XY model

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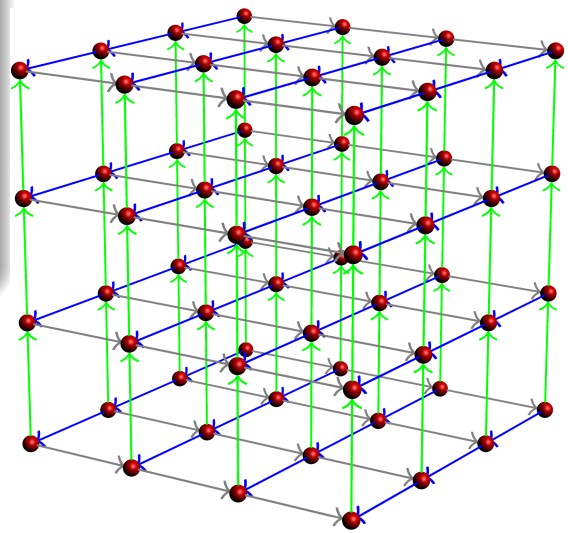
Lattice models

Definition

A *lattice model* is a physical model defined on a discrete space called a lattice, a subset of $\mathbb{R}^n$ isomorphic to $\mathbb{Z}^n$, as opposed to the continuum of spacetime.



Introduced in condensed matter physics as atoms in a crystal approximate very well a lattice. Very useful in computational physics, where discretization of space become necessary.

n-vector model

Definition

A *n-vector model* is a system of spins described by a n-dimensional unit-lenght vector, located on a lattice site

$$H = -J \sum_{n.n.} \mathbf{s}_j \cdot \mathbf{s}_i \tag{1}$$

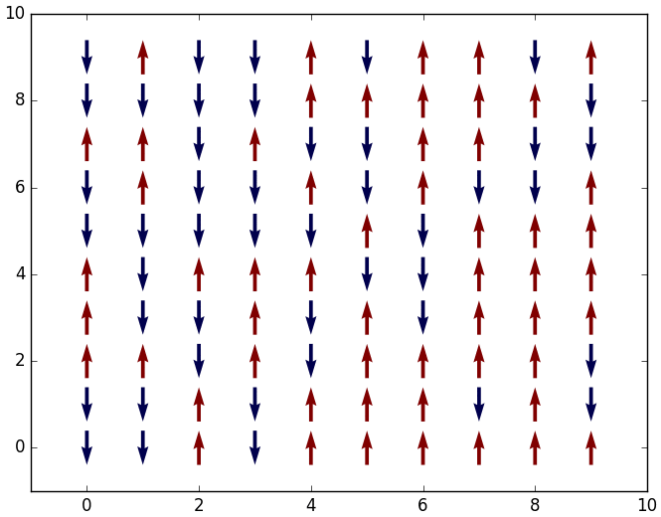
- $n = 1$ Ising model
- $n = 2$ XY model
- $n = 3$ Heisenberg model

Ising model

From equation 1 we can see that the difference between the two possible configurations of neighbouring spins is

$$\Delta E = E_{\uparrow\uparrow} - E_{\uparrow\downarrow} = -2J$$

then *ferromagnetic* phemonena could arise if $J > 0$, while *antiferromagnetic* phenomena could happen if $J < 0$.

