Scaling Theory

Roger Herrigel
Advisor: Helmut Katzgraber

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Outline

- The scaling hypothesis
  - Critical exponents
  - The scaling hypothesis
  - Derivation of the scaling relations
- Heuristic explanation
  - Kadanoff construction (1966)
  - Scaling for the correlation function
- Universality
  - Finite size scaling
  - Disordered systems / Harris criterion (1974)
- Polymer statistics

Critical exponents

Summery of the critical exponents for a magnetic system

$$t = \frac{T - T_c}{T_c} \qquad h = \frac{H}{k_B T_c}$$

Exponent	Definition	Description
α	$C_H \sim \lvert t \rvert^{-\alpha}$	specific heat at $H = 0$
β	$M \sim \lvert t \rvert^{\beta}$	magnetization at $H = 0$
γ	$\chi \sim \lvert t \rvert^{-\gamma}$	isothermal susceptibility at $H = 0$
δ	$M \sim h^{\frac{1}{\delta}}$	critical isotherm
ν	$\xi \sim \lvert t \rvert^{-\nu}$	correlation length
η	$G(r) \sim \lvert r \rvert^{-(d-2+\eta)}$	correlation function

- Fundamental thermodynamics $\Rightarrow$ Exponent inequalities such as

$$\alpha + 2\beta + \gamma \geq 2 \qquad \text{(Rushbrooke)}$$

Critical exponents

The critical exponent λ of a function $f(t)$ is

$$\lambda = \lim_{t \to 0} \frac{\ln f(t)}{\ln t}$$

- The function $f(t)$ near critical temperature T_C ($t \to 0$) is dominated by t^{λ}

$\Rightarrow$ t^{λ} describes $f(t)$ at the transition.

The scaling hypothesis

- The singular part of the free energy density f is a homogeneous function near a second-order phase transition.

Homogeneous functions

1 dim $f(\lambda r) = g(\lambda) f(r)$

the scaling factor g is of the from $g(\lambda) = \lambda^p$

n dim $f(\lambda \vec{r}) = g(\lambda) f(\vec{r})$

Generalized homogeneous functions

(i) $\lambda f(x, y) = f\left(\lambda^a x, \lambda^b y\right) \Leftrightarrow$

(ii) $\lambda^c f(x, y) = f\left(\lambda^a x, \lambda^b y\right)$

The scaling hypothesis

- The singular part of the free energy density f is a homogeneous function near a second-order phase transition.
- The reduced temperature t and the order parameter h rescale by different factors.

$$f(t,h) = b^{-d} f\left(b^{y_t} t, b^{y_h} h\right)$$

- If f is a homogeneous function then also its Legendre transform
  $\Rightarrow$ all thermodynamical potentials are homogeneous.

Derivation of the scaling relations I

The scaling hypothesis postulates that the free energy is homogeneous

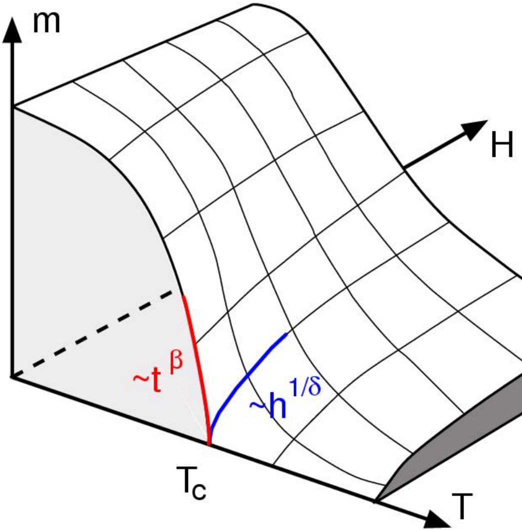
$$f\left(t,h\right)=b^{-d}f\left(b^{y_t}t,b^{y_h}h\right)$$

