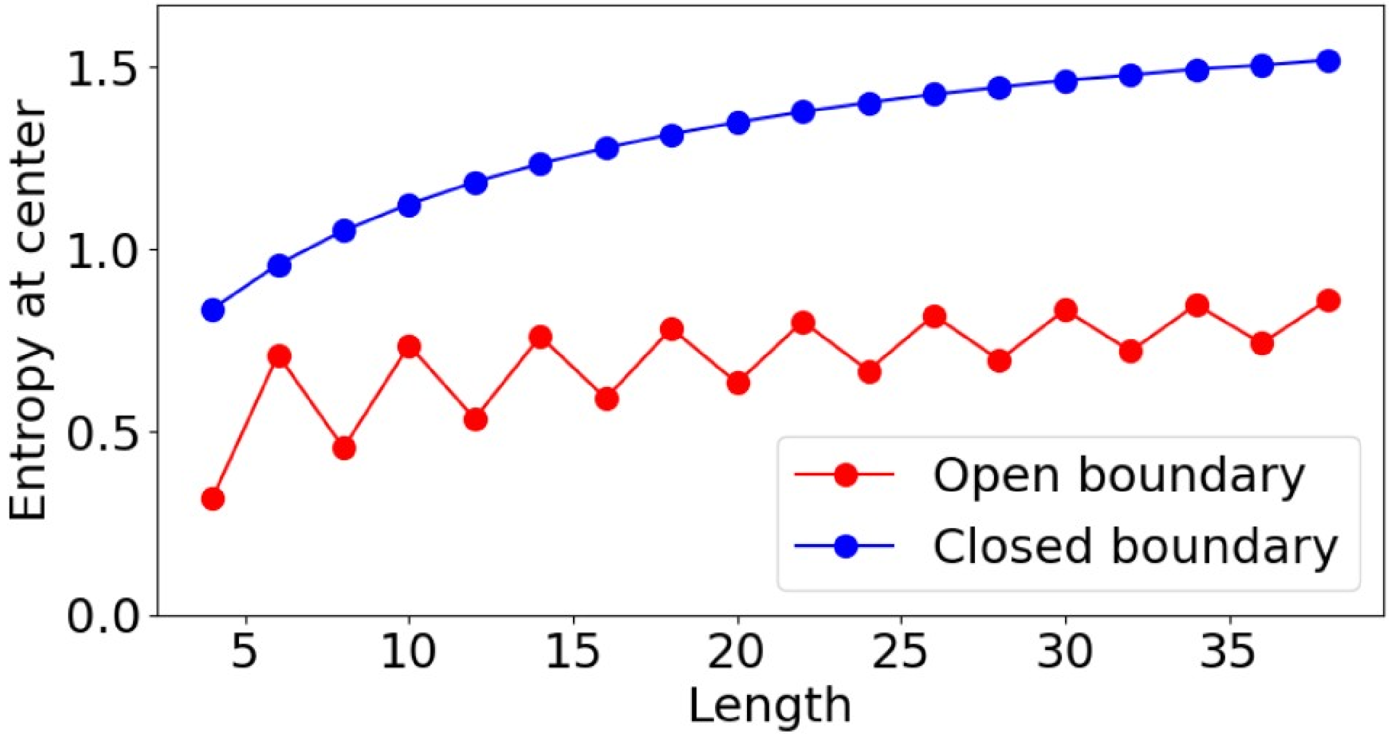
Closed boundary conditions



Closed boundary conditions lead to higher entanglement entropy

The importance of the boundary conditions in the entropy

When we consider a 1D Hamiltonian we can choose open or closed boundary conditions



Quantum magnets in the thermodynamic limit

Fractionalization in quantum spin chains

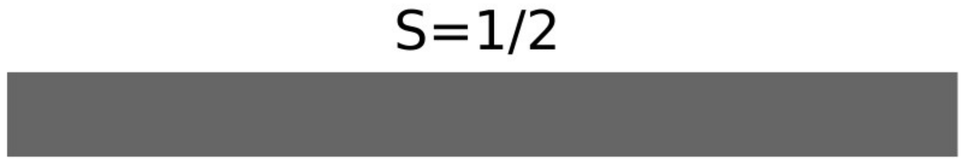
When considering a Heisenberg model, we could use S=1/2 or S=1 operators

