4. Classical degeneracies and order by disorder

4.1. Classical degeneracies

< discrete
< continuous

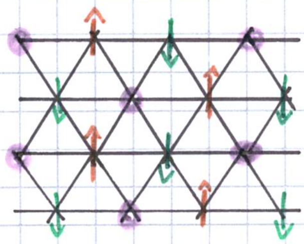
Frustration can produce manifold of lowest-energy states which still have extensive set of degrees of freedom left.

Example triangular-lattice Ising AF

Lowest energy requires ↑↑↓ or ↓↓↑ in each triangle.

One family of lowest-energy states can be constructed by putting

A sublattice ↑
B sublattice ↓
C sublattice arbitrary !



⇒ Ground-state manifold contains at least (!) $2^{N/3}$ states

⇒ residual entropy density $S/N\,(T\to 0) \geq \frac{1}{3} k_B \ln 2$

Full result (Wannier 1950): $S/N\,(T\to 0) \approx 0.338\, k_B$

Example classical (spin) ice (see Chapter 5)

Ising spins on corner-sharing tetrahedra (pyrochlore), lowest energy requires „2in, 2out" („ice rule", 6 possible states for single tetrahedron)

Full result (Pauling 1938 + later):

$$S/N\,(T\to 0) = \frac{1}{2} \ln \frac{3}{2}\, k_B$$

+ 1% correction

Example pyrochlore Heisenberg spins

Single tetrahedron $H = J/_2 \; \vec{S}_{tot}^{\,2} + \text{const}$; $\vec{S}_{tot} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \vec{S}_4$

Consider states with $S_{tot} = 0$. Count angle degrees of freedom:

$$\underbrace{4}_{\text{4 spins}} \times \underbrace{2}_{\text{spin orientation}} - \underbrace{3}_{\text{vector sum} = 0} - \underbrace{3}_{\substack{\text{global rotations}\\ \text{(symmetry)}}} = 2$$

$\leadsto$ 2 angles free (in addition to global rotation!)

For pyrochlore lattice : $2N \times 2$ orientations, $N \times 3$ constraints $\Big\}$ N angles free (extensive!)

System with extensive residual classical degrees of freedom are called strongly (or highly) frustrated;
as opposed to weakly frustrated system (eg triangular-lattice Heisenberg).

ATTN: Weakly frustrated — only degenerate w.r.t. global symmetry trafo + discrete, finite degeneracies

subextensive set of degeneracies (like J_1-J_2 square lattice)

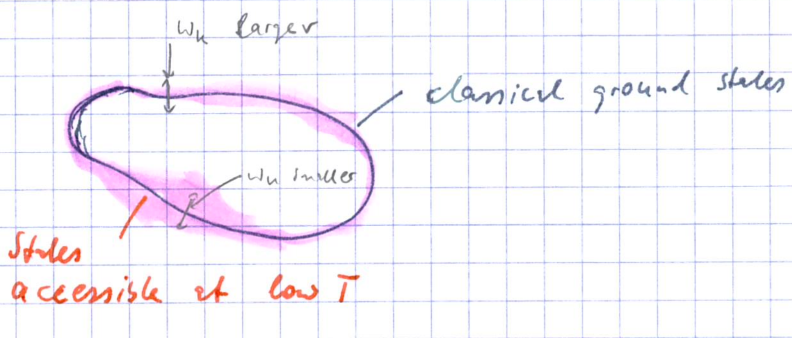
Note The above (Maxwellian) counting argument,
degrees of freedom in ground state = total # degrees of freedom − # constraints,
is not exact, because
(i) the constraints may not be independent,
(ii) There may be lattices on which not all constraints can be fulfilled.

Example kagome Heisenberg   Naive counting yields zero (extensive) d.o.f.,

4.2. Order by disorder

Fluctuations may lift degeneracy among classically degenerate states. < quantum corrections to energy / entropy $F = E - TS$ at finite T

Phase-space picture:

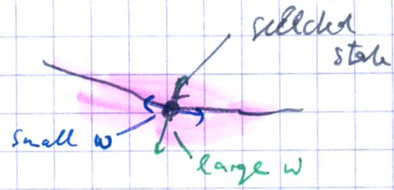


Different classical states differ in their excitation spectrum ω_k.
Fluctuation effects typically select // prefer those classical states with low excitation energies, because those yield small zero-point energy (recall $H_2 = \sum_k \omega_k (\alpha_k^\dagger \alpha_k + \frac{1}{2})$) and large low-$T$ entropy. The selected state is usually one with LRO.

As a result of this selection, fluctuation effects may enhance the tendency to long-range order
$\hat{=}$ „order by disorder" < quantum (via zero-point energy) / thermal (via entropy)

Often thermal and quantum fluctuations select same state.

If long-range order is established as a result of order by disorder, this state will have excitation modes with particularly low energy corresponding to fluctuations within classically degenerate manifold.
Classically these modes are at zero energy, but quantum effects produce finite ω.



→ mode energy not $\propto TS$.

Thermal order by disorder:

Small temperature $0 < T \ll JS^2$ may or may not lead to long-range order: „too many" soft modes destroy order for any T, while „few" soft modes produce obd (need detailed calculation).

Larger temperature $T \gtrsim JS^2$ will destroy order anyway. (see mean-field theory)

Quantum order by disorder

Small quantum fluctuations can be achieved for large S, hence one expects long-range order generically (!) for $1 \ll S < \infty$. For smaller S quantum fluctuations may destroy order (in favor of spin liquids, valence-bond solids etc).

