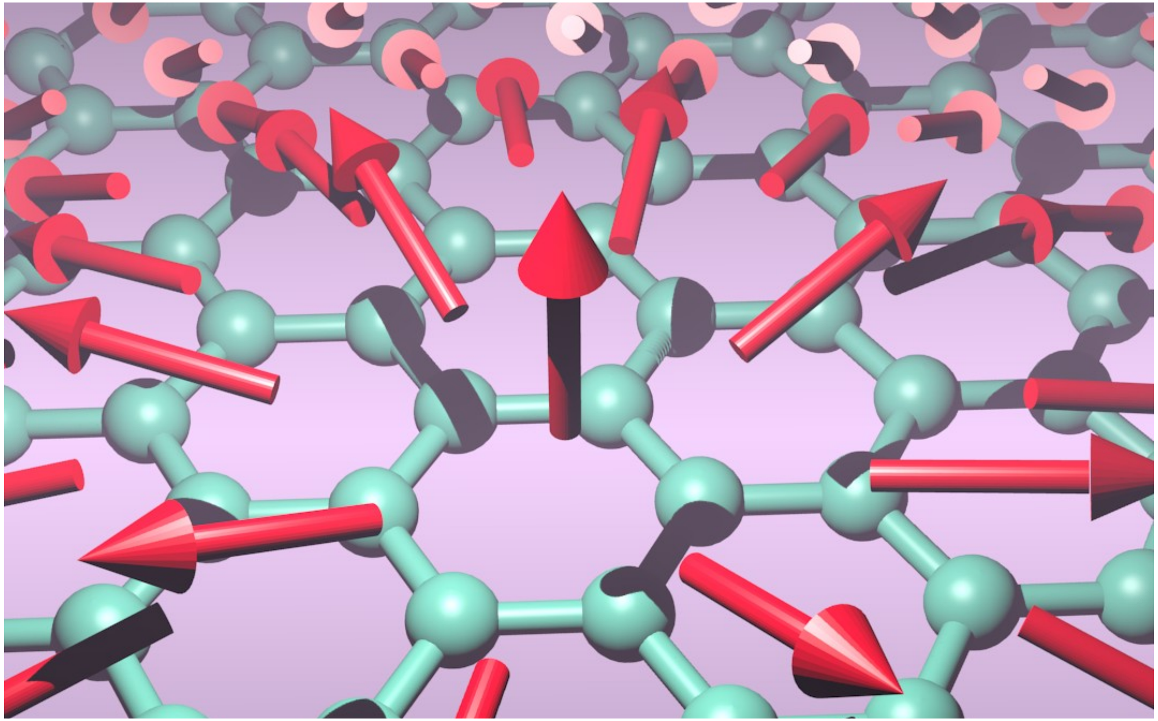
Magnetism, magnons, quantum magnetism and spinons



