Magnetism, magnons, quantum magnetism and spinons



May 2nd 2023

Today's learning outcomes

- Derive minimal models for magnetism
- Identify the quantum excitations of ordered magnets
- Identify the quantum excitations of quantum spinliquids
- Identify the fundamental physics of Kondo lattice models

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



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

Broken crystal symmetry Charge density wave



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

Broken gauge symmetry Superconductors



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

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



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 simple interacting Hamiltonian

$$\begin{aligned} \text{Free Hamiltonian} & \text{Interactions} \\ \text{(Hubbard term)} \\ H &= \sum_{ij} t_{ij} [c^{\dagger}_{i\uparrow} c_{j\uparrow} + c^{\dagger}_{i\downarrow} c_{j\downarrow}] + \sum_{i} Uc^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} \end{aligned}$$

What is the ground state of this Hamiltonian?

U > 0

Magnetism

$$U < 0\,$$
 Superconductivity

The mean-field approximation

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

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

$$Uc_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} \approx U\langle c_{i\uparrow}^{\dagger}c_{i\uparrow}\rangle c_{i\downarrow}^{\dagger}c_{i\downarrow} + \dots + h.c_{i\downarrow}$$
$$Uc_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow} \approx M\sigma_{ss'}^{z}c_{i,s}^{\dagger}c_{i,s'} + h.c.$$

Magnetic order

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

For U > 0 i.e. repulsive interactions

The mean-field approximation

The non-collinear mean-field Hamiltonian

$$Uc_{n\uparrow}^{\dagger}c_{n\uparrow}c_{n\downarrow}^{\dagger}c_{n\downarrow} \approx M_{n}^{\alpha}\sigma_{ss'}^{\alpha}c_{n,s}^{\dagger}c_{n,s'} + h.c.$$

Non-collinear magnetic order

$$M_n^z \sim \langle c_{n\uparrow}^{\dagger} c_{n\uparrow} \rangle - \langle c_{n\downarrow}^{\dagger} c_{n\downarrow} \rangle$$
$$M_n^x \sim \langle c_{n\uparrow}^{\dagger} c_{n\downarrow} \rangle + \langle c_{n\downarrow}^{\dagger} c_{n\uparrow} \rangle$$
$$M_n^y \sim i \langle c_{n\uparrow}^{\dagger} c_{n\downarrow} \rangle - i \langle c_{n\downarrow}^{\dagger} c_{n\uparrow} \rangle$$

A Hamiltonian for a weakly correlated magnet

$$\begin{array}{ll} \textit{Free Hamiltonian} & \textit{Exchange term} \\ H = \sum_{ij} t_{ij} [c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}] + M \sum_{i} \sigma_{s,s'}^{z} c_{i,s}^{\dagger} c_{i,s'} \\ \end{array}$$

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



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



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? $\langle S_z angle eq 0$

In general, in the weak coupling limit magnetism appears when

Repulsive interaction

Density of states

The critical interaction for magnetic ordering

Magnetic instabilities occur once interactions are strong enough



For interactions below a threshold, no magnetic order occurs

The strongly localized limit and the Heisenberg model

From a weak magnet to the strongly localized limit

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

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



Let us start with a Hubbard model dimer

$$H = t[c_{0\uparrow}^{\dagger}c_{1\uparrow} + c_{0\downarrow}^{\dagger}c_{1\downarrow}] + \sum_{i} Uc_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}c_{i\downarrow} + h.c.$$
Now in the limit $U \gg t$ Levels 0 1
The full Hilbert space at half filling is

The full millert space at fiall filling is



Let us start with a Hubbard model dimer

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

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



Let us start with a Hubbard model dimer

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

The low energy manifold is



Just one electron in each site for

r $U \gg t$

Local S=1/2 at each site

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

$$\begin{split} H &= H_0 + V \\ H_0 &= \sum_i U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} \\ \text{"pristine" Hamiltonian} \\ \text{(Hubbard)} \end{split} V = t [c_{0\uparrow}^{\dagger} c_{1\uparrow} + c_{0\downarrow}^{\dagger} c_{1\downarrow}] + \text{h.c.} \end{split}$$