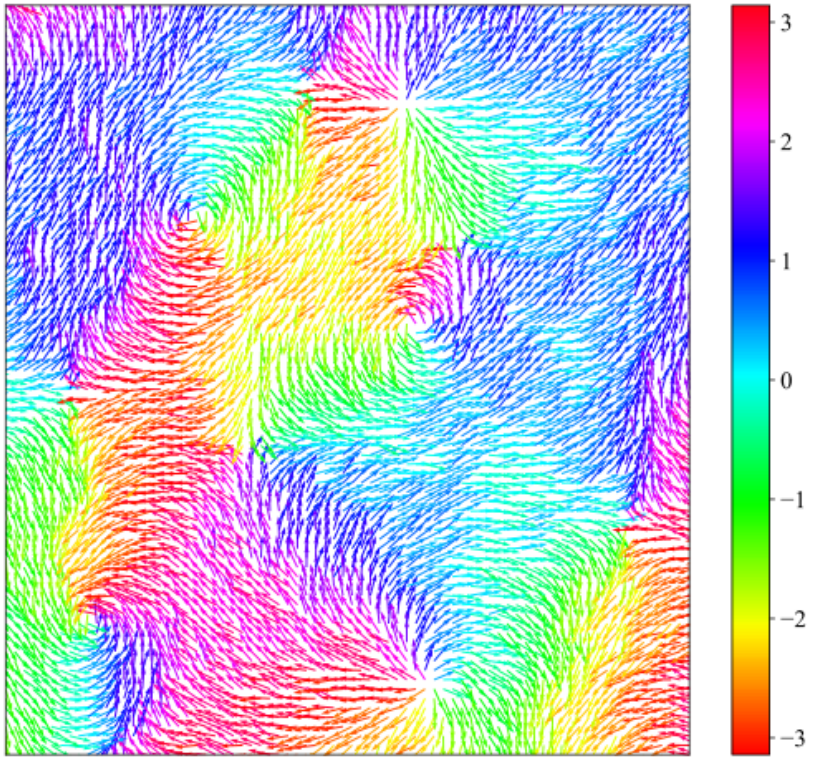


Invented much before Stanley's formalization of n-vector models by Wilhelm Lenz. In 1925 Ising solved the 1D case and showed that no pahse transitions are allowed.

2D XY model

A very interesting case because an infinite-order transition occurs at $k_B T_c/J \simeq 0.88$: a transition between a quasi-ordered phase at low temperatures and a disordered phase at high temperatures.

At high temperatures vortices will form, while at $T < T_c$ vortices will try to annihilate with antivortices. Vortices and antivortices formations are clearly visible in the Monte Carlo simulation color map of the spin configuration at $k_B T/J = 0.4$ on the right.



3D XY model

The most physically interesting situation as experimental data, Monte Carlo simulation results and theoretical estimates can be compared.

A ferromagnet-paramagnet phase transition happens at $T_c \simeq 2.22$ and around this temperature *critical exponents* can be extrapoleted. Critical exponents are a useful tool to describe the system behaviour around the critical point.

Monte Carlo simulations

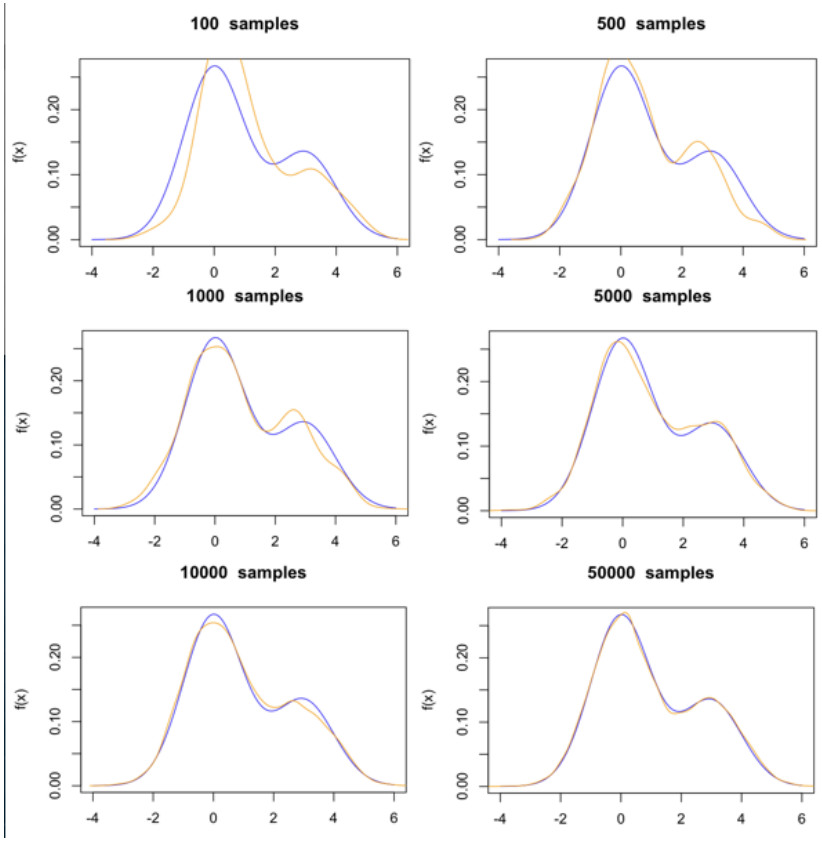
Used to solve deterministic problems via a probabilistic approach. Based on the central limit theorem, it's used in dynamical simulation where observables are averaged over values computed on samples of the system.