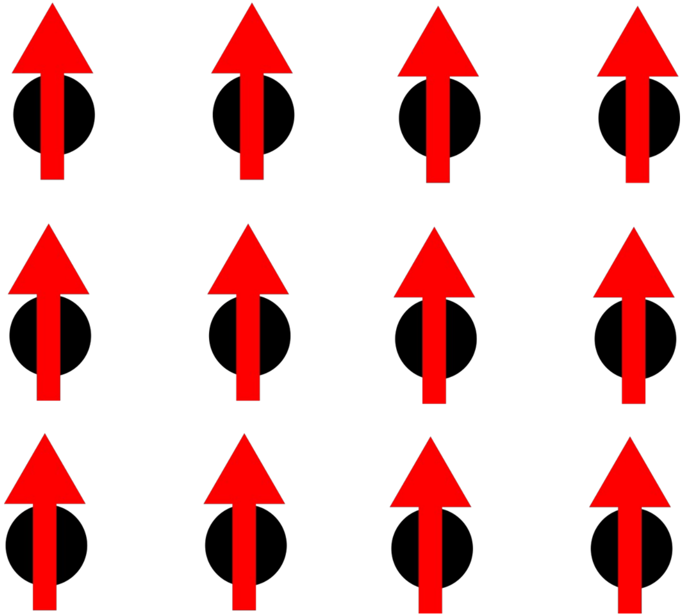
May 10th 2021

Today’s learning outcomes

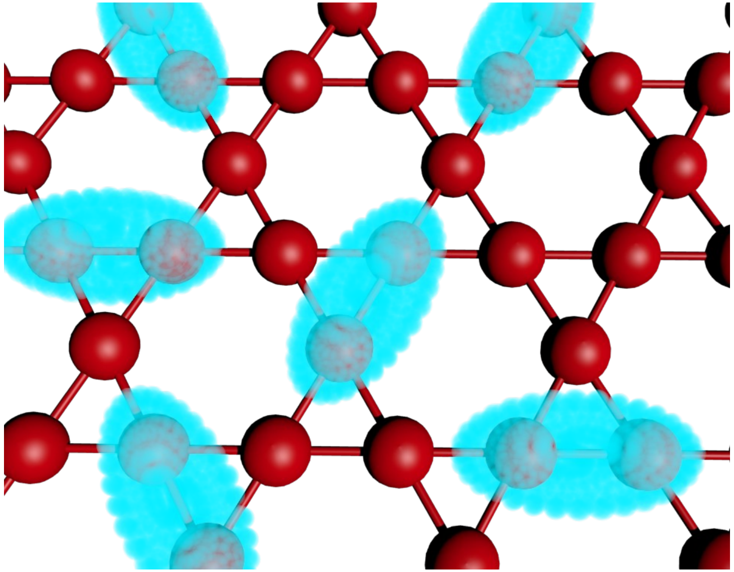
- The physical nature of magnetism
- The quantum excitations of ordered magnets
- The basics of quantum spin-liquids
- The quantum excitations of quantum spin-liquids

