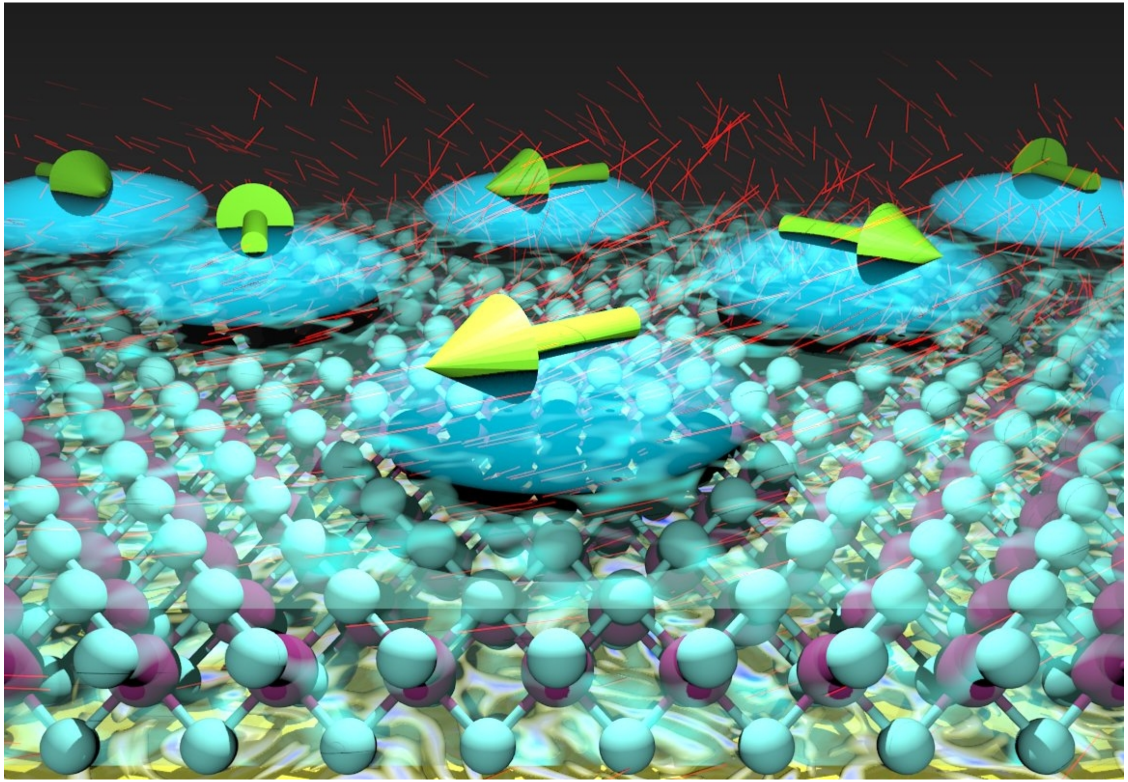
Magnetic 2D materials



Jyväskylä Summer School "Emergent Quantum Matter in Artificial Two-dimensional Materials"

Wednesday August 10th 2022

Schedule for the lecture

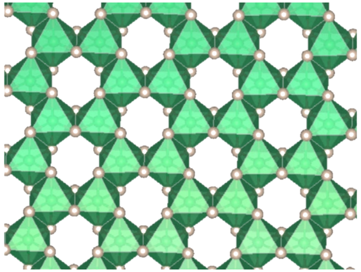
- 40 min lecture
- 15 min break
- 40 min lecture
- 15 min break
- 40 min lecture

Today’s plan

- The origin of magnetic exchange
- Antiferromagnets, ferromagnets and multiferroics
- Magnetic order and magnons in 2D materials
- Van der Waals quantum spin liquids
- Van der Waals heavy-fermion Kondo insulators

Van der Waals magnetic materials

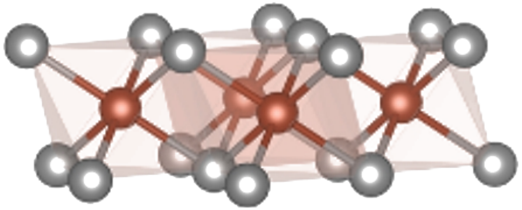
Ferromagnet, antiferromagnets



CrI_3, $CrCl_3$, $CrBr_3$

Break time-reversal

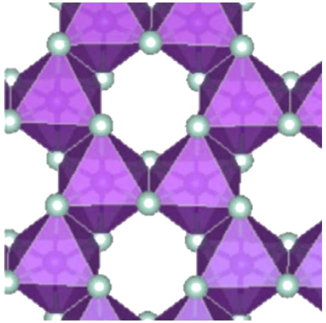
Multiferroics



NiI_2

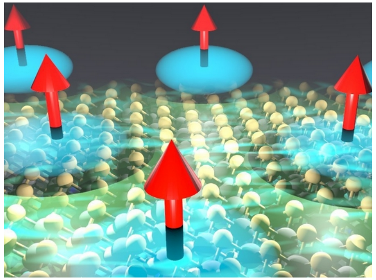
Break time-reversal and inversion symmetry

(proximal) Quantum spin-liquids



$RuCl_3$, 1T-TaS_2

Heavy-fermion Kondo insulators

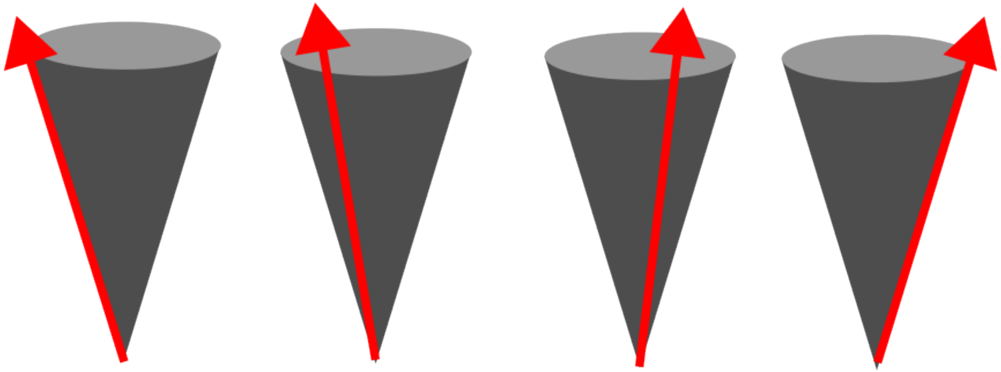


1T-TaS_2/1H-TaS_2

Do not break time-reversal

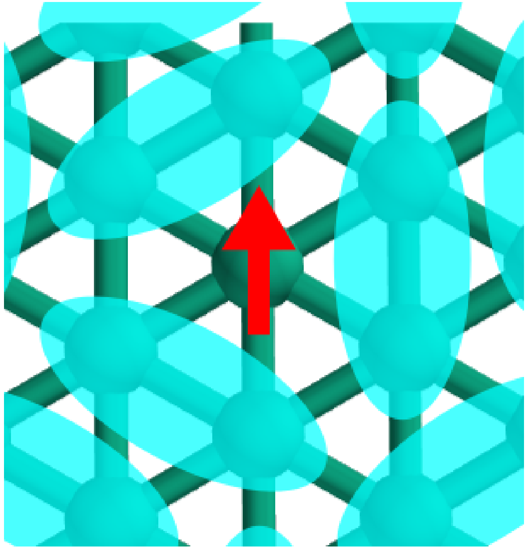
Emergent excitations in van der Waals magnets

Magnons



S=1
No charge

Spinons



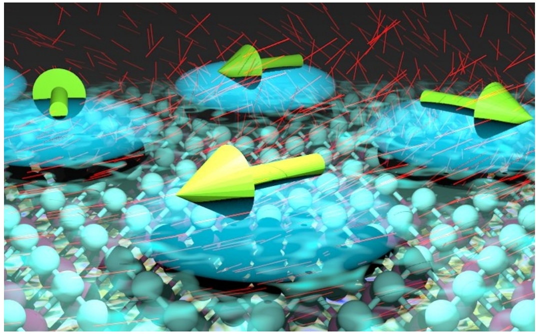
S=1/2
No charge

The role of electronic interactions

Electronic interactions are responsible for symmetry breaking

Broken time-reversal symmetry

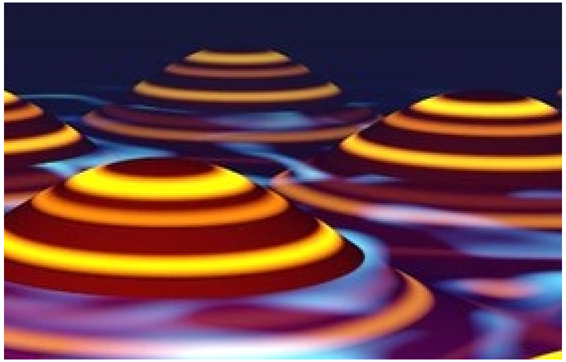
Classical magnets



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

Broken crystal symmetry

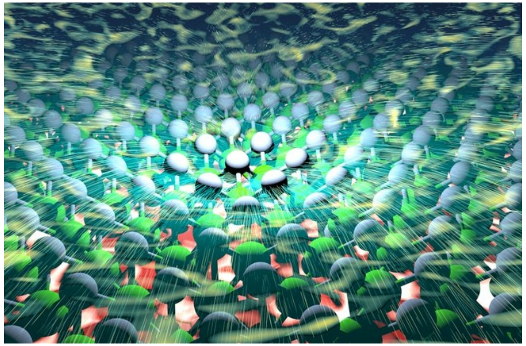
Charge density wave



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

Broken gauge symmetry

Superconductors



$$\langle c_\uparrow c_\downarrow \rangle \rightarrow e^{i\phi} \langle c_\uparrow c_\downarrow \rangle$$

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

<u>Magnetism is promoted by repulsive interactions</u>

A simple interacting Hamiltonian

Free Hamiltonian

Interactions (Hubbard term)

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

What is the ground state of this Hamiltonian?

$U < 0$ Superconductivity

$U > 0$ Magnetism

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

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

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

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

A Hamiltonian for a weakly correlated magnet

Free Hamiltonian ***Exchange term***

$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + M \sum_i \sigma^z_{s,s'} c^\dagger_{i,s} c_{i,s'}$$

Her we assume that interactions are weak (in comparison with the kinetic energy)

What if interactions are much stronger than the kinetic energy?

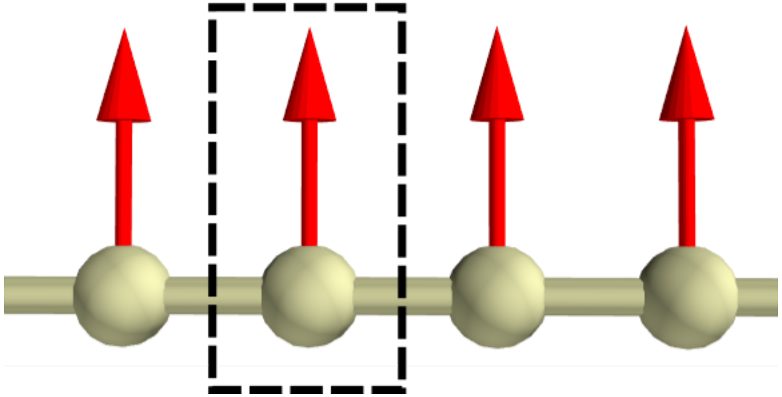
Solving the interacting model at the mean-field level in a 1D chain

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

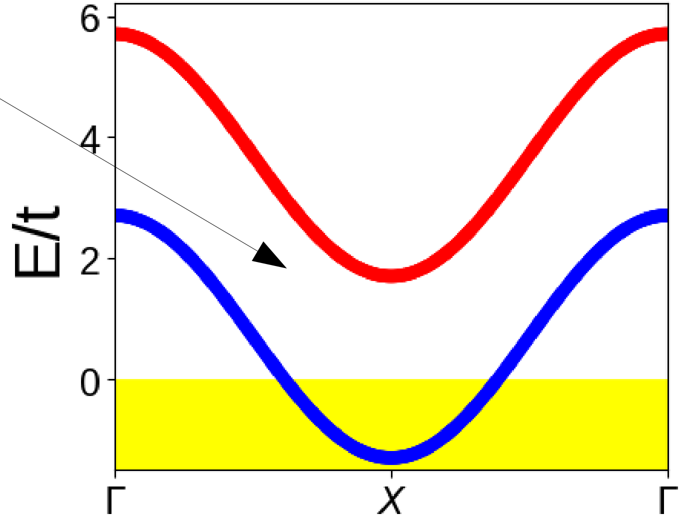
$$H = \sum_{ij} t_{ij} [c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{i\downarrow} c_{j\downarrow}] + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Filling 0.2 (full would be 1)

Interaction-induced splitting



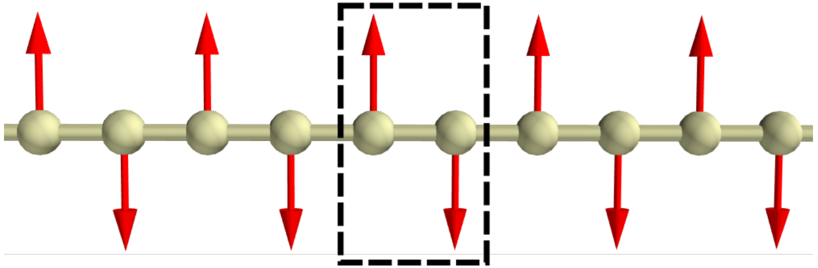
$U = 8t$

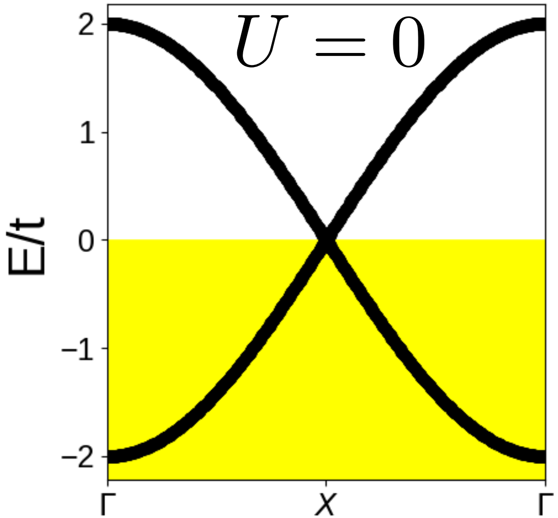


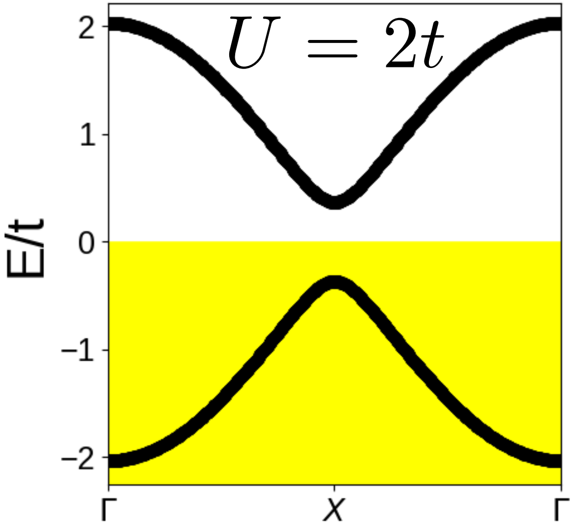
Solving the interacting model at the mean-field level in a 1D chain

