Tensor networks for many-body fermionic models

Learning outcomes

- Rationalize quantum phase transitions in large fermionic models
- Understand the relationship between fermionic and spin models in tensor networks
- Rationalize spin-charge separation in Hubbard models

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?

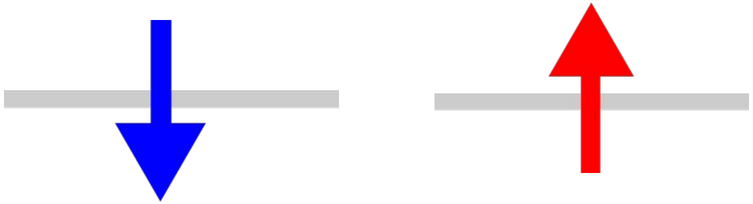
Fermionic and spin many-body-Hamiltonians

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

The matrix-product state ansatz

In the spin basis $$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L}|s_1,s_2,\ldots s_L\rangle$$

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)

Wavefunction is parametrized in the spin basis, observables are transformed to the real basis

Quantum phase transition in a spinless fermionic model

Let us look at a minimal interacting fermionic model

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

Two limiting cases

$$V = 0$$

Non-interacting chain (metal)

$$V \to \infty$$

Charge density wave (insulator)

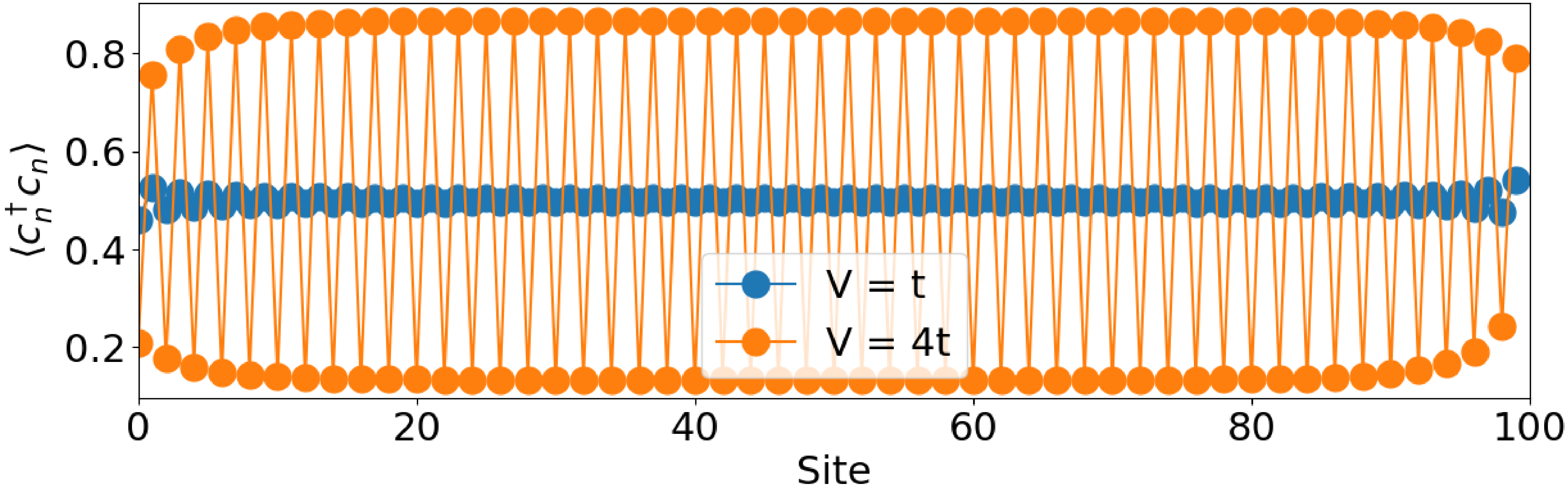
How can we observe such a phase transition?

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



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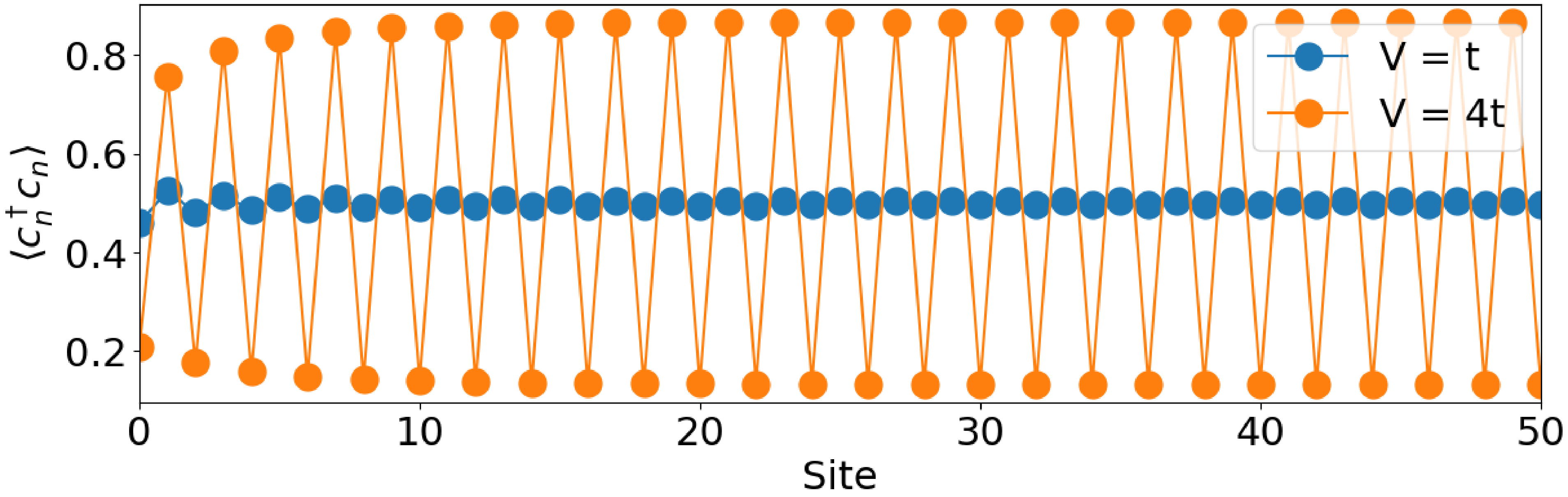
Kinetic

