Ising model and descendents [tln93]

The importance of the Ising model is connected to its simplicity.

- The Ising spin is a classical degree of freedom of the simplest kind. It becomes a quantum degree of freedom in some contexts, e.g. in the presence of a transverse magnetic field.
- The interaction between Ising spins has the simplest possible structure.
- The Ising coupling is employed to represent many different physical couplings between physical degrees of freedom associated with atoms or molecules on a lattice of any symmetry or dimensionality.
- Solutions of the Ising model can be transcribed to a multitude of physical applications via rigorous mappings, e.g. between uniaxial magnets and lattice gases.
- In computational studies, the Ising model is favorite discrete representation for the simulation of continuum models.
- The structural simplicity of the Ising model facilitates the study of universal features in cooperative phenomena, specifically features that depend on the lattice dimensionality.
  - ▷ With increasing dimensionality $\mathcal{D}$ of the lattice, the ordering tendency are stronger and the thermal fluctuations are weaker.
  - ▷ In $\mathcal{D} = 1$ there is only one lattice type. An analytic solution is available by several methods. That solution can be extended to ladders and lattices with no connected loops (Bethe lattice).
  - ▷ In $\mathcal{D} = 2$ an exact solution is available for several lattice types. This is one of only few exactly solvable models exhibiting a second order phase transition in the face of correlated fluctuations.
  - ▷ The Ising model in $\mathcal{D} = 2$ on a triangular lattice is an ideal model for the study of geometric frustration (realized when antiparallel alignment of Ising spins is energetically favored).
  - ▷ An exact solution for any lattice in $\mathcal{D} = 3$ has been tantalizingly out of reach to any attempts. Extensive numerical studies and approximations have produced many results of consistent accuracy.
  - ▷ In the limit $\mathcal{D} = \infty$ methodological simplifications can be put into place (equivalent-neighbor model) which produce an exact solution. The role of fluctuations is reduced to irrelevance.

Further-neighbor coupling:

The standard Ising model involves an interaction between nearest-neighbor (nn) sites of a lattice. An obvious generalization includes a coupling between next-nearest-neighbor (nnn) sites.

The $T = 0$ phase diagram of an Ising chain with nn and nnn coupling is discussed in [tln96].

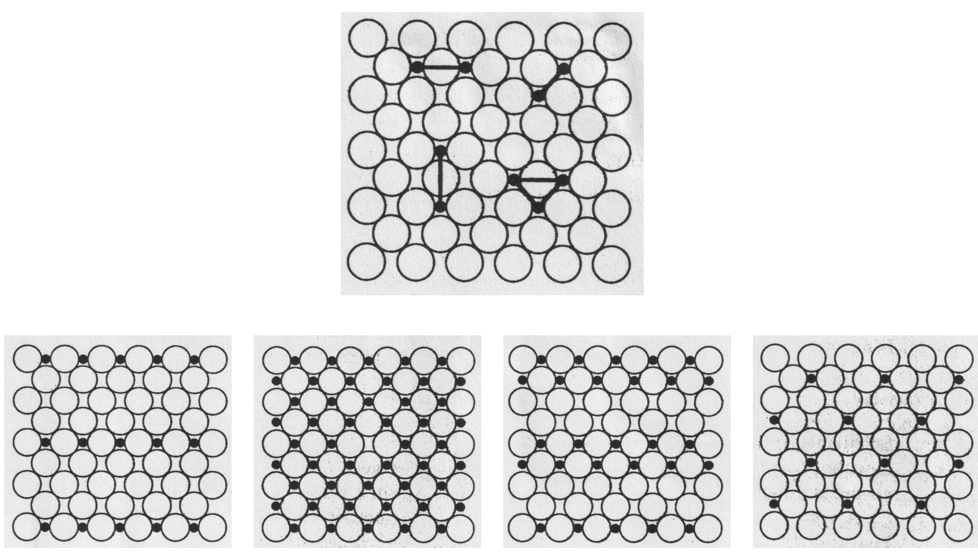
An application of the Ising model on a square-lattice ($\mathcal{D} = 2$) with nn and nnn coupling pertains to hydrogen atoms adsorbed to a (110) surface of iron ordered in a bcc lattice.

A simplified scenario depicts the Fe atoms on the surface as big open circles on a square lattice and the H atoms as small closed circles occupying the centers of the squares as shown.

