PHY 341/641
Thermodynamics and Statistical Physics

Lecture 20

Methodologies of statistical mechanics. (Chapter 5 in STP)

- Phase transitions in spin systems
- Mean field approximation

9	2/06/2012	Probability distributions	3.4-3.5	HW 9	2/8/2012
10	2/08/2012	Continuous distributions/Central limit theorem	3.6-3.10	HW 10	2/10/2012
11	2/10/2012	Introduction to statistical mechanics	4.1-4.2	HW 11	2/13/2012
12	2/13/2012	Enumeration of microstates	4.3	HW 12	2/15/2012
13	2/15/2012	Many particle systems	4.4-4.5	HW 13	2/17/2012
14	2/17/2012	Microcanonical ensemble	4.6	HW 14	2/20/2012
15	2/20/2012	Canonical ensemble	4.7-4.8	HW 15	2/22/2012
16	2/22/2012	Grand canonical ensemble	4.9-4.12	HW 16	2/24/2012
17	2/24/2012	Introduction to magnetic systems	5.1-5.5		
	2/27/2012	APS -- no class; take-home exam			
	2/29/2012	APS -- no class; take-home exam			
	3/02/2012	APS -- no class; take-home exam			
18	3/05/2012	Exam due -- Ising model	5.5	HW 17	03/07/2012
19	3/07/2012	Ising model	5.6-5.7	HW 18	03/09/2012
20	3/09/2012	Phase transformation	5.8-5.10		
	3/12/2012	*Spring Break*			
	3/14/2012	*Spring Break*			
	3/16/2012	*Spring Break*			
21	3/19/2012	Many particle systems	6.1-6.2		

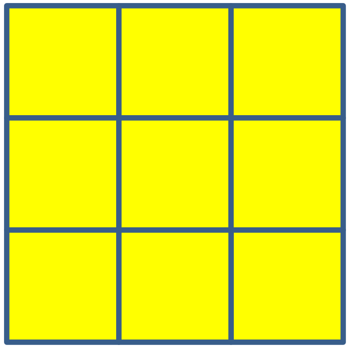
Ising model in various lattices – mean field solutions

Microstates :

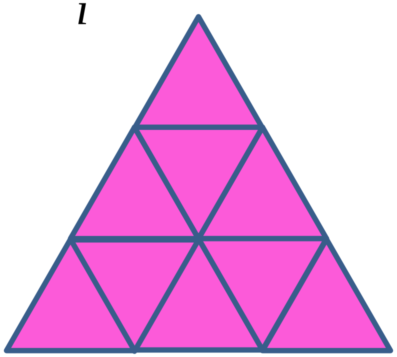
$$E_s = -J \sum_{i,j(nn)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i$$

Mean fields approximation :

$$E_s^{MF} = -J \sum_{i}^{N} s_i \, q \langle s_j \rangle - H \sum_{i=1}^{N} s_i$$



q=4/2



q=6/2

$$\langle H_{eff} \rangle = Jq \langle s_j \rangle + H \equiv Jqm + H$$

Note: textbooks differ with counting neighbors q without double counting. Here q implies “unique” neighbors.

Self-consistency condition for mean field treatment

$$\left\langle H_{eff} \right\rangle = Jq\left\langle s_j \right\rangle + H \equiv Jqm + H$$

