Tutorial on Basic Statistical Physics

IPAM 6/02

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Outline

I)

A) Preliminaries

Thermodynamics + Stat Mech

B) Models

Spin Models : Ising & Potts

CS Models as Spin Models

C) Infinite Volumes & States

Thermodynamic Limit

Gibbs States

D) Phase Transitions

Order of Transition

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II)

A) Mean-Field Approximation for the Ising Model

B) Potts Model on the Complete Graph

Part I:

A) Preliminaries

1) Thermodynamics

In thermodynamics, we calculate interesting macroscopic properties of systems. The fundamental quantity is the

$$\underline{\text{free energy}} \qquad f(\underset{\text{inv. temp.}}{\beta}, \underset{\text{field}}{h})$$

Derivatives of the free energy give us the macroscopic properties, e.g.

magnetization (order parameter) $\quad m = \dfrac{-\partial f}{\partial h}$

internal energy $\quad u = \dfrac{\partial}{\partial \beta}(\beta f)$

entropy $\quad s = \beta f - \beta u$

(Second der's wrt h and β give susceptibility and the specific heat.)

Problems of combinatorial optimization (e.g. k-SAT) are zero-temp., mean-field random spin systems. Here u gives the optimal energy (e.g. max-k-SAT = min # of unsat. clauses) and s gives the number of solutions with this energy.

2) Statistical Mechanics

Statistical mechanics is an attempt to derive thermodynamics from microscopic models.

space: Λ

States: $s \in \Omega_\Lambda$

Hamiltonian: $H_\Lambda(s)$ energy of state s

Fundamental assumption:

$$\text{Prob}\left(\begin{matrix}\text{system in state } s \\ \text{at inv. temp } \beta\end{matrix}\right) \propto e^{-\beta H_\Lambda(s)}$$

expectations:

$X : \Omega_\Lambda \to \mathbb{R}$ function

$$\mu_\Lambda(X) \equiv \langle X \rangle_\Lambda = \frac{1}{Z_\Lambda} \sum_{s \in \Omega_\Lambda} X(s)\, e^{-\beta H_\Lambda(s)}$$

normalization:

partition function: $$Z_\Lambda = \sum_{s \in \Omega_\Lambda} e^{-\beta H_\Lambda(s)}$$

free energy $$f_\Lambda(\beta) = -\frac{1}{\beta}\frac{1}{|\Lambda|} \log Z_\Lambda(\beta)$$

$$f(\beta) = \lim_{\Lambda \nearrow \mathbb{L}} f_\Lambda(\beta)$$

B) Models

Consider only lattice models : $\Omega \subset \mathbb{L}$

Graph $G_\Lambda = (\Lambda, E(\Lambda))$

(or for k-body interactions, k-uni. hypergraph)

1) Spin Models

$\sigma = \{\sigma_x \mid x \in \Lambda\} \in \Omega$ spin configuration

$H_\Lambda(\sigma)$ Hamiltonian

a) Ising

$\sigma_x \in \{-1, +1\}$ $\qquad\qquad \Omega = \{-1, +1\}^\Lambda$

$$H_\Lambda(\sigma) = -\sum_{(x,y)\in E(\Lambda)} J_{xy}\,\sigma_x \sigma_y - \sum_{x\in\Lambda} h_x \sigma_x$$

uniform: $h_x = h$

$J_{xy} = J > 0$ ferromagnetic

$= -J < 0$ antiferromagnetic

$$Z_\Lambda(\beta, h) = \sum_\sigma e^{\beta J \sum_{(x,y)} \sigma_x \sigma_y}\, e^{\beta h \sum_x \sigma_x}$$

<u>order parameter</u>

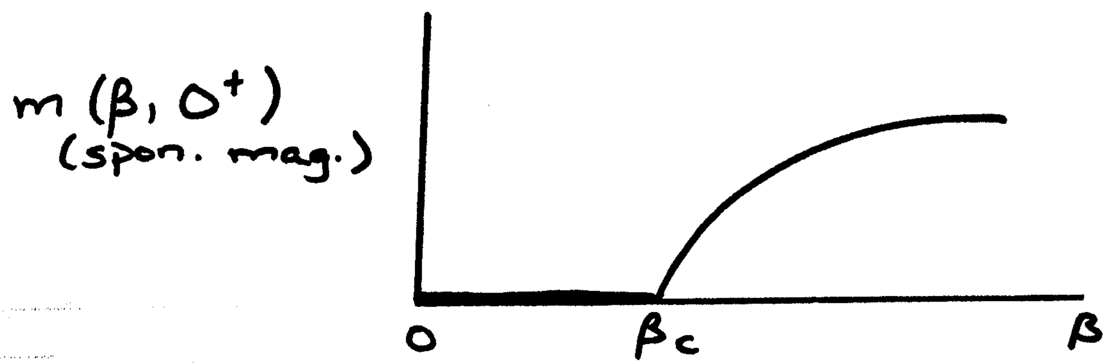
$$m_\Lambda(\beta, h) = \frac{1}{\beta}\frac{\partial}{\partial h}\frac{1}{|\Lambda|}\log Z_\Lambda(\beta, h)$$