Interaction

Pinning



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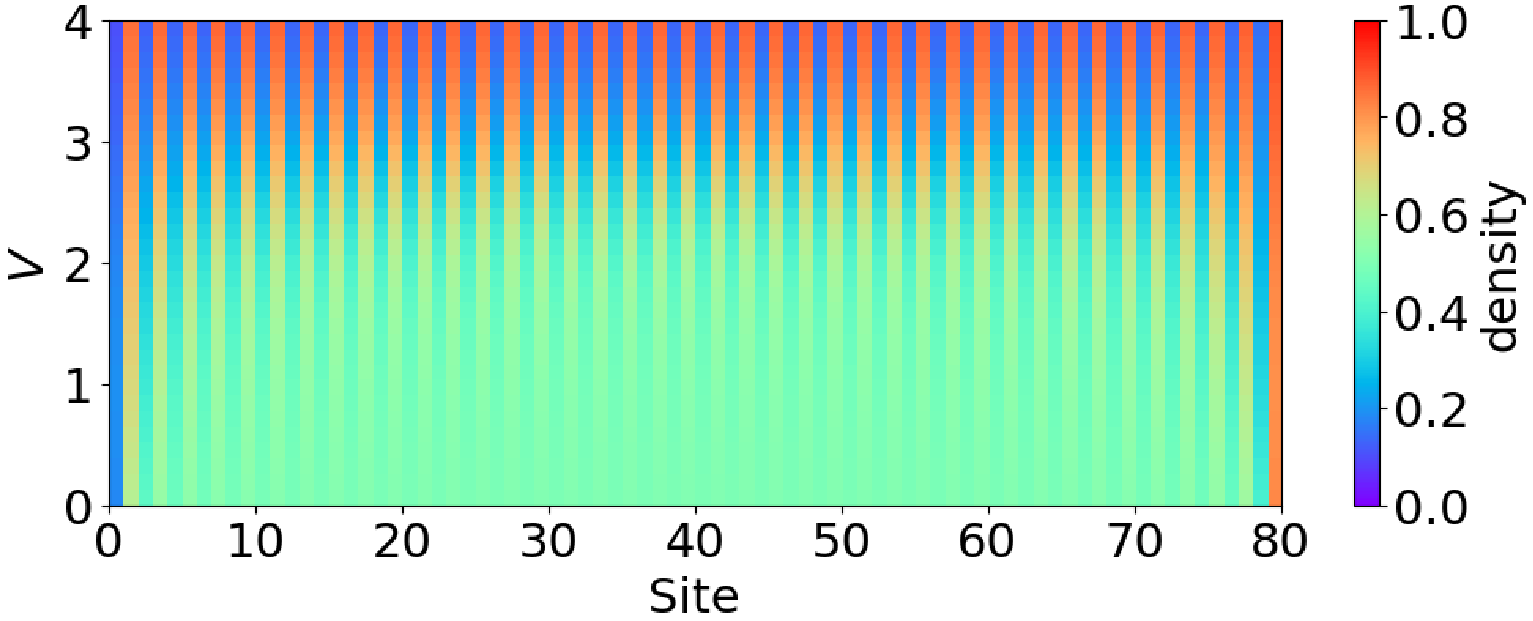


Fermionic correlation functions

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

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

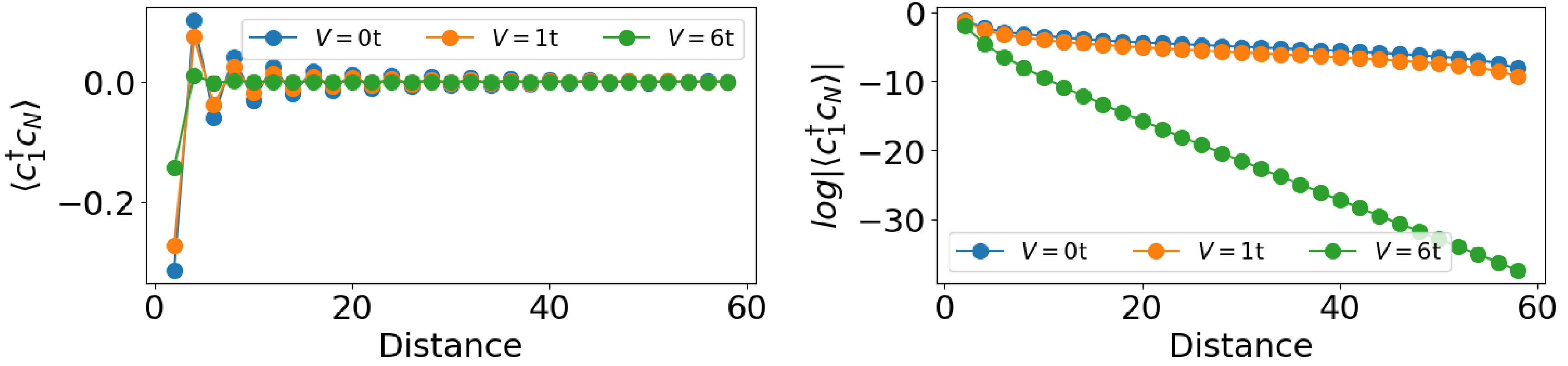
Insulator

Particle fluctuations in a spinless model

We take an interacting fermionic model

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

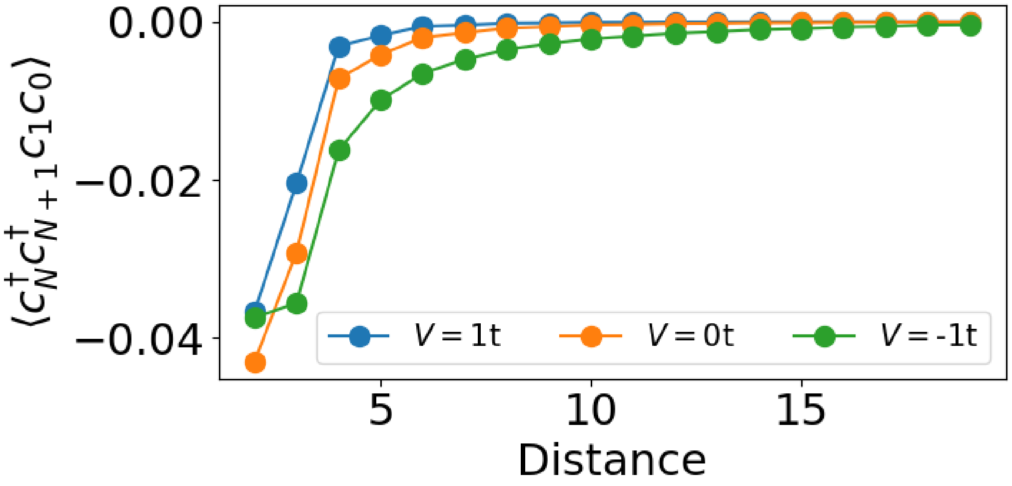
And compute the non-local particle-particle correlator $\chi_{ij} \equiv \langle c_i^\dagger c_j \rangle$

