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Tensor networks for spin and fermionic quantum many-body, and billion-size single particle super-moire materials

Training Workshop: Modelling Layered Materials, INL, Portugal

October 14th 2025

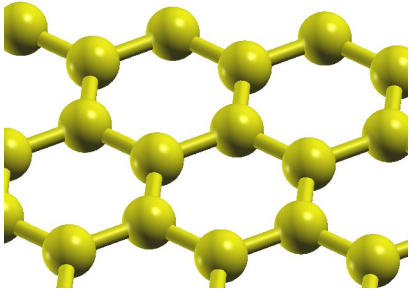
Plan for today

- Billion-size single particle super-moire materials with tensor networks
- Many-body quantum magnetism
  - Expectation values, phase transitions
  - Thermodynamic limit with tensor networks
- Many-body fermionic models
  - Expectations values, entanglement
  - Thermodynamic limit with tensor networks

The two-dimensional materials world

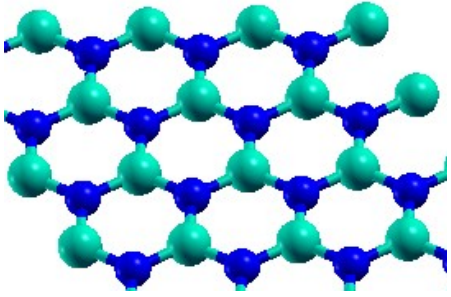
Semimetal

Graphene



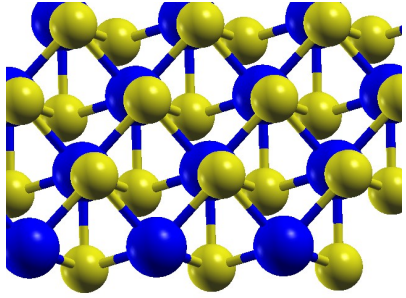
Insulator

BN



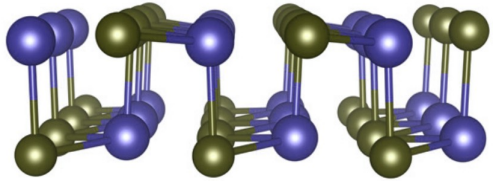
Superconductor

$NbSe_2$



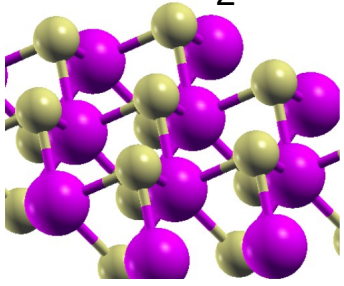
Ferroelectric

SnTe



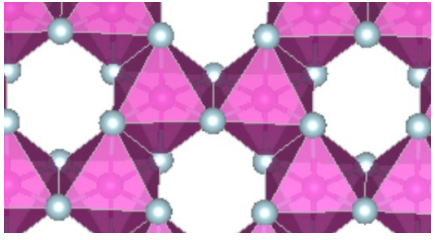
Semiconductor

WS_2



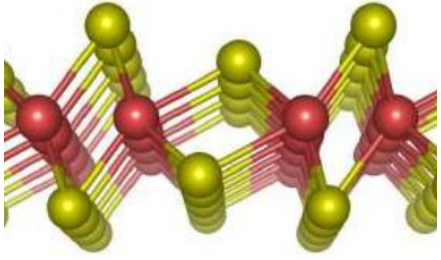
Ferromagnet

CrI_3



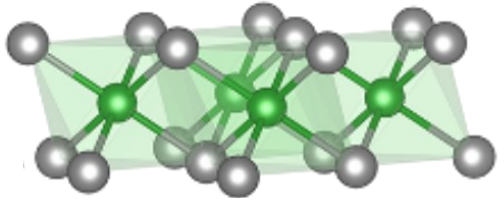
Quantum spin Hall insulator

WTe_2



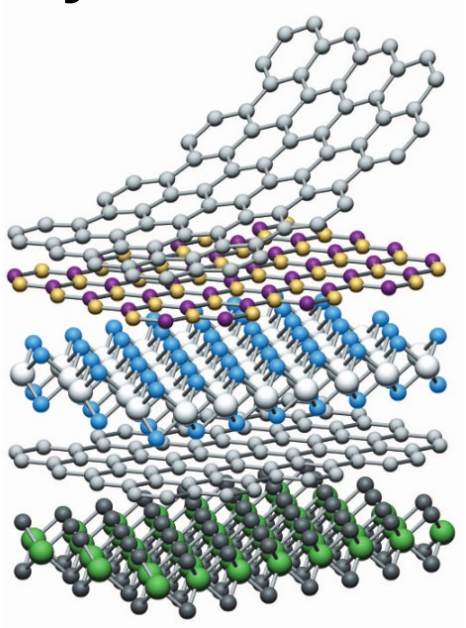
Multiferroic

NiI_2



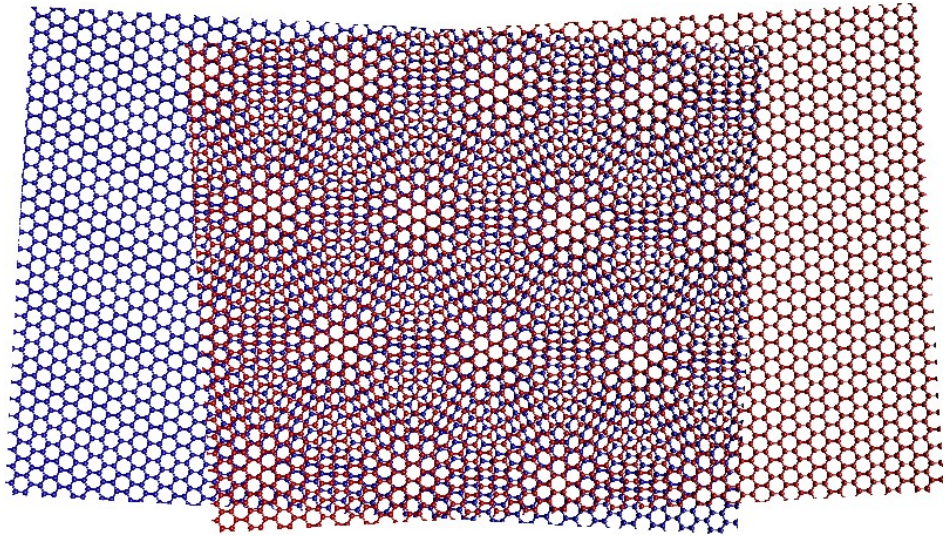
The flexibility of two-dimensional materials

They can be stacked



Nature 499, 419–425 (2013)

They can be rotated

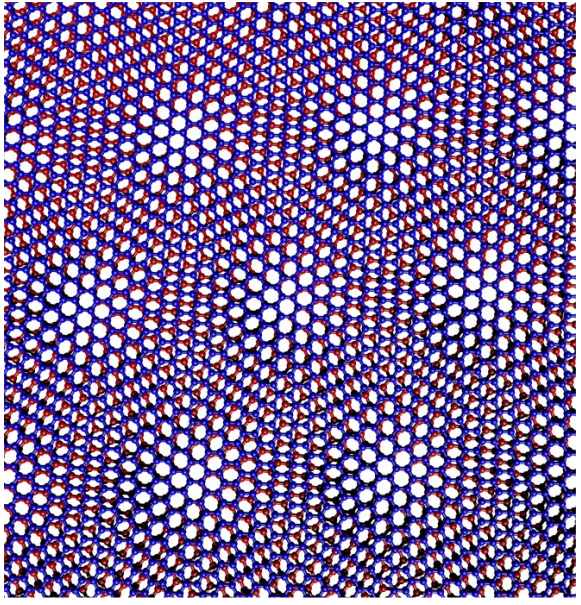


Science 361, 6403, 690-693 (2018)

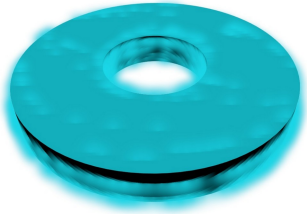
These are unique features of two-dimensional materials

The tunability of twisted van der Waals materials

Twisted bilayer graphene

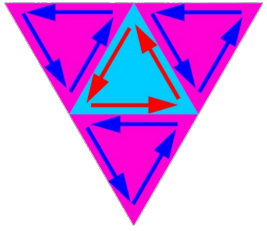


Superconductivity



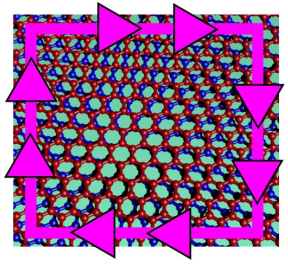
Nature 556, 43–50 (2018)

Topological networks



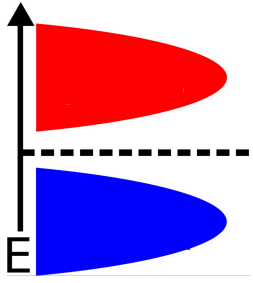
Nano Lett. 18, 11, 6725-6730 (2018)

Chern insulators



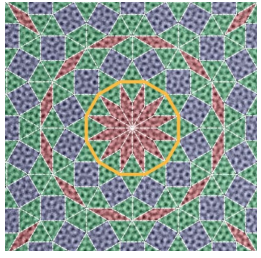
Science 365, 605-608 (2019)

Correlated insulators



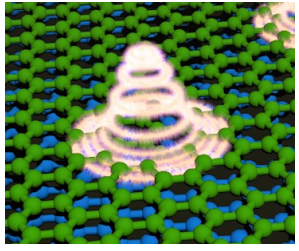
Nature 556, 80–84 (2018)

Quasicrystalline physics



Science 361, 782-786 (2018)

Proximal fractional Chern insulators

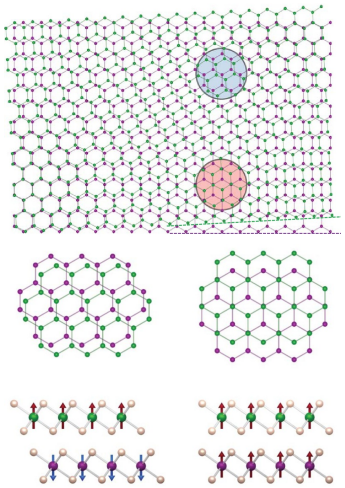


Nature 600, 439–443 (2021)

Twisted multilayers provide a powerful platform for emergent phenomena

Artificial quantum matter in moire van der Waals heterostructures

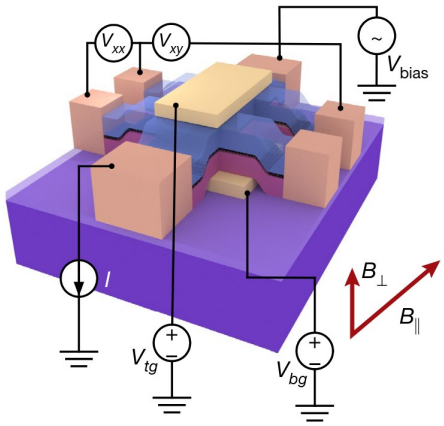
Unconventional magnets



Twisted $CrBr_3$

Science, 374(6571), 1140-1144 (2021)

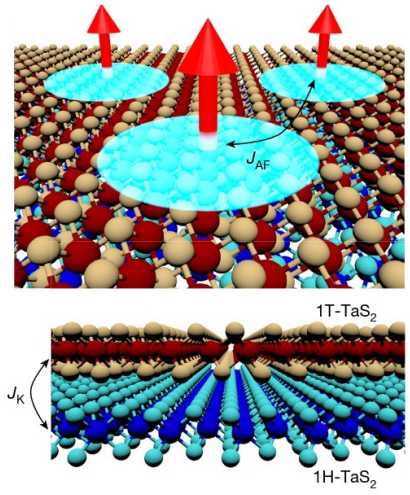
Unconventional superconductors



Twisted trilayer graphene

Nature 595, 526–531 (2021)

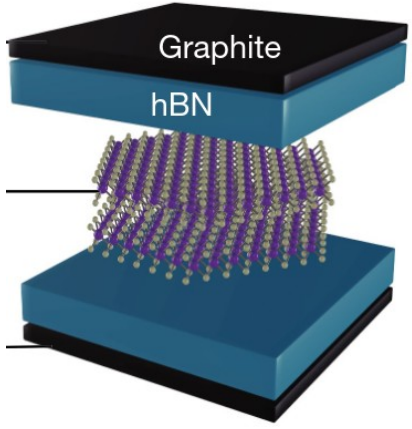
Heavy-fermion quantum materials



1H-1T TaS_2

Nature 599, 582–586 (2021)

Fractional topological matter

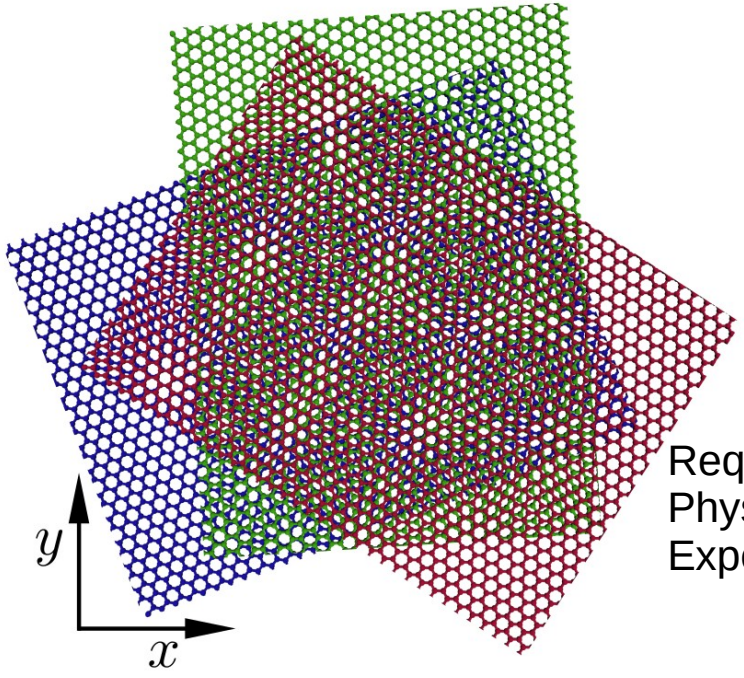


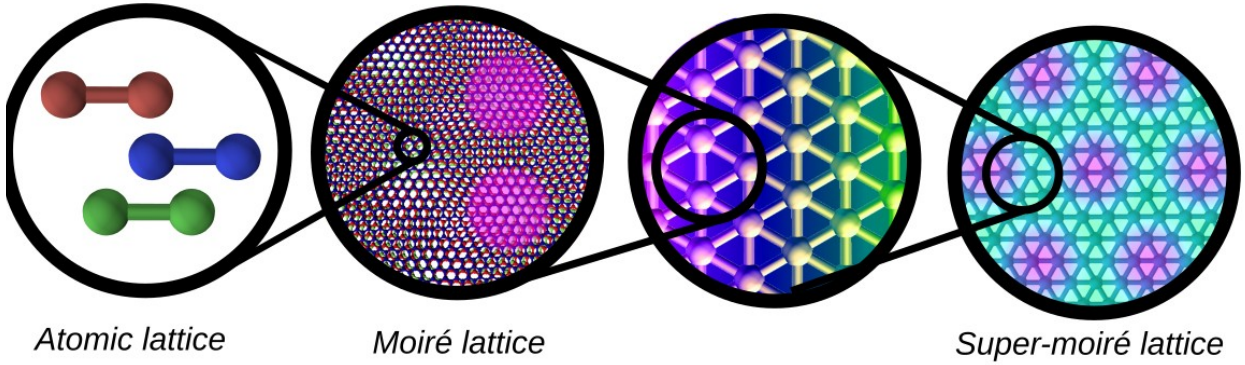
Twisted $MoTe_2$

Nature 622, 63–68 (2023)

Super-moire materials

Moire-of-moire materials





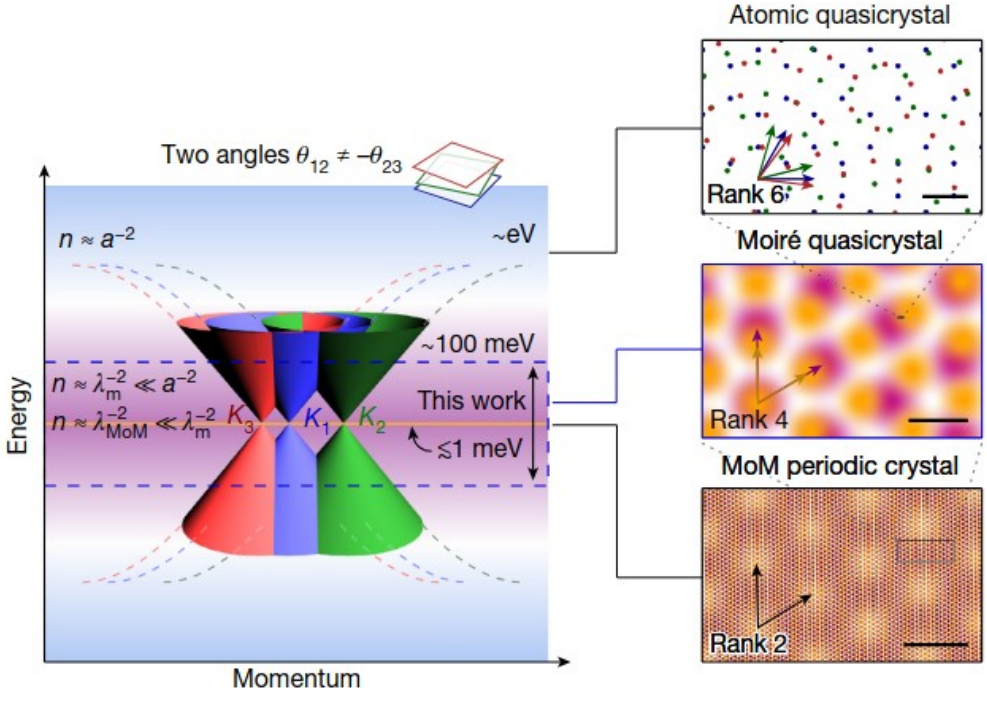
Requires computing up to a billion sites (10^9)
Physics at several length scales (atomic, moire, and super-moire)
Experiments showing correlations and unconventional superconductivity

Nature 620, 762–767 (2023)
Nature 625, 494–499 (2024)
Nature 641, 896–903 (2025)

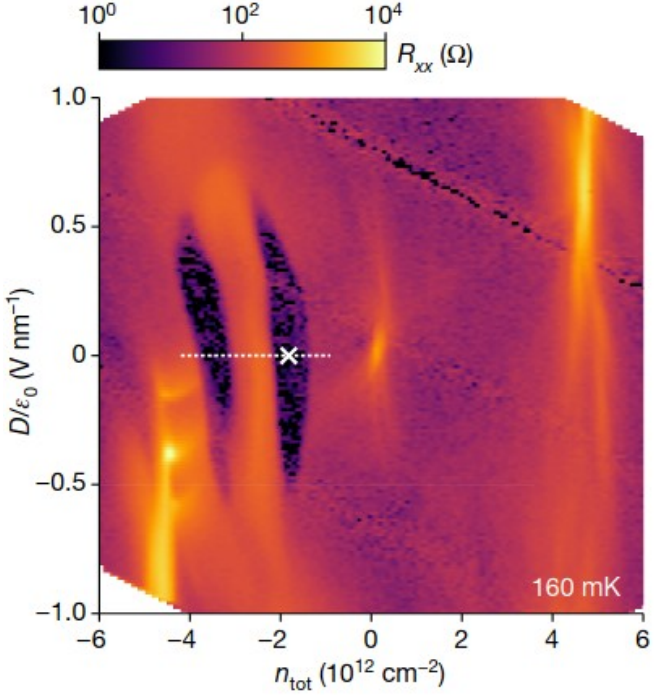
How can we compute the electronic structure of exceptionally large systems?

Super-moire materials, experimentally

Moire quasicrystal in twisted trilayer graphene

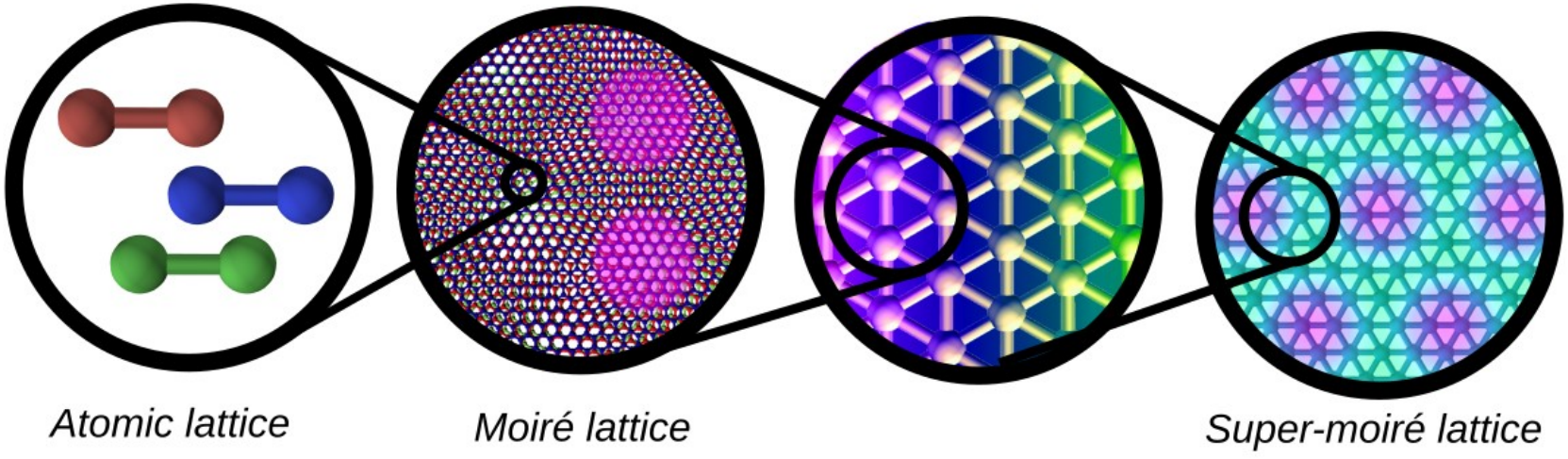


Coexisting correlations and superconductivity



Nature 620, 762–767 (2023)

Why super-moire materials are hard (for theorists)



Moire systems **N=10^5 sites**, calculations taking around 1 minute
Computational cost grows as **N** (best case) or **N^3** (worst case)
Super-moire **N=10^9 sites**, calculations taking 10 days – 1000000 years

Is there a way to solve exceptionally large electronic structure problems?

(even going beyond usual memory limitations of conventional methods)

Behind the scenes

Yitao Sun

Tiago Antão

Marcel Niedermeier

Adolfo Fumega

Correlated states in super-moiré materials with a kernel polynomial quantics tensor cross interpolation algorithm, AO Fumega, M Niedermeier, JL Lado, **2D Materials 12 (1), 015018 (2025)**

Self-consistent tensor network method for correlated super-moire matter beyond one billion sites, Y Sun, M Niedermeier, TVC Antão, AO Fumega, JL Lado, **arXiv:2503.04373 (2025)**

Tensor network method for real-space topology in quasicrystal Chern mosaics, TVC Antão, Y Sun, AO Fumega, JL Lado, **arXiv:2506.05230 (2025)**

Tensor networks for super-moire materials

Tensor network for single particle tight binding problems

We can identify a many-body space with a very large single particle one

Many-body basis $|\uparrow\uparrow\uparrow\rangle$ $|\uparrow\uparrow\downarrow\rangle$ $|\uparrow\downarrow\uparrow\rangle$ $|\uparrow\downarrow\downarrow\rangle$ $|\downarrow\uparrow\uparrow\rangle$ $|\downarrow\uparrow\downarrow\rangle$ $|\downarrow\downarrow\uparrow\rangle$ $|\downarrow\downarrow\downarrow\rangle$

Single particle basis $c_1^\dagger|\Omega\rangle$ $c_2^\dagger|\Omega\rangle$ $c_3^\dagger|\Omega\rangle$ $c_4^\dagger|\Omega\rangle$ $c_5^\dagger|\Omega\rangle$ $c_6^\dagger|\Omega\rangle$ $c_7^\dagger|\Omega\rangle$ $c_8^\dagger|\Omega\rangle$

We can use tensor networks to solve very large tight binding problem

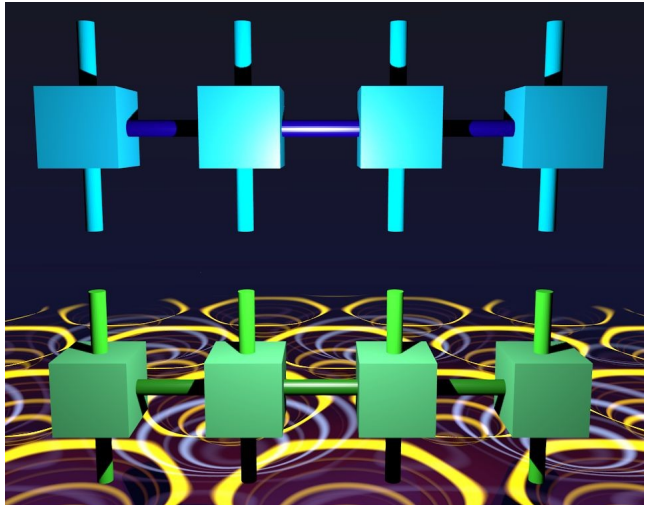
2D Materials 12 (1), 015018 (2025) *arXiv:2503.04373 (2025)* *arXiv:2506.05230 (2025)*

Dealing with very large spaces with tensor networks

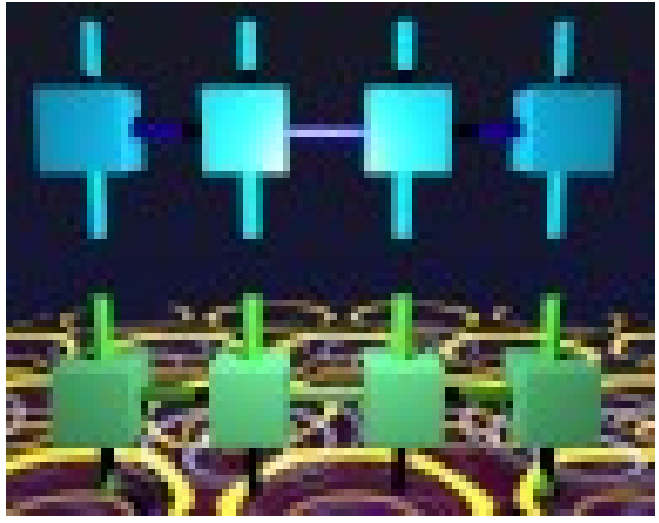
A many-body wavefunction a is a very high dimensional object (2^L coefficients)

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

Tensor-networks allow “compressing” exponentially large information with linear resources



“True wavefunction”



“Tensor-network wavefunction”

Dealing with very large spaces with tensor networks

Typical many-body wavefunction $|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L} |s_1, s_2, \ldots s_L\rangle$

We need to determine in total 2^L coefficients

Is there an efficient way of storing so many coefficients?

Tensor networks allow parametrizing many-body wavefunctions as

$$|\Psi\rangle = \sum_{\{s\}} \mathrm{Tr}\left[M_1^{(s_1)} M_2^{(s_2)} \cdots M_N^{(s_N)}\right] |s_1 s_2 \ldots s_N\rangle$$

$L\chi^2$ parameters

Full wavefunction  *Matrix product state*

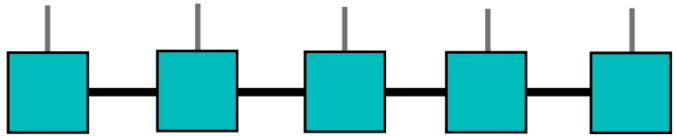
Tensor networks allow to drastically reduce the memory required to store a many-body state

Annals of Physics 326, 96 (2011)

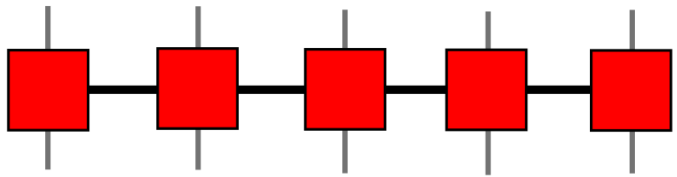
Exponentially large algebra with tensor networks

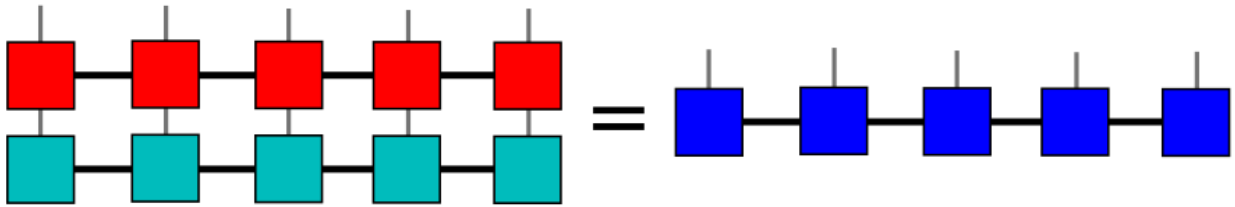
Tensor network allow to (approximately) operate in exponentially large vector spaces

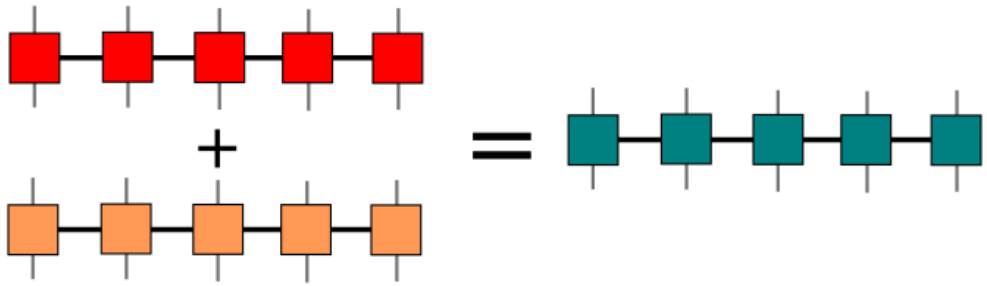
vector

$|\Psi\rangle \equiv$ 

matrix

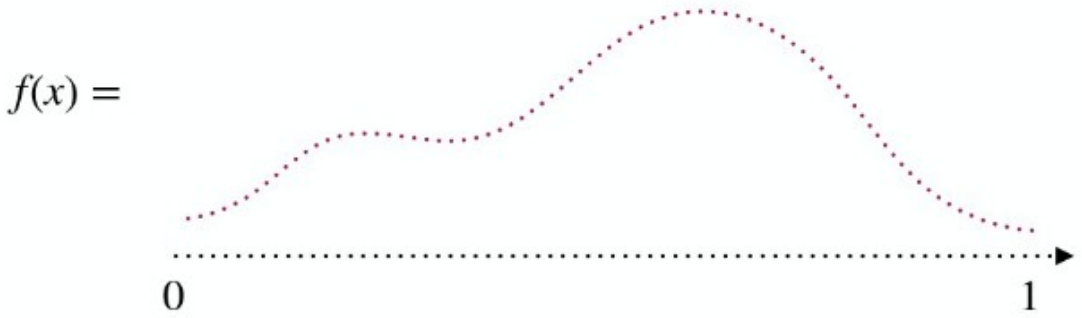
$\hat{A} \equiv$ 

$|\Psi_2\rangle = \hat{A}|\Psi_1\rangle \equiv$ 

$\hat{A}_3 = \hat{A}_1 + \hat{A}_2 \equiv$ 

Tensor networks for non quantum-many body

Imagine that you have a function with an exponentially large number of points



We could store all those values with a tensor network

$$c_{s_1,s_2,\ldots,s_L} = M^{s_1} M^{s_2} \ldots M^{s_L}$$

$$x = \sum_n 2^{-n} s_n \qquad f(x) = c_{s_1,s_2,\ldots,s_L} \qquad s_n = 0, 1$$

There is an algorithm (tensor cross interpolation) that enables to systematically build the MPS

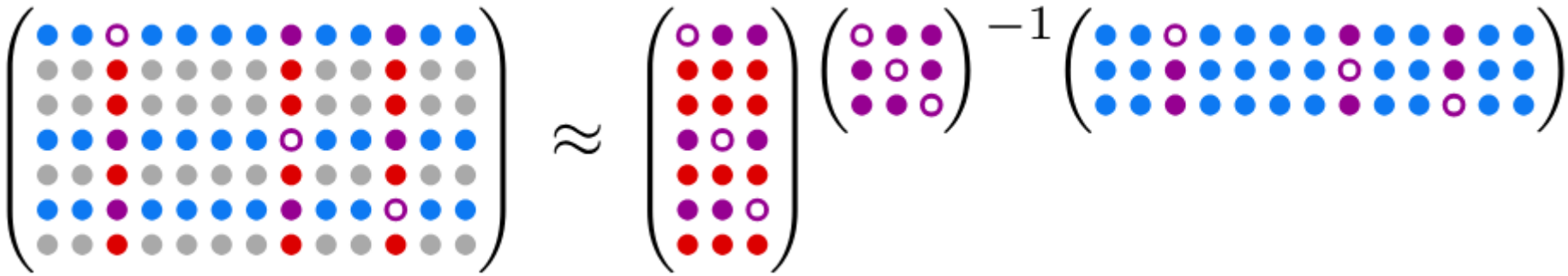
Quantum-inspired active learning algorithm

Learning the tensor network representation

We need to represent all the tight binding terms as tensor networks

- In some cases, we can build the initial tensor network explicitly

- In other cases, we learn the tensor network with quantics tensor cross interpolation



Phys. Rev. Lett. 132, 056501 (2024)

SciPost Phys. 18, 104 (2025)

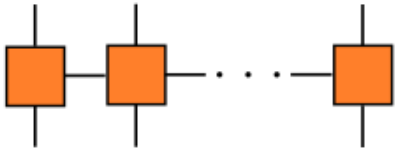
Self-consistent electronic interactions with tensor networks

Super-moire interacting Hamiltonian

$$H = H_0 + H_V = \sum_{\alpha\beta} t_{\alpha\beta} c^\dagger_\alpha c_\beta + \sum_{\alpha\beta} V_{\alpha\beta} c^\dagger_\alpha c_\alpha c^\dagger_\beta c_\beta$$

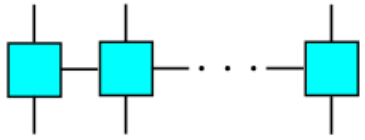
Mean-field decoupled Hamiltonian

$$H^{MF} = \sum_{\alpha\beta} (t_{\alpha\beta} + \chi_{\alpha\beta}) c^\dagger_\alpha c_\beta = \sum_{\alpha\beta} H^{MF}_{\alpha\beta} c^\dagger_\alpha c_\beta \qquad \mathcal{H}^{MF}_{\alpha\beta} \equiv$$



Tensor network representation of the correlators

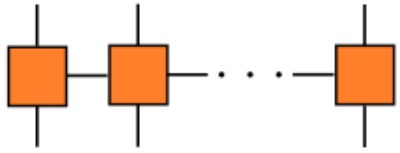
$$\langle c^\dagger_\alpha c_\beta \rangle = \langle \alpha | \Xi(\mathcal{H}^{MF}) | \beta \rangle \equiv$$



Self-consistent electronic interactions with tensor networks

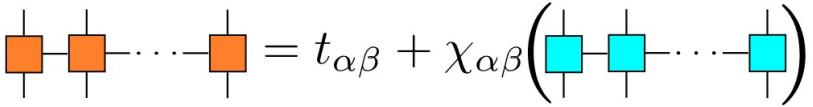
We represent the super-moire electronic Hamiltonian as a tensor-network

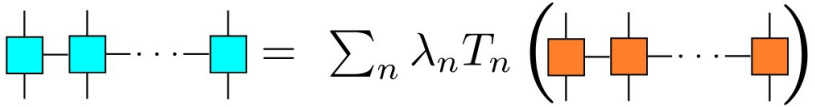
$$\mathcal{H}^{MF}_{\alpha\beta} \equiv \Gamma^{(1)}_{s_1,s_1'}\Gamma^{(2)}_{s_2,s_2'}\Gamma^{(3)}_{s_3,s_3'}...\Gamma^{(L)}_{s_L,s_L'}$$

$\mathcal{H}^{MF}_{\alpha\beta} \equiv$ 

The mean-field problem can be reformulated purely with tensor networks

Tensor Network SCF loop

$\mathcal{H}^{MF}_{\alpha\beta} \equiv$ 

$\langle c^\dagger_\alpha c_\beta \rangle \equiv$ 

arXiv:2503.04373 (2025)

Spectral functions with the kernel polynomial method

Let us expand a delta function in Chebyshev polymials

$$\delta(\omega - \mathcal{H}) = \sum_n \lambda_n(\omega) T_n(\mathcal{H})$$

Chebyshev relation

$$T_n(\mathcal{H}) = 2\mathcal{H}T_{n-1}(\mathcal{H}) - T_{n-2}(\mathcal{H})$$

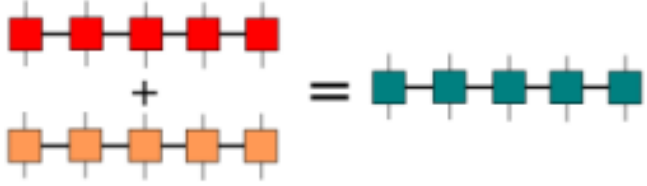
Expansion coefficients for delta function

$$\lambda_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

Rev. Mod. Phys. 78, 275 (2006)

KPM can be implemented with tensor networks by using tensor network algebra

Phys. Rev. B 83, 195115 (2011)
Phys. Rev. Research 1, 033009 (2019)



Spectral functions with tensor networks

Local spectral function of the mean-field Hamiltonian

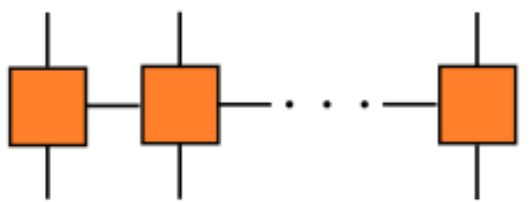
$$D(\omega,\alpha) = \langle\alpha| \left[\sum_n T_n(\mathcal{H}^{MF}) P_n(\omega) \right] |\alpha\rangle$$

With a tensor network Chebyshev algorithm

$$P_n(\omega) = \frac{2T_n(\omega)}{\pi\sqrt{1-\omega^2}}$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

$$\mathcal{H}^{MF}_{\alpha\beta} \equiv$$



Rev. Mod. Phys. 78, 275 (2006)

arXiv:2503.04373 (2025)

Tensor network representation of a super-moire Hamiltonian

We can identify a many-body space with a very large single particle one

Many-body basis $|\uparrow\uparrow\uparrow\rangle \; |\uparrow\uparrow\downarrow\rangle \; |\uparrow\downarrow\uparrow\rangle \; |\uparrow\downarrow\downarrow\rangle \; |\downarrow\uparrow\uparrow\rangle \; |\downarrow\uparrow\downarrow\rangle \; |\downarrow\downarrow\uparrow\rangle \; |\downarrow\downarrow\downarrow\rangle$

Single particle basis $c_1^\dagger|\Omega\rangle \; c_2^\dagger|\Omega\rangle \; c_3^\dagger|\Omega\rangle \; c_4^\dagger|\Omega\rangle \; c_5^\dagger|\Omega\rangle \; c_6^\dagger|\Omega\rangle \; c_7^\dagger|\Omega\rangle \; c_8^\dagger|\Omega\rangle$

In the tight binding basis uniform hopping takes the form

$$H_{0,NN} = \sum_{\alpha,s}^{N-1} t(c^\dagger_{x_{\alpha+1},s} c_{x_\alpha,s} + h.c.)$$