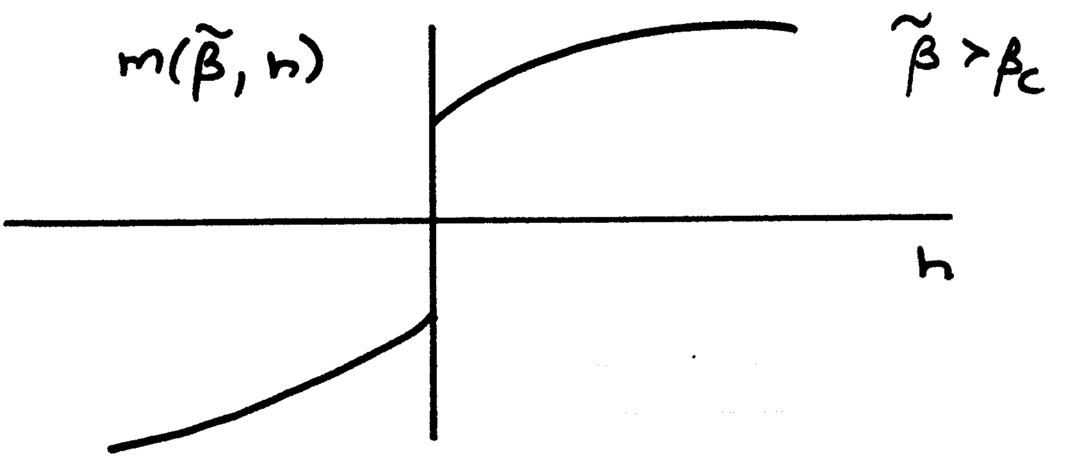
$$= \frac{1}{|\Lambda|}\frac{1}{Z_\Lambda}\sum_{\sigma, x}\sigma_x e^{-\beta H}$$

$$= \frac{1}{|\Lambda|}\sum_x \langle \sigma_x \rangle_\Lambda (\beta, h)$$

infinite-volume limit (discuss later)

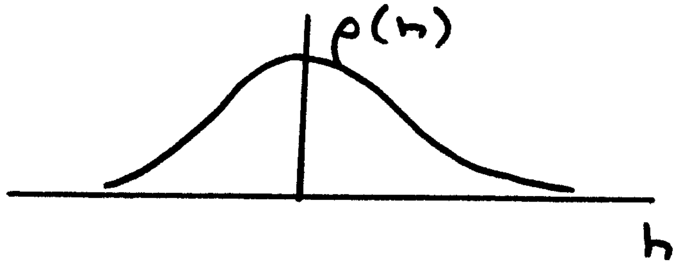
$$m(\beta, h) = \lim_{\Lambda \uparrow \mathbb{L}} m_\Lambda(\beta, h)$$



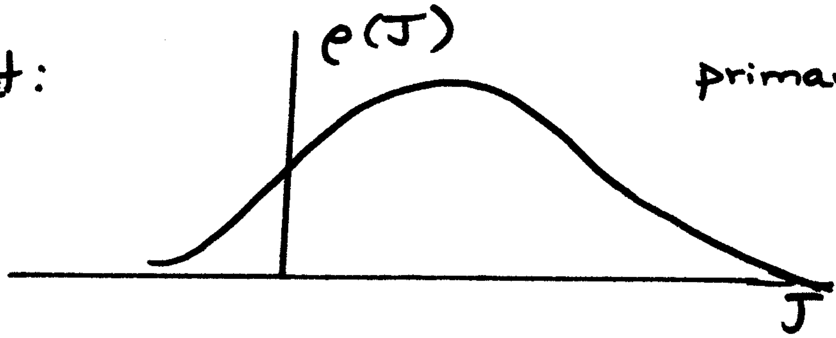


random: h_x and/or J_{xy} i.i.d. r.v.'s

random field:

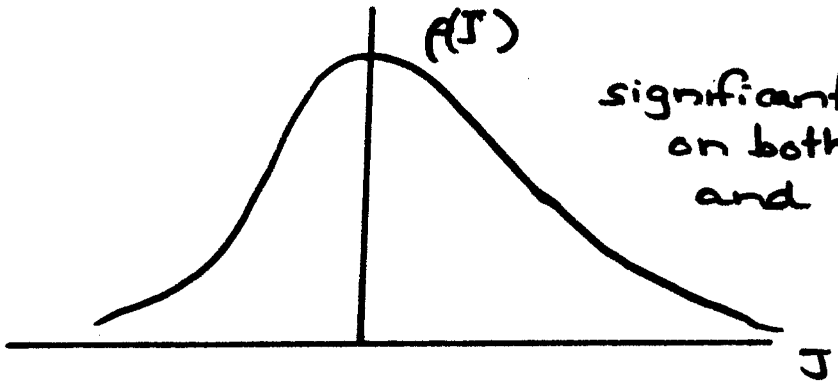


random ferromagnet:



primarily $J>0$

spin glass:



significant weight on both $J>0$ and $J<0$

Now we have another measure ρ. Let E denote expectation wrt ρ.