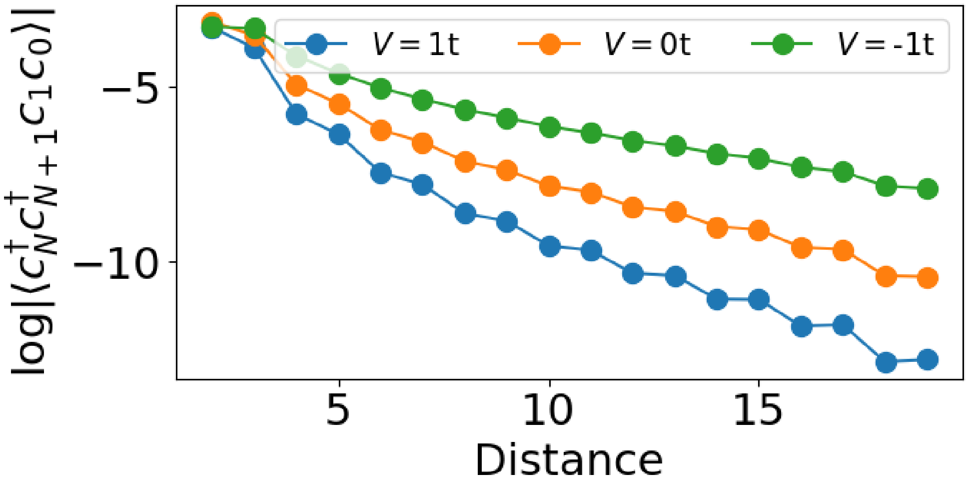


Pairing correlations in an interacting model

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

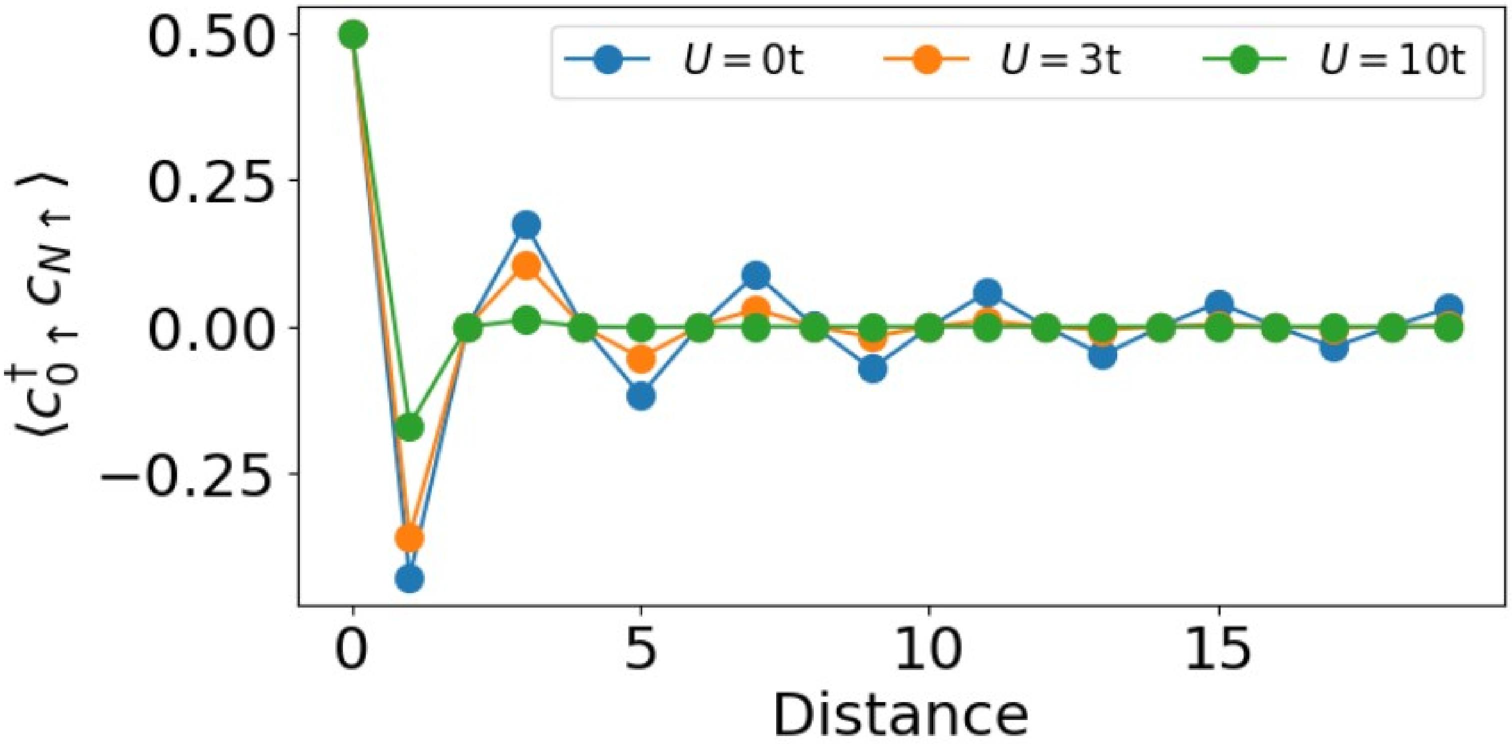
At strong interaction, the system becomes a gapped electric insulator

