Symmetry and ergodicity breaking, mean-field study of the Ising model

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Topics

Introduction

Formalism

The model system: Ising model

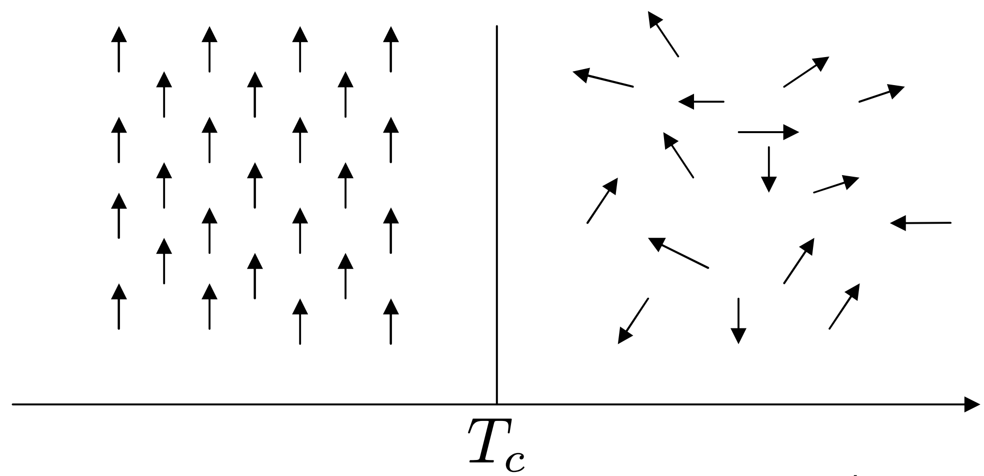
Solutions in one and more dimensions

Symmetry and ergodicity breaking

Conclusion

Introduction

phase A

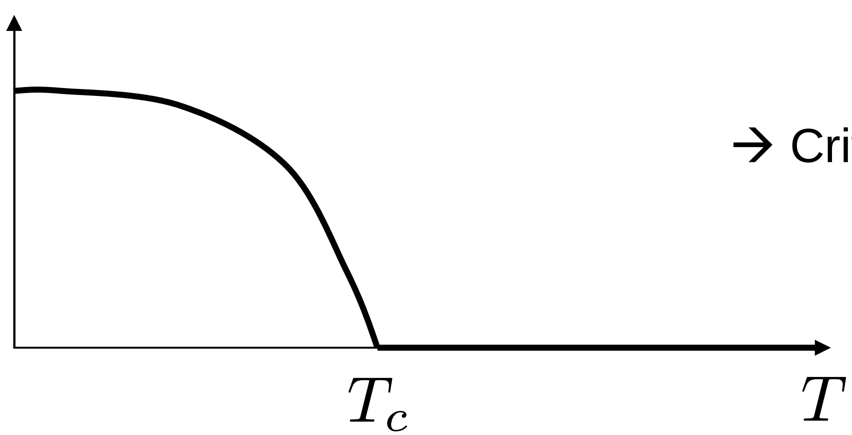


phase B

temperature T

phase transition

order parameter



→ Critical exponents

Formalism

Statistical mechanical basics

sample region Ω

i) certain dimension d

ii) volume $V(\Omega)$

iii) number of particles/sites $N(\Omega)$

iv) boundary conditions

Hamiltonian defined on the sample region

$$-\frac{H_\Omega}{k_B T} = \sum_n K_n \Theta_n$$

Θ_n: Depending on the degrees of freedom

K_n: Coupling constants

Partition function

$$Z_\Omega[\{K_n\}] = Tr\,\exp^{-\beta H_\Omega(\{K_n\},\{\Theta_n\})} \qquad \beta = \frac{1}{k_B T}$$

Free energy

$$F_\Omega[\{K_n\}] = F_\Omega[K] = -k_B T log Z_\Omega[\{K_n\}]$$

Free energy per site

$$f_b[K] = \lim_{N(\Omega)\to\infty} \frac{F_\Omega[K]}{N(\Omega)}$$

i) Non-trivial existence of limit

ii) Independent of Ω

iii) $$\lim_{N(\Omega)\to\infty} \frac{N(\Omega)}{V(\Omega)} = const$$

Phases and phase boundaries

Supp.: - $f_b[K]$ exists

- there exist D coulping constants: $\{K_1, \ldots, K_D\}$

- $f_b[K]$ is analytic almost everywhere
- non-analyticities of $f_b[\{K_n\}]$ are points, lines, planes, hyperplanes in the phase diagram