annealed $\qquad f_\Lambda = -\frac{1}{\beta}\frac{1}{|\Lambda|} \log E(Z_\Lambda) \qquad$ both J's and σ's relax

quenched $\qquad f_\Lambda = -\frac{1}{\beta}\frac{1}{|\Lambda|} E(\log Z_\Lambda) \qquad$ J's are essentially frozen

b) <u>Potts</u>

$$\sigma_x \in \{1, \ldots, q\}$$

$$H_\Lambda(\sigma) = -J \sum_{(x,y)\in E(\Lambda)} \delta(\sigma_x, \sigma_y) - h \sum_{x \in \Lambda} \delta(\sigma_x, 1)$$

$$\delta(\sigma_x, \sigma_y) = \begin{cases} 1 & \sigma_x = \sigma_y \\ 0 & \sigma_x \neq \sigma_y \end{cases}$$

<u>Note:</u> $J \to -\infty$ (zero-temp antiferromag. Potts)

$=$ <u>coloring problem</u>

Notice that zero-temp. models are optimization problems. I won't have time to show you, but the independent set model is a zero-temp Ising lattice gas. And, as we'll now see, random k-SAT and random integer partitioning are like zero-temp spin systems.

4) Comb. Opt. Problems as Zero-Temp Random Spin Model

e.g. **Max k-SAT Problem**

$x_1, \ldots, x_N \in \{0,1\} = \{\text{false}, \text{true}\}$

$\bar{x}_i = 1 - x_i$

$C = x \vee y \vee z$

$F = C_1 \wedge \cdots \wedge C_M$

Q: Find $x_1, \ldots, x_N$ s.t. max # of clauses satisfied

<u>Equivalent k-Body Random Spin Model</u>

$\sigma = \{x_1, \dots, x_N\} \in \{0,1\}^N$

$c = x \vee y \vee z$

$$E_c(\sigma) = \bar{x}\,\bar{y}\,\bar{z} = \begin{cases} 0 & \text{if } c(\sigma) = \text{true} \\ 1 & \text{if } c(\sigma) = \text{false} \end{cases}$$

$$H_F(\sigma) = \sum_{c \in F} E_c(\sigma) = \sum_{(x,y,z) \in E^{(3)}} J_{xyz}\, E_{xyz}(\sigma)$$

$J_{xyz} \in \{0,1)$

Note: $|E^{(3)}| = \binom{N}{k} \sim N^k \gg M \Rightarrow$ dilute model

$H_F(\sigma) = 0 \iff F(\sigma) = \text{true}$

$$Z_F(\beta) = \sum_\sigma e^{-\beta H_F(\sigma)}$$

$\beta \to \infty \iff$ Find σ s.t. $H_F(\sigma) = \min$ (max k-SAT)

Max k-SAT = <u>Zero-temp dilute k-body spin glass</u>

c) Infinite Volumes and Gibbs States

i) Thermodynamic Limit and Existence of Free Energy

"Thm:" Suppose $\mathbb{L}$ amenable

Suppose Λ is a van Hove sequence : $\frac{|\partial\Lambda|}{|\Lambda|} \to 0$

Then for many models*

$$\lim_{\Lambda \to \mathbb{L}} \frac{1}{|\Lambda|} f_\Lambda = f \text{ exists}$$

Note: For random models, f is a.s. independent of $\{J_{xy}\}$ and $\{h\}$.

"f is self-averaging"

* models s.t.

$$|H_{\Lambda_1 \cup \Lambda_2} - H_{\Lambda_1} - H_{\Lambda_2}| \le c_1 |\delta(\Lambda_1, \Lambda_2)|$$

$$|H_\Lambda| \le c_2 |\Lambda|$$

2) Gibbs States

a) Boundary Conditions and Finite-Volume Measures

$$H_\Lambda = H_\Lambda(\sigma_\Lambda \mid \sigma_{\Lambda^c})$$

$$= H_\Lambda(\sigma_\Lambda) + \sum_{\substack{(x,y):\\ x\in\Lambda\\ y\in\Lambda^c}} H_{xy}(\sigma_x, \sigma_y)$$

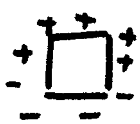
Common b.c.:

free

periodic

$+, -$ Ising

$1, \dots, q$ Potts


Dobrushin (Ising)

