Quantum many-body fermionic Hamiltonians

Learning outcomes

- Understand the difference between single particle and many-body fermionic systems
- Rationalize the meaning of expectation values in an interacting fermionic model
- Identify phase transitions in interacting fermionic models

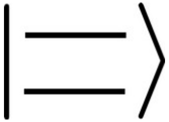
From single particle to many-body fermions

The fermionic many-body dimer

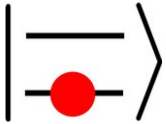
Let us take a minimal interacting fermionic Hamiltonian with 2 sites

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

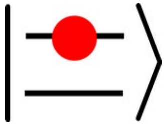
The different many-body states are

$$|\Omega\rangle =$$ 

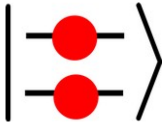
The “vacuum” state

$$c_0^\dagger|\Omega\rangle =$$ 

One particle in level #0

$$c_1^\dagger|\Omega\rangle =$$ 

One particle in level #1

$$c_0^\dagger c_1^\dagger|\Omega\rangle =$$ 

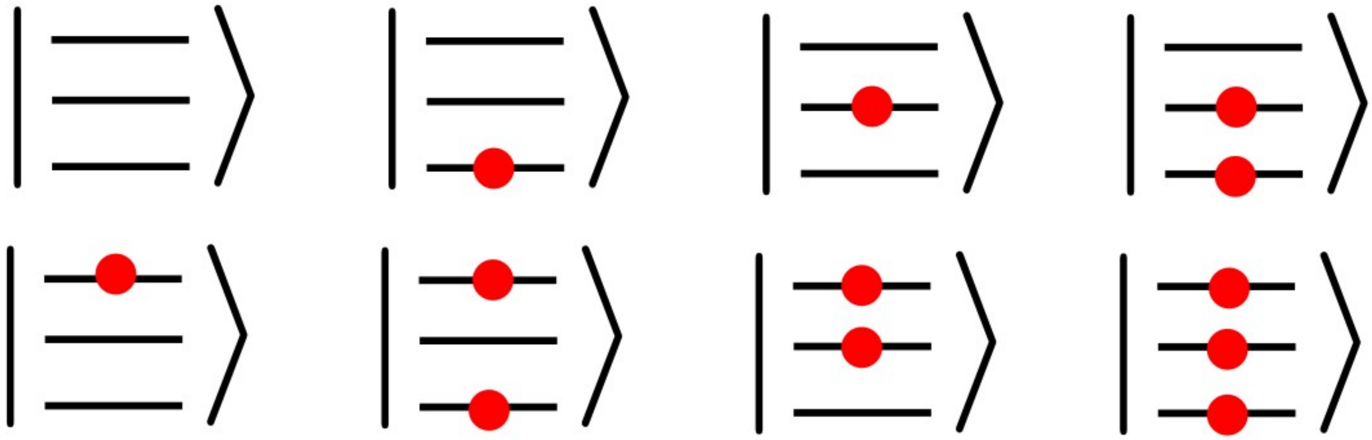
Two particles in level #0 & #1

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



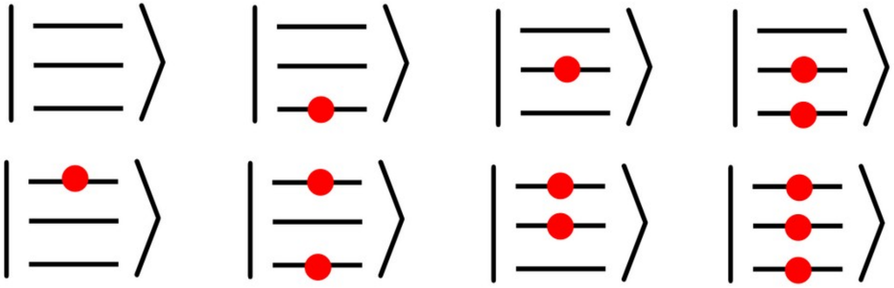
The fermionic quantum many-body problem

For a fermionic many-body problem with L sites

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

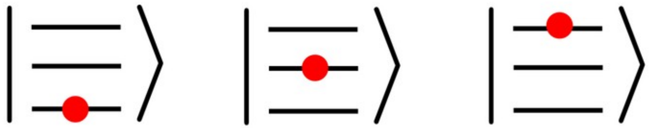
The dimension of the
full Hilbert space grows as