The system configuration is seen as a random variable defined on the phase space, seen as the sample space. The samples are picked based on the probability function of the random variable: in this case for example the canonical distribution as defined below.

$$P = \frac{\exp(-\beta H)}{Z} \tag{2}$$

Markov chain sampler

It is the algorithm that samples the configurations based on the propability function in equation 2. Starting from a random configuration a slightly different one is created and is accepted or not as a new sample based on the comparison of the probabilities of the two configuration.



Every step is a link in the chain and in the limit of an infinite chain the samples will approach the probability function as in the figure.

Metropolis-Hastings algorithm

Invented in 1953 by Metropolis and Rosenbluth and extended to a more general case in 1970 by Hastings, is the first Monte Carlo algorithm invented.

Based on the Markov chain sampler it means it violates one of the central limit theorem hypothesis: the indipendence of the samples.

To account for it the Markov chain limit theorem is used which is basically the same as the original one but it accounts for correlation when estimating the error on the function value.

Implementation

The Metropolis-Hastings algorithm is used in 3D case, on a cube of $L = 6$. Every spin is changed at every step instead of just one, as can be found in most of the previous work, to dicrease computational time and correlation.

The order of magnitude of the change in the angle of the spin is controlled by Δ in the following way

$$\theta_i^{\mathsf{mc}} = \theta_i + \Delta(\xi - 0.5)$$

where ξ is a random number with uniform distribution in $[0, 1]$.

Implementation

The configurations of interest are the one at equilibrium, then 10k inital Monte Carlo steps are dedicated to reach equilibrium and to update the value of Δ to reduce correlation. Other 190k steps are executed to obtain observable values.

Values of C_v and M where obtained at different temperatures and different values of the external field h. The study is focused on the properties evolution near the critical point.

Critical exponents

They are defined as the exponents of the power laws describing the behaviour of some physical quantities around the critical temperature. They come from the assumption that the system is described by an order parameter m that vanishes at T_c.

So a ordered phase and a disordered phase can be distingiushed: a ordering field h is then defined as the parameter which opposes the disordering of the system at high temperature.

It is believed, on strong experimental basis, that they do not depend on the particular of the physical systema, but only on some general properties:

- the dimensionality of the system
- the dimensionality of the spin
- the range of the interaction

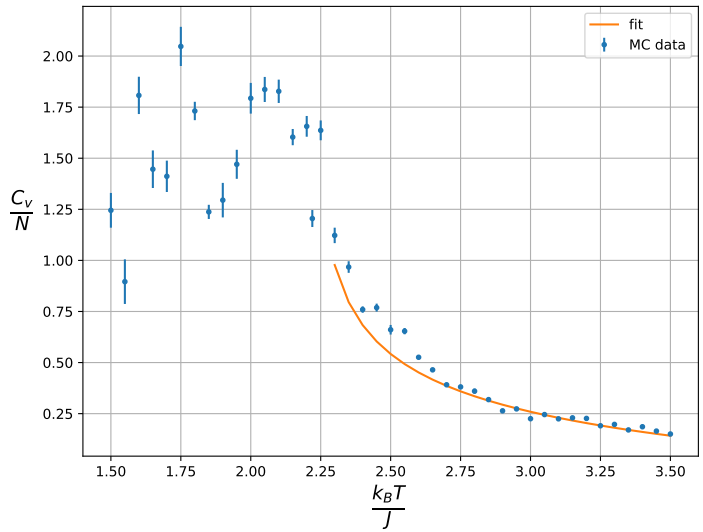
In the case of the ferromagnets the parameter m correspond to the magnetization squared and h to external field.