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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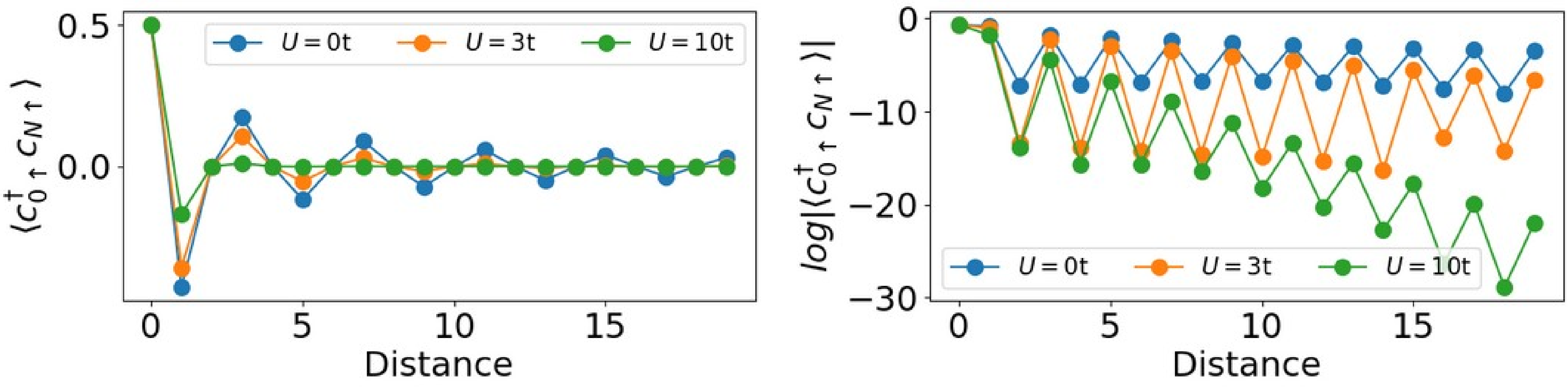
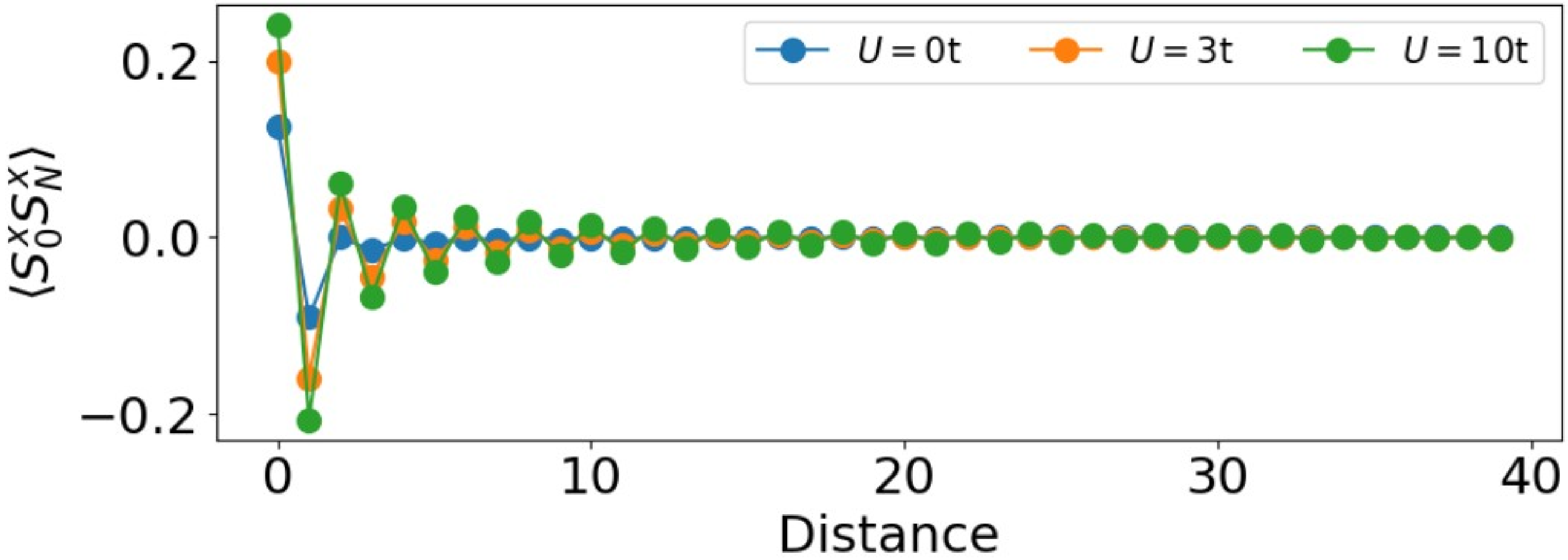