In the tensor-network pseudospin basis, uniform hopping takes the form

$$\mathcal{H}_{0,NN} = \sum_{l,s}^{L} t(\sigma^+_{l,s} \bigotimes_{m>l} \sigma^-_{m,s} + h.c.)$$

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Single particle basis $c_1^\dagger|\Omega\rangle \; c_2^\dagger|\Omega\rangle \; c_3^\dagger|\Omega\rangle \; c_4^\dagger|\Omega\rangle \; c_5^\dagger|\Omega\rangle \; c_6^\dagger|\Omega\rangle \; c_7^\dagger|\Omega\rangle \; c_8^\dagger|\Omega\rangle$

The tensor-network moire hopping can be built as

Find the MPS representation fo the modulation and store in a diagonal MPO $\mathcal{T}$

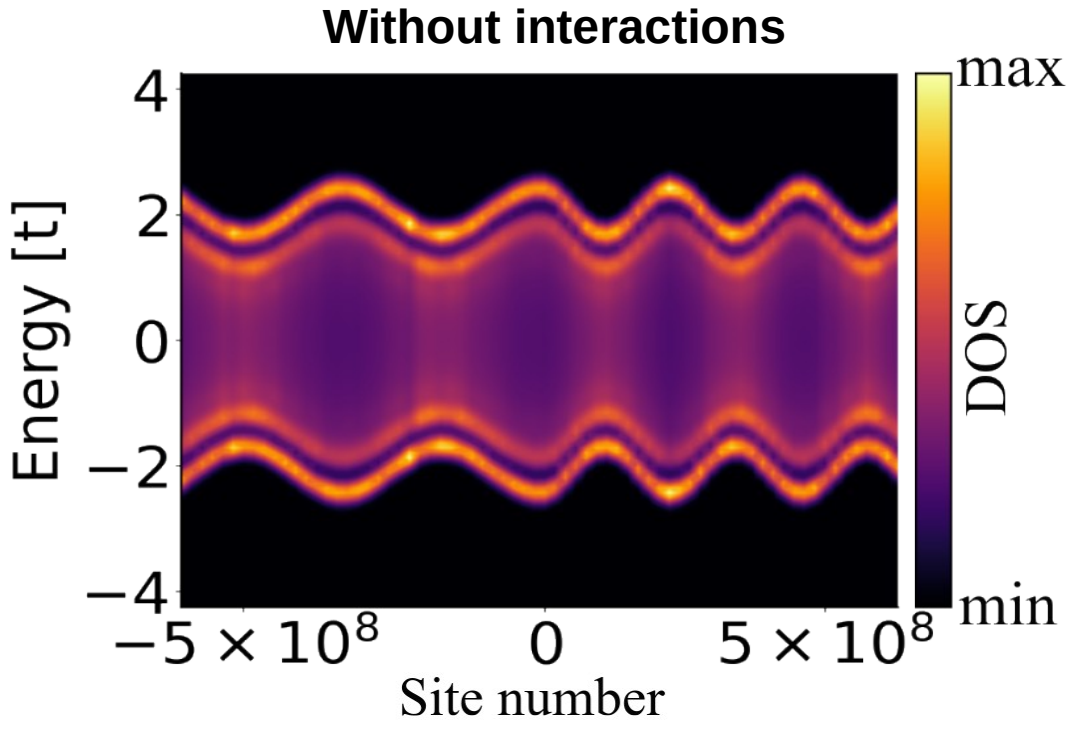
$$|\tau\rangle = \sum M_{s_1}^{(1)} M_{s_2}^{(2)} M_{s_3}^{(3)} ... M_{s_L}^{(L)} \, |s_1, s_2, ..., s_L\rangle$$

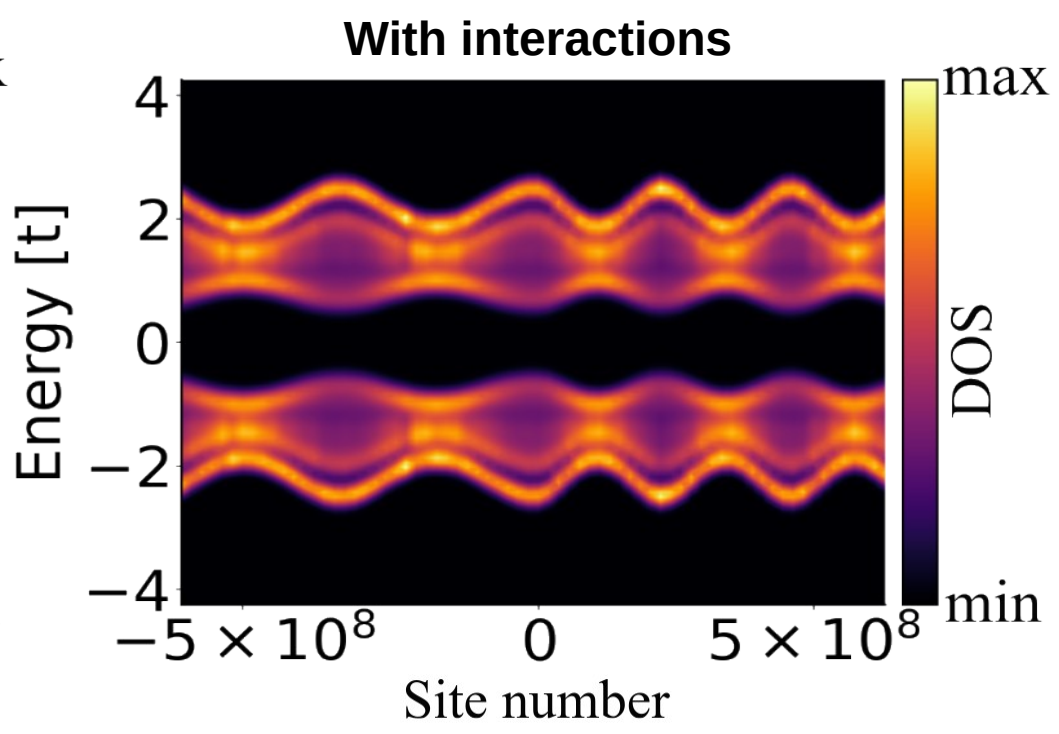
Quantics tensor cross interpolation

Modulated super-moire by constraction

$$\mathcal{H}_0 = \{[\mathcal{T} \sum_{l,s}^{L} (\sigma_{l,s}^{+} \bigotimes_{m>l} \sigma_{m,s}^{-})] + h.c.\}$$

Solving billion-size super-moire materials

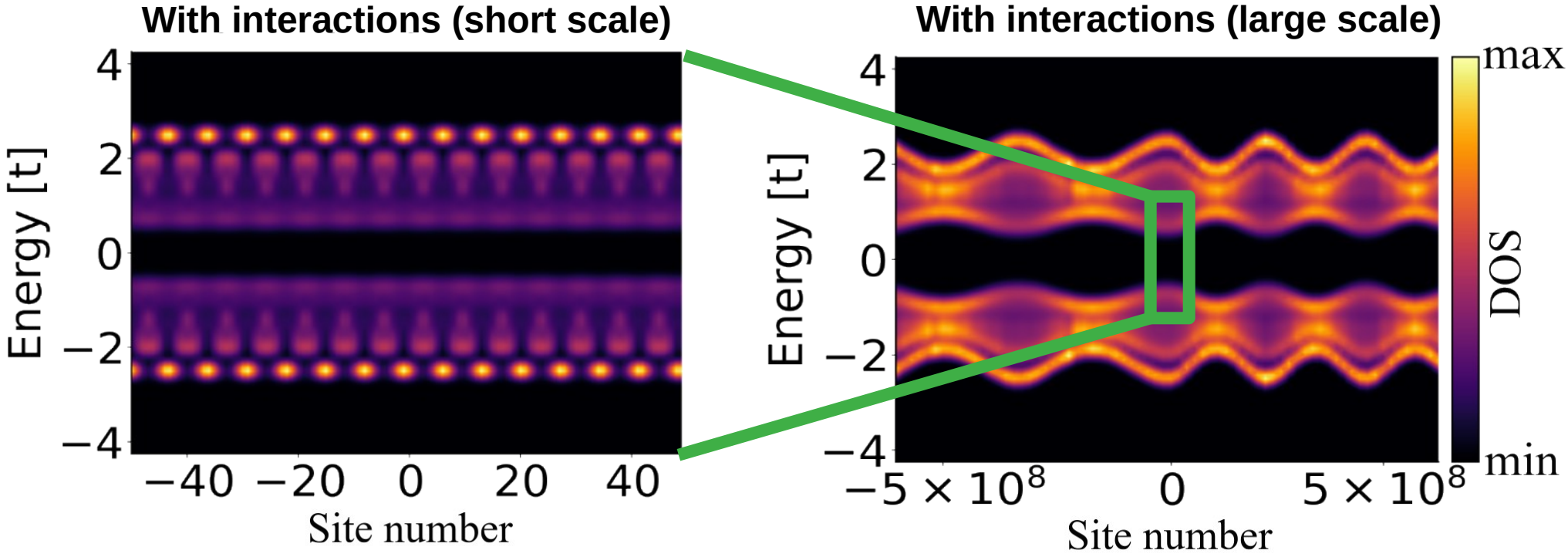




Tensor networks allow to solve selfconsistently a super-moire with one billion sites

arXiv:2503.04373 (2025)

Solving billion-size super-moire materials



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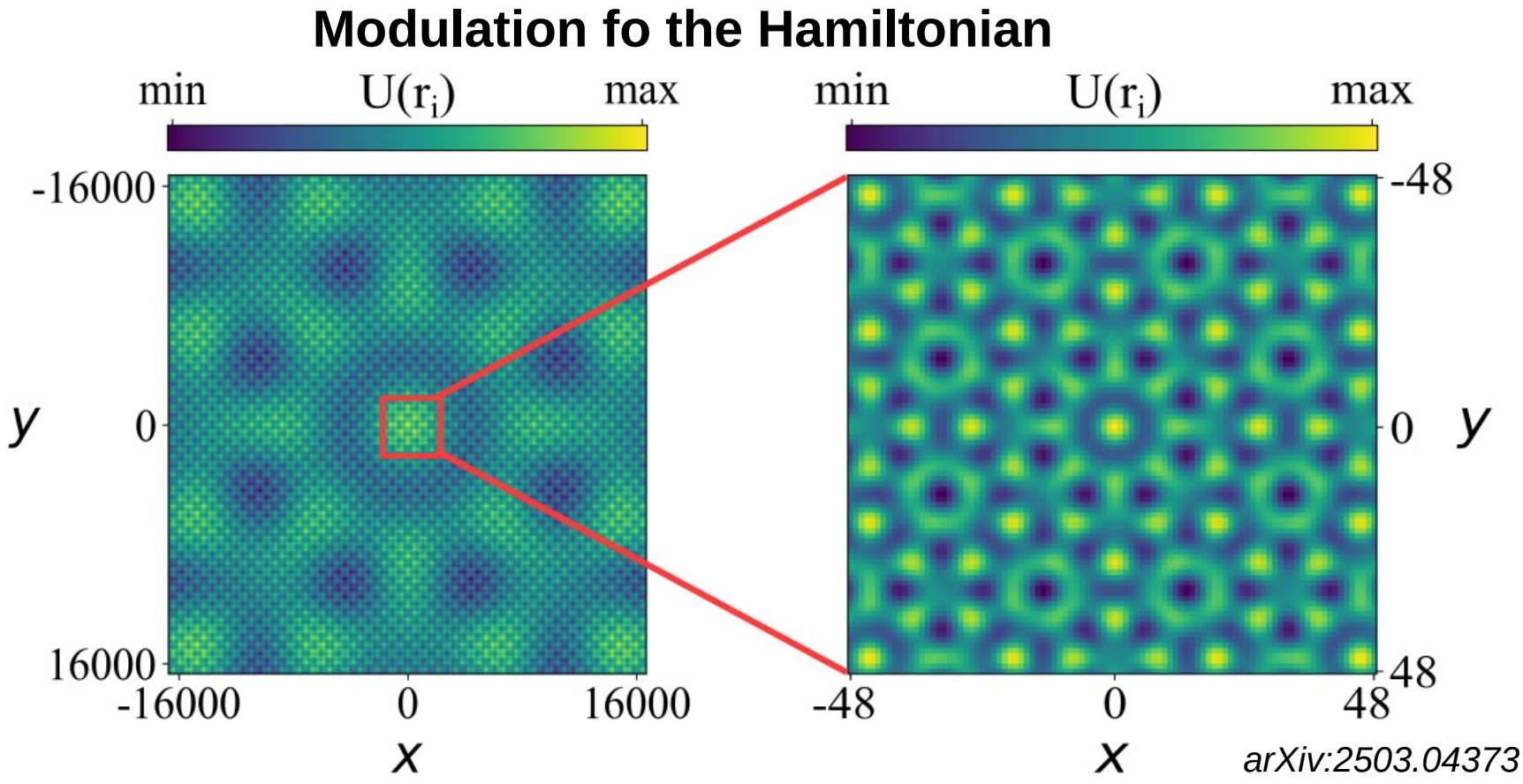
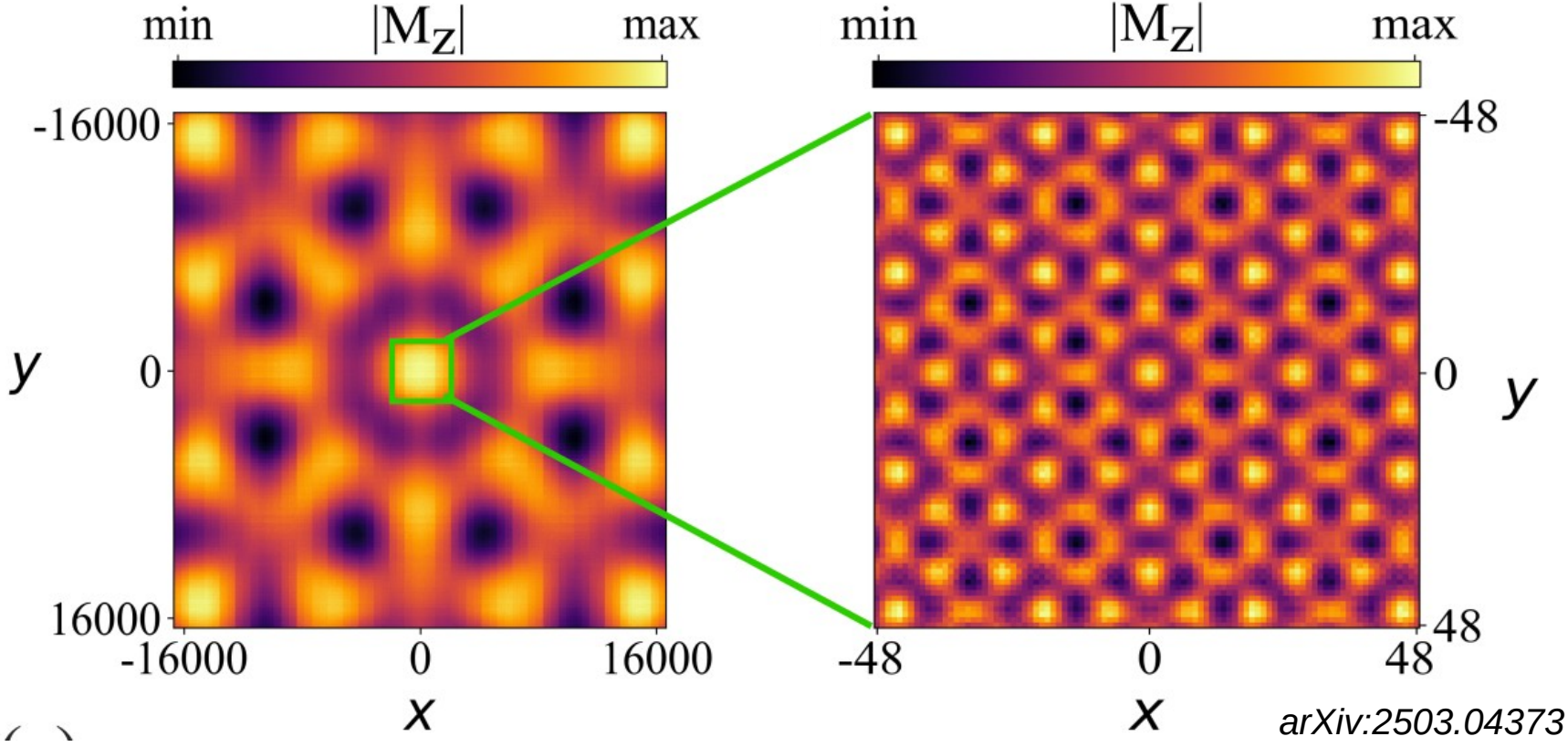
Two-dimensional billion size interacting super-moire



arXiv:2503.04373 (2025)

Two-dimensional billion size interacting super-moire

Selfconsistent symmetry broken order (magnetization)



arXiv:2503.04373 (2025)

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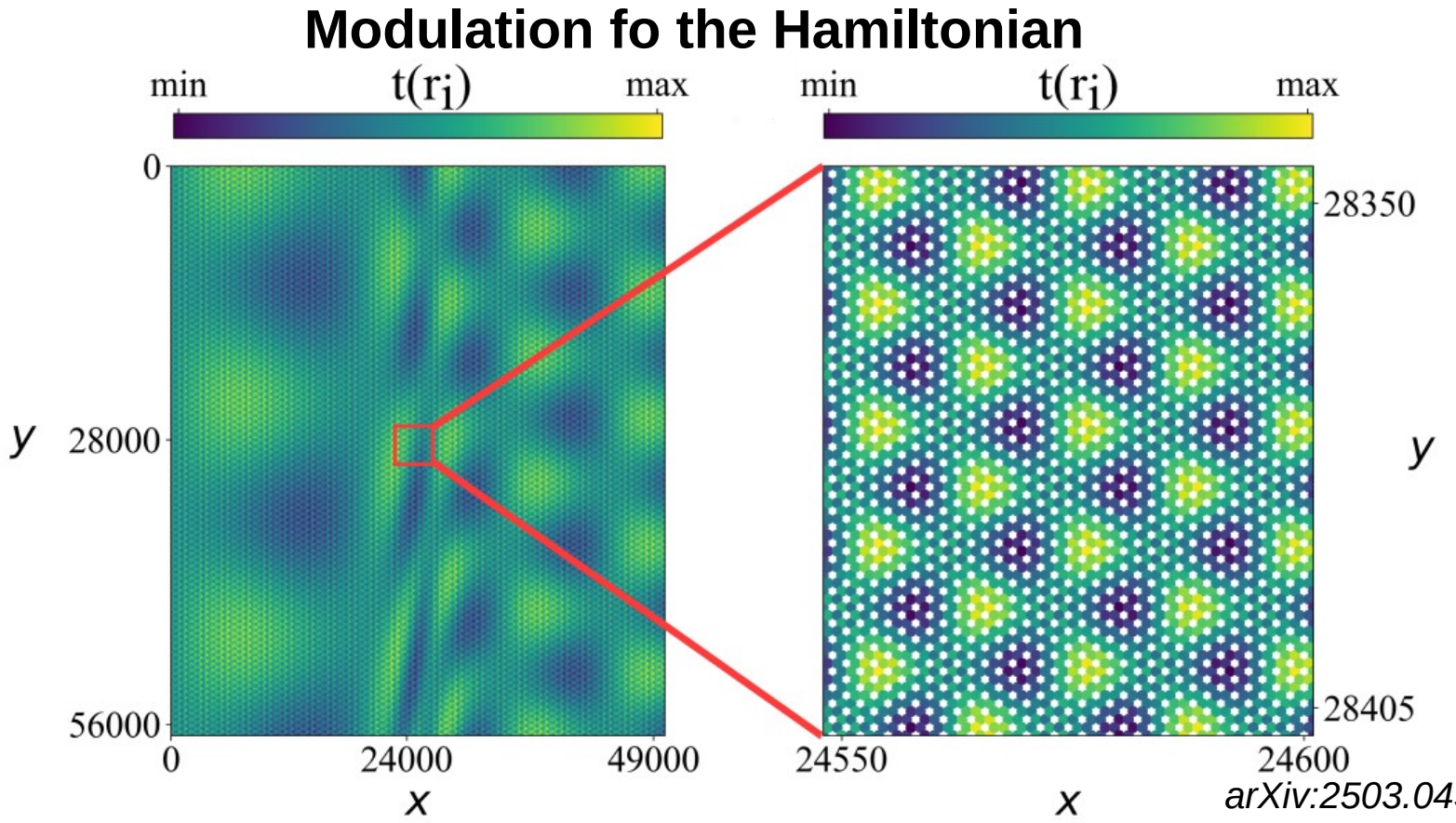

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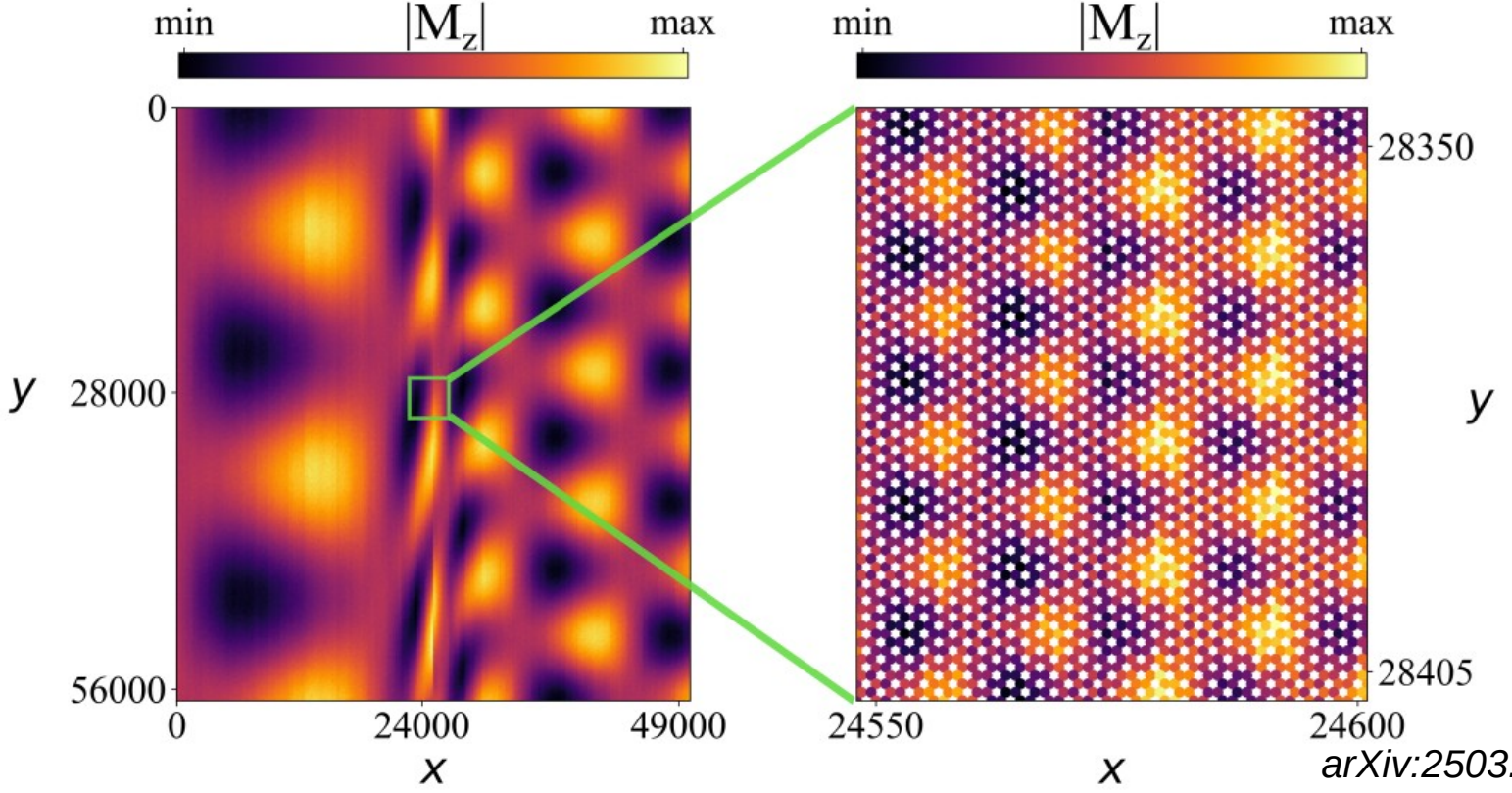


arXiv:2503.04373 (2025)

Tensor networks for topological super-moire materials

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

Hamiltonian

$$H(\mathbf{k})$$

Wavefunction

$$|\Psi(\mathbf{k})\rangle$$

$$A_\mu^\alpha = i\langle \partial_{k_\mu} \Psi_\alpha | \Psi_\alpha \rangle$$

$$\Omega = \nabla \times \mathbf{A}|_z$$

Metric (Berry curvature)

$$C = \int_{BZ} \Omega d^2\mathbf{k}$$

Topological invariant (Chern number)

Real space topological invariants

Topological invariants are often defined in reciprocal space

$$C = \int_{BZ} \Omega d^2\mathbf{k}$$

$$\Omega_\alpha = \partial_{k_x} A_y^\alpha - \partial_{k_y} A_x^\alpha$$

$$A_\mu^\alpha = i\langle \partial_{k_\mu} \Psi_\alpha | \Psi_\alpha \rangle$$

Is it possible to define them in real space?

Real-space Chern number

$$C_\alpha = 2\pi i \langle \alpha | \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} | \alpha \rangle$$

$$\hat{P} = \int_{-\infty}^{\epsilon_F} \delta(\omega - H) d\omega$$

$$\hat{Q} = 1 - \hat{P}$$

Phys. Rev. B 84, 241106® (2011)

Kernel polynomial for topological invariants in real-space

The density matrix of a super-moire system can be expressed as a tensor network

$$\hat{\mathcal{P}} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega = \sum \Xi^{(1)}_{s_1,s_1'} \Xi^{(2)}_{s_2,s_2'} \cdots \Xi^{(L)}_{s_L,s_L'} |s\rangle\langle s'|$$

With a kernel polynomial tensor network algorithm

$$\hat{\mathcal{P}} = \sum_n T_n(\hat{\mathcal{H}}) \int_{-\infty}^{\varepsilon_F} d\omega \frac{T_n(\omega)}{\sqrt{1-\omega^2}},$$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

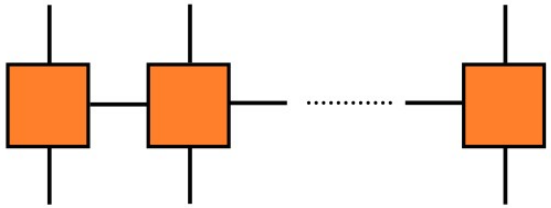
$$T_0 = 1 \text{ and } T_1(x) = x$$

arXiv:2506.05230 (2025)

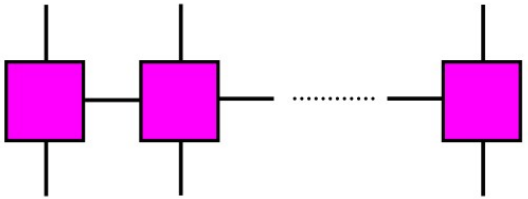
Phys. Rev. B 84, 241106® (2011)

Computing Chern numbers with tensor networks

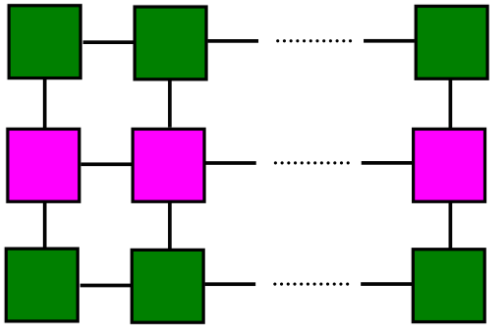
Density matrix as tensor network $\hat{P} = \int_{-\infty}^{\varepsilon_F} \delta(\omega - \hat{H}) d\omega =$



Topological marker as tensor network $\hat{\Gamma} = \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} =$



Chern number from tensor network contraction $C_\alpha = 2\pi i \langle \alpha | \hat{\Gamma} | \alpha \rangle =$



arXiv:2506.05230 (2025)

Tensor network topological marker

Real-space Chern number (Chern marker)

$$C_\alpha = 2\pi i \langle \alpha | \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} | \alpha \rangle$$

Tensor-network Chern marker

$$\hat{\mathcal{C}}_\alpha = 2\pi i \left(\begin{array}{c} \hat{\mathcal{Q}} \\ \hat{\mathcal{Y}}_\alpha^\Lambda \\ \hat{\mathcal{P}} \\ \hat{\mathcal{X}}_\alpha^\Lambda \\ \hat{\mathcal{Q}} \end{array} \right. \left. - \begin{array}{c} \hat{\mathcal{P}} \\ \hat{\mathcal{Y}}_\alpha^\Lambda \\ \hat{\mathcal{Q}} \\ \hat{\mathcal{X}}_\alpha^\Lambda \\ \hat{\mathcal{P}} \end{array} \right)$$

arXiv:2506.05230 (2025)

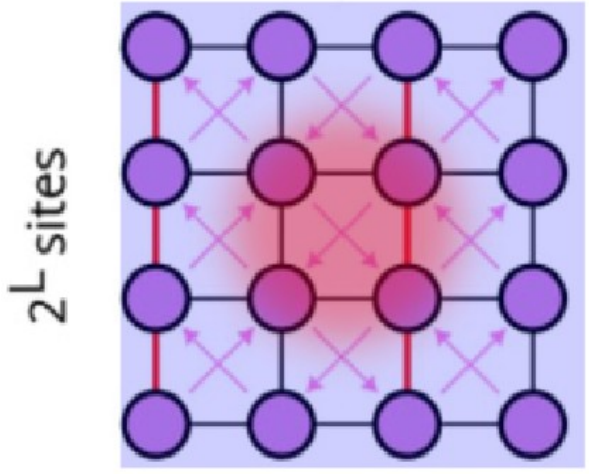
Topological domain with tensor networks

arXiv:2506.05230 (2025)

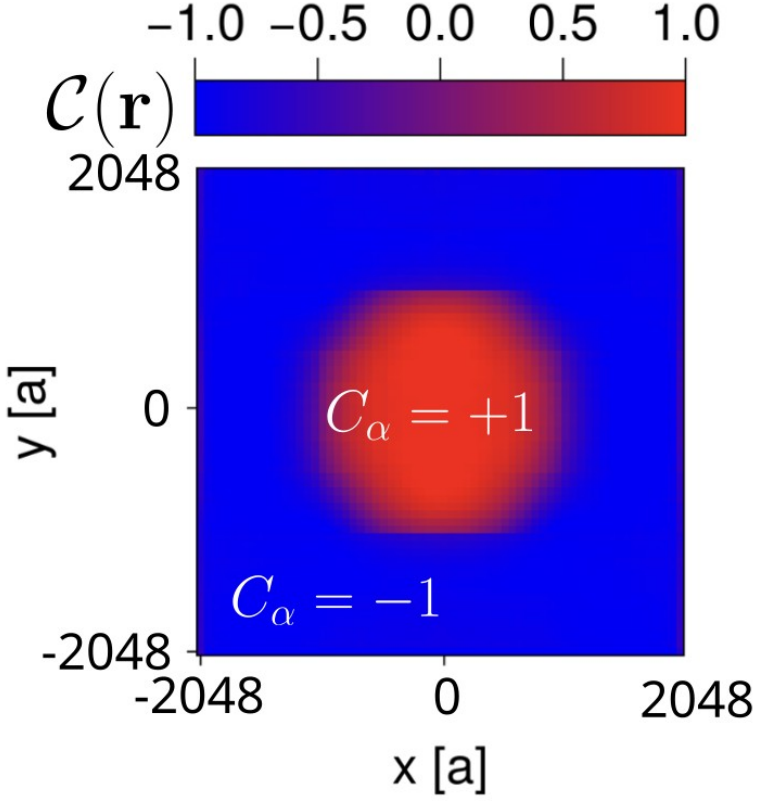
Topological marker

$$C_\alpha = 2\pi i \langle \alpha | \hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P} | \alpha \rangle$$

In a spatially modulated topological Hamiltonian

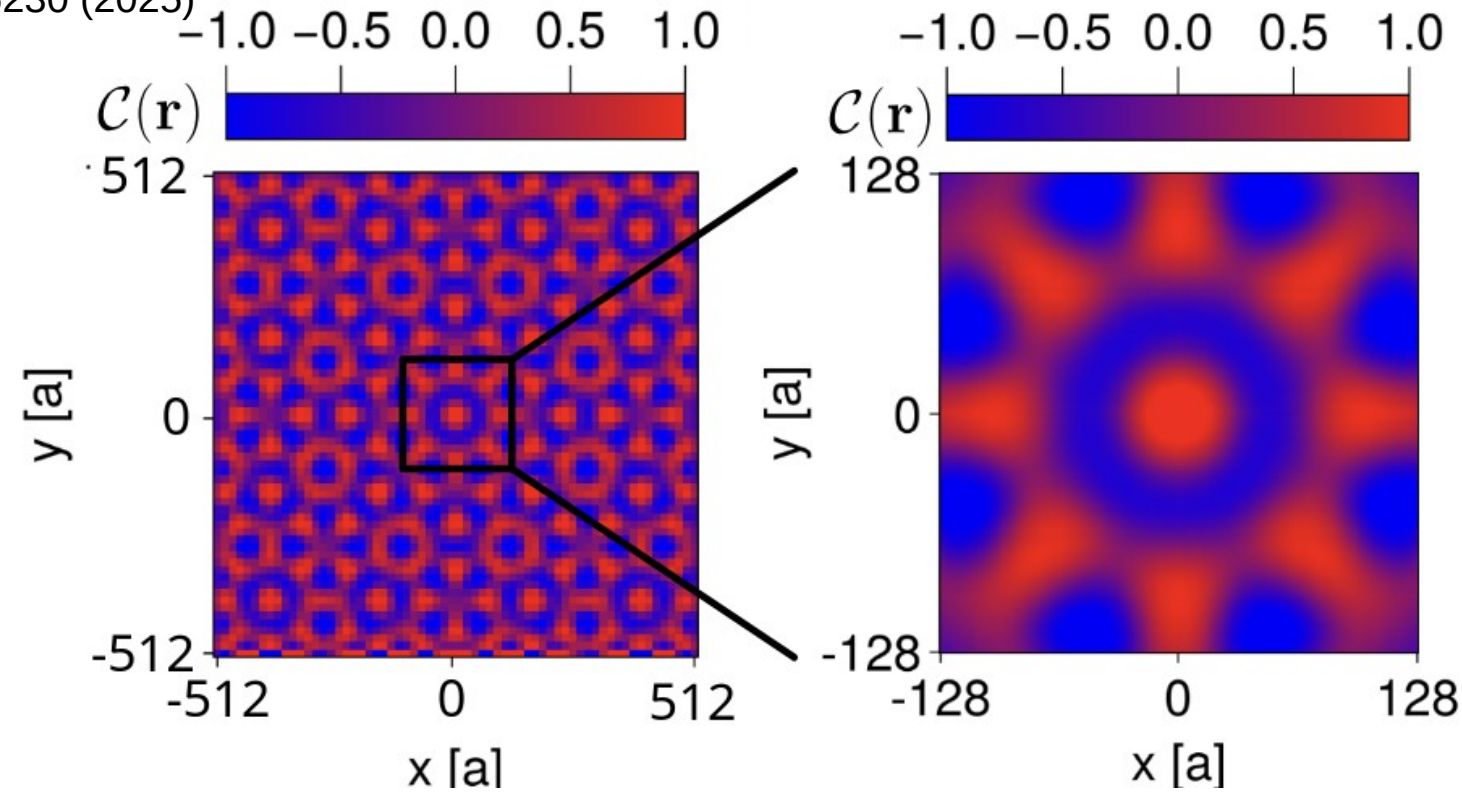


Chern number



Chern mosaic in a 8-fold topological quasicrystal

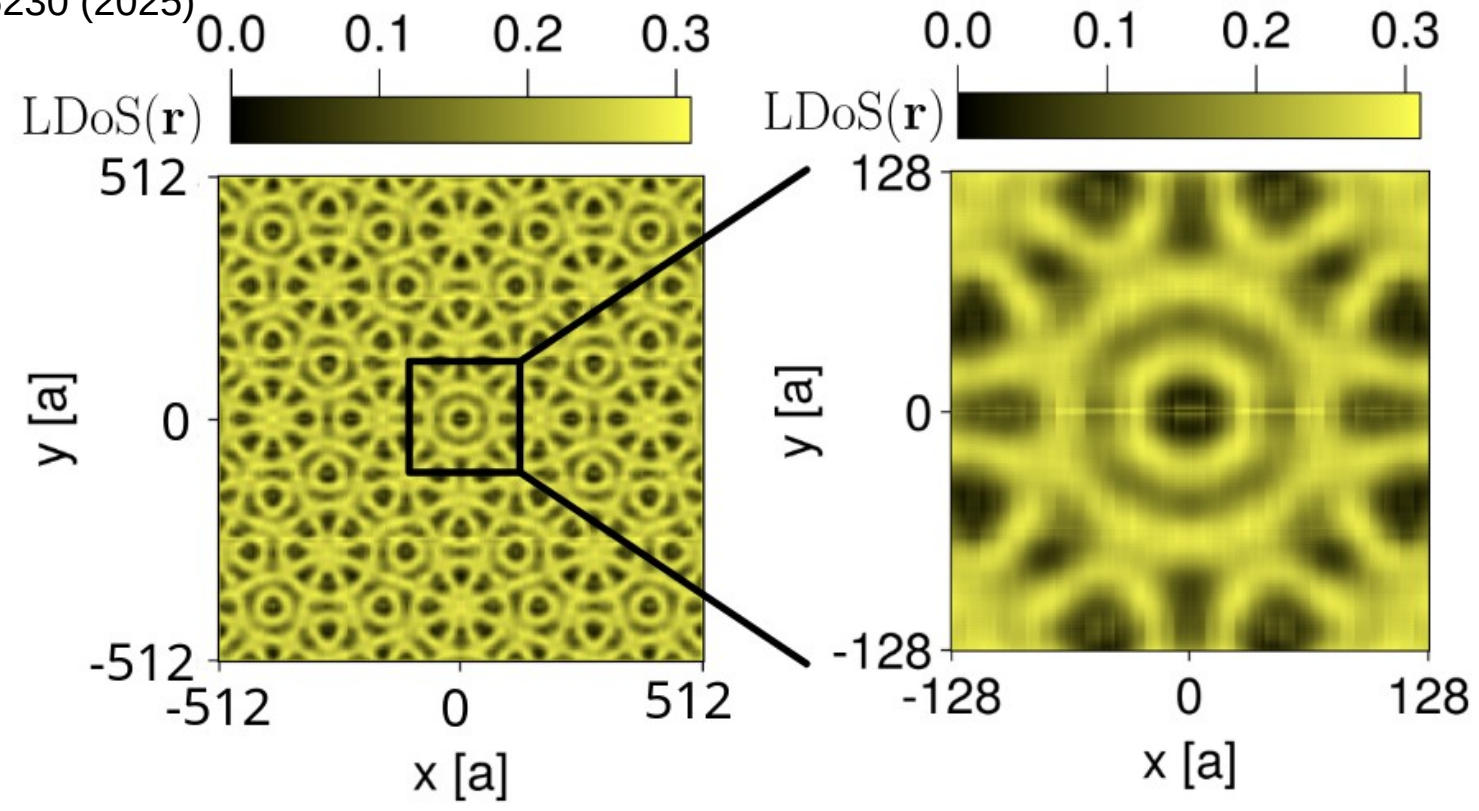
arXiv:2506.05230 (2025)



Domains with different topological invariants can be directly computed in real space