$\Longrightarrow$ Finite-volume states:

e.g. $\langle \quad \rangle_{\Lambda,\text{free}}$

$\langle \quad \rangle_{\Lambda,+}$

$\langle \quad \rangle_{\Lambda,-}$

$$\mu_{\Lambda,\sigma_{\Lambda^c}}(\cdot) = \frac{1}{Z_{\Lambda,\sigma_{\Lambda^c}}} \mathbb{1}_{\sigma_{\Lambda^c}} e^{-\beta H_\Lambda(\cdot \mid \sigma_{\Lambda^c})}$$

b) Infinite-Volume States (Gibbs States)

Def 1 (Weak Compactness) – too abstr. for application

$\mu \in \mathcal{G}$ if $\exists$ seq. Λ_n, $\sigma_{\Lambda_n^c}$ s.t.

$$\mu = \lim_{n\to\infty} \mu_{\Lambda_n, \sigma_{\Lambda_n^c}}$$

Def 2 (DLR)

$\mu \in \mathcal{G}$ if

$$\mu(\cdot \mid \sigma_{\Lambda^c}) = \mu_{\Lambda, \sigma_{\Lambda^c}}(\cdot)$$

(i.e. The system should be in macroscopic equilibrium, i.e all parts of the system are in equil. wrt their exteriors)

Def 3 (Integrated DLR)

$\mu \in \mathcal{G}$ if $\forall$ local $A \in \mathcal{F}$

$$\mu(A) = \int d\mu(\sigma)\, \mu_{\Lambda, \sigma_{\Lambda^c}}(A)$$

Under certain circumstances (quasi-locality, etc.), these three def's are equivalent.

D) Phase Transition

1. Def. (Infinite system)

A phase transition is a point of non-analyticity of $f(\beta, h)$.

"$\Longleftrightarrow$" qualitative change in the space of Gibbs states

2. Order of Phase Transition

a) Continuity

A phase transition is second-order if all of the "rel. quantities" (relevant der's of f) are continuous.

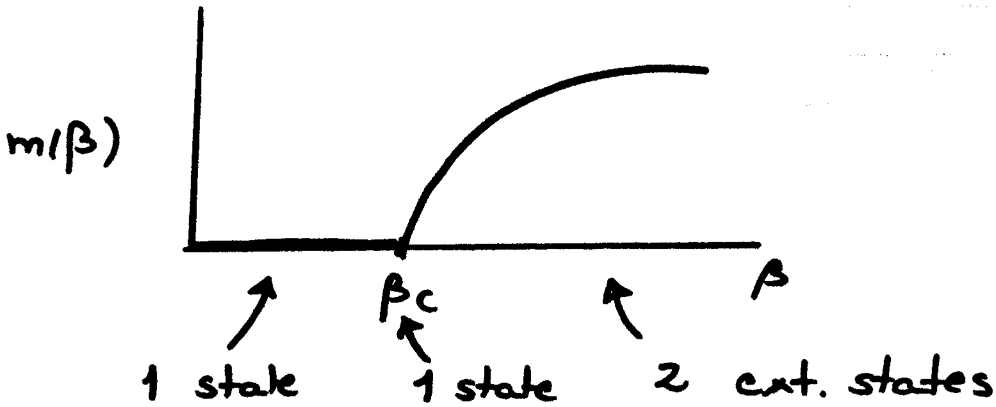
It is first-order if some of the relevant quantitie are discontinuous.

b) Gibbs States

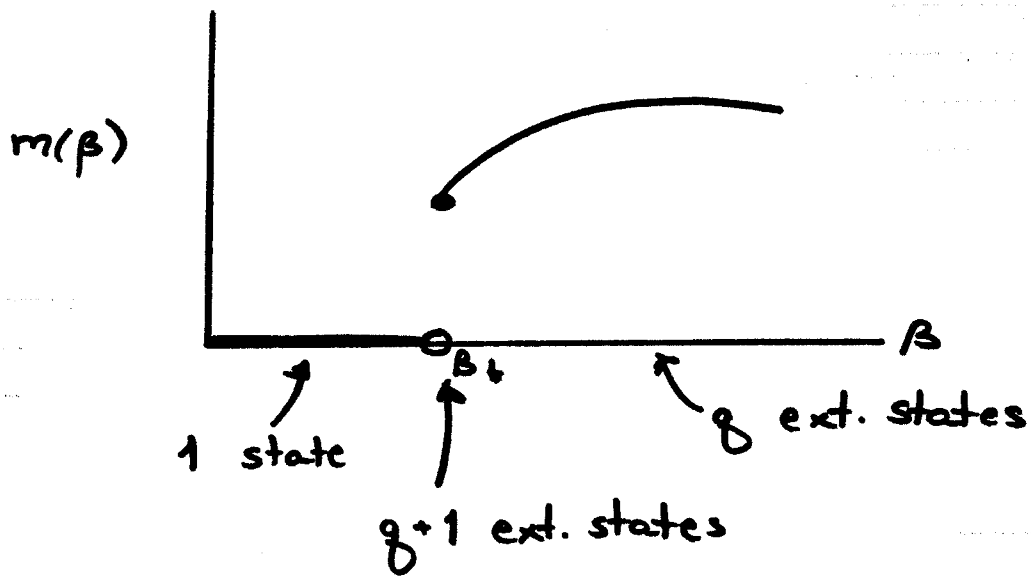
At a second-order transition, there is only one Gibbs state.

