Many-body interactions and classical symmetry-broken magnetism

Learning outcomes

- Understand the origin of magnetism
- Identify the classical ground state of simple interacting Hamiltonians
- Rationalize how magnetic states emerge from interacting fermionic Hamiltonians

Different kinds of Hamiltonians

Single particle Hamiltonians $H = \sum_{ij} t_{ij} c_i^\dagger c_j$

Insulators, semiconductors, metals

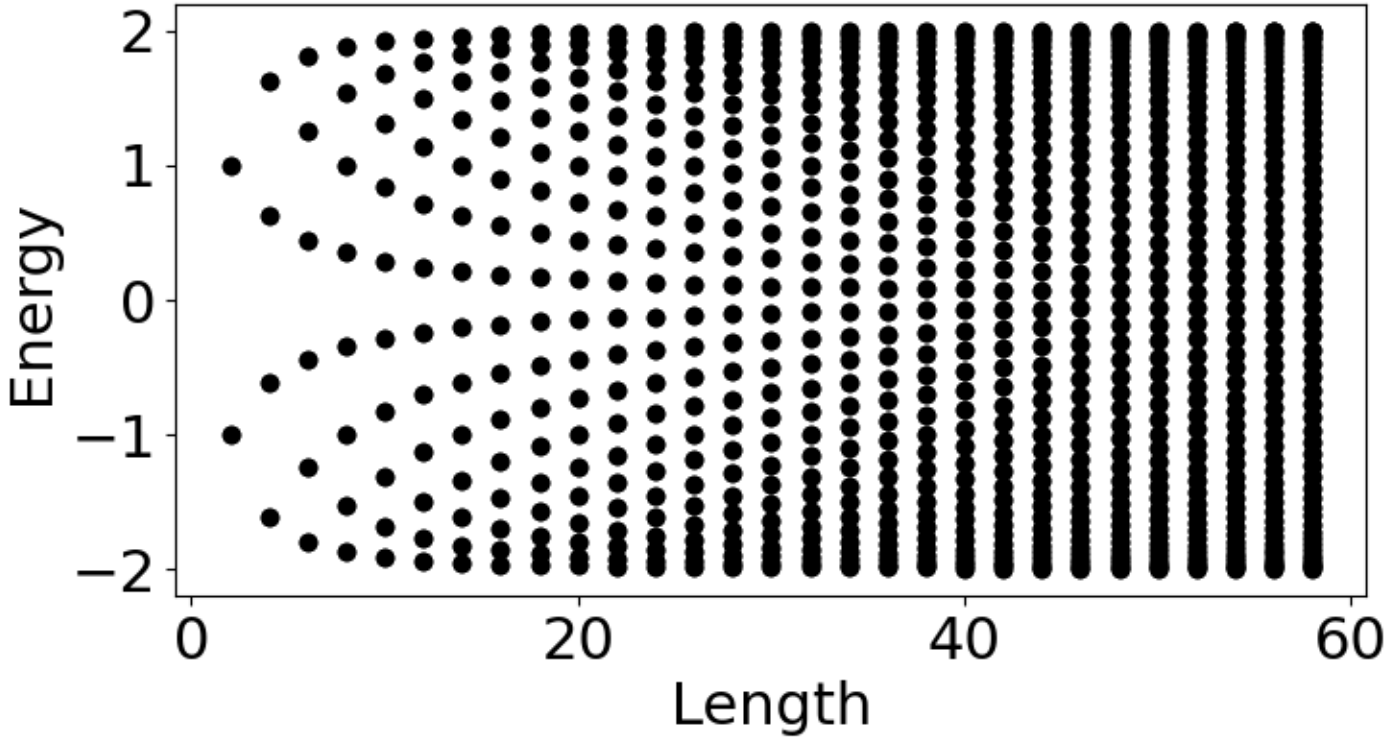
Many-body Hamiltonian $H = \sum_{ijkl} V_{ijkl} c_i^\dagger c_j c_k^\dagger c_l$

Classical and quantum magnets, charge density waves, superconductors

With second quantization, both cases can be treated on the same footing

Finite size effects in quantum systems

Let us consider a finite size fermionic system $H = \sum_{n=1,L} c_n^\dagger c_{n+1} + h.c.$