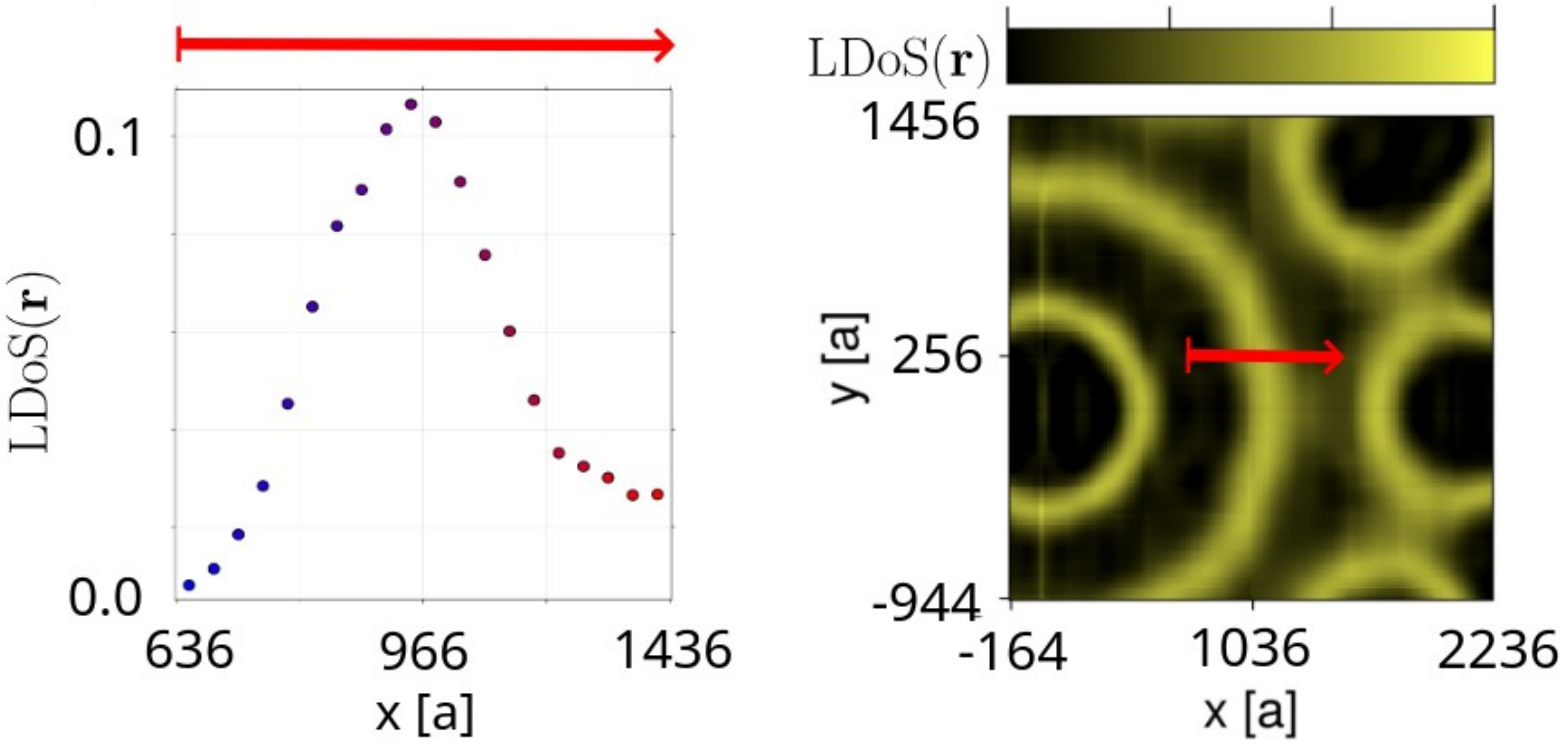
Topological modes in a 8-fold topological quasicrystal

arXiv:2506.05230 (2025)



Topological modes appear between topological domains in real space

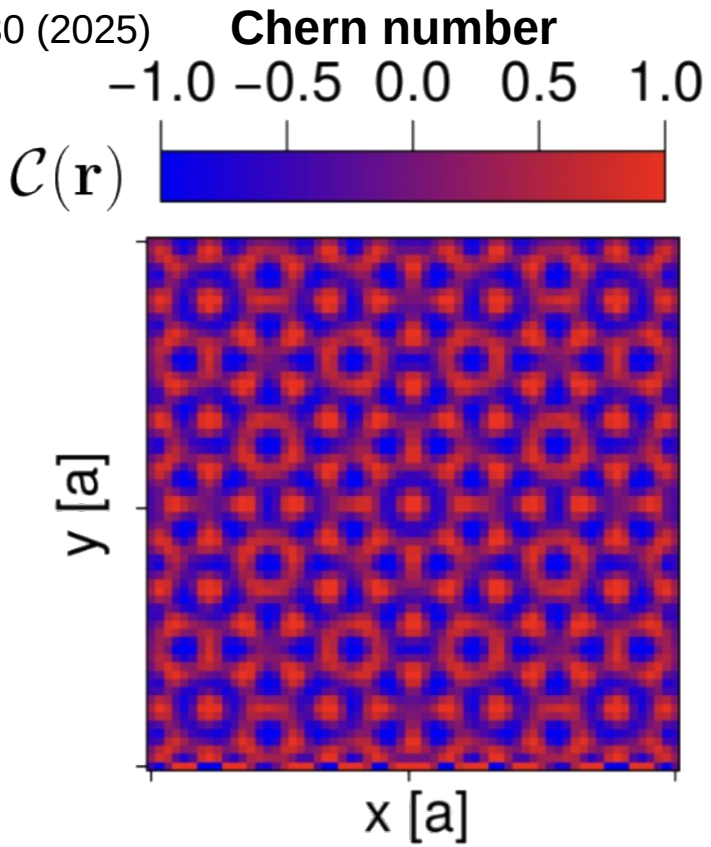
Zero modes across topological quasicrystalline domain

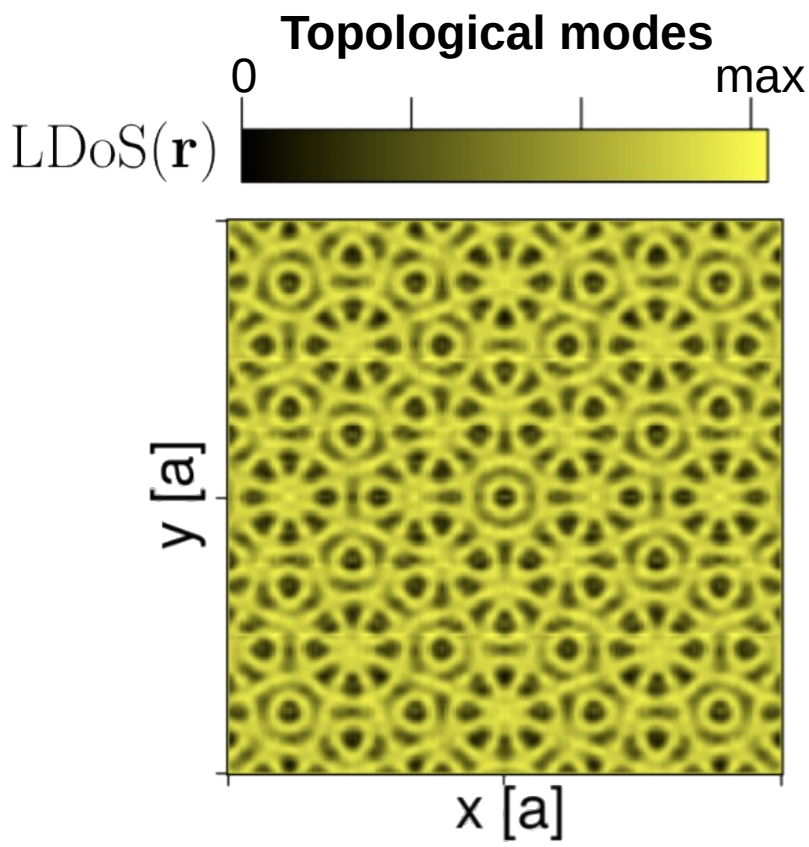


The real space distribution of topological states can be mapped in real space

Chern mosaic and topological modes in a quasicrystal

arXiv:2506.05230 (2025)





Tensor networks allow computing topology in exceptionally large super-moire systems

Many body quantum magnetism

The Ising dimer

What is the ground state of this Hamiltonian

$$\mathcal{H} = S_0^z S_1^z$$

The Hamiltonian has two ground states (related by time-reversal symmetry)

$$|GS_1\rangle = |\uparrow\downarrow\rangle \qquad |GS_2\rangle = |\downarrow\uparrow\rangle$$

Each ground state breaks time-reversal symmetry

A symmetry broken antiferromagnet is a macroscopic version of this

The quantum Heisenberg dimer

What is the ground state of this quantum Hamiltonian?

$$\mathcal{H} = \vec{S}_0 \cdot \vec{S}_1$$

The ground state is unique, and does not break time-reversal

$$|GS\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \qquad \langle \vec{S}_i \rangle = 0$$

The state is maximally entangled

How does this generalize to a macroscopic system?

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

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 L=4 sites, the elements of the basis are

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

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

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

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

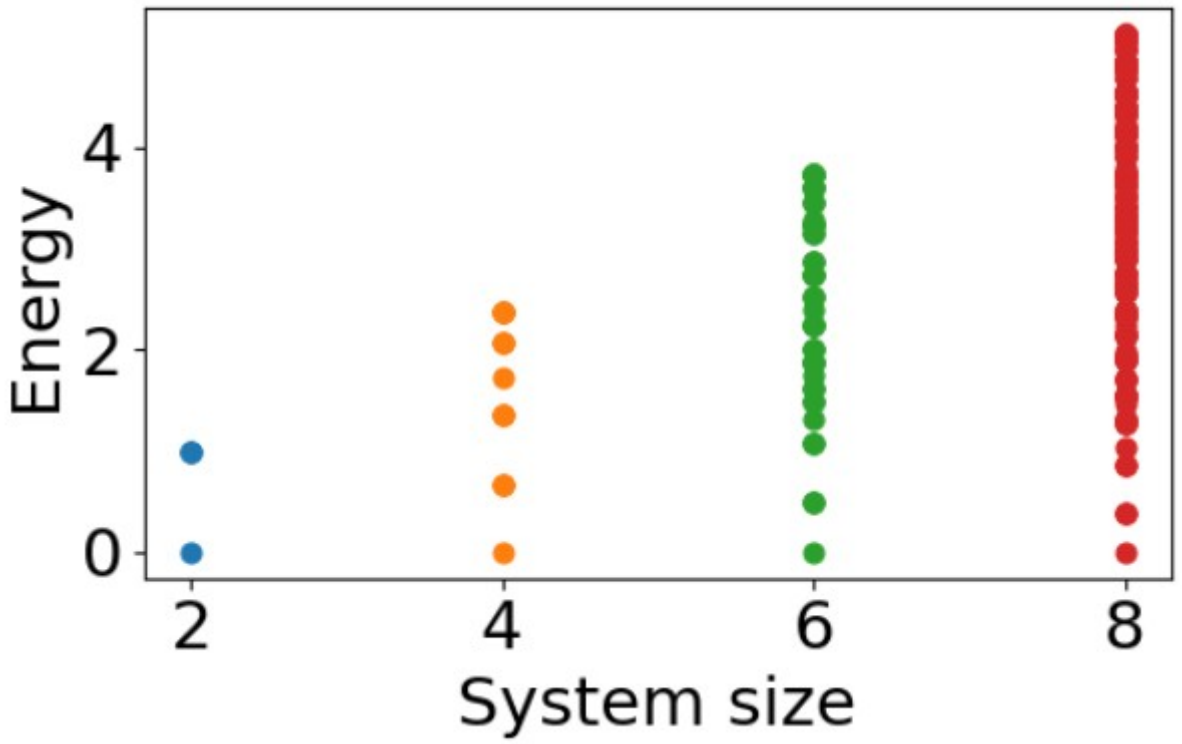
We need to determine in total 2^L coefficients

The Hamiltonian is a $2^L \times 2^L$ matrix

Understanding the many-body spectra

Energies of a many-body model

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



From classical to quantum magnetism

Let us take a modified Heisenberg model

$$H = \sum_n J_{xy} S_n^x S_{n+1}^x + J_{xy} S_n^y S_{n+1}^y + S_n^z S_{n+1}^z$$

For $J_{xy} = 0$ we have an Ising model

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

For $J_{xy} = 1$ we have a Heisenberg model

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

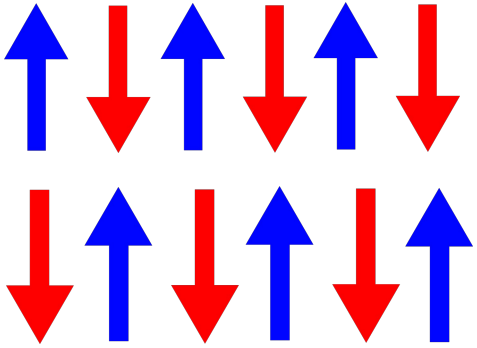
From classical to quantum magnetism

Let us take a modified Heisenberg model

$$H = \sum_n J_{xy} S_n^x S_{n+1}^x + J_{xy} S_n^y S_{n+1}^y + S_n^z S_{n+1}^z$$

Ising model

Two ground states



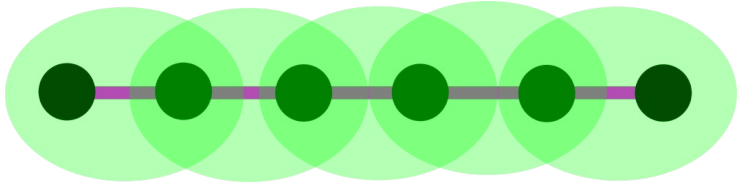
Transition at

$$J_{xy} = 0.5$$

in the thermodynamic limit

Heisenberg model

One ground state

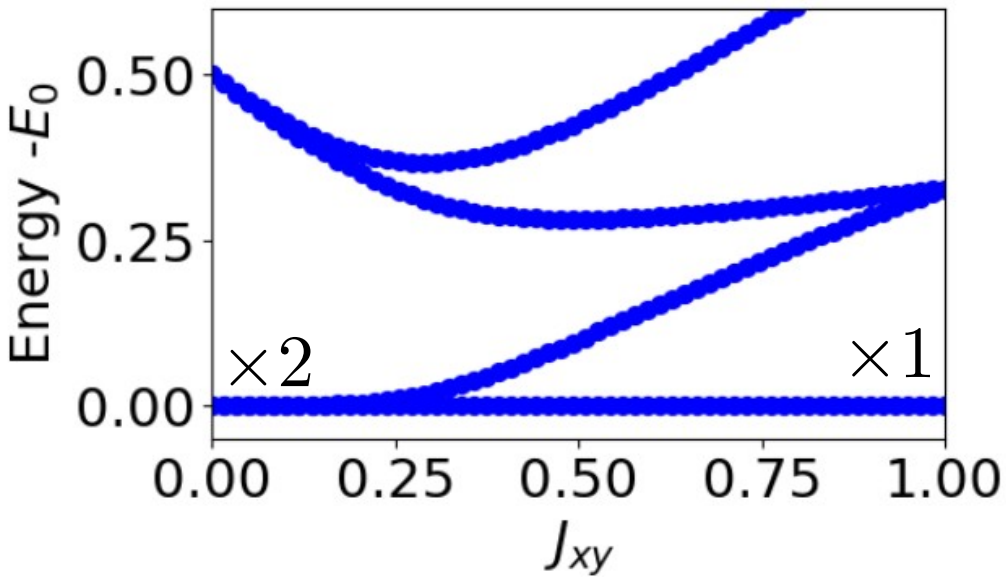


From classical to quantum magnetism

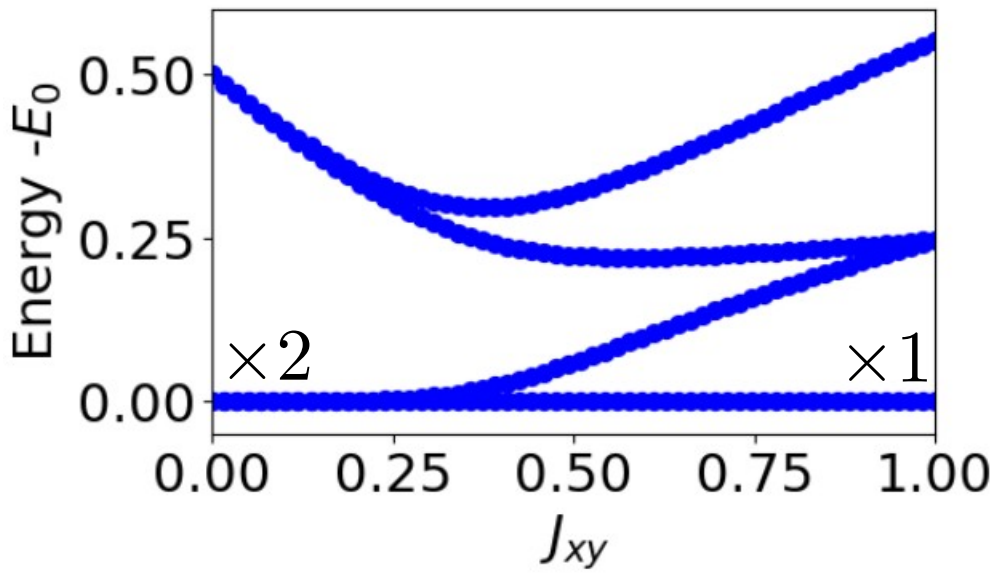
Let us take a modified Heisenberg model

$$H = \sum_n J_{xy} S_n^x S_{n+1}^x + J_{xy} S_n^y S_{n+1}^y + S_n^z S_{n+1}^z$$

$L = 10$



$L = 14$



A minimal quantum magnet

Let us start by taking the Heisenberg dimer

$$H = \vec{S}_0 \cdot \vec{S}_1 \qquad S = 1/2$$

We can define a collective spin as

$$\vec{L} = \vec{S}_0 + \vec{S}_1$$

So that the Hamiltonian takes the form

$$H \sim \vec{L} \cdot \vec{L} \sim l(l+1) \qquad L = 0, 1$$

$l = 0$ singlet

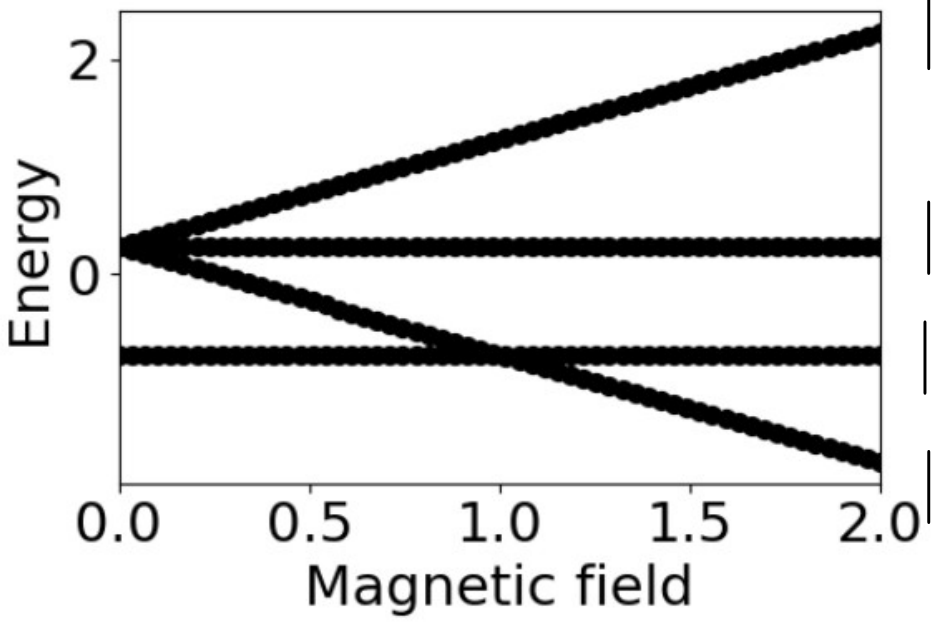
$l = 1$ triplet

Energies of a many-body model

Let us look how the energies depend on the external magnetic field

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

$$L = 2$$



$$|T, +1\rangle = |\uparrow\uparrow\rangle$$

$$|T, 0\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \right)$$

$$|S\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

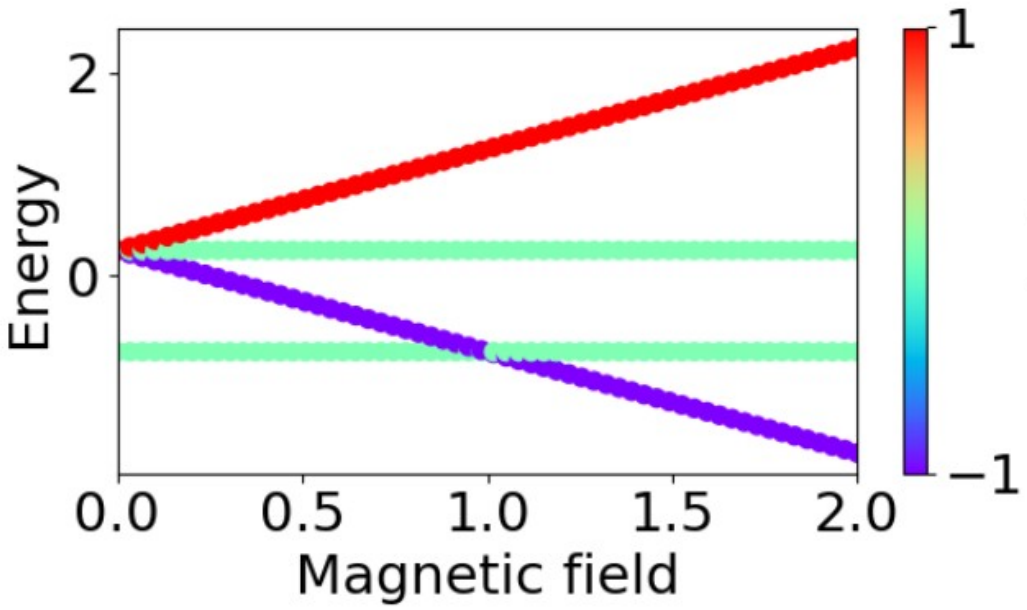
$$|T, -1\rangle = |\downarrow\downarrow\rangle$$

Energies of a many-body model

Let us look how the energies depend on the external magnetic field

$$\langle S_z \rangle = \langle \Omega_n | \sum_n S_n^z | \Omega_n \rangle \qquad H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$$

$$L = 2$$



$$|T,+1\rangle = |\uparrow\uparrow\rangle$$

$$|T,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|S\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

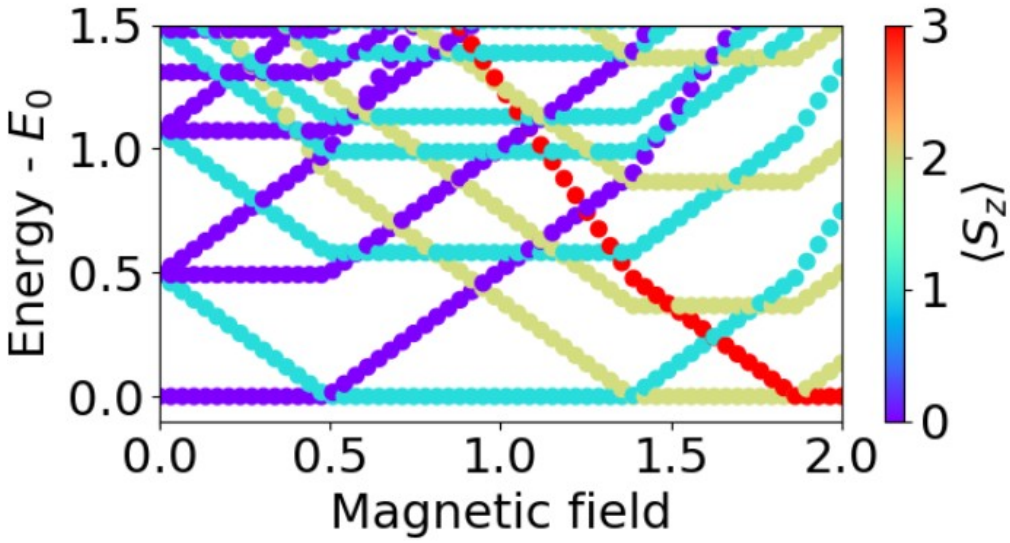
$$|T,-1\rangle = |\downarrow\downarrow\rangle$$

Energies of a many-body model

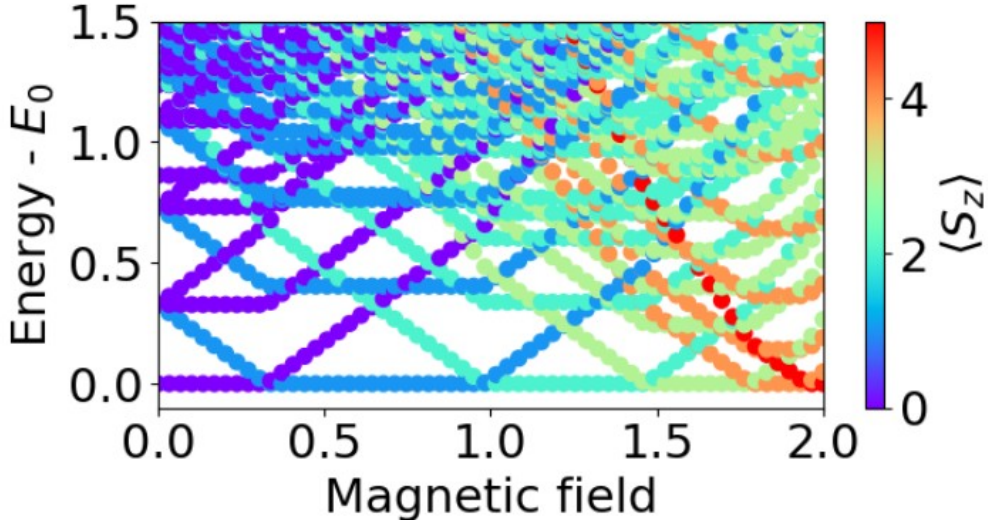
Let us now look at bigger systems

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

$L = 6$



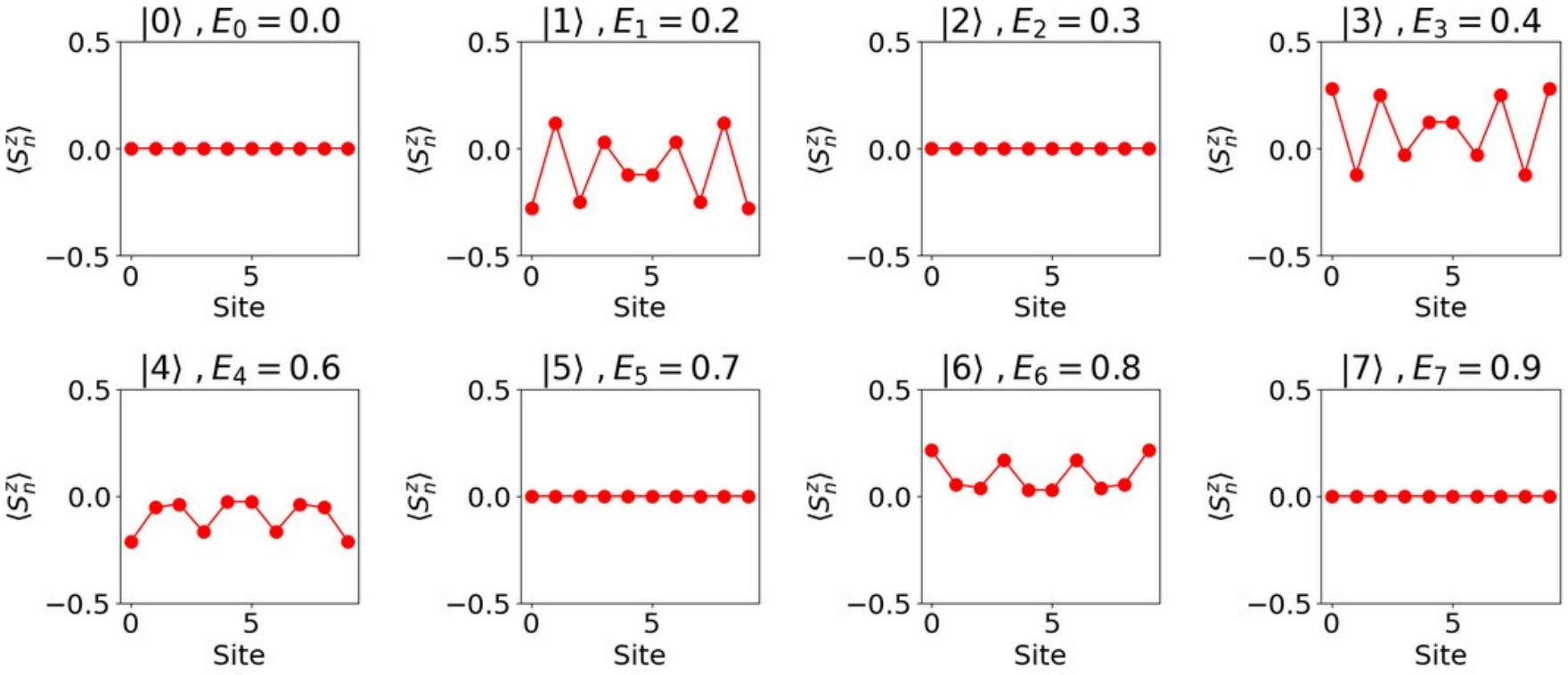
$L = 10$



Excitation energies and magnetization

Let us now consider a system with L=10

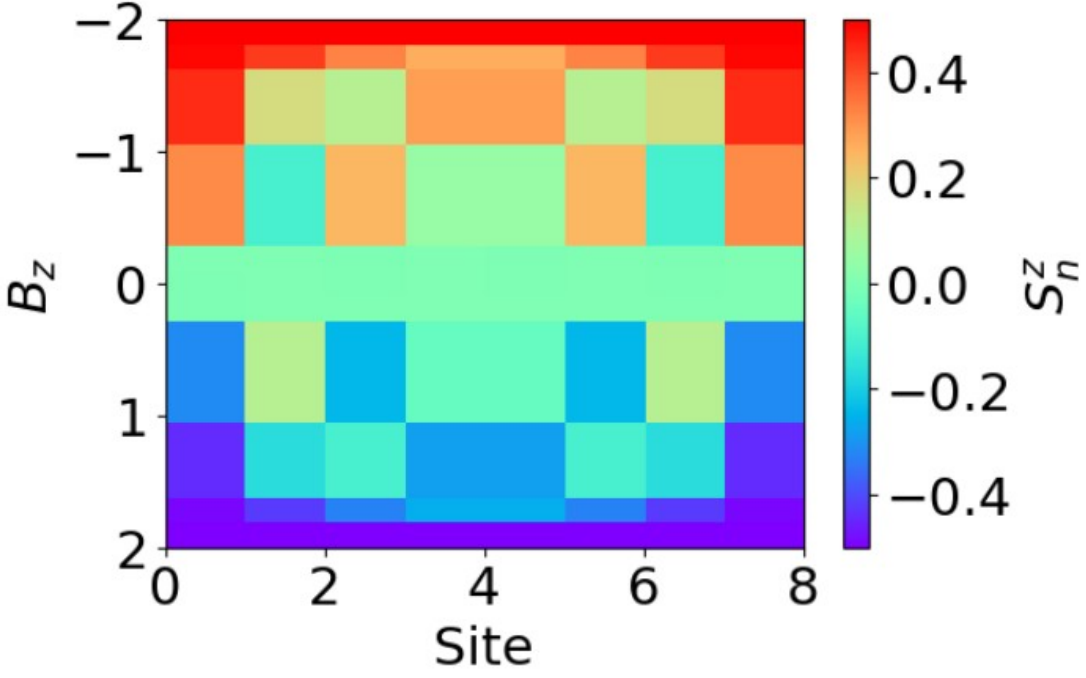
$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S_n^z$$



Ground state of a many-body model

Let us look how the ground state depends on the external magnetic field

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



$$H|\Omega_n\rangle = E_0|\Omega_n\rangle$$

$$\langle S_n^z\rangle = \langle\Omega_n|S_n^z|\Omega_n\rangle$$

Dynamical spin correlators

The many-body excitations of spin Hamiltonian can be characterized by the dynamical spin correlator

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

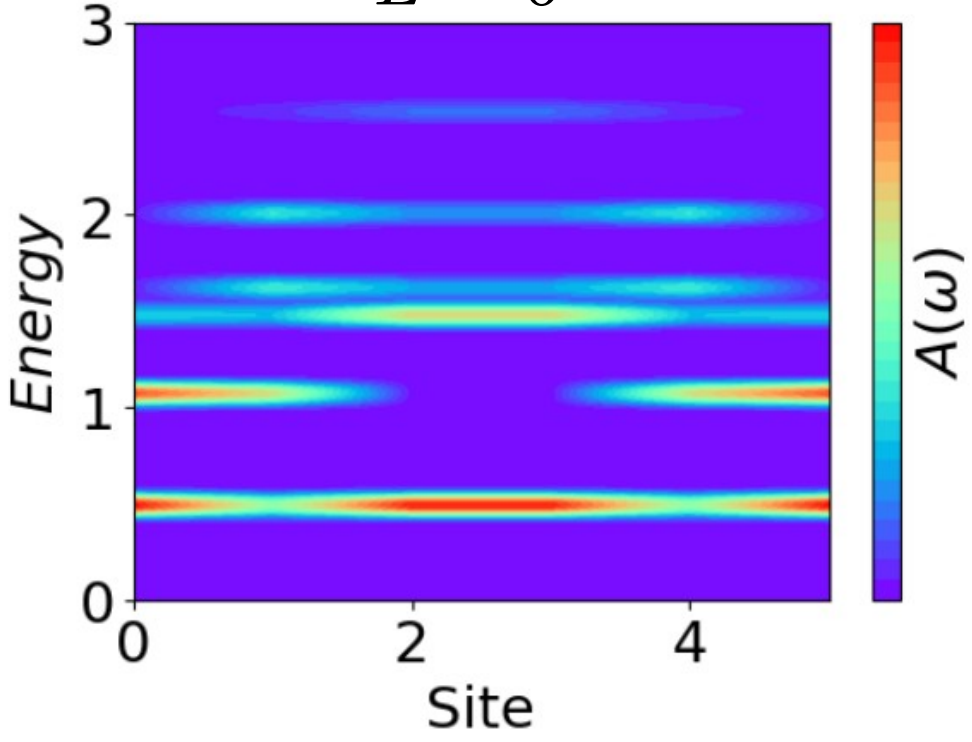
The spectral function above signal excited states that have one more spin excitation than the ground state

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

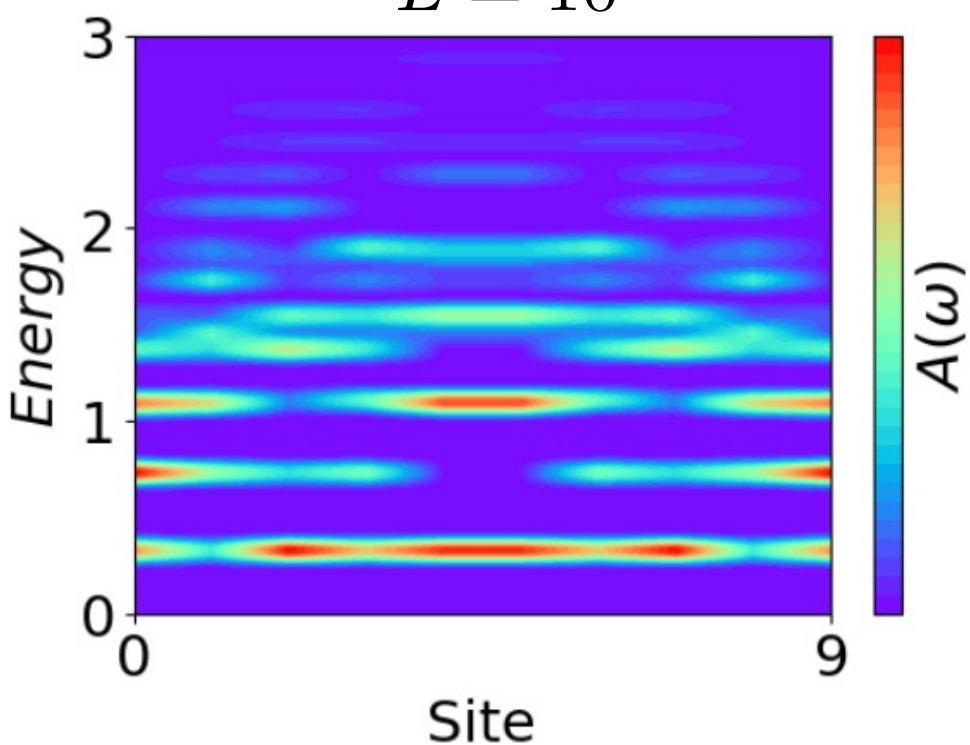
Dynamical correlator of the Heisenberg model

Lets look at the Heisenberg model with $S = 1/2$ $\quad H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$

$L = 6$



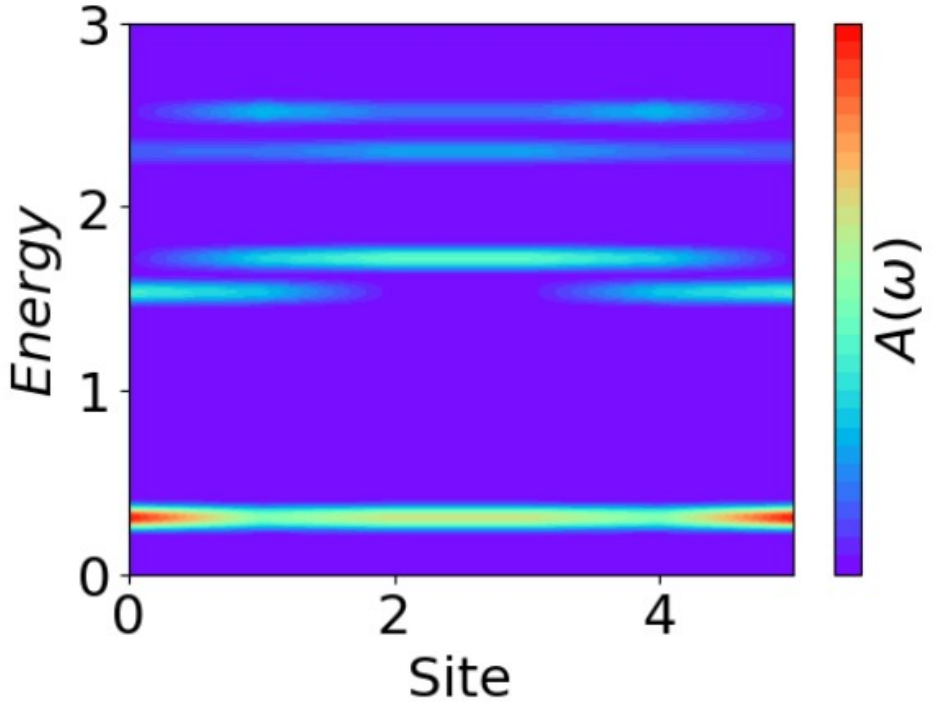
$L = 10$



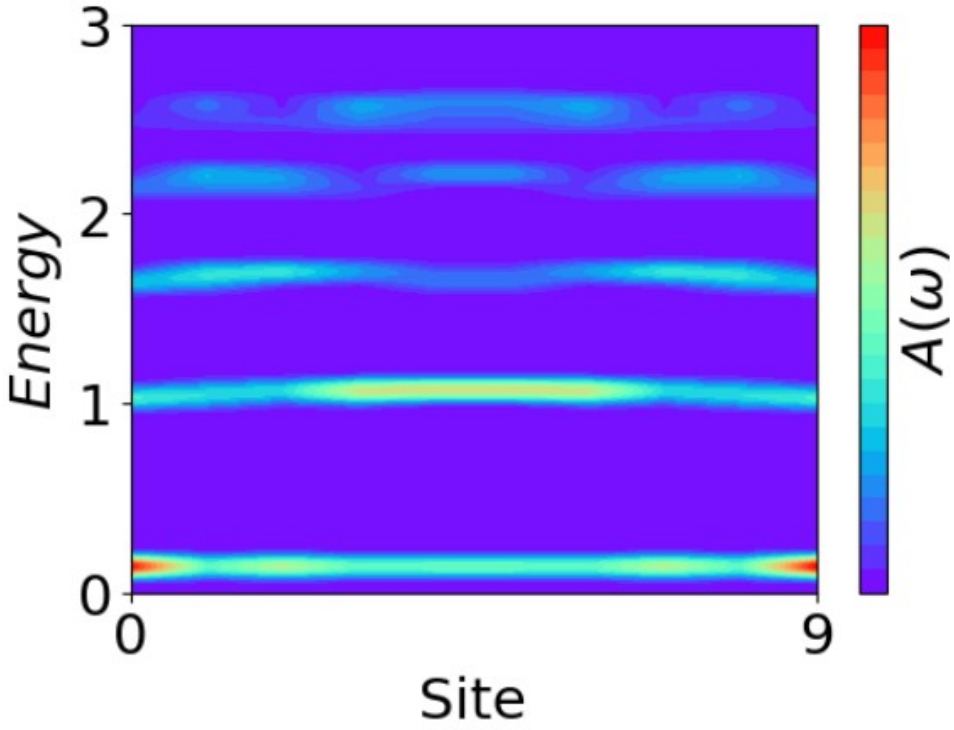
Dynamical correlator of the Heisenberg model

