First order phase transition

In the thermodynamic limit:
A first derivative of the free energy density becomes discontinuous.
Recall that the free energy is given by

$$f = -k_B T \lim_{L \to \infty} \frac{1}{L^3} \ln Z$$

A simple example that we know already:
The Ising model and also the ϕ^4-model in general undergoes a transition in the external field h. At $h = 0$ the magnetisation jumps from $-m$ to m as we increase h.
Special: The two phases are related by Z_2-Symmetry; Therefore we know exactly that the transition occurs at $h = 0$

Lattice Models discussed in the Literature

q-state Potts model:

$$H = -J \sum_x \sum_\mu \delta_{\sigma_x, \sigma_{x+\hat{\mu}}}$$

with $\sigma \in \{1, 2, ..., q\}$. For $q = 2$ we get the Ising model.

In 2 dimensions: First order transition for $q > 4$;
Often used to probe ideas to locate first order transition.

In 3 dimensions: First order transition for $q > 2$;
$q = 3$ studied intensively about 25 years ago due to some analogy with lattice-QCD

Blume-Capel model:

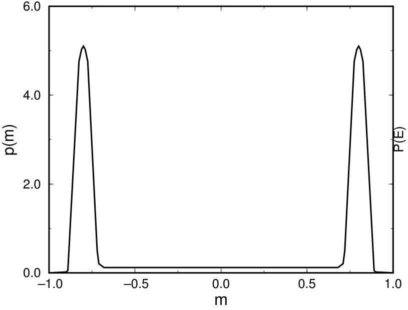
$$S = -\beta \sum_x \sum_\mu s_x s_{x+\hat{\mu}} + D \sum_x s_x^2 - h \sum_x s_x$$

with $s \in \{-1, 0, 1\}$. For $D \to -\infty$ we recover the Ising model. For $h = 0$ and fixed D the model undergoes a phase transition from paramagnetic to ferromagnetic behaviour a certain $\beta_c(D)$. For $D \leq D_{tri}$ the transition is second order while for $D > D_{tri}$ is first order.

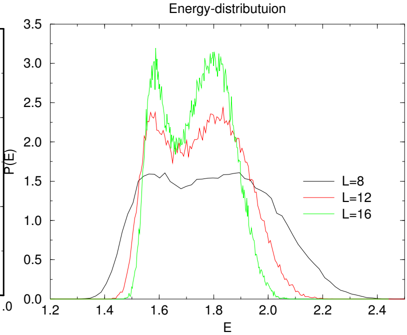
In three dimensions: $D_{tri} = 2.0313(4)$, Y. Deng and H. W. J. Blöte, Phys. Rev. E **70**, 046111 (2004).

First order transitions and finite lattices

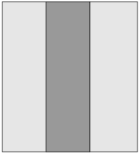
Ising model, Histogram of the magnetisation,
sketch

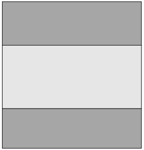


3-state Potts model in 3 dimensions at the transition temperature.



Explanation of these histograms; in particular contribution between the two peaks





Configurations that have two regions that can be assigned to two different phases. There are two interfaces between these two regions of the total area $2L^2$. Such mixed configurations are surpressed by the factor (leading contribution)

$$\exp(-2\sigma L^2)$$

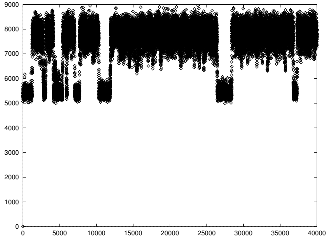
where σ is the interface tension.

Determination of the transition temperature:

At the transition, all phases have equal weight. Degeneracies have to be taken into account. E.g. in the Potts model we have q ordered phases.

4-state Potts model in 3 dimensions close to the transition temperature. The transition is stronger than in the 3-state case

16^3-lattice, Monte-Carlo-time evolution of the energy, Metropolis algorithm.



It takes a long time to go from one phase to an other.

A way out of this problem is provided by the proposal of
B. Berg and T. Neuhaus
Multicanonical Ensemble:
A New Approach to Simulate First-order Phase Transitions,
hep-lat/9202004, Phys. Rev. Lett. 68 (1992) 9.
Instead of generating the configurations with the Boltzmann factor as weight we use some modified (artificial) weight:

$$P(X) \propto \exp(-\beta H(X)) \times P_M(H(X))$$

Where $P_M(H(X))$ should be chosen such that the minimum between the peaks is lifted. $P_M(H(X))$ has to be determined numerically. The Metropolis algorithm has to be adopted to the modified weight. The proposal for a new value of the spin is done in the same way as before. The modified weight has to be taken into account in the acceptance probability:

$$A(X', X) = \min\left(1\ ,\ \exp(-\beta(H(X') - H(X))\frac{P_M(H(X'))}{P_M(H(X))}\right)$$

To get expectation values (and also the histogram) we have to remove $P_M(H(X))$ by reweighting:

$$\langle A\rangle \approx \frac{\sum_i A_i P_M(H_i)^{-1})}{\sum_i P_M(H_i)^{-1})}$$

Related methods:
Simulated Tempering: A New Monte Carlo Scheme,
by Enzo Marinari and Giorgio Parisi,
hep-lat/9205018, Europhys. Lett. 19 (1992) 451-458

Here the temperature (or inverse temperature) is used as dynamical variable. In addition to "standard" update-steps there are updates of the inverse temperature β.

Parallel Tempering:
Optimized Monte Carlo Methods
Enzo Marinari
cond-mat/9612010, Lectures given at the 1996 Budapest Summer School on Monte Carlo Methods.
even older references