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

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

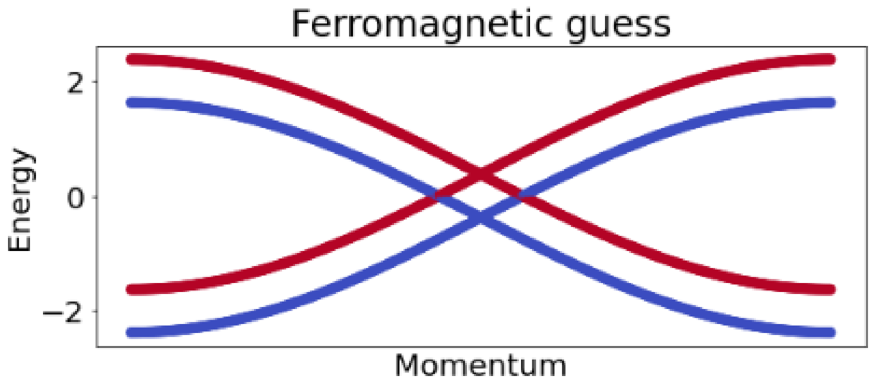


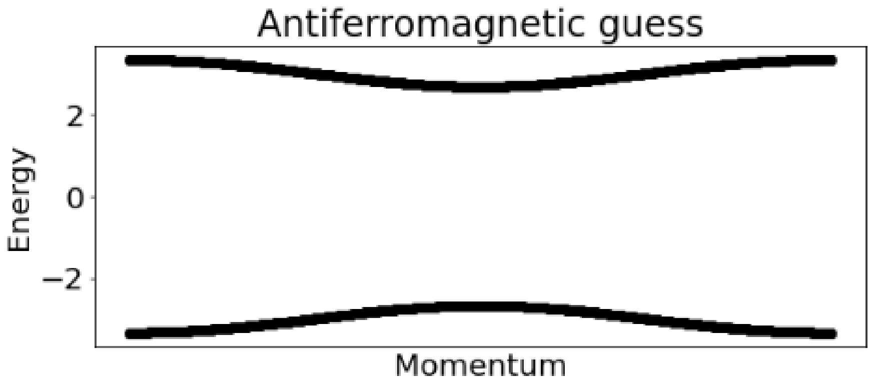


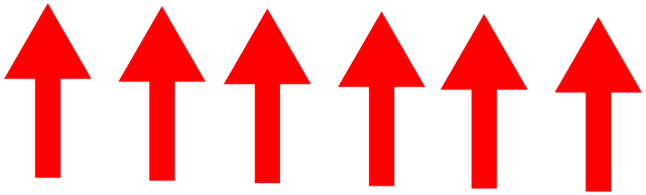


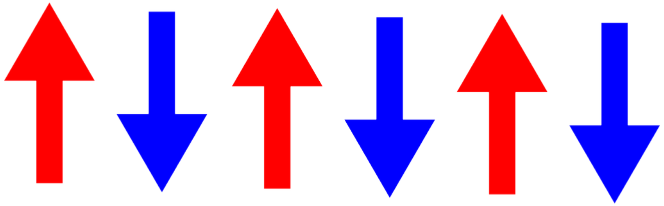
Competing solutions for a magnetic state

Let us now consider two selfconsistent solutions for the interacting model





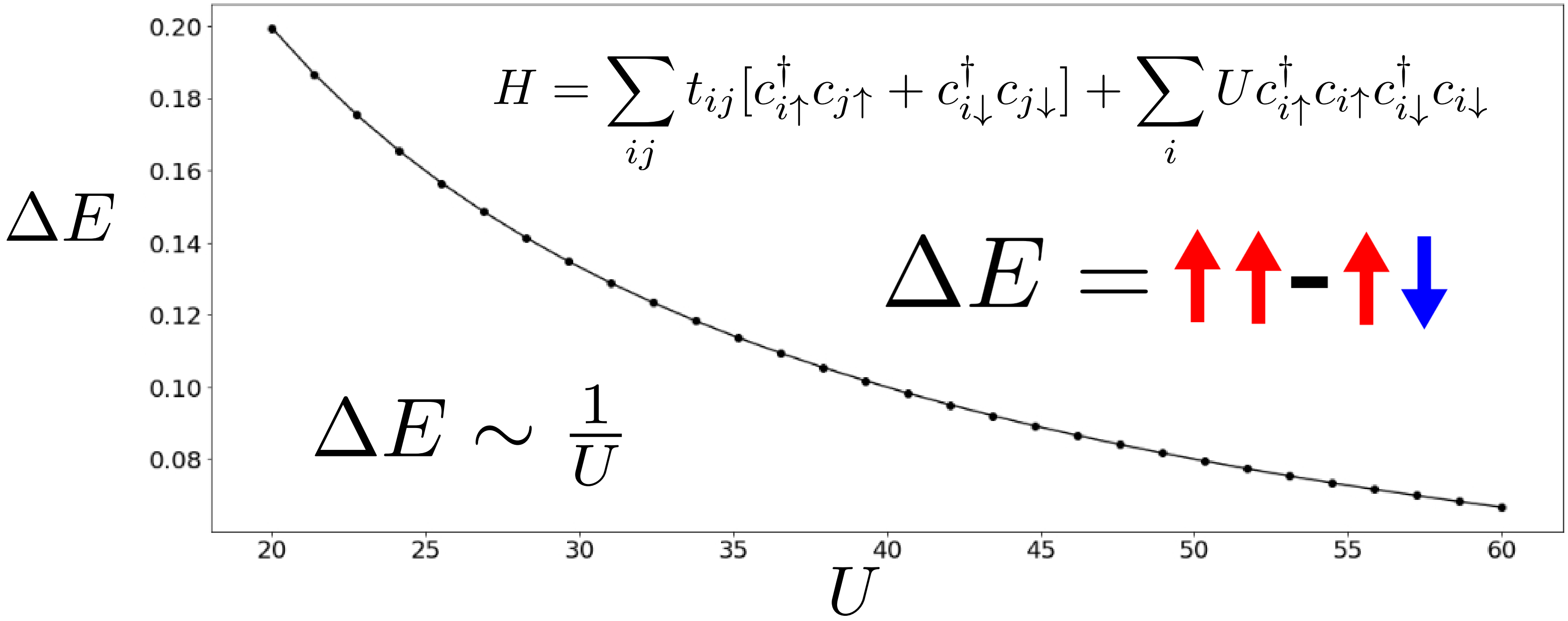




Only once of them is the true ground state, but which one it is?

Competing solutions for a magnetic state

Let us now compute the energy difference between the two configurations



For strong interactions, the AF configuration always has lower energy

The critical interaction for magnetic ordering

Lets take the Hamiltonian

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

Do we have magnetism for any value of U? $\langle S_z \rangle \neq 0$

In general, in the weak coupling limit magnetism appears when

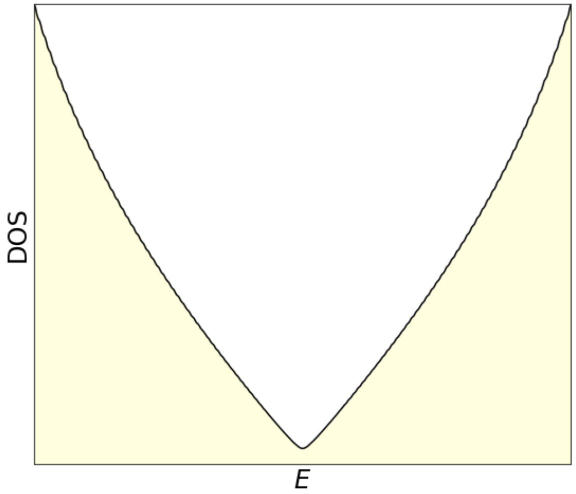
$$UD(\omega) > 1$$

Repulsive interaction

Density of states

The critical interaction for magnetic ordering

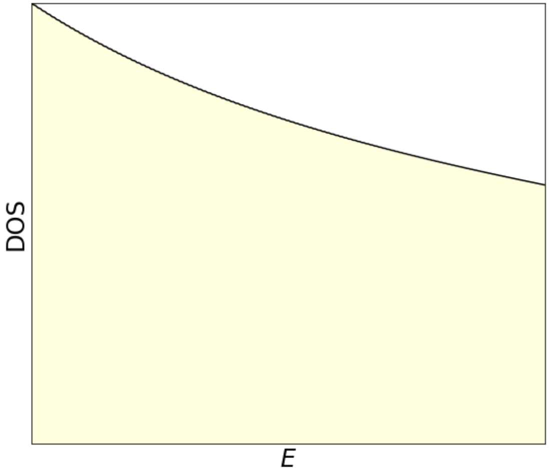
Semimetals



No low coupling instability

$$U_C \gg t$$

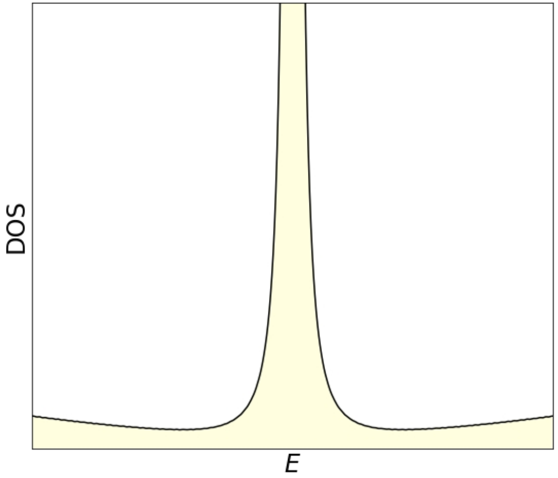
Metals



Controlled by DOS

$$U_C \sim \frac{1}{D(E_F)}$$

Flat bands

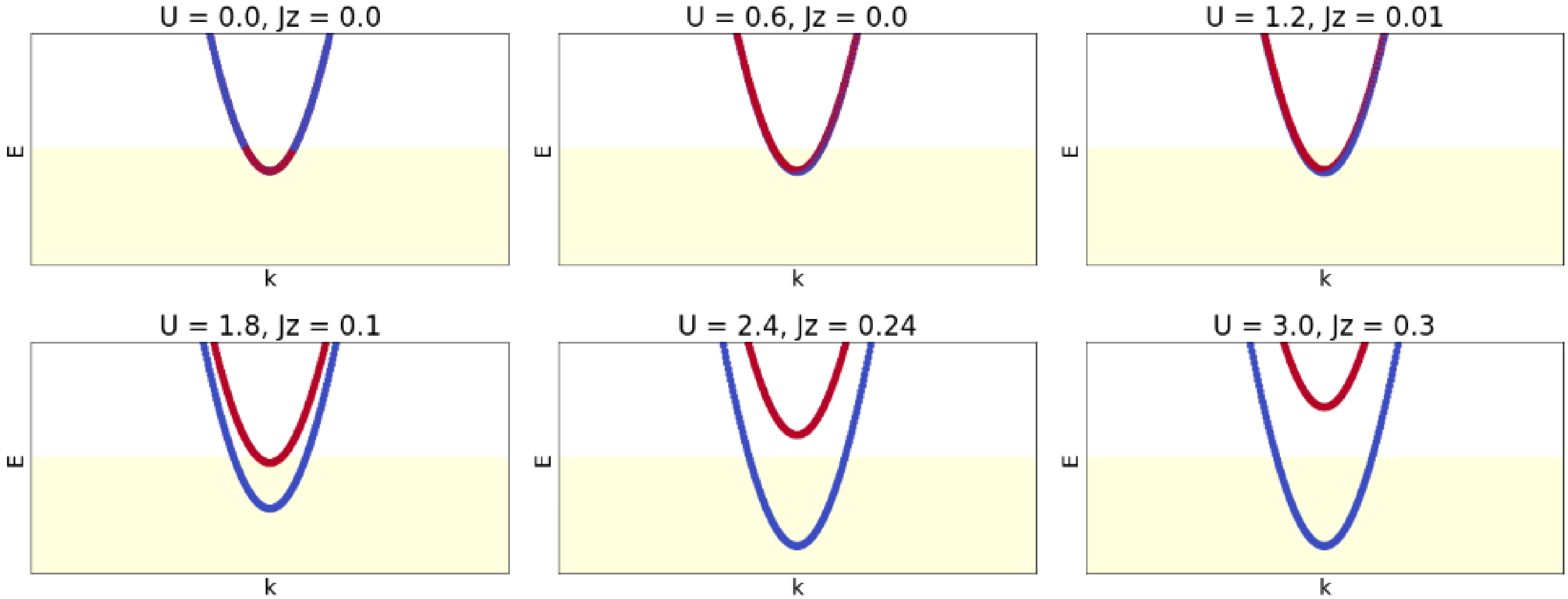


Arbitrarily small interactions

$$U_C \to 0$$

The critical interaction for magnetic ordering

Magnetic instabilities occur once interactions are strong enough



For interactions below a threshold, no magnetic order occurs

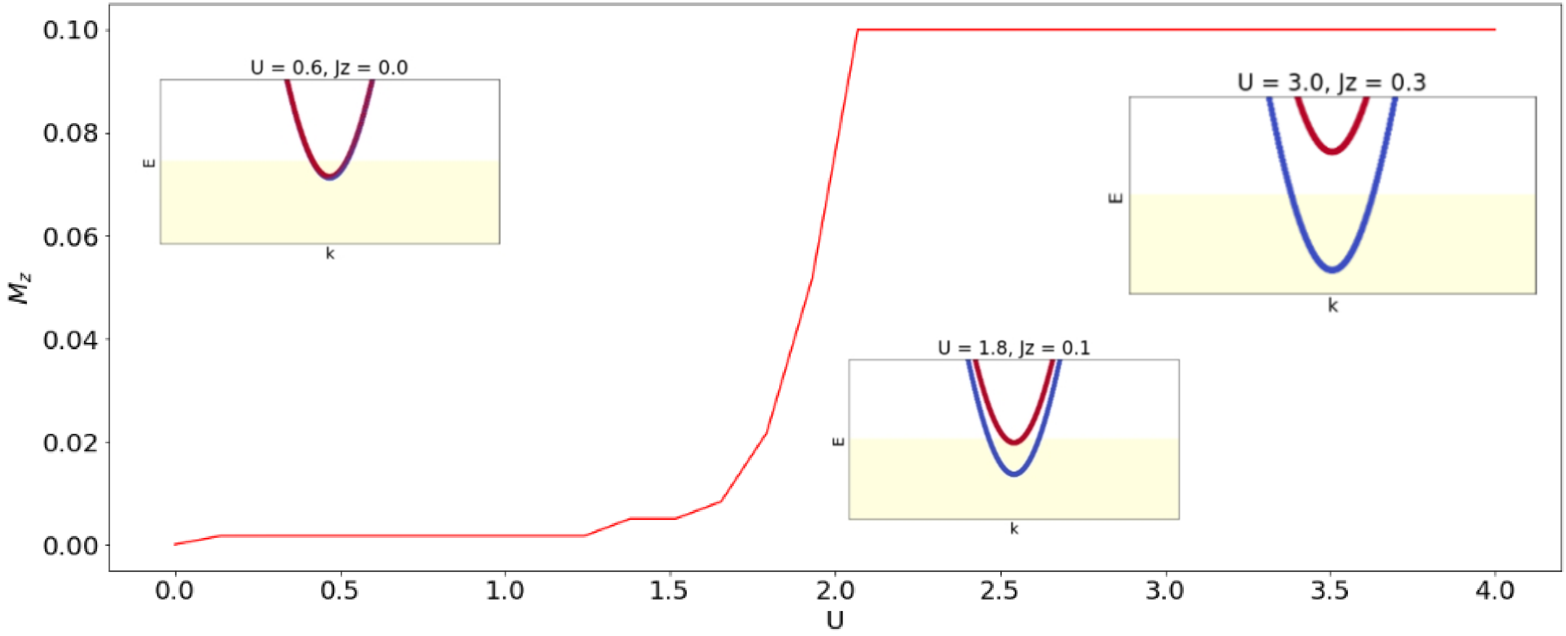
The critical interaction for magnetic ordering

Depending on the strength of interactions, we can have three different regimes

No magnetism

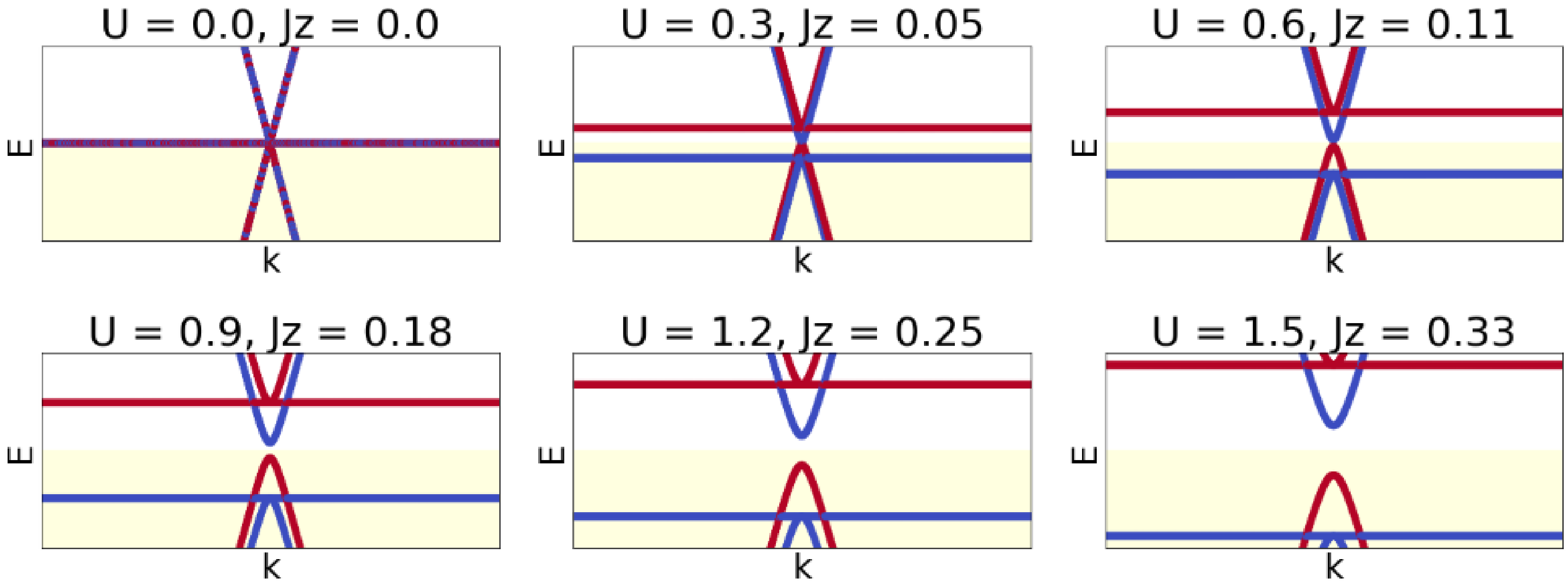
Non-saturated magnetization

Saturated magnetization (half metal)