$$d = 2^L$$



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

$|\circ\circ\rangle$ fully empty

$|\circ\downarrow\rangle$ down electron

$|\uparrow\circ\rangle$ up electron

$|\uparrow\downarrow\rangle$ fully filled

Spinless fermions

$|\circ\rangle$ empty

$|\bullet\rangle$ filled

Spins

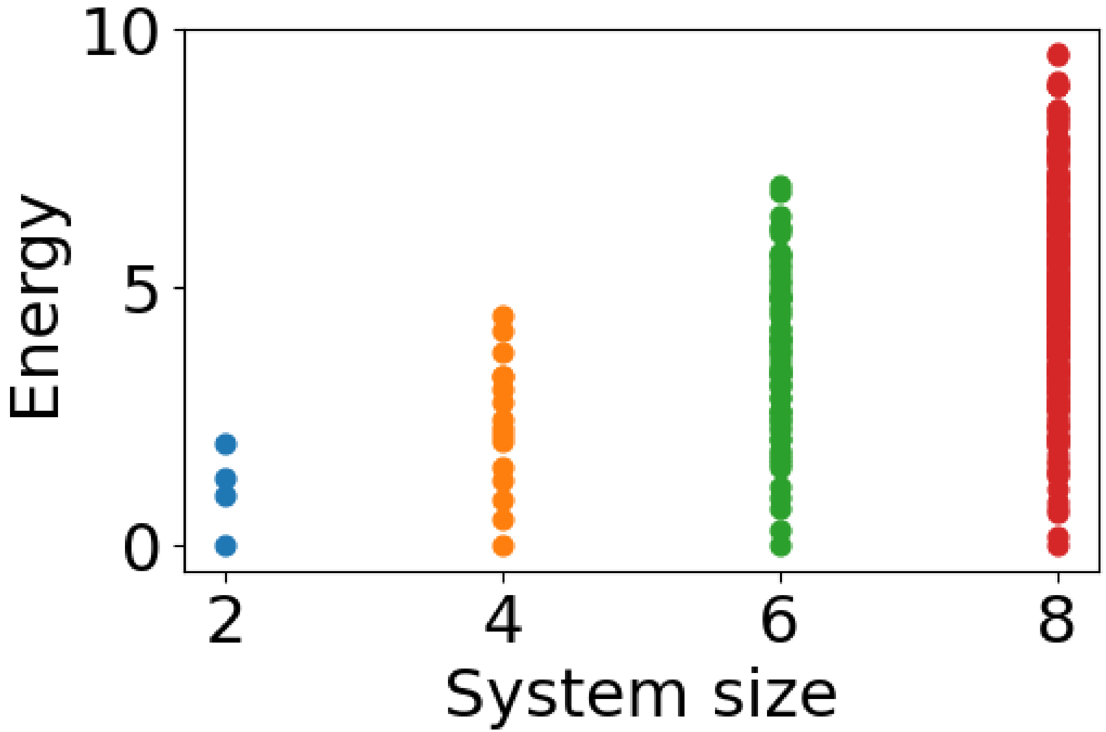
$|\downarrow\rangle$ down

$|\uparrow\rangle$ up

Understanding the fermionic many-body spectra

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

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

Two limiting cases

$$V = 0$$

Non-interacting chain (metal)

$$V \to \infty$$

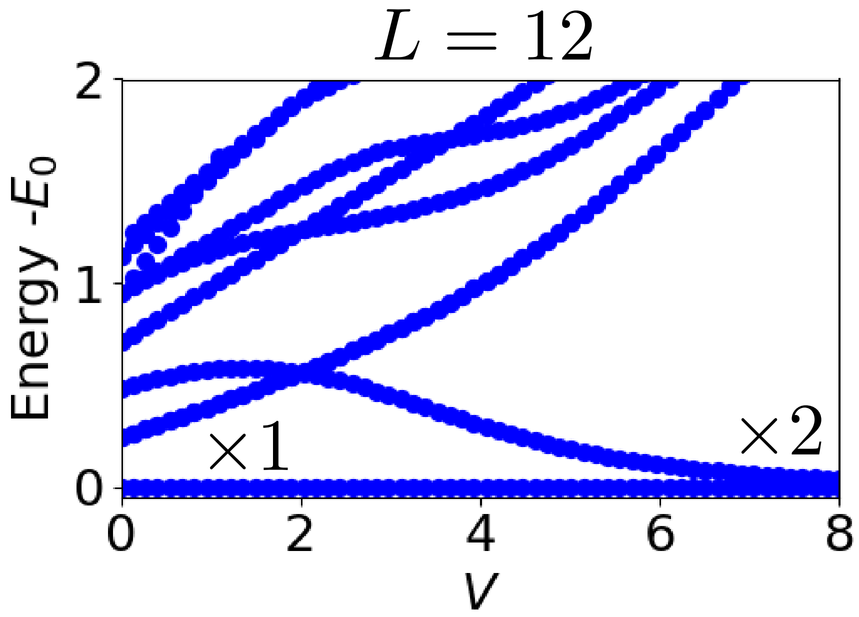
Charge density wave (insulator)

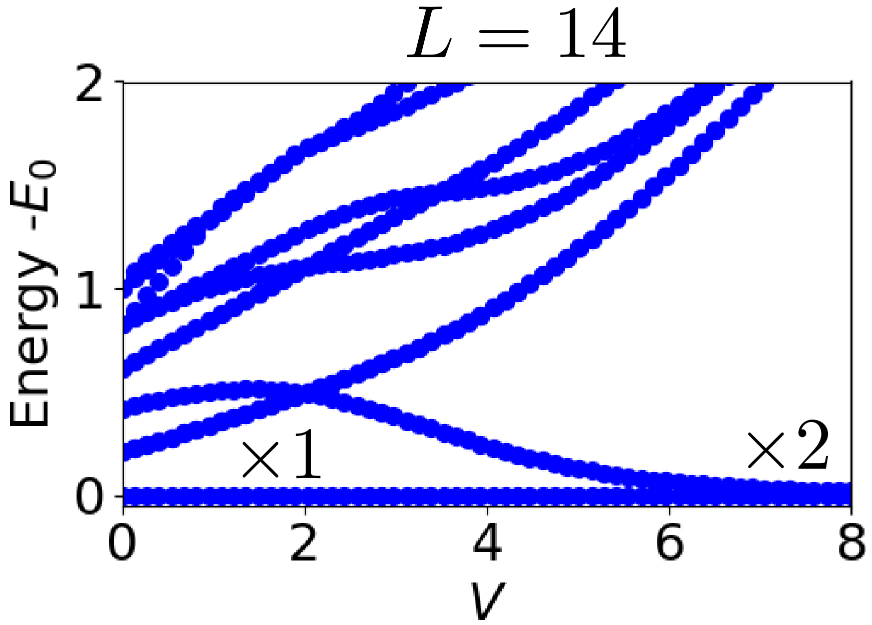
How can we observe such a phase transition?