→ Dimension of these singular loci: $D_s = 0, 1, 2, \ldots$

Codimension C for each type of singular loci: $C = D - D_s$

Phase: region of analyticity of $f_b[K]$

Phase boundaries: loci of codimension C = 1

Types of phase transitions

$f_b[K]$ is everywhere continuous.

Two types of phase transitions:

a) Discontinuity across the phase boundary of $\frac{\partial f_b[K]}{\partial K_i}$

first-order phase transition

b) All derivatives of the free energy per site are continuous across the phase boundaries

Continuous phase transition

Overview

$$Z_\Omega[K] = Tr\, \exp^{-\beta H_\Omega(K,\{\Theta_n\})}$$

↓

$$F_\Omega[K] = -k_B T log Z_\Omega[K]$$

↓

$$f_b[K] = \lim_{N(\Omega)\to\infty} \frac{F_\Omega[K]}{N(\Omega)}$$

↙ ↘

$$\epsilon_{in}[K] = \frac{\partial}{\partial\beta}(\beta f_b[K])$$

internal energy

↓

$$C[K] = \frac{\partial \epsilon_{in}[K]}{\partial T}$$

heat capacity

$$M[K] = -\frac{\partial f_b[K]}{\partial H}$$

magnetization

↓

$$\chi_T[K] = \frac{\partial M[K]}{\partial H}$$

magnetic susceptibility

Critical exponents

How do the measurable quantities change in the neighbourhood of a critical point?

Critical temperature T_C $$t = \frac{T - T_C}{T_C}$$

$$\left.\begin{array}{lll} \text{heat capacity} & & C \sim |t|^{-\alpha} \\ \text{Order parameter (t < 0)} & & M \sim |t|^{\beta} \\ \text{susceptibility} & & \chi \sim |t|^{-\gamma} \end{array}\right\} \quad \text{for } H \equiv 0$$

Equation of state $M \sim H^{1/\delta}$

Correlation length

- Length scale over which the fluctuations of the microscopic degrees of freedom are significantly correlated with each other

(Cardy: Scaling and Renormalization in Statistical Physics)

- Strong dependence on temperature near a phase transition diverging to infinity at the transition itself

Critical exponents for the correlation function

$$\Gamma(r) \quad \xrightarrow{t \to 0} \quad r^{-p} e^{-r/\xi}$$

Correlation length $\qquad \xi \sim |t|^{-\nu}$

Power-law decay (t=0) $\qquad p = d - 2 + \eta$

The model system: Ising model

- attempt to simulate a domain in a ferromagnetic material
- Spontaneous magnetization in absence of an external magnetic field
- Critical temperature: Curie temperature

Importance of Ising model

- Equivalent models (lattice gas, binary alloy)
- The only non-trivial example of a phase transition that can be worked out be mathematical rigor in statistical mechanics
- Compare computer simulations of the model with exact solution

Characterization of the Ising model

i) Periodic lattice Ω in d dimensions

ii) Lattice contains $N(\Omega)$ fixed points called lattice sited

iii) For each site: classical spin variable S_i = +/- 1 (i = 1, …, N) in a definite direction (degrees of freedom)

iv) Most general Hamiltonian

$$-H_\Omega = \sum_{i\in\Omega} H_i S_i + \sum_{i,j} J_{ij} S_i S_j + \sum_{i,j,k} K_{ijk} S_i S_j S_k + \ldots$$

v) Number of possible configurations: $2^{N(\Omega)}$

$$Tr \equiv \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \cdots \sum_{S_{N(\Omega)}=\pm 1} \equiv \sum_{\{S_i=\pm 1\}}$$