Let: $\quad b=|t|^{\frac{1}{y_t}}$

$$\Rightarrow \qquad f\left(t,h\right)=|t|^{\frac{d}{y_t}}\,f\left(\pm 1,|t|^{-\frac{y_h}{y_t}}\,h\right)$$

$$\Rightarrow \qquad f\left(t,h\right)=|t|^{\frac{d}{y_t}}\,\phi\left(|t|^{-\frac{y_h}{y_t}}\,h\right)$$

Derivation of the scaling relations II



Derivation of the scaling relations III

$$f\left(t,h\right) = |t|^{\frac{d}{y_t}}\,\phi\left(|t|^{-\frac{y_h}{y_t}}\,h\right)$$

1. Magnetization: $M \sim |t|^{\beta}$

$$M = \frac{1}{k_B T}\,\frac{\partial f}{\partial h}\Big|_{h=0} = \frac{1}{k_B T}\,|t|^{\frac{d-y_h}{y_t}}\,\phi'\left(|t|^{-\frac{y_h}{y_t}}\,h\right) \sim |t|^{\frac{d-y_h}{y_t}}$$

$$\Rightarrow \quad \boxed{\beta = \frac{d-y_h}{y_t}}$$

2. Critical Isotherm: $M \sim h^{\frac{1}{\delta}}$

M should remain finite as $t \longrightarrow 0 \quad \Rightarrow \quad \phi'\left(x\right) \sim x^{\frac{d}{y_h}-1}$

because then

$$M \sim |t|^{\frac{d-y_h}{y_t}}\,\frac{h^{\frac{d-y_h}{y_h}}}{|t|^{\frac{y_h(d-y_h)}{y_h y_t}}} \quad \Rightarrow \quad \boxed{\delta = \frac{y_h}{d-y_h}}$$

Derivation of the scaling relations IV

$$f(t,h) = |t|^{\frac{d}{y_t}} \phi\left(|t|^{-\frac{y_h}{y_t}} h\right)$$

3. Heat capacity: $C \sim |t|^{-\alpha}$

$$C = \left.\frac{\partial^2 f}{\partial t^2}\right|_{h=0} \sim |t|^{\frac{d}{y_t}-2} \Rightarrow \boxed{\alpha = \frac{d}{y_t} - 2}$$

4. Magnetic susceptibility: $\chi \sim |t|^{\gamma}$

$$\chi = \left.\frac{1}{k_B T}\frac{\partial M}{\partial h}\right|_{h=0} = \left.\frac{1}{(k_B T)^2}\frac{\partial^2 f}{\partial h^2}\right|_{h=0} \sim |t|^{\frac{d-2y_h}{y_t}} \Rightarrow \boxed{\gamma = \frac{d-2y_h}{y_t}}$$

Hyperscaling I

$$G(r) = b^{-2(d-y_h)} G\left(\frac{r}{b}, b^{y_t} t\right)$$

$$G(r) = |t|^{\frac{2(d-y_h)}{y_t}} \Phi\left(\frac{r}{|t|^{-\frac{1}{y_t}}}\right)$$

5. Correlation length: $\xi \sim |t|^{-\nu}$

We have $G \sim e^{\frac{r}{\xi}}$ $\forall t$ also for $t \neq 0$

$$\xi \sim |t|^{-\frac{1}{y_t}} \quad \Rightarrow \quad \boxed{\nu = \frac{1}{y_t}}$$

Hyperscaling II

6. Correlation function: $G \sim |r|^{-(d-2-\eta)}$

$$G(r) = b^{-2(d-y_h)} G\left(\frac{r}{b}, b^{y_t} t\right)$$

choose $b = r$ and $t = 0$

$$G(r) \sim r^{-2(d-y_h)} \quad \Rightarrow \quad \boxed{\eta = d + 2 - 2y_h}$$

Scaling relations

We got the following equations:

$$\alpha = \frac{d}{y_t} - 2 \qquad \beta = \frac{d - y_h}{y_t}$$
$$\gamma = \frac{d - 2y_h}{y_t} \qquad \delta = \frac{y_h}{d - y_h}$$
$$\nu = \frac{1}{y_t} \qquad \eta = d + 2 - 2y_h$$

$\Rightarrow$ we can cancel the y_h and y_t which have no experimental relevance.