From single particle to correlated fermions

Let us look at a minimal interacting fermionic model

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





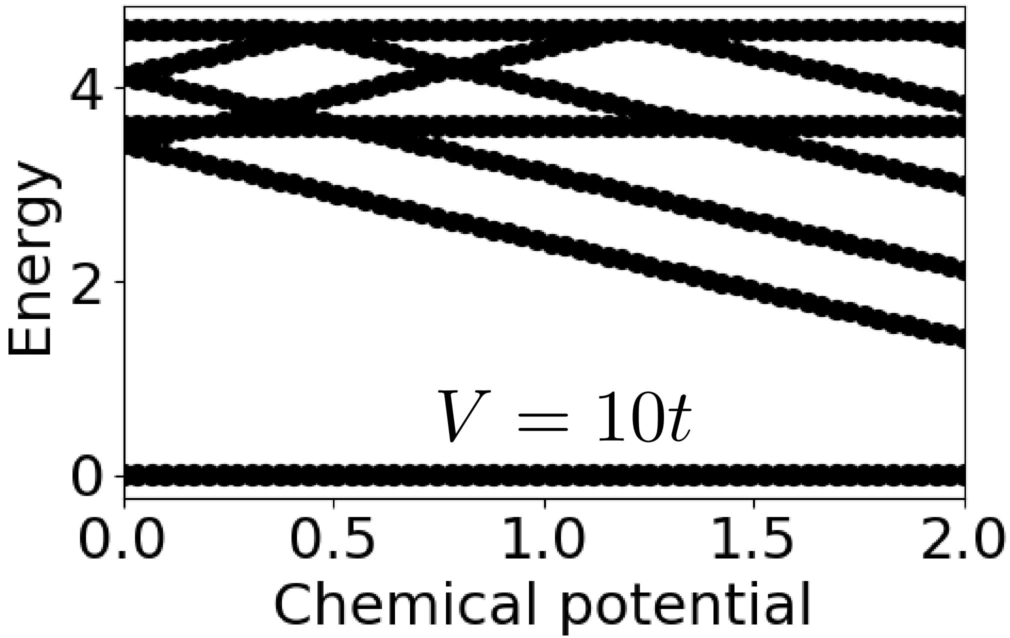
The chemical potential

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

Kinetic energy

Interaction

Chemical potential



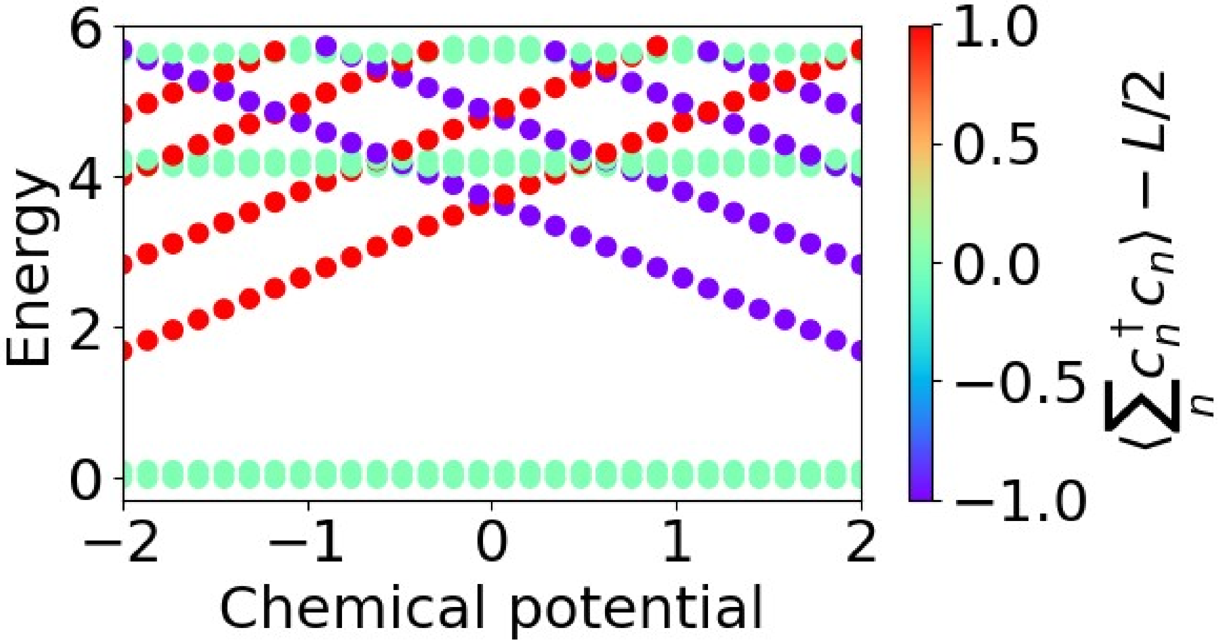
The occupation number

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

Kinetic energy

Interaction