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

$$S = 1/2$$

Gapless quantum magnet

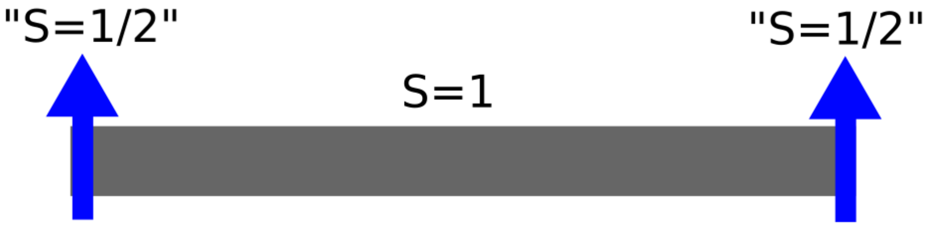
Gapless spinons



$$S = 1$$

Gapped quantum magnet

Topological fractional edge modes

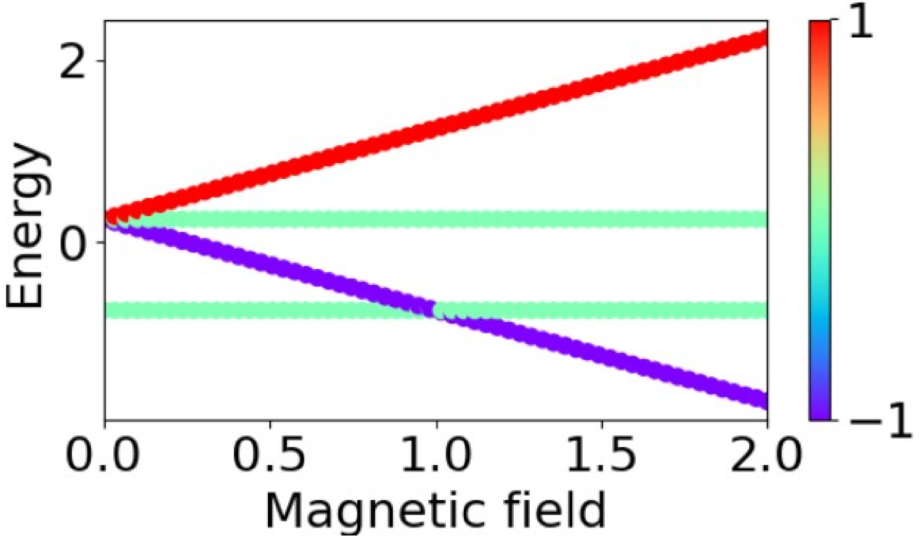


The gapless spectra of S=1/2

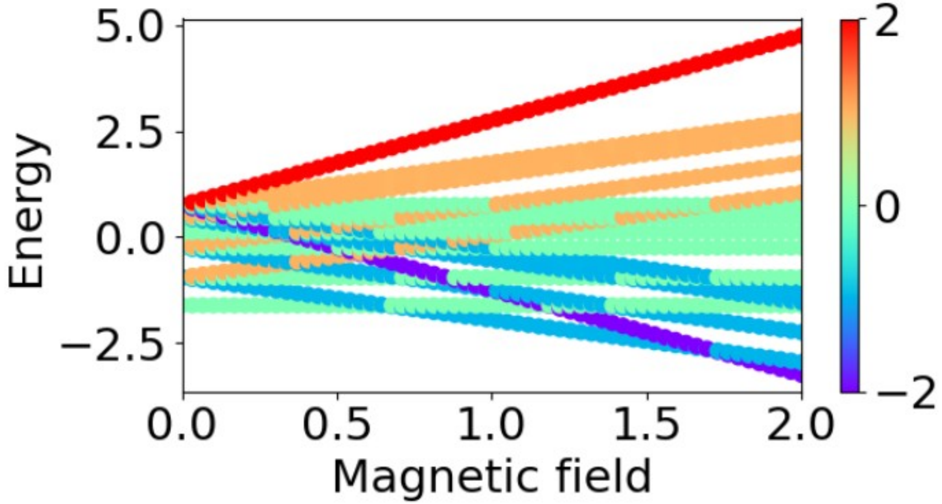
Let us look at the many-body spectra at finite field for $S = 1/2$