Lets look at the Heisenberg model with $S = 1$ $H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$

$L = 6$



$L = 10$



Two types of spin chains

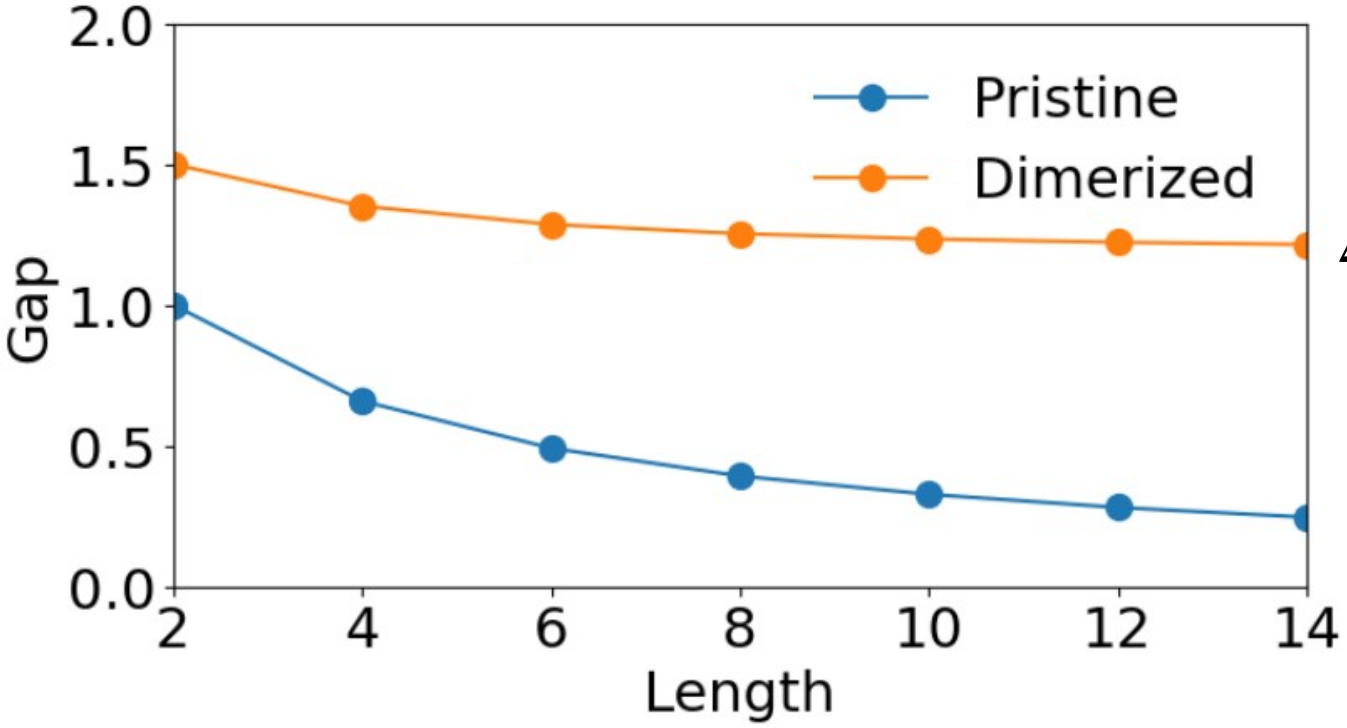
Let us consider two different types of many-body spin chains

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

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

Pristine and dimerized chains

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



$$\Delta(L) \sim \Delta_0 + \Delta_1 e^{-\lambda L}$$

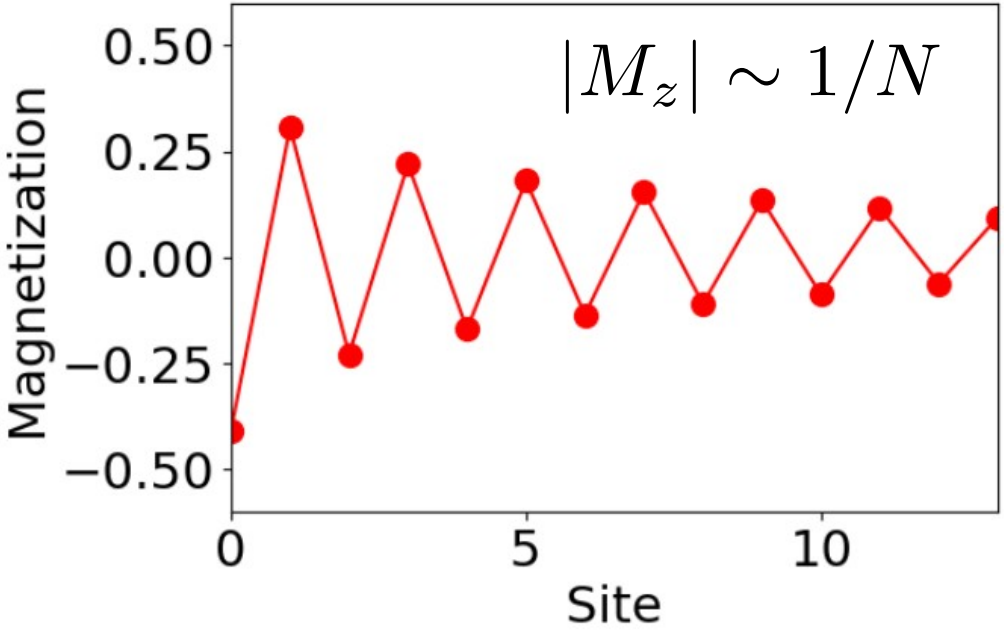
$$\Delta(L) \sim 1/L$$

Response of a quantum magnet to a magnetic impurity

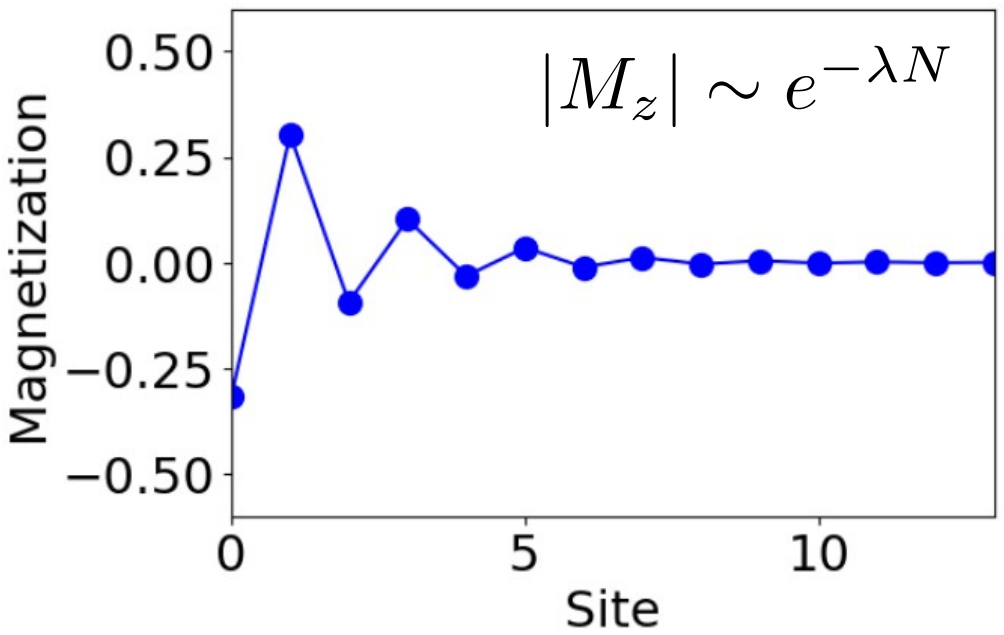
Quantum chain with a local field

$$H = J_{ij} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + B_z S_0^z$$

Uniform chain



Dimerized chain



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

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

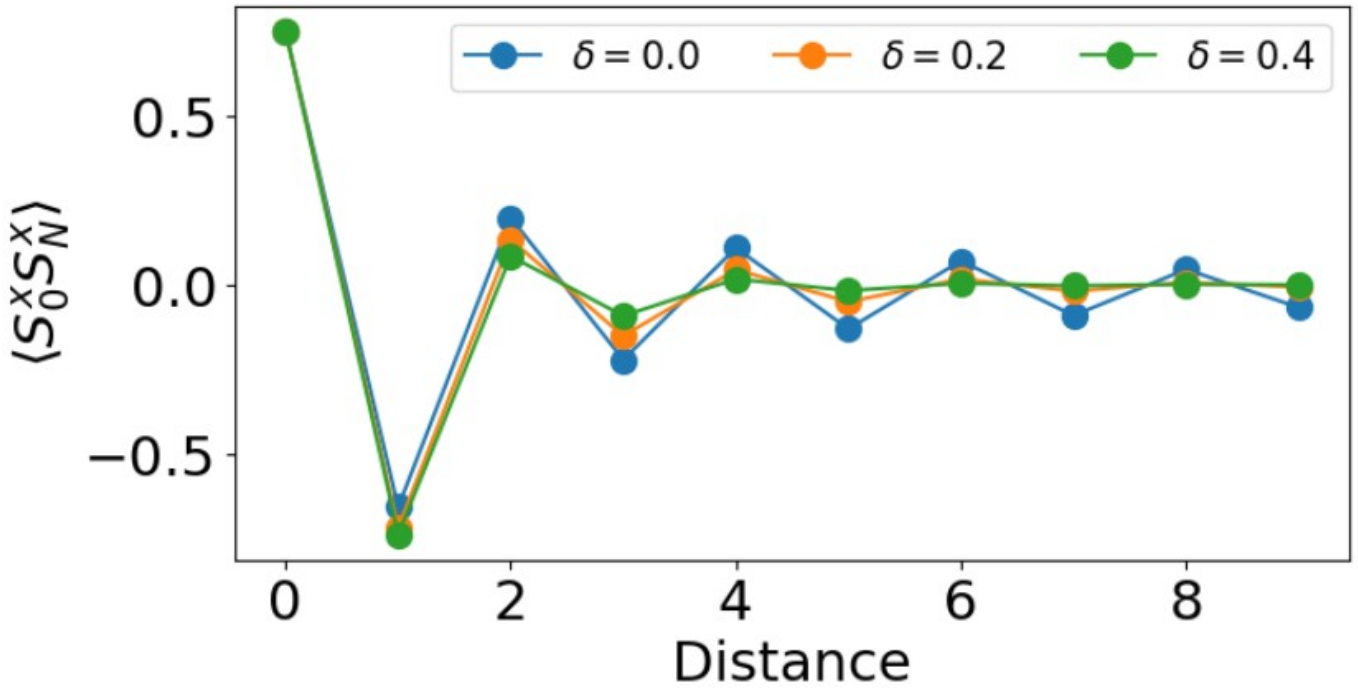
Gapless spectrum

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

Gapped spectrum

Non-local static correlators

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



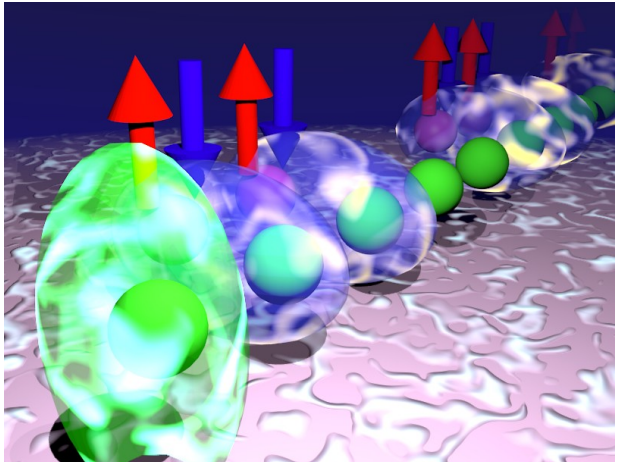
Matrix product states and tensor networks

The fundamental idea of tensor-networks

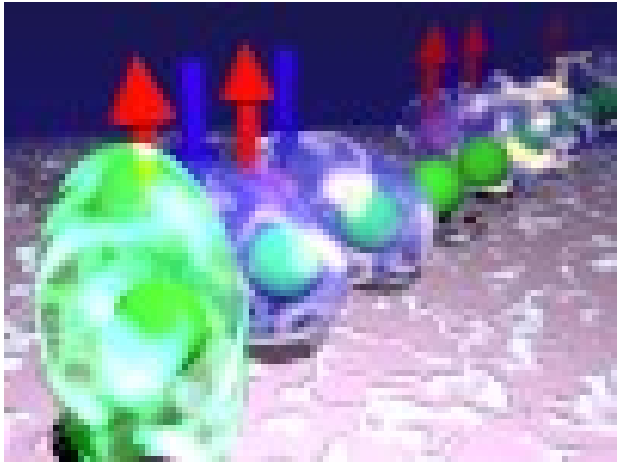
A many-body wavefunction a is a very high dimensional object

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

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



“True wavefunction”



“Tensor-network wavefunction”

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

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

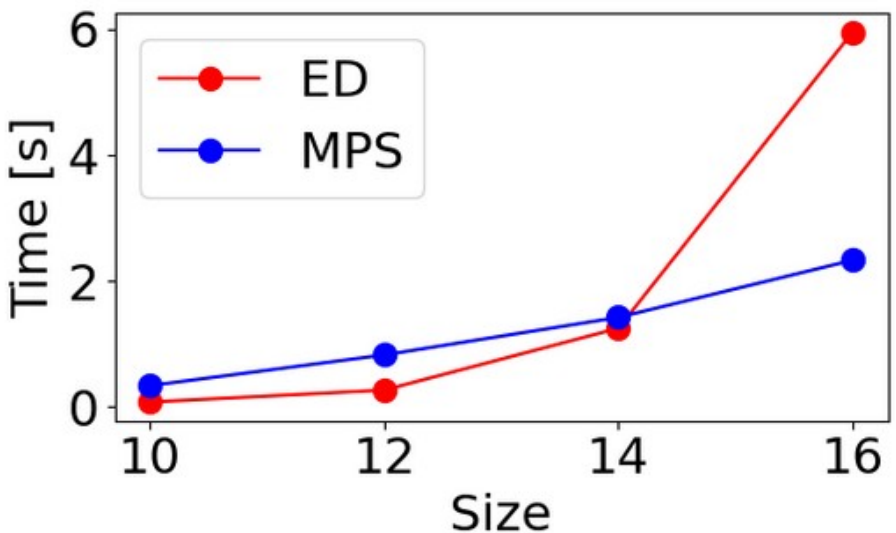
This ansatz can be generalized for time-evolution, excited states, open systems.

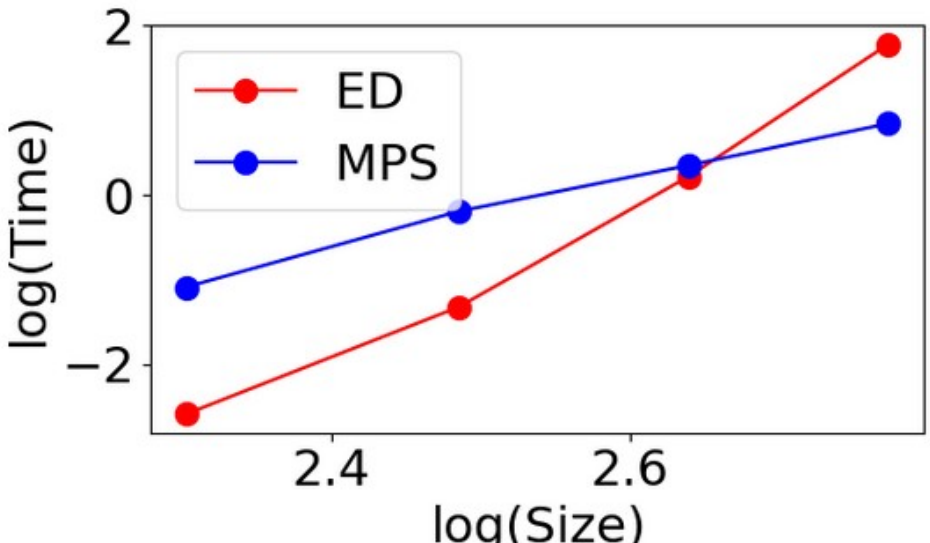
Computational complexity of matrix product states

Matrix product states provide a highly favorable scaling with system size

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

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





Computational complexity of matrix product states

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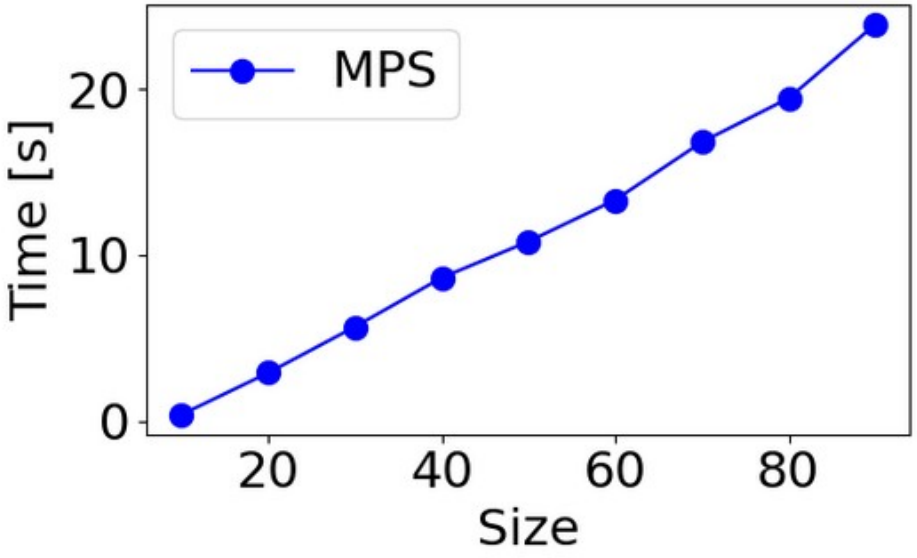
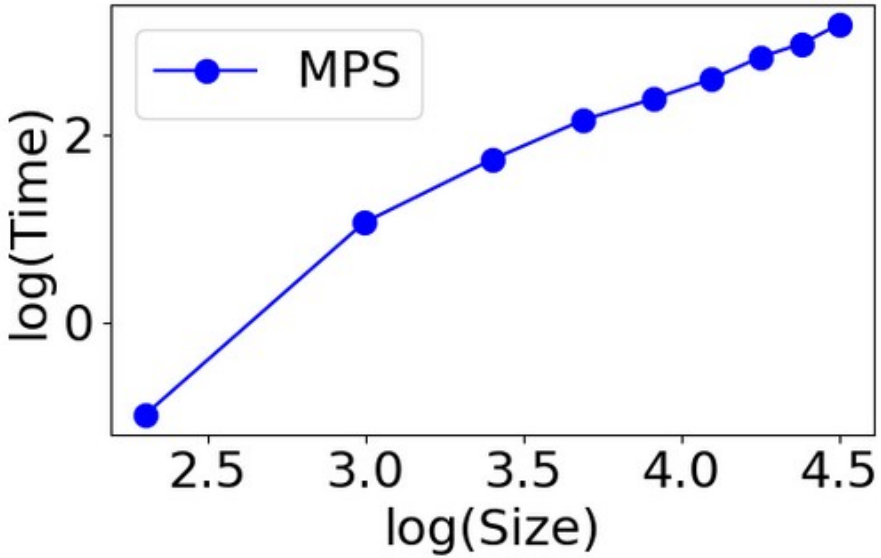
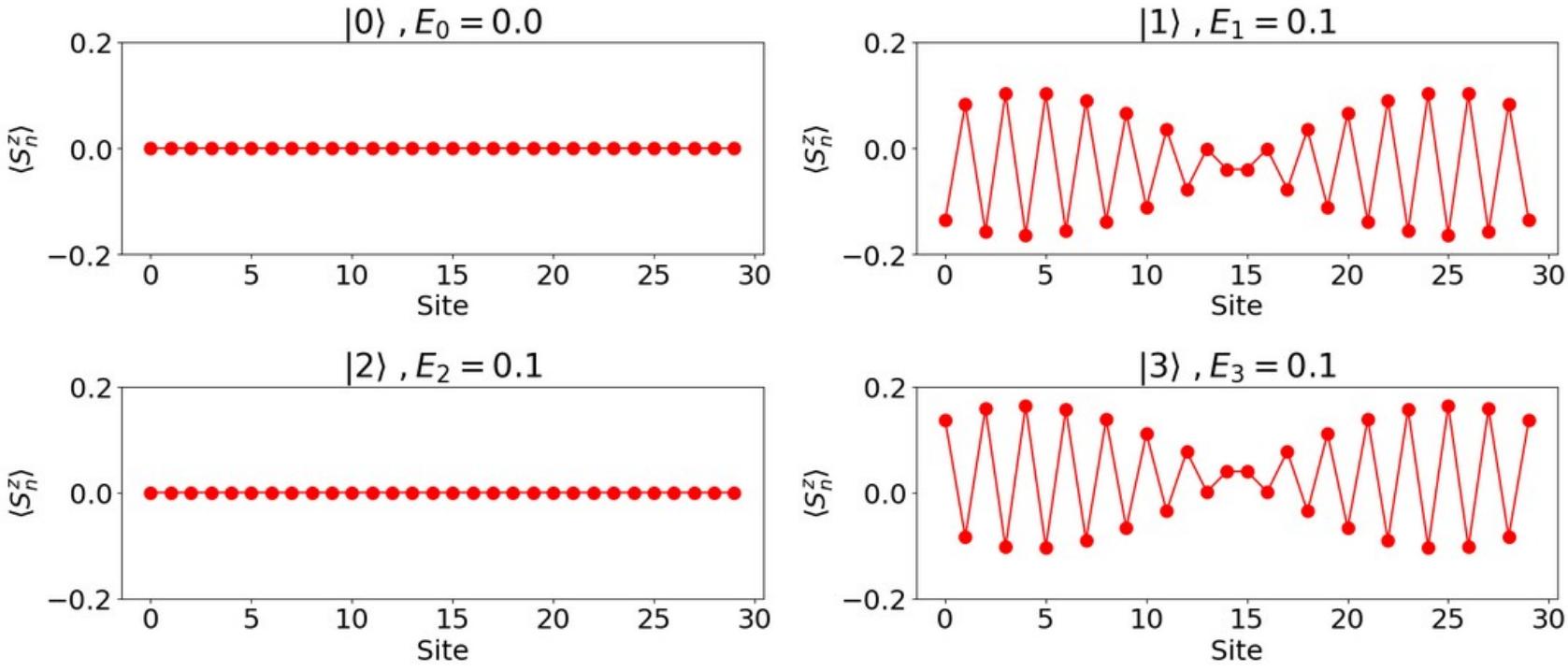




Magnetization in excited states of long chains

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

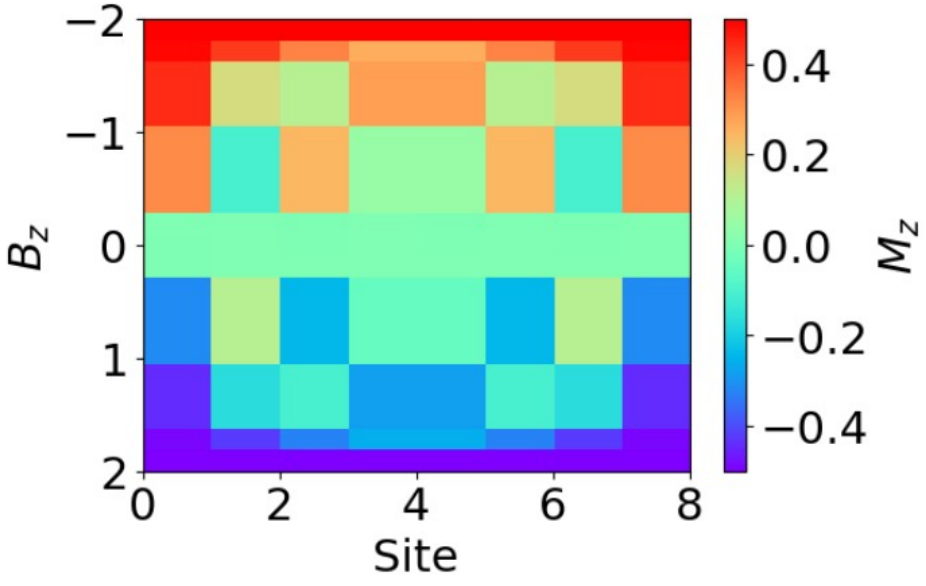


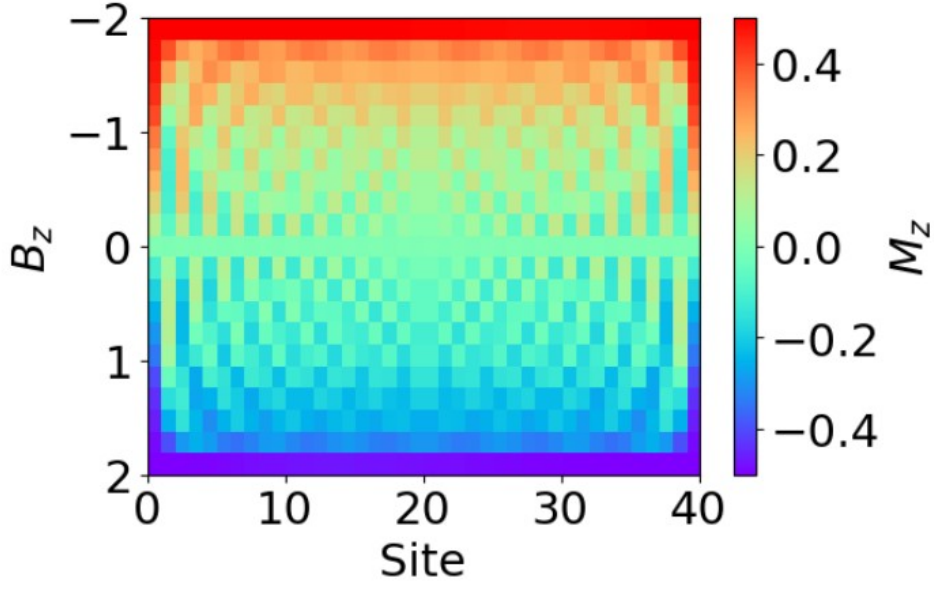
Level crossing with matrix product states

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



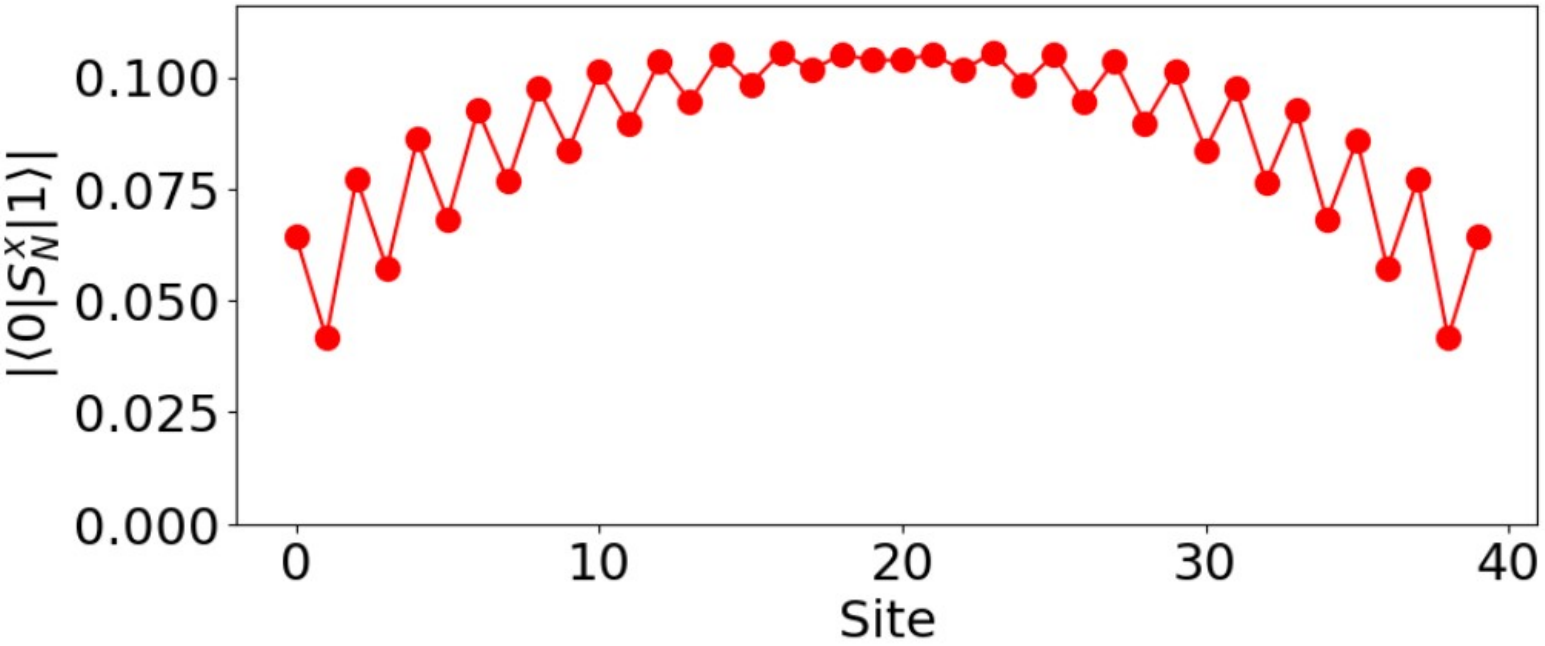


Matrix elements between ground state and excited states

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

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

$$M_{0\to 1} = |\langle 1|S_n^x|0\rangle|$$



Matrix elements between ground state and excited states

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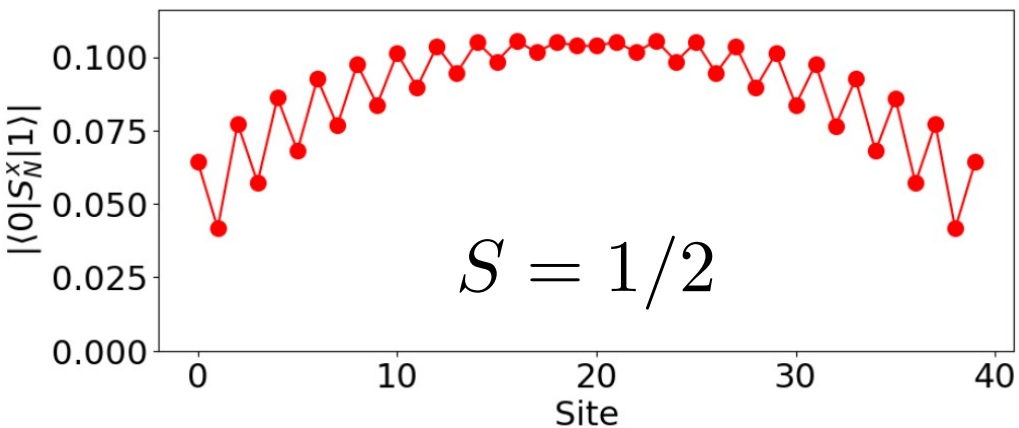
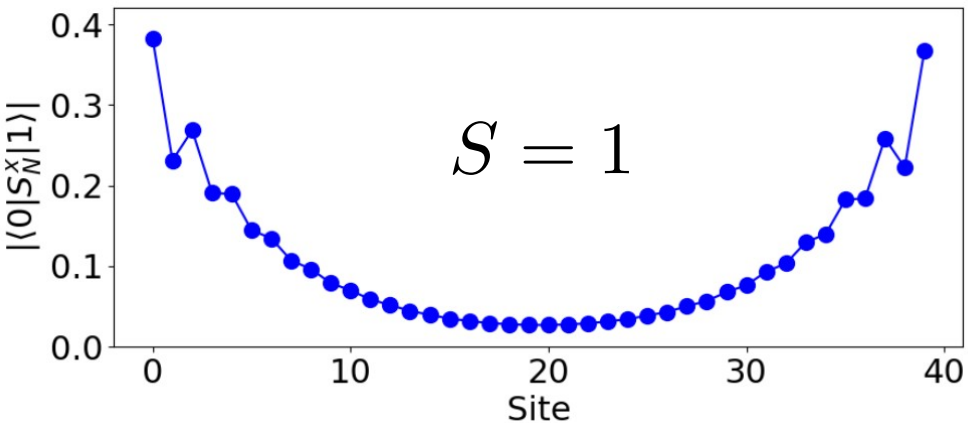
$$H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + B_z \sum_n S^z_n$$

$$M_{0\to 1} = |\langle 1|S^x_n|0\rangle|$$

Bulk excitation



Edge excitation

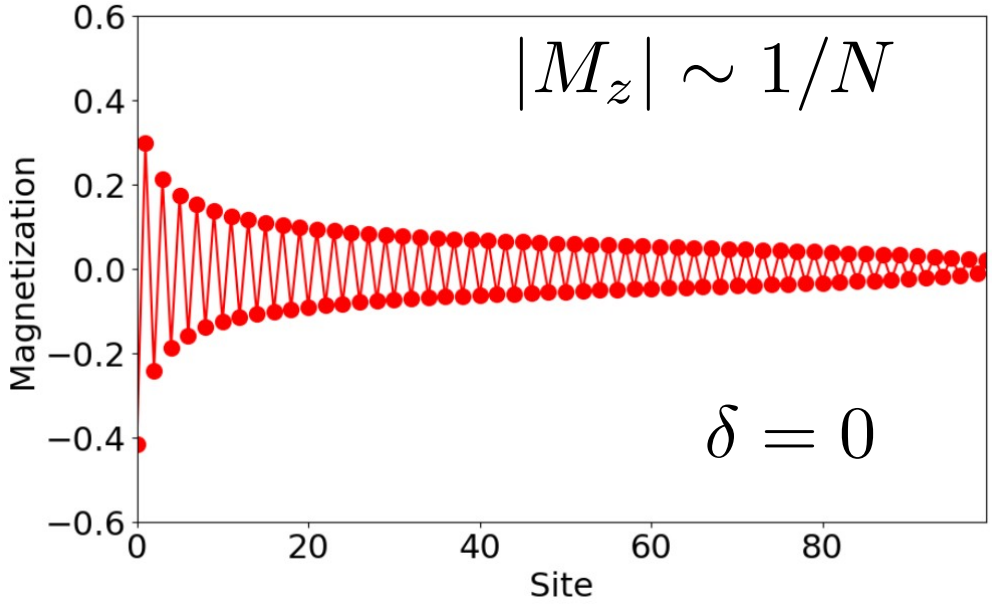


Response of a large quantum magnet to a magnetic impurity

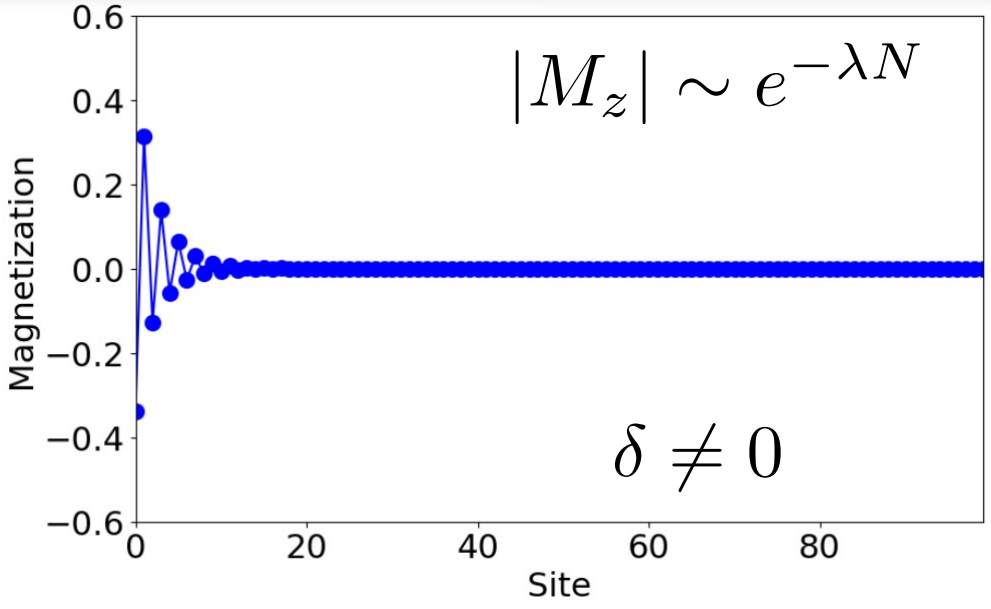
Quantum chain with a local field

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

Uniform chain

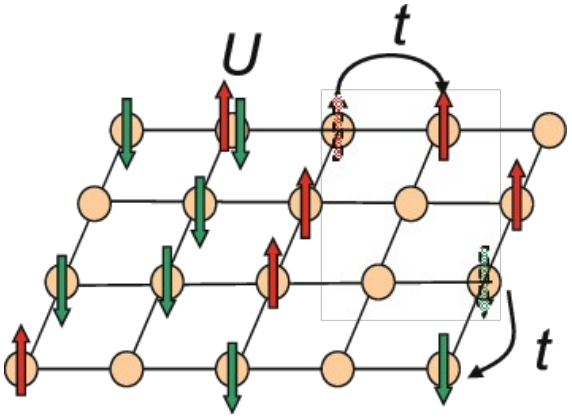


Dimerized chain



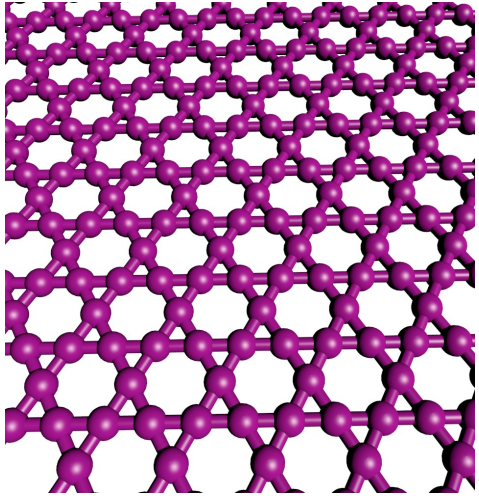
Some paradigmatic quantum materials tackled with tensor networks

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



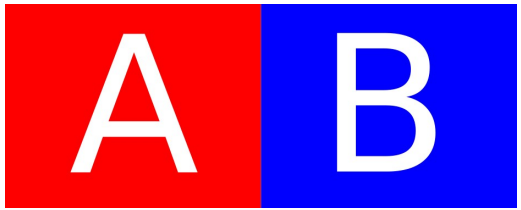
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

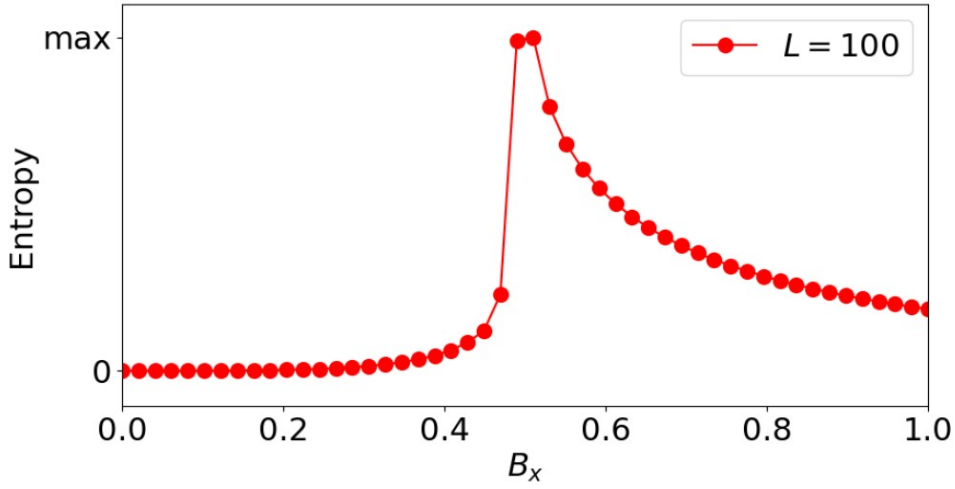
Can such a phase transition be observed from the entanglement entropy?