Assumptions

i) two-spin coupling only $K_{ijk} = 0, \ldots$

ii) External magnetic field spatially constant $H_i \equiv H$

iii) Nearest-neighbour interactions only $\sum_{i,j} \to \sum_{<ij>}$

iv) Isotropic interactions $J_{ij} \equiv J$

v) Hypercubic lattice $z = 2d$

vi) Ferromagnetic material $J > 0$

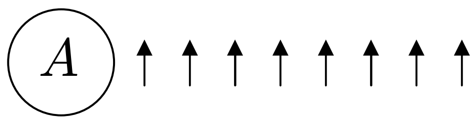
$$-H_\Omega = H \sum_{i \in \Omega} S_i + J \sum_{<i,j>} S_i S_j$$

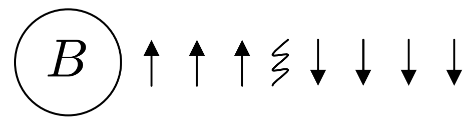
$$Z_\Omega[H,T,J] = \sum_{\{S_i = \pm 1\}} exp^{\beta(H \sum_{i\in\Omega} S_i + J \sum_{<i,j>} S_i S_j)}$$

Arguments for phase transition in d = 1,2 dimensions with H = 0

$$F_\Omega[K] = E_{in}[K] - TS_\Omega[K] = -J \sum_{<i,j>} S_i S_j - T k_B log(\sharp(states))$$

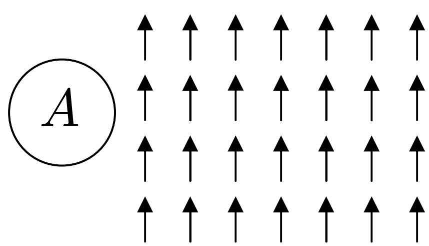
d = 1

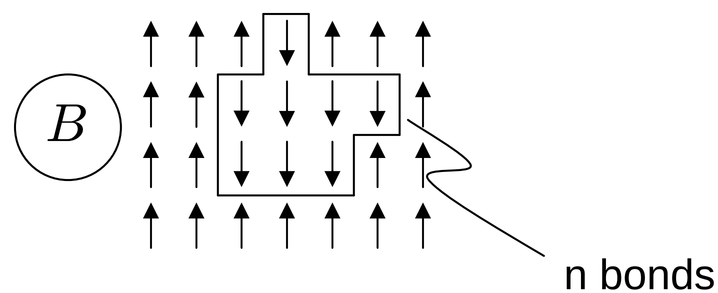




$$F_{N,B} - F_{N,A} = 2J - k_B T log(N-1) \stackrel{N \to \infty}{\to} -\infty$$

d = 2





$$F_{N,B} - F_{N,A} = [2J - log(z-1) k_B T] n$$

$$T_C = \frac{2J}{k_B log(z-1)}$$

Long range order ←→ short range order

- nearest neighbour interaction: short range interaction

- What about:

$$J_{ij} = \frac{J}{|r_i - r_j|^\sigma}$$

Answer:

$\sigma < 1$	thermodynamic limit does not exist
$1 \leqslant \sigma \leqslant 2$	long range order persist for $0 < T < T_C$
$2 \leqslant \sigma$	short-range interaction: no ferromagnetic state for $T > 0$

Solutions in one and more dimensions

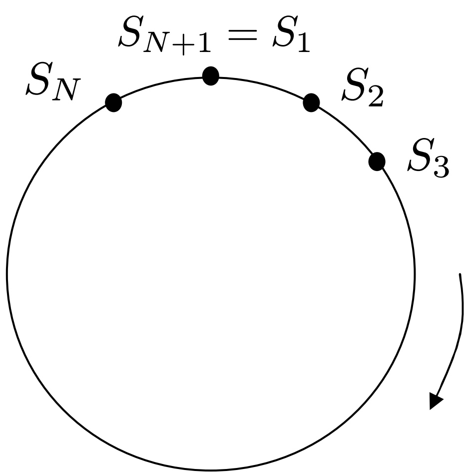
$d = 1$	$H = 0$	- ad hoc methods - recursion method
	$H \neq 0$	- transfer matrix method (Kramers, Wannier 1941)
$d = 2$	$H = 0$	- low temperature expansion - Onsager solution (1944)
$d = 1, 2, 3$	$H \neq 0$	- mean-field method (Weiss)