An example of a critical exponent could be δ, defined as

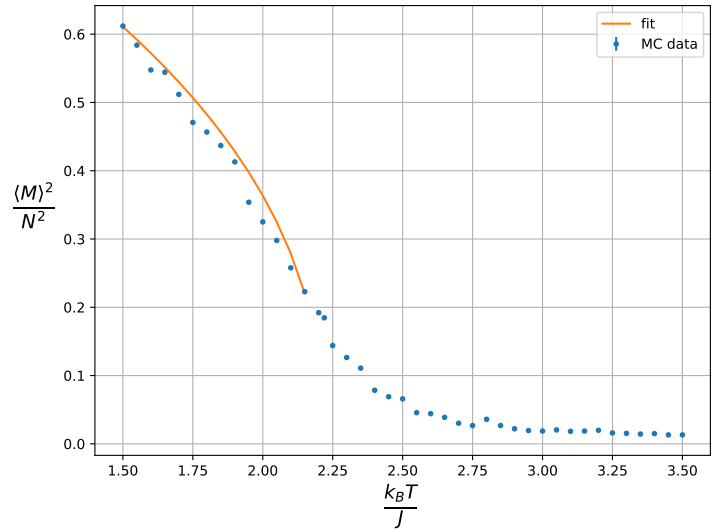
$$m \sim h^{1/\delta} \quad \text{for } T = T_c \text{ as } h \to 0$$

Results

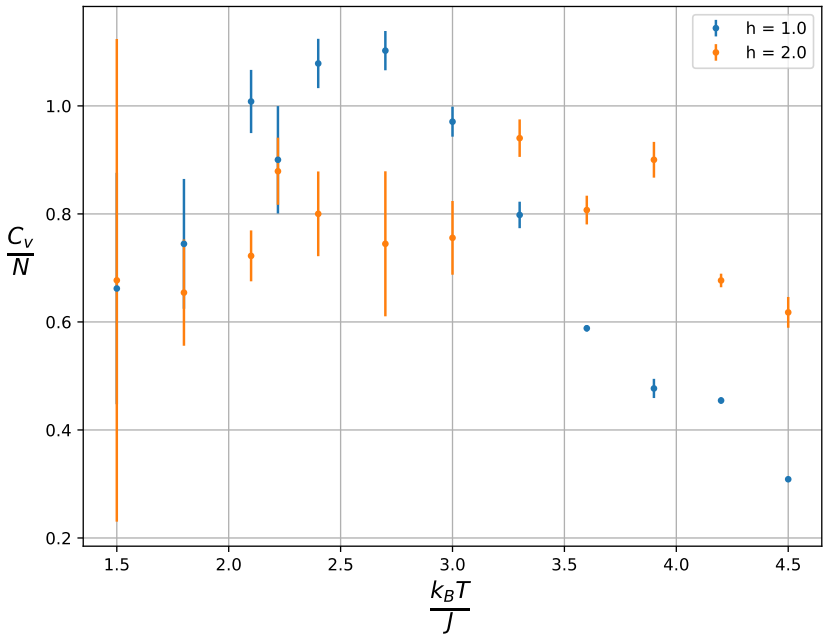
Graphs of C_v and M^2 in respect of T, with $h = 0$ are reported. The specific heat has a divergence around $k_B T_c / J \simeq 2.22$ as expected, while for $T > T_c$ the magnetization rapidly fades off.