$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$$

$L = 2$



$L = 4$



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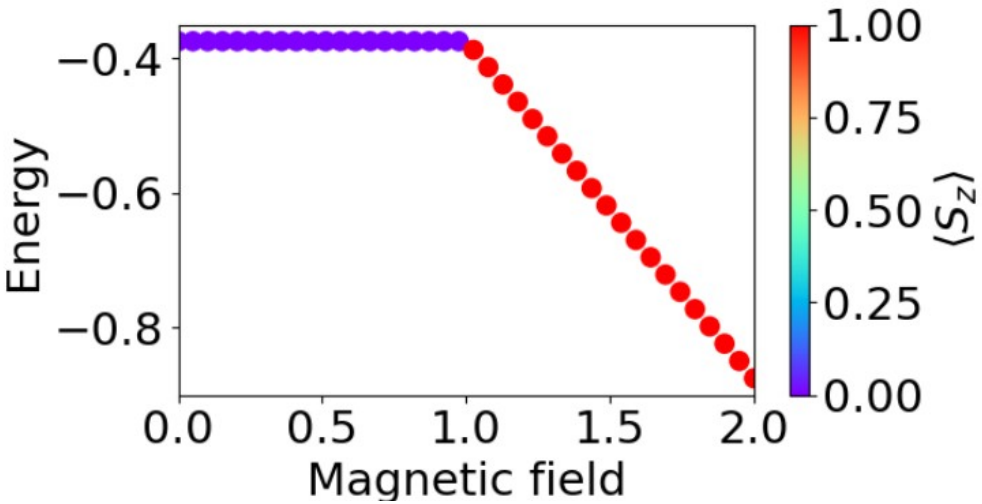
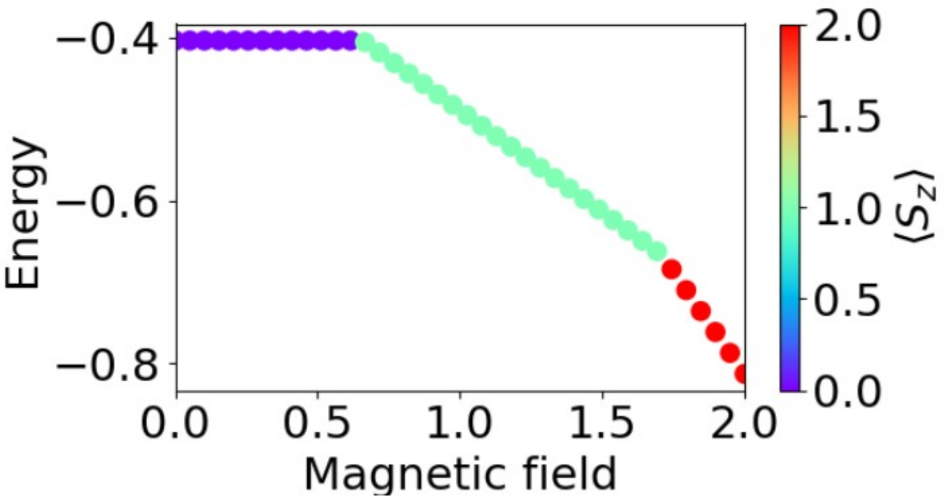
$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$$