$d = 1$	$H \neq 0$

Transfer matrix method

Reduce the problem of calculating the partition function to the problem of finding the eigenvalues of a matrix

Assumption: $S_{N+1} = S_1$



$$Z_\Omega[H, J] = Tr \exp^{-\beta H_\Omega(H, J, \{S_i\})}$$

$$H_\Omega(H, J, \{S_i\}) = -H \sum_{i \in \Omega} S_i - J \sum_{<i,j>} S_i S_j$$

$h := \beta H$ $\quad$ $K := \beta J$

$$Z_\Omega[h, K] = \sum_{S_1} \dots \sum_{S_N} e^{h \sum_i S_i + K \sum_i S_i S_{i+1}}$$

Calculation: $$det\begin{pmatrix} e^{h+K}-\lambda & e^{-K} \\ e^{-K} & e^{-h+K}-\lambda \end{pmatrix} \equiv 0$$

$$\Rightarrow \quad \lambda_{1,2} = e^{K}(\cosh(h) \pm \sqrt{\sinh(h)^2 + e^{-4K}})$$

$$\Rightarrow \quad \boxed{f_b(h,K,T) = -Jk_B T log(cosh(h) + \sqrt{sinh(h)^2 + e^{-4K}})}$$

Spatial correlation in one dimension (T > 0)

$d = 1$	$H = 0$

Definition: two point correlation function

$$G(i,j) := \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

$$G(i,i+j) = \langle S_i S_{i+j} \rangle = (tanh(K))^j$$

$$G(i,i+j) = e^{-j log(coth(K))} \equiv e^{-j/\xi}$$

$$\Rightarrow \xi = \frac{1}{log(coth)K))} \cong 1/2 \quad e^{J/(k_B T)}$$

Onsager solution

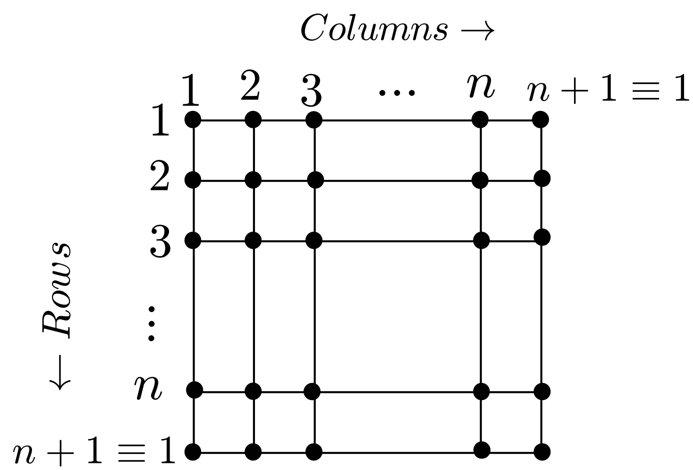
$d = 2$	$H = 0$

Notation and boundary conditions:

$$\mu_\alpha = \{s_1, s_2, \ldots, s_n\}_{\alpha th\ row}$$

$$s_{n+1} = s_1 \ , \ \mu_{n+1} = \mu_1$$

$$N = n^2$$



Elements of the Hamiltonian:

$$E(\mu, \mu') = -\epsilon \sum_{k=1}^{n} s_k s'_k$$

$$E(\mu) = -\epsilon \sum_{k=1}^{n} s_k s_{k+1} - H \sum_{k=1}^{n} s_k$$

Partition function:

$$Z_\Omega[H, T] = \sum_{\mu_1} \cdots \sum_{\mu_n} e^{-\beta \sum_{\alpha=1}^{n} [E(\mu_\alpha, \mu_{\alpha+1}) + E(\mu_\alpha)]}$$

Properties of the matrix P:

- $\langle \mu | P | \mu' \rangle := e^{-\beta[E(\mu,\mu')+E(\mu)]}$
- $P : 2^n \times 2^n matrix$
- $Z_\Omega[H,T] = TrP^n$

$$\Rightarrow \quad \lim_{N\to\infty} \frac{1}{N} log(Z_\Omega[H=0,T]) = \lim_{n\to\infty} \frac{1}{n} log(\lambda_{max})$$

largest eigenvalue of P

$$f_b[H=0,T] = \lim_{N(\Omega)\to\infty} \frac{F_\Omega[0,T]}{N(\Omega)} = \lim_{N(\Omega)\to\infty} \frac{-k_B T log Z_\Omega[0,T]}{N(\Omega)} = -k_B T \lim_{n\to\infty} \frac{1}{n} log(\lambda_{max})$$

$$\Rightarrow \quad \boxed{\beta f_b[0,T] = -\log\left(2\cosh 2\beta\epsilon\right) - \frac{1}{2\pi}\int_0^\pi d\phi \log \frac{1}{2} 1 + \sqrt{1-\kappa^2 sin^2\phi}}$$

$$\kappa = 2[\cosh 2\phi \; coth 2\phi]^{-1}$$

Mean-field theory

Arguments for mean-field theory:

- Simplest treatment of an interacting statistical mechanical system

- often gives a qualitatively correct picture of the phase diagram of a given model

- „the“ mean-field theory

Hamiltonian

$$-H_\Omega = H \sum_{i \in \Omega} S_i + J \sum_{<i,j>} S_i S_j$$

Partition function

$$Z_\Omega[H,T,J=0] = \sum_{\{S_i = \pm 1\}} exp^{\beta(H \sum_{i\in\Omega} S_i)} =$$

$$= \prod_{k=1}^{N} \sum_{S_k = \pm 1} exp^{\beta H S_k} = (e^{\beta H} + e^{-\beta H})^N = (2\cosh \beta H)^N$$

Assumption: d-dimensional hypercubic lattice $z = 2d$

Postulate: effective field due to the magnetic moments of all other spins

$$-H_\Omega = H \sum_{i\in\Omega} S_i + J \sum_{<i,j>} S_i S_j = \sum_{i\in\Omega} S_i [H + J \sum_{j\ n.n.} S_j]$$

$$\sum_{j\ n.n.} S_j = \underbrace{\sum_{j\ n.n.} \langle S_j \rangle}_{\text{mean field}} + J \underbrace{\sum_{j\ n.n.} (S_j - \langle S_j \rangle}_{\text{fluctuation in the mean field}} \cong \sum_{j\ n.n.} \langle S_j \rangle = 2dM$$

$$-H_\Omega = \sum_{i\in\Omega} S_i [H + J \sum_{j\ n.n.} S_j] = \sum_{i\in\Omega} S_i [H + 2dJM] \equiv H_{eff} \sum_{i\in\Omega} S_i$$

$$\Rightarrow \boxed{Z_\Omega[H,T] = (2\cosh\beta H_{eff})^N = (2\cosh\beta[H + 2dJM])^N}$$

