Ising model: critical temperatures

dim	lattice	q	$k_B T_c / J$	$k_B T_c / Jq$
1	chain/ring	2	0	0
2	honeycomb	3	~ 1.52	~ 0.5
	square	4	2.269	0.57
	triangular	6	~ 3.64	~ 0.61
3	diamond	4	~ 2.704	~ 0.68
	cubic	6	~ 4.512	~ 0.75
	bcc	8	~ 6.35	~ 0.79
	fcc	12	~ 9.79	~ 0.82
4	hypercubic	8	~ 6.68	~ 0.84
∞	"	∞	∞	1.0

Note:
- phase transition for all lattices in $d > 1$
- $T_c \xrightarrow{q \to \infty} k_B J q$

Practical aspects of Monte Carlo

Unit of dynamics: „sweep" ≡ „Monte Carlo step/site"

$N = L^d$ attempts of flipping 1 spin

Sequential/random spin-flips: it is saver to randomly select spins that can be flipped, but also costlier. Alternative: select all spins sequentially.
→ different dynamics; usually same distribution

Acceptance rule: Metropolis rule alway accepts changes that lower the energy or leave energy unchanged (highest acceptance rate)

$$P(i \to j) = \min\{1, e^{-\beta \Delta E}\}; \quad \Delta E = E_j - E_i$$

alternative: heat-bath acceptance rule (≡ Glauber dynamics)

$$P(i \to j) = \frac{e^{-\beta \Delta E}}{e^{-\beta \Delta E} + e^{\beta \Delta E}} = \frac{1}{2}\left[1 + \tanh(-\beta \Delta E)\right]$$

reaches local equilibrium in single step

(→ e.g. decay of magnetization in $T=\infty$ Ising model)

Parallelization: possible using checkerboard decomposition: (i) try flips of "white" sites
(ii) try flips of "black" sites

Finite-size scaling

LB Fig 4.1

For homogeneous systems and within a single phase one expects* scaling relationships of the forms

$$F(L,T) = L^{-(2-\alpha)/\nu}\, \mathcal{F}(\varepsilon L^{1/\nu}) \; ; \quad \varepsilon = |1 - \tfrac{T}{T_c}|$$

depends only on combination of L and T

$$\Rightarrow \quad M = L^{-\beta/\nu} M^0(\varepsilon L^{1/\nu})$$

$$\chi = L^{\gamma/\nu} \chi^0(\varepsilon L^{1/\nu})$$

$$C = L^{\alpha/\nu} C^0(\varepsilon L^{1/\nu})$$

Here, all exponents have their infinite-lattice values.

Practical application: for estimate of T_c and applicable exponents, plot scaled observable vs. its argument, e.g. $M^0(x)$, where $M^0 = M_L L^{\beta/\nu}$; $x = \varepsilon L^{1/\nu}$

These curves should asymptotically fall on top of each other for $T<T_c$ and $T>T_c$, respectively.

How to get T_c?

E.g. by looking at intersection points of Binder's cumulant $U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$ when evaluated for range of linear sizes L.

$$U_4 \xrightarrow{L\to\infty} \begin{cases} \frac{2}{3} & \text{for } T<T_c \\ U^* & \text{for } T=T_c \\ 0 & \text{for } T>T_c \end{cases}$$

Υ motivation: correlation length: $\xi = \xi_0 \, \varepsilon^{-\nu}$

$\Rightarrow$ dimensionless length $\frac{L}{\xi} = \xi_0^{-1} \varepsilon^{\nu} L$

rescale: $\left(\frac{L}{\xi} \xi_0\right)^{1/\nu} = \varepsilon L^{1/\nu}$

derivation of susceptibility using second argument in $\mathcal{F}$: $\mathcal{F}(\varepsilon L^{1/\nu}, B L^{(\gamma+\beta)/\nu})$

Exponents are not independent, but related e.g. by thermodynamic relations:

Rushbrooke equality $\qquad \alpha + 2\beta + \gamma = 2$

Hyperscaling $\qquad d\nu = 2 - \alpha$

(square lattice Ising: $\alpha = 0, \beta = \frac{1}{8}, \gamma = \frac{7}{4} \Rightarrow \nu = 1$)

Note: scaling holds only for small $\varepsilon L^{1/\nu}$; further away from T_c and for too small L, corrections to scaling become important!

LB Fig 4.4

So far: 2^{nd} order transitions. Different analysis necessary for 1^{st} order transitions!

Tradeoff: Smaller systems allow for longer run times (in terms of autocorrelation time)