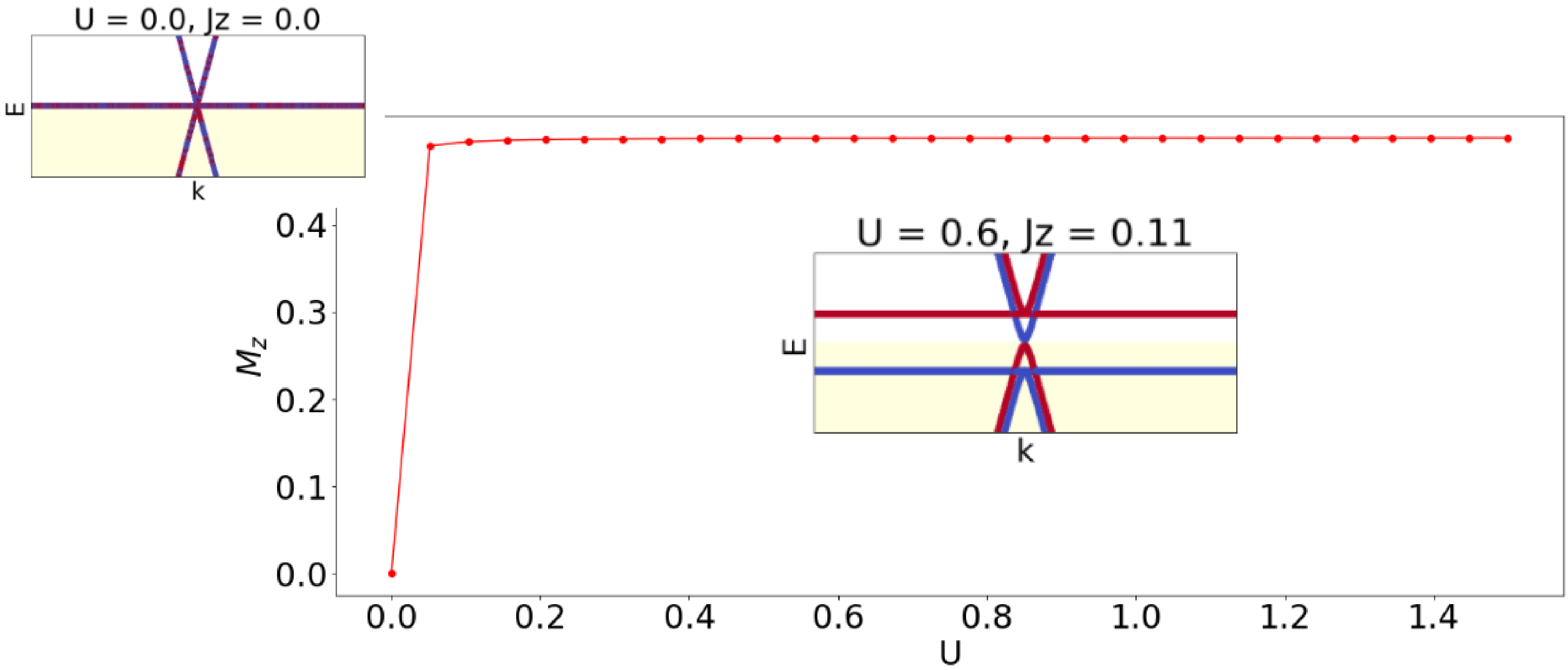
Magnetic instabilities in a flat band system

Magnetic instabilities occur for arbitrarily small interactions



Magnetic instabilities in a flat band system

In the flat band regime, any non-zero interaction gives rise to a magnetic instability

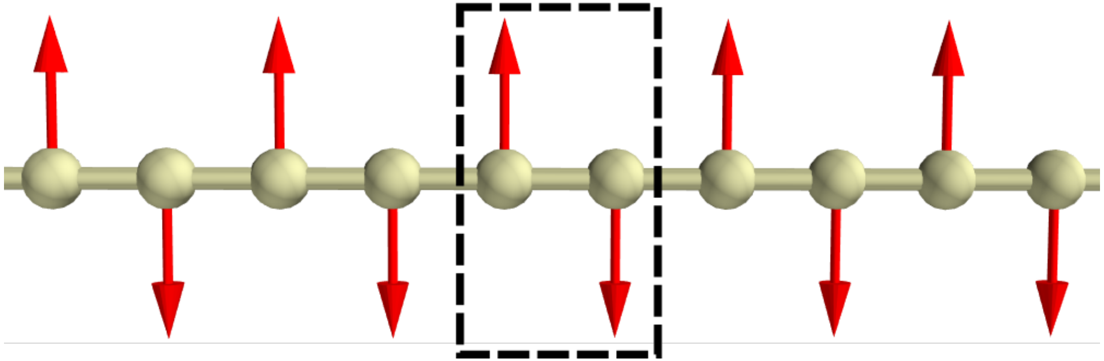


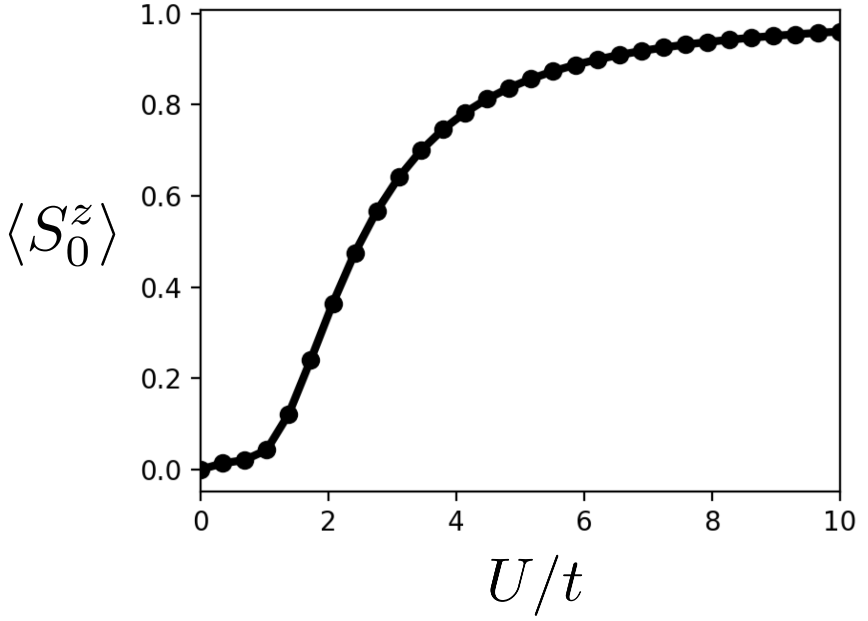
The strongly localized limit and the Heisenberg model

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

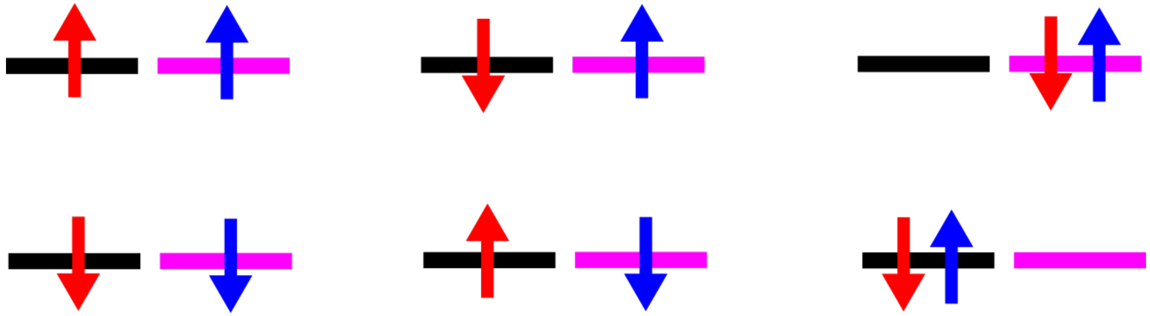
Let us start with a Hubbard model dimer

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

Now in the limit $U \gg t$

Levels

The full Hilbert space at half filling is

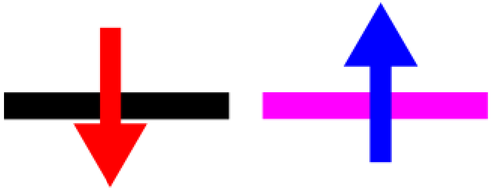


The strongly localized limit

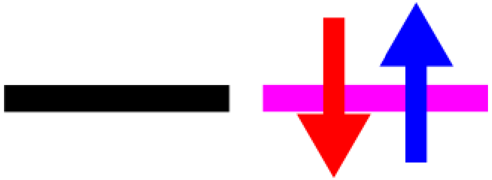
Let us start with a Hubbard model dimer

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

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



~ 0



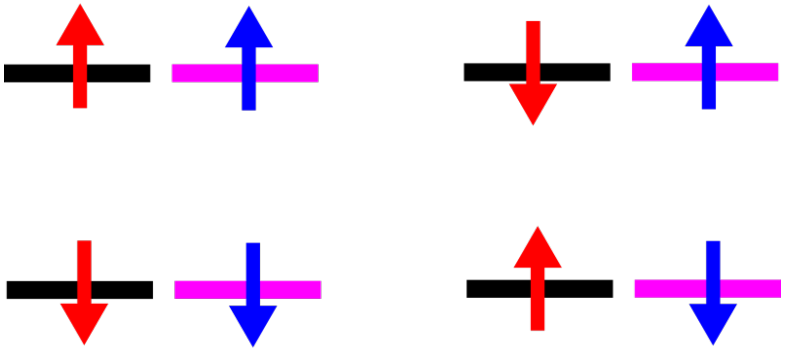
$\sim U$

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

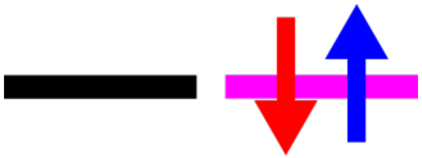
We can compute J using second order perturbation theory

$$H = H_0 + V$$

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

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

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

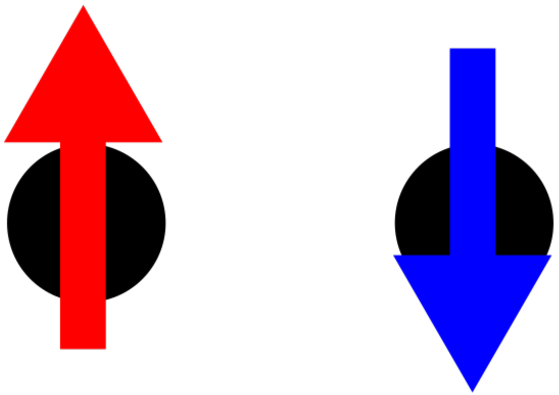
The Heisenberg model

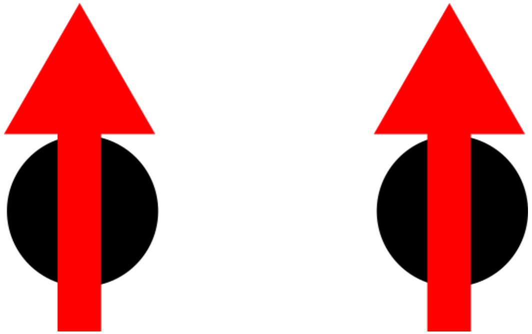
$$J_{ij} > 0$$

Antiferromagnetic coupling

$$J_{ij} < 0$$

Ferromagnetic coupling

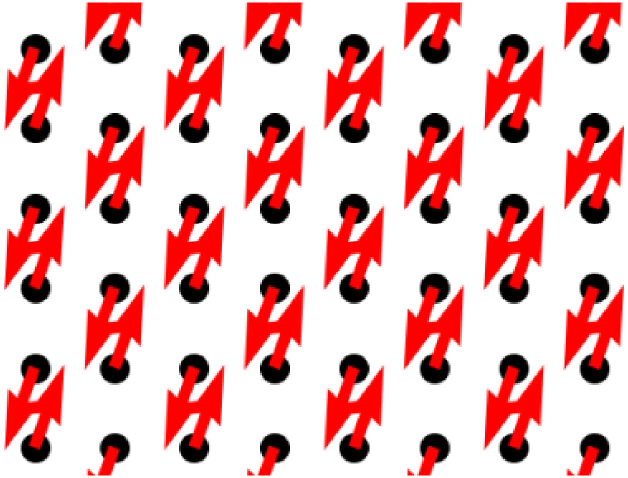




Classical ground states

Antiferromagnetism driven by superexchange

In the square lattice



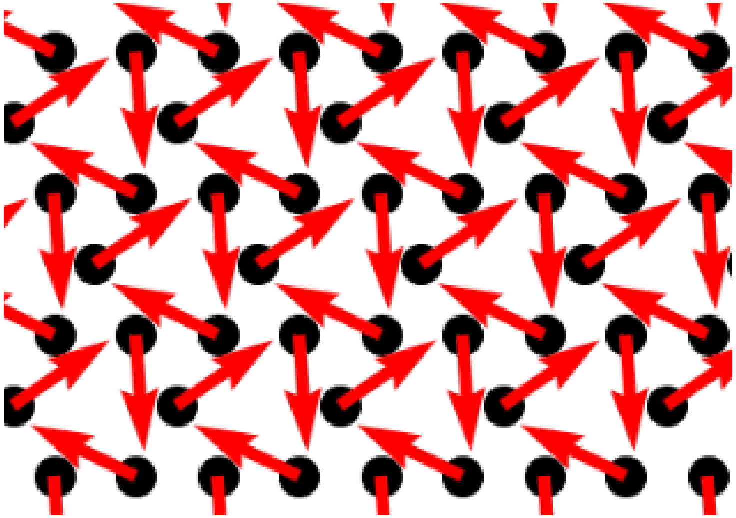
In the honeycomb lattice

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

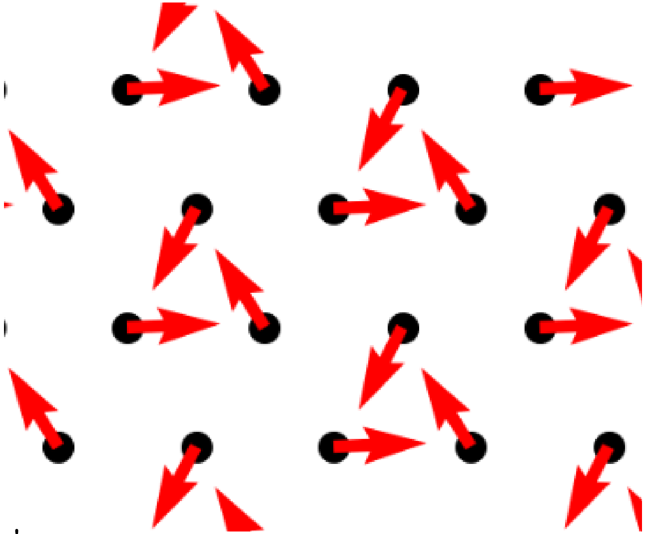
In bipartite lattices, the magnetization is collinear