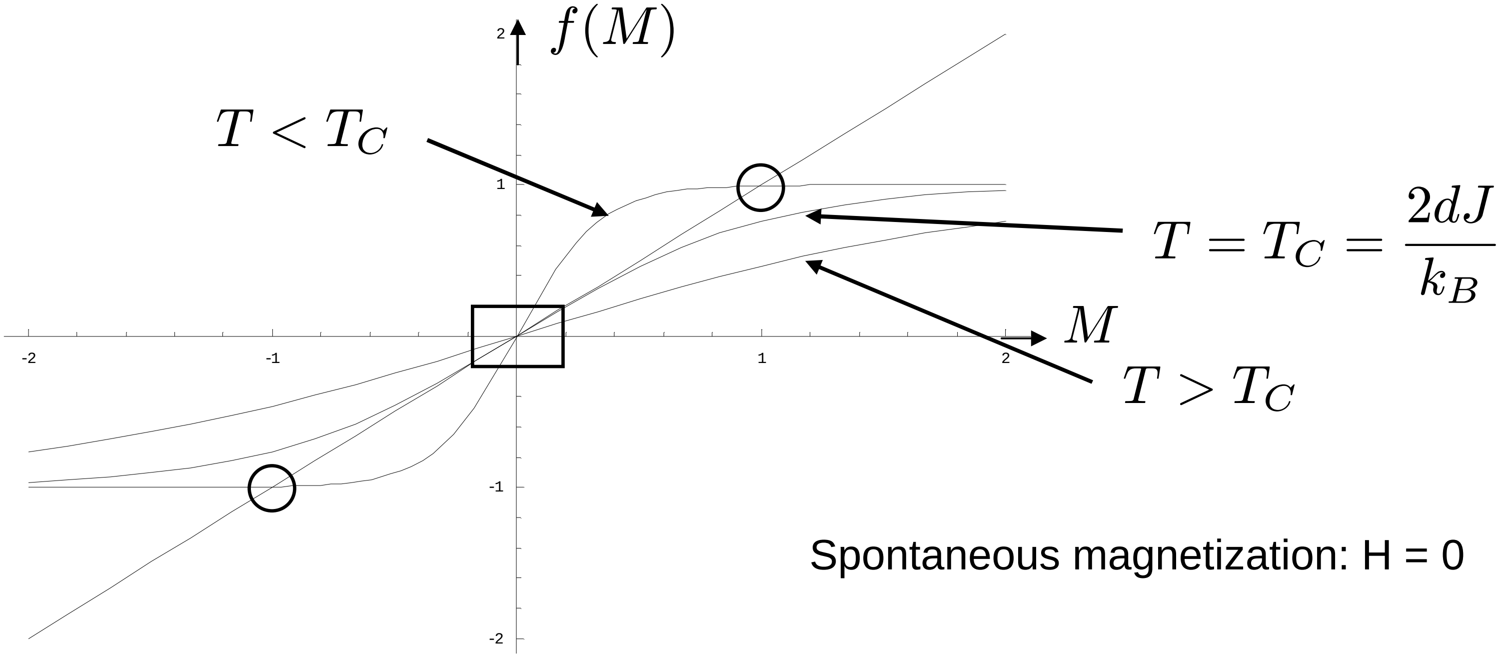
Free energy per site

$$f_b[H,T] = \lim_{N(\Omega)\to\infty} \frac{-k_B T log Z_\Omega[H,T]}{N(\Omega)} = \lim_{N(\Omega)\to\infty} \frac{-k_B T log(2\cosh\beta[H+2dJM])^{N(\Omega)}}{N(\Omega)}$$

$$\Rightarrow \boxed{f_b[H,T] = -k_B T \log 2\cosh\beta[H+2dJM]}$$

magnetization per site

$$M[K] = -\frac{\partial f_b[K]}{\partial H} = \tanh\frac{H+2dJM}{k_B T}$$



Spontaneous magnetization: H = 0

Critical exponents for mean-field theory of the Ising model

$$M = \tanh \frac{H + 2dJM}{k_B T} = \frac{\tanh \frac{H}{k_B T} + \tanh M\tau}{1 + \tanh \frac{H}{k_B T} \tanh M\tau}$$

$$\tau = \frac{T_C}{T}$$

Expand for small H,M:

$$\boxed{\frac{H}{k_B T} = M(1-\tau) + M^3(\tau - \tau^2 + \frac{\tau^3}{3} + \ldots) + \ldots}$$

$\boxed{H = 0}$ $$M^2 = 3\frac{T - T_C}{T_C} + \ldots \Rightarrow \boxed{\beta = \frac{1}{2}}$$

$\boxed{\tau = 1}$ $$\frac{H}{k_B T} = M^3 + \ldots \Rightarrow \boxed{\delta = 3}$$

$\boxed{M = 0}$ $$\frac{1}{k_B T} = \chi_T(1-\tau) + 3M^2\chi_T(\tau - \tau^2 + \frac{\tau^3}{3}) + \ldots \Rightarrow \boxed{\gamma = 1}$$

Symmetry and ergodicity breaking

The ergodic hypothesis

dynamical degrees of freedom $\eta_i(t)$

Any observable $A(\{\eta_i(t)\})$

time average
$$\langle A \rangle_{ta} \;:=\; \lim_{t\to\infty} \frac{1}{t} \int_0^t dt' A(\{\eta_i(t')\})$$

expectation value
$$\langle A \rangle_{eqm} \;:=\; \int \prod_i d\eta_i P_{eqm}(\{\eta_i\}) A(\{\eta_i)\})$$