Today's materials

Ferromagnet & antiferromagnets

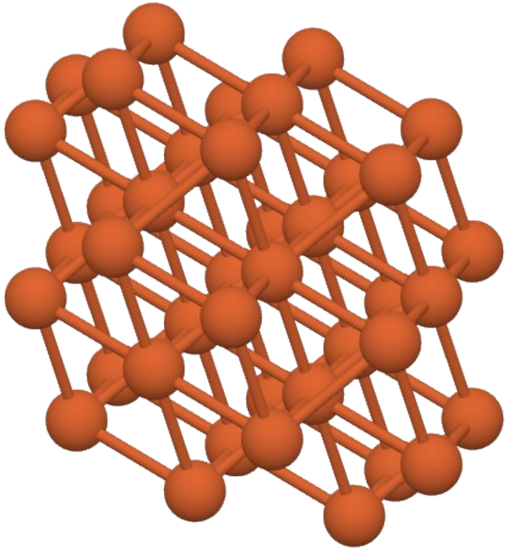


Quantum spin-liquids



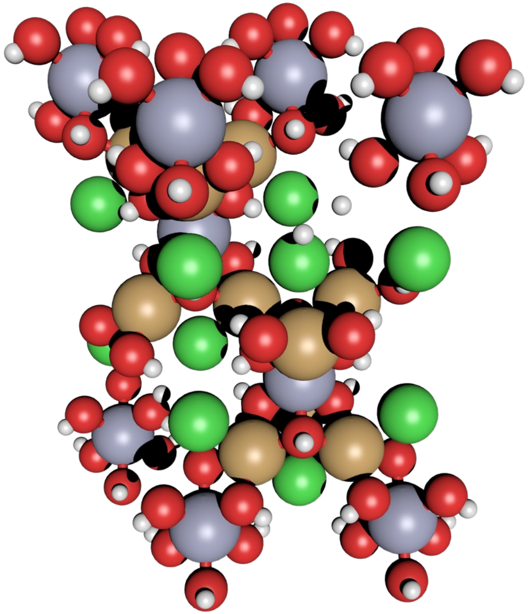
Today’s materials

Ferromagnet & antiferromagnets



Iron

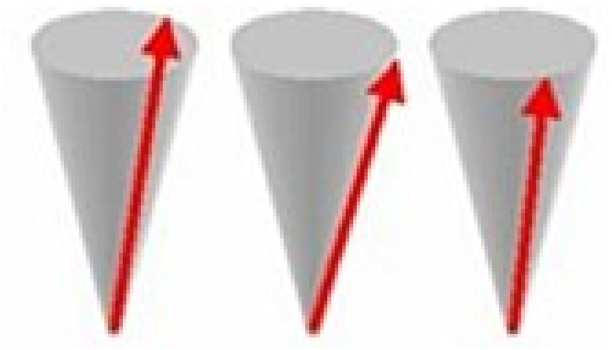
Quantum spin-liquids



Herbertsmithite

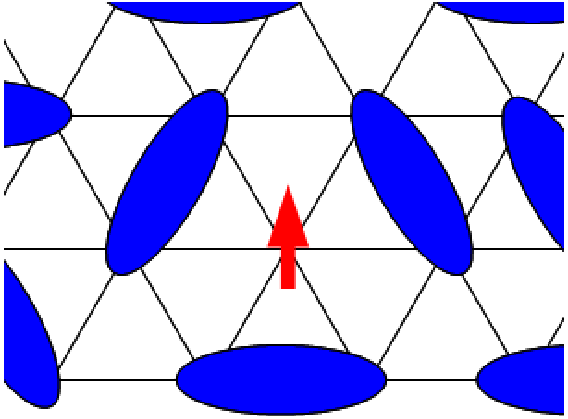
Today’s quasiparticles

Magnons



S=1
No charge

Spinons



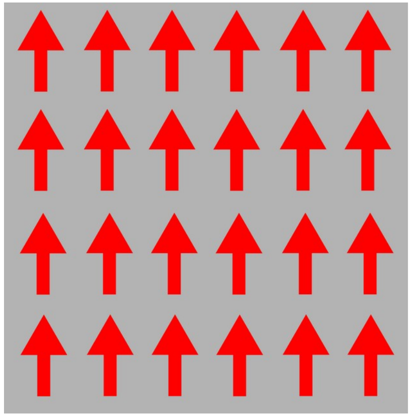
S=1/2
No charge

A reminder from previous sessions

Electronic interactions are responsible for symmetry breaking

Broken
time-reversal symmetry

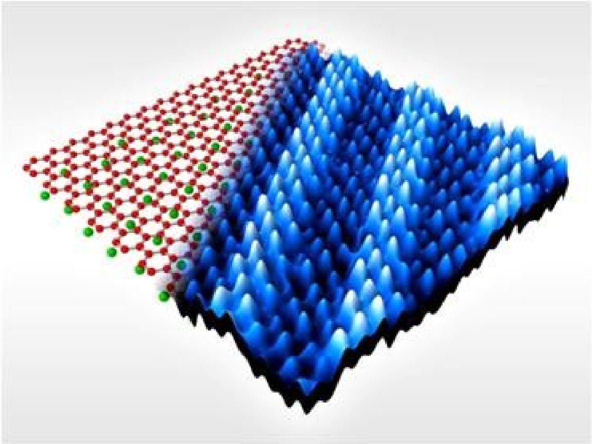
Classical magnets



$$\mathbf{M} \to -\mathbf{M}$$

Broken
crystal symmetry

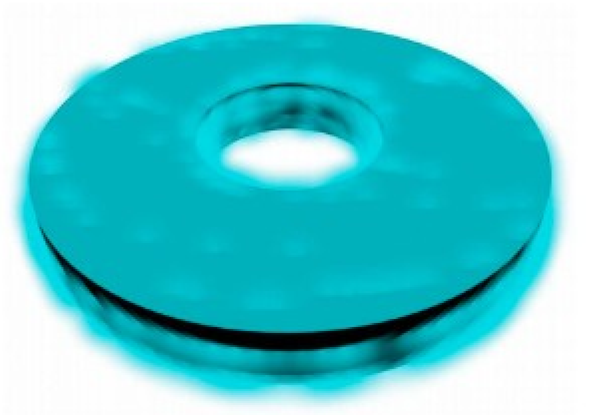
Charge density wave



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

Broken
gauge symmetry

Superconductors



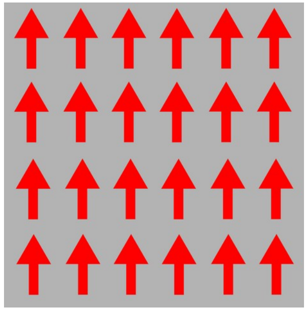
$$\langle c_\uparrow c_\downarrow \rangle \to e^{i\phi} \langle c_\uparrow c_\downarrow \rangle$$