Antiferromagnetism driven by superexchange

In the Kagome lattice



In the triangular lattice



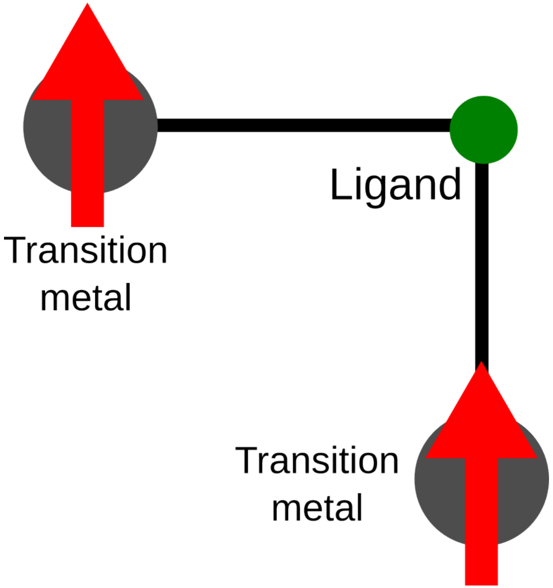
$$H = \sum_{ij,s} t_{ij} c^\dagger_{i,s} c_{j,s} + \sum_i U c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + h.c.$$

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

The origin of ferromagnetic coupling

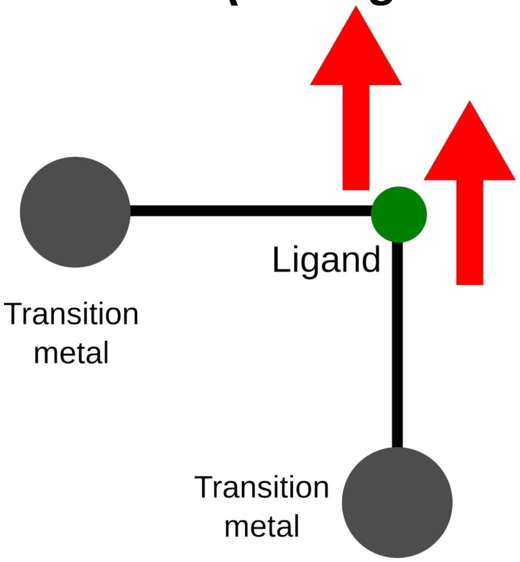
Exchange interactions can be ferromagnetic if mediated by an intermediate site

Low energy manifold



$CrCl_3, CrBr_3, CrI_3$

Virtual state (among others)



The sign of the coupling depends on the filling of the d-shell and the angle

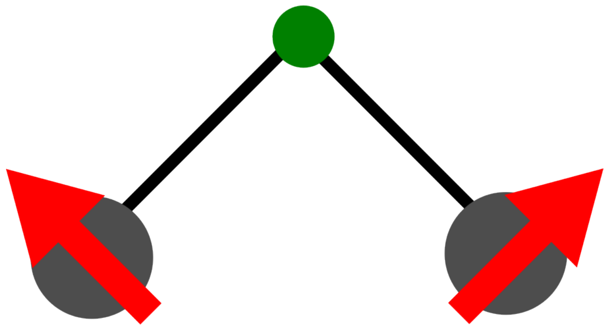
Goodenough-Kanamori rules

Non-isotropic exchange coupling

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

Antisymmetric exchange

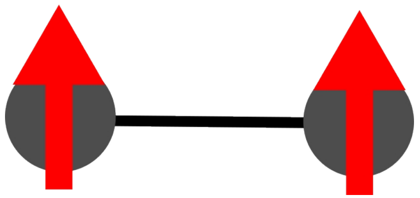
$$(\mathbf{r}_{ik} \times \mathbf{r}_{kj}) \cdot \vec{S}_i \times \vec{S}_j$$



Promotes
non-collinear order

Anisotropic exchange

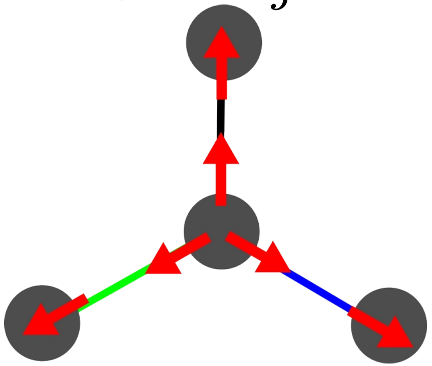
$$S_i^z S_j^z$$



Promotes
easy axis/plane

Kitaev interaction

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



Promotes
frustration

Break

10-15 min break

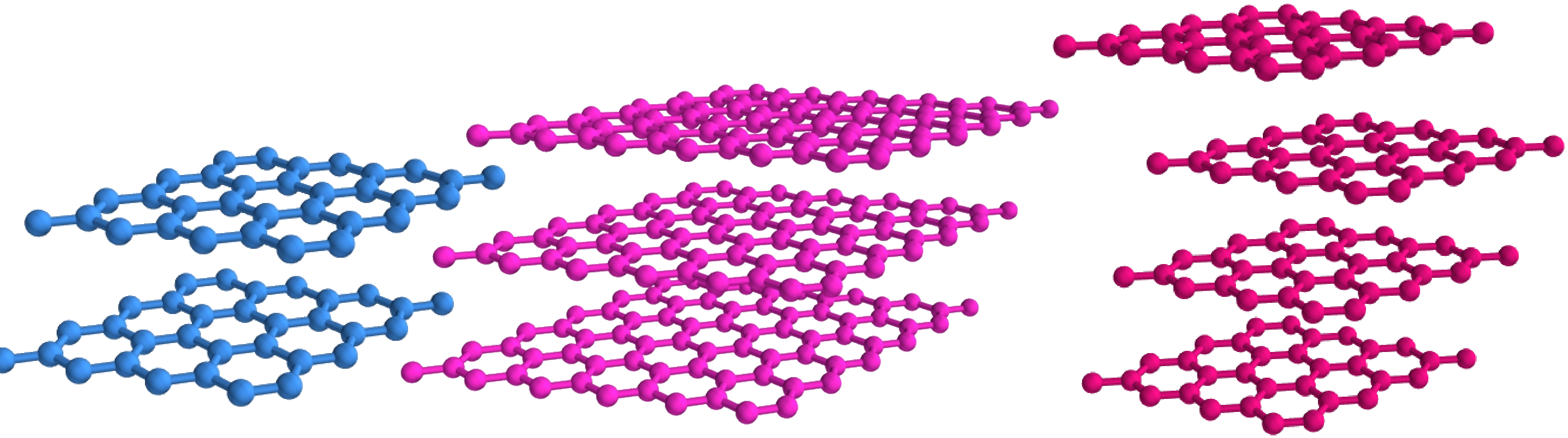
(optional) to discuss during the break

Which type of magnetic order fulfills

$$\langle c^\dagger_{n\uparrow} c_{n\downarrow} \rangle \neq 0 \qquad Im\left[\langle c^\dagger_{n\uparrow} c_{n\downarrow} \rangle\right] = 0 \qquad Re\left[\langle c^\dagger_{n\uparrow} c_{n\downarrow} \rangle\right] = 0$$

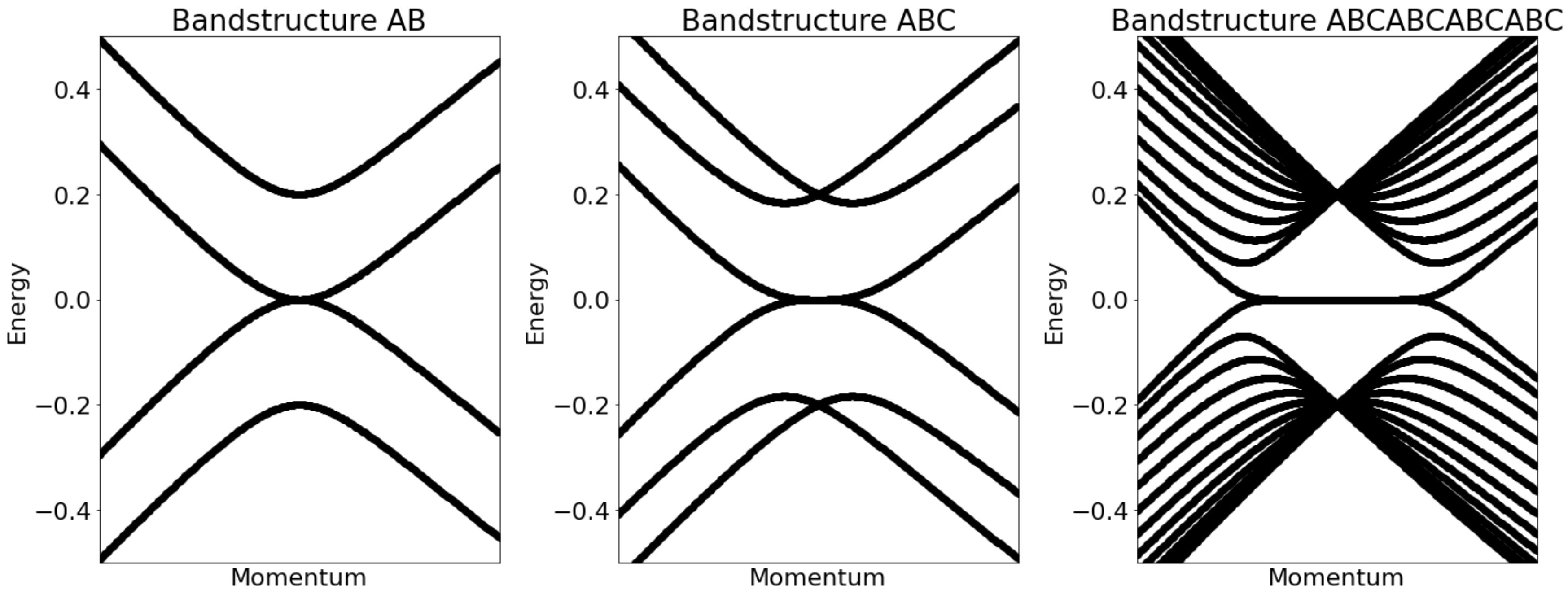
Symmetry breaking in graphene multilayers

Magnetic symmetry breaking in graphene multilayers



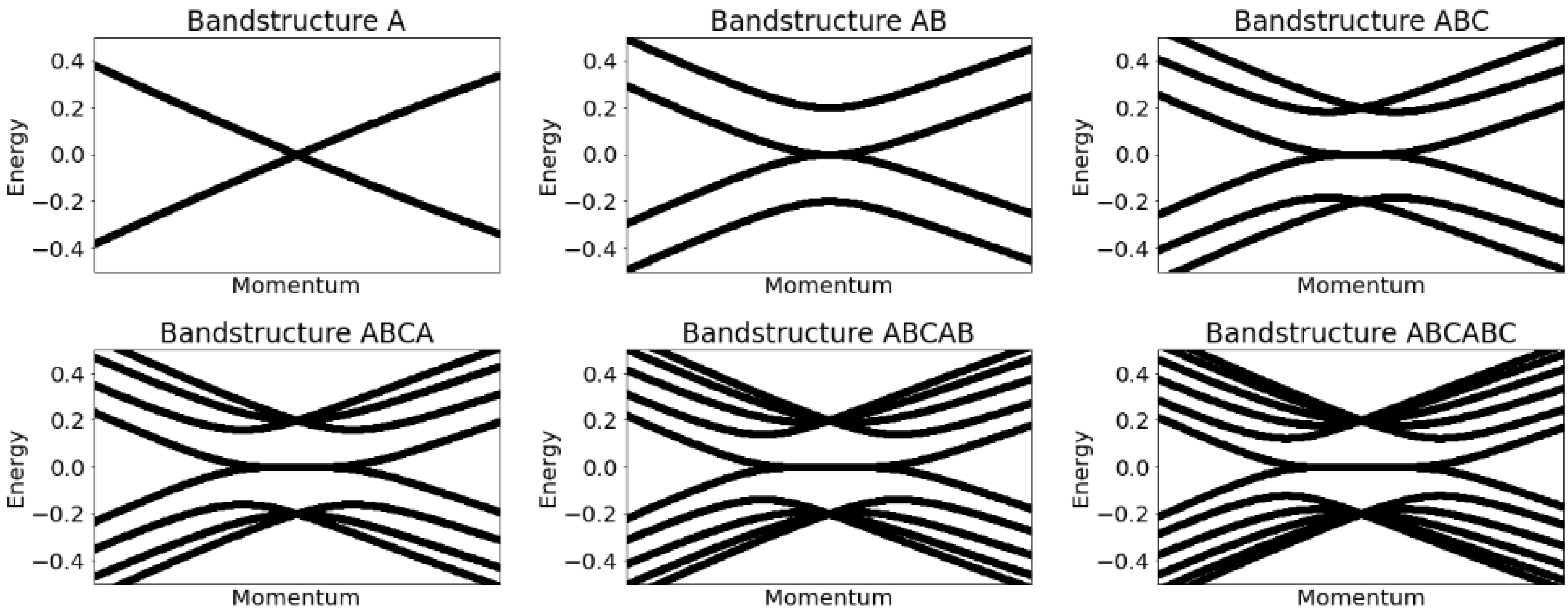
Magnetism in graphene multilayers

Graphene trilayers can have magnetic instabilities driven by repulsive interactions