Chemical potential



The number of electrons is given by

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

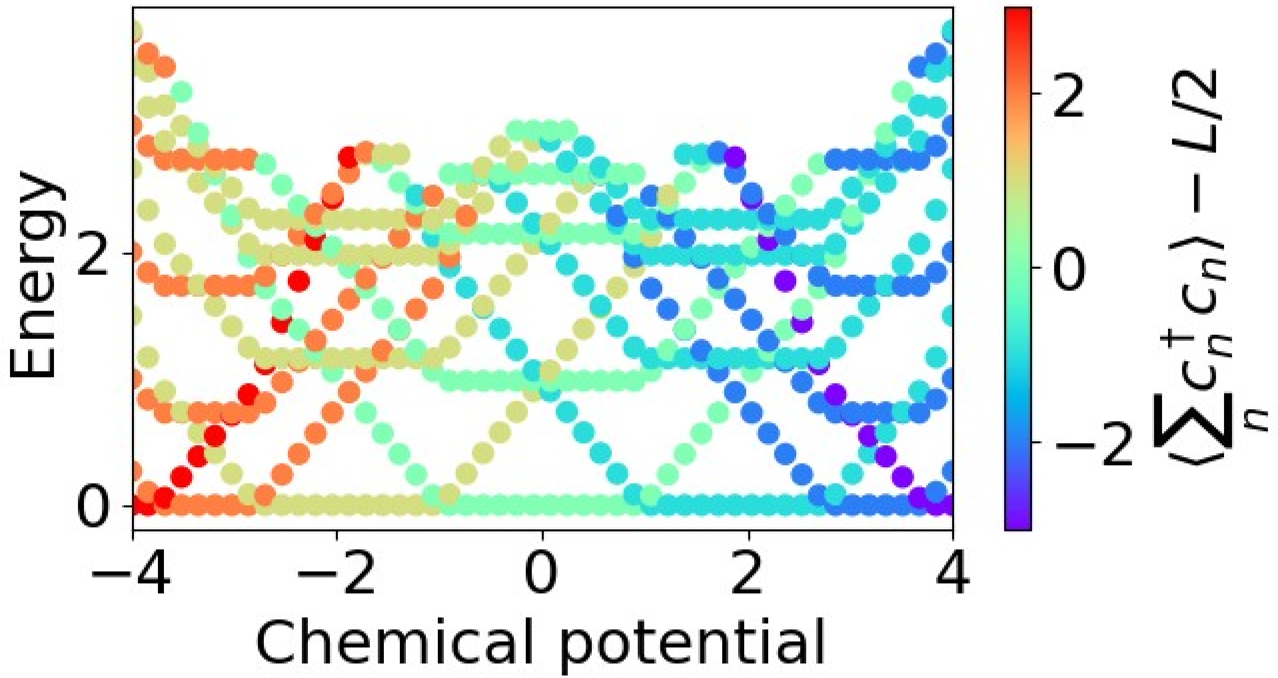
The occupation number

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

Kinetic energy

Interaction

Chemical potential



The number of electrons is given by

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

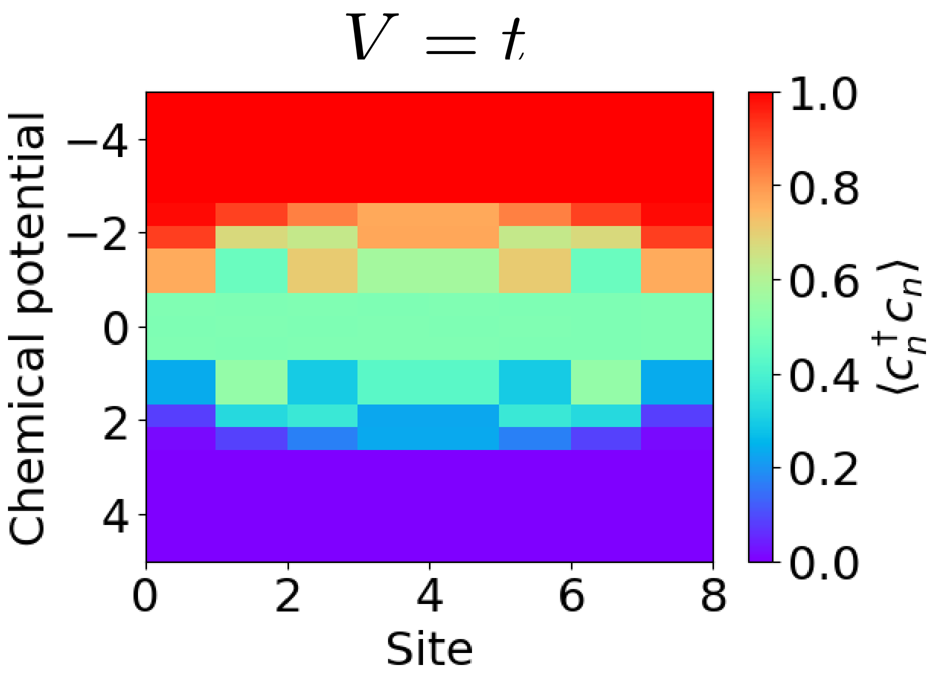
Electronic density as a function of the chemical potential