Entanglement entropy and phase transitions

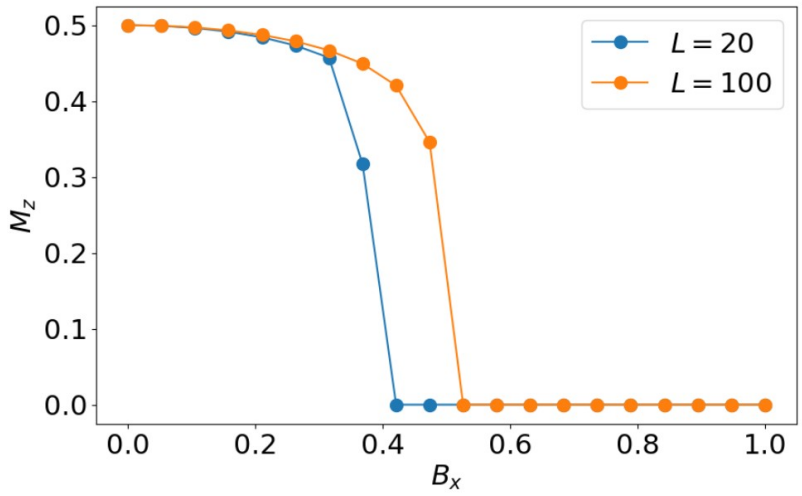
Let us look at the transverse field Ising model

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

Phase transition from entropy

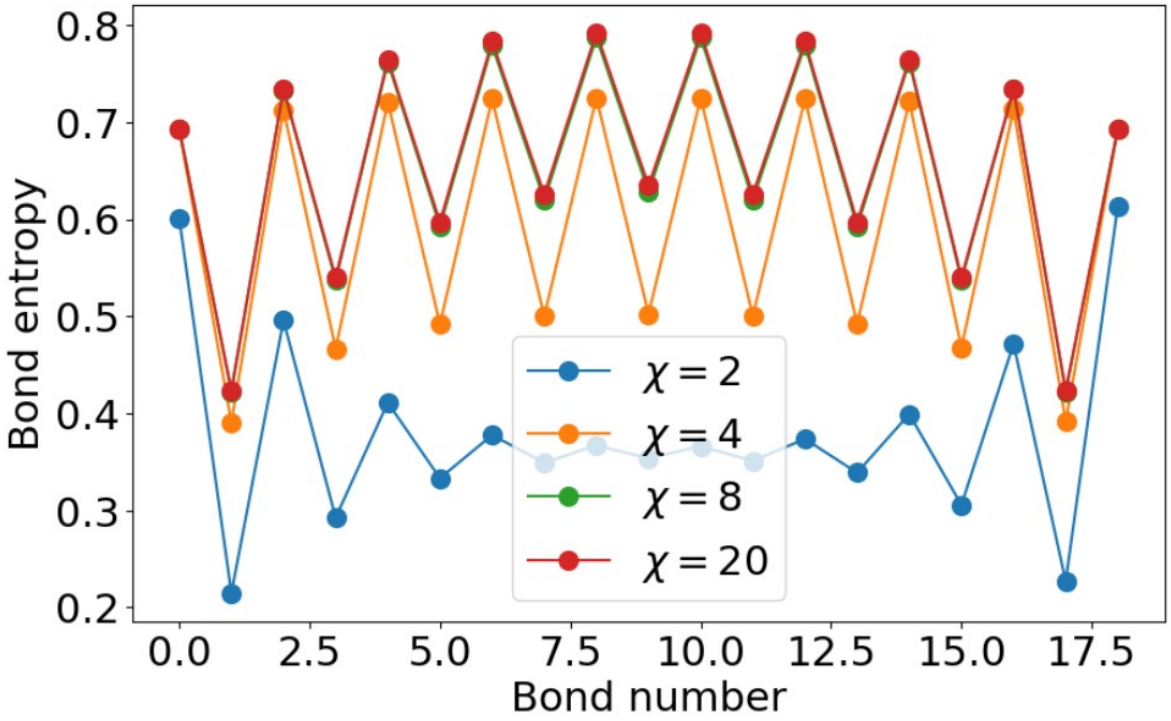


Phase transition from order parameter



Entanglement entropy in space and the bond dimension

The bond dimension determines the maximal entanglement entropy



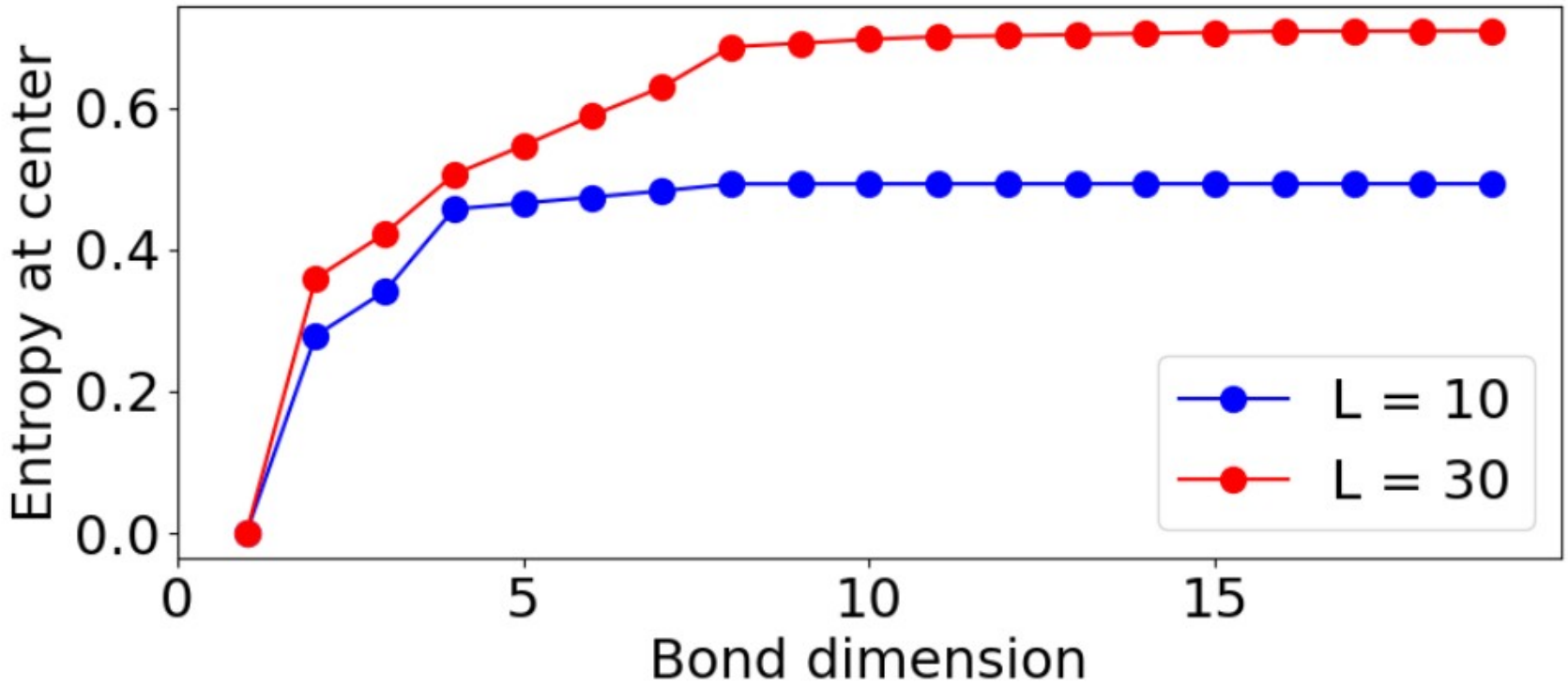
Heisenberg model

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

Entanglement entropy and the bond dimension

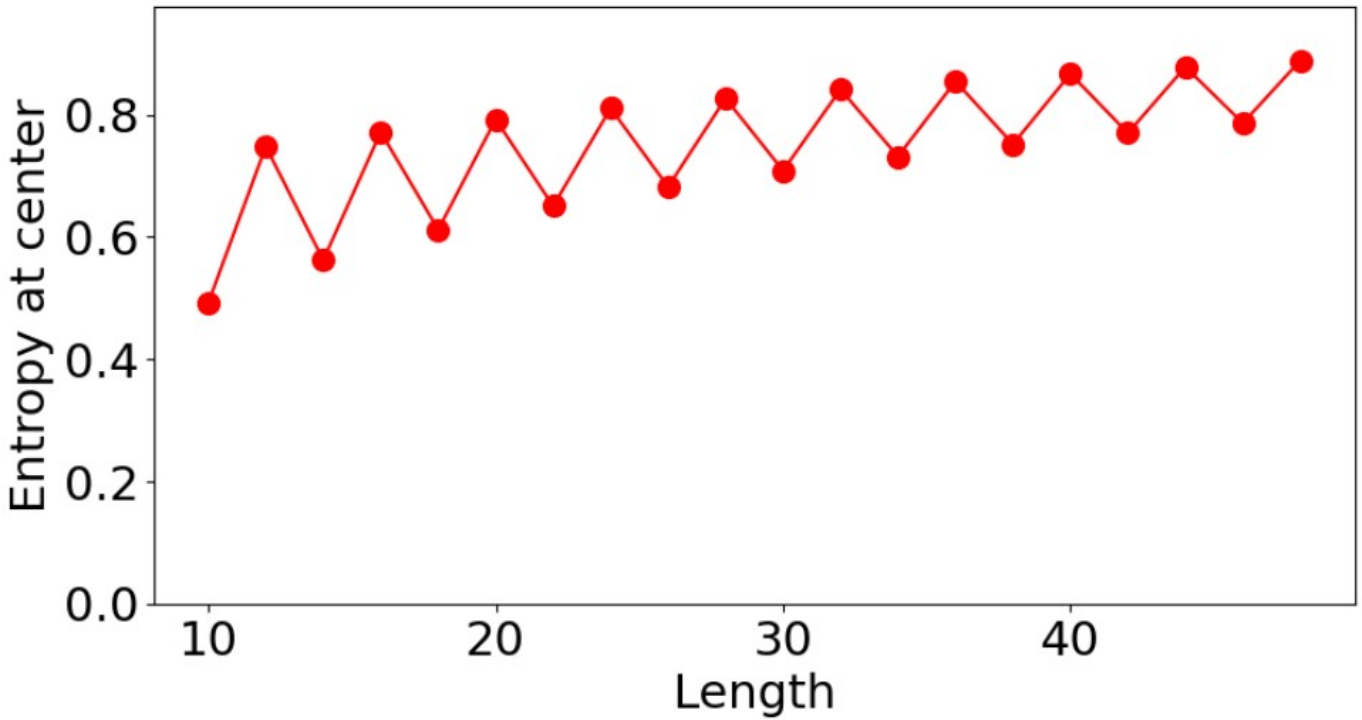
The entanglement of the MPS saturates with the bond dimension

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



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 $H = \sum_n J \vec{S}_{2n} \cdot \vec{S}_{2n+1}$

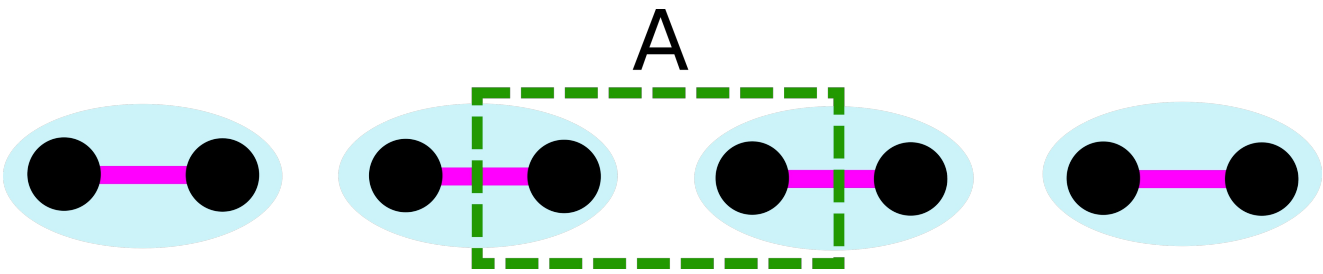
The many-body wavefunction is just a product of singlet between dimers

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

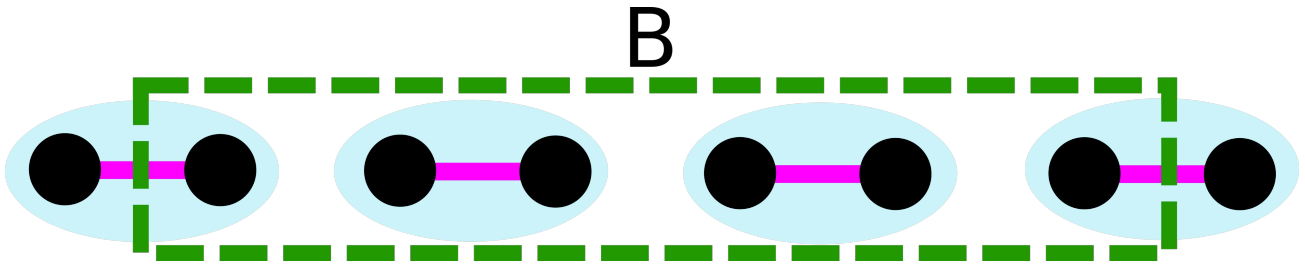
What is the entanglement entropy when making a bipartition?

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

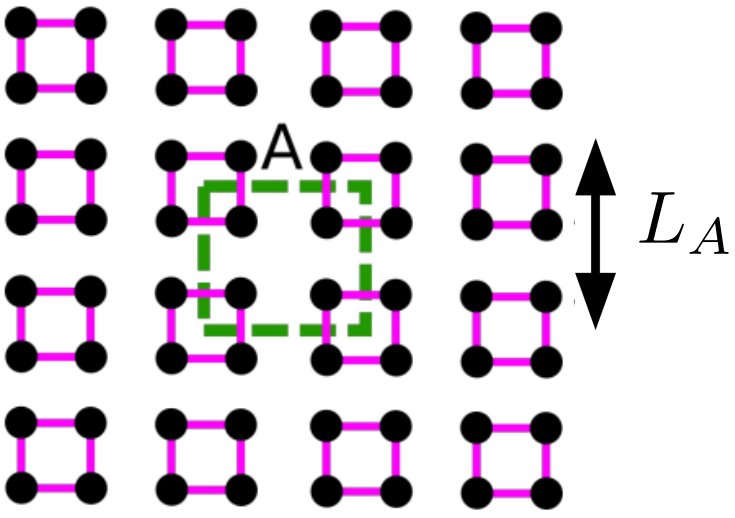


The entanglement entropy does not depend on the size of the partition $S_A \sim S_B \sim 2\log(2)$

The entanglement entropy of a gaped 2d model

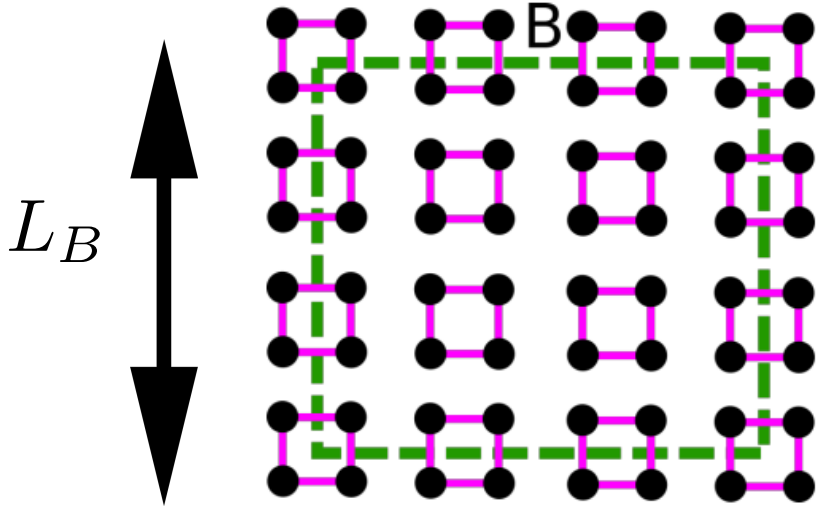
Let us consider the analogous Heisenberg model dimerized in 2D $H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Partition A



$S_B > S_A$

Partition B

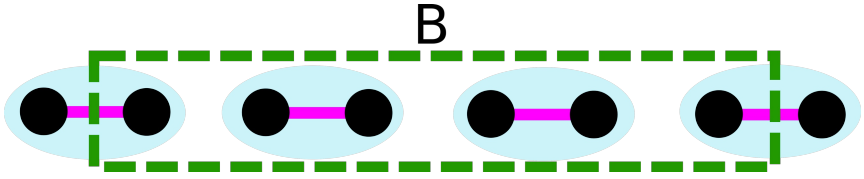


$S_A \sim L_A \sim \partial A$

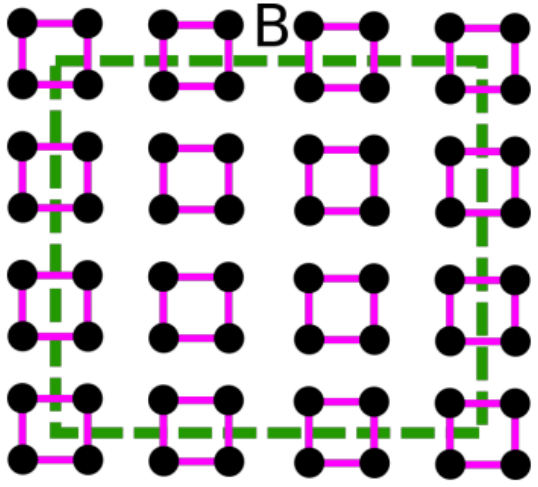
$S_B \sim L_B \sim \partial B$

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

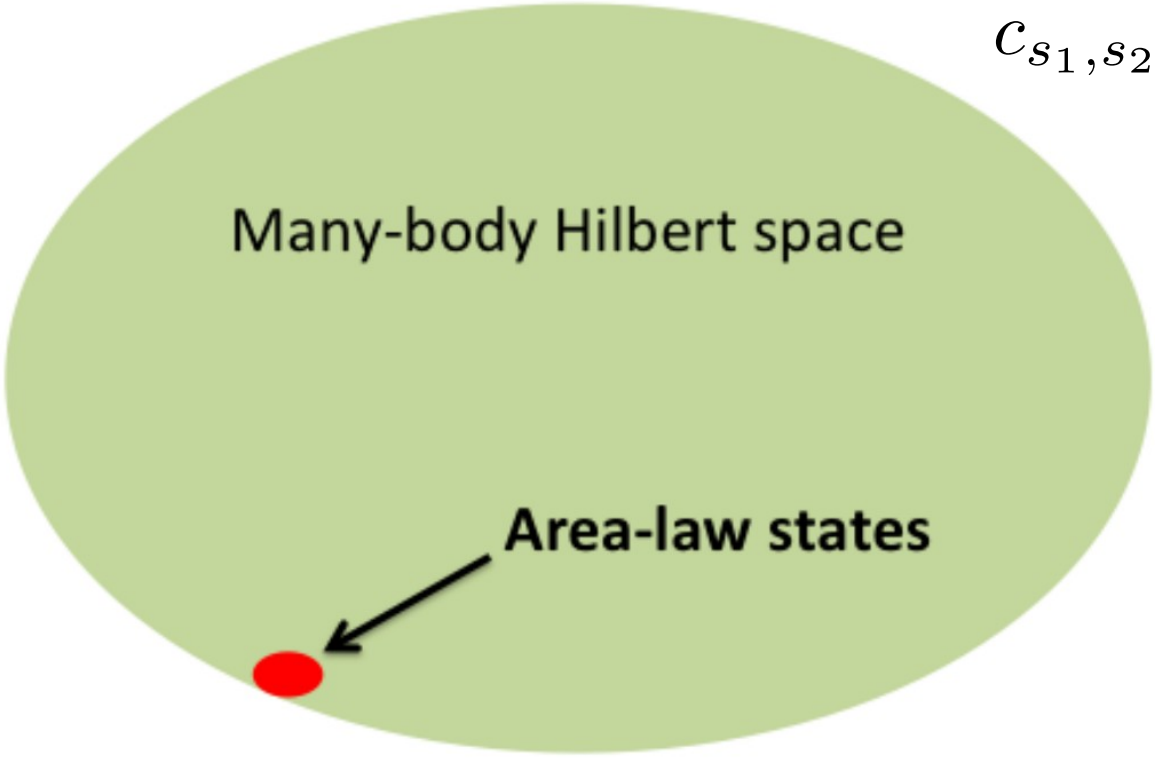


In 2D, it grows linearly with the size of the subsystem

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

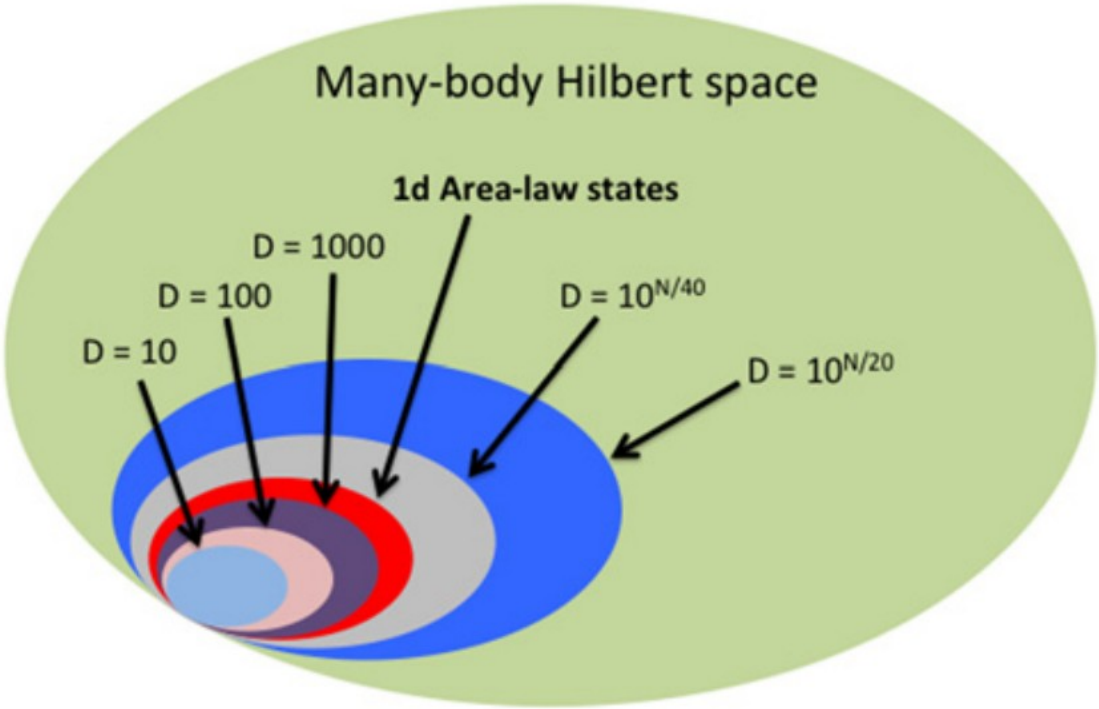
$$S_A \sim \log(m)$$

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?

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

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

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

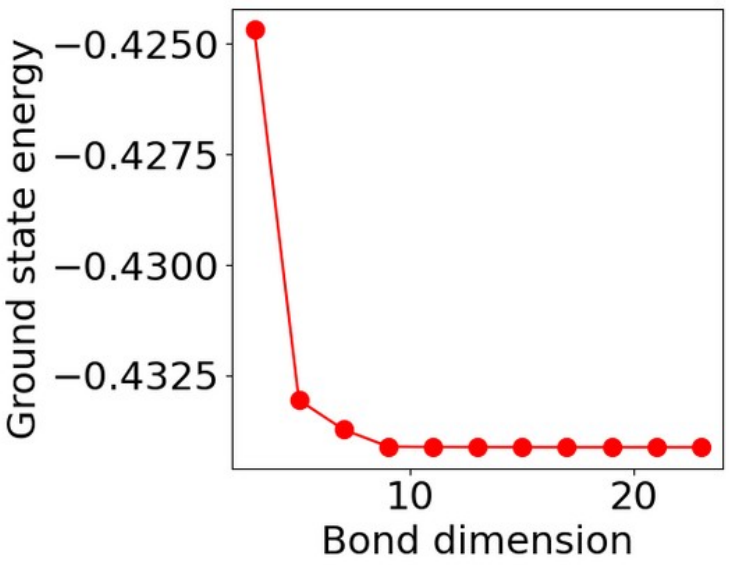
A non-zero fluctuation means that the variational state has some mixing with an excited state

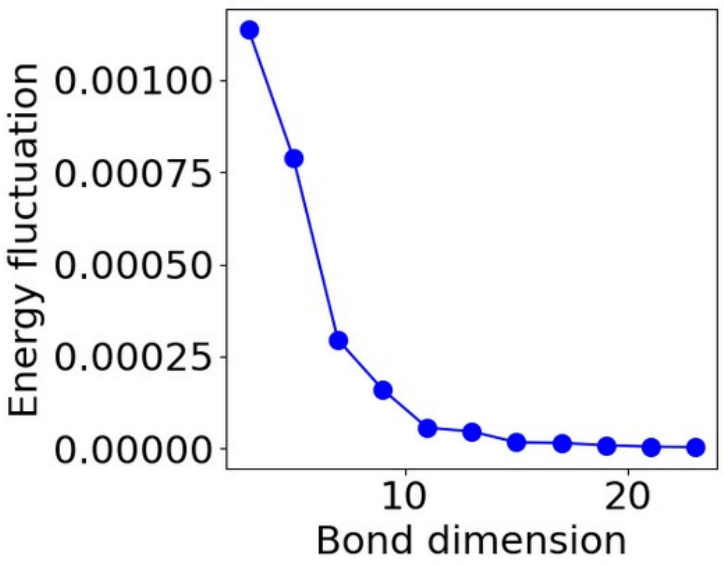
The importance of the bond dimension, ground state

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

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



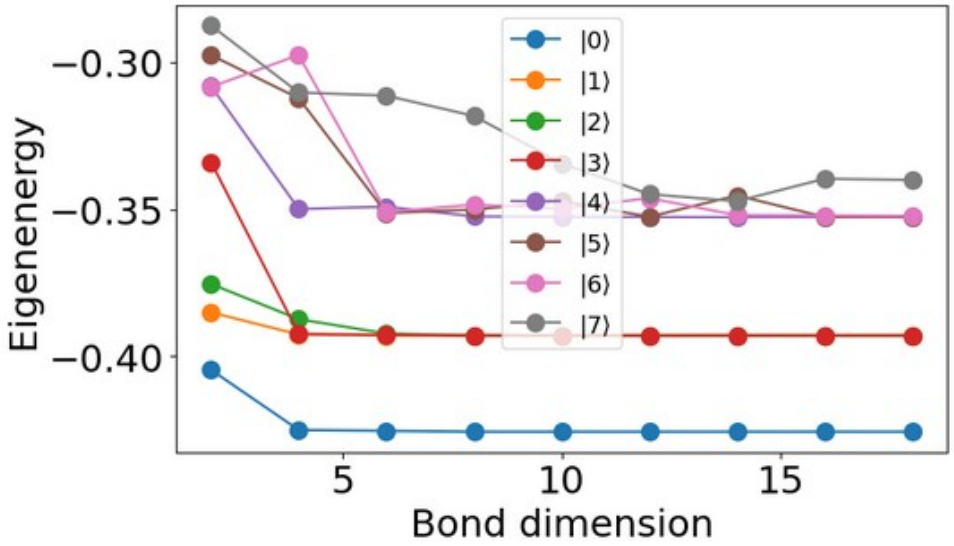


The importance of the bond dimension, excited states

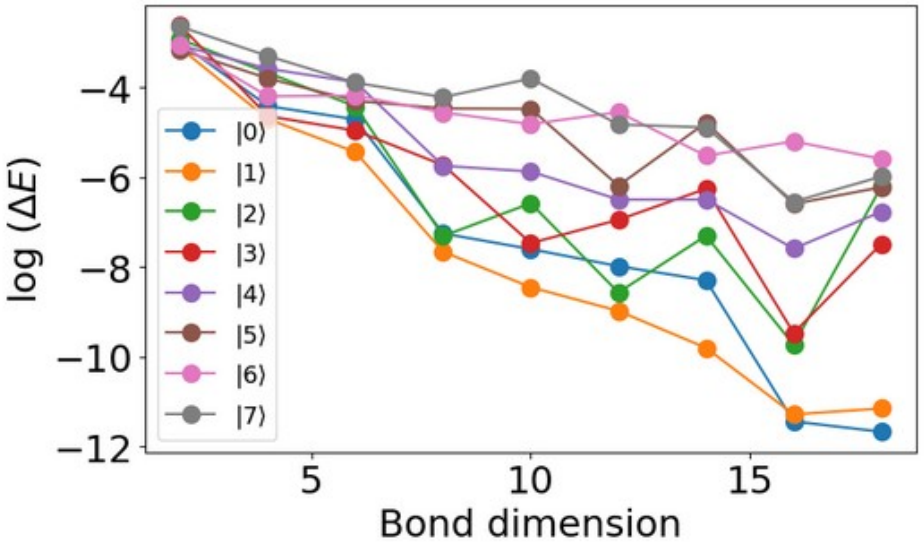
We will now look at excited states $H = \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$

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

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



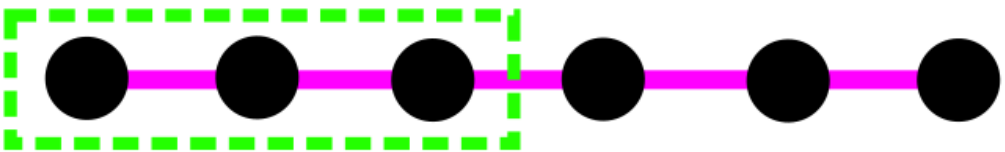
$\sqrt{\langle n|H^2|n\rangle - (\langle n|H|n\rangle)^2}$



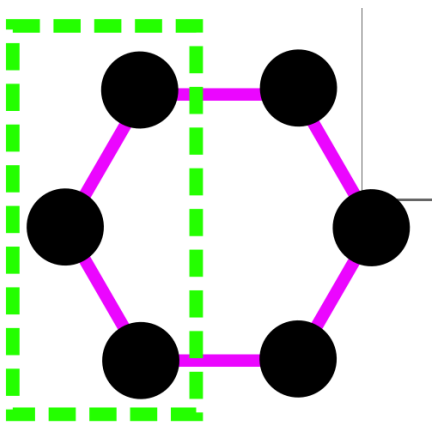
The importance of the boundary conditions in the entropy

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

Open boundary conditions



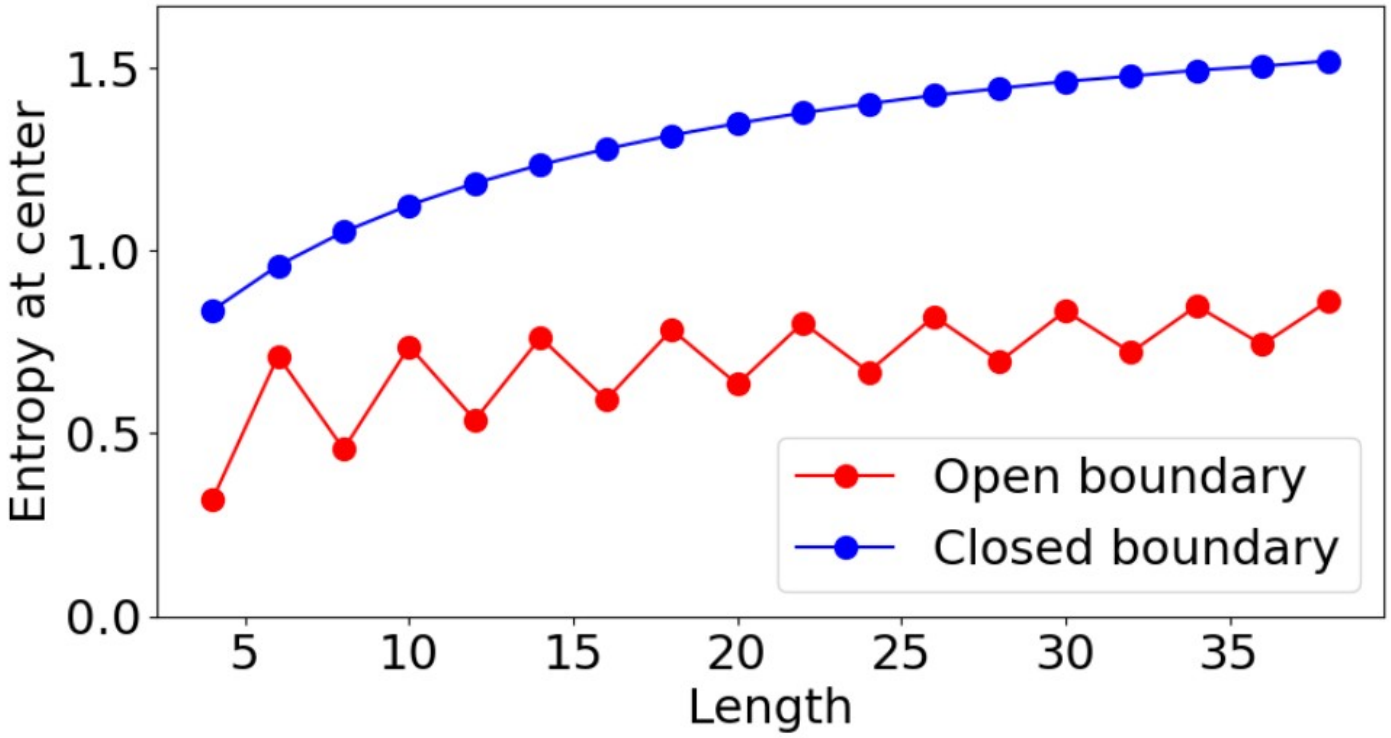
Closed boundary conditions



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

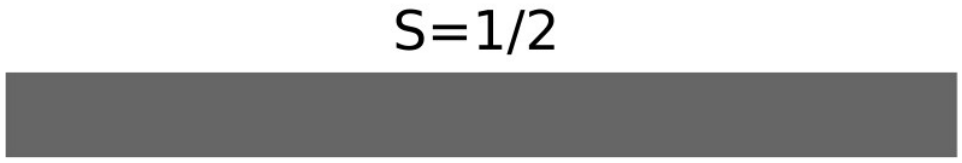
When considering a Heisenberg model, we could use S=1/2 or S=1 operators

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

$S = 1/2$

Gapless quantum magnet

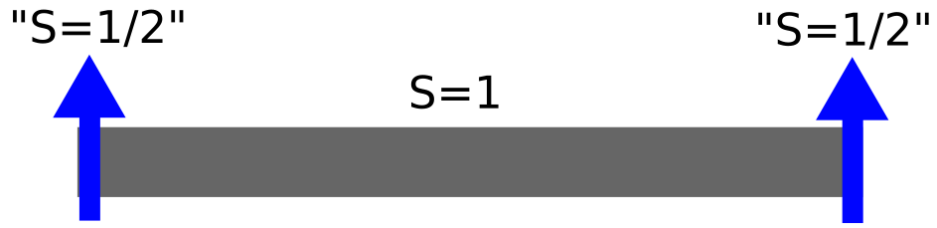
Gapless spinons



$S = 1$

Gapped quantum magnet

Topological fractional edge modes

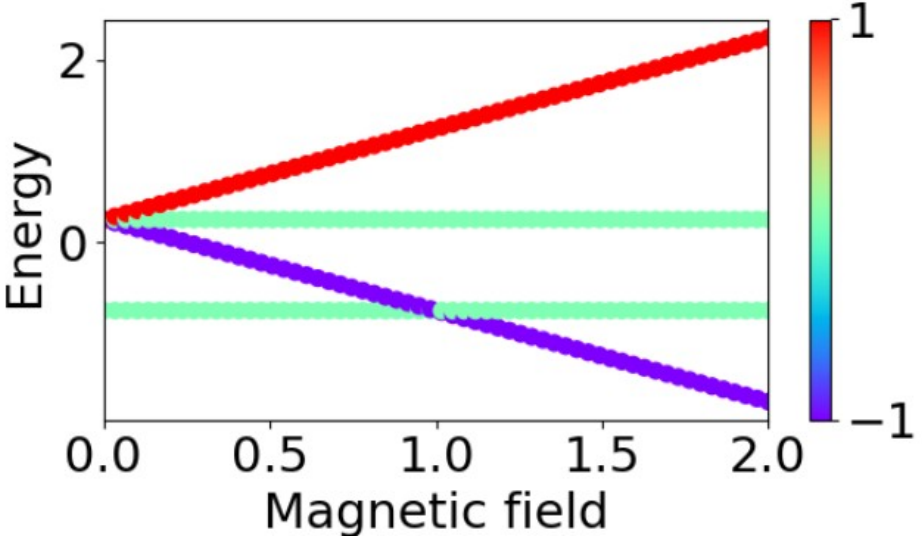


The gapless spectra of S=1/2

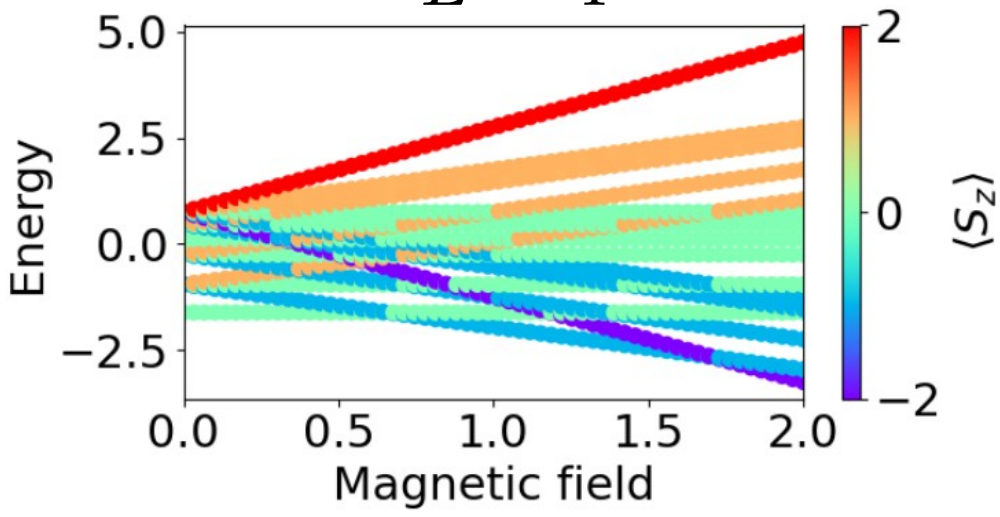
Let us look at the many-body spectra at finite field for $S = 1/2$