$L = 2$



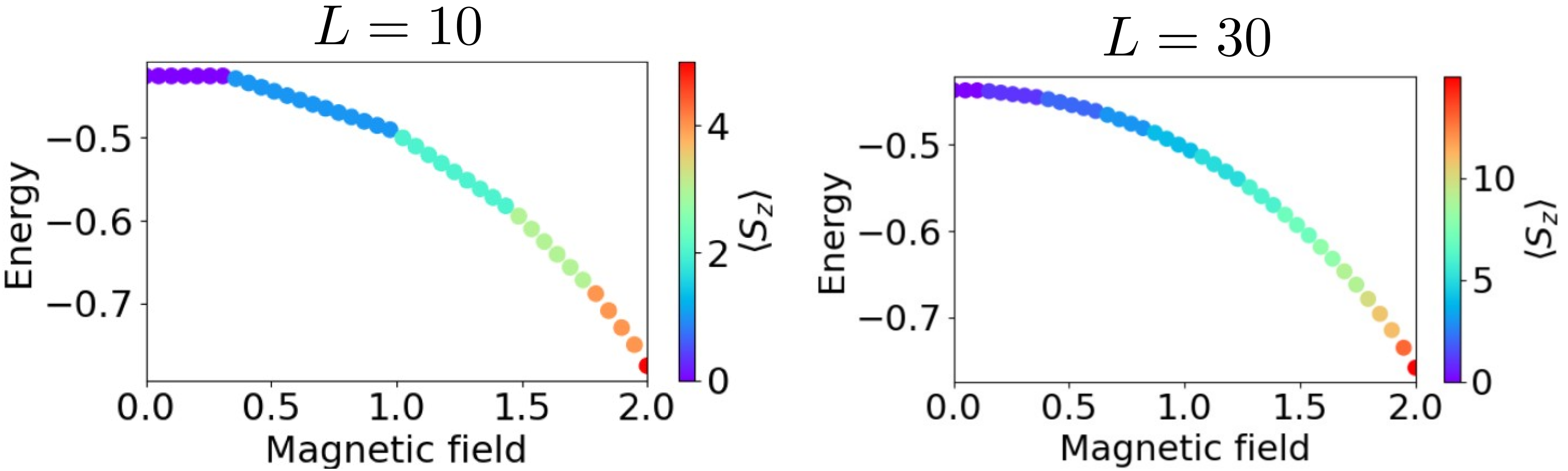
$L = 4$



The gapless spectra of S=1/2

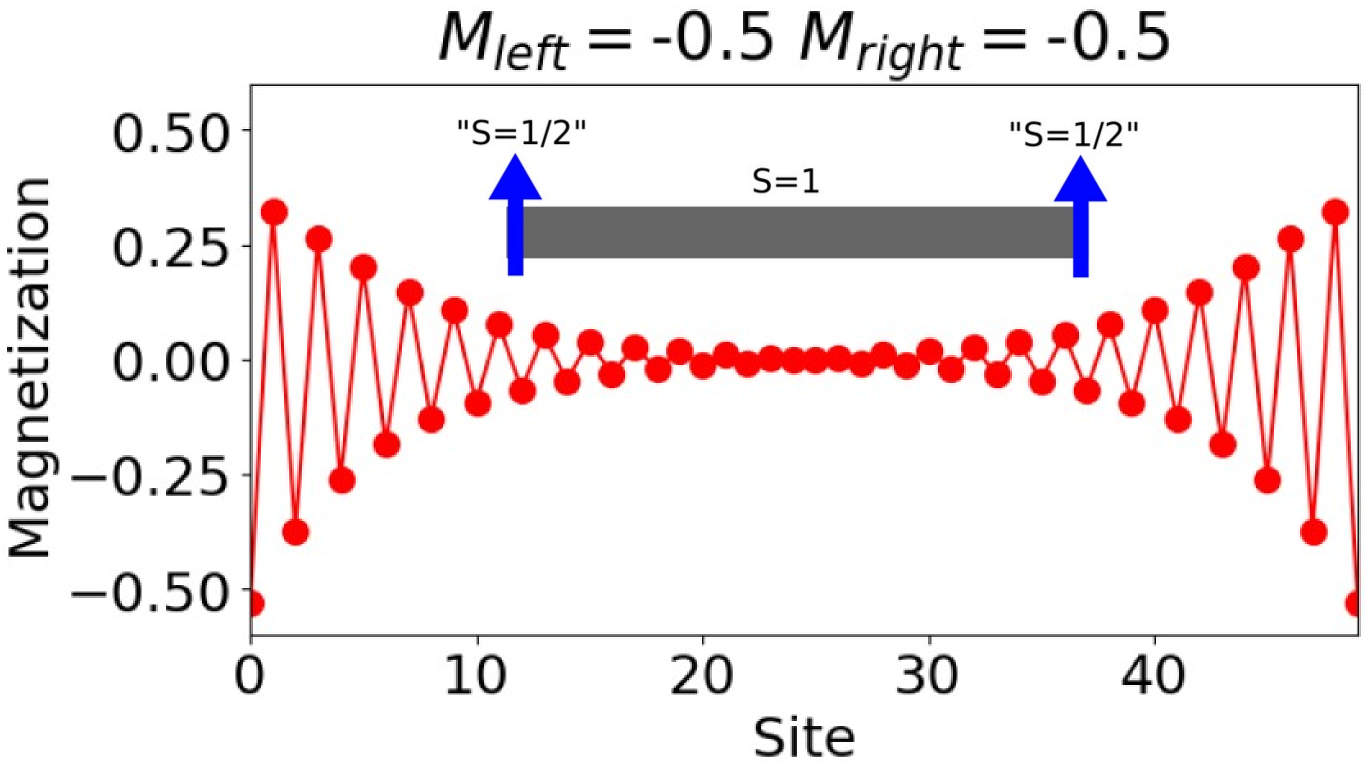
Let us look at the many-body spectra at finite field for $S=1/2$