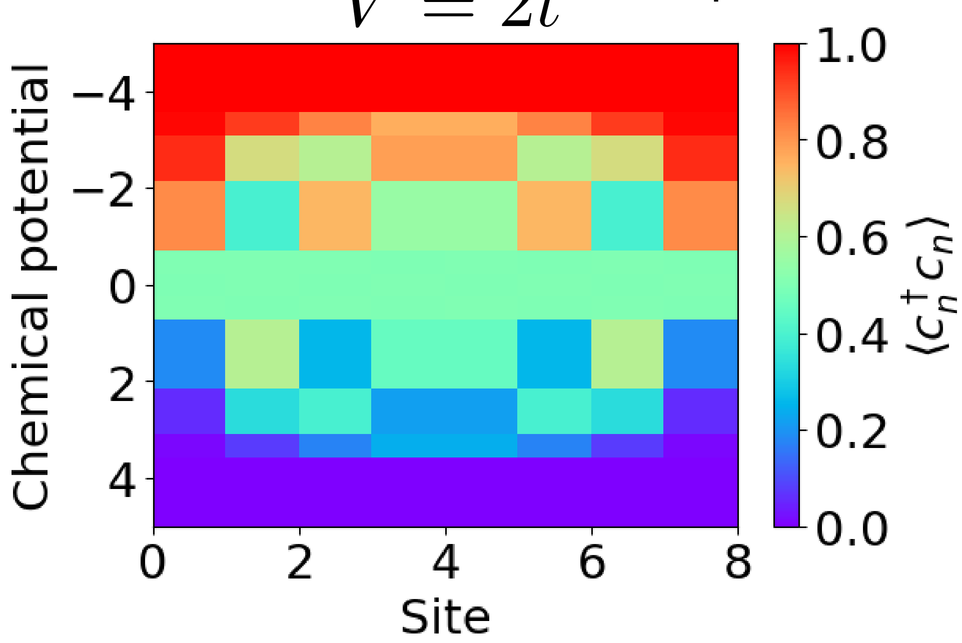
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right) \left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right) + \mu \sum_n c_n^\dagger c_n$$

Kinetic energy

Interaction

Chemical potential

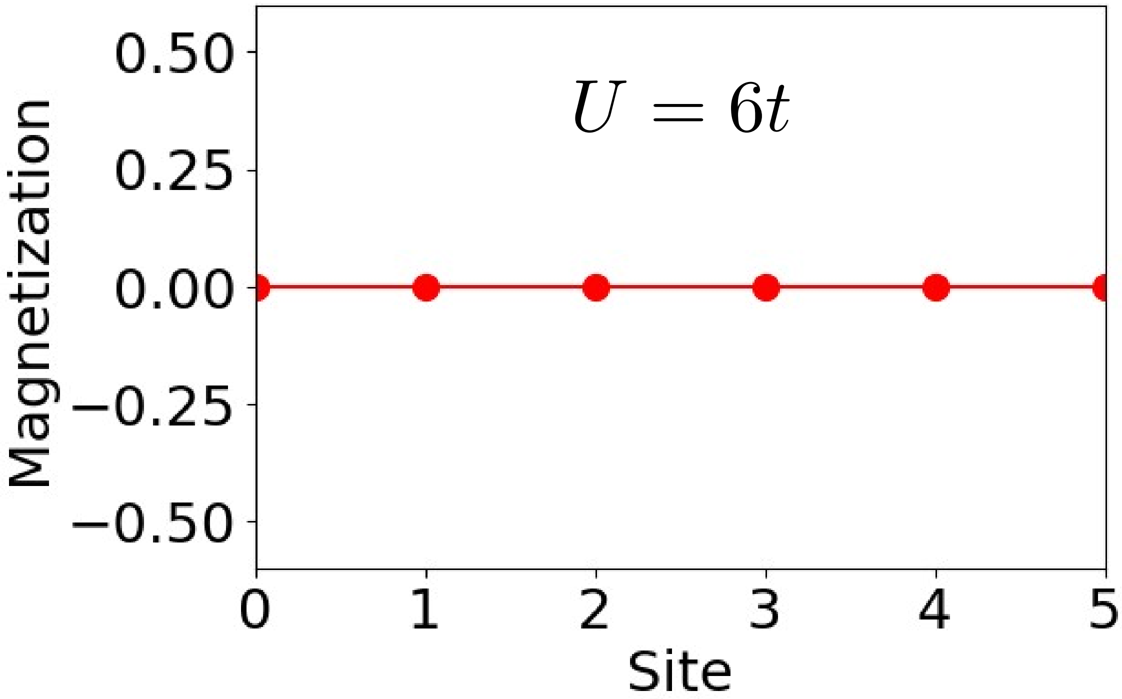




The many-body Hubbard model

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

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

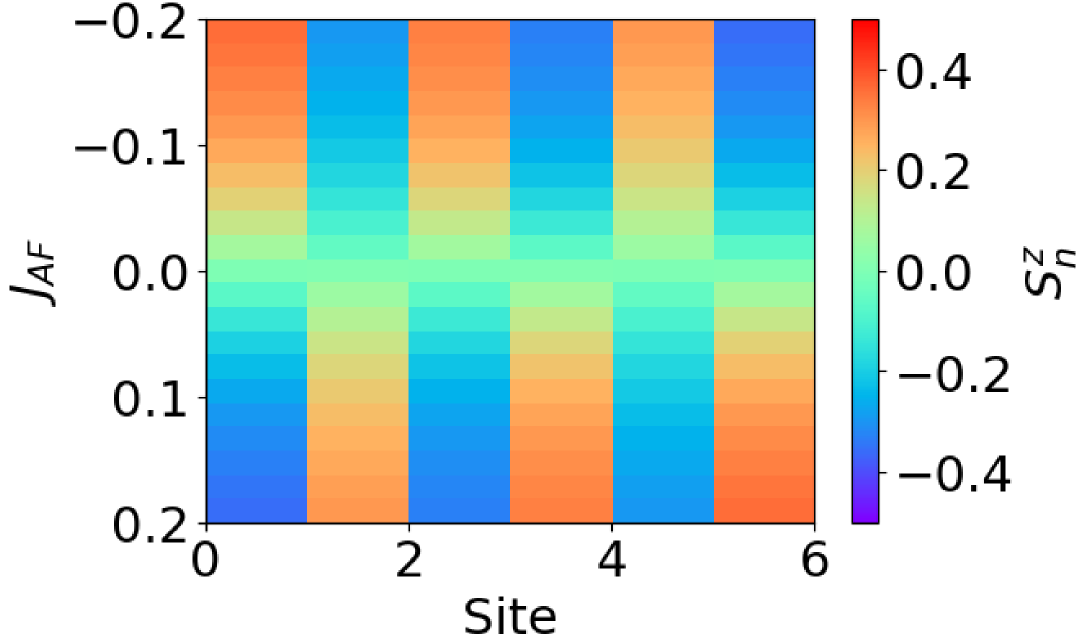
The Hubbard model, quantum and classical solution