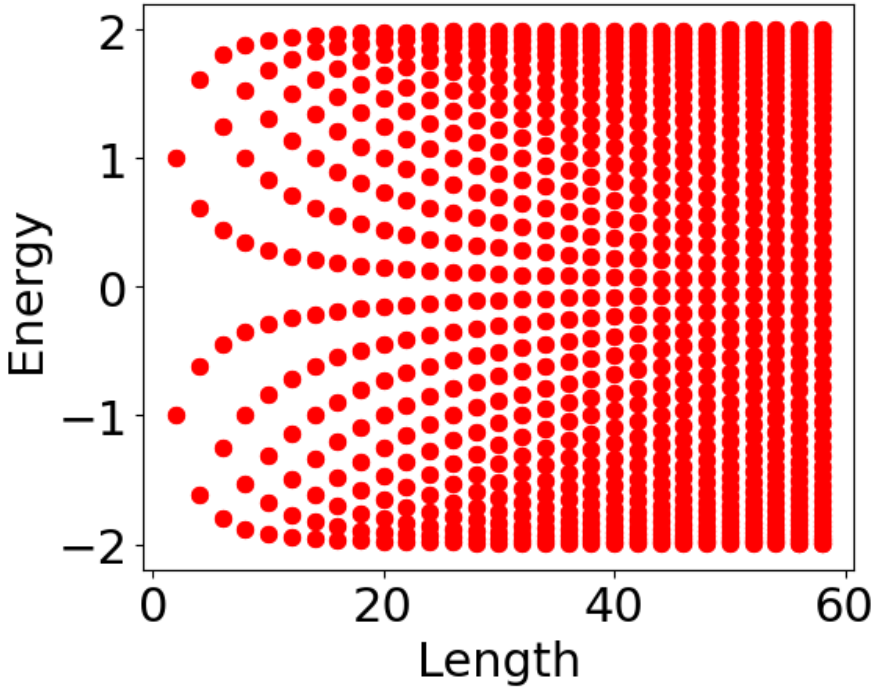


$$H|\psi_\alpha\rangle = \epsilon_\alpha|\psi_\alpha\rangle$$

Finite size effects in quantum systems

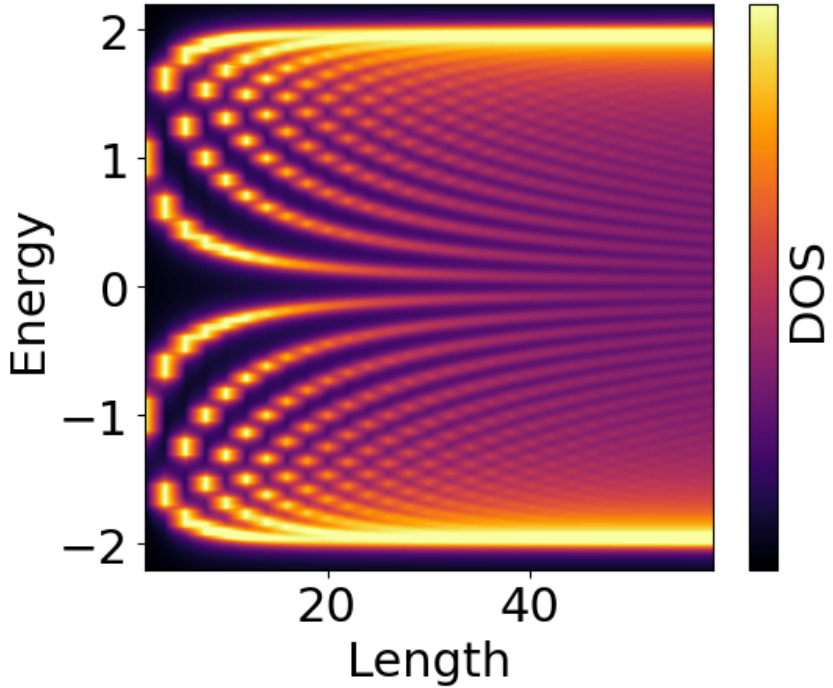
Hamiltonian

$$H = \sum_{n=1,L} c_n^\dagger c_{n+1} + h.c.$$



The density of states

$$D(\omega) = \mathrm{Tr}[\delta(\omega - H)]$$

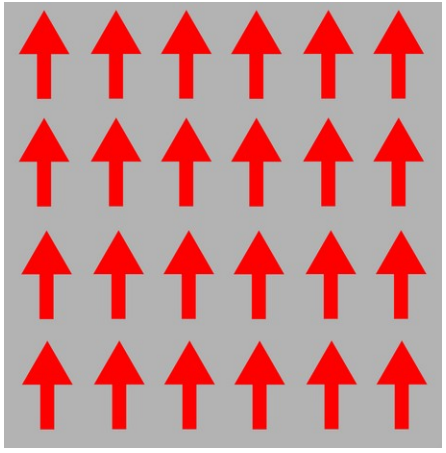


Electronic interactions in quantum systems

Electronic interactions are responsible for symmetry breaking

Broken time-reversal symmetry

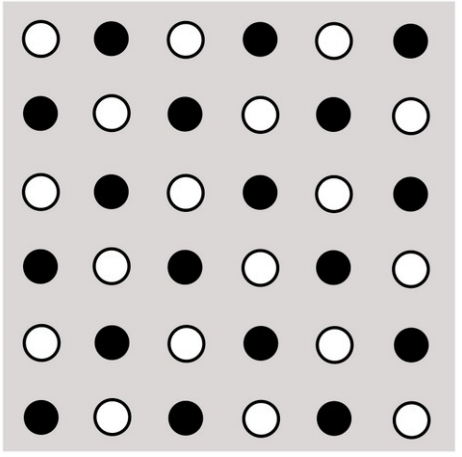
Classical magnets



$$\mathbf{M} \rightarrow -\mathbf{M}$$

Broken crystal symmetry

Charge density wave



$$\mathbf{r} \rightarrow \mathbf{r} + \mathbf{R}$$

Fundamentals of second quantization

Define operators that can create or destroy particles

c_i Annihilation operator, destroys a particle in site i

$c_i^\dagger$ Creation operator, creates a particle in site i

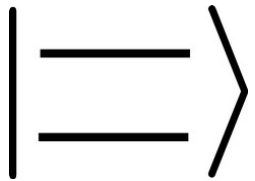
The empty vacuum state $|\Omega\rangle$ is defined as $c_i|\Omega\rangle = 0$

The Hamiltonian is written in terms of creation and annihilation operators

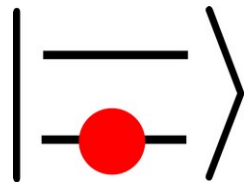
$$H = c_0^\dagger c_1 + h.c.$$

Fundamentals of second quantization

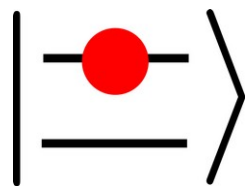
Lets see some examples using the two-levels presented before

$|\Omega\rangle =$ 

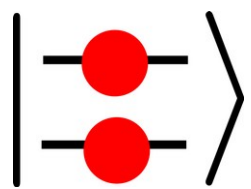
The “vacuum” state

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

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

Fermionic quantum statistics in second quantization

Fermi-Dirac statistics for electrons

→ Wavefunctions are antisymmetric with respect to interchanging labels

→ There can only be 0 or 1 fermion per level

$$\{c_i^\dagger, c_j\} = c_i^\dagger c_j + c_j c_i^\dagger = \delta_{ij} \qquad \{c_i, c_j\} = 0$$

Anti-symmetric wavefunction $c_0^\dagger c_1^\dagger |\Omega\rangle = -c_1^\dagger c_0^\dagger |\Omega\rangle$

At most one fermion per site $c_0^\dagger c_0^\dagger |\Omega\rangle = 0$

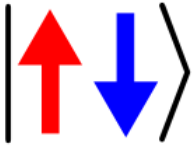
Three types of many-body sites

Spinful fermions

fully empty

down electron

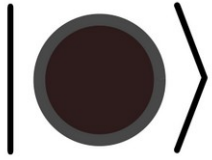
up electron



fully filled

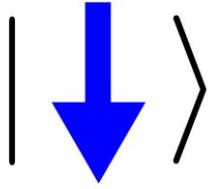
Spinless fermions

empty

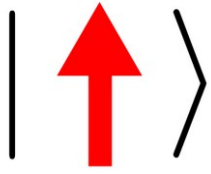


filled

Spins



down



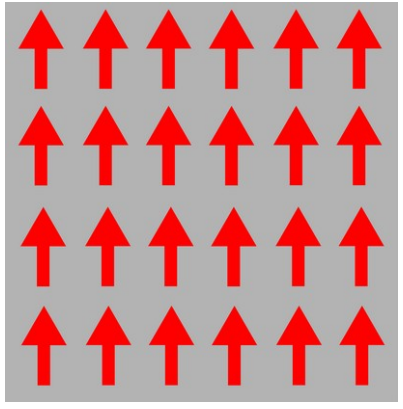
up

Many-body interactions and emergent states

Some quantum states can be approximately described by mean field theories

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

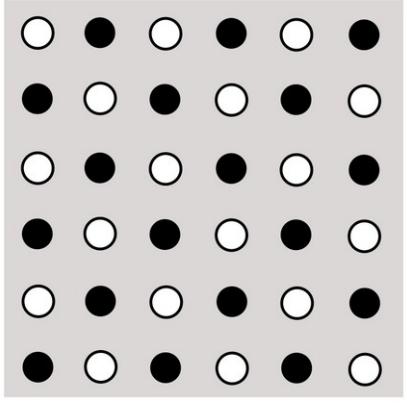
Magnets



Hubbard interaction

$$H \sim c_{\uparrow,n}^\dagger c_{\uparrow,n} c_{\downarrow,n}^\dagger c_{\downarrow,n}$$

Charge density waves



Nearest-neighbor repulsion

$$H \sim c_n^\dagger c_n c_{n+1}^\dagger c_{n+1}$$

Interactions and mean field

Free Hamiltonian ***Interactions***

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

What are these interactions coming from?

- Electrostatic (repulsive) interactions
- Mediated by other quasiparticles (phonons, magnons, plasmons,...)

The net effective interaction can be attractive or repulsive

Magnetism is promoted by repulsive interactions

A spinful interacting Hamiltonian

Free Hamiltonian ***Interactions (Hubbard term)***

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

How can we solve this many-body Hamiltonian in an approximate way?