$$H=\sum_n \vec{S}_n\cdot\vec{S}_{n+1}+B_z\sum_n S_n^z$$



Emergent fractional S=1/2 in the Heisenberg S=1 chain

Lets take an S=1 chain with a small magnetic field $H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$

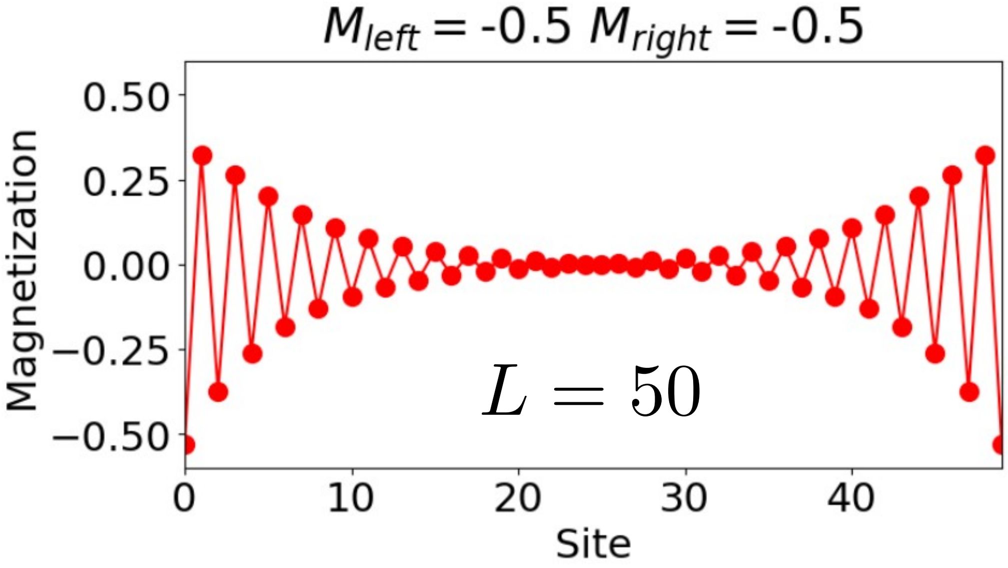


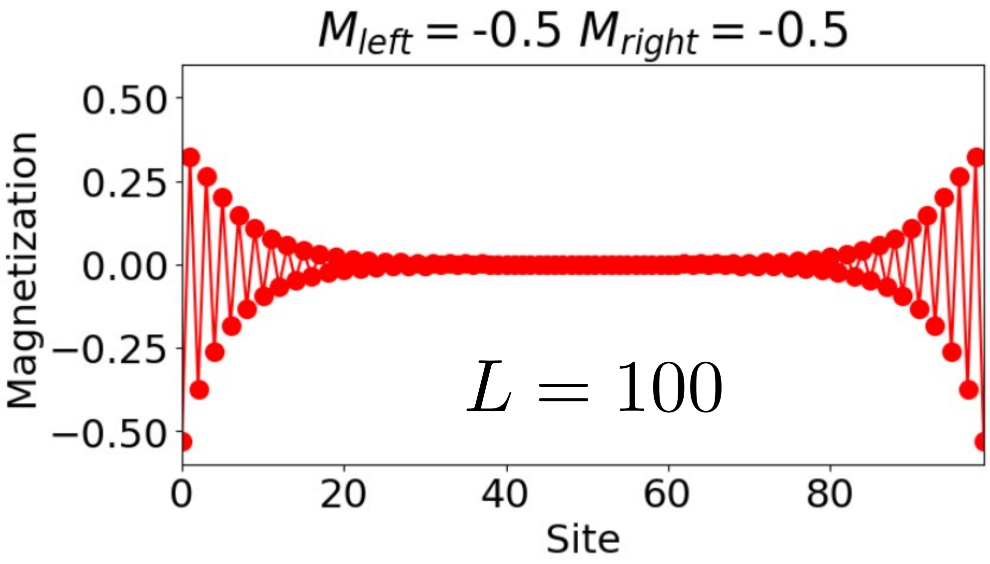
$S = 1$

Emergent fractional S=1/2 in the Heisenberg S=1 chain

Lets take an S=1 chain with a small magnetic field $H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$

Emergent fractional edge modes appear in the thermodynamic limit





Non-local static correlators

The non-local static correlator allows probing how the many-body wavefunction is entangled between different regions of the system

$$\chi_{ij} \equiv \langle \vec{S}_i \cdot \vec{S}_j \rangle - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle$$

