Phase transition and critical phenomena

- order to disorder transition occur discontinuous

- may be first order or continous

- universal behavior near continuous phase transitions

- depend on (broken) symmetries, range of interactions, lattice/dimension

- Spin models are useful “minimal” description

Heisenberg Model

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

XY-Model

$$H = \sum_{\langle i,j \rangle} J_{ij} (S_i^x \cdot S_j^x + S_i^y \cdot S_j^y)$$

Ising-Model

$$H = \sum_{\langle i,j \rangle} J_{ij} S_i^z \cdot S_j^z$$

Free energy is minimized $F = E - TS$

Ordered phase

Disordered phase

Order parameter:
measurable quantity with characteristically different value for each phase.

Examples:

“density”

“structure factor”

“condensate fraction”

“superfluid density”

“magnetization”

Ehrenfest classification:

A first order phase transition shows a discontinuity in the derivative of the free energy and in the order parameter as a function of temperature, pressure (and/or another control parameter).

A continuous phase transition has no discontinuity in the derivative of the free energy, but may be discontinuous in second or higher order. The change of order parameter is continuous, but (often) non-analytically.

Critical exponents: Power-laws near continuous phase transitions

Specific heat: $c_V \propto |T - T_c|^{-\alpha}$

Order parameter: $m \propto (T_c - T)^{\beta}$

Response: $\chi = \left.\frac{\partial m}{\partial B}\right|_{B=0} \propto |T - T_c|^{-\gamma}$

Order parameter: $m \propto |B|^{1/\delta}$

Hyper-Scaling laws

$$\alpha + 2\beta + \gamma = 2$$

$$\gamma = \beta(\delta - 1) \, .$$

TABLE 12.1. THE VALUES OF THE CRITICAL INDICES (compiled on the basis of a review article by Kadanoff *et al.* (1967), in which a detailed bibliography of the original works is also given)*

Critical index	Theoretical values: mean field approximation	Theoretical values: Ising model 2-dim.	Theoretical values: Ising model 3-dim.	Experimental values: ferromagnetic transition	Experimental values: gas–liquid transition
β	$\frac{1}{2}$	$\frac{1}{8}$	0.313 ± 0.004	0.33 ± 0.03	0.346 ± 0.01
γ	1	$\frac{7}{4}$	1.250 ± 0.001 (a)	1.33 ± 0.03	1.37 ± 0.2
γ'	1	$\frac{7}{4}$	1.31 ± 0.05	(1.0 ± 0.1) (b)	1.0 ± 0.3
δ	3	15	5.2 ± 0.15	4.1 ± 0.1	4.4 ± 0.4
α	$= 0$ } (c)	$\to 0$ } (d)	0.1 ± 0.1	$\lesssim 0.16$	0.2 ± 0.2
α'	$= 0$	$\to 0$	$0.07^{+0.16}_{-0.04}$	$\lesssim 0.16$	0.12 ± 0.12

General energy with two-body interaction U

$$E = \sum_{j=1}^{N} \frac{\vec{p}_j^{\,2}}{2m} + \sum_{j=1}^{N} \sum_{i \neq j} U(\vec{r}_i - \vec{r}_j)$$

Partition function

$$Z_N = \frac{1}{(2\pi\hbar)^{3N} N!} \int \left(\prod_{j=1}^{\mathrm{N}} \mathrm{d}^3\vec{r}_j \mathrm{d}^3\vec{p}_j \right) \exp(-\beta E)$$

Discretized approximation: Hard-core with potential box:

Phase transition as function of chemical potential

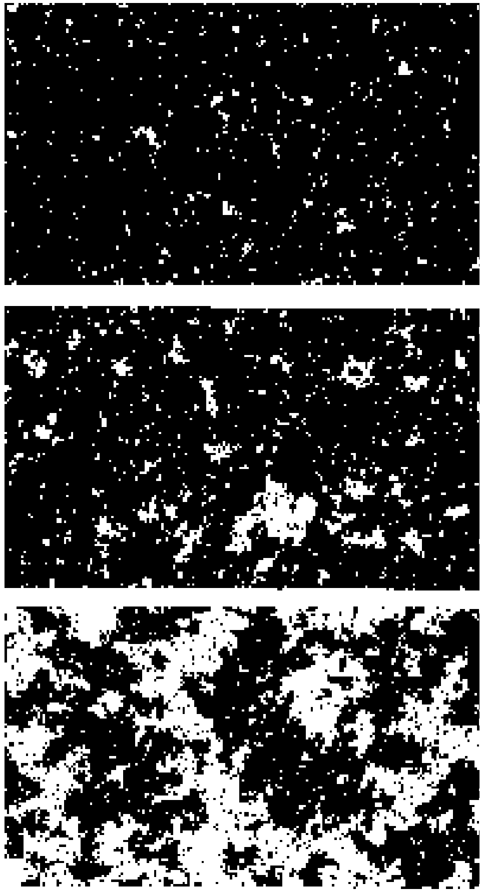
$$H_{\text{int}} = -U \sum_{\langle l,m \rangle} n_l n_m - \mu \sum_l n_l$$

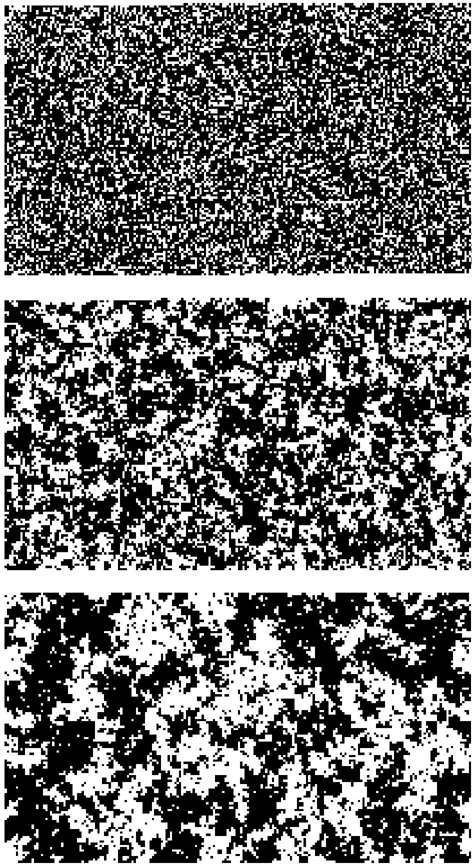
Phase transition in the Ising model

$$H = \sum_{\langle i,j \rangle} J_{ij} S_i^z \cdot S_j^z - B \sum_j S_j^z$$

Domain walls

Scale invariance: Numerical simulations





Fractal dimensions

$$V = L^D \qquad D = \frac{\log V}{\log L}$$

Scaling dimension:

near critical point, each quantity changes with a characteristic powerlaw under rescaling with λ

Free energy is self-similar function of $t = T - T_c$ and $h = B - B_c$

$$G(t,h) = \lambda G(\lambda^s t, \lambda^r h)$$

$$m = -\frac{\partial G}{\partial h} = \lambda^{r+1} m(\lambda^s t, \lambda^r h)$$

$$\chi(t,h) = \lambda^{2r+1}\chi(\lambda^s t, \lambda^r h)$$

$$C_h(t,h) = \lambda^{2s+1} C_h(\lambda^s t, \lambda^r h)$$

Scaling for $h=0$ and/or $t=0$

$$
\begin{aligned}
C_h(t,0) &= |t|^{-(2s+1)/s}\, C_h(\pm 1,0) \\
m(t,0) &= (-t)^{-(r+1)/s} m(-1,0) \\
\chi(t,0) &= |t|^{-(2r+1)/s}\, \chi(\pm 1,0) \\
m(0,h) &= |h|^{-(r+1)/r}\, m(0,\pm 1)
\end{aligned}
$$

$$
\begin{aligned}
\alpha &= \frac{2s+1}{s} \\
\beta &= -\frac{r+1}{s} \\
\gamma &= \frac{2r+1}{s} \\
\delta &= -\frac{r}{r+1}
\end{aligned}
$$