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

$L = 2$



$L = 4$



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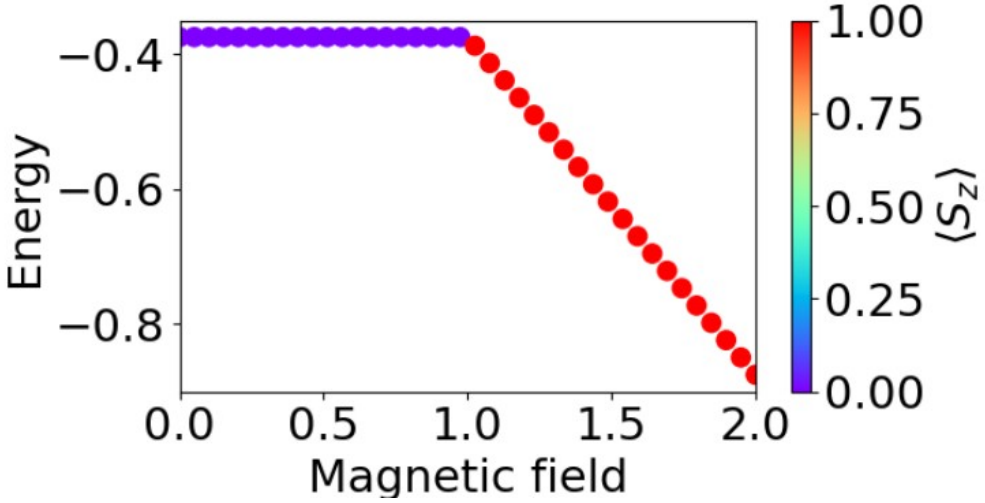
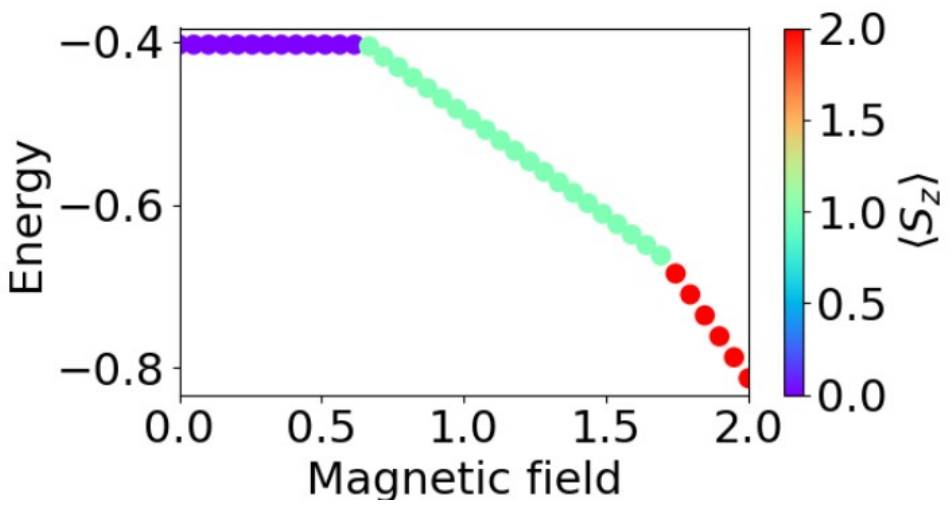


$L = 4$

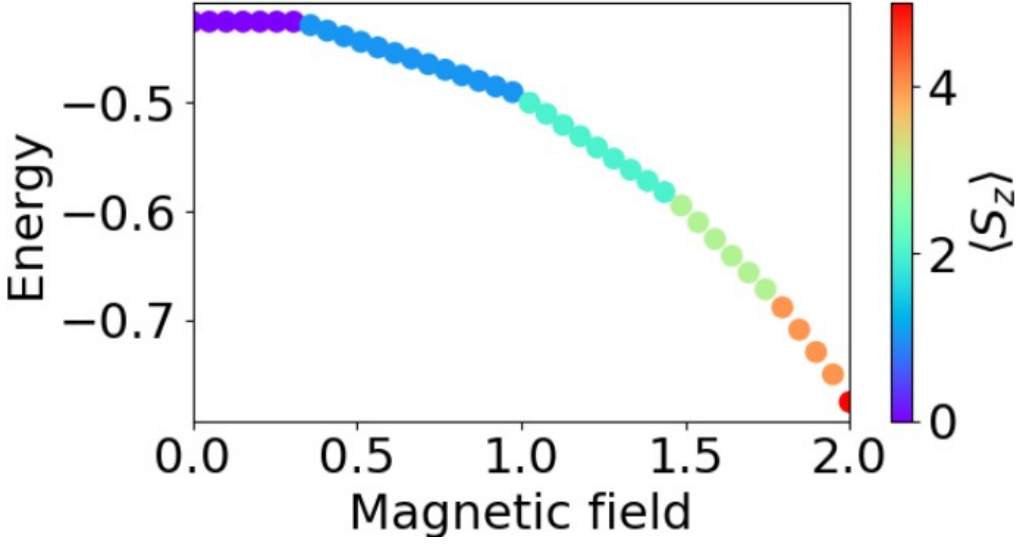


The gapless spectra of S=1/2

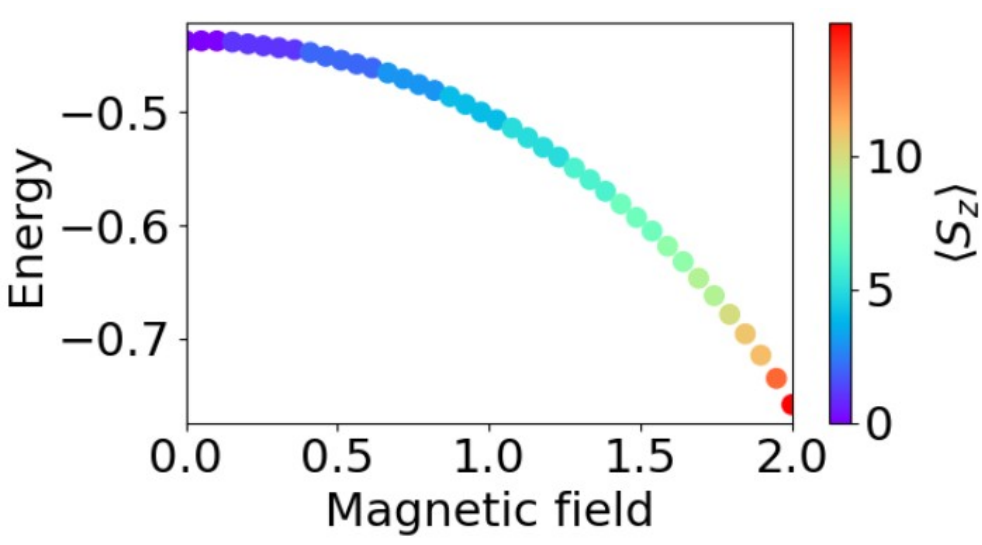
Let us look at the many-body spectra at finite field for $S = 1/2$

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

$L = 10$



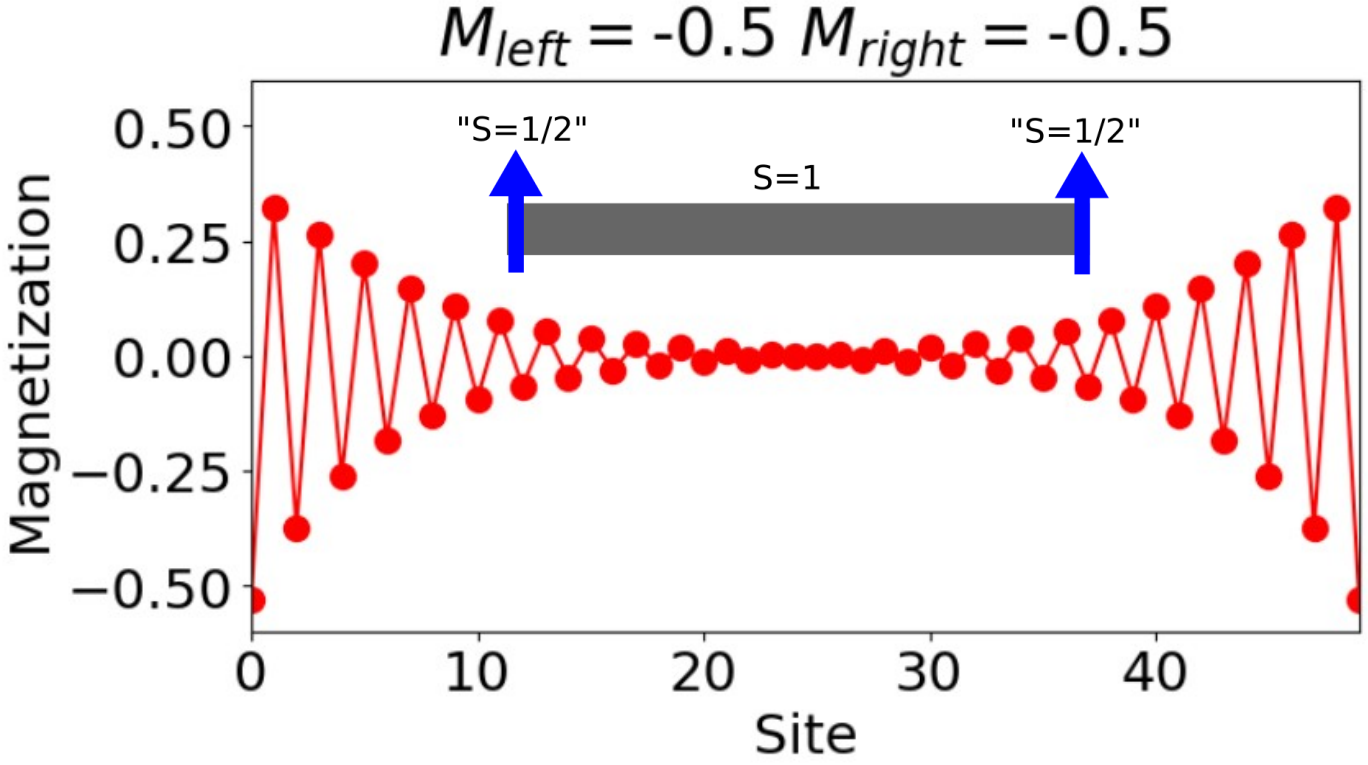
$L = 30$



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

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

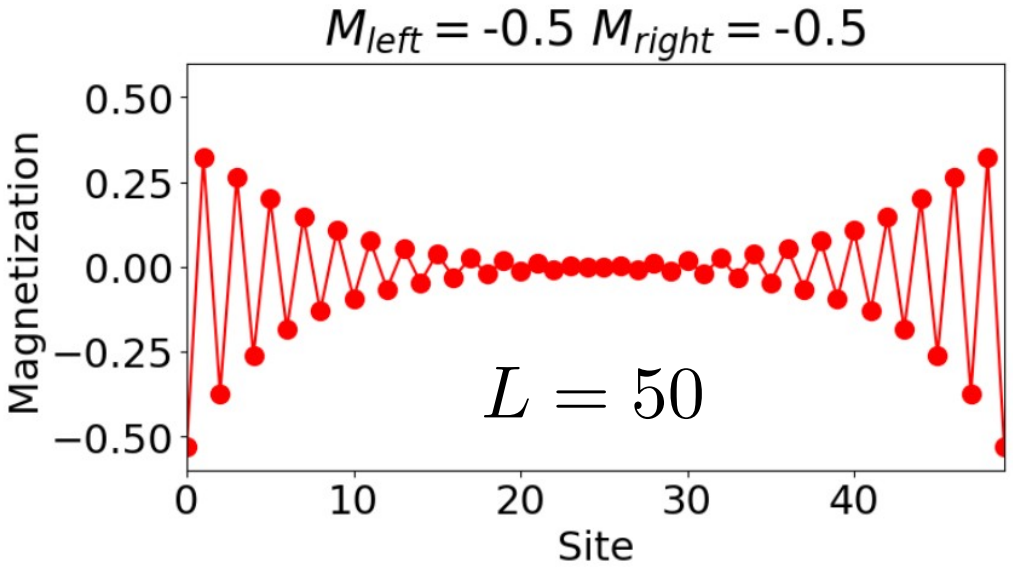
$S = 1$

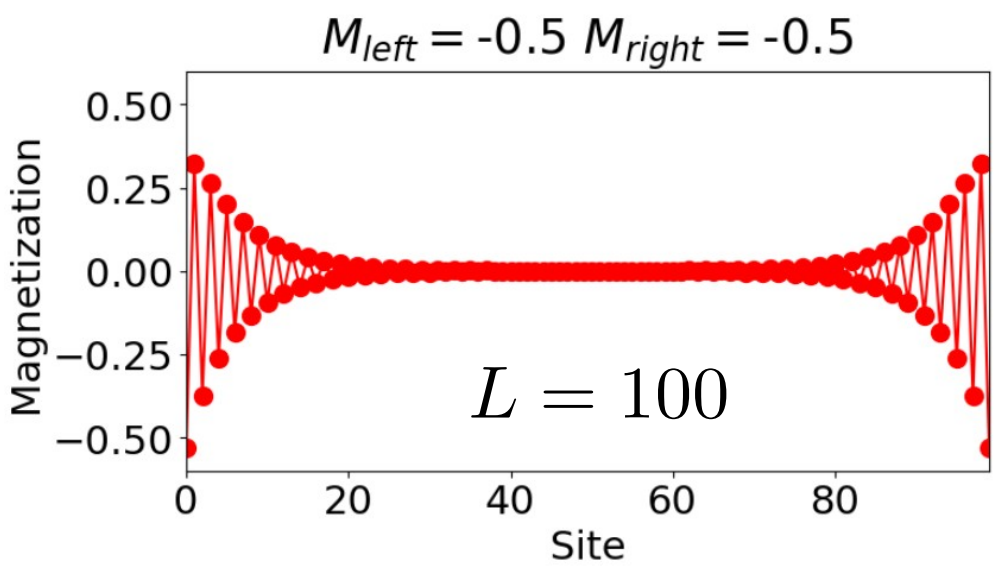


Emergent fractional S=1/2 in the Heisenberg S=1 chain

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

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

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

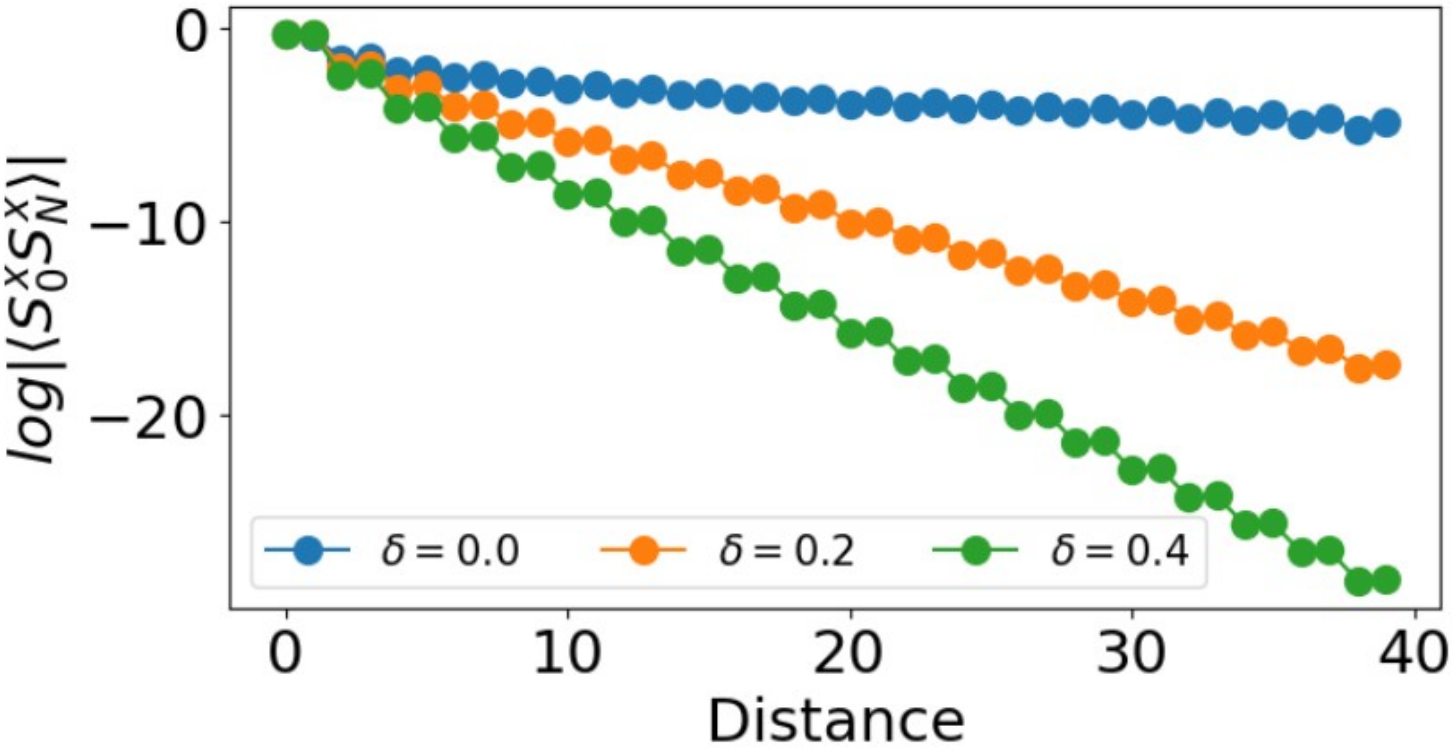
Gapless spectrum

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

Gapped spectrum

Non-local static correlators

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



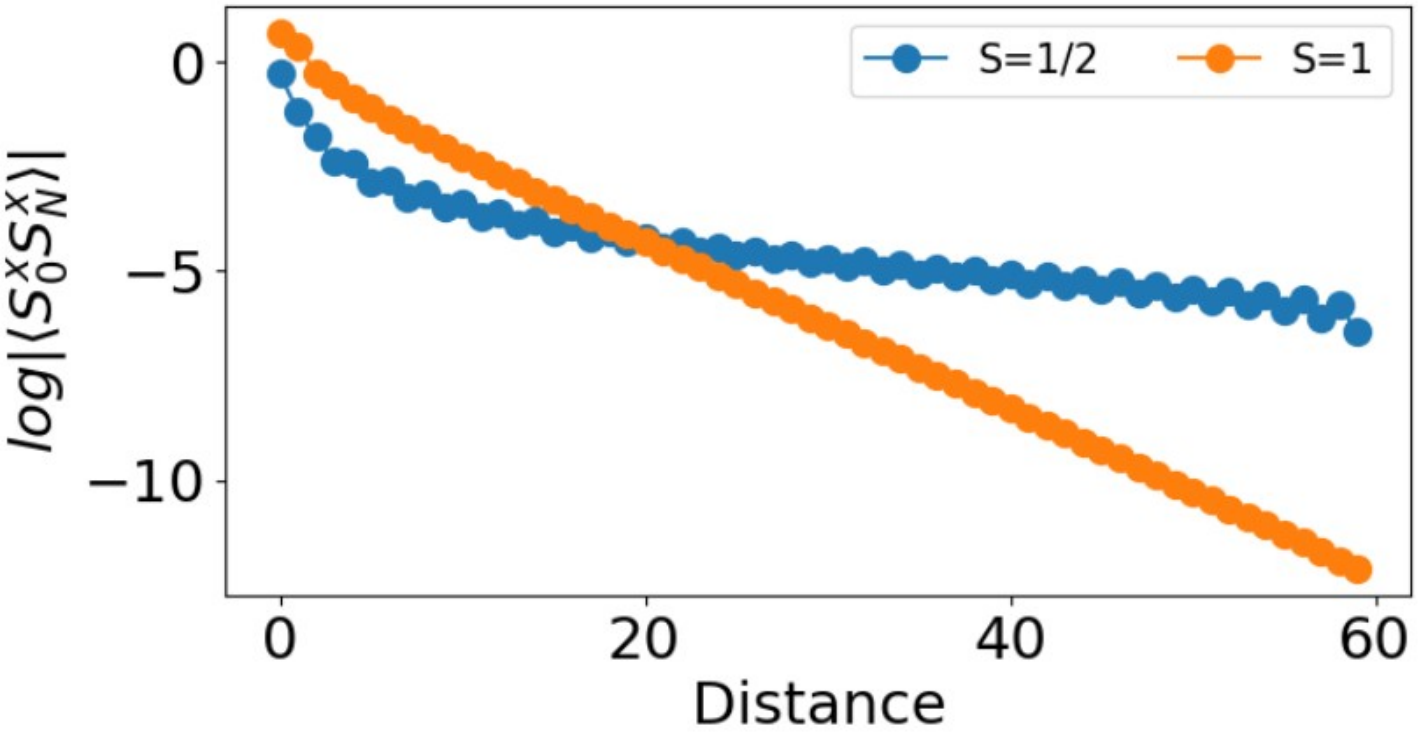
$\chi_{ij} \sim 1/|r_i - r_j|$

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

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

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

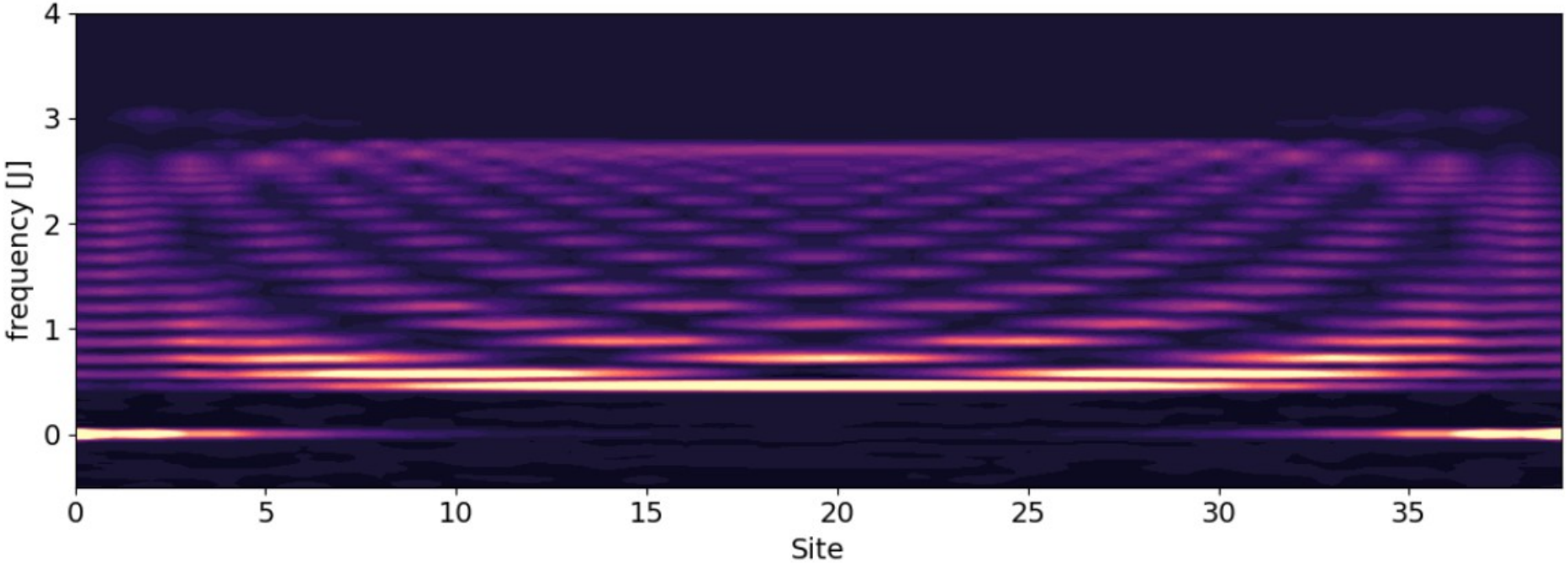
for $S = 1$

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

Gapped

Fractional edge modes from the dynamical correlator for S=1

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



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

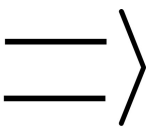
Many-body fermionic models

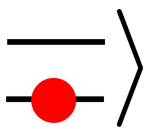
The fermionic many-body dimer

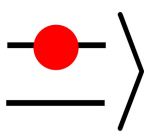
Let us take a minimal interacting fermionic Hamiltonian with 2 sites

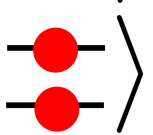
$$H = c_0^\dagger c_1 + c_1^\dagger c_0 + V c_0^\dagger c_0 c_1^\dagger c_1$$

The different many-body states are

$|\Omega\rangle =$  The "vacuum" state

$c_0^\dagger|\Omega\rangle =$  One particle in level #0

$c_1^\dagger|\Omega\rangle =$  One particle in level #1

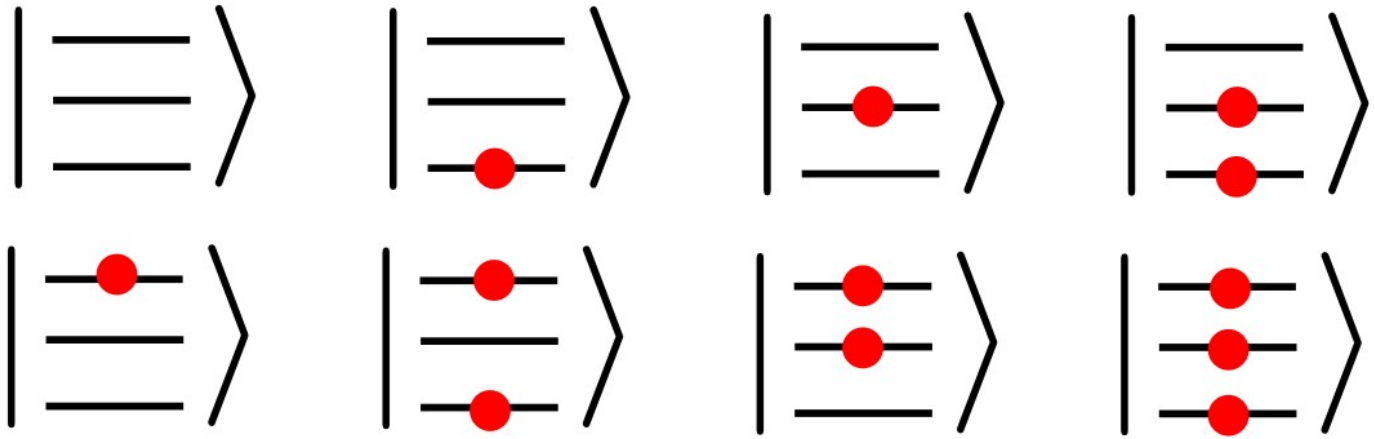
$c_0^\dagger c_1^\dagger|\Omega\rangle =$  Two particles in level #0 & #1

The fermionic many-body dimer

Let us take a minimal interacting fermionic Hamiltonian with 3 sites

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$$

The different many-body states are



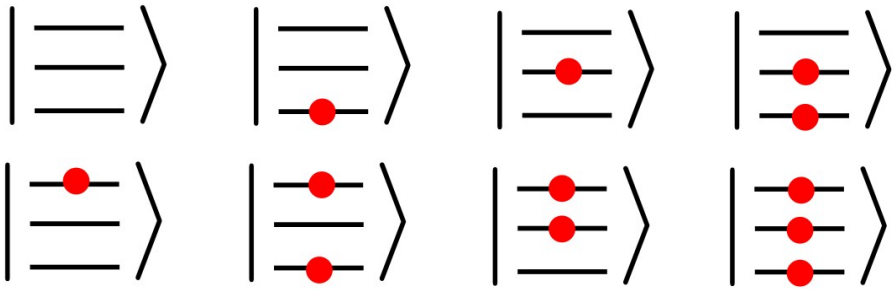
The fermionic quantum many-body problem

For a fermionic many-body problem with L sites

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$$

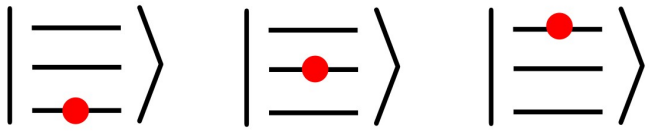
The dimension of the full Hilbert space grows as

$$d = 2^L$$



The dimension of the single particle space grows as

$$d = L$$



The fermionic quantum many-body problem

For an interacting fermionic many-body problem

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$$

A typical wavefunction is written as

$$|\Psi\rangle = \sum c_{n_1,n_2,\ldots,n_L} |n_1, n_2, \ldots n_L\rangle$$

We need to determine in total 2^L coefficients

The Hamiltonian is a $2^L \times 2^L$ matrix

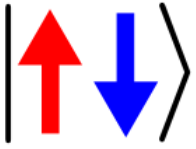
Fermionic sites and spins

Spinful fermions

fully empty

down electron

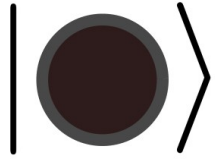
up electron



fully filled

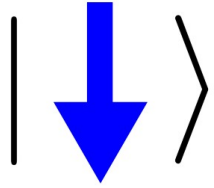
Spinless fermions

empty

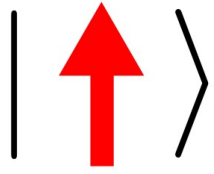


filled

Spins



down



up

Fermionic and spin many-body-Hamiltonians

We can have two types of many-body Hamiltonians

Many-body fermionic Hamiltonians

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$$

Many-body spin Hamiltonians

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

Can we systematically map spin and fermionic Hamiltonians?

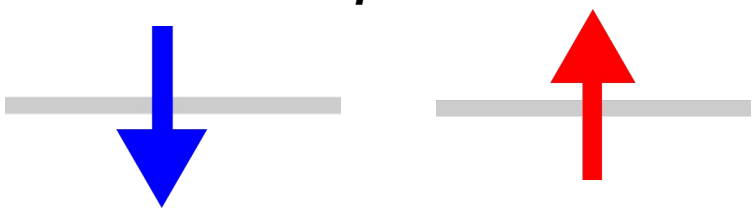
Fermionic and spin many-body-Hamiltonians

For a single site, the local Hilbert space is similar

Fermionic

empty full

Spin



down up

Leading to identifying the operators as $c^\dagger \sim S^+ \qquad c \sim S^-$

However, between different sites, fermionic operators anticommute, whereas spin commute

The right algebra can be recovered adding a properly chosen filling-dependent sign

The equivalence between fermionic and spin Hamiltonians

If we have a generic fermionic Hamiltonian, we can transform it into a spin Hamiltonian with

$$S_i^+ = c_i^\dagger e^{i\pi \sum_{i<j} c_j^\dagger c_j} \qquad S_i^- = c_i e^{-i\pi \sum_{i<j} c_j^\dagger c_j} \qquad S_i^z = c_i^\dagger c_i - \frac{1}{2}$$

Jordan-Wigner transformation

spin = fermion x string

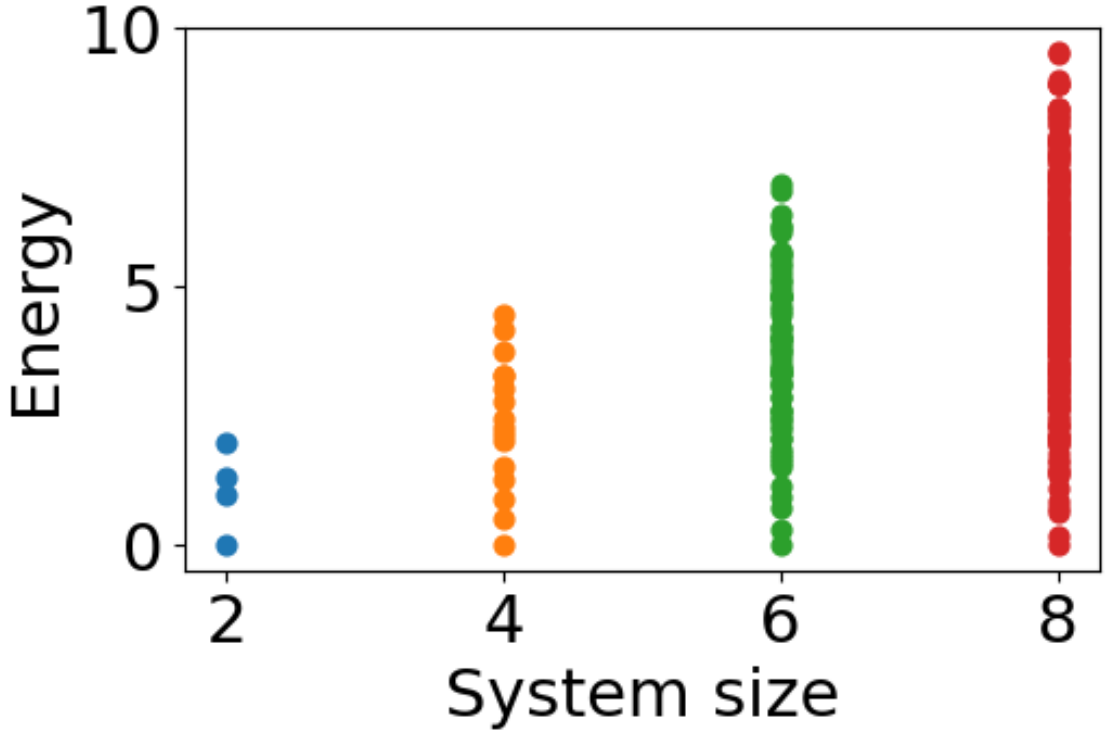
$$S_i^+ \qquad c_i^\dagger \qquad e^{-i\pi \sum_{i<j} c_j^\dagger c_j}$$

This transformation fulfills the algebraic relations of spins and fermions

In practice, we can solve a fermionic model by using a tensor network in the transformed spin model

Energies of a many-body fermionic model

Let us take a fermionic model $H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$



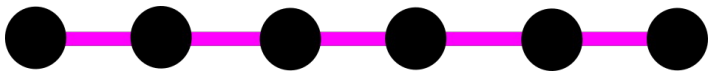
Quantum phase transition in a spinless fermionic model

Let us look at a minimal interacting fermionic model

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$

Two limiting cases

$V = 0$



Non-interacting chain (metal)

$V \to \infty$

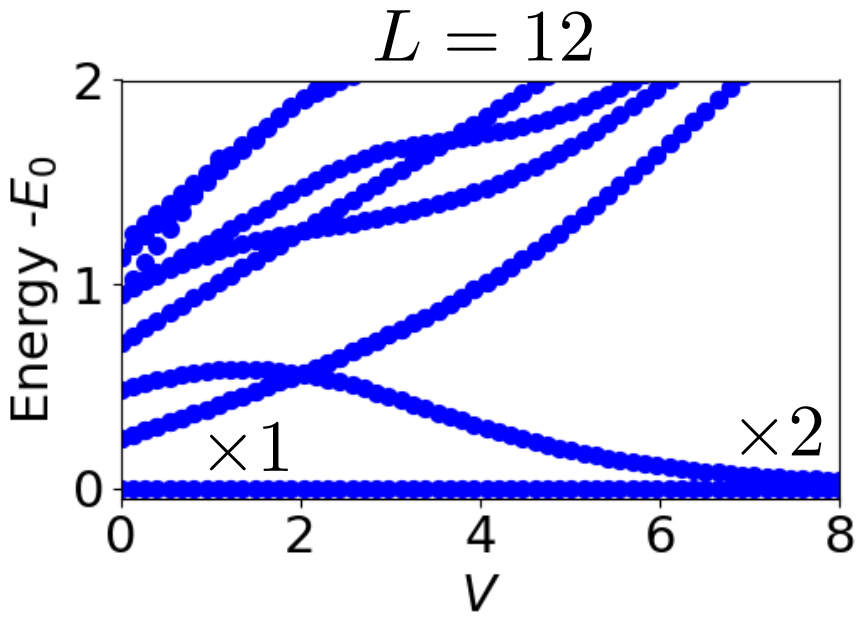
Charge density wave (insulator)

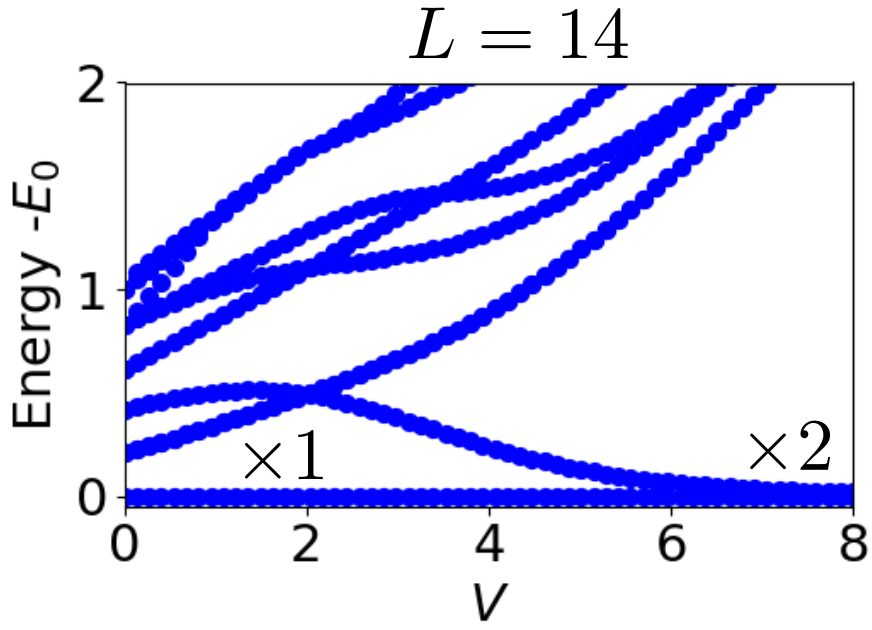
How can we observe such a phase transition?