Real system at finite T:

Quantum fluct win for $T \ll JS$.

Thermal obd active for $JS \ll T \ll JS^2$

energy of single mode

classical ground-state energy

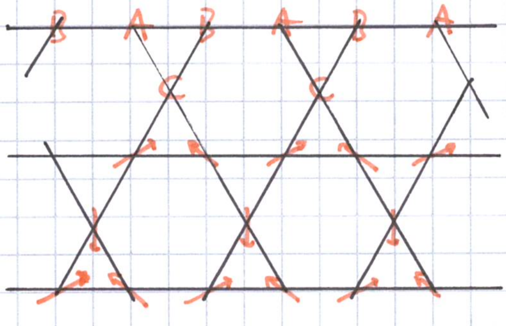
Note: The temperature window for thermal obd, $JS \ll T \ll JS^2$, only exists for large S.

For small S (e.g. $S = 1/2$) thermal obd is never realized ! (because quantum effects win at low T, and thermal fluct destroy all order at higher T)

4.3. Order by disorder: Examples

(A) Strongly frustrated systems

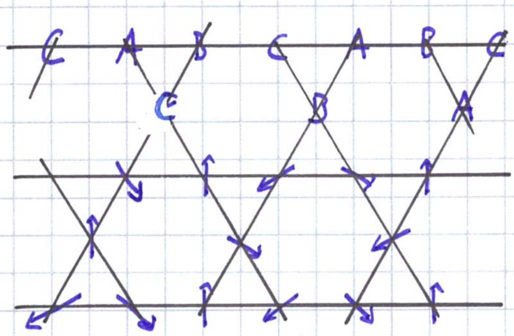
- Classical kagome Heisenberg AF



„$q=0$" state

Ground-state manifold has extensive continuous set of d.o.f.

Fluctuations select (to leading order) coplanar states. Two ordered candidates are „$q=0$" and „$\sqrt{3}\times\sqrt{3}$".



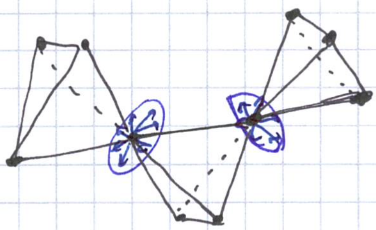
„$\sqrt{3}\times\sqrt{3}$" state

Numerics indicates weak selection of $\sqrt{3}\times\sqrt{3}$ order at very low T.

↷ classical kagome Heisenberg AF displays long-range order as $T\to 0$ (but not at $T=0$!!)

- Classical pyrochlore Heisenberg AF

No thermal obd.



- Classical pyrochlore XY AF:

Pyrochlore lattice has 4 spins per unit cell.

Crystalline symmetry dictates local anisotropy axes!

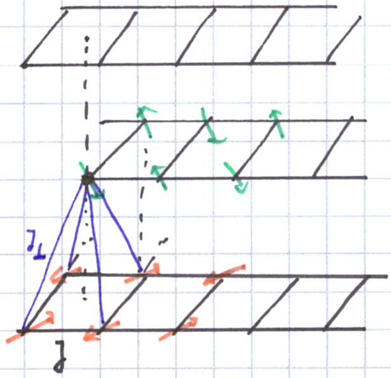
XY $\hat{=}$ spins preferentially $\perp$ axis connecting centers of neighboring tetrahedra

Ground-state manifold has one continuous d.o.f.

Fluctuations select discrete (non-coplanar) ordered states, labelled ψ_2 (or ψ_3, depending on parameters) at low T.

Example: $Er_2Ti_2O_7$

(B) Weakly frustrated systems



- Classical body-centered tetragonal Heisenberg AF

  Assume $J_\perp \ll J$.

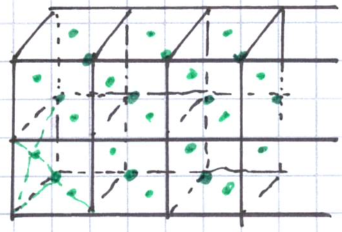
  Each layer has (π,π) AF order,

  but ground-state manifold has subextensive

  continuous d.o.f. $\hat{=}$ relative orientation

  between layers.

  Fluctuations select collinearly ordered states.



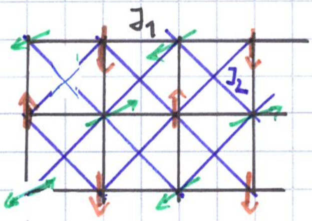
- Classical fcc Heisenberg AF

  Depending on ratio of

  first / second / third-neighbor couplings,

  various different states can appear.

  In all cases, fluctuations select collinear states.



- $J_1 - J_2$ square-lattice Heisenberg AF (↝ exercise)

  Assume $J_2 \gg J_1$ (!!).

  System consist of two interpenetrating

  square (sub) lattices, each with AF order.

  red green

  Ground-state manifold has one

  continuous d.o.f. $\hat{=}$ relative orientation ϕ of two subsystems

  Fluctuations select collinear state.

  Quantum o.b.d. can be computed using spin waves:

  Energy correction is $\Delta E \simeq - J N S \cos^2 \phi$ (effective biquadratic interaction $(\vec{S}\cdot\vec{S})^2$)

  ↝ $\phi = 0, \pi$ preferred $\hat{=}$ collinear order