Is there an effective single particle Hamiltonian that describes the same ground state?

$$H_{MF} = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_{ijss'} \chi_{ijss'} c^\dagger_{is} c_{js'}$$

The mean-field approximation

Mean field: *Approximate four fermions by two fermions times expectation values*

Four fermions (not exactly solvable) ***Two fermions (exactly solvable)***

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx U \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle c^\dagger_{i\downarrow} c_{i\downarrow} + ... + h.c.$$

$$U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \approx M \sigma^z_{ss'} c^\dagger_{i,s} c_{i,s'} + h.c.$$

For $U > 0$
i.e. repulsive interactions

Magnetic order
$$M \sim \langle c^\dagger_{i\uparrow} c_{i\uparrow} \rangle - \langle c^\dagger_{i\downarrow} c_{i\downarrow} \rangle$$

The mean-field approximation

The non-collinear mean-field Hamiltonian

$$U c^\dagger_{n\uparrow} c_{n\uparrow} c^\dagger_{n\downarrow} c_{n\downarrow} \approx M^\alpha_n \sigma^\alpha_{ss'} c^\dagger_{n,s} c_{n,s'} + h.c.$$

Non-collinear magnetic order

$$M^z_n \sim \langle c^\dagger_{n\uparrow} c_{n\uparrow} \rangle - \langle c^\dagger_{n\downarrow} c_{n\downarrow} \rangle$$

$$M^x_n \sim \langle c^\dagger_{n\uparrow} c_{n\downarrow} \rangle + \langle c^\dagger_{n\downarrow} c_{n\uparrow} \rangle$$

$$M^y_n \sim i\langle c^\dagger_{n\uparrow} c_{n\downarrow} \rangle - i\langle c^\dagger_{n\downarrow} c_{n\uparrow} \rangle$$

The mean-field approximation

The mean-field approximation is equivalent to finding a variational wavefunction of the form

$$|GS\rangle = \prod_\alpha \psi_\alpha^\dagger |\Omega\rangle$$

$$\psi_\alpha^\dagger = \sum_n \chi_{\alpha,n} c_n^\dagger$$

Such that it minimizes the expectation value of the energy

$$E = \langle GS|H|GS\rangle \qquad \frac{\delta E}{\delta \chi} = 0 \qquad \frac{\delta E}{\delta \langle c_i^\dagger c_j \rangle} = 0$$

This assumption, leads to a selfconsistent problem for the mean-field Hamiltonian

$$H^{MF}_{(1)} \rightarrow \langle c_i^\dagger c_j \rangle_{(1)} \rightarrow H^{MF}_{(2)} \rightarrow \langle c_i^\dagger c_j \rangle_{(2)} \rightarrow H^{MF}_{(3)} \rightarrow \ldots$$

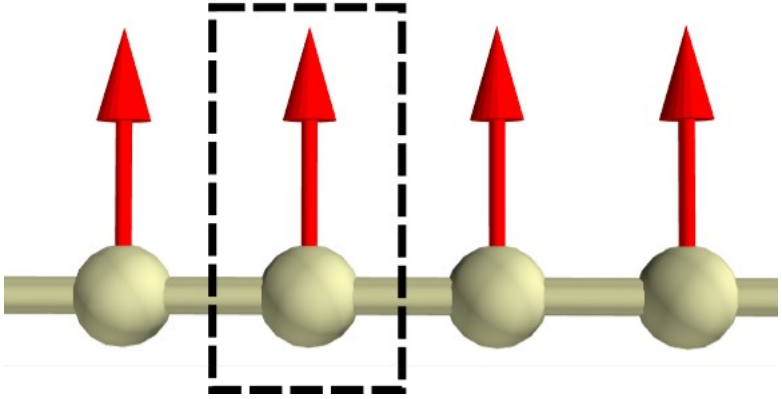
Solving the interacting model at the mean-field level in a 1D chain

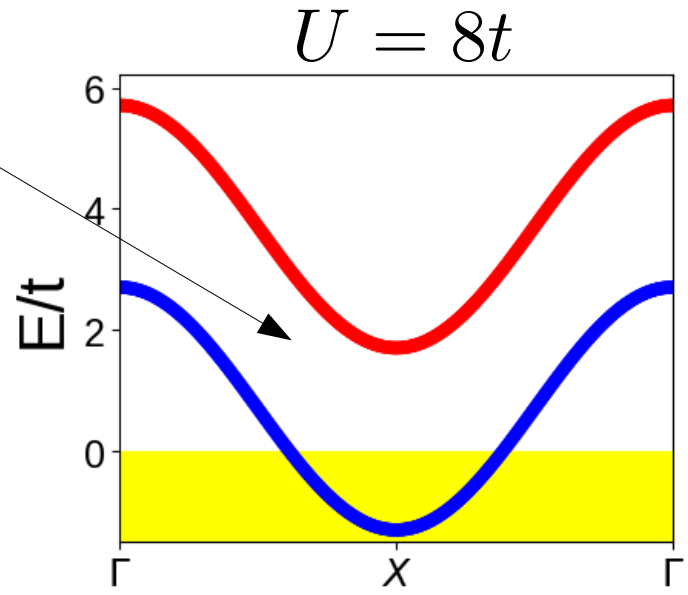
We will take the interacting model and solve it at the mean field level

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

Filling 0.2 (full would be 1)

Interaction-induced splitting

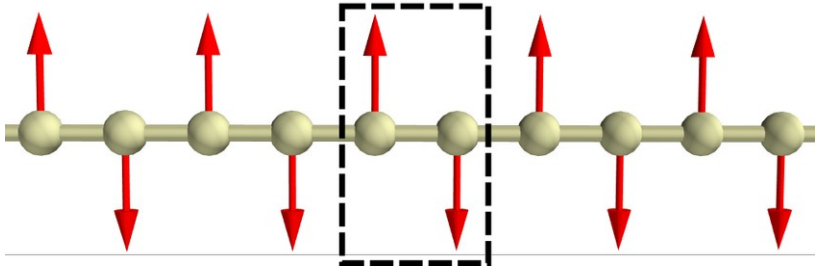


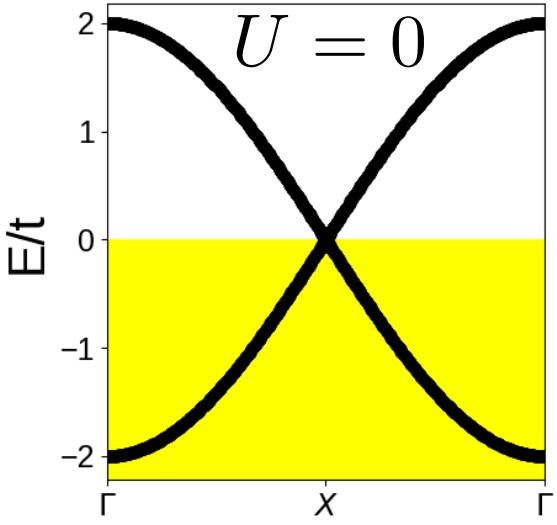


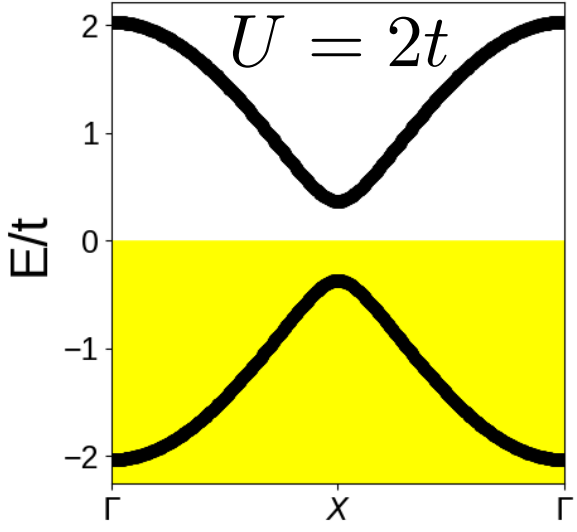
Solving the interacting model at the mean-field level in a 1D chain