At a first-order transition, there is more than one Gibbs state. (If there are N ordered extremal states and 1 disordered stat, there are N+1 extremal Gibbs states at the transition

Ising (h=0)



Potts (h=0)



3) Universality & Critical Exponents for 2^{nd}-Order Transitions

a) Critical Exponents

The way the relevant quantities tend to 0 or ∞ as $T \to T_c$, or the way the quantities behave at T_c is given by critical exponents

e.g.

$$u(T) \sim |T - T_c|^{1-\alpha} \qquad T \to T_c$$

$$m(T) \sim |T - T_c|^{\beta} \qquad T \to T_c$$

$$\chi(T) \sim |T - T_c|^{-\gamma} \qquad T \to T_c$$

$$\langle \sigma_0 \sigma_x \rangle \sim \frac{1}{|x|^{d-2+\eta}} \qquad T = T_c$$

(d = spatial dim e.g. on $\mathbb{Z}^d$)

b) "Universality"

Exponents depend only on the "symmetry" of the model and the spatial dimension.

c) Upper critical dimension

Above a certain dimension, the exponents stop changing with dimension and assume the values they have "in mean field." — Christian's lecture

Almost all of this is at the level of folklore.

PART II -

A) The Mean-Field Approx. for the Ising-Model

$G = (\Lambda, E)$ regular, degree D

Consider σ_x and the measure

$$\mu(\sigma_x \mid \sigma_{\Lambda \setminus \{x\}}) = \frac{1}{Z_x} e^{-\beta H(\sigma_x \mid \sigma_{\Lambda \setminus \{x\}})}$$

$$H(\sigma_x \mid \sigma_{\Lambda\setminus\{x\}}) = -\sum_{y : \langle xy \rangle \in E} \sigma_x \sigma_y - h\sigma_x$$

$$= -\sigma_x \Big(h + \sum_y \sigma_y\Big)$$

M.F. Approx.

$$\approx -\sigma_x \big(h + D \langle \sigma_y \rangle\big)$$

$$= -\sigma_x (h + DM)$$

$\Longrightarrow$

$$\mu(\sigma_x \mid \dots) \approx \frac{e^{\beta(h+DM)\sigma_x}}{2\,\mathrm{ch}\,\beta(h+DM)}$$

$\Rightarrow$

$$\boxed{\mu \approx \mu_{MF} = \prod_x \frac{e^{\beta(h+DM)\sigma_x}}{2\,\mathrm{ch}\,\beta(h+DM)}} \qquad (1)$$

Selfconsistency:

$$\langle \sigma_x \rangle_{MF} = M$$

<u>Mean Field Equation</u>

$$\boxed{M = \mathrm{th}\,\beta(h+DM)}$$

<u>Q.</u>: What happens if this has several solutions?

Variational Approach

$$Z \quad \sum_{\sigma_\Lambda} e^{\beta H(\sigma_\Lambda)}$$

$$\log Z \quad \mathrm{m\ n}_{\rho} \left[\beta \langle H \rangle_\rho \quad S(\rho) \right]$$

<u>MF-Appr</u> Cons der onl, ρ of the form (

$$\Rightarrow \quad \log Z - \beta |\Lambda| \inf_{M} V_{eff}(M)$$

Mean Field Eff Potent al

$$\boxed{V_{eff}(M) = dM^2 - \frac{1}{\beta} \log 2\, \mathrm{ch}\, \beta(h + DM)}$$

2)