Scaling relations

From these six equations of the critical exponents one obtains:

$$\boxed{\alpha + 2\beta + \gamma = 2}$$ Rushbrook's Identity

$$\boxed{\delta - 1 = \frac{\gamma}{\beta}}$$ Widom's Identity

$$\boxed{2 - \alpha = d\nu}$$ Josephson's Identity

$$\boxed{\gamma = \nu\,(2 - \eta)}$$

$\Rightarrow$ **There are only 2 independent Exponents**

Onsager solution 1944

$$H_\Omega = -J \sum_{\langle ij \rangle}^{N} s_i s_j - H \sum_{i}^{N} s_i$$

The exponents of the Onsager solution for the 2-dim Ising model.

$$\alpha = 0 \quad \beta = \frac{1}{8} \quad \gamma = \frac{7}{4}$$
$$\delta = 15 \quad \nu = 1 \quad \eta = \frac{1}{4}$$

equations	values
$\alpha + 2\beta + \gamma = 2$	$0 + 2\frac{1}{8} + \frac{7}{4} = 2$
$\delta - 1 = \frac{\gamma}{\beta}$	$15 - 1 = \frac{7}{4}\frac{8}{1}$
$2 - \alpha = d\nu$	$2 - 0 = 2 \cdot 1$
$\gamma = \nu\left(2 - \eta\right)$	$\frac{7}{4} = 1\left(2 - \frac{1}{4}\right)$

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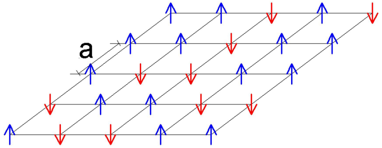
Kadanoff construction 1966

Motivation:

- heuristic explanation $\Rightarrow$ Idea of Renormalization group

Ising model:



$$H_\Omega = -J \sum_{\langle ij \rangle}^{N} s_i s_j - H \sum_{i}^{N} s_i$$

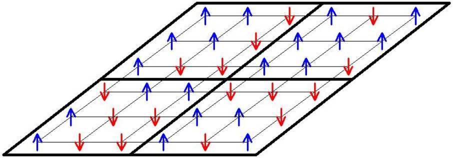
- dimension d
- lattice of N sites with distance a
- spins $s_i = \pm 1$
- only nearest neighbor interactions

For $T \to T_C \Rightarrow \xi \to \infty$

Kadanoff construction

Block spin transformation

- Partition the lattice into blocks of side ba
- Each block is associated with a new spin $\tilde{s}$. Set $\tilde{s}$ to majority of spins in the block.



	cells	cell length
original lattice	N	a
lattice of blocks	$N' = b^{-d}N$	$a' = ba$

Each block contains b^d sites of the original lattice

Kadanoff construction

Assumption 1:

- Block spin interacts only with nearest neighbor block spin and an effective external field

$$H_\Omega = -J \sum_{\langle ij \rangle}^{N} s_i s_j - H \sum_{i}^{N} s_i$$

$$\tilde{H}_\Omega = -\tilde{J} \sum_{\langle ij \rangle}^{Nb^{-d}} \tilde{s}_i \tilde{s}_j - \tilde{H} \sum_{i}^{Nb^{-d}} \tilde{s}_i$$

Since Hamiltonians have the same structure
$\Rightarrow$ free energy same with (different parameters)

$$Nf\left(t, h\right) = Nb^{-d} f\left(\tilde{t}, \tilde{h}\right)$$

Kadanoff construction

$$Nf\left(t,h\right) = Nb^{-d} f\left(\tilde{t},\tilde{h}\right)$$

$$f\left(t,h\right) = b^{-d} f\left(\tilde{t},\tilde{h}\right)$$

We expect that $\tilde{h} = \tilde{h}\left(h,b\right)$ and $\tilde{t} = \tilde{t}\left(t,b\right)$. From the above equation we conclude:

$$\tilde{h} \propto h \qquad \tilde{t} \propto t$$

Assumption 2:

$$\tilde{h} = b^{y_h} h \qquad \tilde{t} = b^{y_t} t$$

$$\Rightarrow \qquad f\left(t,h\right) = b^{-d} f\left(b^{y_t} t, b^{y_h} h\right)$$

Scaling for the correlation function

Consider Hamiltonian with non-uniform external field h not changing significantly over distances ba.