Let us do again a 1D, but now with 2 sites per unit cell and at half filling

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

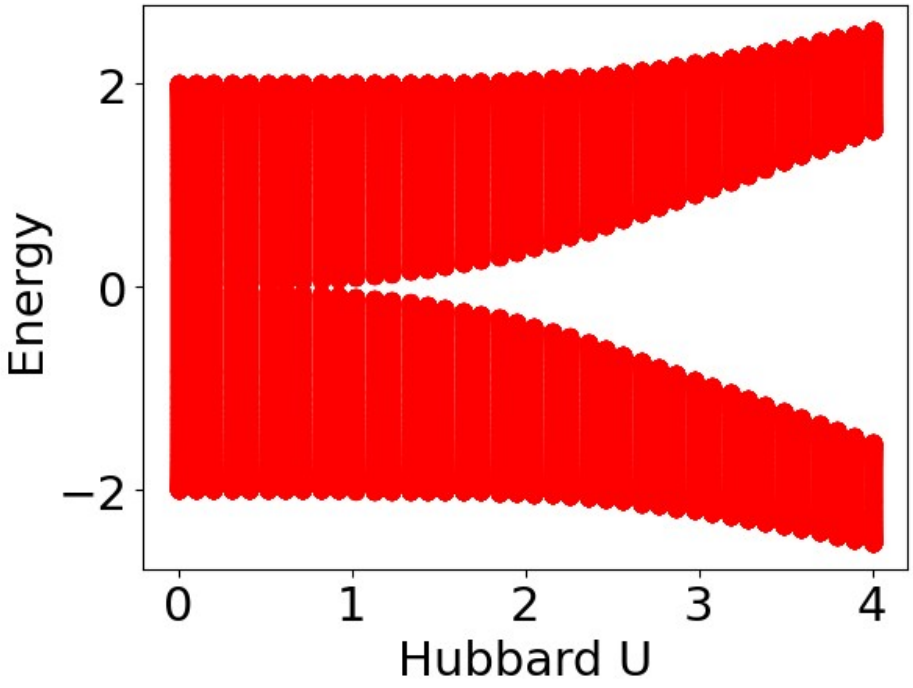


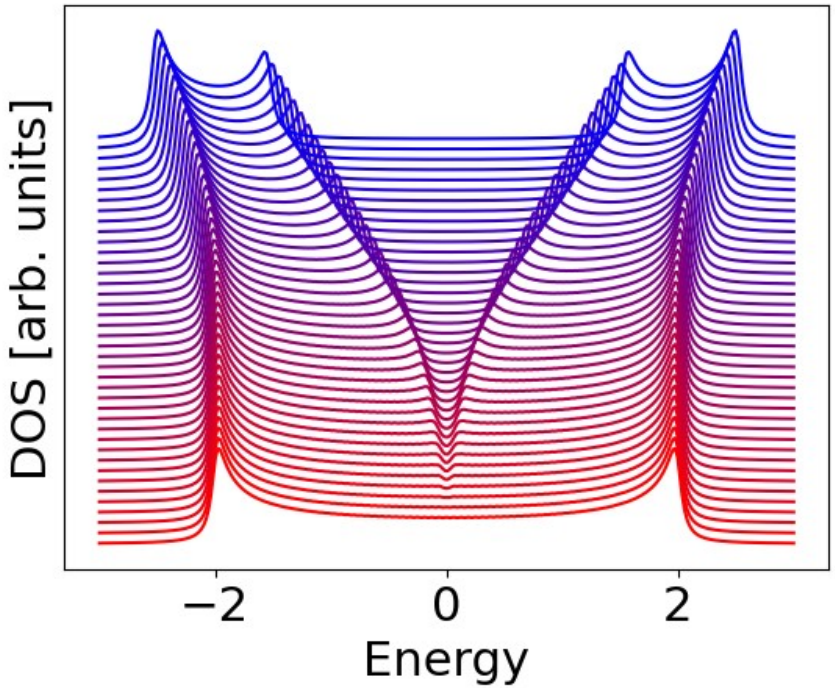




Interaction-induced gap opening

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



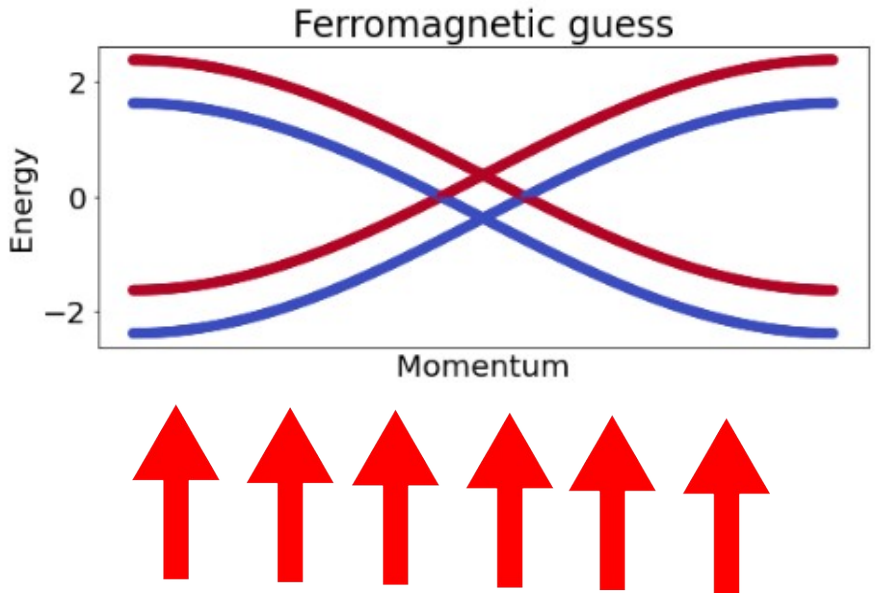


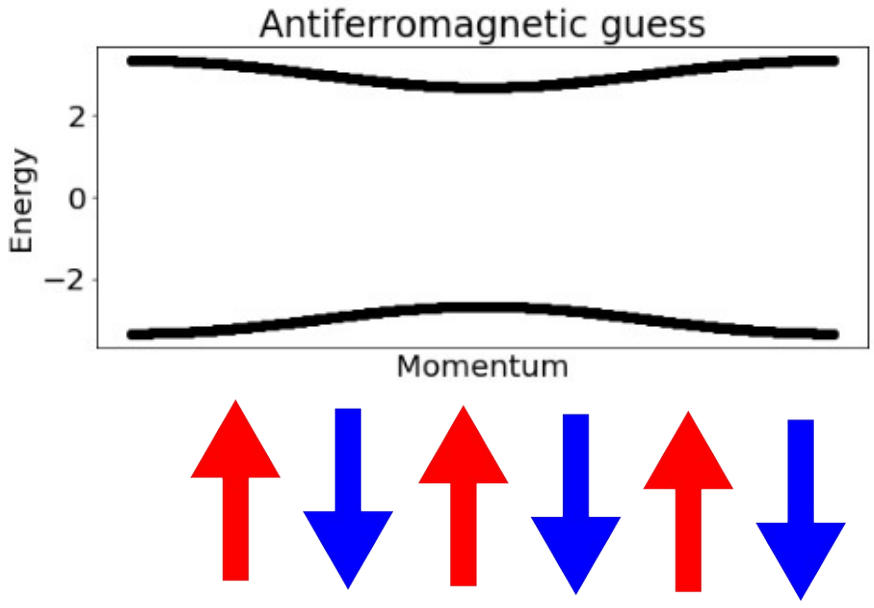
$U = 4t$

$U = 0$

Competing magnetic solutions

Let us now consider two selfconsistent solutions for the interacting model

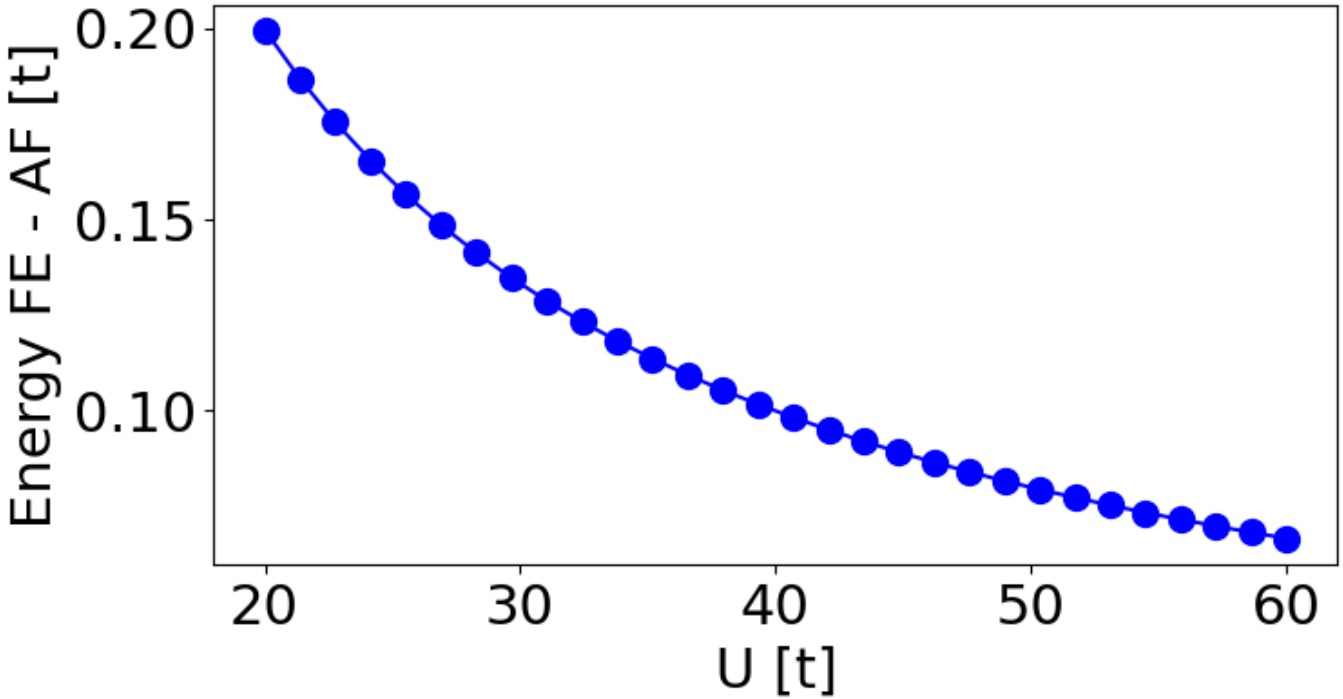




Only once of them is the true ground state, but which one it is?

Competing magnetic solutions

Let us now compute the energy difference between the two configurations



$\Delta E =$ ↑↑ - ↑↓

$\Delta E \sim \frac{1}{U}$

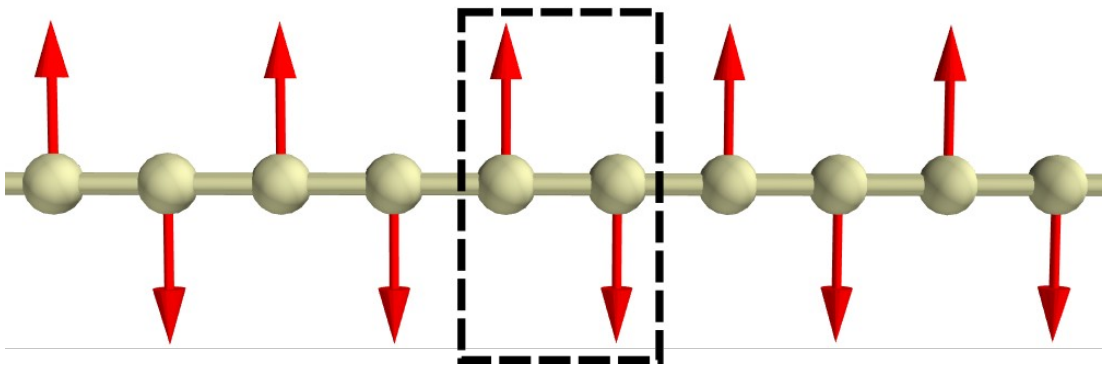
For strong interactions, the AF configuration always has lower energy