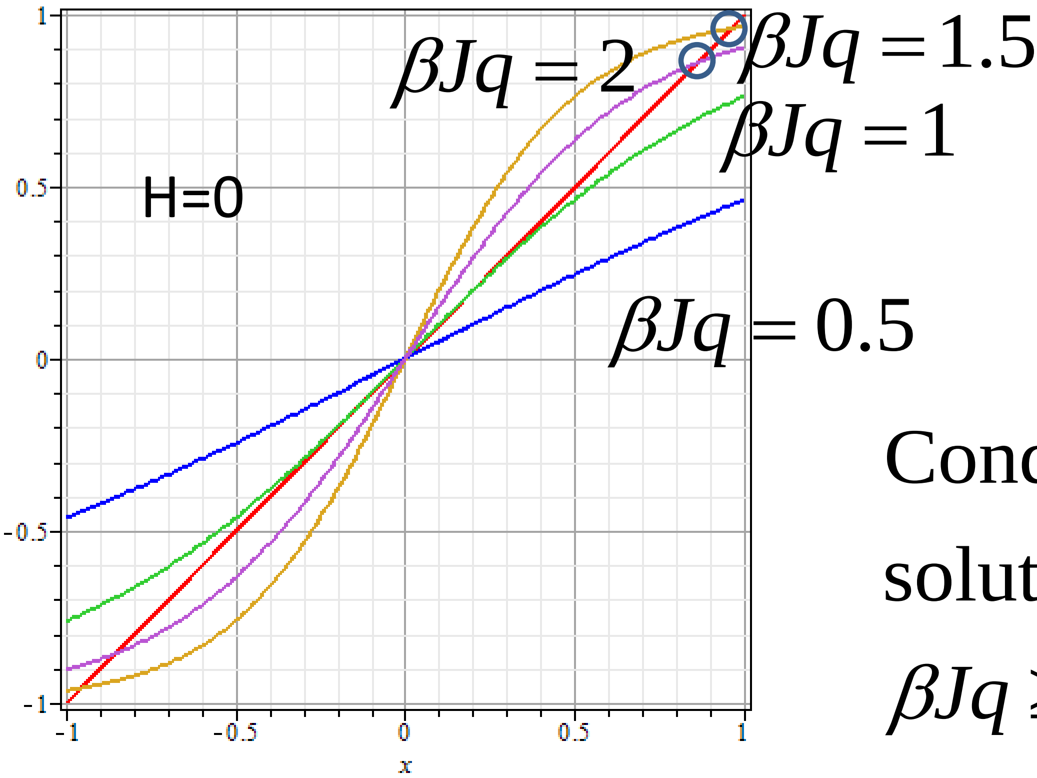
$$Z_1 = \sum_{s_1=\pm 1} e^{-\beta\left\langle H_{eff} \right\rangle s_1} = 2\cosh\left(\beta\left(Jqm + H\right)\right)$$

$$\frac{F}{N} = -kT \ln Z_1$$

$$m = -\frac{1}{N}\frac{\partial F}{\partial H} = \tanh\left(\beta\left(Jqm + H\right)\right)$$

Mean field self-consistency condition:

$$m = \tanh(\beta(Jqm + H))$$



Condition for non-trivial solution for m at $H = 0$:

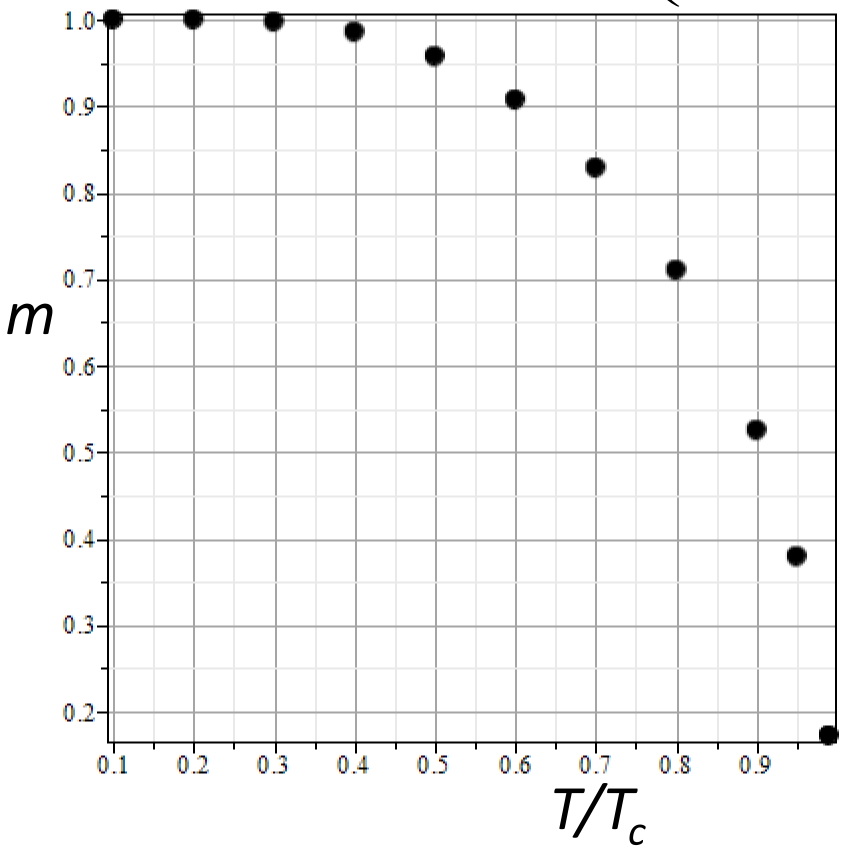
$\beta Jq \geq 1$

➔Mean field solutions exhibit "critical behavior" (phase transition) at $\beta_c Jq=1$.