For a product state, the correlator above is zero

Two different types of decays are possible in the correlator

$$\chi_{ij} \sim 1/|r_i - r_j|$$

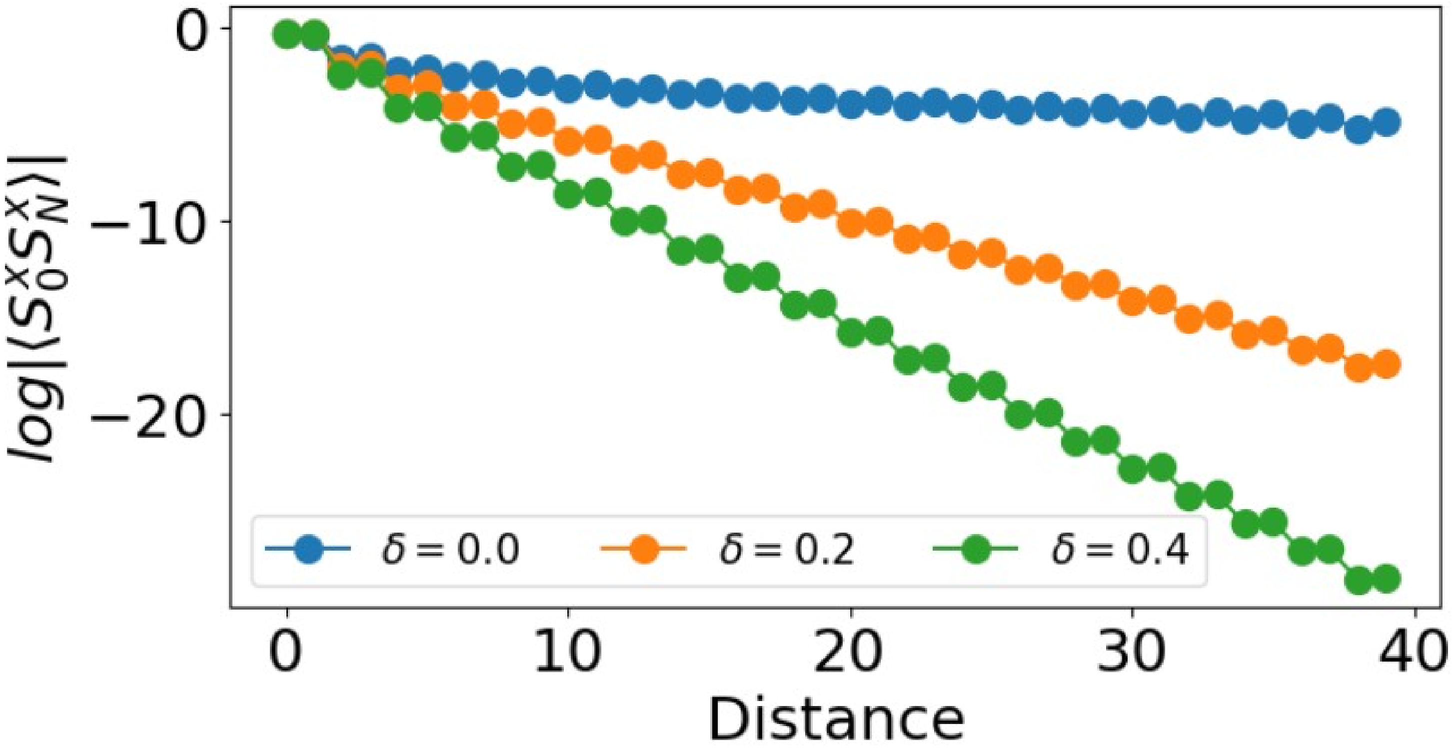
Gapless spectrum

$$\chi_{ij} \sim e^{-\lambda |r_i - r_j|}$$

Gapped spectrum

Non-local static correlators

Let us now take an S=1/2 Heisenberg model $H = \sum_n (1+\delta(-1)^n)\vec{S}_n \cdot \vec{S}_{n+1}$