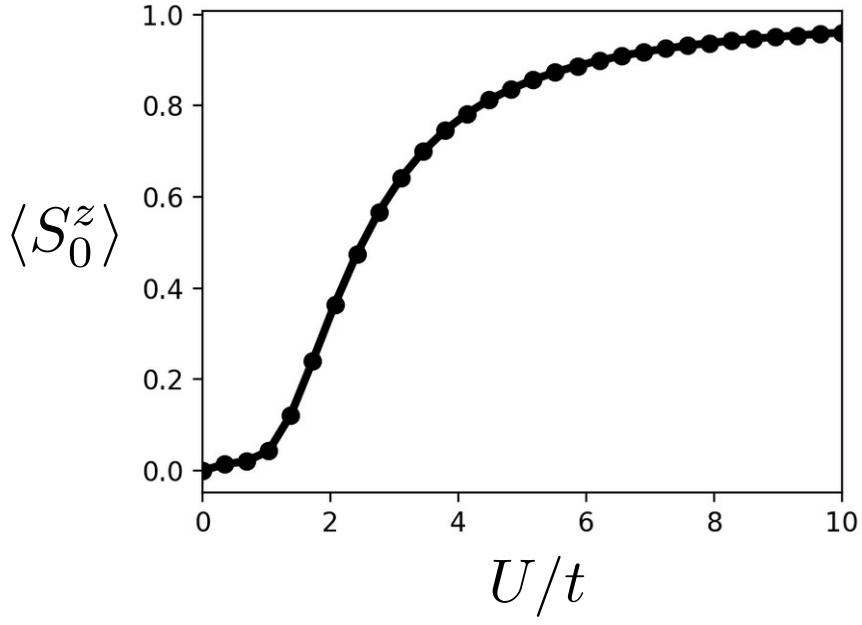
The strongly localized limit and the Heisenberg model

From a weak magnet to the strongly localized limit

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

For large interaction strength, the system develops a local quantized magnetic moment





The strongly localized limit

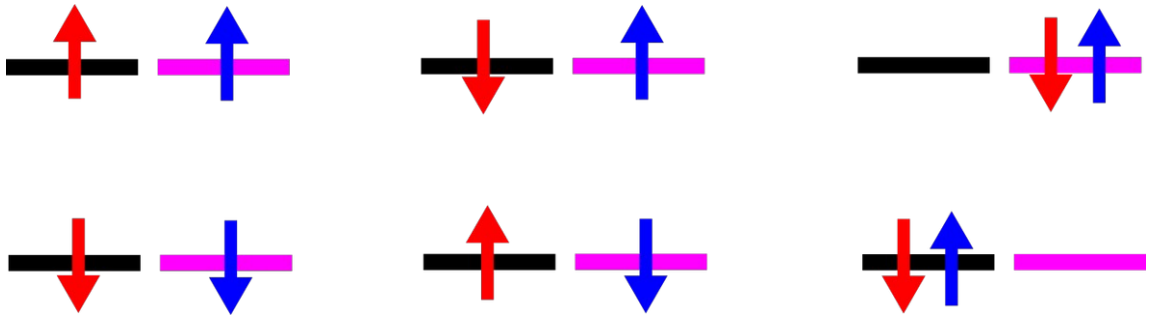
Let us start with a Hubbard model dimer

$$H = t[c^\dagger_{0\uparrow} c_{1\uparrow} + c^\dagger_{0\downarrow} c_{1\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + h.c.$$

Now in the limit $U \gg t$

Levels

The full Hilbert space at half filling is



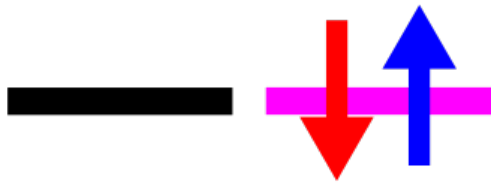
The strongly localized limit

Let us start with a Hubbard model dimer

$$H = t[c^{\dagger}_{0\uparrow}c_{1\uparrow} + c^{\dagger}_{0\downarrow}c_{1\downarrow}] + \sum_i U c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow} + h.c.$$