The nearest-neighbor coupling between H atoms is indicated by short slanted lines and the nnn coupling by longer vertical or horizontal lines.

Depending on the relative strength and sign of the two couplings the Ising model thus generalized predicts several different ordering patterns including the ones shown.

Some of these ordered phases are observable by experiments. What phase is realized depends on the temperature and on the fraction of sites occupied.

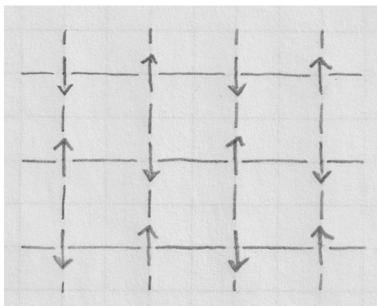


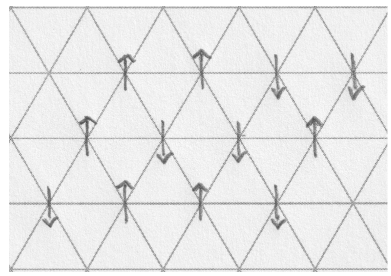
[image from Yeomans 1992]

Geometric frustration:

Bipartite lattices can be split into two interpenetrating sublattices such that all nn couplings are inter-sublattice couplings.

In dimension $\mathcal{D} = 2$, for example, the square lattice is bibartite, but the triangular lattice is not.





Consider the Ising model with nn coupling and no magnetic field:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i^z S_j^z, \quad S_i^z = \pm\tfrac{1}{2}.$$

Spin alignment, which is favored if $J > 0$, is readily accommodated at low temperature, irrespective of whether the lattice bipartite or not.

Spin anti-alignment, on the other hand, which is favored if $J < 0$, is only accommodated at low temperature for bipartite lattices. In lattices which are not bipartite, the nn coupling with $J < 0$ is frustrated geometrically.

In the triangular lattice, for example, the the spins on the corners of each triangle, which are mutually nn coupled, can be completely aligned, but not completely anti-aligned. Anti-alignment is frustrated by geometry.

The Ising model on a square-lattice undergoes a phase transition at low temperature to a ferromagnetic phase if $J > 0$ and to an antiferromagnetic phase if $J < 0$.

On a triangular lattice, by contrast, the Ising model still orders ferromagnetically if $J > 0$, but does not order antiferromagentically if $J < 0$. The macrostate of the latter remains disordered down to zero temperature.

Disorder in interacting spin systems can originate in thermal fluctuations, quantum fluctuations, competing interactions, or geometric frustration, further analyzed in different modules.

Potts model:

Hamiltonian: $\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}, \quad \sigma_i = 1, 2, \ldots, q.$

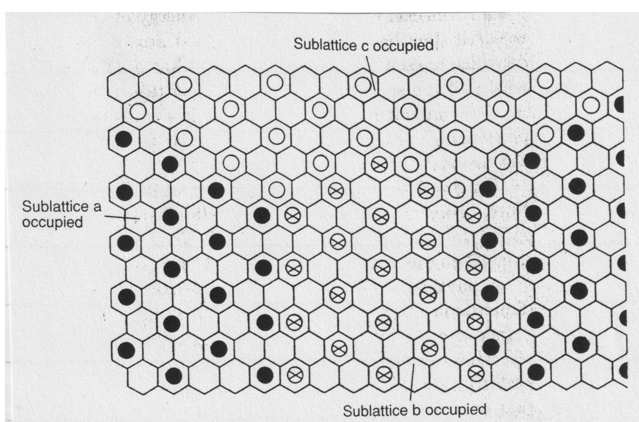
For $q = 2$ the Potts model is equivalent to the Ising model.

The q-state Potts model in $\mathcal{D} = 2$ dimensions exhibits an order-disorder transition which is continuous if $2 \leq q \leq 4$ and discontinuous if $q > 4$.

One application of the 3-state Potts model $\mathcal{D} = 2$ pertains to krypton atoms adsorbed on a (hexagonal) graphite layer.

- The favorable position of Kr atoms is at the center of carbon rings.
- The size of Kr renders nearest-neighbor (nn) occupancies unfavorable.
- The hexagonal lattice can be split into three sublattices such that all nearest-neighbor hexagons belong to different sublattices.
- Hexagons of triplets around each vertex belong to different sublattices.
- Single occupancy of triplets around vertex i is describable by the Potts variable σ_i.
- The repulsive nn interaction between Kr atoms is (effectively) modeled by the 3-state Potts model with $J > 0$.
- A higher energy is associated with nn vertices associated with $\sigma_i \neq \sigma_j$. They produce occupancies in nn hexagons.