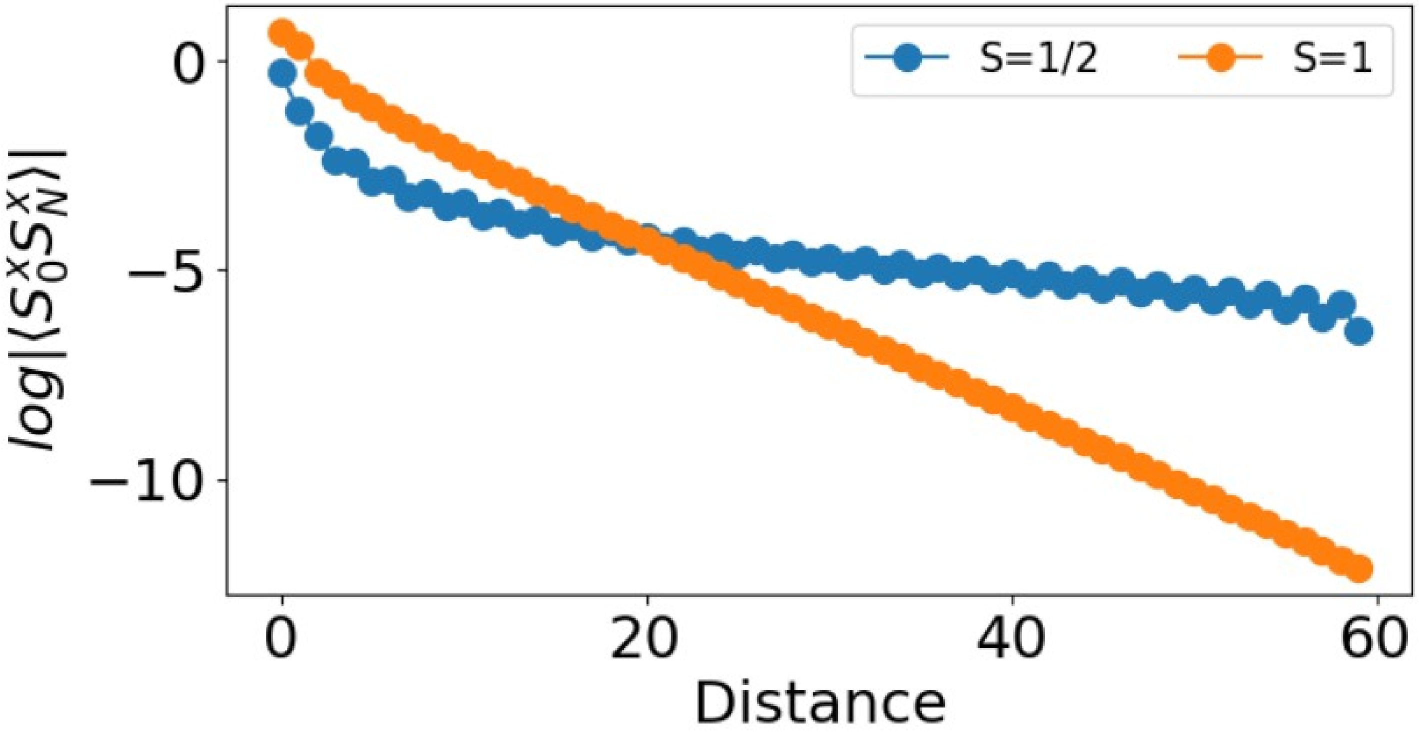
$$\chi_{ij} \sim 1/|r_i - r_j|$$

$$\chi_{ij} \sim e^{-\lambda|r_i - r_j|}$$

$$\chi_{ij} \sim e^{-\lambda|r_i - r_j|}$$

Non-local static correlators

Let us now take a uniform Heisenberg model $H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$



for $S = 1/2$

$$\chi_{ij} \sim 1/|r_i - r_j|$$