The more layers a stacking has, the flatter the dispersion

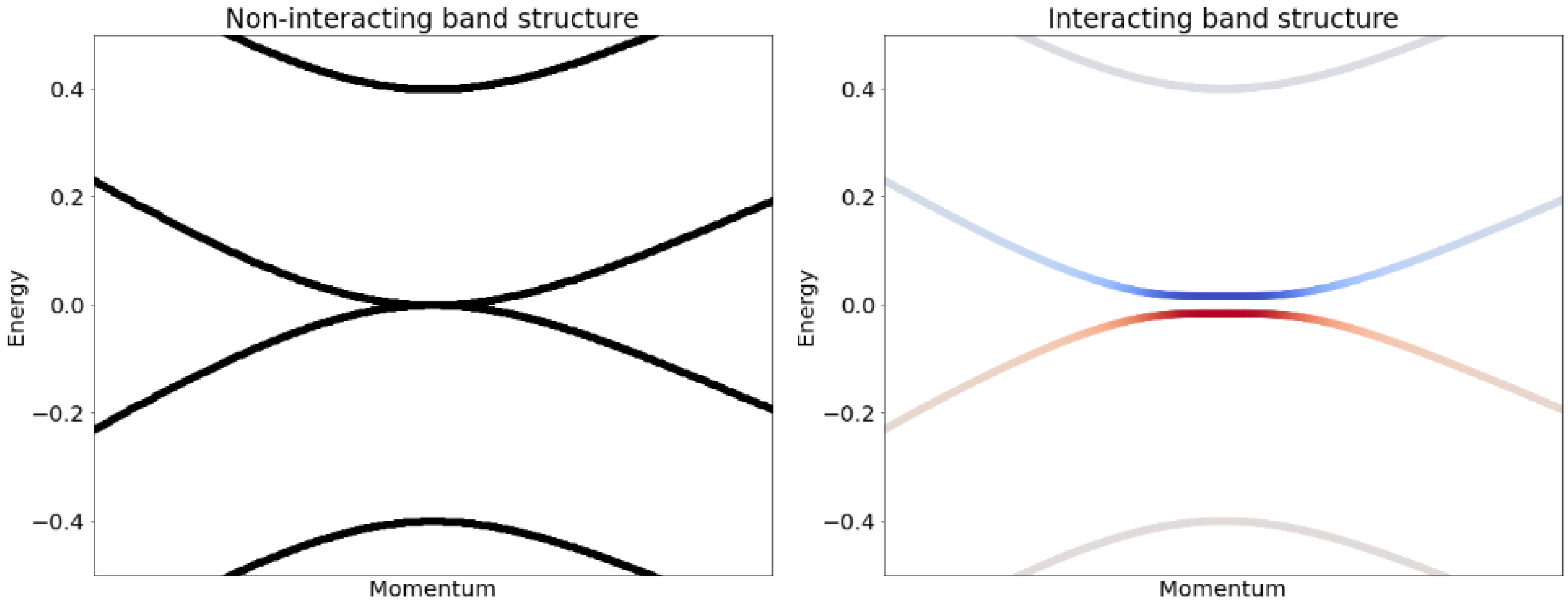
Magnetism in graphene multilayers



The more layers a stacking has, the flatter the dispersion

Magnetism in graphene bilayers

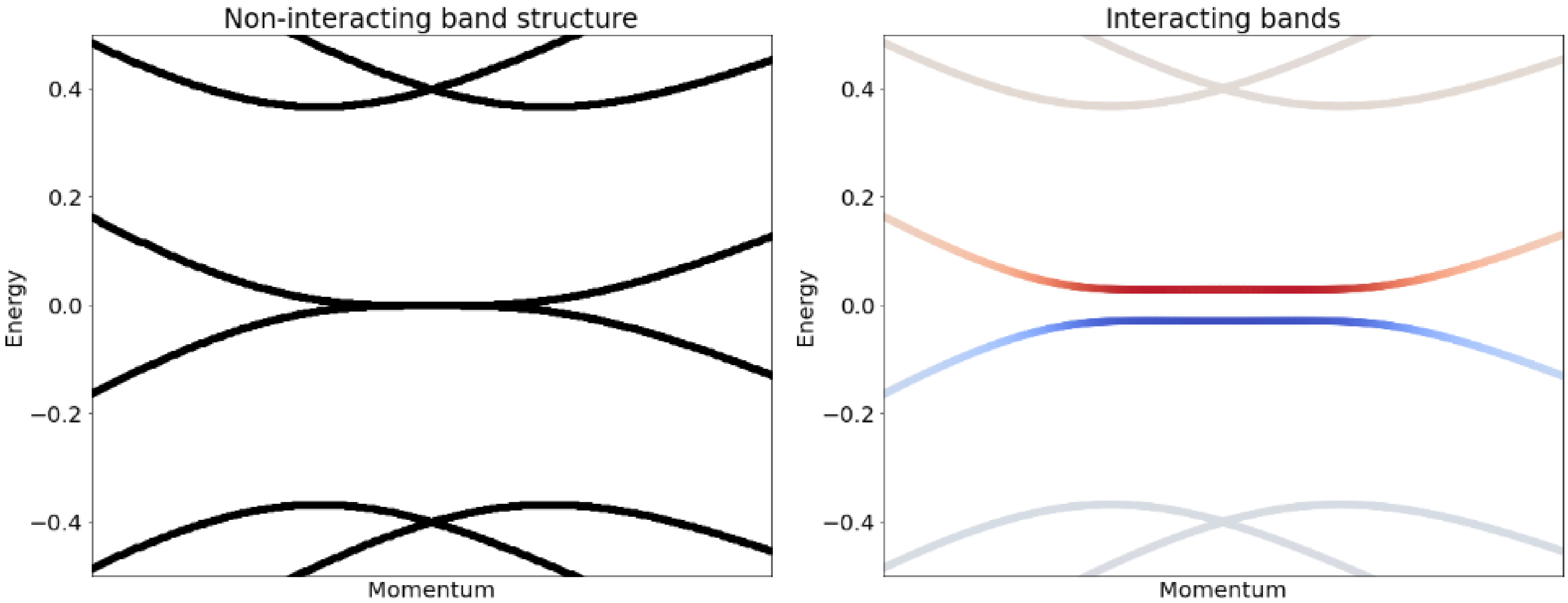
Graphene bilayers can have magnetic instabilities driven by repulsive interactions



AB graphene bilayer

Magnetism in graphene trilayers

Graphene trilayers can have magnetic instabilities driven by repulsive interactions

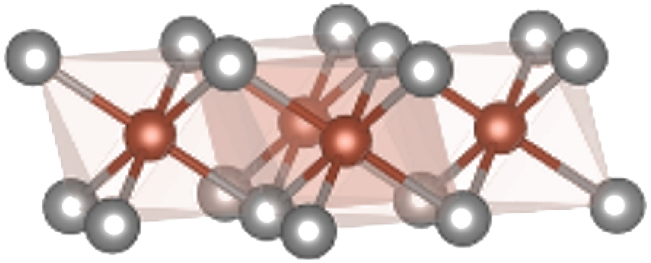


ABC graphene trilayer

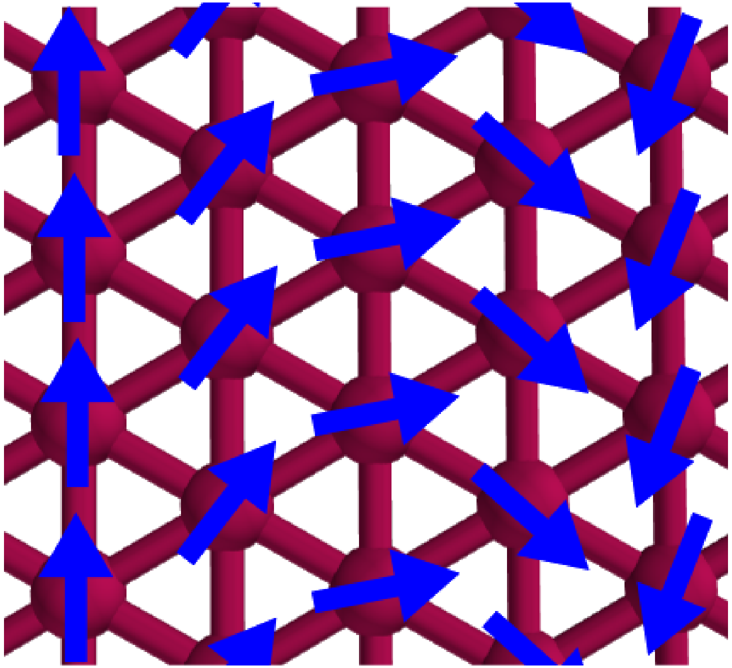
Multiferroic van der Waals materials

Electric polarization in a magnetic material

Multiferroics host, simultaneously, magnetism and electric polarization



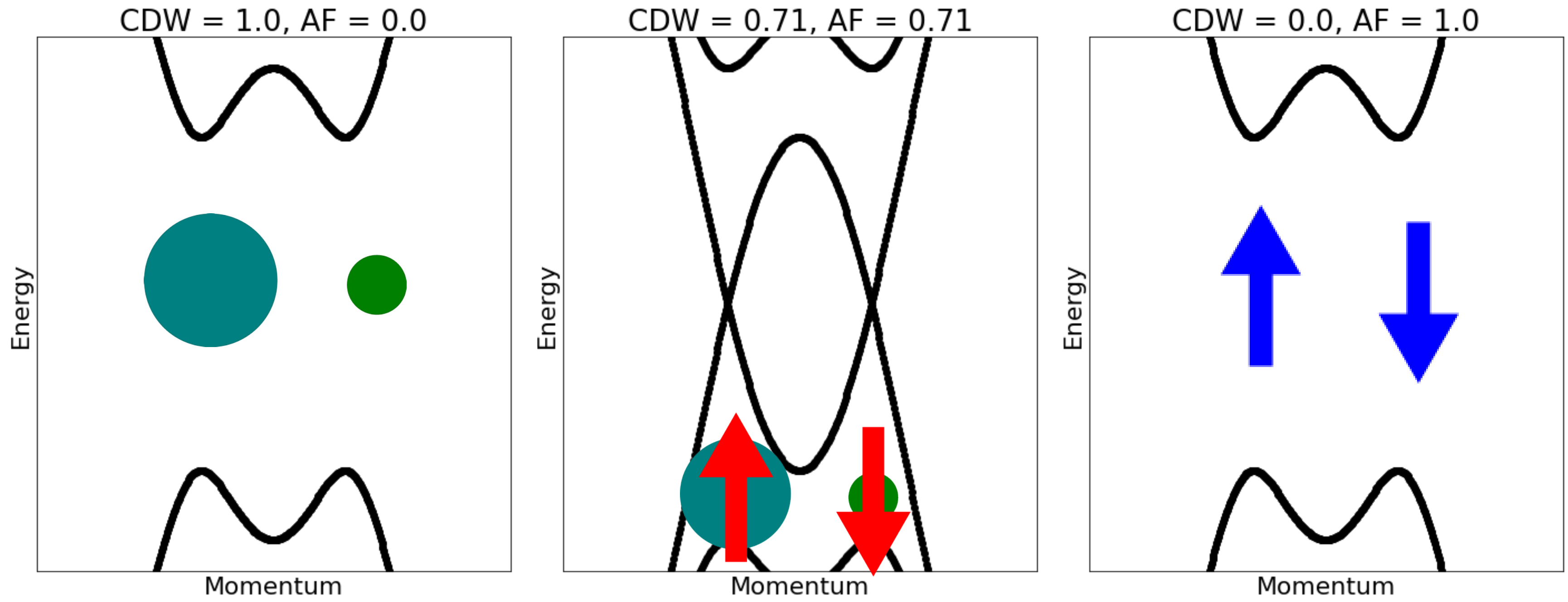
NiI_2



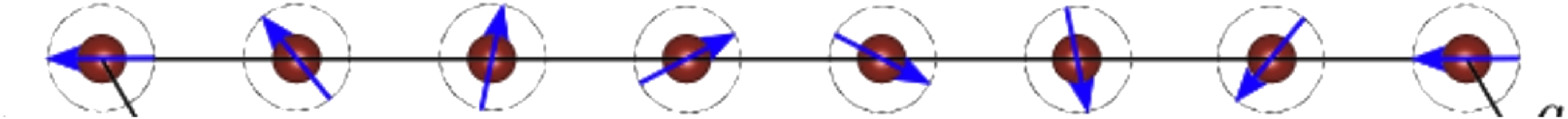
Why are multiferroics rare

If we want both electric and magnetic polarization, interactions must drive both simultaneously

However, magnetic and charge order often compete to open gaps



Coupling between magnetism and polarization



$$\mathbf{P} = \xi \mathbf{q} \times \mathbf{e}$$

Electric polarization

SOC driven

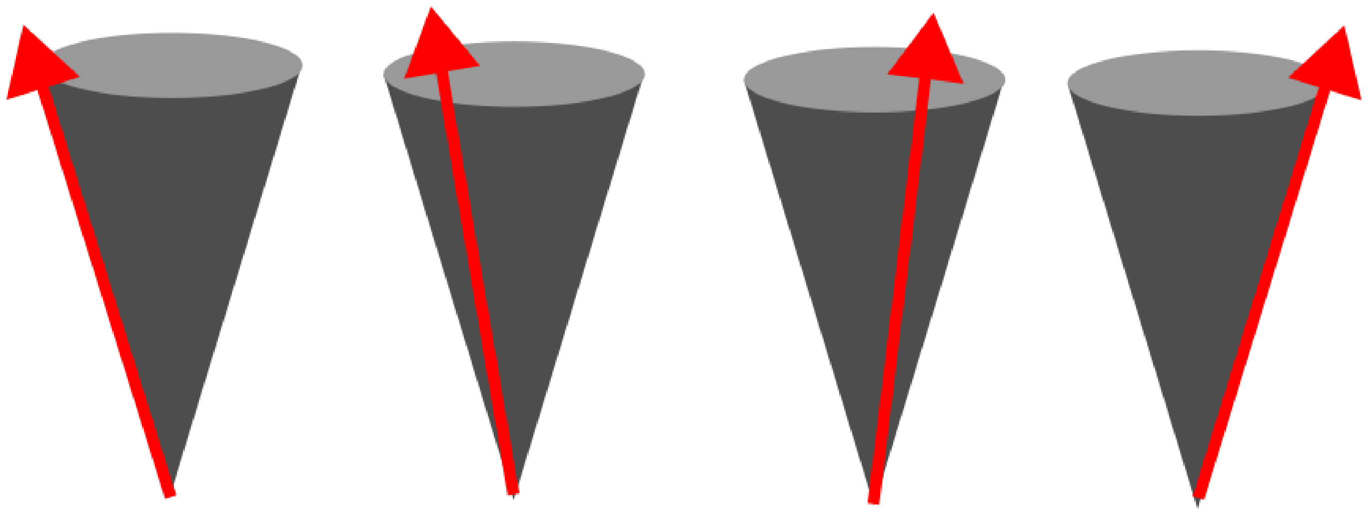
Wavevector of the spin spiral

Spin rotation axis

Excitations in 2D magnets

Excitations in a ferromagnet

Qualitatively, magnons are the fluctuations of the order parameter



Excitations in the Heisenberg model

The Heisenberg model is a full-fledged many-body problem

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

Algebraic commutation relations $$[S_j^\alpha, S_j^\beta] = i\epsilon_{\alpha\beta\gamma} S_j^\gamma$$

$$S = 1/2, 1, 3/2, 2, ...$$

How do we compute its many-body excitations?

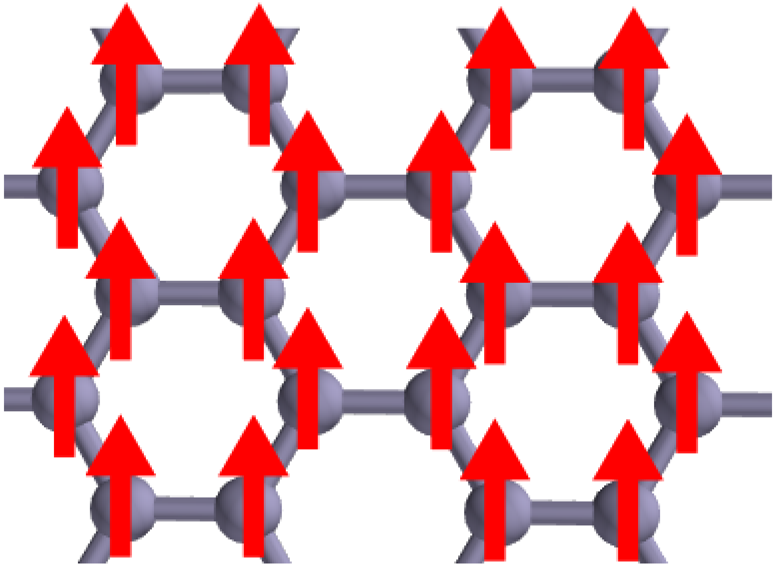
The ferromagnetic Heisenberg model

In the case of a ferromagnetic Heisenberg model, we know the ground state

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

$$J_{ij} < 0$$

$$|GS\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow \ldots\rangle$$



But how do we compute the excitations?

The Holstein–Primakoff transformation

Replace the spin Hamiltonian by a bosonic Hamiltonian

$$S_+ = \sqrt{2s}\sqrt{1 - \frac{a^\dagger a}{2s}}\,a, \quad S_- = \sqrt{2s}a^\dagger\sqrt{1 - \frac{a^\dagger a}{2s}}, \quad S_z = (s - a^\dagger a)$$

Make the replacement and decouple with mean-field assuming $\langle a_i^\dagger a_i \rangle \ll s$

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \longrightarrow \mathcal{H} = \sum_{ij} \gamma_{ij} a_i^\dagger a_j$$

Spins **Magnon**

Magnons in a nutshell

Increase the spin $S_i^+ \sim a_i$ Destroy a magnon

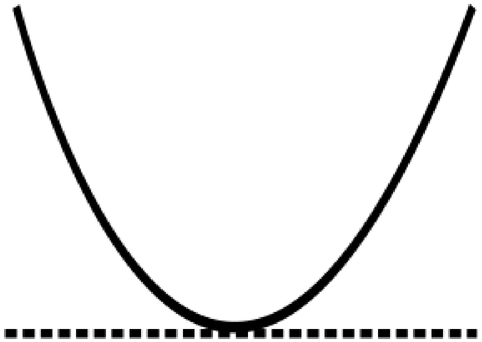
Decrease the spin $S_i^- \sim a_i^\dagger$ Create a magnon

Net magnetization $\langle S_i^z \rangle = S - \langle a_i^\dagger a_i \rangle$ Maximal minus the magnons

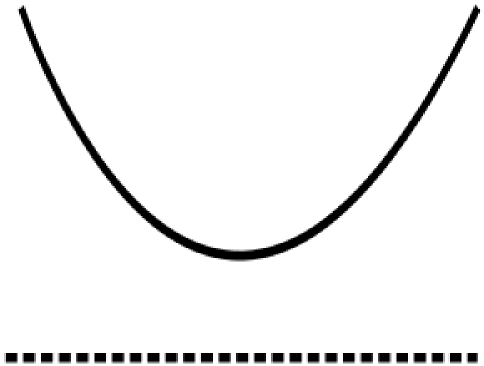
Magnons are S=1 excitations that exist over the symmetry broken state