$$\frac{dV_{eff}}{dM} = 0 \Rightarrow$$

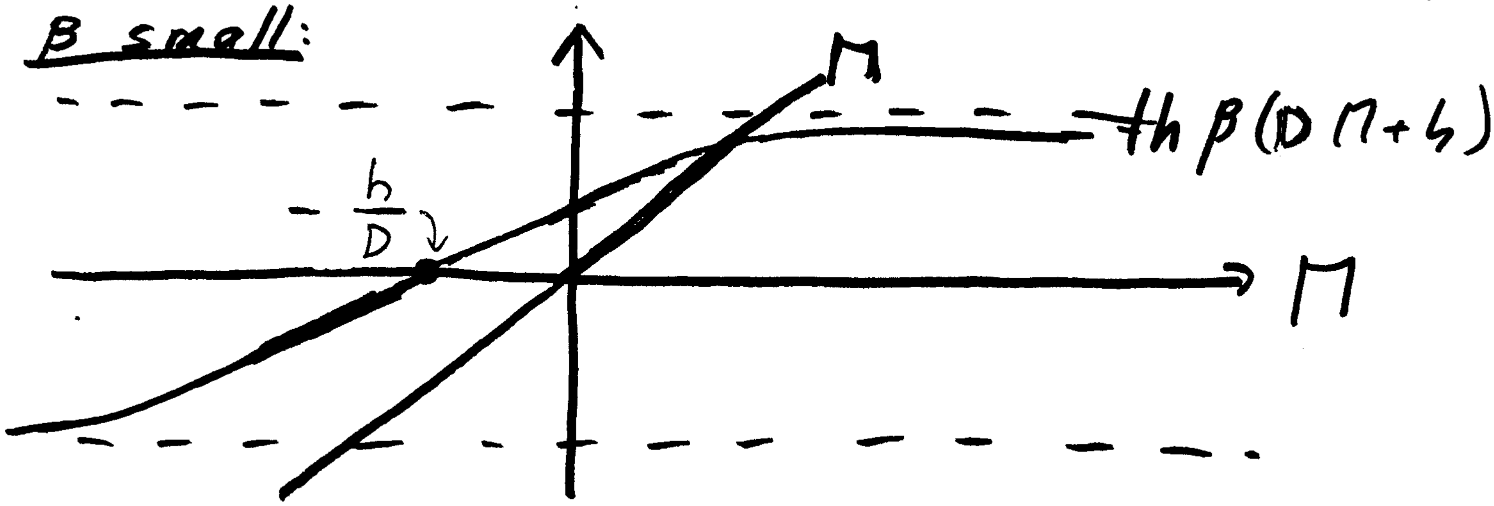
<u>Saddle-Point Equation</u>

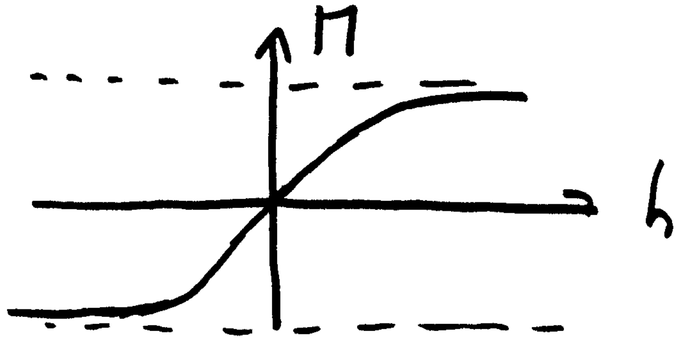
$$\boxed{M = \cancel{th}\ \beta(h + DM)} \qquad (3)$$

If (3) has several solutions, choose that one which minimizes V_{eff}. For $h>0$, this turns out to be the largest solution of (3).

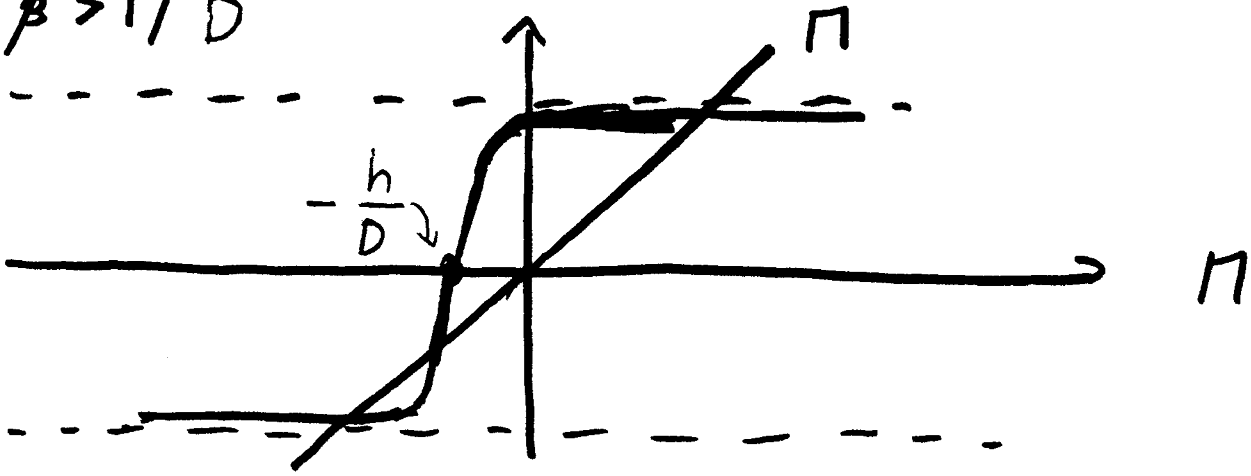
Solutions of the MF-Equations

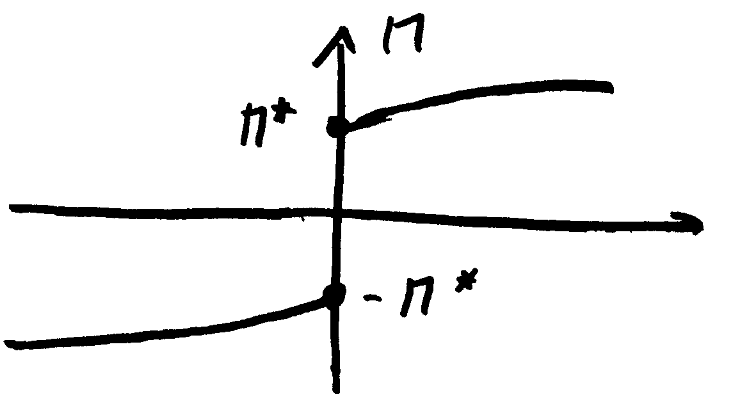
β small:

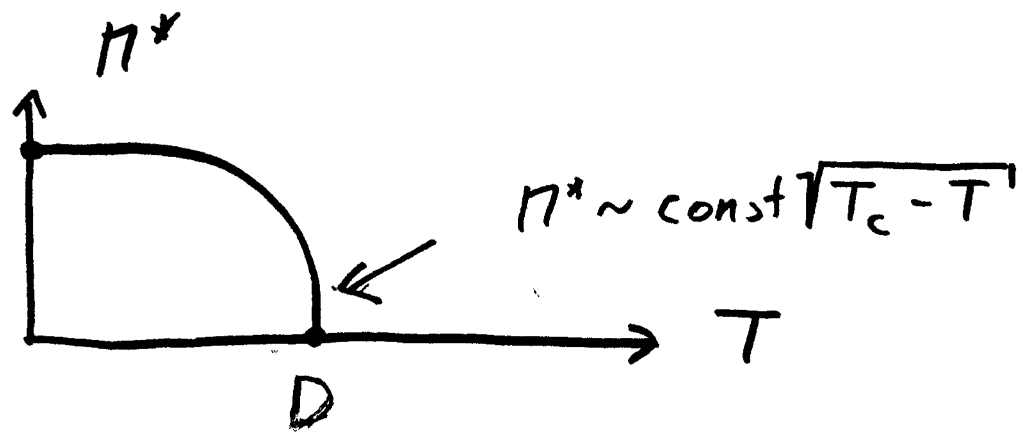




$\beta > 1/D$







Critical Exponents

$\alpha = 0$

$\beta = 1/2$

$\gamma = 1$

B) The Potts Model on the Complete Graph

We want to calculate the large n asymptotics of

$$Z_n = \sum_{\sigma \in \{1,\cdots,q\}^n} e^{-\beta H(\sigma)}$$

$$H(\sigma) = -\frac{1}{2n} \sum_{i,j=1}^{n} \delta(\sigma_i, \sigma_j)$$

Step 1:

$$-H(\sigma) = \frac{1}{2n} \sum_{m=1}^{q} \sum_{i,j} \delta(\sigma_i, m)\, \delta(\sigma_j, m)$$

$$= \frac{1}{2n} \sum_{m=1}^{q} \Big[\sum_{i} \delta(\sigma_i, m) \Big]^2$$

step 2:

$$e^{x^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{x\phi} e^{-\frac{\phi^2}{2}} \, d\phi$$

Step 3:

$$\sum_{\sigma} e^{\sum_{m=1}^{q} \alpha_m \sum_{i=1}^{n} \delta(\sigma_i, m)}$$

$$= \prod_{i=1}^{n} \sum_{\sigma_i} e^{\sum_m \alpha_m \delta(\sigma_i, m)}$$

$$= \left(\sum_{m=1}^{q} e^{\alpha_m} \right)^n$$

This gives

$$\boxed{Z_n = \left(\frac{\beta n}{2\pi} \right)^{q/2} \int d\vec{\phi}\, e^{-n\beta V_{eff}(\vec{\phi})}} \quad (4)$$

$$\vec{\phi} = (\phi_1, \cdots, \phi_q)$$

$$\boxed{V_{eff}(\vec{\phi}) = \frac{1}{2} \vec{\phi}^{\,2} - \frac{1}{\beta} \log \sum_{m=1}^{q} e^{\beta \phi_m}} \quad (5)$$

$\Rightarrow$

$$\boxed{-\frac{1}{n} \log Z_n \longrightarrow \beta \min_{\vec{\phi}} V_{eff}(\vec{\phi}) = \beta f}$$

Saddle Point Equations

$$\boxed{\phi_m = \frac{e^{\beta \phi_m}}{\sum_{k=1}^{q} e^{\beta \phi_k}}} \qquad (6)$$

Symmetric Ansatz:

$\vec{\phi}$ is symm. under permutations

$\Rightarrow \quad \phi_m = \frac{1}{q}$

Symmetry Breaking

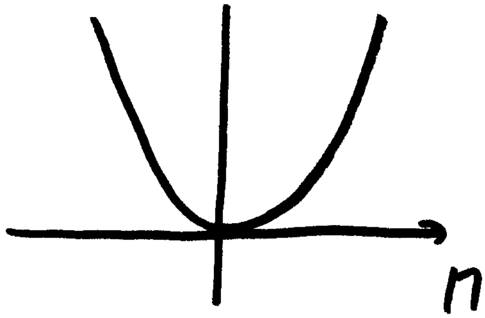
Ansatz

$$\phi_m = \begin{cases} \frac{1}{q}(1-M) & m \neq 1 \\ \frac{1}{q}(1+(q-1)M) & m = 1 \end{cases}$$

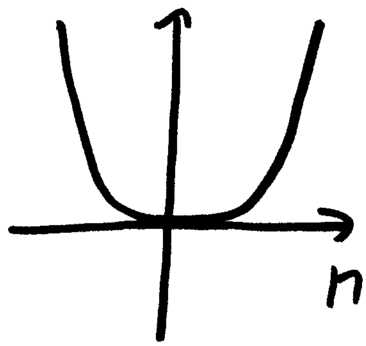
Saddle Point Equation

$$M = \frac{1-e^{-\beta M}}{1+(q-1)e^{-\beta M}}$$

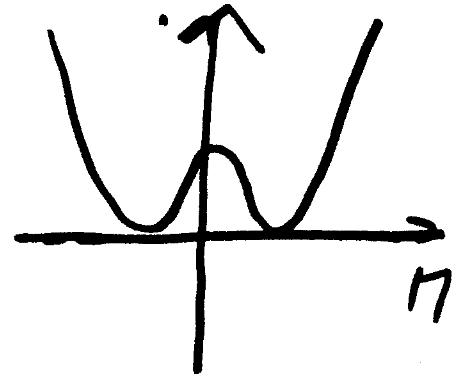
$\boxed{q=2}$



$\beta < q$

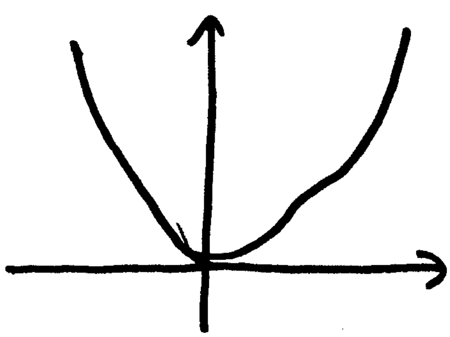


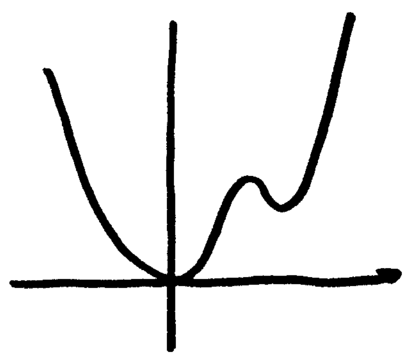
$\beta = q$



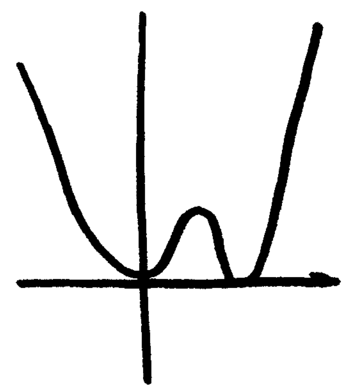
$\beta > q$

$\boxed{q>2}$

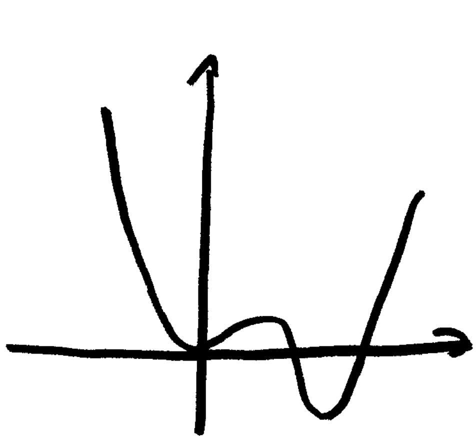


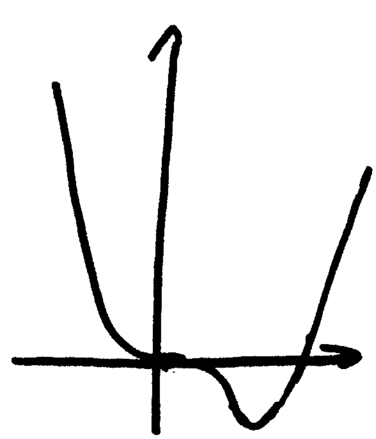


$\beta < \beta_c$



$\beta = \beta_c$





$\beta > \beta_c$

One finds

$$M = 0 \qquad \beta < \beta_0 = 2\,\frac{q-1}{q-2}\log(q-1)$$

$$M \geq M(\beta_0) = \frac{q-2}{q-1} \qquad \beta \geq \beta_0$$