Correlations and mean field

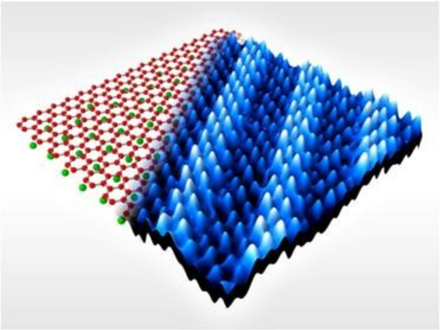
Many quantum states can be approximately described by mean field theories

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

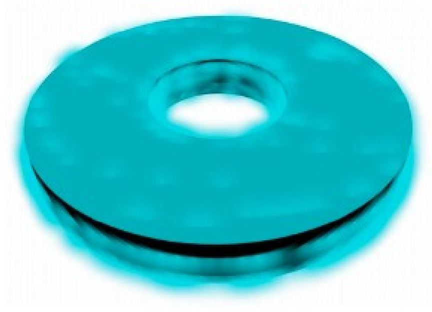
Magnets



Charge density waves



Superconductors



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)

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

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

For $U > 0$

i.e. repulsive interactions

Magnetic order

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

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?

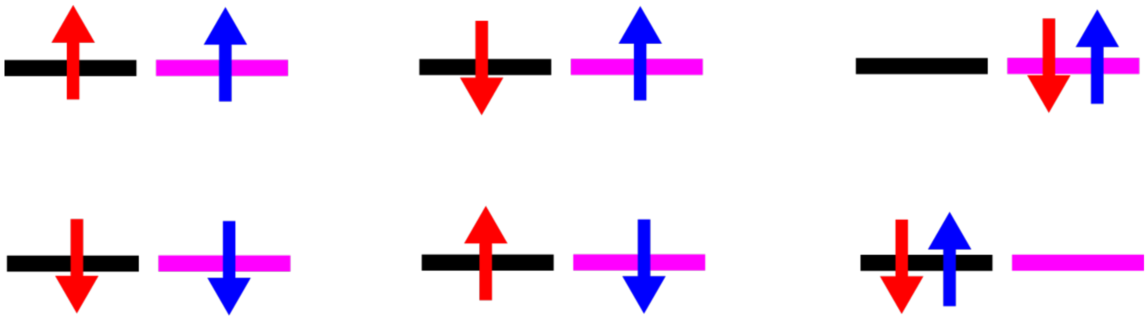
The strongly localized limit

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 $U \gg t$

The full Hilbert space at half filling is

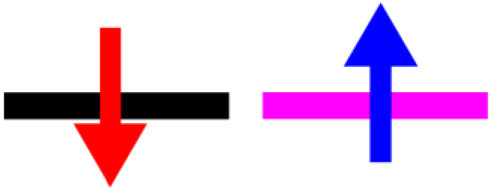


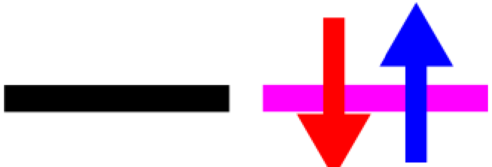
The strongly localized limit

Let us start with a Hubbard model dimer

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

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





The strongly localized limit

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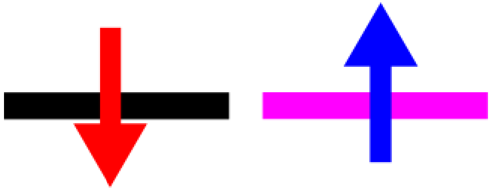
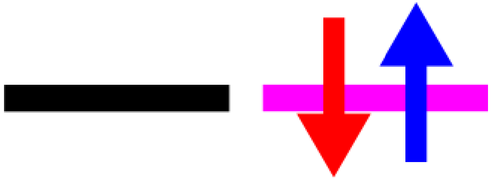