Define: $\tilde{r} = r/b$

$$\beta H_{\Omega} = \beta H_{\Omega 0} - \sum_{r} h(r)\, s(r)$$

$$\beta \tilde{H}_{\Omega}(\tilde{s}) = \beta \tilde{H}_{\Omega 0}(\tilde{s}) - \sum_{\tilde{r}} \tilde{h}(\tilde{r})\, \tilde{s}(\tilde{r})$$

If Z is the partition function the 2-point correlation function is given by

$$\begin{aligned} G(r_1 - r_2, H_{\Omega}) &= \langle s(r_1)\, s(r_2)\rangle - \langle s(r_1)\rangle \langle s(r_2)\rangle \\ &= \left.\frac{\partial^2}{\partial h(r_1)\, \partial h(r_2)} \ln Z \right|_{h(r)=0} \end{aligned}$$

Scaling for the correlation function

$$\frac{\partial^2}{\partial \tilde{h}(\tilde{r}_1)\,\partial \tilde{h}(\tilde{r}_2)} \ln \tilde{Z}\left(\tilde{h}\right) = \frac{\partial^2}{\partial \tilde{h}(\tilde{r}_1)\,\partial \tilde{h}(\tilde{r}_2)} \ln Z(h)$$

LHS: $G(\tilde{r}_1 - \tilde{r}_2, \tilde{H}_\Omega)$

RHS: If $r = |r_1 - r_2| \gg ba \quad \Rightarrow \quad b^{-2y_h} b^{2d} G(r, H_\Omega)$

$$\Rightarrow \qquad G\left(\frac{r}{b}, \tilde{H}_\Omega\right) = b^{2d-2y_h} G(r, H_\Omega)$$

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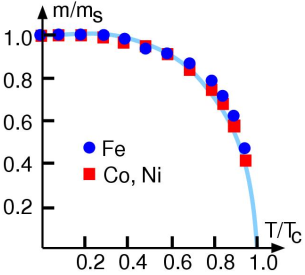
Universality classes I

Universality is a prediction of the renormalization group theory

Definition: Systems whose properties near 2nd order phase transition are controlled by the same renormalization group fixed point are in the same universality class.

Properties:

- have the same (relevant) critical exponents
- can have different transition temperatures



3D Heisenberg	β
Fe	0.34(4)
Ni	0.378(4)
CrB_3	0.368(5)
EuO	0.36(1)
Monte Carlo	0.364(4)

Universality classes II

Universality classes are characterized by:

- spatial dimension
- symmetry of the order parameter
- range and symmetry of Hamiltonian

- The details of the form and magnitude of interactions is not relevant.

If the above properties of a system are the same of an other (well known) system, we already known its critical exponents!

Finite size scaling

- All numerical calculations use finite systems.
- Calculate quantities such as C, M,χ for different lattice size.
- Near the critical temperature.

$$C_L = L^{\frac{\alpha}{\nu}} \widetilde{C}\left(L^{\frac{1}{\nu}} t\right)$$

- $\widetilde{C}$ is independent of lattice site but depends on T_c, α and ν.
- If these parameters are chosen correctly and we plot $C_L L^{-\alpha/\nu}$ against $L^{\frac{1}{\nu}} t$ the curve will collapse.

Disordered systems

What happens if the system contains impurities?

- ordered phase is destroyed
- system remains ordered

Harris criterion (1974)
The critical behavior of a quenched disordered system does not differ form that of the pure system if

$$d\nu > 2$$

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Polymers

- A polymer is a chain of monomers.