Spin-spin correlators in the Hubbard model

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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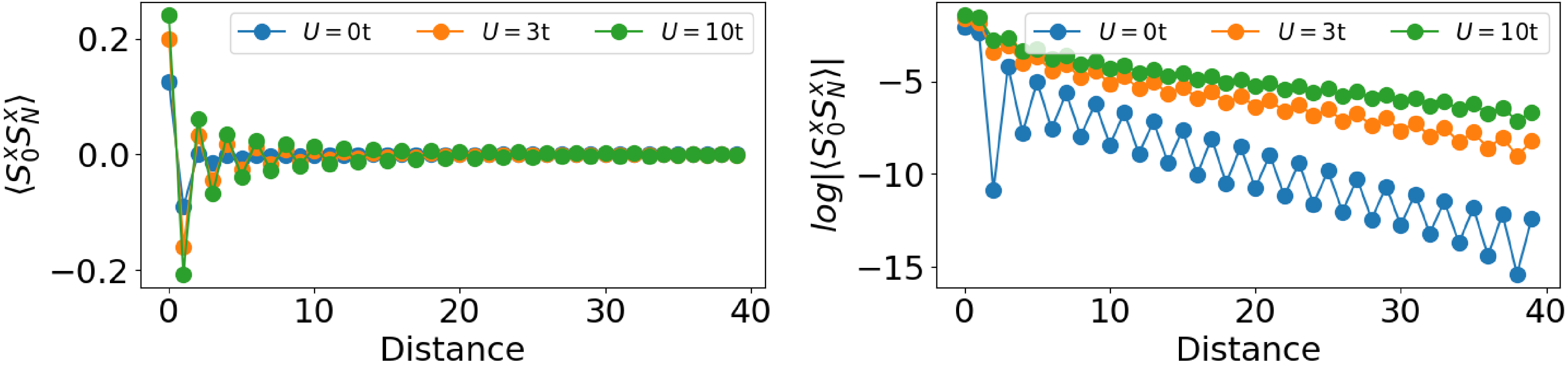
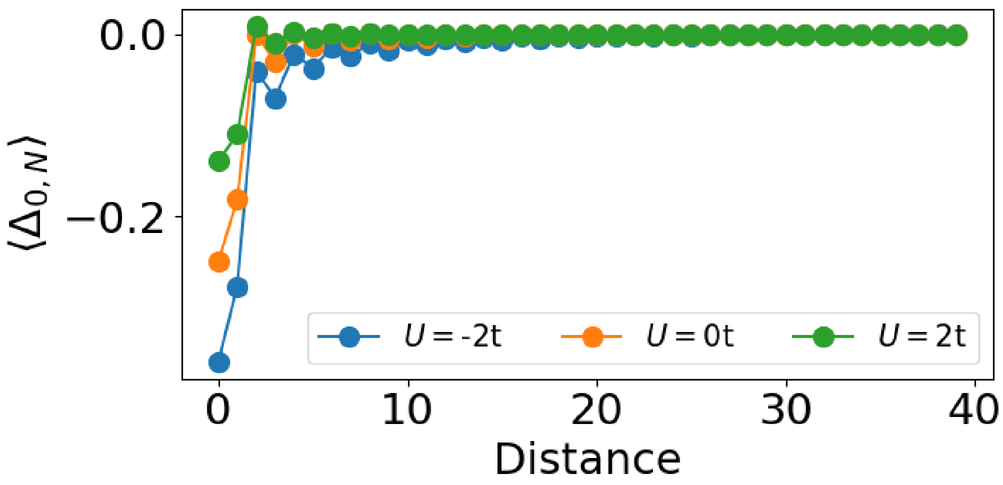
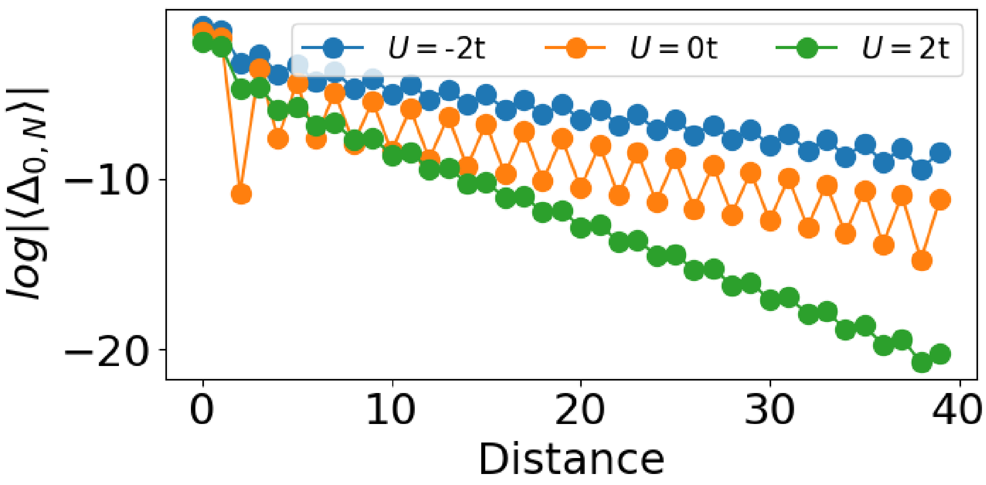


Pairing interaction in the Hubbard model

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

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

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

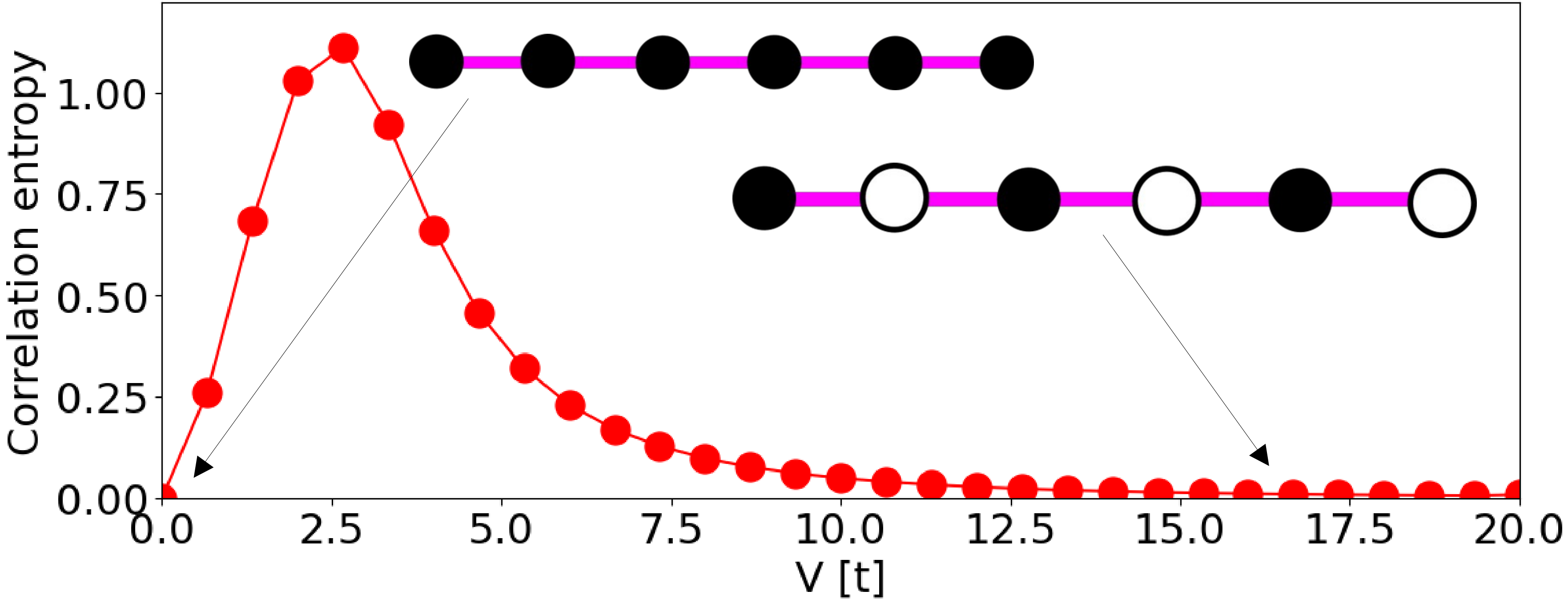
$S = -\sum_\alpha \lambda_\alpha \log(\lambda_\alpha)$ where $\chi|v\rangle = \lambda_\alpha |v\rangle$