Magnon dispersions

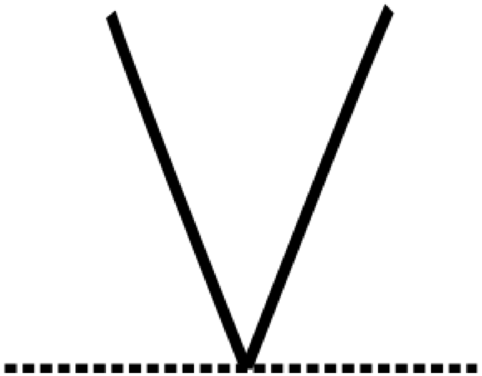
Gapless magnons



Gapped magnons



Dirac magnons



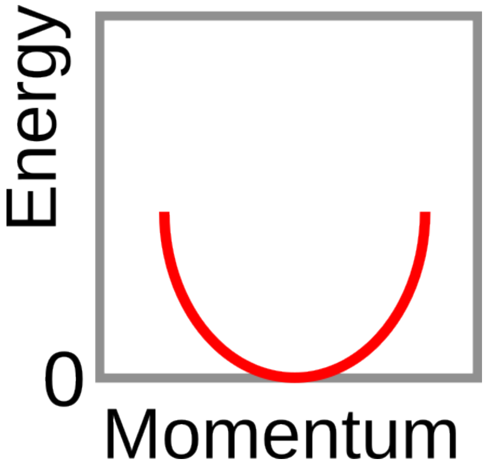
$$\mathcal{H} = \sum_{ij} \gamma_{ij} a_i^\dagger a_j$$

$$\mathcal{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

Magnons in the presence and absence of anisotropy

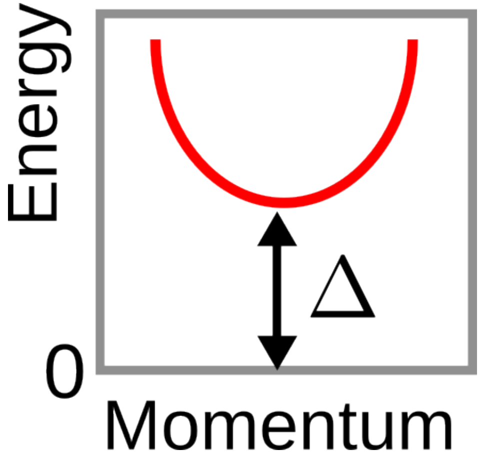
Without anisotropy

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



With anisotropy

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - K \sum_{\langle ij \rangle} S_i^z S_j^z$$



$$\Delta \sim K$$

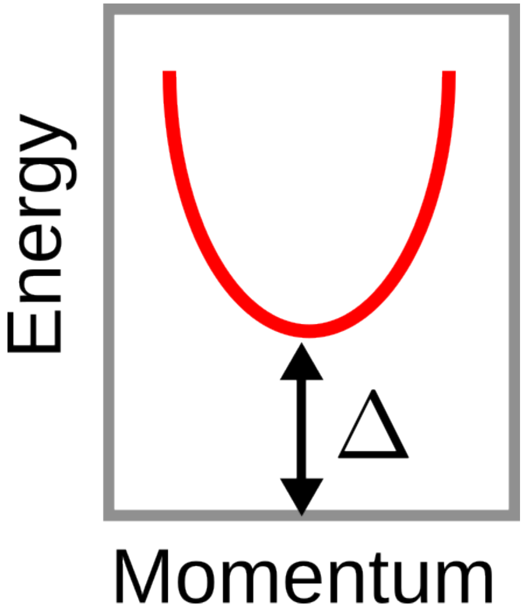
Anisotropy in the spin model generates a magnon gap

The role of magnons in 2D magnets

$$S_z = s - a^\dagger a$$

Correction from magnon population

$$\delta M_z = \langle a^\dagger a \rangle$$



Magnons renormalize the total magnetization

$$\delta M_z \sim T \int_0^{k_c} \frac{k\,dk}{\Delta + k^2}$$

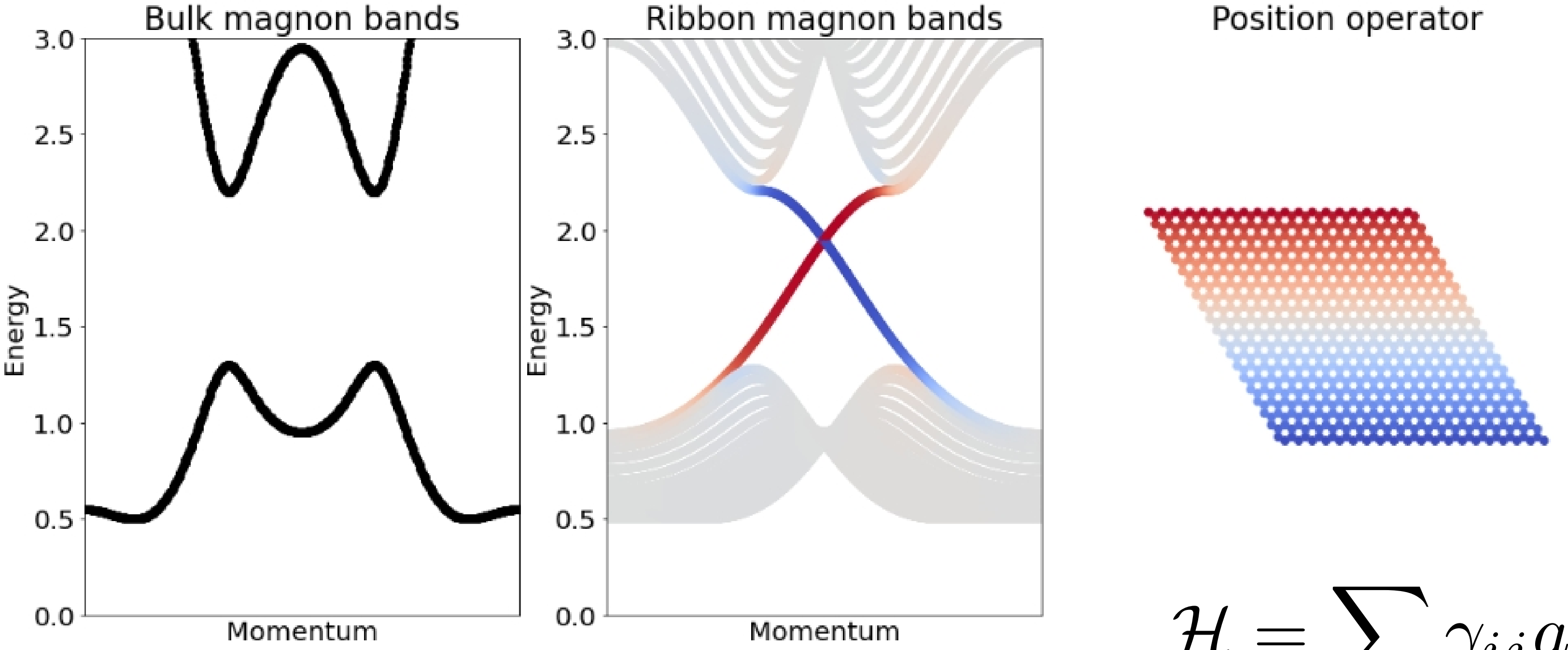
Temperature

In the absence of a magnon gap, the correction to the magnetization is infinite

$$\delta M_z \sim T \int_0^{k_c} \frac{dk}{k} \to \infty$$

Topological magnons

A magnon dispersion can have topological gaps at high energies, leading to topological modes



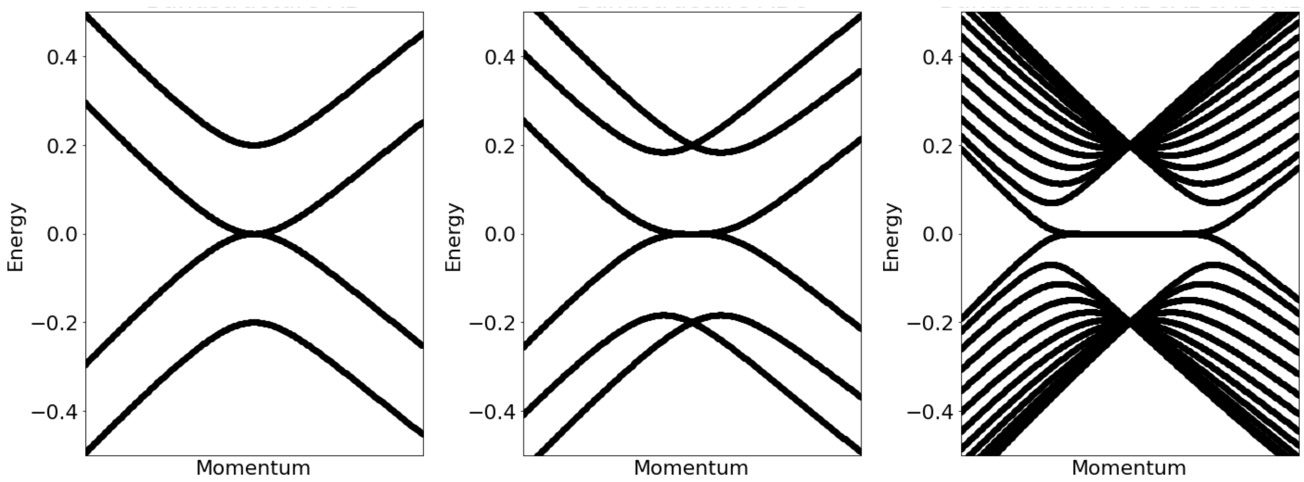
$$\mathcal{H} = \sum_{ij} \gamma_{ij} a_i^\dagger a_j$$

Break

10-15 min break

(optional) to discuss during the break

Which one of these electronic structures has the strongest magnetic instability?



Van der Waals quantum spin liquids

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

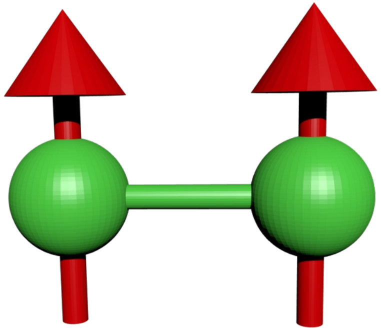
$$|GS\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \qquad \langle \vec{S}_i \rangle = 0$$

The state is maximally entangled

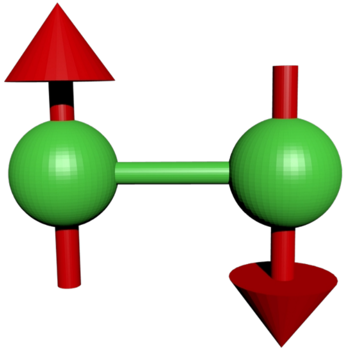
Can we have a macroscopic version of this ground state? $\langle \vec{S}_i \rangle = 0$

Towards quantum-spin liquids

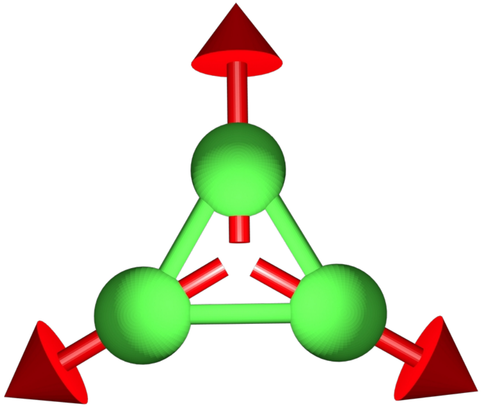
Ferromagnetism



Antiferromagnetism



Frustrated magnetism

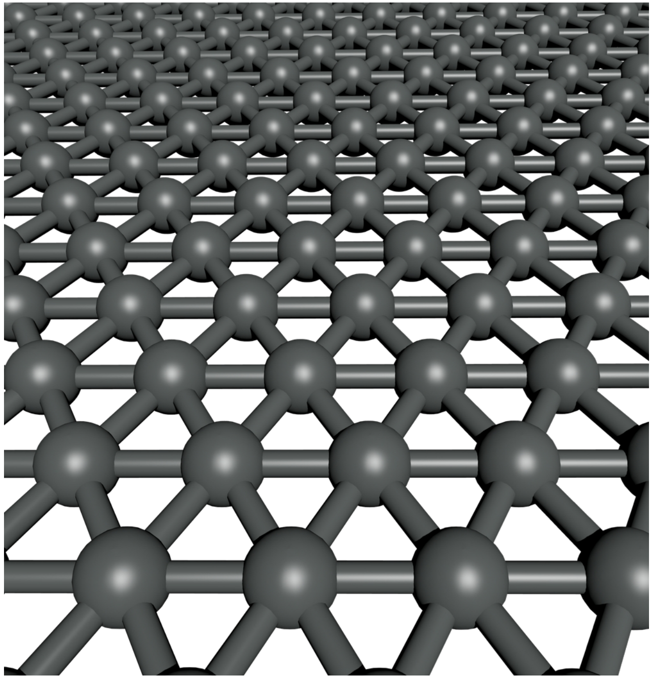


To get a quantum-spin liquid, we should look for frustrated magnetism

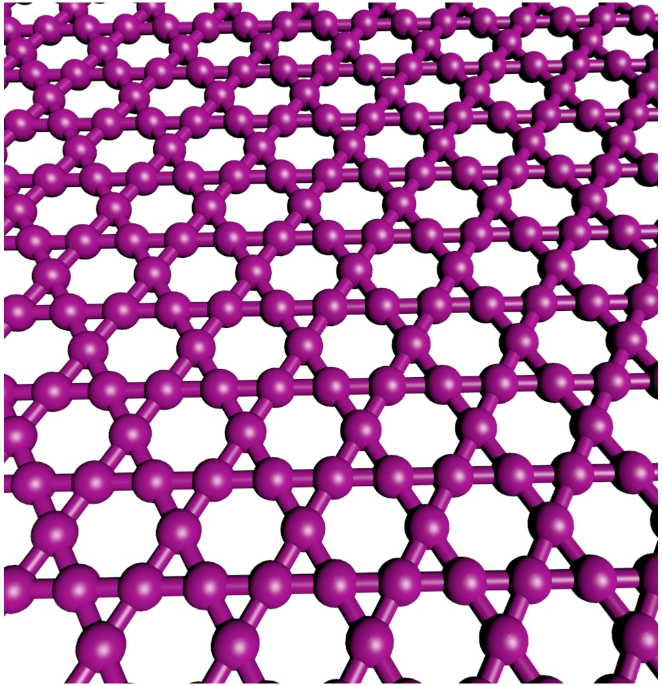
$$\langle \vec{S}_i \rangle = 0$$

Frustrated lattices

Triangular



Kagome



Quasiparticles in a quantum spin-liquid

Let us assume that a certain Hamiltonian realizes a QSL $\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$

Quantum spin liquids require $\langle \vec{S}_i \rangle = 0$

The approximation used for magnons breaks down

$$\langle S_i^z \rangle = S - \langle a_i^\dagger a_i \rangle$$

$$\langle a_i^\dagger a_i \rangle \ll S$$

We need a new approximation for the quantum excitations

The parton transformation

Transform spin operators to auxiliary fermions (Abrikosov fermions)

$$S_i^\alpha = \frac{1}{2}\sigma^\alpha_{s,s'} f^\dagger_{i,s} f_{i,s'}$$

The fermions f (spinons) have S=1/2 but no charge

This transformation artificially enlarges the Hilbert space, thus we have to put the constraint

$$\sum_s f^\dagger_{i,s} f_{i,s} = 1$$

This transformation allow to turn a spin Hamiltonian into a fermionic Hamiltonian

The spinon Hamiltonian

We can insert the auxiliary fermions $S_i^\alpha \sim \sigma^\alpha_{s,s'} f^\dagger_{i,s} f_{i,s'}$

And perform a mean-field in the auxiliary fermions (spinons)

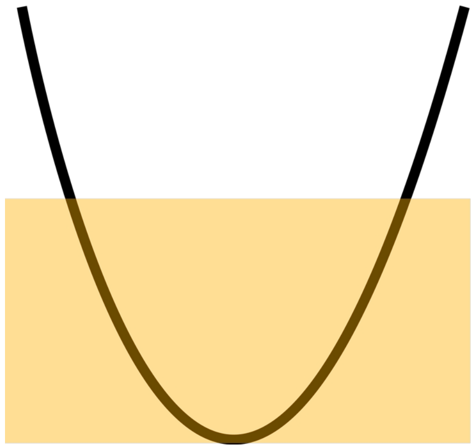
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \longrightarrow \mathcal{H} = \sum_{ij,s} \chi_{ij} f^\dagger_{i,s} f_{j,s}$$

Enforcing time-reversal symmetry $\langle \vec{S}_i \rangle = 0$

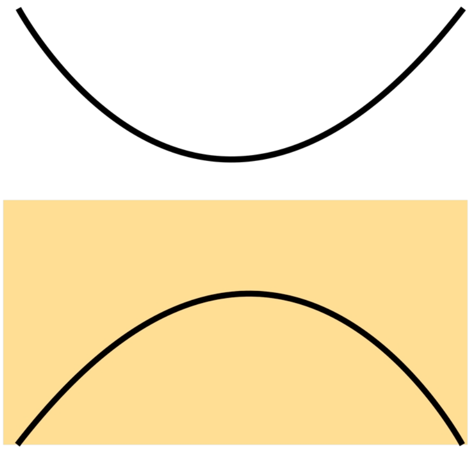
The exitations of the QSL are described by a single particle spinon Hamiltonian