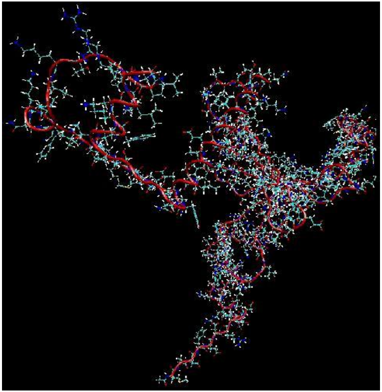


Figure: protein T162

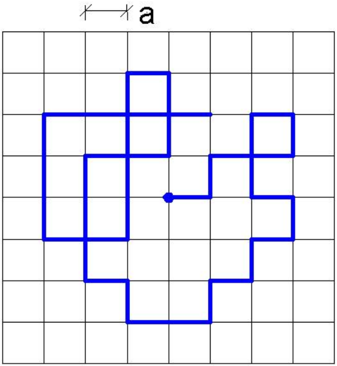
Examples:

- Synthetic Polymers
  - PVC
  - PE
  - PET
- Biopolymers
  - DNA
  - RNA
  - proteins

Random walk: a crude model for a polymer

Random walk

- There is a starting point 0.
- Distance from one point to the next is a constant.
- Direction is chosen at random with equal probability.



Self avoiding random walk

- same but no intersections

Random walk: a crude model for a polymer

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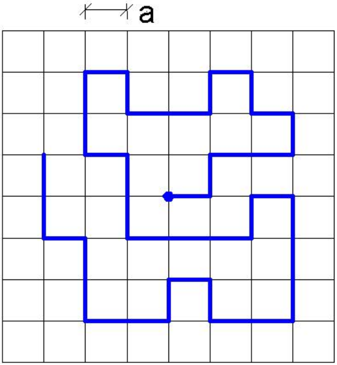


Self avoiding random walk

- same but no intersections

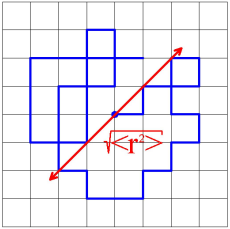
Random walk

Properties of a random walk

- $c_N(\vec{r})$ = number of distinct walks from 0 to $\vec{r}$
- end-to-end vector

$$\vec{r} = \sum_n \vec{a}_n$$

- average square distance



$$\langle r^2 \rangle = \sum_{n=m} \langle \vec{a}_n \vec{a}_m \rangle + \underbrace{\sum_{n \neq m} \langle \vec{a}_n \vec{a}_m \rangle}_{=0} = Na^2$$

What is $\langle r^2 \rangle$ for a polymer (self-avoiding random walk)?

Solution by mapping to a $O(n)$ vector model

Goal:

Find a connection of self-avoiding random walks and the $O(n)$ $n \longrightarrow 0$ model.

Model:

- Hypercubic lattice of dimension d
- Spin on each lattice site has n components. $\vec{S} = \left(S_i^1, S_i^2, .., S_i^n\right)$
- Normalization:

$$\sum_{\alpha}^{n} \left(\vec{S}^{\alpha}\right)^2 = n$$

- only nearest neighbor interactions

Hamiltonian:

$$H_{\Omega} = -K \sum_{\langle ij \rangle, \alpha} S_i^{\alpha} S_j^{\alpha}$$

Moment Theorem

Theorem:
Let $\langle \ldots \rangle_0$ be the average over all spin orientation
For $n \longrightarrow 0$ we have

$$\left\langle S^\alpha S^\beta \right\rangle_0 = \delta_{\alpha\beta}$$

and all other momentum are 0.

Examples:

$$\left\langle S^\alpha S^\beta S^\gamma \right\rangle_0 = 0$$

$$\left\langle S^\alpha S^\alpha S^\alpha S^\beta S^\gamma \right\rangle_0 = 0$$

Mapping to $O(n)$ $n \longrightarrow 0$

The exponent of the Hamiltonian can be written as:

$$\begin{aligned}\exp(-\beta H_\Omega) &= \exp(-\beta K \sum_{\langle ij\rangle,\alpha} S_i^\alpha S_j^\alpha) = \prod_{\langle ij\rangle} \exp(-\beta K \sum_{\alpha} S_i^\alpha S_j^\alpha) \\ &= \prod_{\langle ij\rangle}(1 - \beta K \sum_{\langle ij\rangle,\alpha} S_i^\alpha S_j^\alpha + \frac{1}{2}(\beta K)^2 (\sum_{\langle ij\rangle,\alpha} S_i^\alpha S_j^\alpha)^2 - \ldots)\end{aligned}$$