The energies in the strongly localized limit are $U \gg t$

~ 0



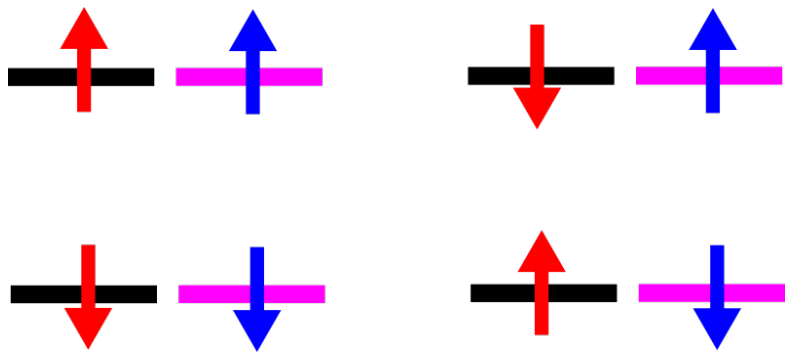
$\sim U$

The strongly localized limit

Let us start with a Hubbard model dimer

$$H = t[c^{\dagger}_{0\uparrow}c_{1\uparrow} + c^{\dagger}_{0\downarrow}c_{1\downarrow}] + \sum_i U c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow} + h.c.$$

The low energy manifold is



Just one electron in each site for $U \gg t$

Local S=1/2 at each site

The strongly localized limit

Effective Heisenberg model in the localized limit $\mathcal{H} = J\vec{S}_0 \cdot \vec{S}_1$

We can compute J using second order perturbation theory

$$H = H_0 + V$$

$$H_0 = \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

"pristine" Hamiltonian
(Hubbard)

$$V = t[c^\dagger_{0\uparrow} c_{1\uparrow} + c^\dagger_{0\downarrow} c_{1\downarrow}] + \text{h.c.}$$

"perturbation" Hamiltonian
(hopping)

The strongly localized limit

Effective Heisenberg model in the localized limit $\mathcal{H} = J\vec{S}_0 \cdot \vec{S}_1$

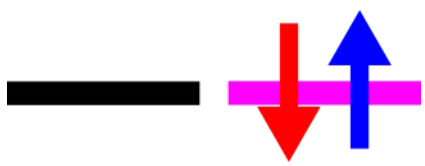
We can compute J using second order perturbation theory

$$H = H_0 + V$$

$$J \sim \frac{t^2}{U}$$

Ground state

Virtual state



The Heisenberg 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

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

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

The Heisenberg model

Non-Hubbard (multiorbital) models also yield effective Heisenberg models

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

In those generic cases, the exchange couplings can be positive or negative

$J_{ij} > 0$

Antiferromagnetic coupling

$J_{ij} < 0$

Ferromagnetic coupling

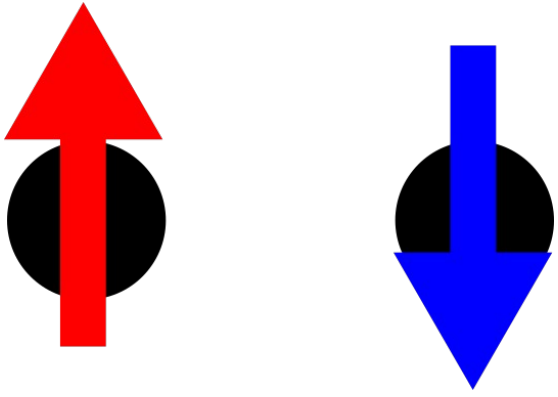
Spin-orbit coupling introduces anisotropic couplings

$$\mathcal{H} = \sum_{ij} J_{ij}^{\alpha\beta} S_i^{\alpha} S_j^{\beta}$$

The Heisenberg model

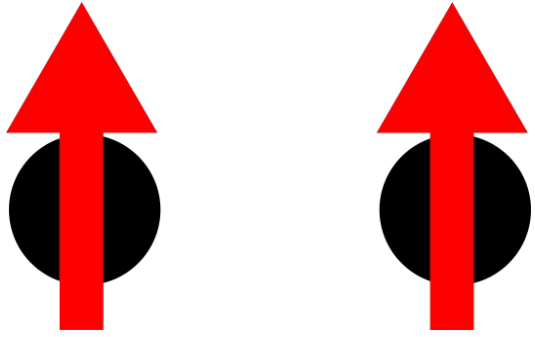
$J_{ij} > 0$

Antiferromagnetic coupling



$J_{ij} < 0$

Ferromagnetic coupling



Classical ground states

Antiferromagnetism driven by superexchange

In the square lattice

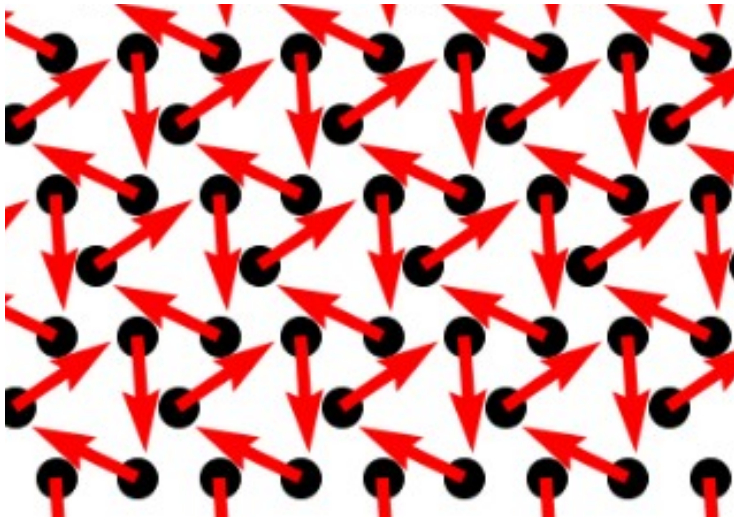
In the honeycomb lattice

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

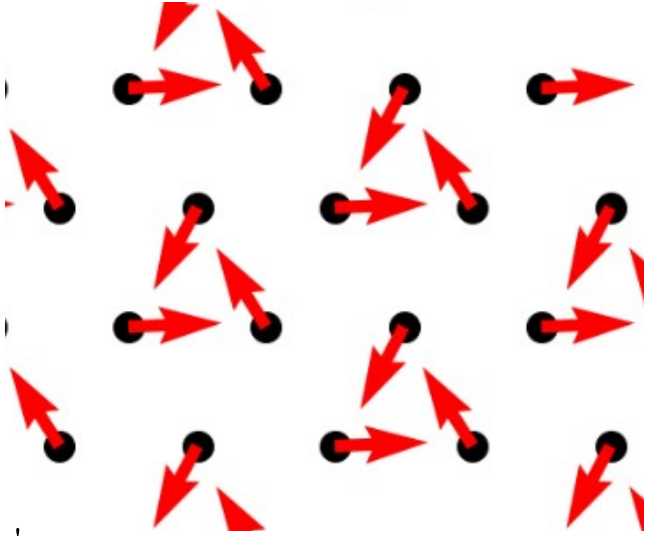
In bipartite lattices, the magnetization is collinear

Antiferromagnetism driven by superexchange

In the Kagome lattice



In the triangular lattice



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

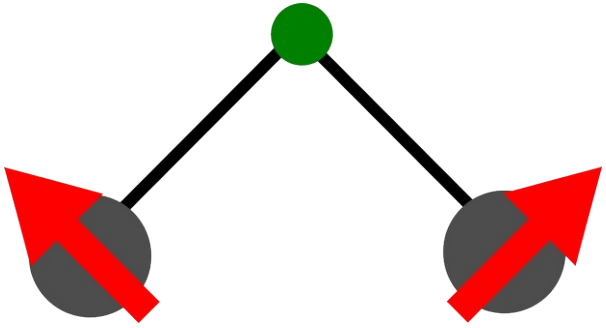
Geometric frustration promotes non-collinear order at the mean-field level