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

Kinetic energy

Many-body interaction

Mean-field stagger magnetization



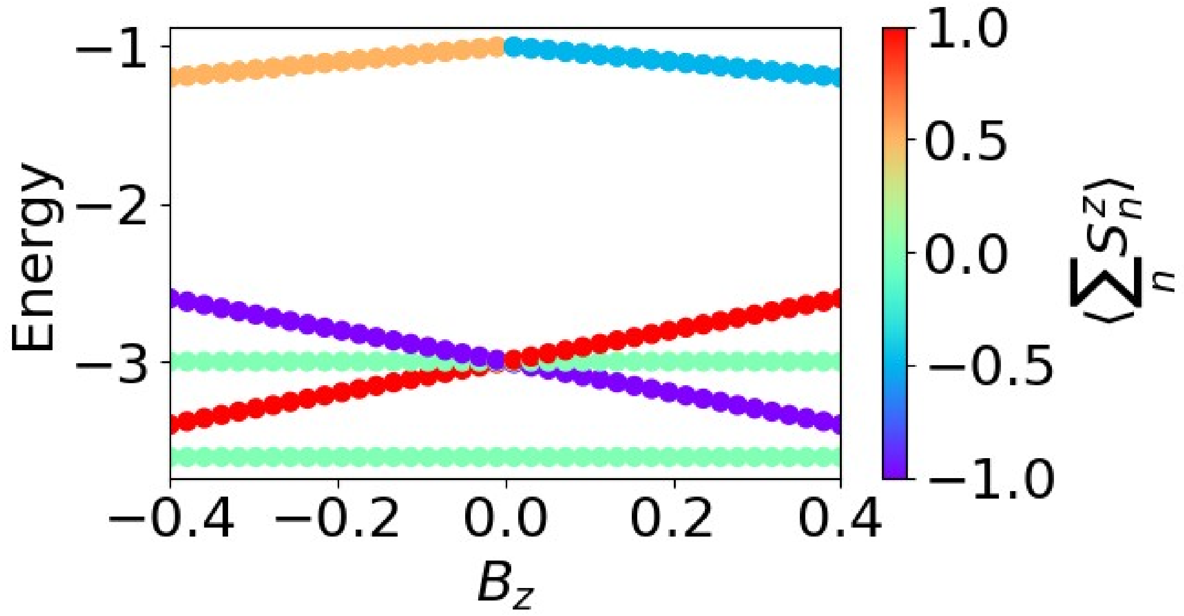
The magnetization is given by

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

The magnetization of the Hubbard dimer

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

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