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

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



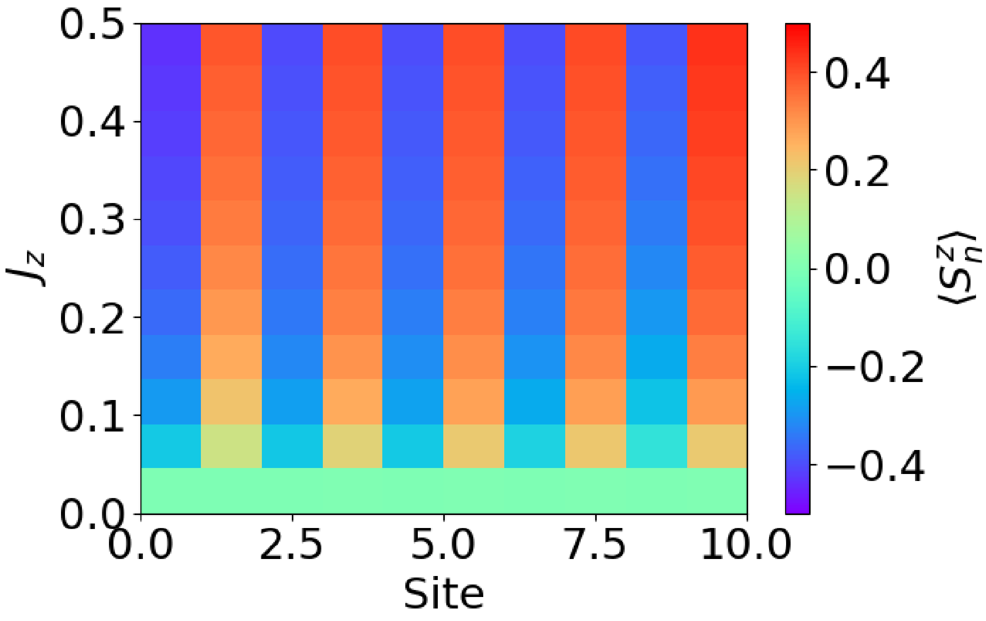
From many-body to mean field in the Hubbard model

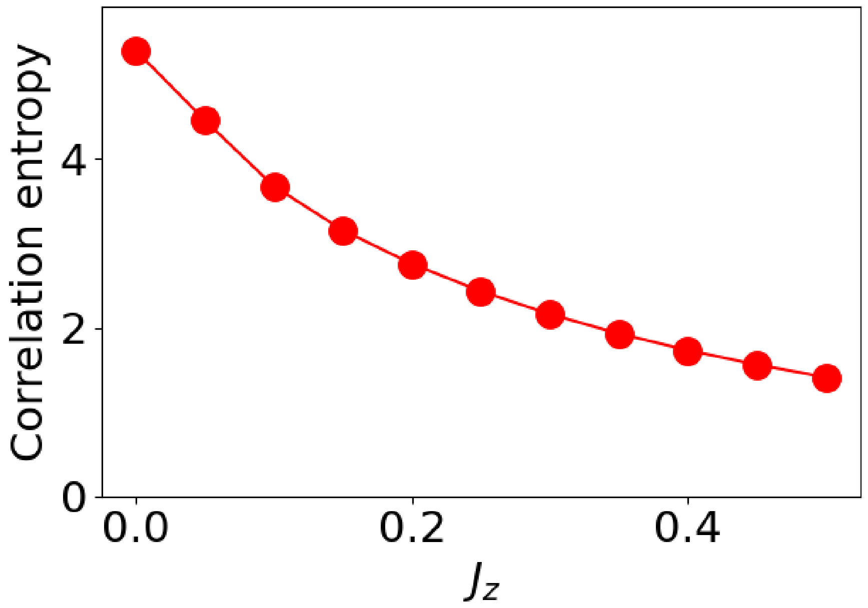
$$H = t\sum_{s,n} c^\dagger_{n,s} c_{n+1,s} + h.c. + U\sum_n \left(c^\dagger_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^\dagger_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right) + J_z \sum_{s,n}(-1)^n \sigma^z_{s,s'} c^\dagger_{n,s}c_{n,s'}$$