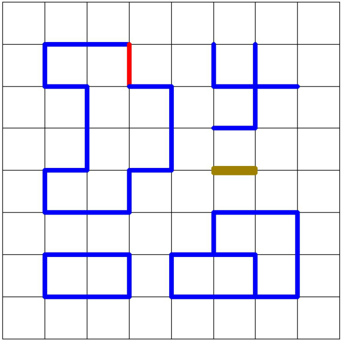
Therefor the partition function Z is given by

$$\begin{aligned}Z &= Tr \exp\left(-\beta H_\Omega\right) = \prod_k \int d\Omega_k \left\langle \exp\left(-\beta H_\Omega\right)\right\rangle_0 \\ &= \Omega \langle \prod_{\langle ij\rangle} (1 - \beta K \sum_{\alpha} S_i^\alpha S_j^\alpha + \frac{1}{2}(\beta K)^2 (\sum_{\alpha} S_i^\alpha S_j^\alpha)^2) - \ldots \rangle_0\end{aligned}$$

where $\Omega = \prod_i \int d\Omega_i$

Diagram Representation

$$Z = \Omega \langle \prod_{\langle ij \rangle} (1 - \beta K \sum_{\alpha} S_i^{\alpha} S_j^{\alpha} + \frac{1}{2} (\beta K)^2 (\sum_{\alpha} S_i^{\alpha} S_j^{\alpha})^2) \rangle_0$$



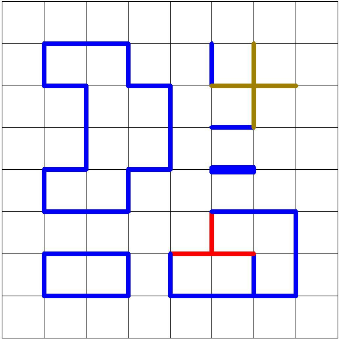
We expand the product over $\langle ij \rangle$

- choose 1 do nothing
- choose $\beta K \sum_{\alpha} S_i^{\alpha} S_j^{\alpha}$ draw a line form i to j
- choose $\frac{1}{2} (\beta K)^2 (\sum_{\alpha} S_i^{\alpha} S_j^{\alpha})^2$ draw smallest loop

$\Rightarrow$ 3^B diagrams

Diagram Representation

$$Z = \Omega \langle \prod_{\langle ij \rangle} (1 - \beta K \sum_{\alpha} S_i^{\alpha} S_j^{\alpha} + \frac{1}{2} (\beta K)^2 (\sum_{\alpha} S_i^{\alpha} S_j^{\alpha})^2) \rangle_0$$



Taking the average

- only vertices with 2 lines survive

$$\langle S_i^{\alpha} S_i^{\alpha} S_i^{\alpha} \rangle_0 = 0$$

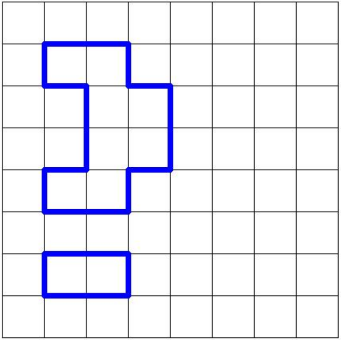
$$\langle S_i^{\alpha} S_i^{\alpha} S_i^{\alpha} S_i^{\alpha} \rangle_0 = 0$$

- index of the spins must be the same

$\Rightarrow$ less than 3^B diagrams

Diagram Representation

$$Z = \Omega \langle \prod_{\langle ij \rangle} (1 - \beta K \sum_{\alpha} S_i^{\alpha} S_j^{\alpha} + \frac{1}{2} (\beta K)^2 (\sum_{\alpha} S_i^{\alpha} S_j^{\alpha})^2) \rangle_0$$