Mean field self-consistency condition for H=0: $m = \tanh(\beta(Jqm))$

$$\text{Define}: \quad \beta_c Jq = 1$$

$$m = \tanh(\beta(Jqm)) = \tanh\left(\frac{\beta}{\beta_c} m\right) = \tanh\left(\frac{T_c}{T} m\right)$$



Summary of results for mean field treatment of Ising model

$$Z_N = \left[2\cosh\left(\beta\left(Jqm + H\right)\right)\right]^N$$

$$F = -kTN \ln\left[2\cosh\left(\beta\left(Jqm + H\right)\right)\right]$$

$$\text{where:} \qquad m = \tanh\left(\beta\left(Jqm + H\right)\right)$$

Internal energy:

$$E = -\frac{\partial \ln Z_N}{\partial \beta}$$

$$= -N\left(Jqm + H\right)\left[\tanh\left(\beta\left(Jqm + H\right)\right)\right]$$

$$= -N\left(Jqm + H\right)m$$

Summary of results for mean field treatment of Ising model (continued)

Internal energy for $H = 0$:

$$E = -NJqm^2$$

where $m = \tanh(\beta(Jqm))$

Heat capacity:

$$C = \left(\frac{\partial E}{\partial T}\right)_N = 2Nk\beta^2 Jqm\left(\frac{\partial m}{\partial \beta}\right)_N$$

$$\left(\frac{\partial m}{\partial \beta}\right)_N = \left(Jqm + \beta Jq\left(\frac{\partial m}{\partial \beta}\right)_N \right)\operatorname{sech}^2(\beta(Jqm))$$

$$\left(\frac{\partial m}{\partial \beta}\right)_N = \frac{Jqm}{\cosh^2(\beta(Jqm)) - \beta Jq}$$

$$C = \frac{2Nk\beta^2 J^2 q^2 m^2}{\cosh^2(\beta(Jqm)) - \beta Jq}$$

Summary of results for mean field treatment of Ising model (continued)

Behavior of heat capacity for $H = 0$

in terms of $T_c = \frac{Jq}{k}$:

$$C = \frac{2Nk\beta^2 J^2 q^2 m^2}{\cosh^2\left(\beta(Jqm)\right) - \beta Jq}$$

$$= \frac{2Nkm^2}{\cosh^2\left(\frac{T_c}{T}m\right) - \left(\frac{T_c}{T}\right)}\left(\frac{T_c}{T}\right)^2$$

Note that: $m = \begin{cases} \tanh\left(\frac{T_c}{T}m\right) & \text{for } T < T_c \\ 0 & \text{for } T > T_c \end{cases}$

Summary of results for mean field treatment of Ising model (continued)

Behavior for T near T_c where m is small

$$m = \begin{cases} \tanh\left(\frac{T_c}{T} m\right) & \text{for } T < T_c \\ 0 & \text{for } T > T_c \end{cases}$$

$$\text{for } T < T_c \text{ and } T \approx T_c :$$

$$m \approx \frac{T_c}{T} m - \frac{1}{3}\left(\frac{T_c}{T} m\right)^3 + \cdots$$

$$m \approx \sqrt{3}\left(\frac{T}{T_c}\right)\left(1 - \frac{T}{T_c}\right)^{1/2}$$

Summary of results for mean field treatment of Ising model (continued) -- behavior for T near T_c where m is small

$$m \approx \sqrt{3}\left(\frac{T}{T_c}\right)\left(1-\frac{T}{T_c}\right)^{1/2}$$

$$C = \frac{2Nkm^2}{\cosh^2\left(\frac{T_c}{T}m\right) - \left(\frac{T_c}{T}\right)}\left(\frac{T_c}{T}\right)^2$$

$$C \equiv 0 \quad \text{for } T > T_c$$

Summary of results for mean field treatment of Ising model (continued) -- behavior for T near T_c where m is small

$$m \approx \sqrt{3}\left(\frac{T}{T_c}\right)\left(1-\frac{T}{T_c}\right)^{1/2}$$

$$C = \frac{2Nkm^2}{\cosh^2\left(\frac{T_c}{T}m\right)-\left(\frac{T_c}{T}\right)}\left(\frac{T_c}{T}\right)^2$$