Hence:

$$\alpha + 2\beta + \gamma = 2$$

$$\gamma = \beta(\delta - 1)\ .$$

Mathematical tool for scale invariance: **The renormalization group (RG)**

- Changing length or energy scales will result in self-similar model

- Microscopic details become less important as length scales are increased

- At very long length scales, short wave length excitations are “lost”

- Integrating out: partial sum over lost degrees of freedom gives new effective model

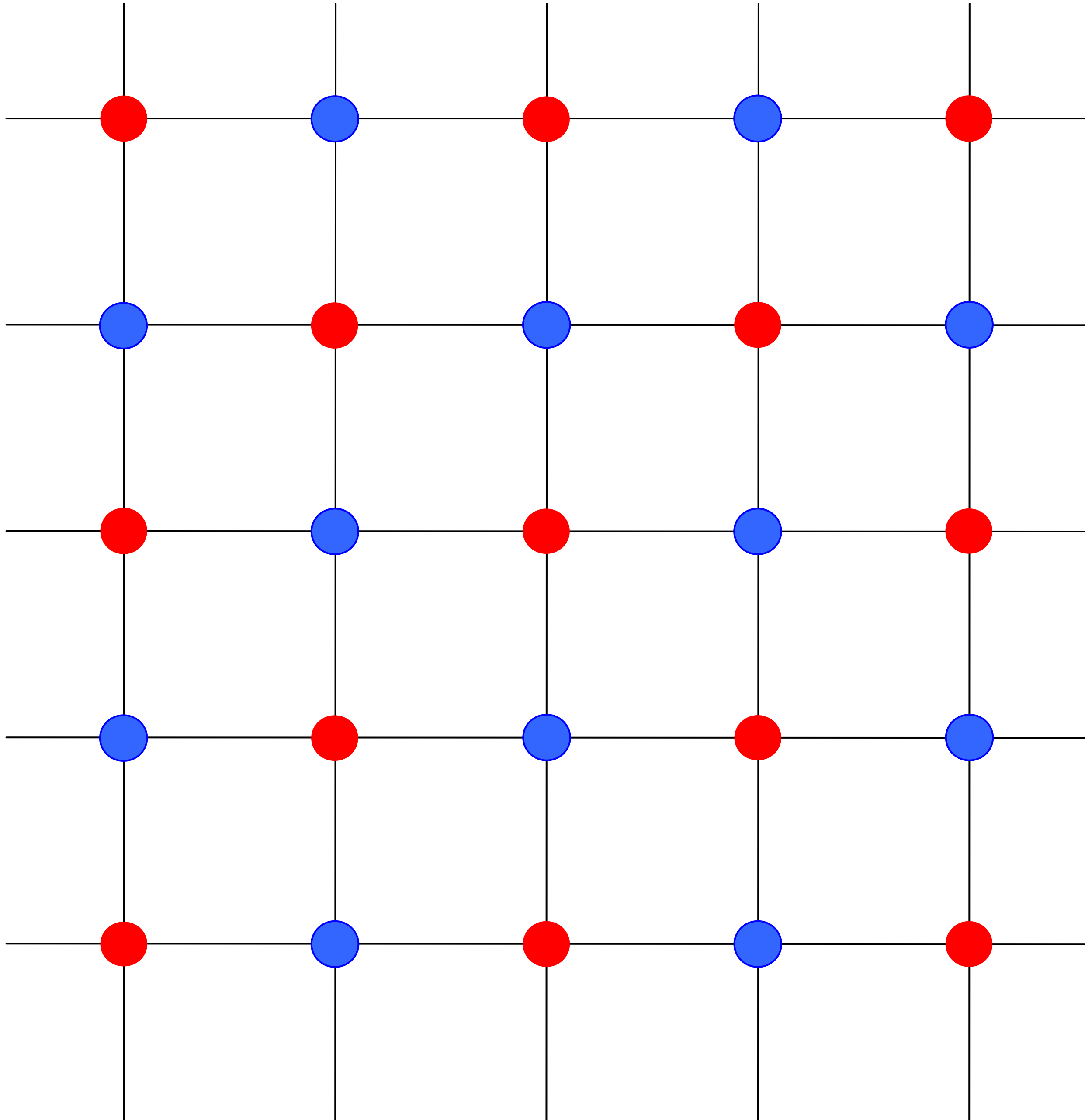
Renormalization group equations: rescaling of parameters under change of “cut-off”