Taking the average

- only vertices with 2 lines survive
- index of the spins must be the same

$\Rightarrow$ less than 3^B diagrams

Mapping to $O(n)$ $n \rightarrow 0$

Taking the average

$$\langle \sum_{\alpha\beta...} S_i^\alpha S_j^\alpha \; S_j^\beta S_k^\beta \; ... \; S_q^\theta S_i^\iota \rangle_0 = \sum_{\alpha\beta...} \delta_{\alpha\beta}\delta_{\beta\gamma}...\delta_{\alpha\iota} = \sum_{\alpha}^{n} 1 = n$$

It follows:

$$Z = \Omega \sum_{loop \;\; conf} n^{number \;\; of \;\; loops} (\beta K)^{number \;\; of \;\; bounds}$$

For $n \rightarrow 0$ we obtain $Z = \Omega$.

Mapping to $O(n)$ $n \rightarrow 0$

Correlation function

$$\begin{aligned} G(i,j) &= \left\langle S_i^1 S_j^1 \right\rangle \\ &= Z^{-1} Tr \prod_{\langle ij \rangle} S_i^1 S_j^1 (1 - \beta K \sum_\alpha S_i^\alpha S_j^\alpha + \frac{1}{2}(\beta K)^2 (\sum_\alpha S_i^\alpha S_j^\alpha)^2) \end{aligned}$$

like before

$\Rightarrow$ surviving diagrams have single line (self-avoiding walk) form i to j

$$\sum_N c_N(r)\, \beta K = \lim_{n \rightarrow 0} G(r, \beta K)$$

This is the important relation which connects a self avoiding random walk to the $O(n)$ $n \rightarrow 0$ model.

Critical behavior

Scaling of c_N

Define: $x = \beta K \qquad c_N = \sum_r c_N(r)$

$$\sum_N c_N x^N = \sum_N \sum_r c_N(r)\, x^N = \lim_{n\to 0} \sum_r G(r,x) = \chi \sim |x - x_c|^{-\gamma}$$

Ansatz: $c_N \propto x_c^{-N} N^{\gamma-1}$

Ansatz is correct since:

$$\begin{aligned}\sum_N c_N x^N &\propto \int_0^\infty dN N^{\gamma-1} \left(\frac{x}{x_c}\right)^N \propto \ln\left(\frac{x}{x_c}\right)^{-\gamma} \\ &= \ln\left(1 + \frac{(x - x_c)}{x_c}\right)^{-\gamma} \sim |x - x_c|^{-\gamma}\end{aligned}$$

Critical behavior

Scaling of $\langle r^2 \rangle$

$$\left\langle r^2 \right\rangle = \sum_{\vec{r}} r^2 \frac{c_N(r)}{c_N}$$

Similar calculations

$$\sum_{\vec{r}} r^2 G(r,x) = \sum_{\vec{r}} \sum_N c_N(r)\, x^N r^2 = \sum_N \sum_{\vec{r}} c_N(r)\, r^2 x^N$$

$$G(r,x) \sim r^{-(d-2+\eta)} e^{-\frac{r}{\xi}} \quad \Rightarrow \quad \sum_{\vec{r}} c_N(r)\, r^2 \sim |x_c - x|^{\gamma - 2\nu}$$

$$\Rightarrow \quad \left\langle r^2 \right\rangle \sim \frac{x_C^{-N} N^{2\nu+\gamma-1}}{x_C^{-N} N^{\gamma-1}} \sim N^{2\nu}$$

Summary

- Near the critical point of a second-order phase transition the thermodynamic potentials are assumed to be homogeneous functions
$$f(t,h) = b^{-d} f(b^{y_t} t, b^{y_h} h)$$

$\Rightarrow$ only 2 independent exponents

- Systems can be grouped into universality classes
- Harris criterion for quenched disordered systems $d\nu > 2$
- Random walk $\langle r^2 \rangle \sim N$
Self-avoiding random walk $\langle r^2 \rangle \sim N^{2\nu}$