~ 0



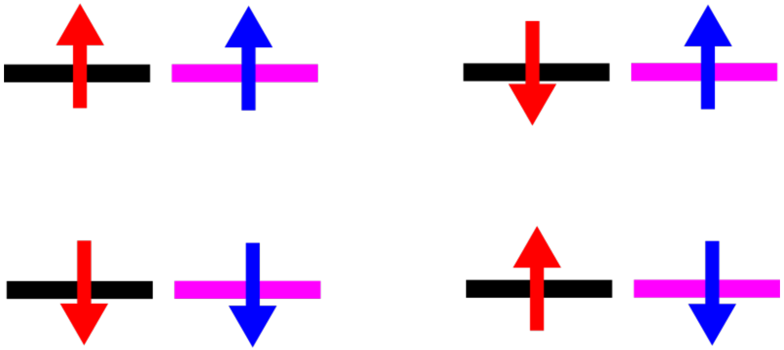
$\sim U$

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

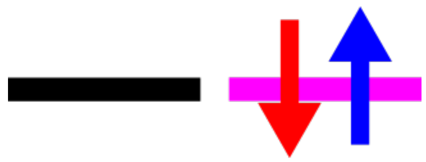
We can compute J using second order perturbation theory

$$H = H_0 + V$$

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

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

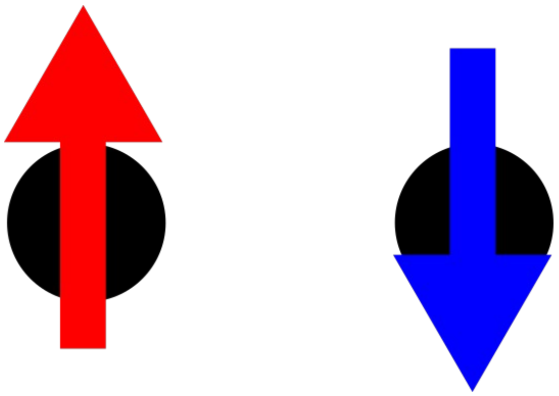
Spin-orbit coupling introduces anisotropic couplings