Spinon dispersions

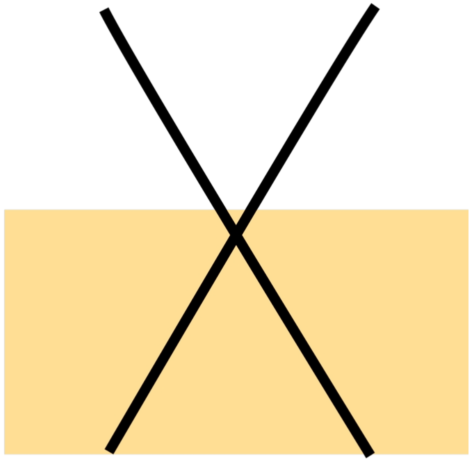
Gapless spinons



Gapped spinons



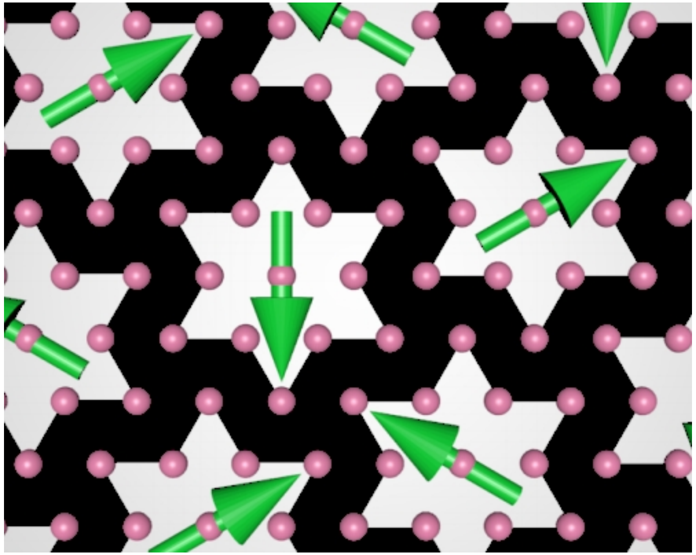
Dirac spinons



$$\mathcal{H} = \sum_{ij,s} \chi_{ij} f^{\dagger}_{i,s} f_{j,s}$$

Frustrated magnetism in 1T-TaS_2

Charge-density wave reconstruction, leading to a localized orbital in a $\sqrt{13} \times \sqrt{13}$ unit cell

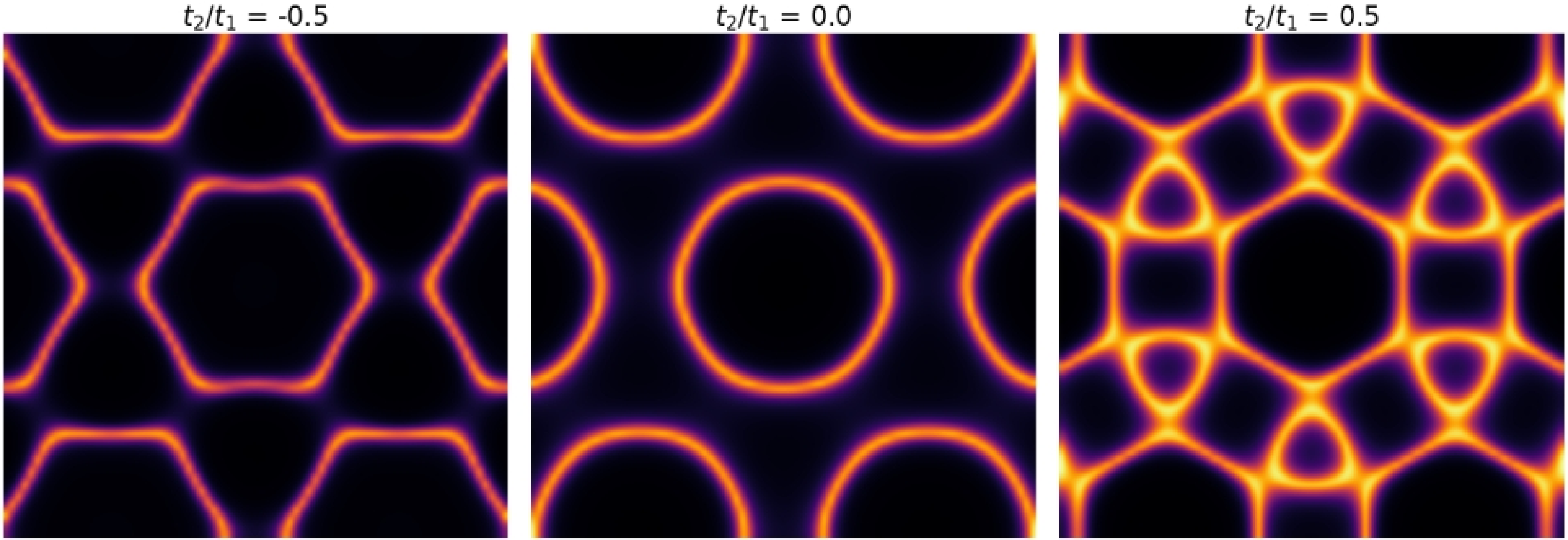


$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Strong interactions give rise to local moment formation

Effectively described by an S=1/2 Heisenberg model in a triangular lattice

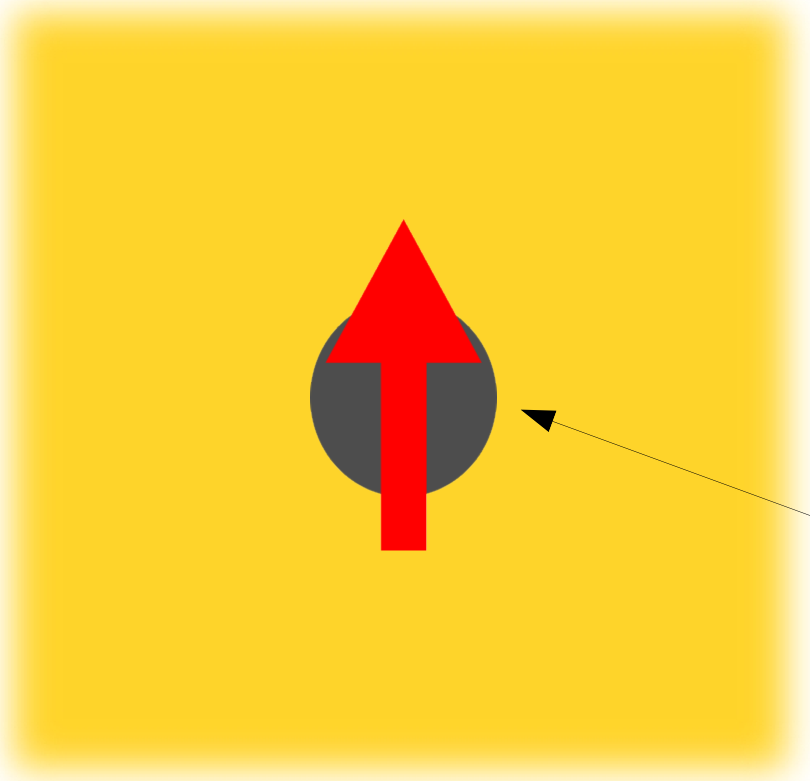
Spinon Fermi surfaces of gapless QSL



In the class of gapless QSL, different Fermi surfaces can appear depending on details of the Hamiltonian

Heavy-fermions in van der Waals materials

The Kondo problem



Conduction electrons

$$H = -t \sum_{(i,j)\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{ H.c} \right)$$

Kondo coupling

$$H_K = \sum_{\alpha\beta} \left(c^\dagger_{0\beta} \vec{\sigma}_{\beta\alpha} c_{0\alpha} \right) \cdot \vec{S}$$

We now take a quantum spin S=1/2

$$|GS\rangle \sim \frac{1}{\sqrt{2}} [| \Uparrow \downarrow\rangle - | \Downarrow \uparrow\rangle]$$

The Kondo lattice problem

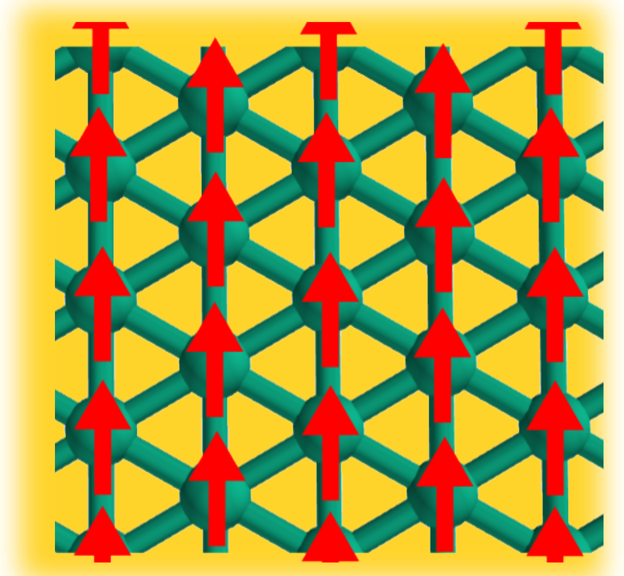
The Kondo lattice problem

$$H = -t \sum_{(i,j)\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{ H.c } \right) + J \sum_{j,\alpha\beta} \left(c^\dagger_{j\beta} \vec{\sigma}_{\beta\alpha} c_{j\alpha} \right) \cdot \vec{S}_j$$

Conduction electrons

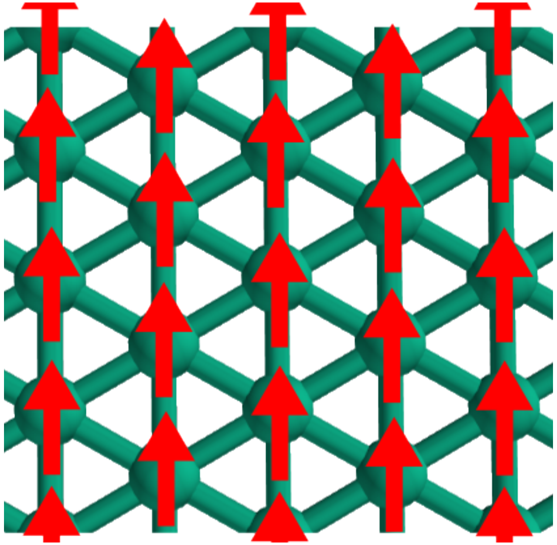
Kondo coupling

Kondo sites



Building an artificial heavy fermion state

Lattice of Kondo impurities



J_K

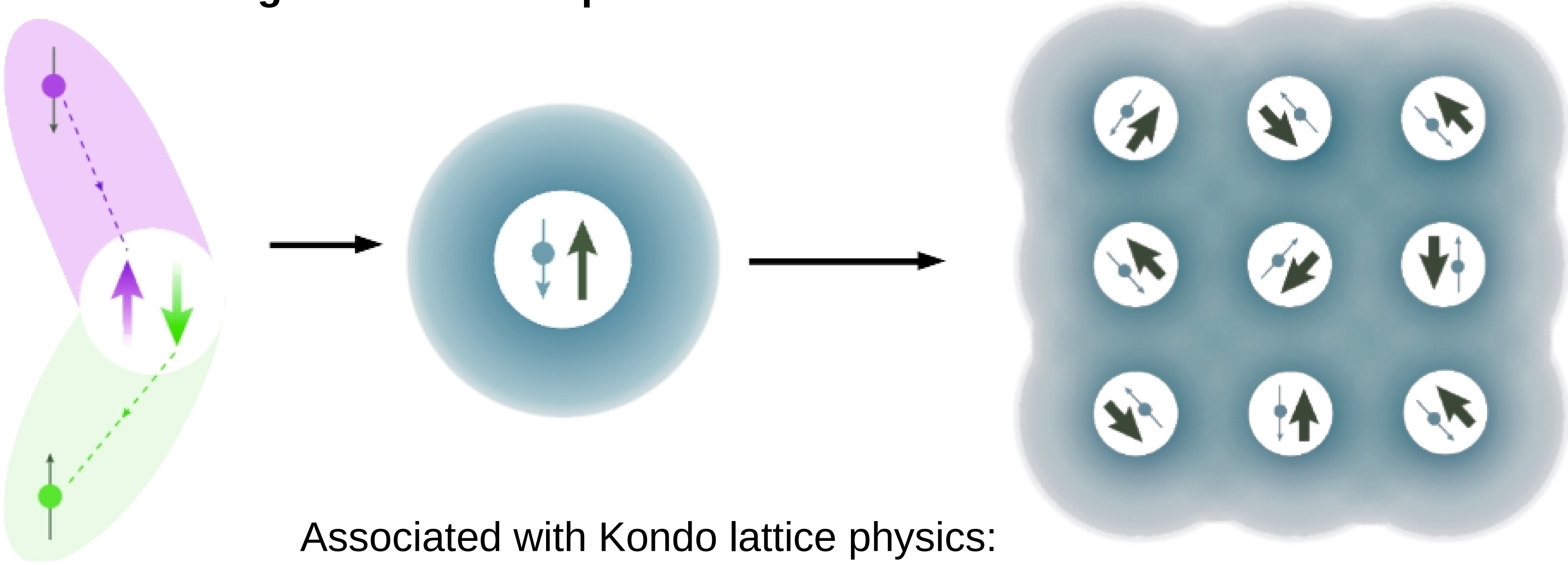
Dispersive electron gas

Both ingredients coupled through Kondo coupling

Building an artificial heavy fermion state

Conduction electrons form Kondo singlets with the impurities

Kondo-lattice model



Associated with Kondo lattice physics:
- Colossal mass enhancement of electrons
- Quantum criticality
- Unconventional (topological) superconductivity

Solving the Kondo lattice problem

$$H = -t\sum_{(i,j)\sigma}\left(c^\dagger_{i\sigma}c_{j\sigma} + \text{ H.c }\right) + J\sum_{j,\alpha\beta}\left(c^\dagger_{j\beta}\vec{\sigma}_{\beta\alpha}c_{j\alpha}\right)\cdot\vec{S}_j$$

Replace the spin sites by auxiliary fermions $S_{\alpha\beta}(j) = f^\dagger_{j\alpha}f_{j\beta} - \frac{n_f(j)}{N}\delta_{\alpha\beta}$

This makes the effective Hamiltonian an “interacting” fermionic Hamiltonian

$$H \sim \sum_{\mathbf{k}\alpha}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha} - J\sum_{j,\alpha\beta}\left(c^\dagger_{j\beta}f_{j\beta}\right)\left(f^\dagger_{j\alpha}c_{j\alpha}\right)$$

Solving the Kondo lattice problem

Now we decouple the fermions with a mean-field approximation

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - J \sum_{j,\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta} \right) \left(f^\dagger_{j\alpha} c_{j\alpha} \right)$$

Obtaining a quadratic Hamiltonian

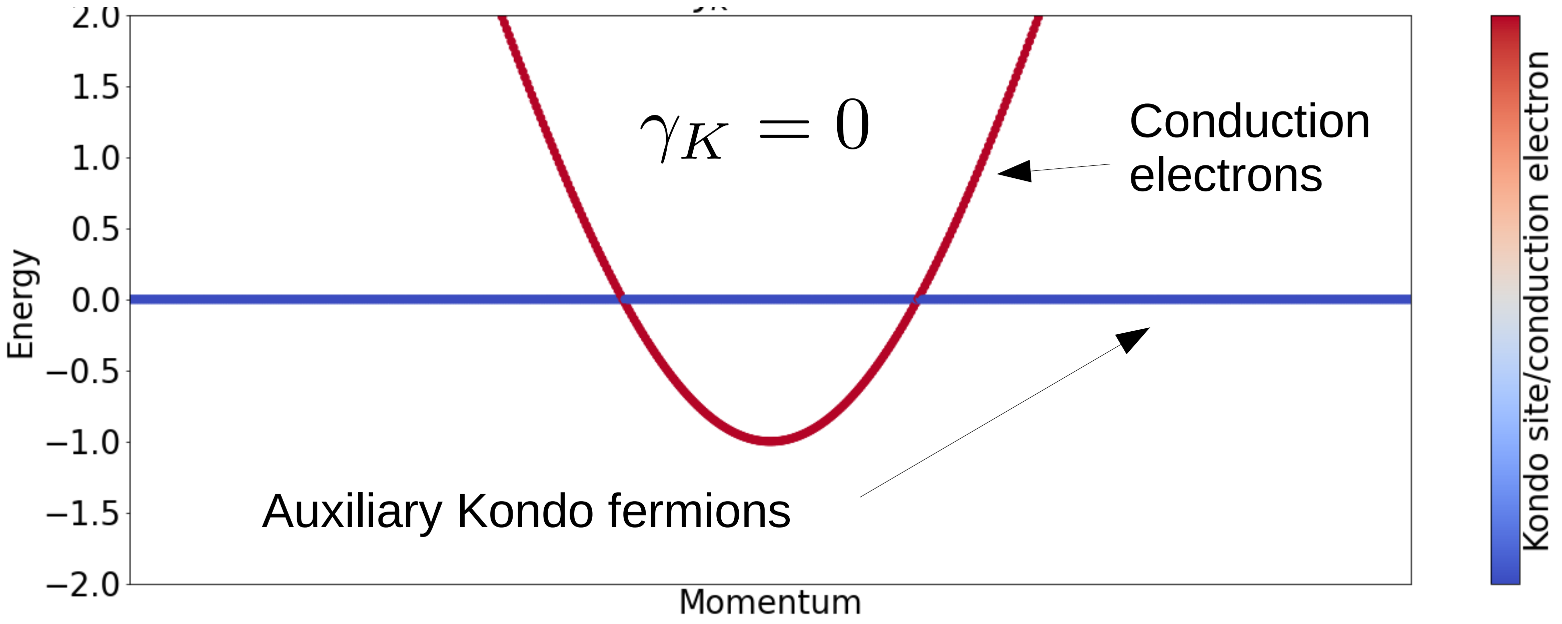
$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha\beta} f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$