Non-isotropic exchange coupling

In the presence of spin-orbit coupling, new terms can appear in the Hamiltonian

Antisymmetric exchange

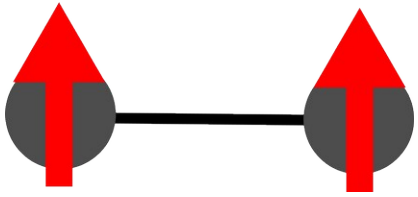
$$(\mathbf{r}_{ik} \times \mathbf{r}_{kj}) \cdot \vec{S}_i \times \vec{S}_j$$



Promotes
non-collinear order

Anisotropic exchange

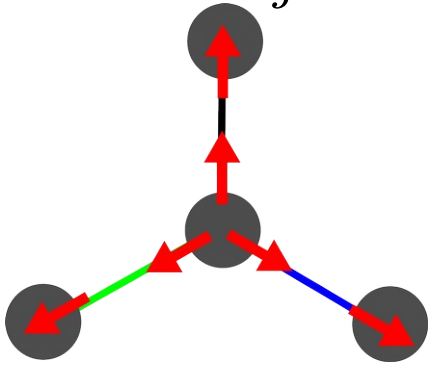
$$S_i^z S_j^z$$



Promotes
easy axis/plane

Kitaev interaction

$$S_i^{\alpha(i)} S_j^{\alpha(j)}$$



Promotes
frustration

Beyond local-interactions

Non-local interactions also lead to many-body correlated states

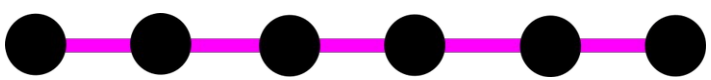
Let us take a spinless model with first neighbor repulsion

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

Two limits

$V = 0$

Non-interacting limit

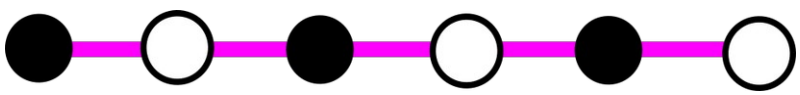


$\langle c_n^\dagger c_n \rangle = 1/2$

Featureless metal

$V \gg t$

Strongly interacting

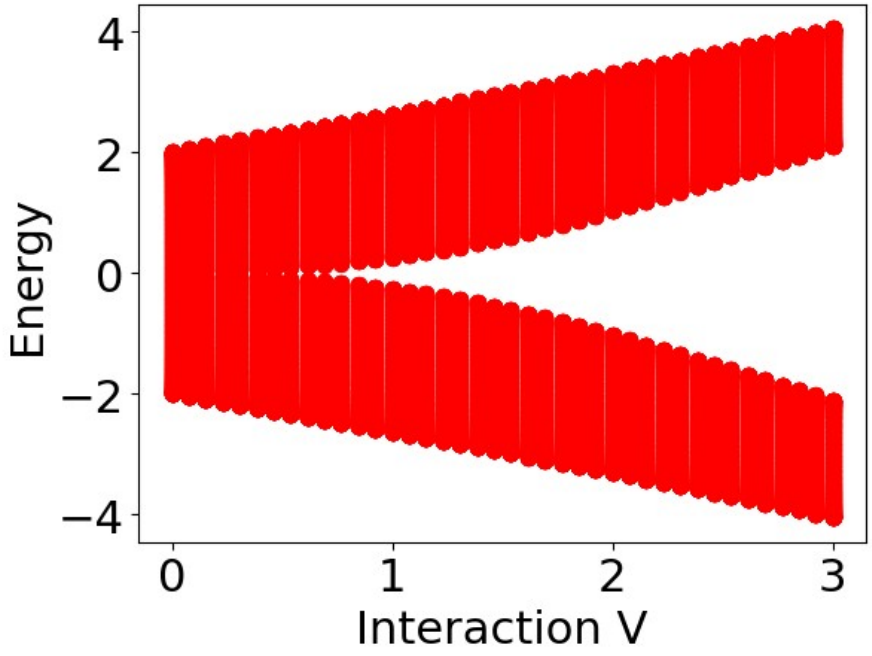


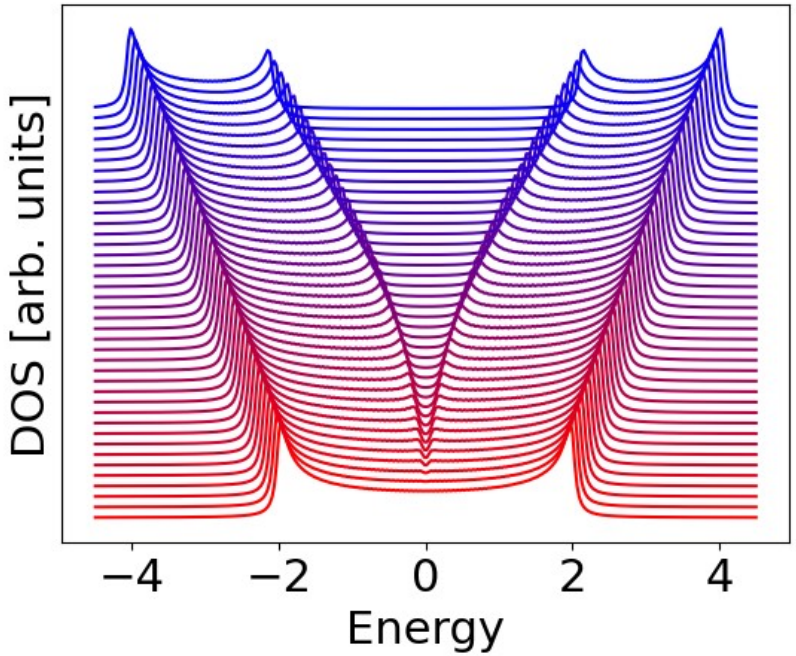
$\langle c_n^\dagger c_n \rangle = 0, 1$