Effective Heisenberg model in the localized limit

We can compute J using second order perturbation theory

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

$$H = H_0 + V$$



The Heisenberg model

For a generic Hamiltonian in a generic lattice

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

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



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



In bipartite lattices, the magnetization is collinear

Antiferromagnetism driven by superexchange

In the Kagome lattice

In the triangular lattice



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



Goodenough-Kanamori rules

Non-isotropic exchange coupling

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



Promotes non-collinear order

Promotes easy axis/plane

Promotes frustration



10-15 min break

(optional) to discuss during the break

Which type of magnetic order fulfills

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

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

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

$$S = 1/2, 1, 3/2, 2, \dots$$

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

$$\mathcal{H} = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$
$$J_{ij} < 0$$
$$GS \rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\dots\rangle$$

But how do we compute the excitations?



The Holstein–Primakoff transformation

Replace the spin Hamiltonian by a bosonic Hamiltonian

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

Magnon

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

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

Spins

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

$$\langle S_i^z
angle = S - \langle a_i^\dagger a_i
angle$$
 Maximal min

Maximal minus the magnons

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

Magnon dispersions



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



Magnons in the presence and absence of anisotropy

Without anisotropy

With anisotropy



Anisotropy in the spin model generates a magnon gap

The role of magnons in 2D magnets

Correction from magnon population

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

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

Magnons renormalize the total magnetization

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

Temperature

Energy T

Momentum

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



Position operator



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

Quantum spin liquids and spinons

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)

 $|GS_1\rangle = |\uparrow\downarrow\rangle \qquad \qquad |GS_2\rangle = |\downarrow\uparrow\rangle$

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



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

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

Frustrated lattices

Triangular







Quasiparticles in a quantum spin-liquid

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

Quantum spin liquids require $~\langle ec{S}_i
angle = 0$

The approximation used for magnons breaks down

ij

$$\begin{split} \langle S_i^z \rangle &= S - \langle a_i^\dagger a_i \rangle \\ \langle a_i^\dagger a_i \rangle \ll S \end{split}$$

We need a new approximation for the quantum excitations

The parton transformation

Transform spin operators to auxiliary fermions (Abrikosov fermions)

$$S_i^{\alpha} = \frac{1}{2} \sigma_{s,s'}^{\alpha} f_{i,s}^{\dagger} f_{i,s'}$$

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

$$\sum_{s} f_{i,s}^{\dagger} f_{i,s} = 1$$

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

The spinon Hamiltonian

We can insert the auxiliary fermions $\int_{-\infty}^{\infty}$

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

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



The Kondo lattice model

The Kondo problem



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

Kondo coupling

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

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



Building an artificial heavy fermion state

Lattice of Kondo impurities



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

X.

₩.

K

Associated with Kondo lattice physics:

- Colossal mass enhancement of electrons
- Quantum criticality
- Unconventional (topological) superconductivity

Solving the Kondo lattice problem

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

Replace the spin sites by auxiliary fermions

$$S_{\alpha\beta}(j) = f_{j\alpha}^{\dagger} f_{j\beta} - \frac{n_f(j)}{N} \delta_{\alpha\beta}$$

This makes the effective Hamiltonian an "interacting" fermionic Hamiltonian

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

Solving the Kondo lattice problem

Now we decouple the fermions with a mean-field approximation

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

Obtaining a quadratic Hamiltonian

$$H \sim \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}} c_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}\alpha} - \gamma_{K} \sum_{\mathbf{k},\alpha\beta} f_{\mathbf{k}\alpha}^{\dagger} c_{\mathbf{k}\alpha} + h.c.$$

Conduction band dispersion

Kondo hybridization

Electronic structure of the Kondo lattice problem





Electronic structure of the Kondo lattice problem



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



Take home

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