Gapless

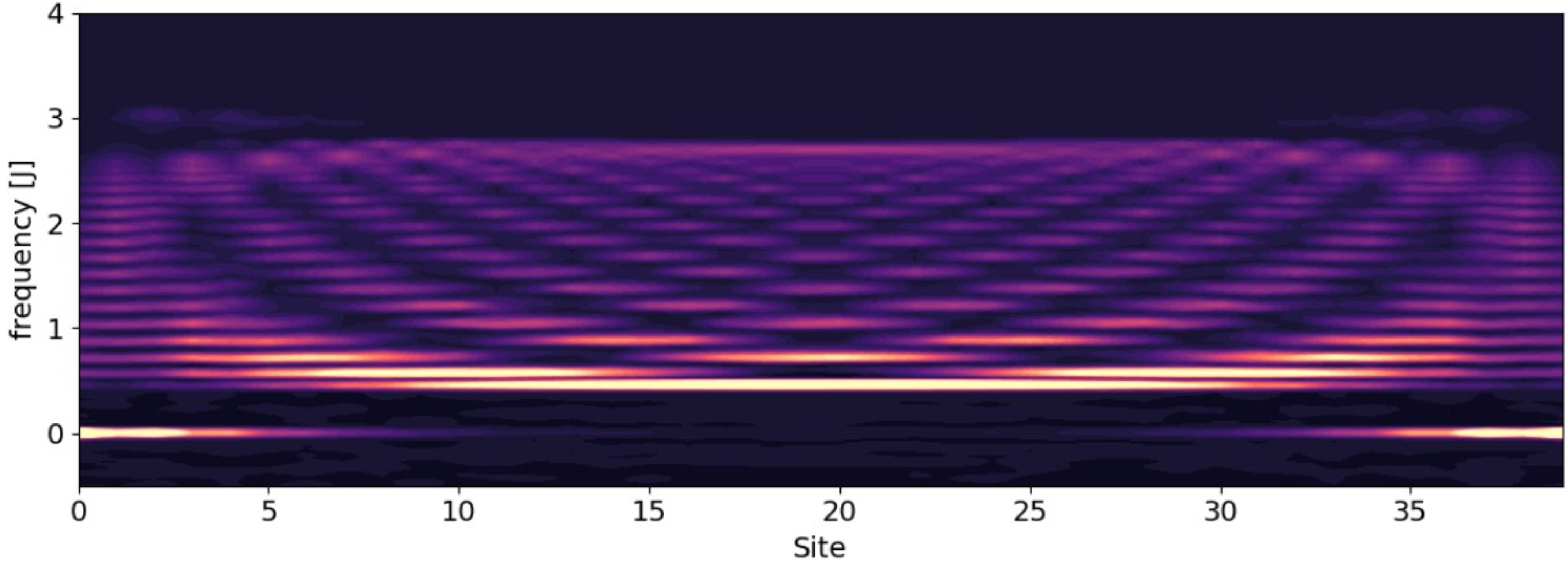
for $S = 1$

$$\chi_{ij} \sim e^{-\lambda |r_i - r_j|}$$

Gapped

Fractional edge modes from the dynamical correlator for S=1

$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$ $\qquad S = 1$



$$A(\omega) = \langle GS | S_n^- \delta(\omega - H + E_{GS}) S_n^+ | GS \rangle$$