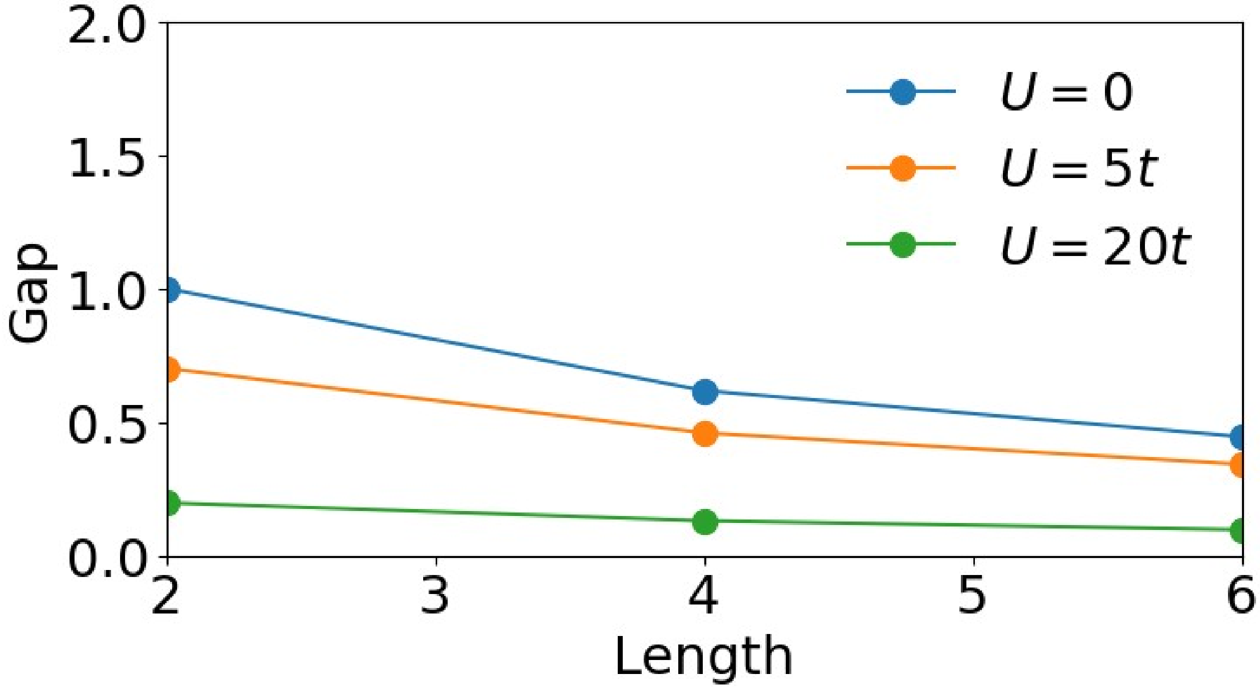


The magnetization is given by

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

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

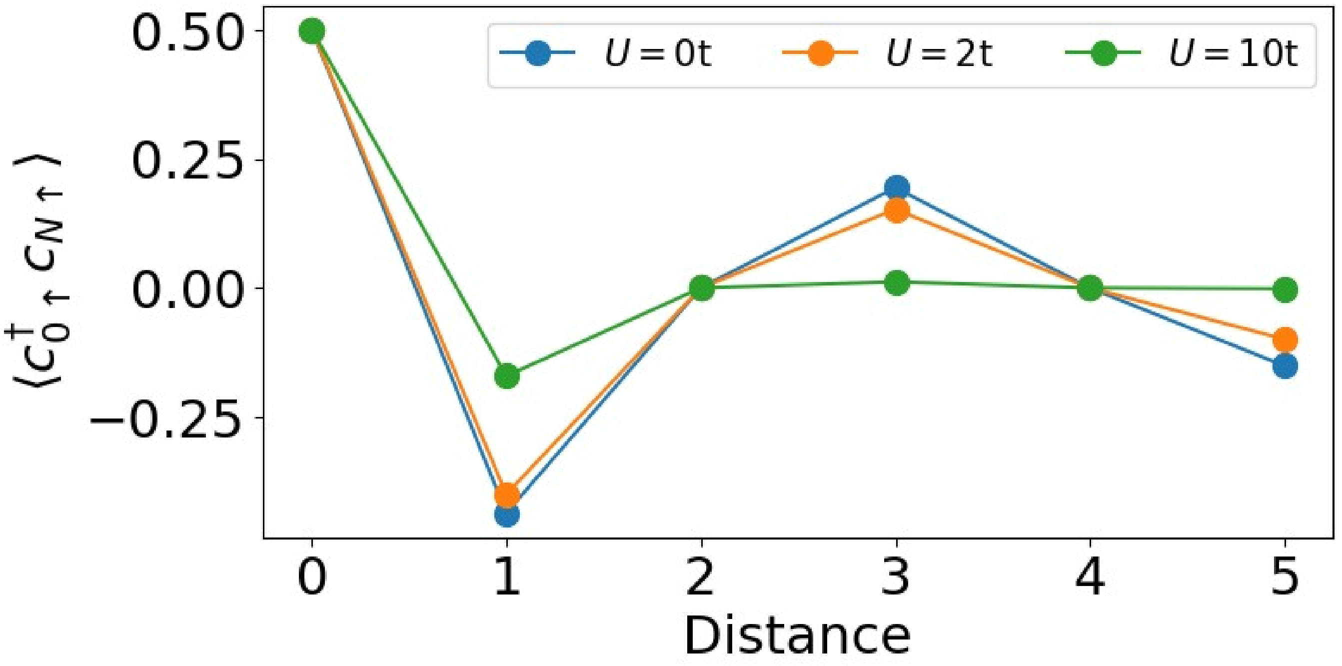
$$\chi_{ij} \sim e^{-\lambda|r_i - r_j|}$$

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

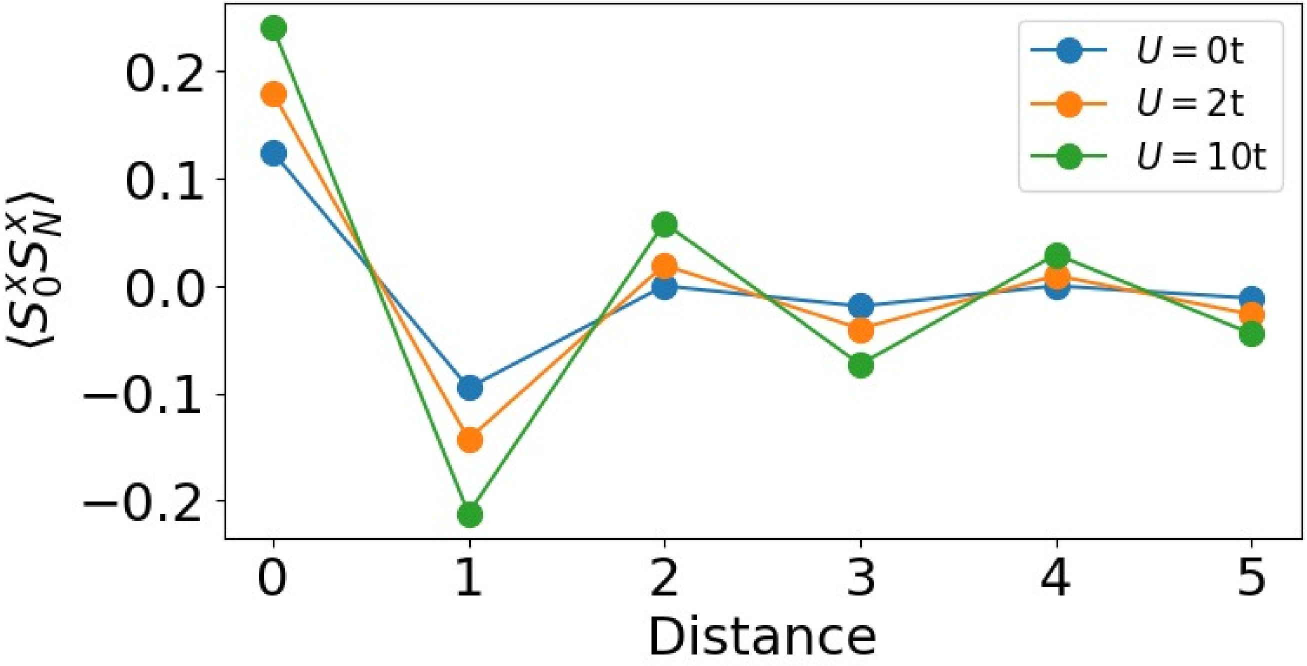
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