From single particle to correlated fermions

Let us look at a minimal interacting fermionic model

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \tfrac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \tfrac{1}{2}\right)$$





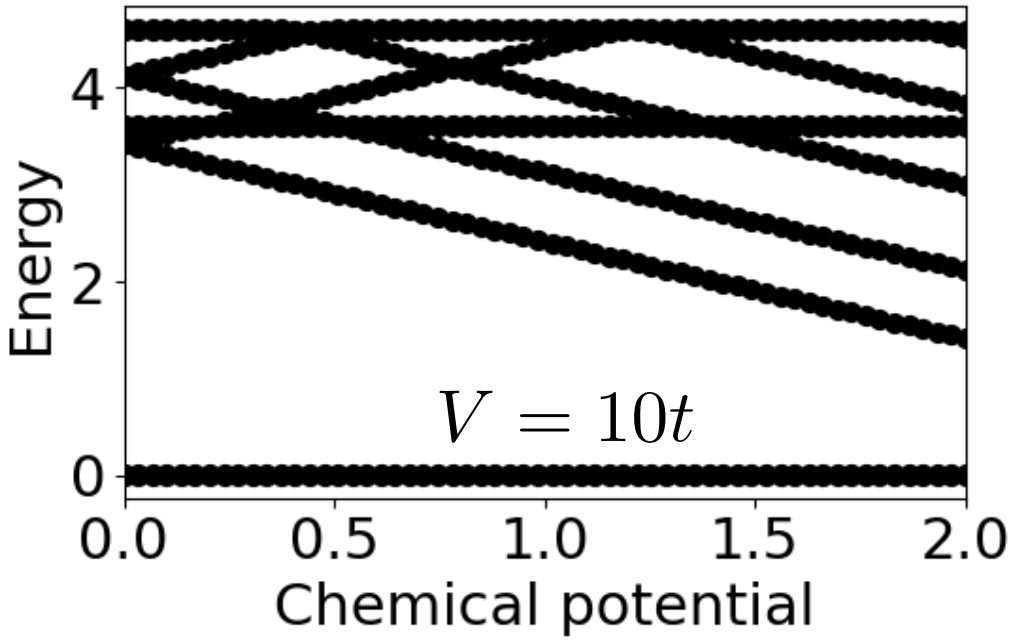
The chemical potential

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \tfrac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \tfrac{1}{2}\right) + \mu \sum_n c_n^\dagger c_n$$

Kinetic energy

Interaction

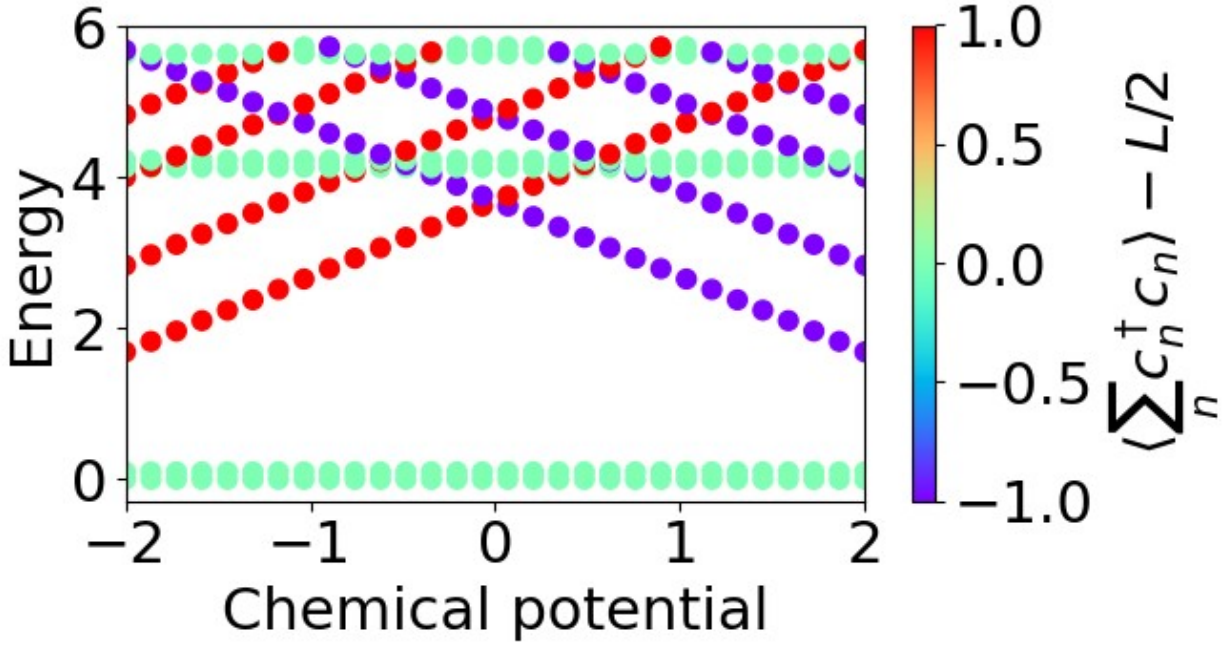
Chemical potential



The occupation number

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \tfrac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \tfrac{1}{2}\right) + \mu \sum_n c_n^\dagger c_n$$

Kinetic energy — Interaction — Chemical potential



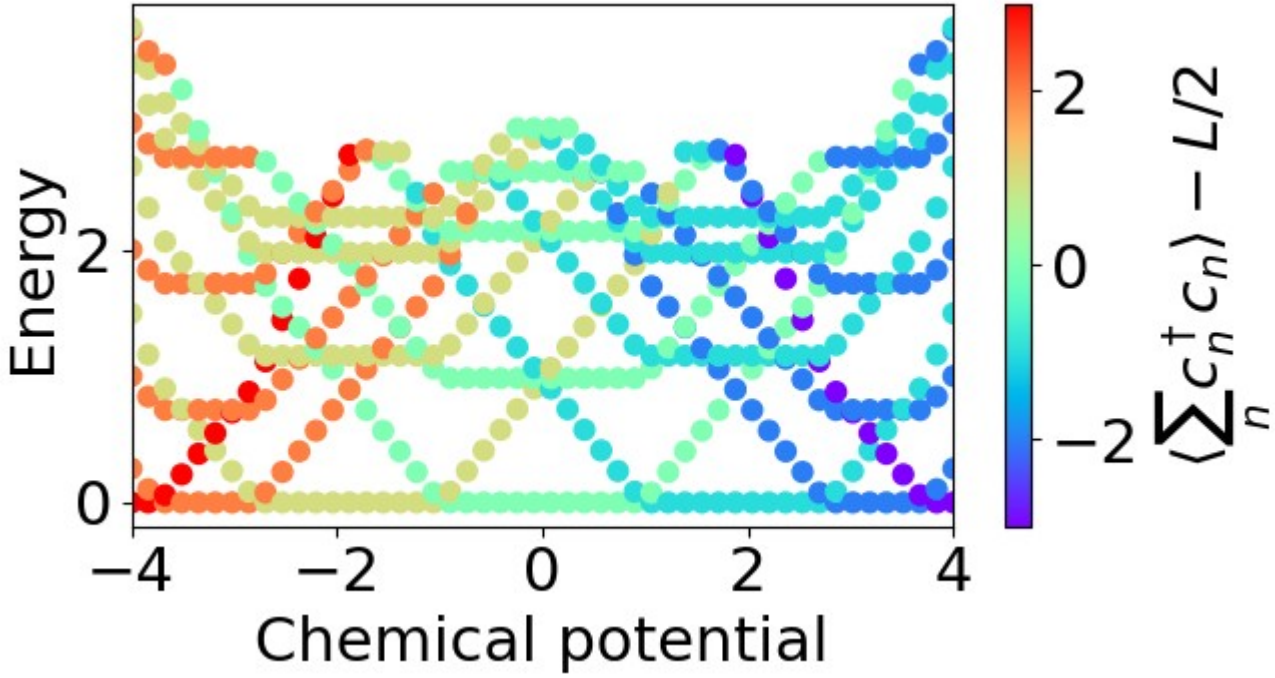
The number of electrons is given by

$$\sum_n \langle c_n^\dagger c_n \rangle$$

The occupation number

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \tfrac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \tfrac{1}{2}\right) + \mu \sum_n c_n^\dagger c_n$$

Kinetic energy — Interaction — Chemical potential



The number of electrons is given by

$$\sum_n \langle c_n^\dagger c_n \rangle$$

Electronic density as a function of the chemical potential

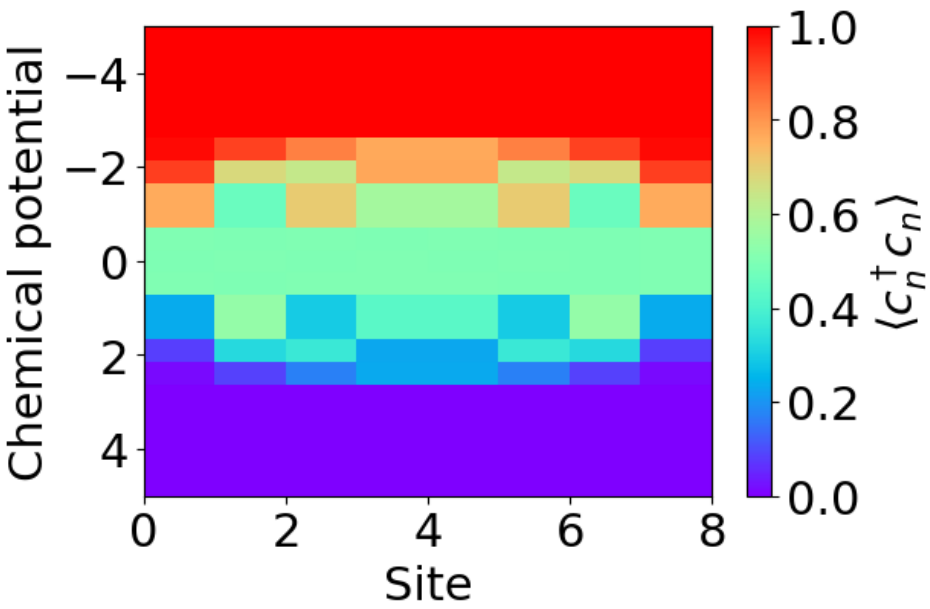
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \tfrac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \tfrac{1}{2}\right) + \mu \sum_n c_n^\dagger c_n$$

Kinetic energy

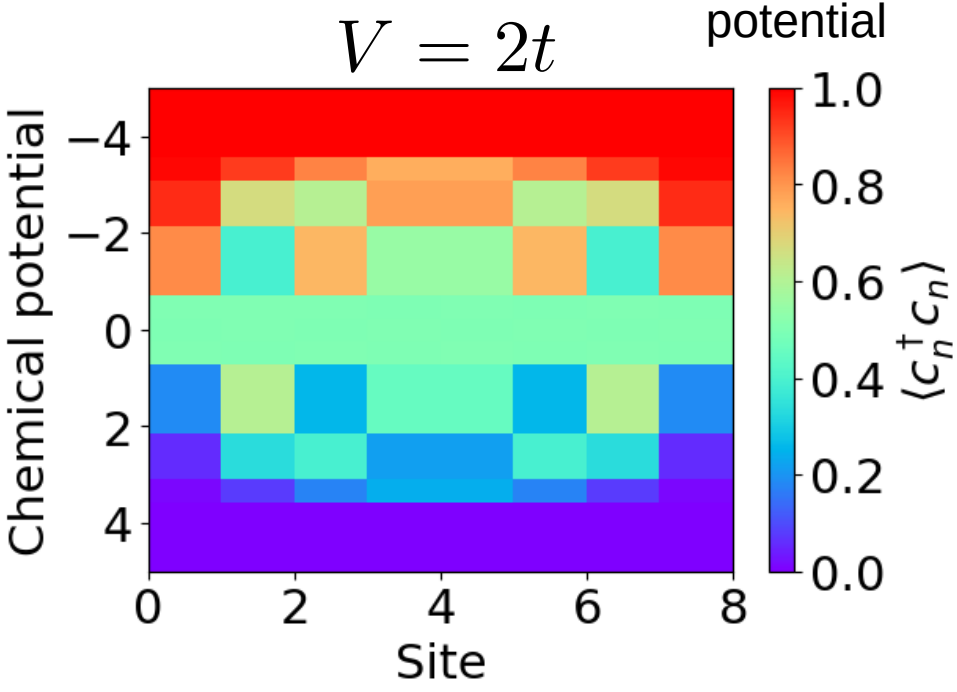
Interaction

Chemical potential

$V = t$



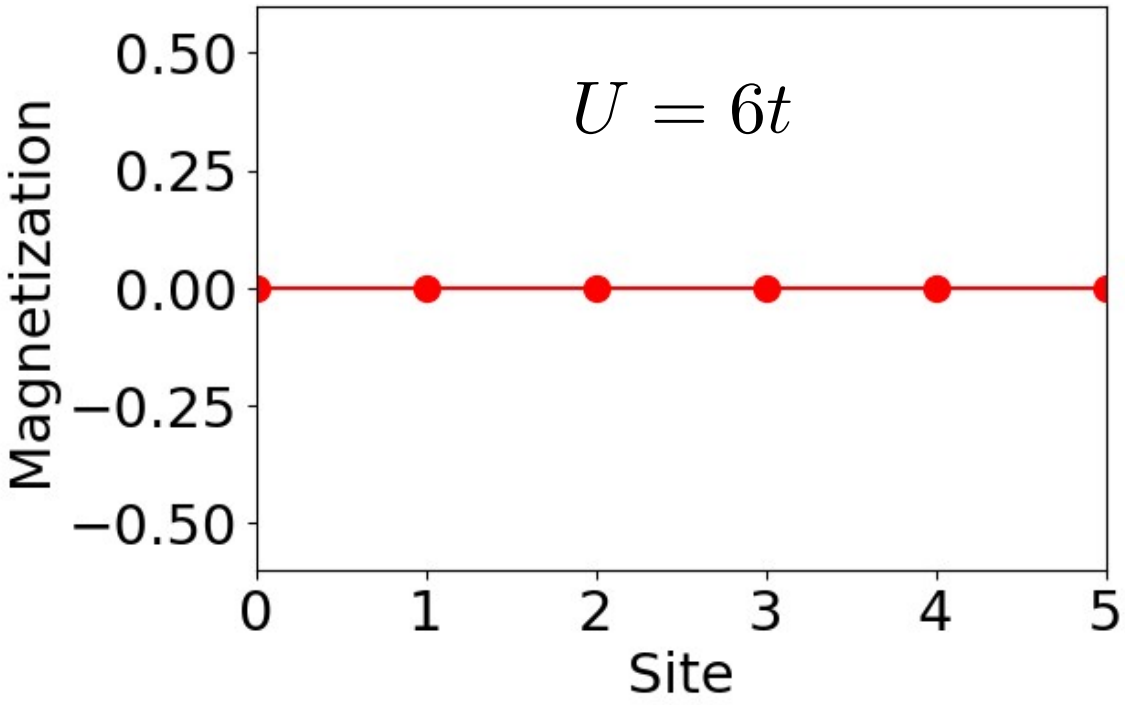
$V = 2t$



The many-body Hubbard model

The Hubbard model

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$$



The magnetization is given by

$$\langle S^z_n \rangle = \frac{1}{2}\sum_{s,s'} \sigma_{s,s'} \langle c^{\dagger}_{n,s} c_{n,s} \rangle$$

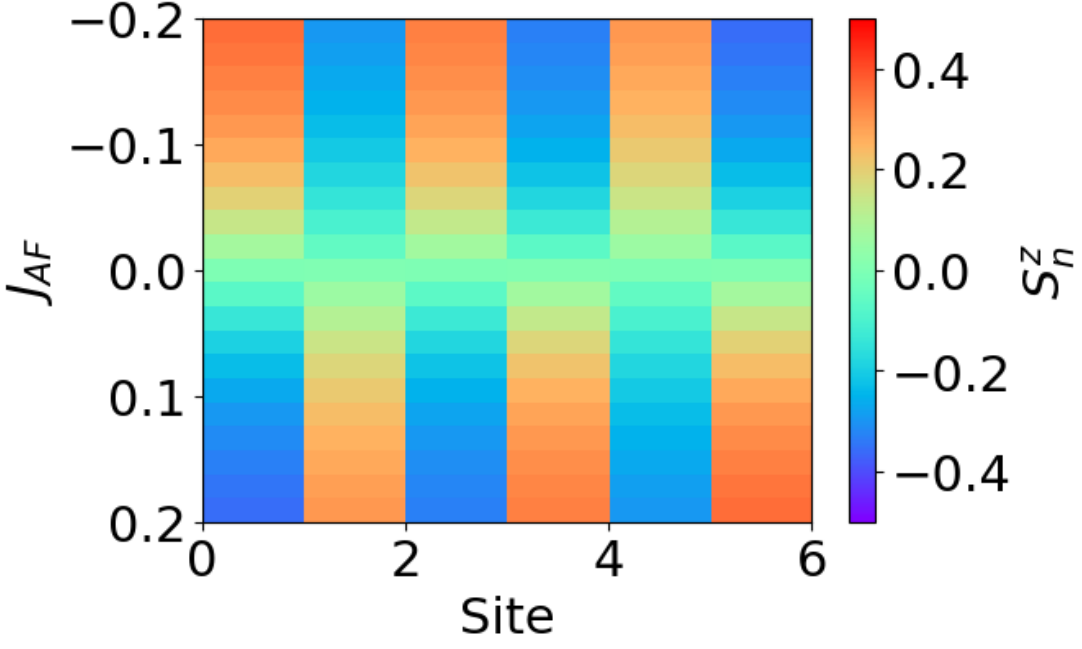
The Hubbard model, quantum and classical solution

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right) + \sum_{n,s,s'}(-1)^{n} J_{AF}\sigma^{z}_{s,s'}c^{\dagger}_{n,s}c^{\dagger}_{n,s'}$$

Kinetic energy

Many-body interaction

Mean-field stagger magnetization



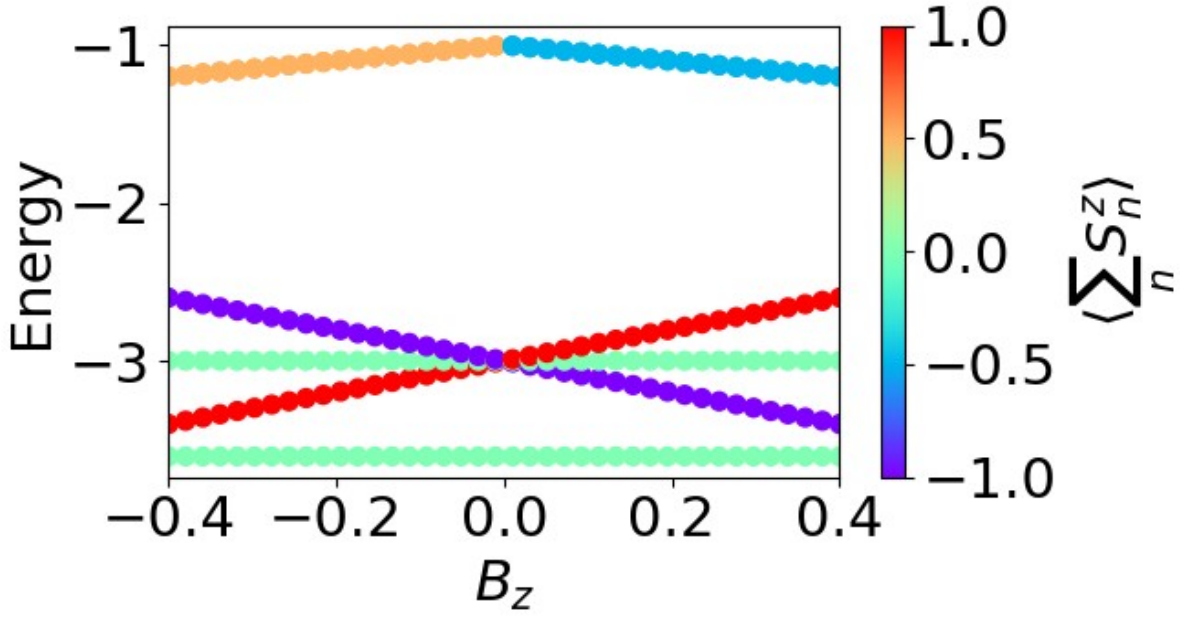
The magnetization is given by

$$\langle S^{z}_{n}\rangle = \frac{1}{2}\sum_{s,s'}\sigma_{s,s'}\langle c^{\dagger}_{n,s}c_{n,s}\rangle$$

The magnetization of the Hubbard dimer

We can now add an external field to split the many-body levels

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right) + B^{z}\sum_{n,s,s'}\frac{1}{2}\sigma_{s,s'}c^{\dagger}_{n,s}c_{n,s}$$

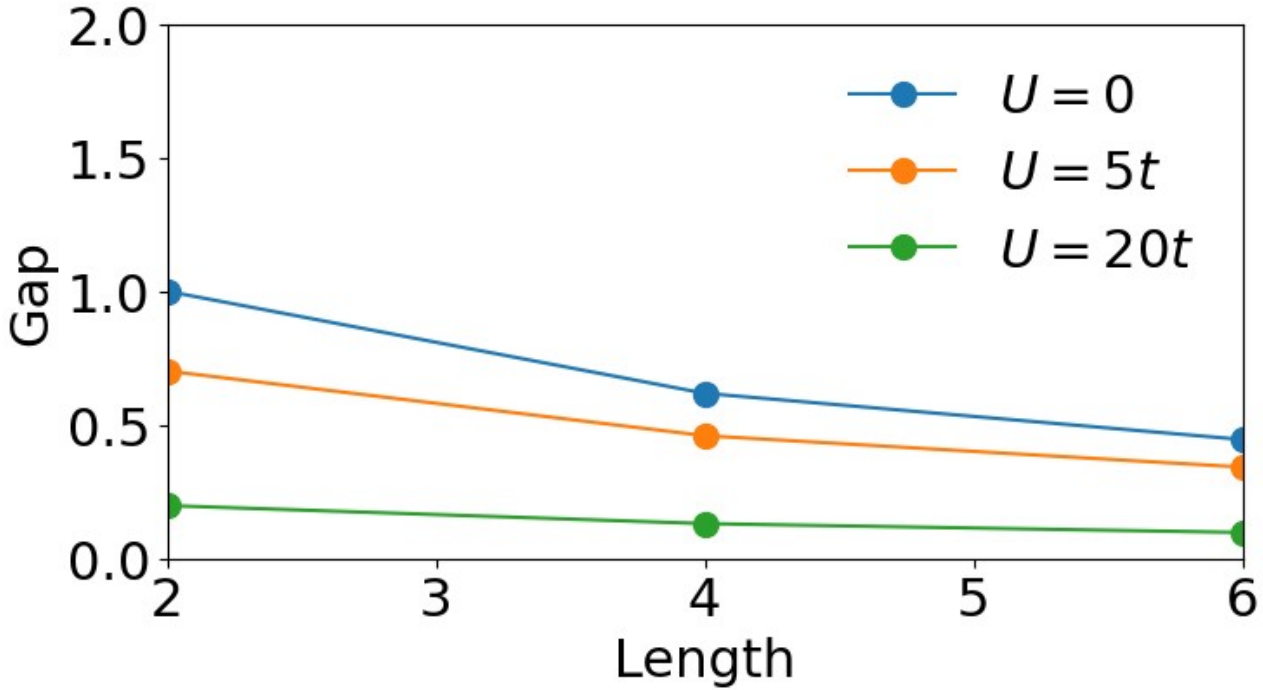


The magnetization is given by

$$\langle S^{z}_{n}\rangle = \frac{1}{2}\sum_{s,s'}\sigma_{s,s'}\langle c^{\dagger}_{n,s}c_{n,s}\rangle$$

The many-body gap in the Hubbard model

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$$



Particle-particle correlators

The non-local static particle-particle allows probing if a system is a metal or an insulator

$$\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$$

Two different types of decays are possible in the correlator

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

Metal

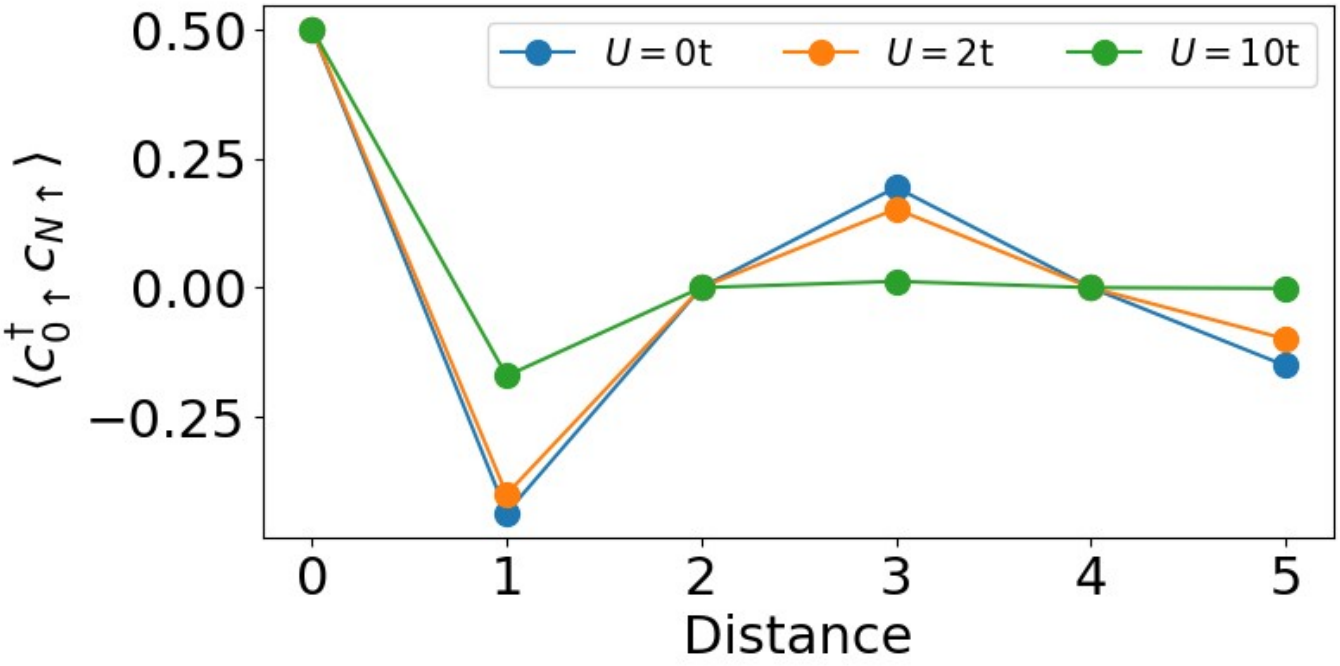
$\chi_{ij} \sim e^{-\lambda |r_i - r_j|}$

Insulator

Particle correlators in the Hubbard model

The particle-particle correlators reflect how metallic a system is

$$\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$$



Spin fluctuations in the Hubbard model

For a generic Hamiltonian in a generic lattice

$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

In the strongly correlated (half-filled) limit we obtain a Heisenberg model

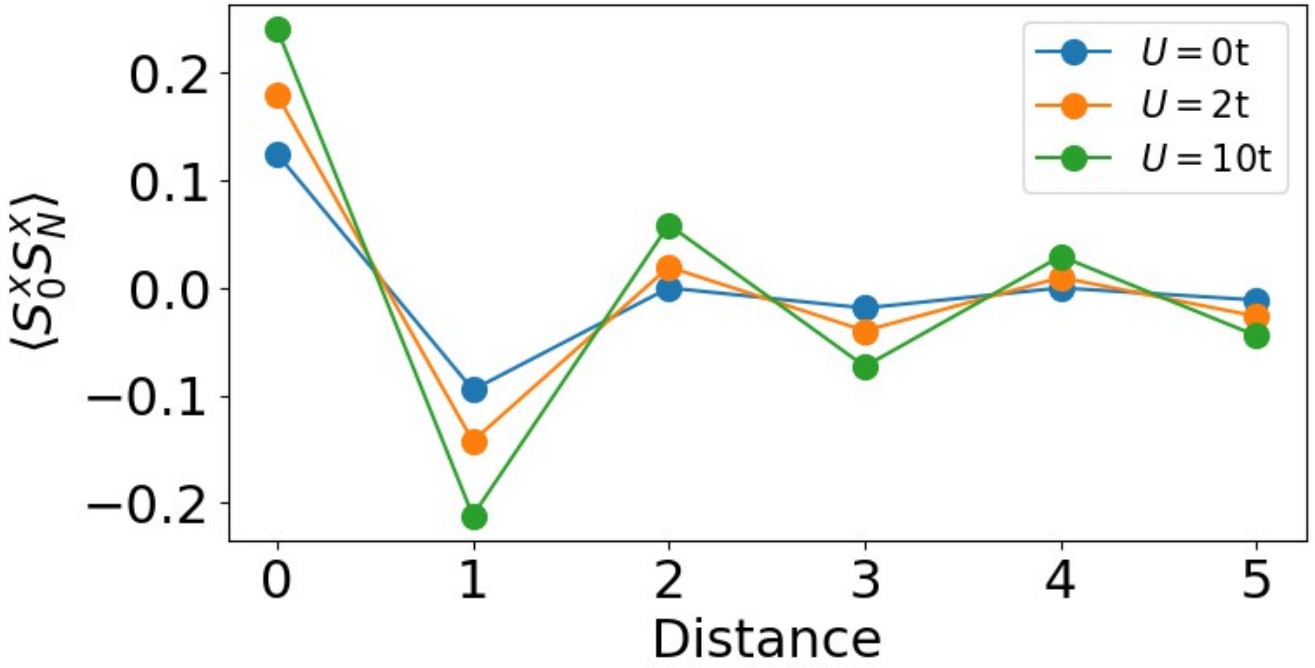
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$J_{ij} \sim \frac{|t_{ij}|^2}{U}$$

Spin-spin correlators in the Hubbard model

The spin-spin correlator reflects the magnetic fluctuations of the system

$$\Xi_{ij} = \langle S_i^x S_j^x \rangle$$



Dynamical correlators for spinful fermions

The many-body excitations of a fermionic Hamiltonian can be characterized by the dynamical correlator

The dynamical spin correlator (spin-excitations)

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

The dynamical particle correlator (charge-excitations)

$$D(\omega) = \langle GS | c_{n,\uparrow} \delta(\omega - H + E_{GS}) c^\dagger_{n,\uparrow} | GS \rangle$$

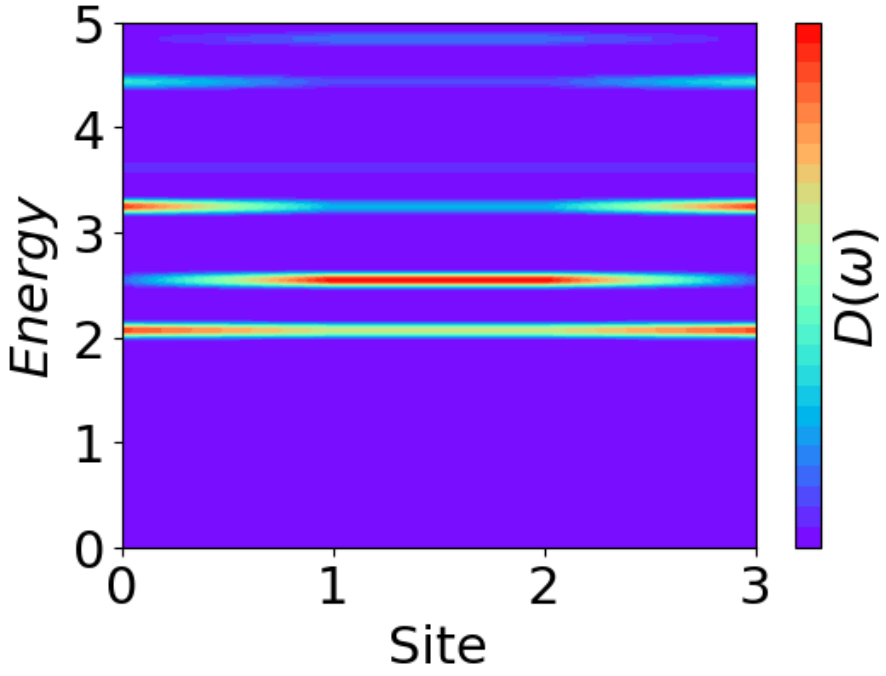
The spectral function above signal excited states that have one more spin excitation than the ground state

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

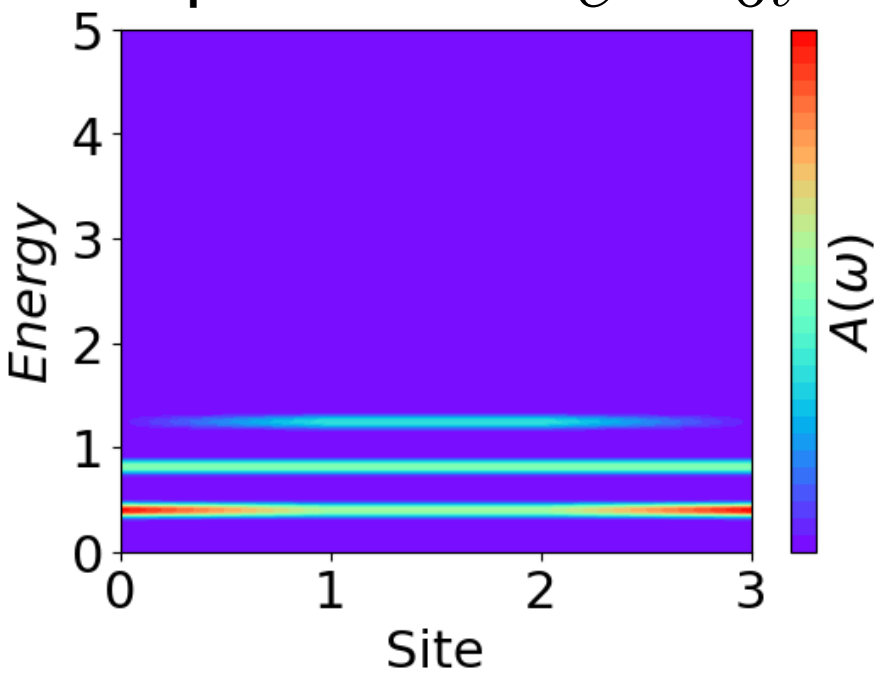
Dynamical correlators of the Hubbard model

$$H = t\sum_{s,n} c^{\dagger}_{n,s} c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$$

Charge correlator $U = 6t$

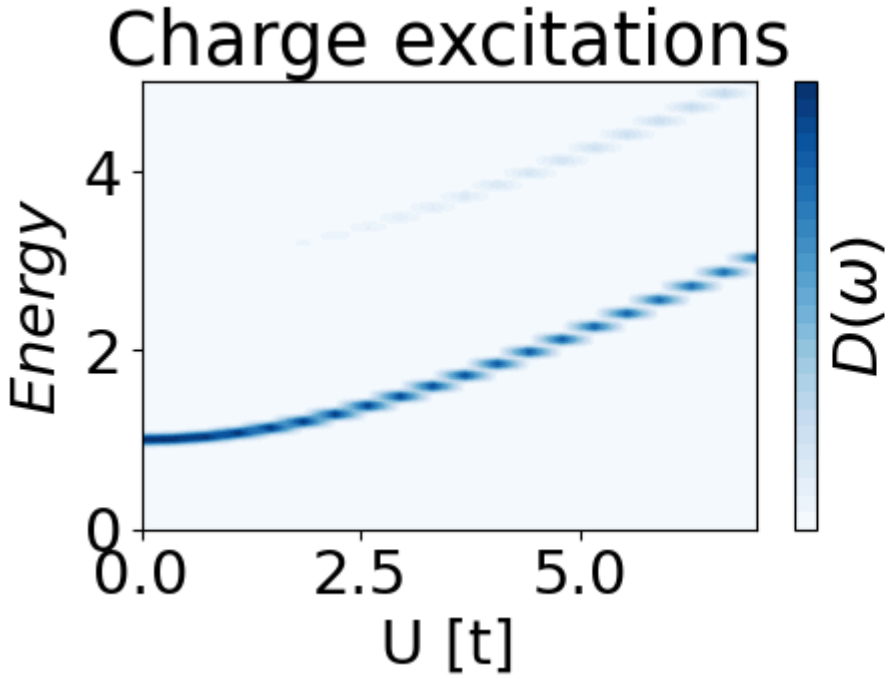


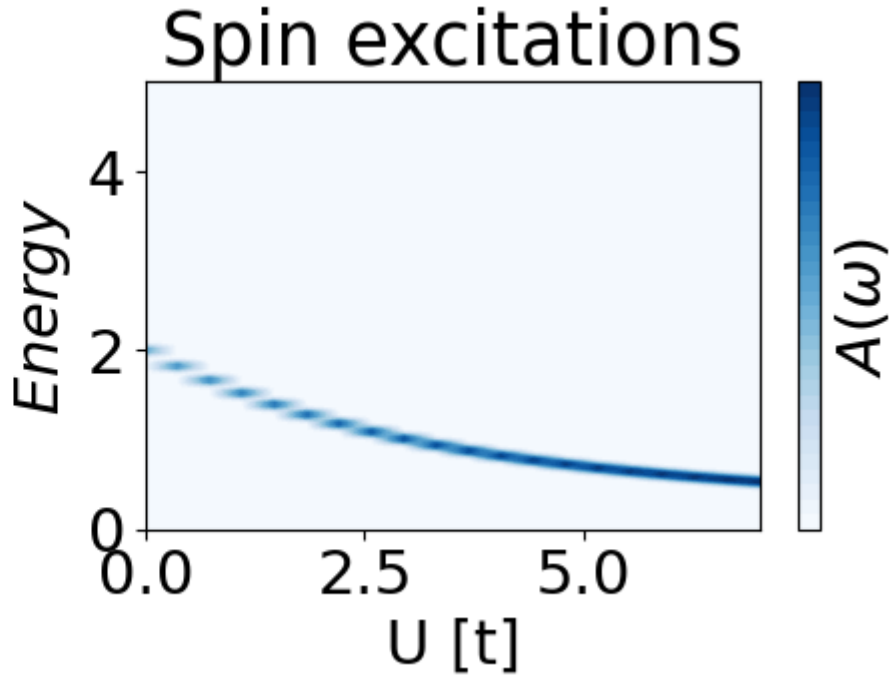
Spin correlator $U = 6t$



Dynamical correlators of the Hubbard model

$$H = t \sum_{s,n} c^{\dagger}_{n,s} c_{n+1,s} + h.c. + U \sum_{n} \left(c^{\dagger}_{n,\uparrow} c_{n,\uparrow} - \frac{1}{2} \right) \left(c^{\dagger}_{n,\downarrow} c_{n,\downarrow} - \frac{1}{2} \right)$$





Thermodynamic limit of many-body fermionic models

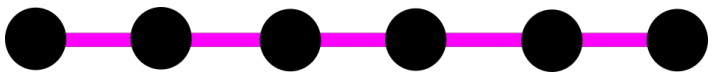
Quantum phase transition in a spinless fermionic model

Let us look at a minimal interacting fermionic model

$$\mathrm{H} = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$

Two limiting cases

$V = 0$



Non-interacting chain (metal)

$V \to \infty$

Charge density wave (insulator)

How can we observe such a phase transition?