$$\boxed{\langle A \rangle_{ta} \stackrel{!}{=} \langle A \rangle_{eqm}}$$

Symmetry of the system at H = 0

$$-H_\Omega(\{S_i\}) = H \sum_{i \in \Omega} S_i + J \sum_{<i,j>} S_i S_j = J \sum_{<i,j>} S_i S_j$$

$$-H_\Omega(\{-S_i\}) = J \sum_{<i,j>} (-S_i)(-S_j) = J \sum_{<i,j>} S_i S_j = -H_\Omega(\{S_i\})$$

statistical mechanical probability of finding the system in the state $\{S_i\}$:

$$P_\Omega(\{S_i\}) = \frac{exp(-\beta H_\Omega(\{S_i\}))}{Z_\Omega[K]}$$

$$\boxed{M \equiv \langle S_i \rangle \ = \ Tr[P_\Omega(\{S_i\}) S_i] \ = \ 0}$$

The restricted ensemble*

divide phase space into components $$\Gamma = \bigcup_\alpha \Gamma_\alpha$$

Assumptions on the properties of components:

(a) Confinement: there is no chance for the phase point for moving from one component to another

(b) Internal ergodicity: ergodic hypothesis for a particular component

Remark: component decomposition depends on the external parameters of the system

→ appearance, disappearance, bifurcation, merge of components

* Palmer, Adv.Phys., (1982), Vol. 31, 669 - 735

Change of component

Definition: cumulative prob. for escape from some component Γ_α : $\mathrm{P}^\alpha(t)$

Assumption: $\boxed{P^\alpha(\tau_0) \ \leq \ p_0}$ $\Rightarrow$ meta-stable component

The Ising model:

Transition probability to a critical cluster

$$(P^\alpha)' \sim \frac{P_A}{P_B} \sim \frac{e^{-\beta F_A}}{e^{-\beta F_B}} \sim e^{-\beta \Delta F} \sim e^{-\beta N^{(d-1)/d}}$$

$$\lim_{N\to\infty} (P^\alpha)'(\tau_0, N) \ = \ 0$$ (for any τ_0 thermodynamical limit for d=2,3)

$$\boxed{\lim_{t\to\infty} \ \lim_{N\to\infty} (P^\alpha)'(t, N) \ = \ 0}$$

Broken symmetry

components do not have the inversion symmetry of the Hamiltonian: $M \neq 0$

broken symmetry	$\Longrightarrow$ $\not\Longleftarrow$	broken ergodicity

So what is special about symmetry breaking?

- Different components are mapped on each other by the symmetry mapping which is broken

- order parameter Φ

$\lvert\Phi\rvert$	magnitude	$\Rightarrow$	degree of freedom
$\Phi/(\lvert\Phi\rvert)$	direction	$\Rightarrow$	component property
$\lvert\Phi\rvert \rightarrow 0$	continuously for continuous phase transition		

Conclusion

Critical exponents for d = 2

	$mean - field$	$Onsager$	Rb_2CoF_4	Rb_2MnF_4
α	$0\ (disc)$	$0\ (log)$	$\simeq 0.8$	4.7×10^{-3}
β	0.5	0.125	0.122 ± 0.008	0.17 ± 0.03
$method$			$neutrons$	$neutrons$

De Jongh, Miedema, Adv.Phys. (1974), Vol. 23, 1 - 260

Critical exponents for d = 3

	$mean-field$	$mean$	$CrBr_3$	$RbMnF_3$
β	0.5	0.312	0.368 ± 0.005	0.316 ± 0.008
δ	3	$\simeq 5$	4.28 ± 0.1	
$method$		$th.\ methods$	$Faraday$	$neutrons$

Concepts to remember

Phase transitions occur in the thermodynamical limit: $f_b[K] = \lim_{N(\Omega)\to\infty} \frac{F_\Omega[K]}{N(\Omega)}$

Ferromagnetic state of the Ising model:

d = 1 no long range order for T > 0 → no ferromagnetic state for T > 0

d > 1 long range order for $T < T_C$ → ferromagnetic state possible

First simple method for a model system calculation: mean-field theory

Broken symmetry: components do not have the inversion symmetry of the Hamiltonian → Introduction of order parameter

Broken ergodicity: divide phase space into components with transition probabilities and internal ergodicity in each component

Questions?