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)

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

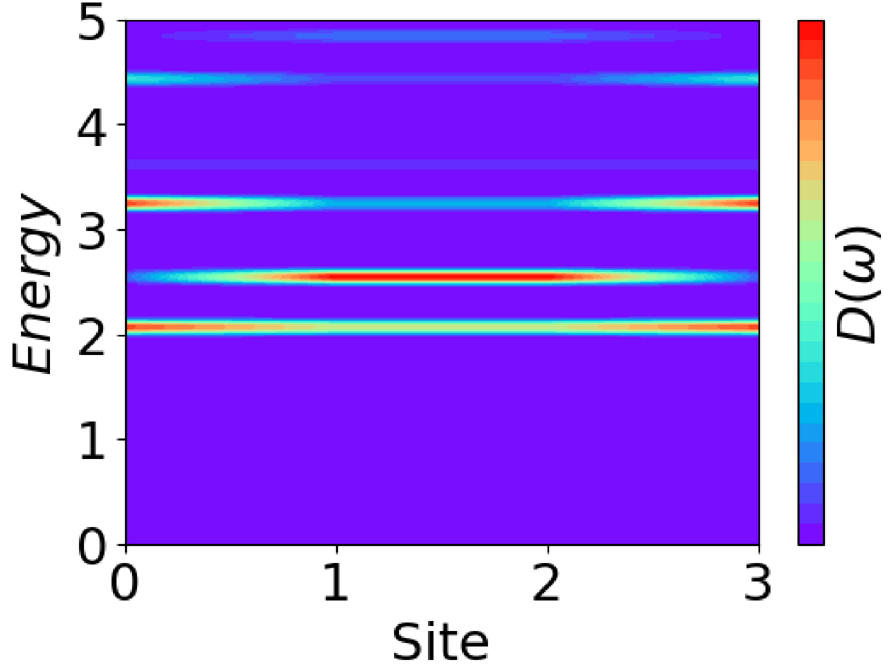
The spectral function above signal excited states that have one more spin excitation than the ground state

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

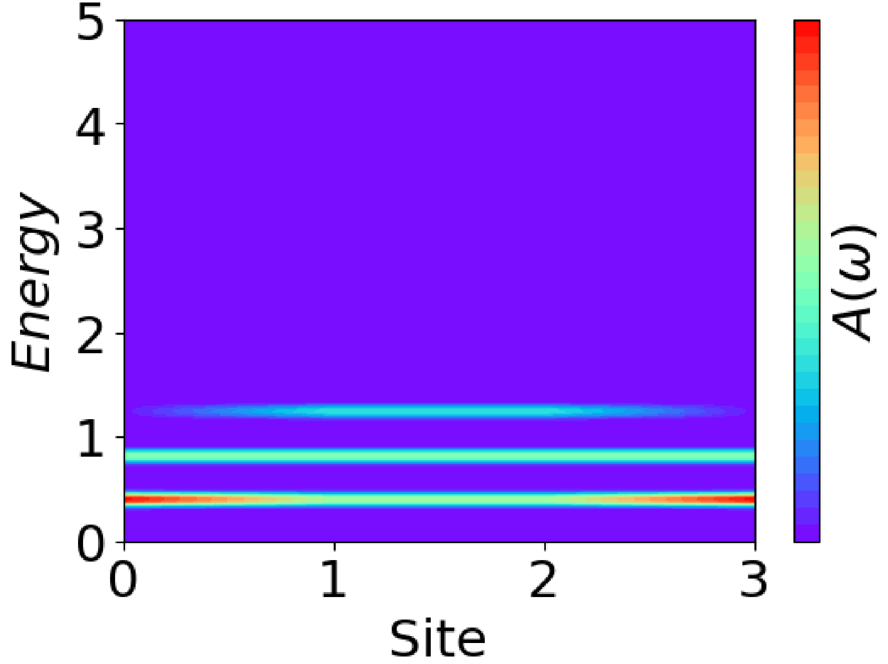
Dynamical correlators of the Hubbard model

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

Charge correlator $U = 6t$



Spin correlator $U = 6t$



Dynamical correlators of the Hubbard model

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