Example: The 2D Ising model at B=0

$$H_{\text{Ising}} = -J \sum_{\langle i,j \rangle} S_i S_j$$

Partition function $Z = \sum_{\{S_j\}} \exp(\beta J \sum_{\langle i,j \rangle} S_i S_j)$

A and B sublattices



Ansatz

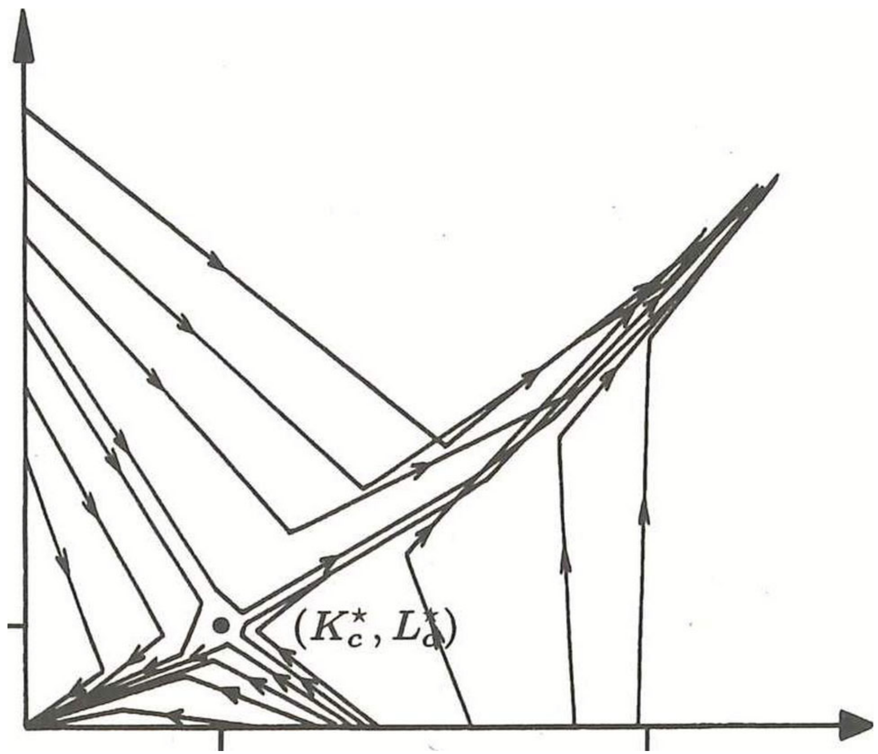
$$Z = \sum_{\{S_j\}_A} \prod_{i_B} 2\cosh \beta J(S_{i+x} + S_{i-x} + S_{i+y} + S_{i-y}) = \sum_{\{S_j\}_A} \prod_{i_B} \exp(-\beta H'(S_{i-x}, S_{i-x}, S_{i+y}, S_{i-y}))$$

$$H'(S_1,S_2,S_3,S_4) = \varepsilon' + \frac{J'}{2}(S_1S_2 + S_2S_3 + S_3S_4 + S_1S_4) + J_2'(S_1S_3 + S_2S_4) + M'(S_1S_2S_3S_4)$$