for $T < T_c$ and $T \approx T_c$:

$$C \approx \frac{2Nk}{1-\left(\frac{T_c}{T}\right)+3\left(1-\frac{T}{T_c}\right)}\left(\frac{T_c}{T}\right)^2 \cdot 3\left(\frac{T}{T_c}\right)^2\left(1-\frac{T}{T_c}\right) \approx \frac{6Nk}{3-\frac{T_c}{T}}$$

$$\approx 3Nk$$

Behavior of magnetic susceptibility (in scaled units):

$$m = \tanh\left(\beta\left(Jqm + H\right)\right)$$

$$\chi(T,H) = \left(\frac{\partial m}{\partial H}\right)_T$$

$$\left(\frac{\partial m}{\partial H}\right)_T = \left(\beta + \beta Jq\left(\frac{\partial m}{\partial H}\right)_T\right)\operatorname{sech}^2\left(\beta\left(Jqm + H\right)\right)$$

$$\chi(T,H) = \left(\frac{\partial m}{\partial H}\right)_T = \frac{\beta}{\cosh^2\left(\beta\left(Jqm + H\right)\right) - \beta Jq}$$

For $H = 0$:

$$\chi(T,0) = \frac{1}{Jq}\frac{\frac{T_c}{T}}{\cosh^2\left(\frac{T_c}{T}m\right) - \frac{T_c}{T}}$$

Behavior of magnetic susceptibility (in scaled units) -- continued:

$$\chi(T,0) = \frac{1}{Jq}\frac{\frac{T_c}{T}}{\cosh^2\left(\frac{T_c}{T}m\right) - \frac{T_c}{T}}$$

For $T > T_c$; $m = 0$

$$\chi(T,0) = \frac{1}{Jq}\frac{\frac{T_c}{T}}{1-\frac{T_c}{T}} = \frac{T_c}{Jq}\frac{1}{T-T_c} \quad \text{Curie-Weiss relation}$$

For $T < T_c$ and $T \approx T_c$; $m \approx \sqrt{3}\left(\frac{T}{T_c}\right)\left(1-\frac{T}{T_c}\right)^{1/2}$

$$\cosh^2\left(\frac{T_c}{T}m\right) \approx 1 + 3\left(1-\frac{T}{T_c}\right)$$

$$\chi(T,0) \approx \frac{1}{Jq}\frac{\frac{T_c}{T}}{\left(1-\frac{T}{T_c}\right)\left(3-\frac{T_c}{T}\right)} \approx \frac{T_c}{2Jq}\frac{1}{T_c-T}$$

Behavior of magnetization at T_c:

$$m = \tanh\left(\beta\left(Jqm + H\right)\right) = \tanh\left(\frac{T_c}{T}m + \frac{H}{kT}\right)$$

At $T = T_c$:

$$m(T_c) = \tanh\left(m(T_c) + \frac{H}{kT_c}\right) \approx m(T_c) + \frac{H}{kT_c} - \frac{1}{3}\left(m(T_c) + \frac{H}{kT_c}\right)^3$$

$$\Rightarrow m(T_c) \approx \left(\frac{3H}{kT_c}\right)^{1/3}$$

Critical exponents:

$$\varepsilon \equiv \left(1-\frac{T}{T_c}\right)$$

		values of the exponents		
Quantity	Critical behavior	$d=2$ (exact)	$d=3$	mean-field theory
specific heat	$C \sim \epsilon^{-\alpha}$	0 (logarithmic)	0.113	0 (jump)
order parameter	$m \sim \epsilon^{\beta}$	1/8	0.324	1/2
susceptibility	$\chi \sim \epsilon^{-\gamma}$	7/4	1.238	1
equation of state ($\epsilon = 0$)	$m \sim H^{1/\delta}$	15	4.82	3
correlation length	$\xi \sim \epsilon^{-\nu}$	1	0.629	1/2
correlation function $\epsilon = 0$	$G(r) \sim 1/r^{d-2+\eta}$	1/4	0.031	0

Table 5.1: Values of the critical exponents for the Ising model in two and three dimensions. The values of the critical exponents of the Ising model are known exactly in two dimensions and are ratios of integers. The results in three dimensions are not ratios of integers and are approximate. The exponents predicted by mean-field theory are discussed in Sections 5.7, and 9.1, pages 256 and 434.