Conduction band dispersion

Kondo hybridization

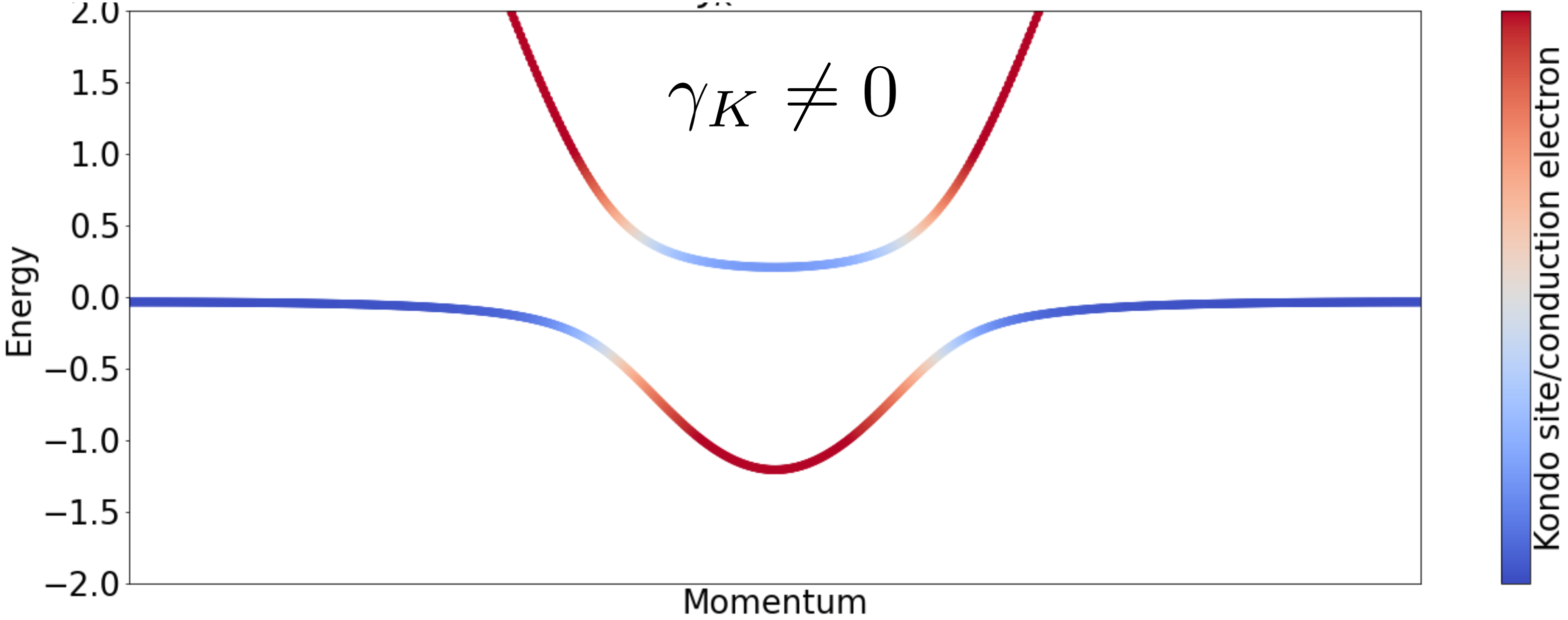
Electronic structure of the Kondo lattice problem

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha\beta} f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$



Electronic structure of the Kondo lattice problem

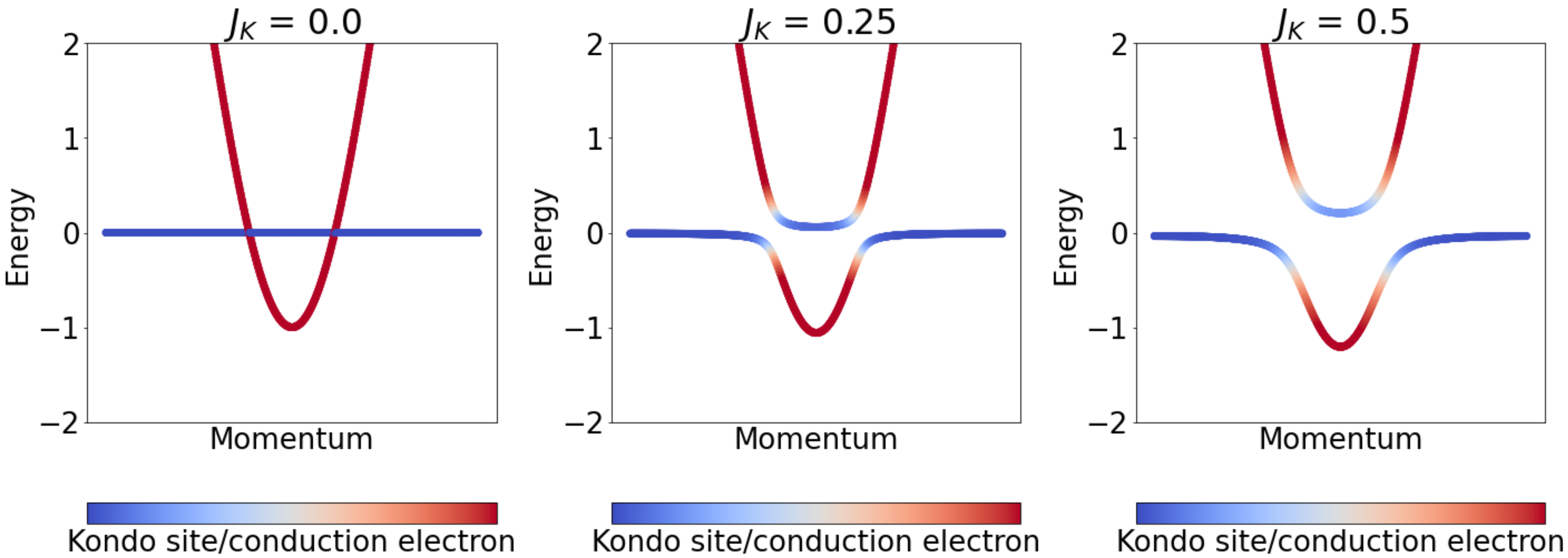
$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} - \gamma_K \sum_{\mathbf{k},\alpha\beta} f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + h.c.$$



The Kondo coupling opens up a gap in the electronic structure

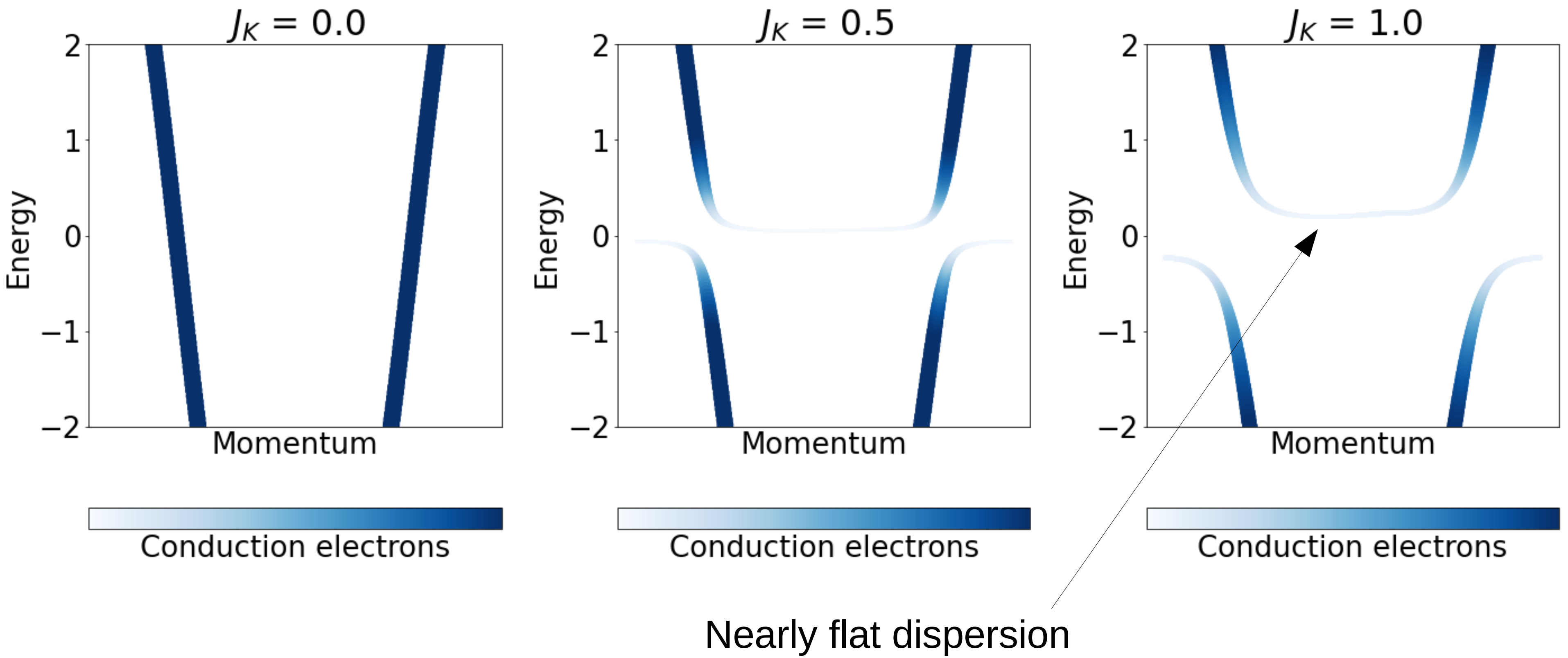
Dependence on the Kondo coupling

The heavy-fermion gap becomes bigger as the Kondo coupling increases



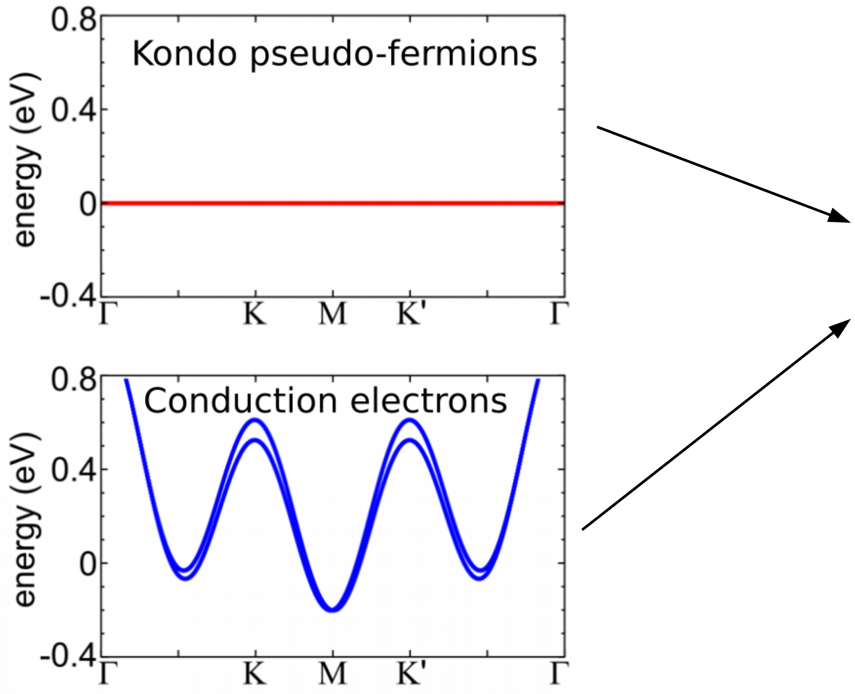
Spectral function of conduction electrons

The conduction electrons develop a heavy mass due to the Kondo coupling

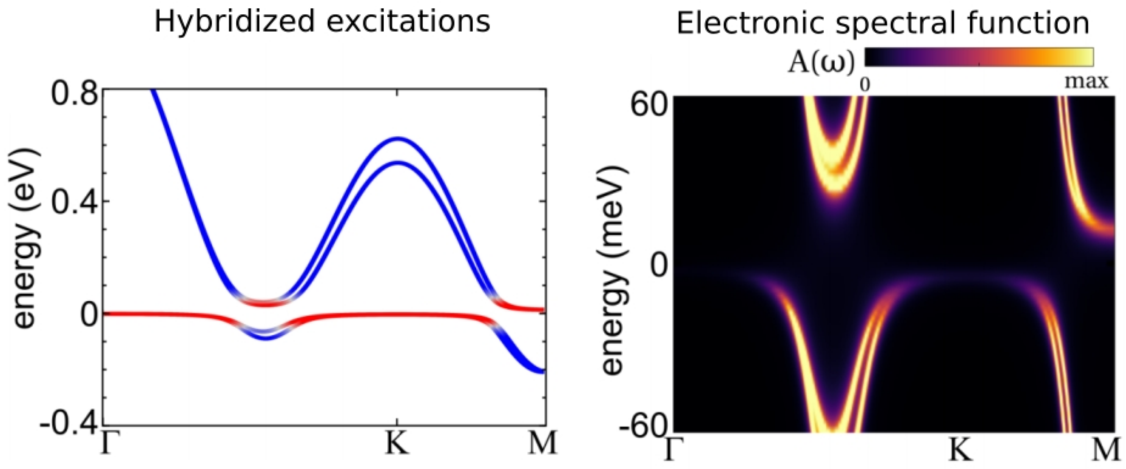


Brief theory of heavy-fermions

Kondo physics introduces resonant pseudo-fermions at the chemical potential



Leading to the opening of a heavy-fermion gap



Heterostructures of 1H-TaS_2/1T-TaS_2

For the exercise session this afternoon

Download the Jupyter-notebook from

https://github.com/joselado/jyvaskyla_summer_school_2022/blob/main/sessions/session3.ipynb

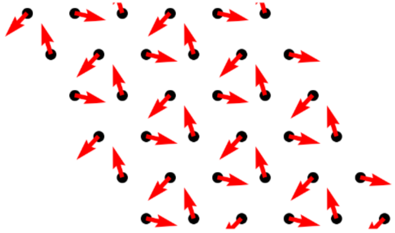
The tasks during the exercise sessions

You will see examples with the code

```
from pyqula import geometry
g = geometry.triangular_lattice() # generate a chain
g = g.get_supercell((3,3)) # make a supercell
h = g.get_hamiltonian() # generate the Hamiltonian

# generate the SCF Hamiltonian
U = 10. # strong Hubbard interaction
h = h.get_mean_field_hamiltonian(U=U,mf="XY",mix=0.9) # solve the interacting problem with a mean-field guess
hs = h.get_supercell(2) # generate a supercell
mx = hs.extract("mx") ; my = hs.extract("my") ; x = hs.geometry.r[:,0] ; y = hs.geometry.r[:,1] # get magnetization
plt.scatter(x,y,c="black",s=400) ; plt.quiver(x,y,mx,my,color="red")  # plot magnetization
plt.axis("equal") ; plt.axis("off")
```

```
(-4.124999999999999, 4.124999999999999, -2.3815698604072066, 2.381569860407206)
```



You have to modify them, and answer questions

Exercise

- Plot the band structure for the SCF solution for the 3x3 supercell, and estimate its gap
- Plot the band structure for the SCF solution for the 1x1 supercell, and estimate its gap
- Can you infer which one is the lowest energy solution, and why?