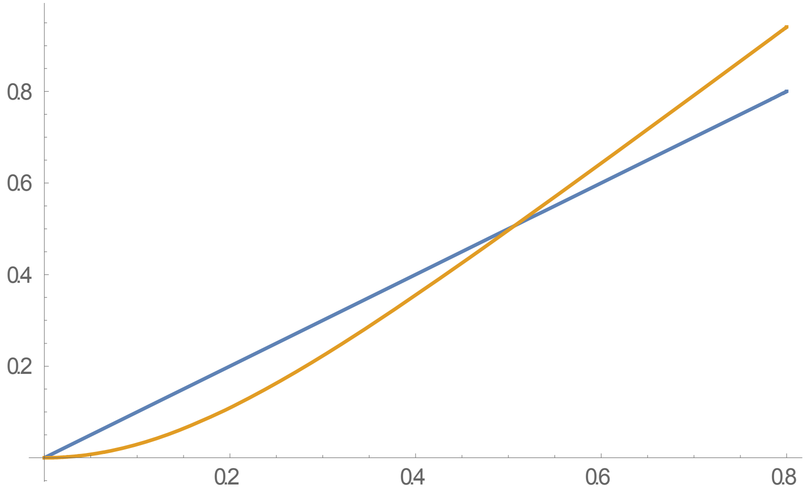
Solution

$$\beta J' = \frac{1}{4}\ln(\cosh 4\beta J) + \beta J_2$$

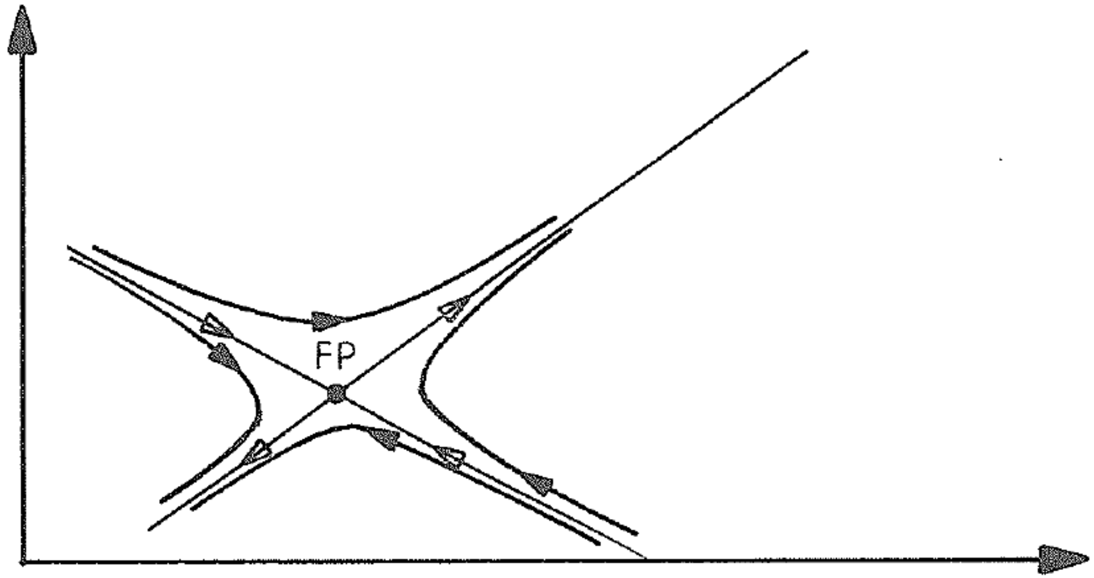
$$\beta J_2' = \frac{1}{8}\ln(\cosh 4\beta J)$$



Critical point $\beta J_c = \frac{3}{8}\ln(\cosh\, 4\beta J_c)$



Flow near fixed point: Linearization



Generalized description of the RG approach:

- rescale energy, momentum or distance cutoff: $\frac{\Lambda}{b} \longrightarrow \Lambda$

  $\Leftrightarrow k \longrightarrow bk\,; \quad x \longrightarrow \frac{x}{b}$

- Scale invariant functions are rescaled according to scaling dimension $\phi(x) \longrightarrow b^{\Delta}\phi(x)$

  $\Leftrightarrow \phi(k) \longrightarrow b^{\Delta-d}\phi(k)$

- All coupling constant are redefined under rescaling. $\vec{g} \longrightarrow \vec{g}' \quad : \quad \vec{g}' = R(\vec{g}, b)$
- Repeated transformation form are possible ("group") $R(R(\vec{g}, b), b') = R(\vec{g}, bb')$

- Finally, find RG flow equations $\frac{d\vec{g}}{dl} = R(\vec{g})$ where $l = ln(b) \qquad d\vec{g} = \vec{g}' - \vec{g}$