Kinetic

Interaction

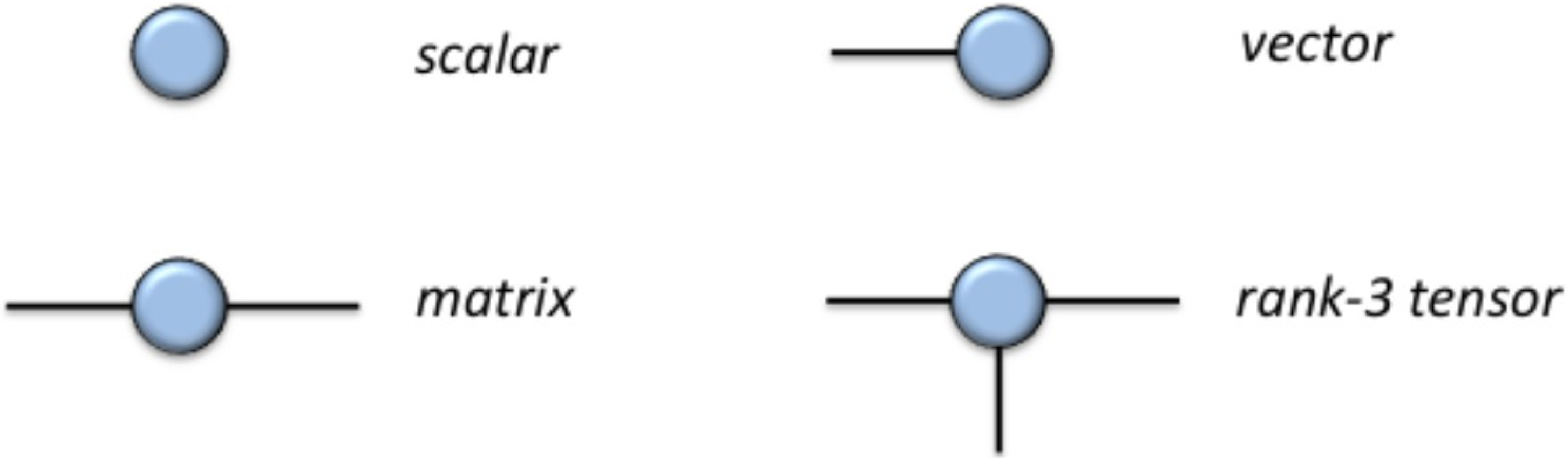
Mean-field antiferromagnetism





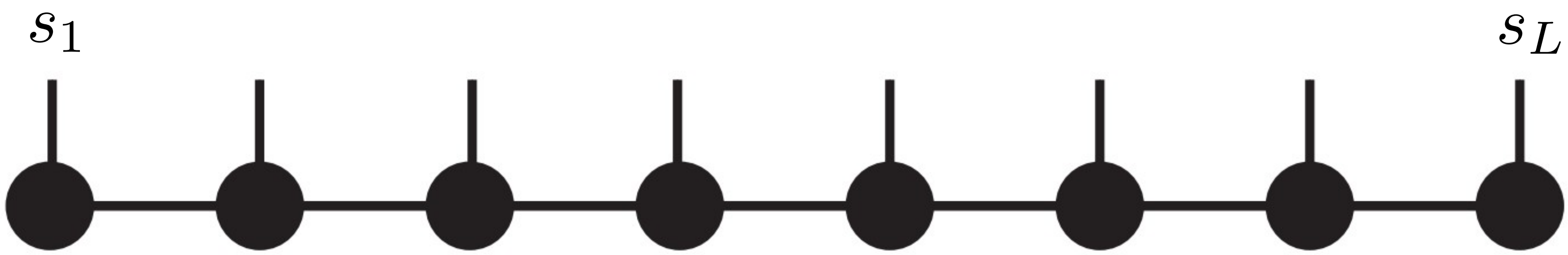
Matrix product state algorithms

The graphical representation of matrix product states



Tensor-network operations can be easily described with diagrams

The matrix product state representation

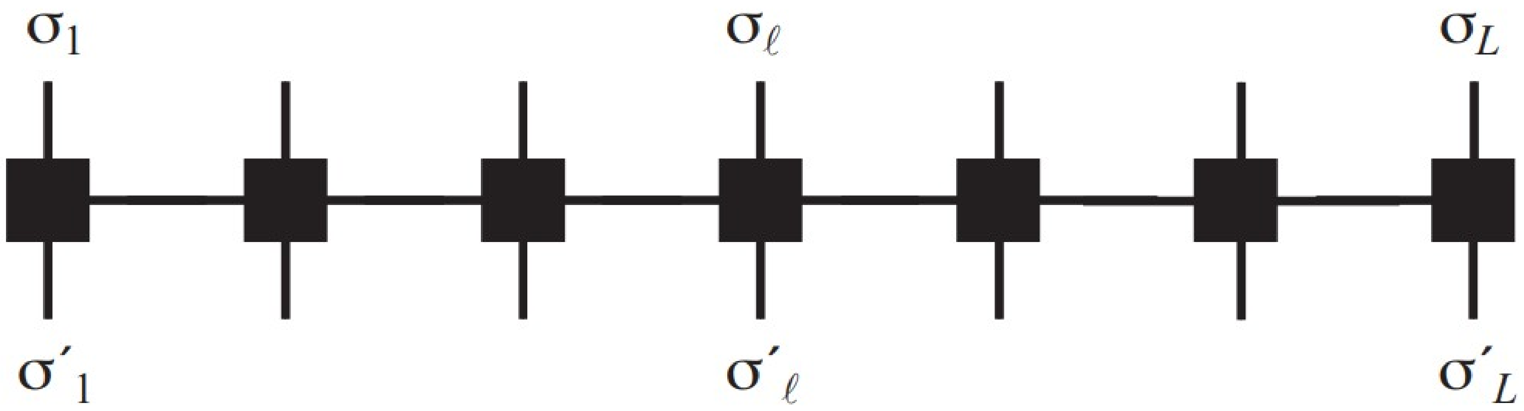


$$|\Psi\rangle = \sum c_{s_1,s_2,\ldots,s_L}|s_1, s_2, \ldots s_L\rangle$$

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

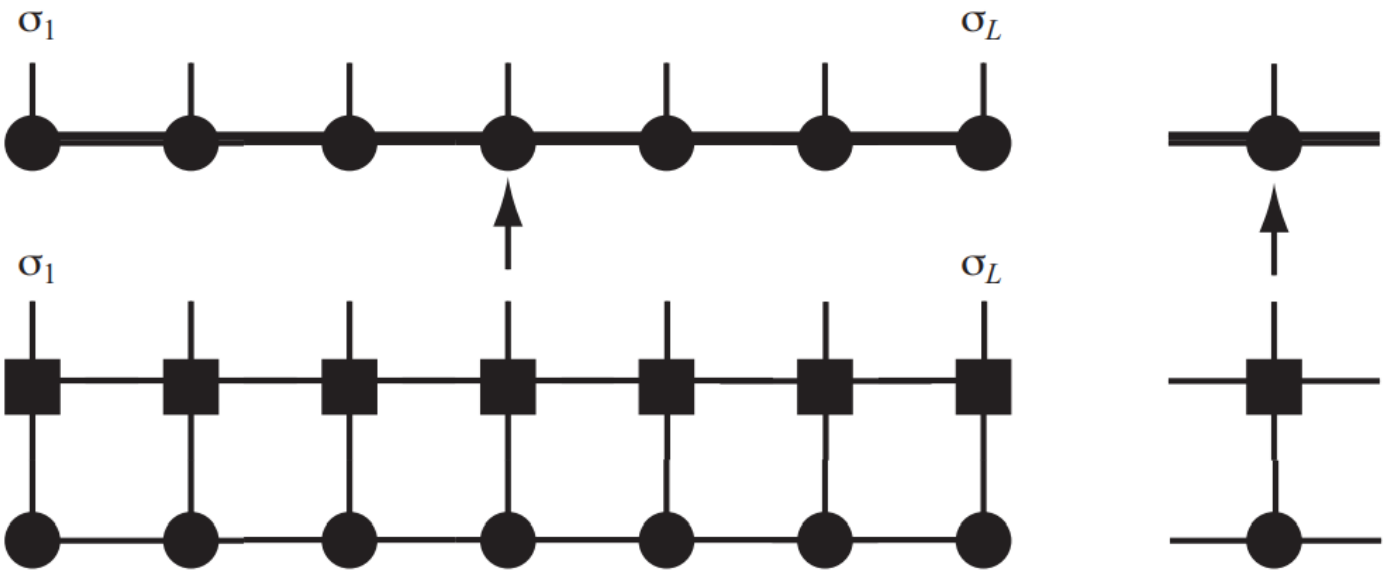
Matrix product operators

Operators can be represented in an analogous form



Operator state product

Products of operators and states can be represented graphically



Ground state calculations