Charge density wave

The impact of non-local interactions in the electronic spectra

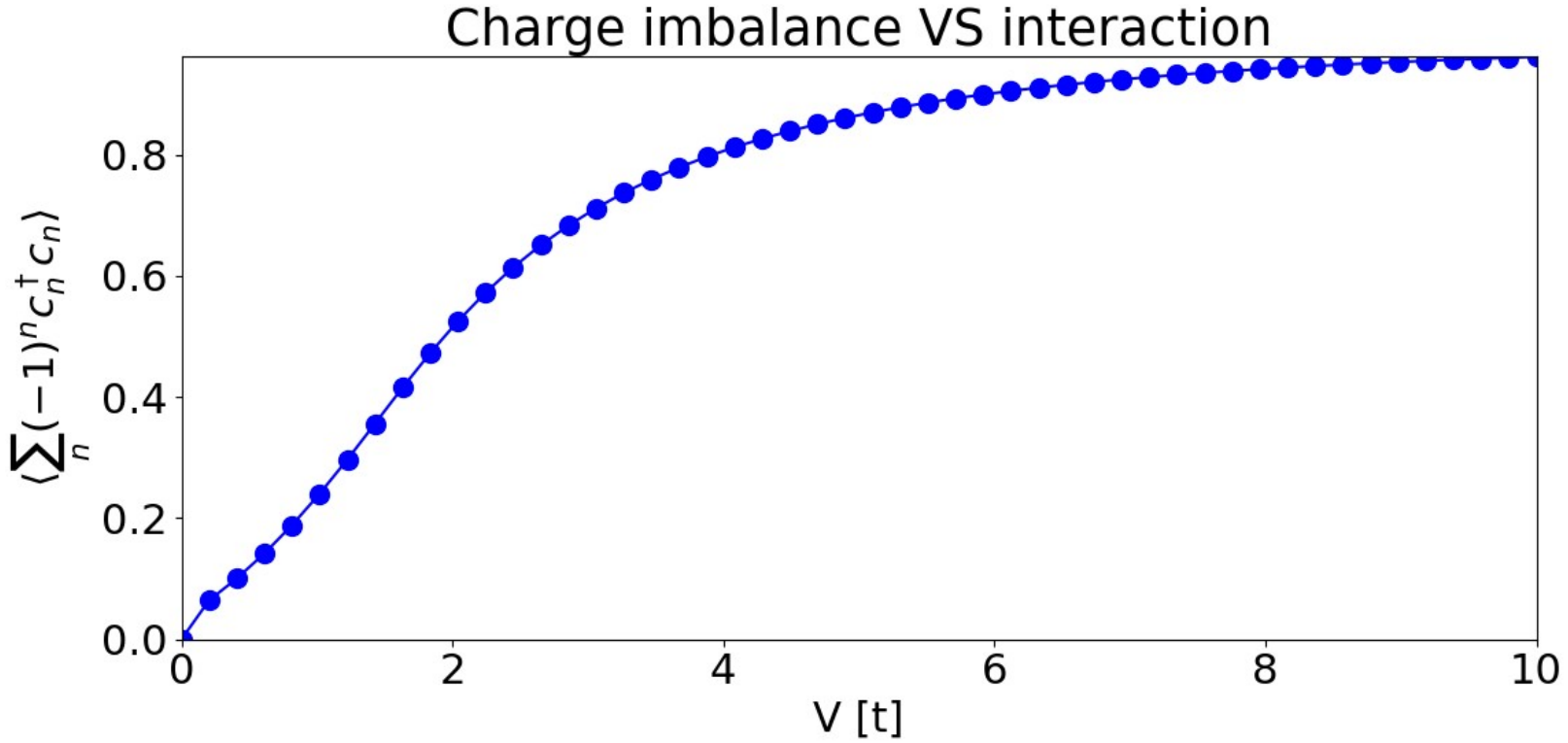
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V \sum_n \left(c_n^\dagger c_n - \frac{1}{2}\right)\left(c_{n+1}^\dagger c_{n+1} - \frac{1}{2}\right)$$





Interaction induced charge density wave

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



The breakdown of mean-field

The limitations of mean-field theory

The true ground state of the Hubbard model in 1D does not break time-reversal symmetry

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

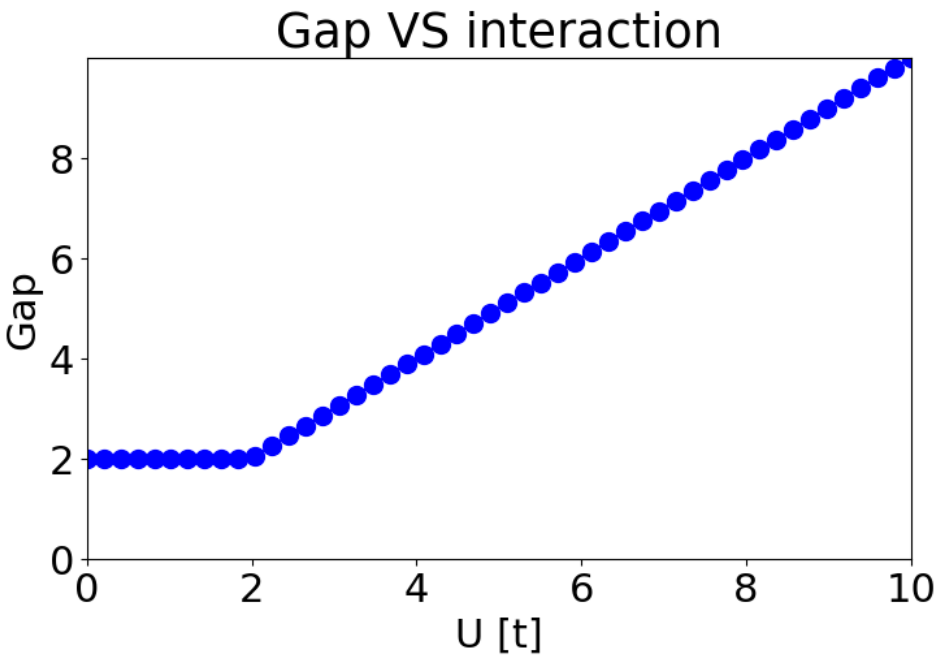
But the mean-field Hamiltonian by construction breaks time reversal symmetry

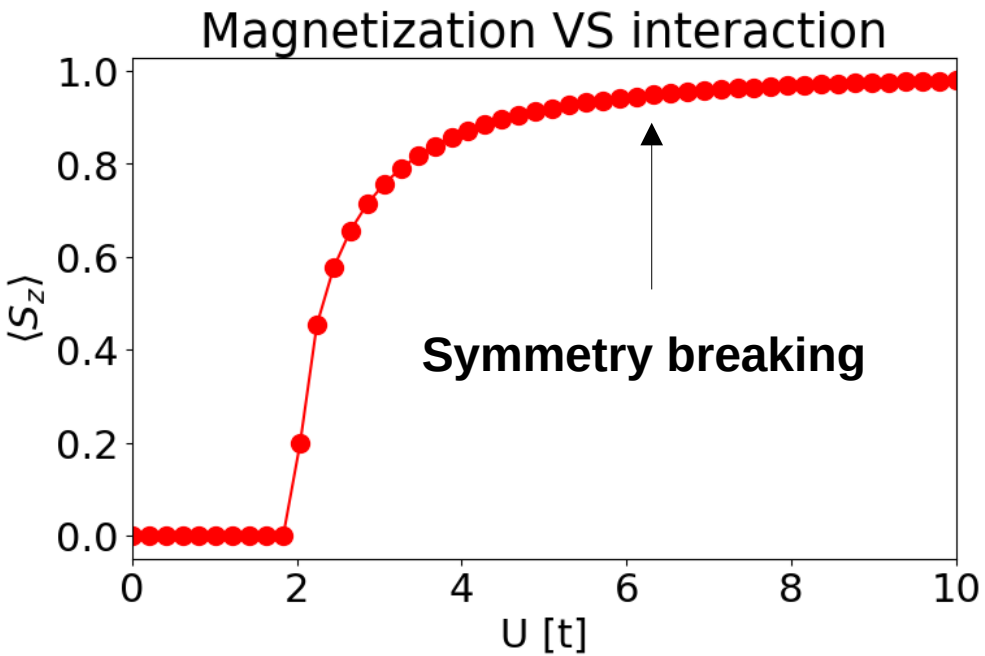
$$H = t\sum_{s,n} c^{\dagger}_{n,s}c_{n+1,s} + h.c. + \sum_{i} M_i \sigma^{z}_{s,s'} c^{\dagger}_{i,s}c_{i,s'}$$

What is the origin of this limitation, and how can we overcome it?

The Hubbard dimer

Let us consider a Hubbard dimer $H = tc^{\dagger}_{1,s}c_{2,s} + h.c. + U\sum_n \left(c^{\dagger}_{n,\uparrow}c_{n,\uparrow} - \frac{1}{2}\right)\left(c^{\dagger}_{n,\downarrow}c_{n,\downarrow} - \frac{1}{2}\right)$





The entangled ground state of the Heisenberg dimer

Let us now take the Hubbard dimer in the strongly interacting limit

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

For $U \gg t$ we obtain the Heisenberg model

$$\mathcal{H} = J\vec{S}_1 \cdot \vec{S}_2$$

Mean field ground state

$$|\Psi_1\rangle = |\uparrow\downarrow\rangle$$

$$|\Psi_2\rangle = |\downarrow\uparrow\rangle$$

True ground state

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

Mean-field cannot describe a strongly localized limit featuring entanglement