Quantum phase transition in a spinless fermionic model

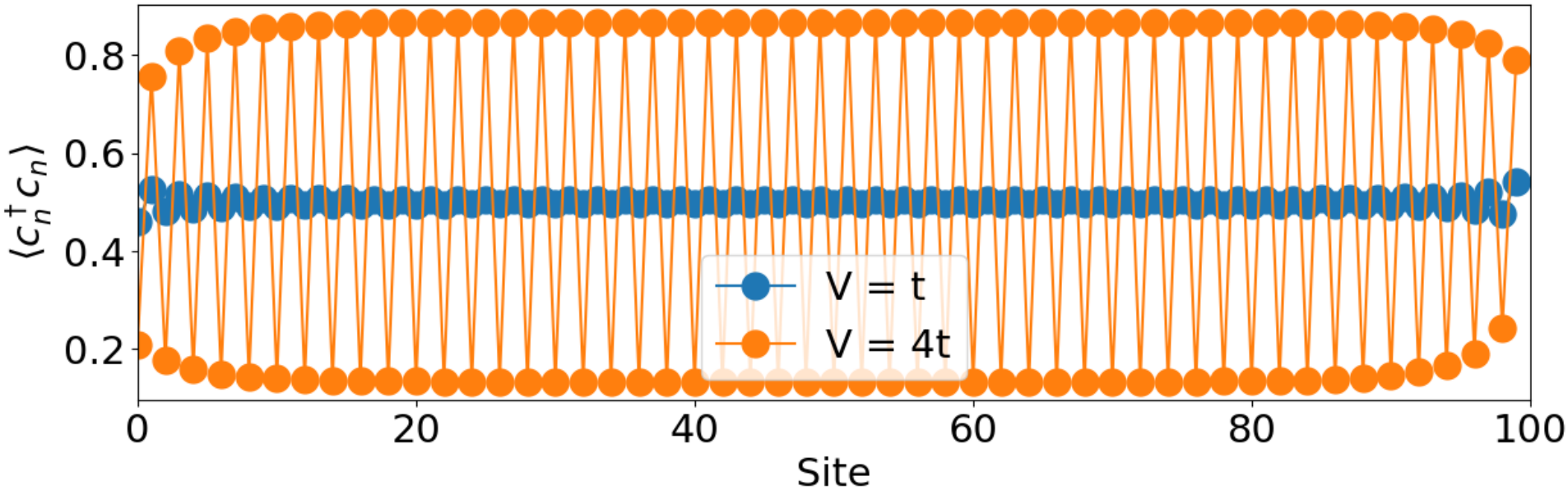
Let us modify the Hamiltonian to pin one the charge density waves

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right) + \lambda(c_1^\dagger c_1 - c_L^\dagger c_L)$$

Kinetic

Interaction

Pinning



Quantum phase transition in a spinless fermionic model

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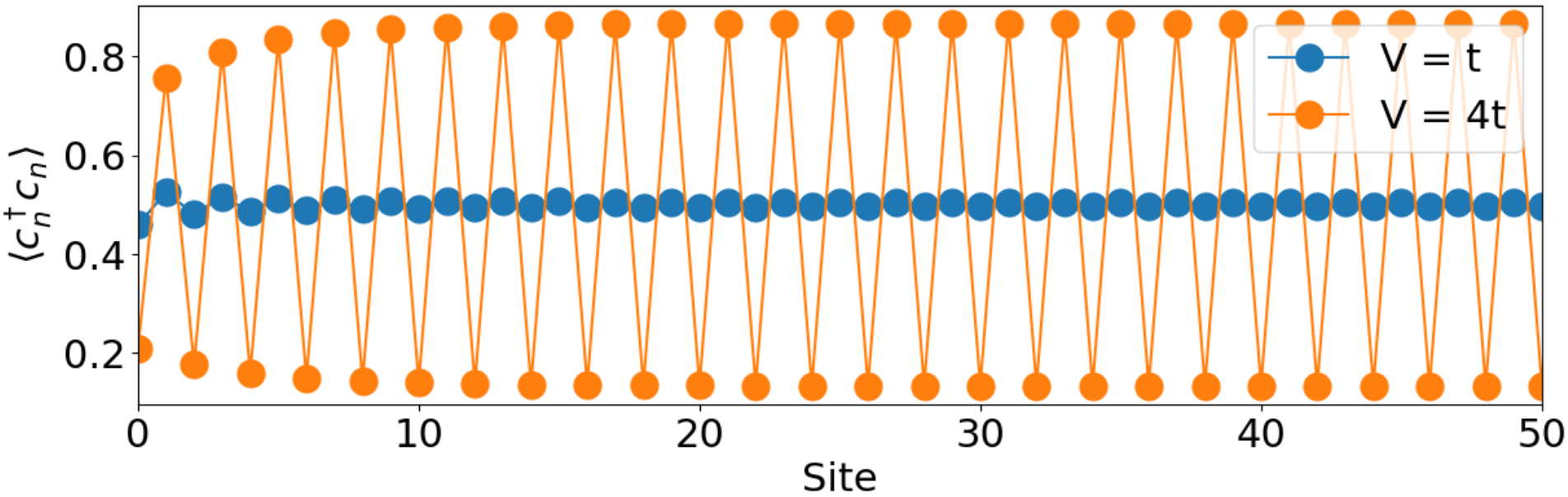
Kinetic

Interaction

Pinning



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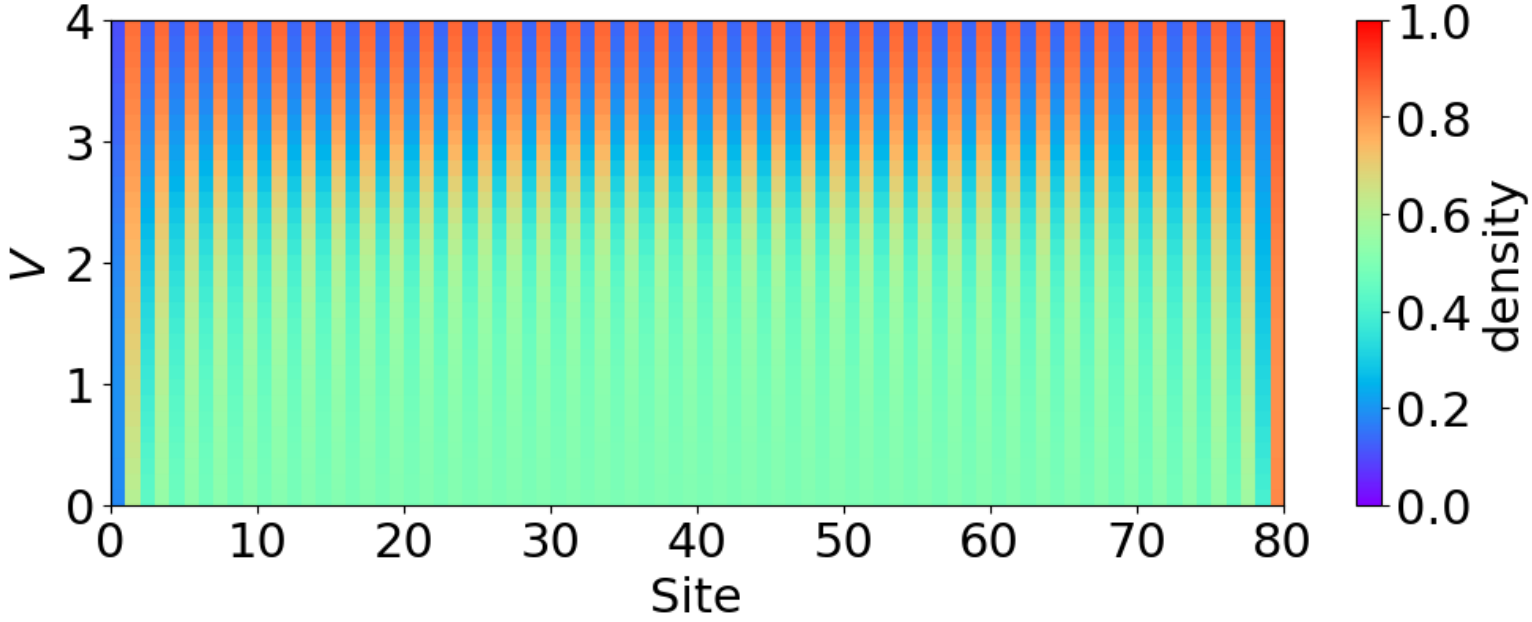
Kinetic

Interaction

Pinning



Fermionic correlation functions

Particle-particle correlators

The non-local static particle-particle allows probing if a system is a metal or an insulator

$$\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$$

Two different types of decays are possible in the correlator

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

Metal

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

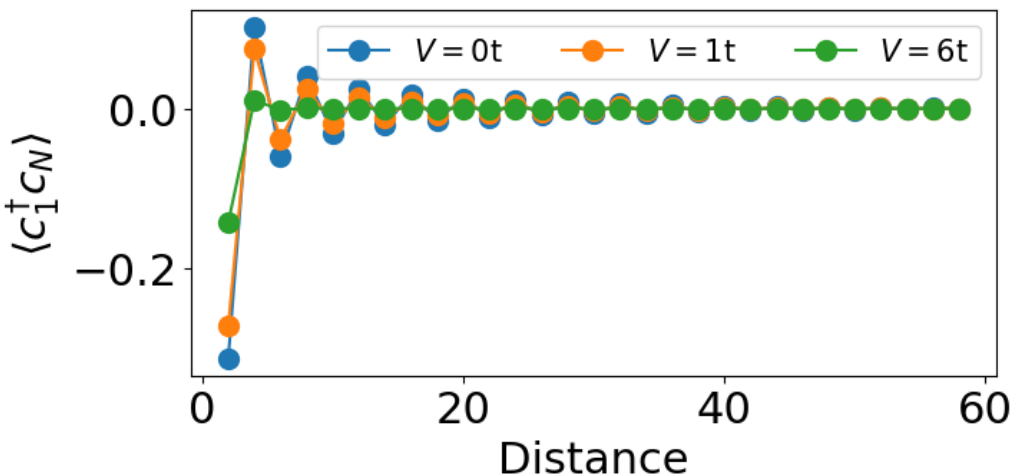
Insulator

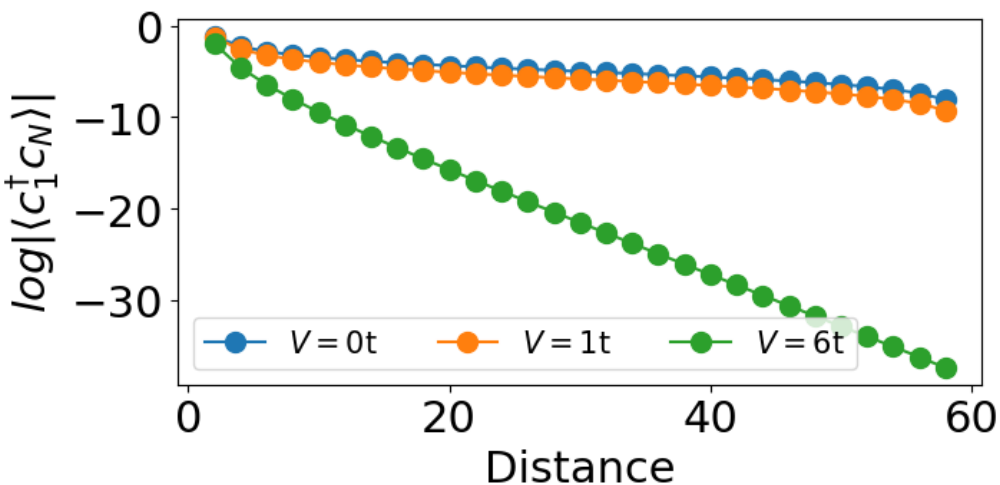
Particle fluctuations in a spinless model

We take an interacting fermionic model

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$

And compute the non-local particle-particle correlator $\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$

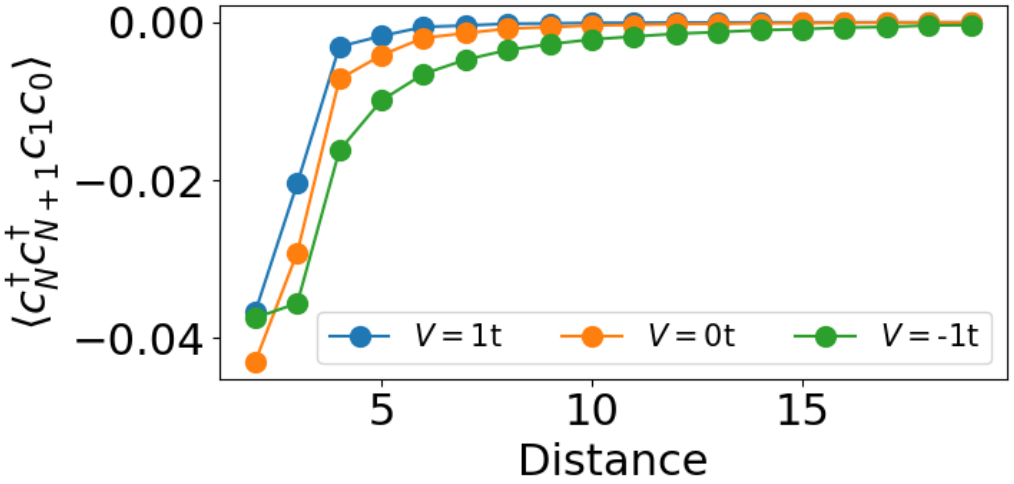


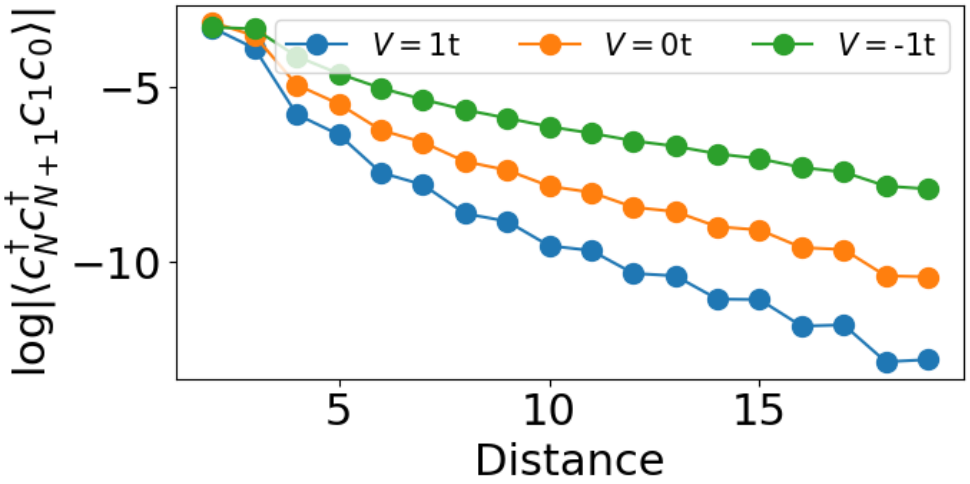


Pairing correlations in an interacting model

The non-local static two-particle correlator allows probing if a system is susceptible to have Cooper pairs

$$\Delta_{ij} \equiv \langle c_i^\dagger c_{i+1}^\dagger c_j c_{j+1} \rangle$$





The Hubbard model

We will now focus on a model of interacting spinful fermions

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$$

Kinetic energy

Interaction

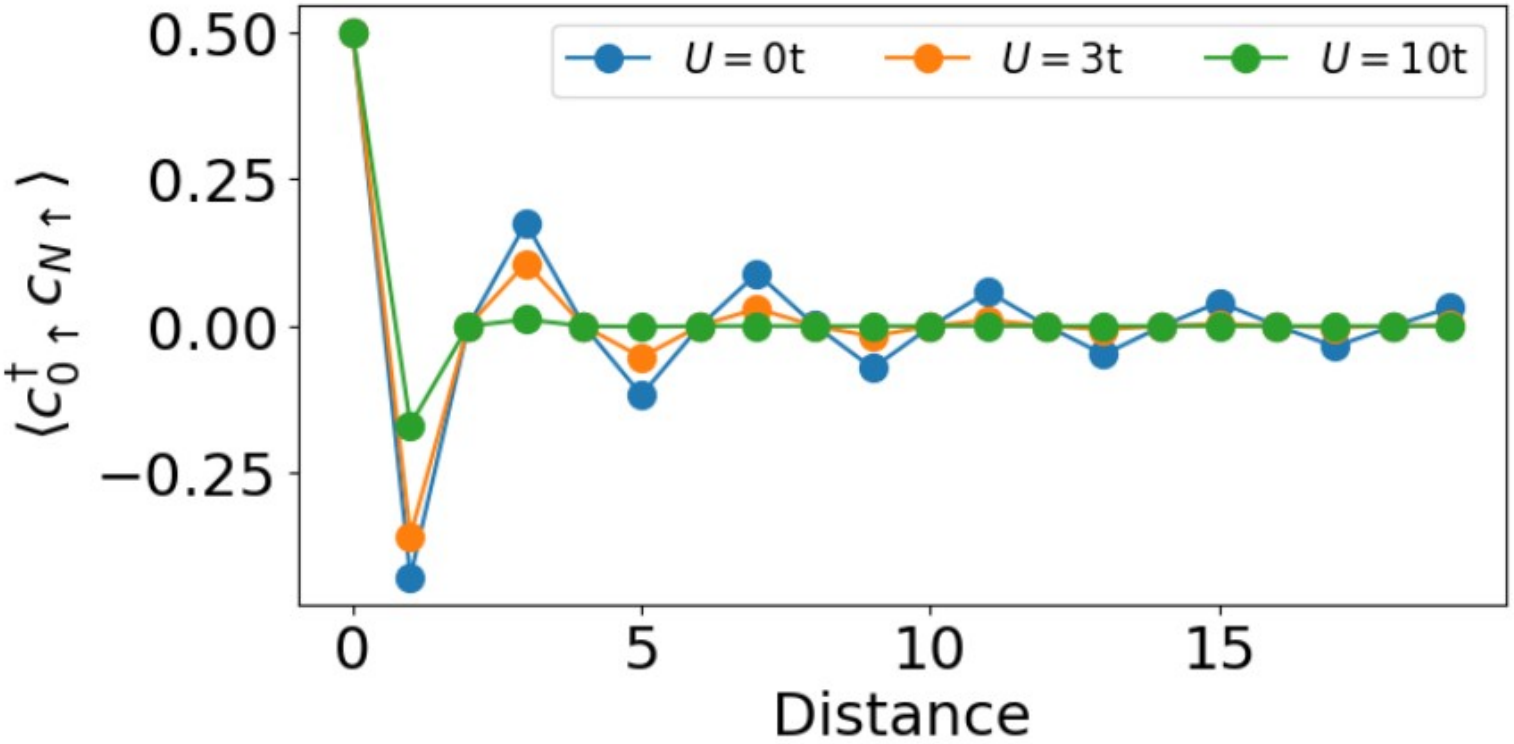
At strong interaction, the system becomes a gapped electric insulator

At strong interaction, the system becomes a gapless quantum magnet

How can we observe this spin-charge separation due to interactions?

Particle-particle correlators in the Hubbard model

$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$$



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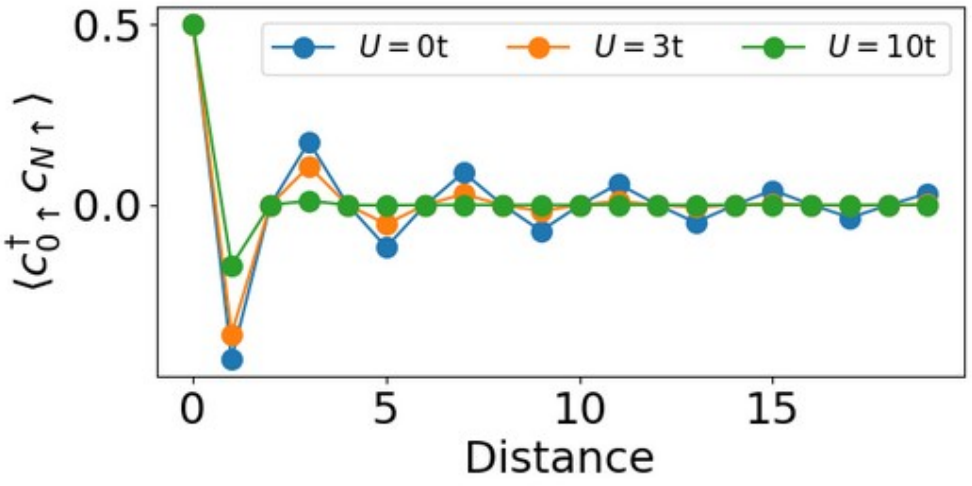
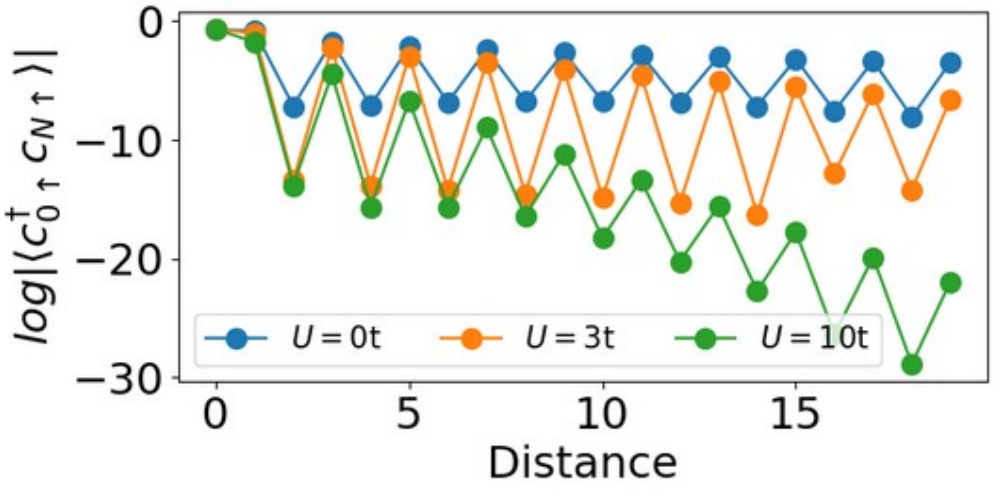
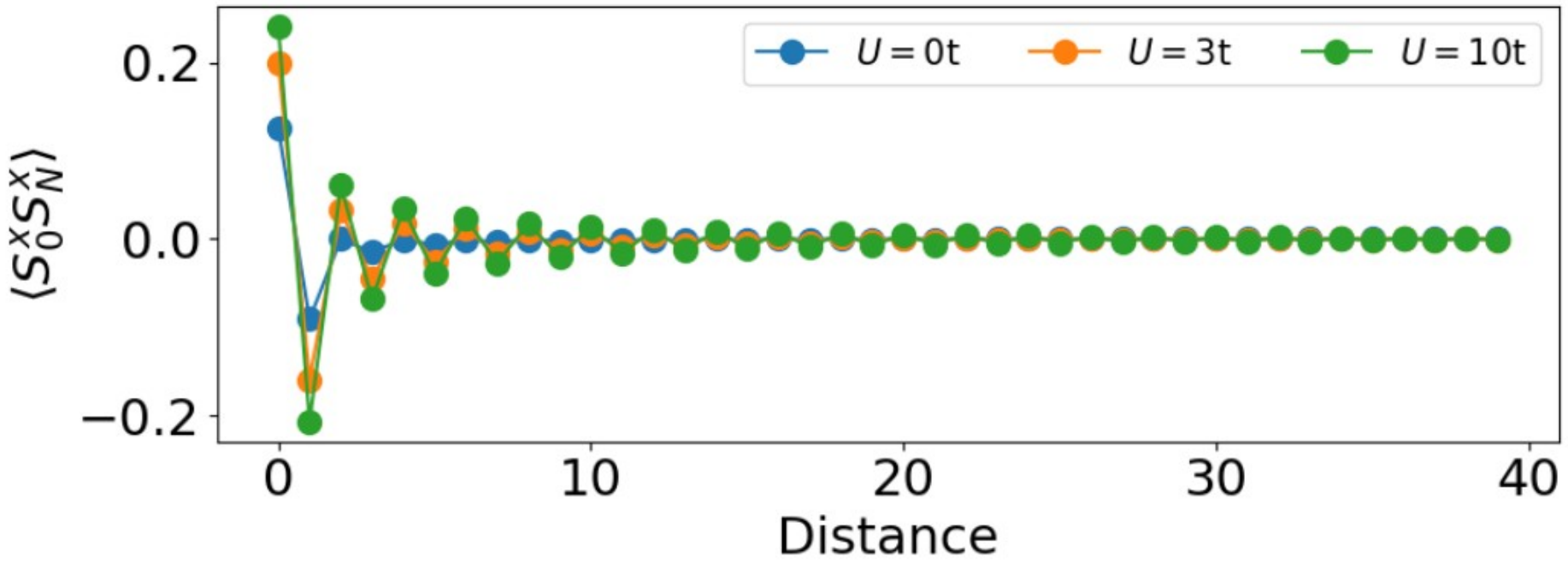




Spin-spin correlators in the Hubbard model

The spin-spin correlator reflects the magnetic fluctuations of the system

$$\Xi_{ij} = \langle S_i^x S_j^x \rangle$$



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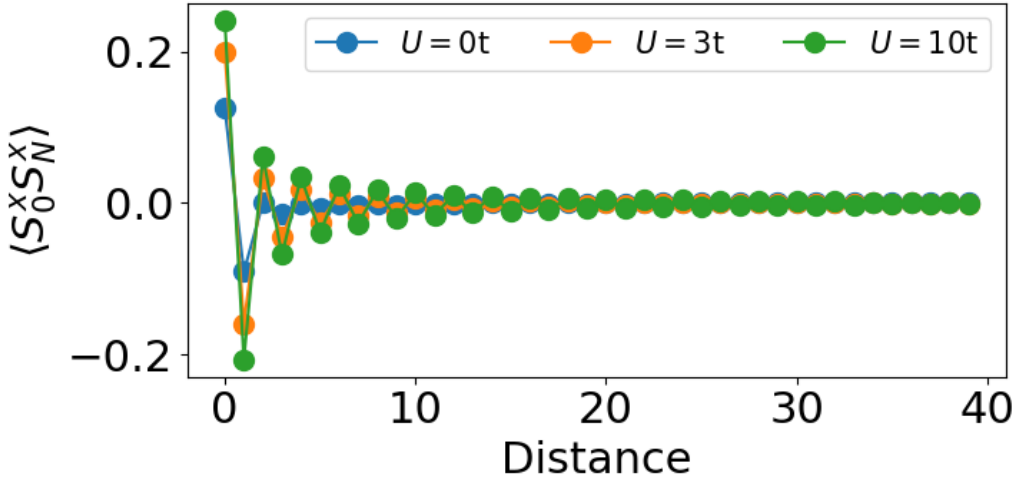
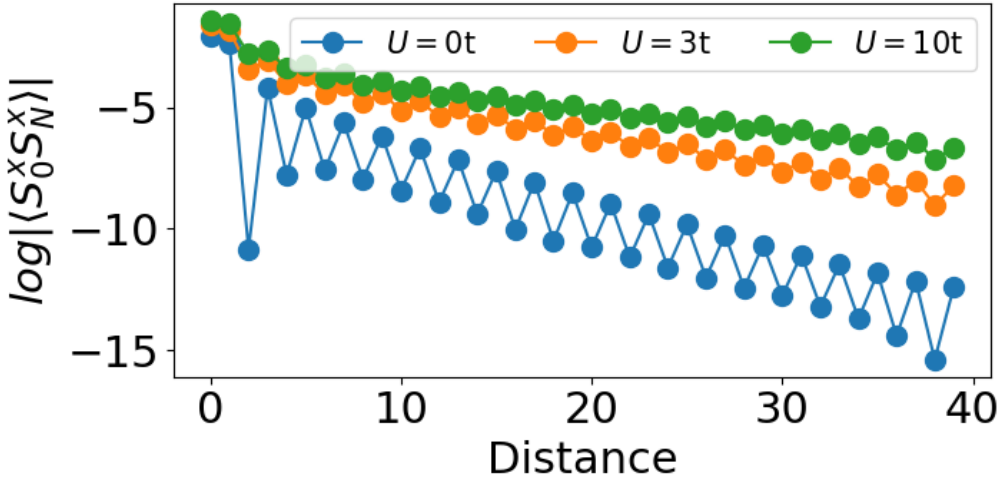
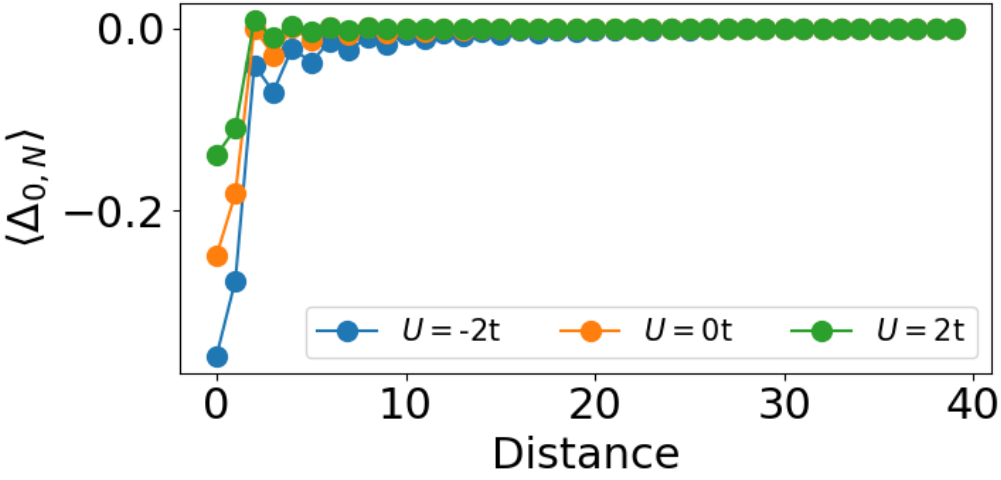


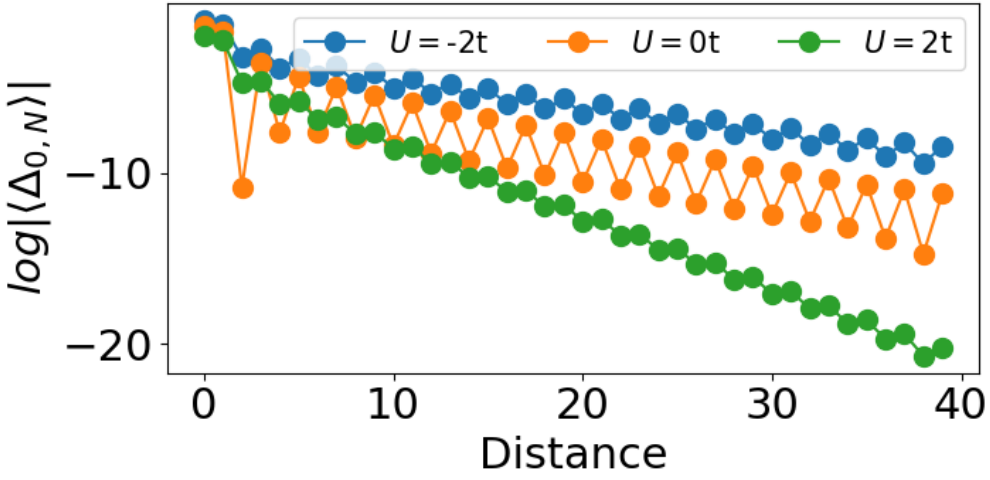


Pairing interaction in the Hubbard model

The pairing correlator reflects the tendency of electrons to form pairs

$$\Delta_{ij} \equiv \langle c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{j,\uparrow} c_{j,\downarrow} \rangle$$





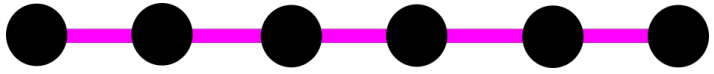
The correlation entropy

Correlated states and mean-field

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$

The two limited cases can be described via mean field theory

$V = 0$



Non-interacting chain (metal)

$$|GS\rangle = \prod_k \Psi_k^\dagger |\Omega\rangle$$

$V \to \infty$

Charge density wave (insulator)

$$|GS\rangle = \prod_{n=1,L/2} c_{2n}^\dagger |\Omega\rangle$$

How can quantify how well a many-body state can be described by a mean-field state?

The fermionic correlation entropy

We can define the correlation matrix as

$$\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$$

We define the correlation entropy as

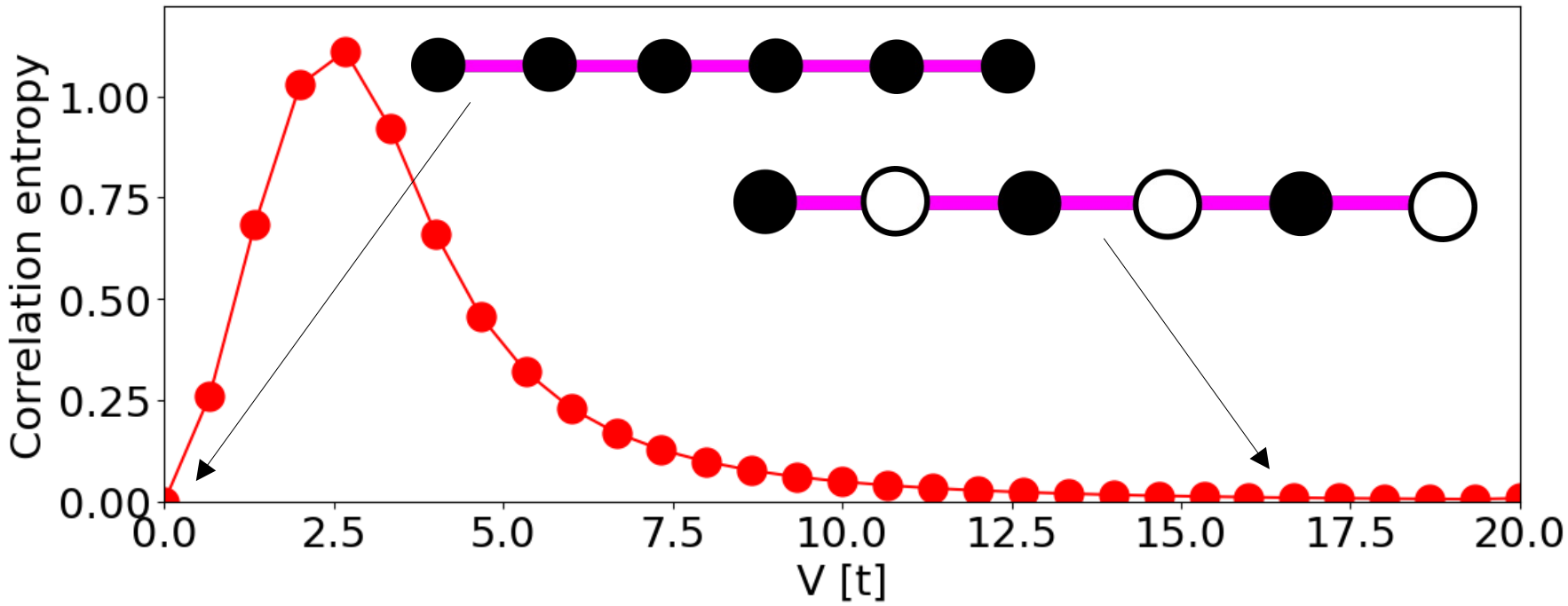
$$S = -\sum_\alpha \lambda_\alpha \log(\lambda_\alpha) \qquad \text{where} \qquad \chi|v\rangle = \lambda_\alpha |v\rangle$$

For mean-field variational fermionic state $|GS\rangle = \prod_k \Psi_k^\dagger |\Omega\rangle$

we have $\lambda_\alpha = 0, 1$ and thus $S = 0$

The correlation entropy of the spinless interacting model

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$



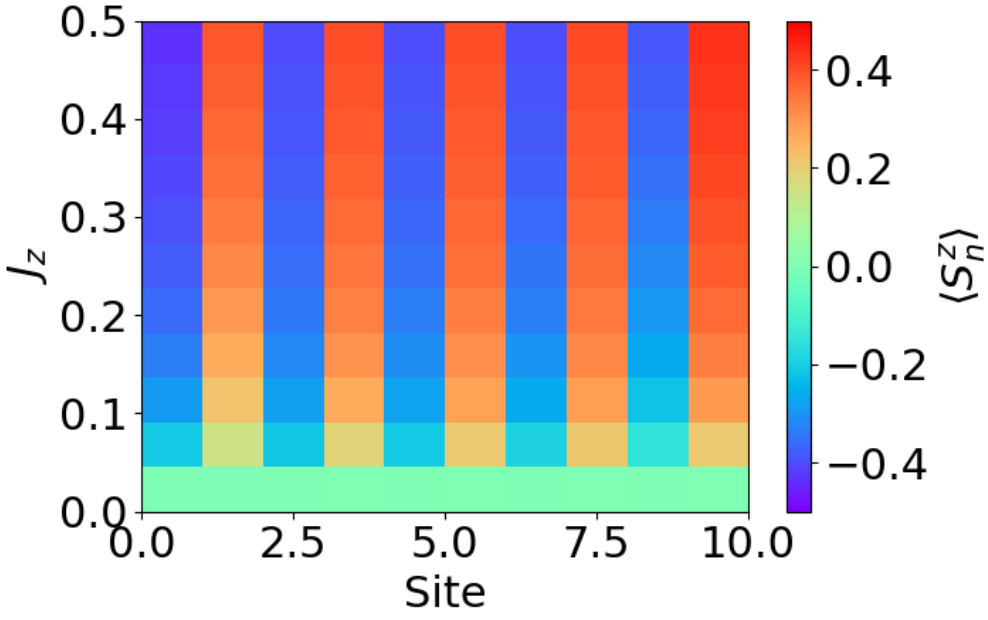
From many-body to mean field in the Hubbard model

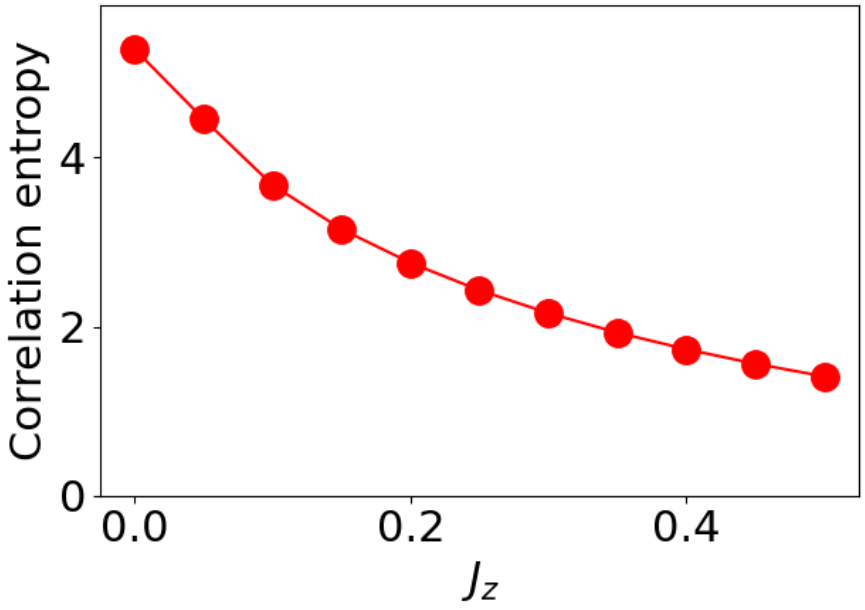
$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + U\sum_{n}\left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right) + J_z\sum_{s,n}(-1)^n\sigma^{z}_{s,s'}c^{\dagger}_{n,s}c_{n,s'}$$

Kinetic

Interaction

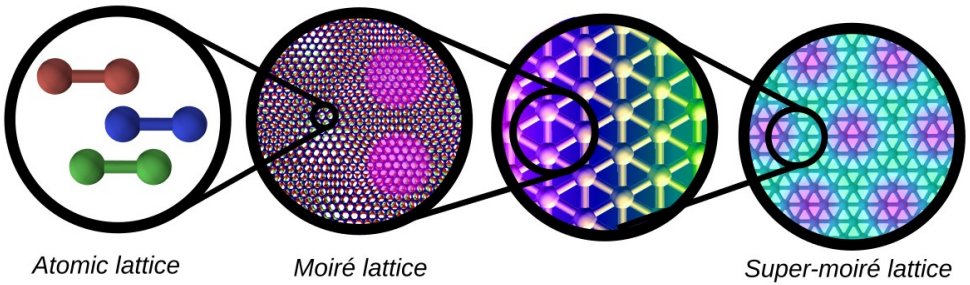
Mean-field antiferromagnetism

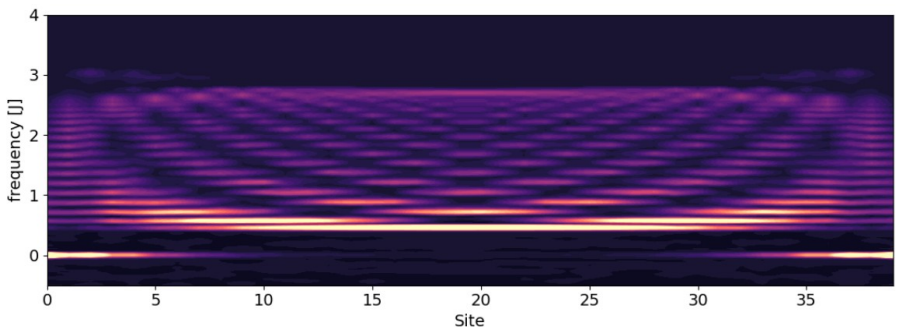




Take home

Tensor network allows solving exponentially large problems, including quantum many-body systems and xceptionally large single particle super-moire materials





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Notebooks for the exercise session

Download the notebooks from

https://github.com/joselado/funlayers_INL_MPS_tutorial

Four different notebooks

Many-body fermionic models with ED
Many-body spin models with ED
Many-body fermionic models with tensor networks
Many-body spin models with tensor networks

Notebooks are independent, you can start from the one you prefer