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

The Heisenberg model

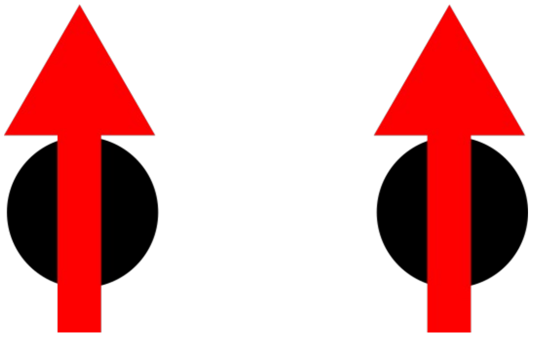
$$J_{ij} > 0$$

Antiferromagnetic coupling



$$J_{ij} < 0$$

Ferromagnetic coupling

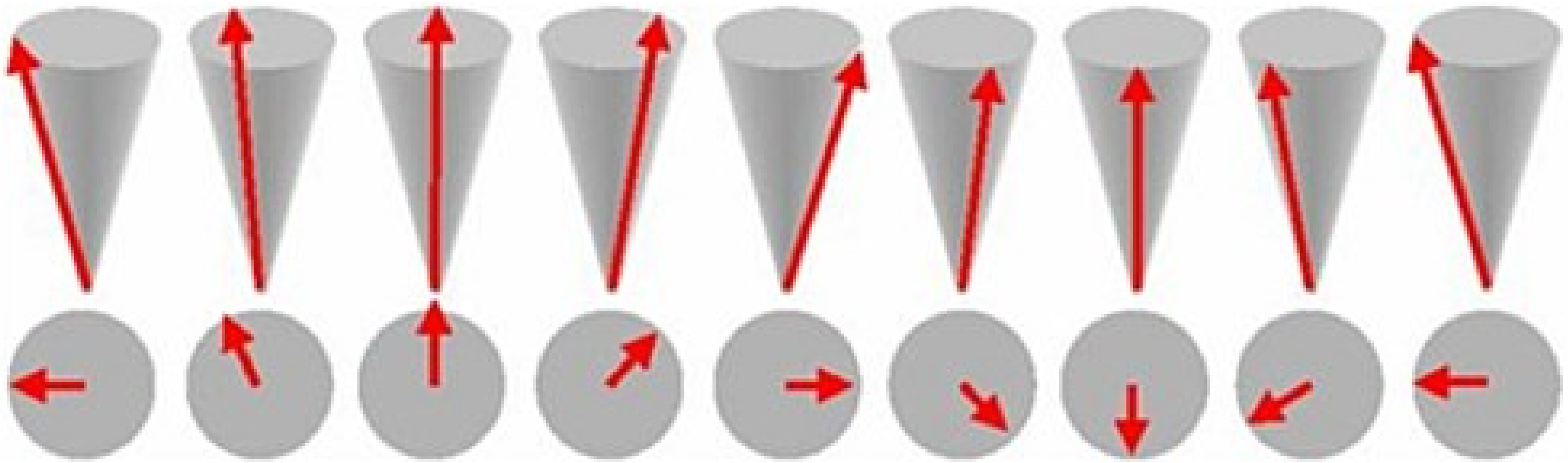


Classical ground states

Magnons

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?

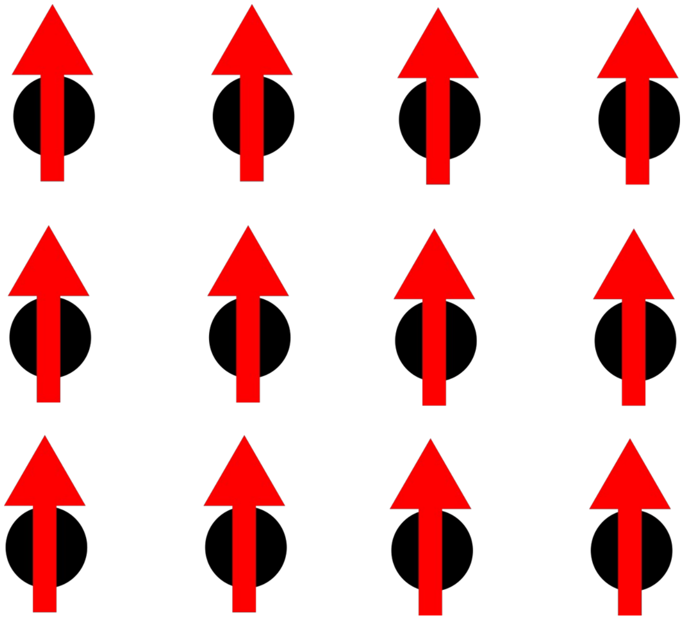
The ferromagnetic Heisenberg model

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

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

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**

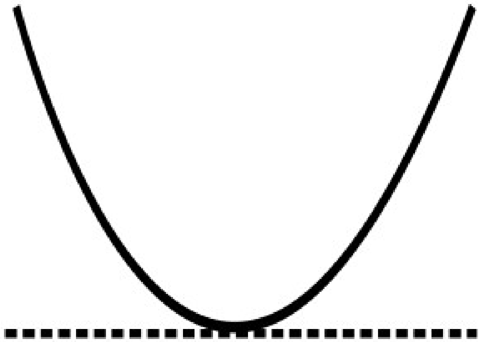
Magnons in a nutshell

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

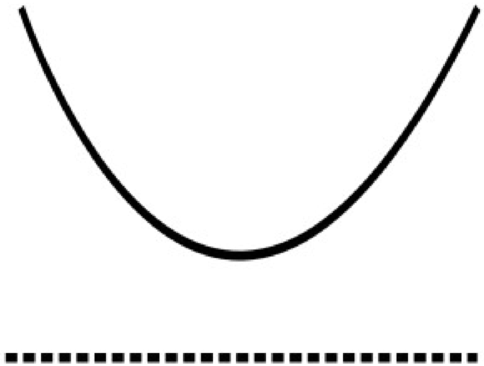
Magnons are S=1 excitations that exist over the symmetry broken state

Magnons dispersions

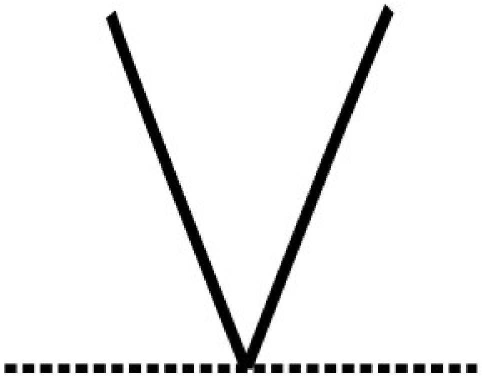
Gapless magnons



Gaped magnons



Dirac magnons



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

Quantum magnets

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 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