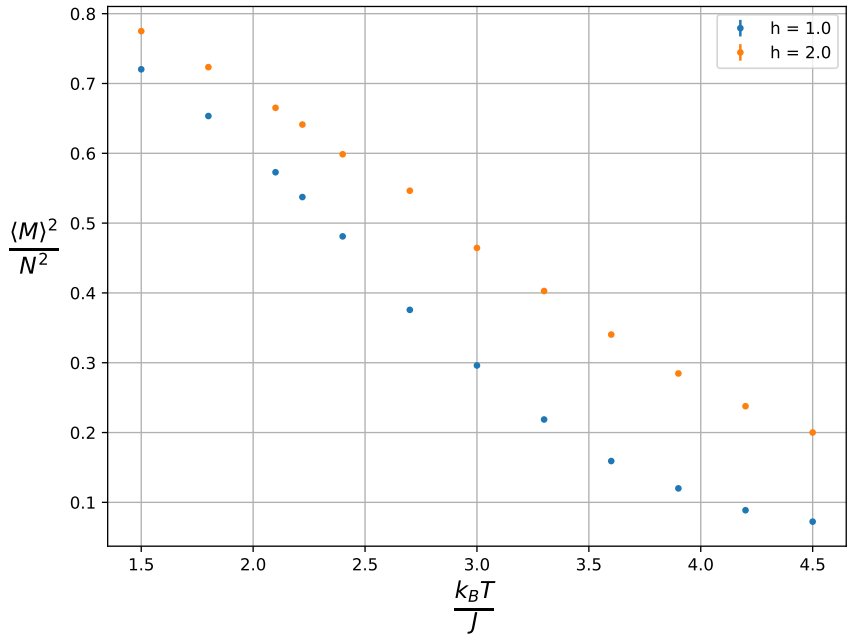


Fluctuations in the region of $T < T_c$ are due to the fact that the system tends to jump between states which are local minima of the system, so the system is stuck in some local minima for quite a few steps.

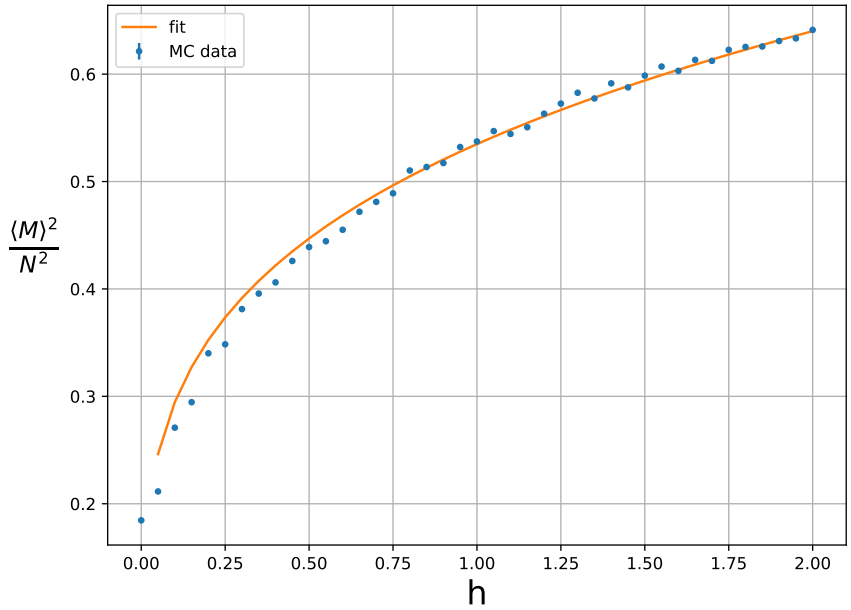


The presence of the ordering field h tends to keep order in the system, above or below the critical temperature: the fluctuations in energy decrease for $T < T_c$ and magnetization do not vanish immidiately after the critical point. Graphs for different values of h are reported below.





A study of the magnetization at $T = T_c$ has been carried to extrapolate the critical exponet δ. The result are reported in the graph on the right.



Every critical exponent obtained is reported below in the table. Theoretical and experimental values coming from prevoius works are also reported.

	α	β	δ	γ	ν
Theorical values		0.362 ± 0.012	4.82 ± 0.12	1.39 ± 0.01	0.705 ± 0.005
Experimental values	0.0-0.2	0.3-0.36	4.2-4.8	4.2-4.8	0.62-0.68
Monte Carlo simulation	0.201 ± 0.004	0.438 ± 0.001	3.86 ± 0.09	0.654 ± 0.008	1.08 ± 0.03
χ_r^2	$\simeq 7 \cdot 10^5$	$\simeq 1 \cdot 10^{12}$	$\simeq 3 \cdot 10^{12}$		

Possible improvements

The simulation is not very accurate near and under the critical point. That is a known fact and varoius techniques can be used to avoid it.

The two major issues are the fluctuation in energy and the presence of local minima of the Hamiltonian near the critical point. They both make the averaging over the step values much less efficient.

Also the fitting function for the critical exponents can be improved by a method called finite-size scaling.