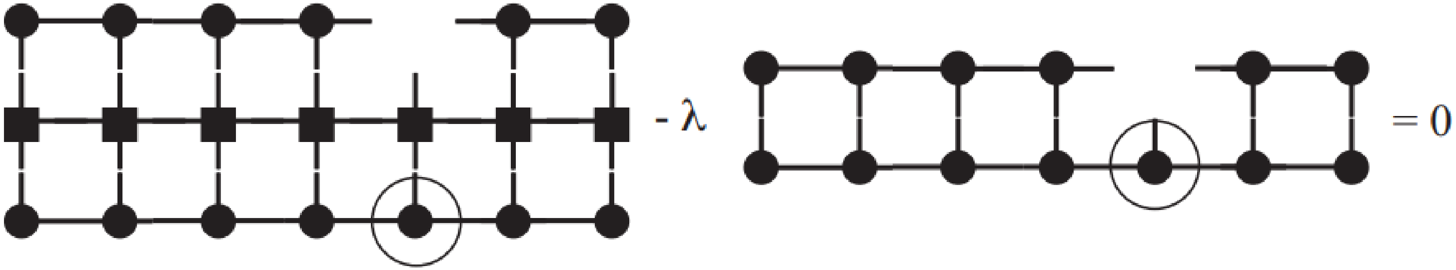
To compute a ground state, we just have to minimize

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$E = \langle \Psi | H | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle$$

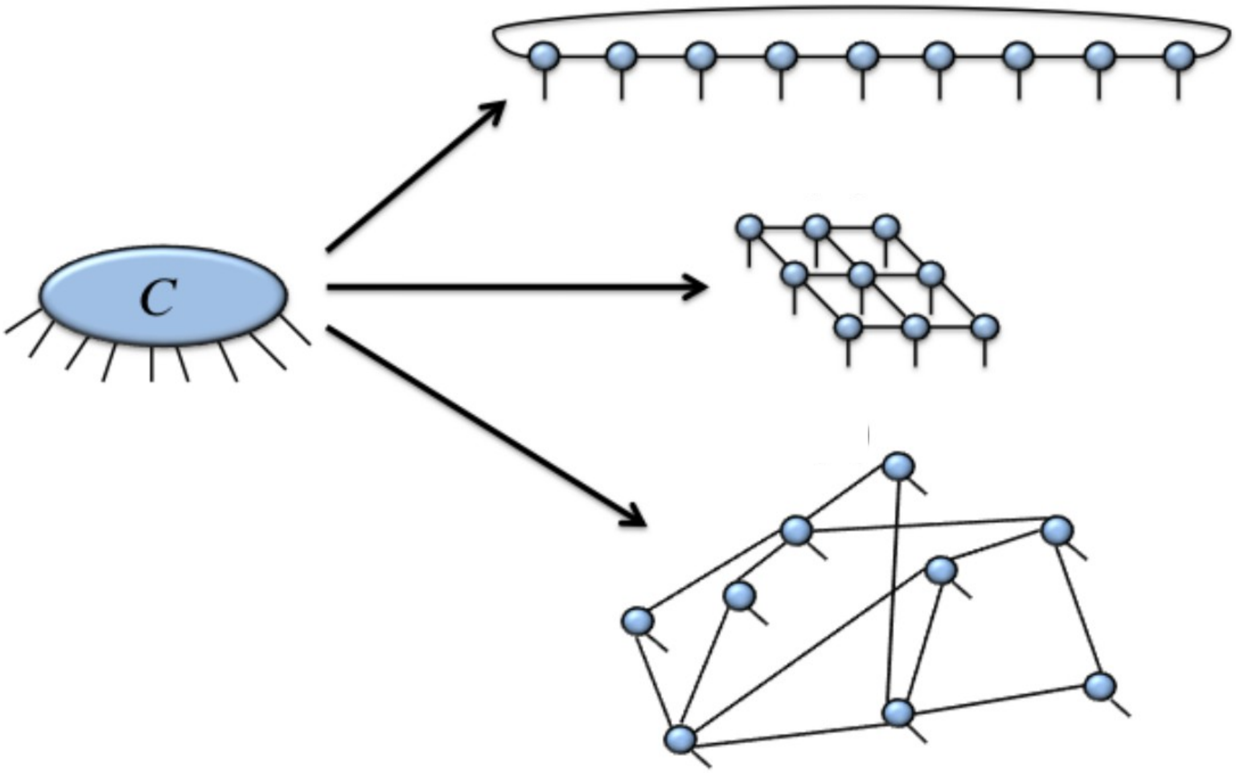
This can be done by minimizing the energy with respect to each matrix

$$\frac{\delta E}{\delta M} = 0$$



This algorithm is known as the density-matrix renormalization group

Beyond matrix-product states

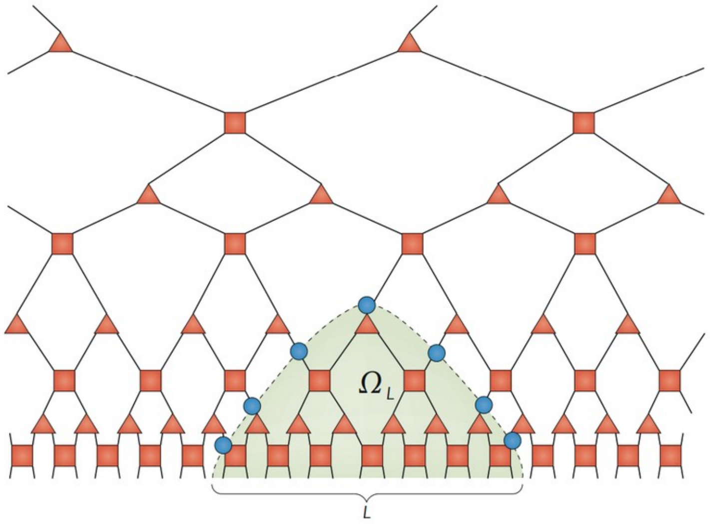


The same tensor can be represented with widely different tensor networks

Beyond matrix-product states

Tensor networks can be extended to deal with higher dimensional/critical systems

Multiscale renormalization ansatz



Projected-entangled pair states