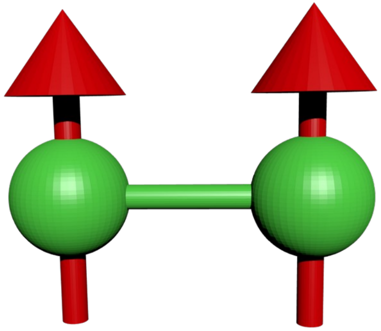
$$|GS\rangle = \frac{1}{2}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle] \qquad \langle \vec{S}_i \rangle = 0$$

The state is maximally entangled

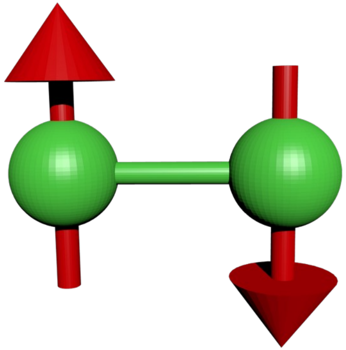
Can we have a macroscopic version of this ground state? $\langle \vec{S}_i \rangle = 0$

Towards quantum-spin liquids

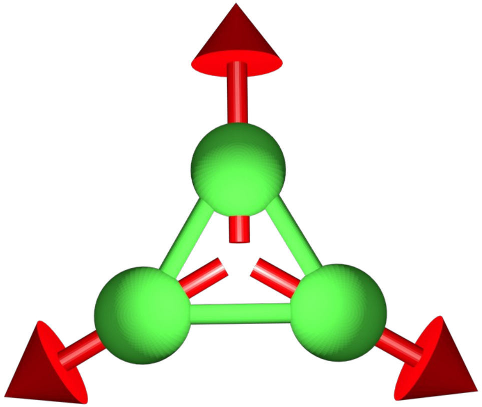
Ferromagnetism



Antiferromagnetism



Frustrated magnetism

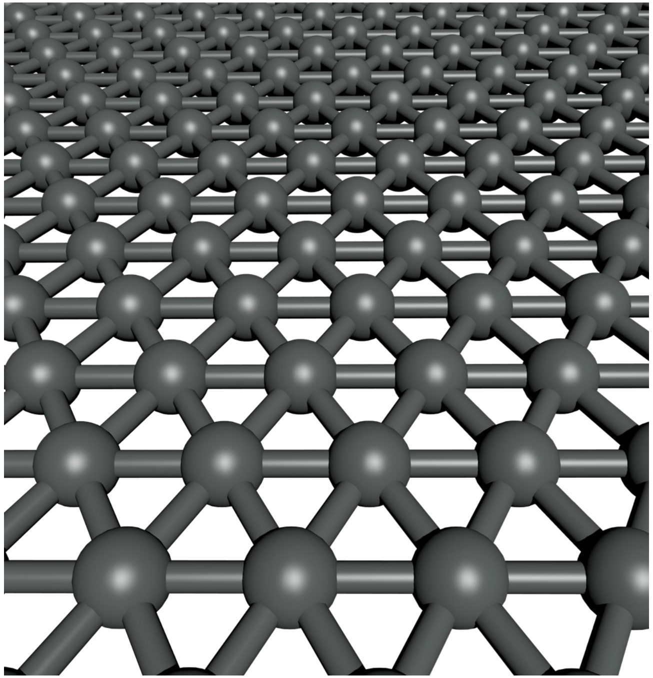


To get a quantum-spin liquid, we should look for frustrated magnetism

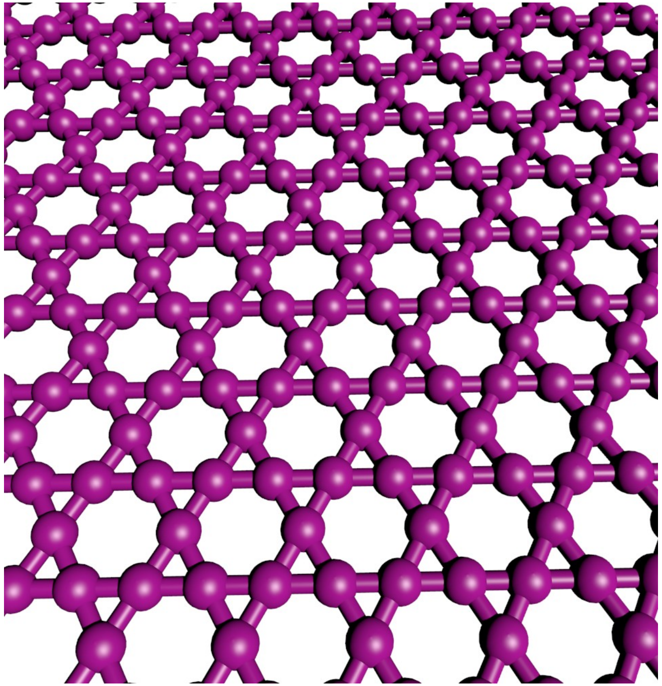
$$\langle \vec{S}_i \rangle = 0$$

Frustrated lattices

Triangular



Kagome



Spinons

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

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 $S_i^\alpha \sim \sigma_{s,s'}^\alpha f_{i,s}^\dagger f_{i,s'}$