The ground state is 3-fold degenerate with all Kr atoms on a single lattice (if vacancies are absent). Low-lying states in macroscopic systems consist of domains with Kr occupying different sublattices.



[image from Yeomans 1992]

n-vector model:

A popular and useful extension of the Ising model works with Ising spins generalized to classical vectors with n components, where $n = 1, 2, 3, \ldots$

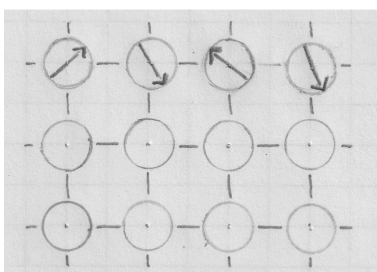
Classical n vector: $\mathbf{S}_i \doteq \left(S_i^{(1)}, \ldots, S_i^{(n)}\right), \quad \sum_{k=1}^{n} \left(S_i^{(k)}\right)^2 = 1.$

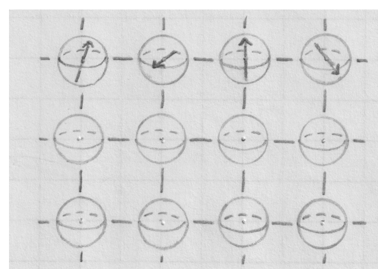
Hamiltonian: $\mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^{(1)}.$

The couplingof strength J is between nearest neighbar sites of some lattice in $\mathcal{D}$ dimensions.

The external magnetic field h is directed along the 1-axis of the n-vector.

The sketches show graphical representation of 2-vectors (left) and 3-vectors (right) on a square lattice. The 1-vector model is the Ising model.





The n-vector model in $\mathcal{D} = 1$ for any n is exactly solvable via the transfer matrix technique (demonstrated for $n = 1$ in [tsc18]) or in other ways.

The limiting case $n \to \infty$ of the n-vector model is known under the name *spherical model* and is amenable to exact solution by different methods.

A discretized version of the 2-vector model,

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j), \quad \theta_i = \frac{2\pi m}{q}, \quad m = 0, 1, \ldots, q-1.$$

known under the name *clock model*, is (in some ways) a halfway station toward the q-state Potts model.

XYZ model:

The XYZ model is an important quantum extension of the Ising model:

$$\mathcal{H} = \sum_{\langle ij \rangle} \left[J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z \right] - h \sum_i S_i^z \quad : \ s = \tfrac{1}{2}.$$

The main source of additional complexity relative to the Ising model is the presence of non-commuting operators in the Hamiltonian.

Two agents of disorder are present. At high T, thermal fluctuations are dominant. At low T, quantum fluctuations become more pronounced.

Quantum fluctuations persist at $T = 0$ under most circumstances and give rise to nontrivial states of spin ordering.

The XYZ model in $\mathcal{D} = 1$ is special because it is exactly solvable. Exact solutions will be explored in later modules.

- The Ising chain is recovered in the case $J_x = J_y = 0$.
- The case $J_z = 0$ is known under the name XY model. It can be mapped onto a system of free spinless fermions and solved exactly.
- The Heisenberg model, $J_x = J_y = J_y$, was exactly solved by the original Bethe ansatz.
- The XXZ model, $J_x = J_y = J$, $J_z = \Delta J$, which includes uniaxial exchange anisotropy, is still amenable to the Bethe ansatz as a method of exact analysis.
- The transverse Ising model, $J_y = J_z = 0$, $h \neq 0$, is the simplest extension of the Ising chain which exhibits nontrivial intrinsic dynamics.
- The general XYZ model with biaxial exchange anistotropy is still exactly solvable $T = 0$ via a mapping to the transfer matrix of classical lattice models.
- The general XYZ model includes special disorder points in the space of parameters J_x, J_y, J_z, h, where the ground state has a simple product nature.
- The spectrum of the XX model, the case $J_x = J_y$, $J_z = 0$ can be generated from different reference states (pseudo-vacua) as configurations of particles with different statistics.
  - ▷ fermions from the ground state (physical vacuum) at $h = J$,
  - ▷ semionic spinons from the ground state at $h = 0$.