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

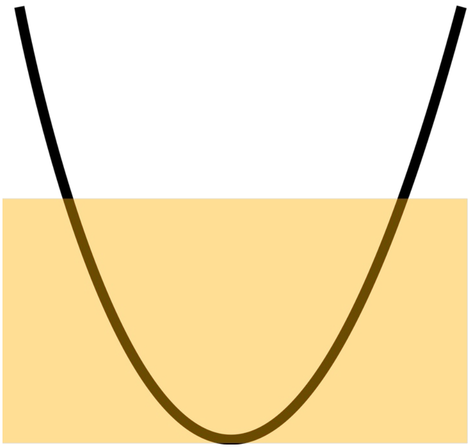
$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \longrightarrow \mathcal{H} = \sum_{ij,s} \chi_{ij} f_{i,s}^\dagger f_{j,s}$$

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

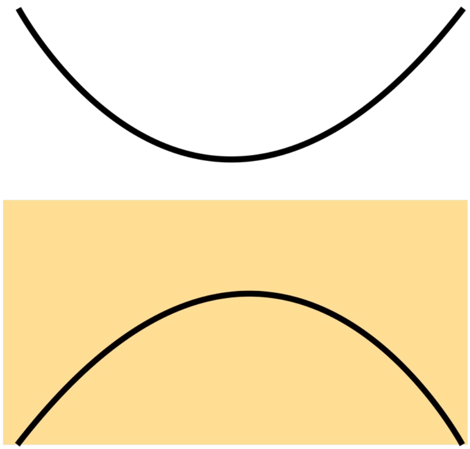
The exitations of the QSL are described by a single particle spinon Hamiltonian

Spinon dispersions

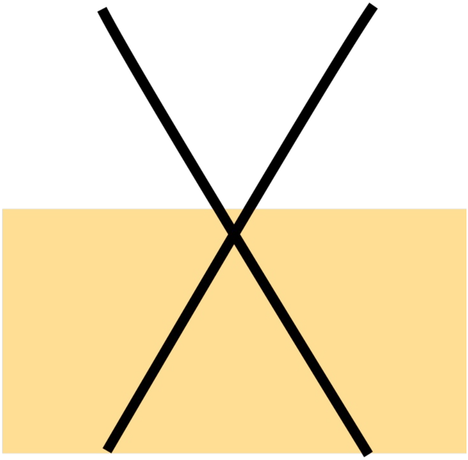
Gapless spinons



Gaped spinons



Dirac spinons



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

Take home

- Magnetism arises from repulsive interactions
- The fundamental excitations of magnets are magnons and have S=1
- Frustrated magnetic models can display quantum spin-liquid behavior
- The fundamental excitations of QSL have S=1/2

Reading material

- Steven Simon, Oxford solid-state basics, pages 225-229
- Notes Titus Neupert, pages 125-137