PHY 341/641
Thermodynamics and Statistical Physics

Lecture 19

Methodologies of statistical mechanics. (Chapter 5 in STP)

Ising model systems

a. Definition
b. Exact solution for 1-dimension
c. Mean field solution for 1-d
d. Ising model for 2 dimensions

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

Microstates:

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

For one-dimensional system with periodic boundary conditions:

$$E_s = -J \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$$

Exact solution for 1-dimensional Ising system of N spins with periodic boundary conditions ($s_{N+1}=s_1$)

$$Z_N = \mathrm{Tr}\left(\mathbf{T}^N\right) = \lambda_1^N + \lambda_2^N = \lambda_1^N\left(1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right)$$

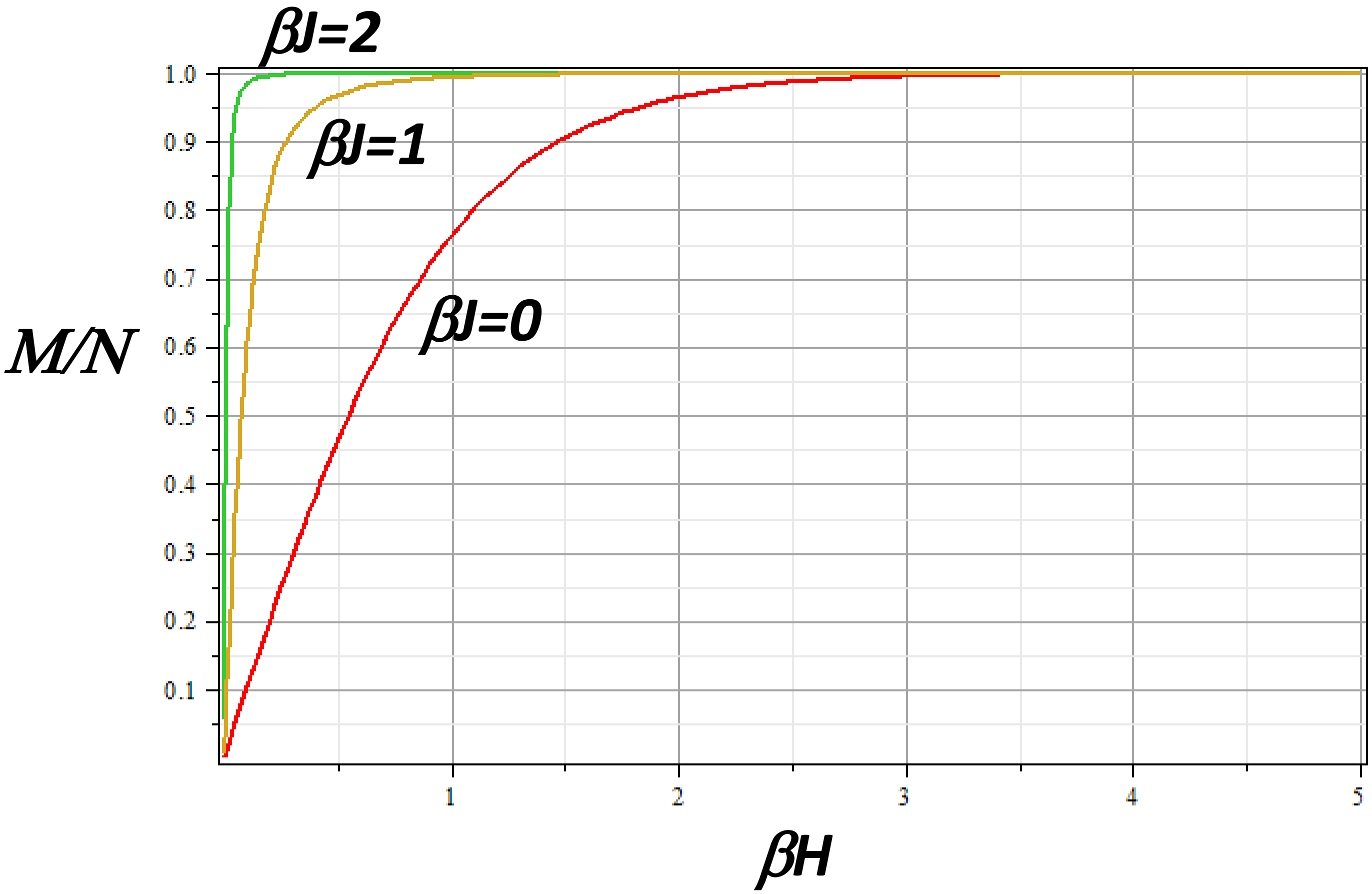
$$F(T,J,H) = -kT\ln Z_N = -NkT\ln\lambda_1 - kT\ln\left[1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right]$$

$$\approx -NkT\ln\lambda_1$$

$$= -NJ - kT\ln\left[\cosh\left(\beta H\right) + \left[\sinh^2\left(\beta H\right) + e^{-4\beta J}\right]^{1/2}\right]$$

$$M(T,J,H) = -\frac{\partial F}{\partial H} = \frac{N\sinh\left(\beta H\right)}{\left[\sinh^2\left(\beta H\right) + e^{-4\beta J}\right]^{1/2}}$$

$$M(T,J,H)=\frac{N\sinh(\beta H)}{\left[\sinh^2(\beta H)+e^{-4\beta J}\right]^{1/2}}$$



Mean field approximation for 1-dimensional Ising model

Exact macrostate energy:

$$E_s = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$$

Mean field macrostate energy:

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

$$= -\left(J\langle s_i \rangle + H\right)\sum_{i=1}^{N} s_i$$

$$\equiv -H_{eff}\sum_{i=1}^{N} s_i$$

Mean field partition function and Free energy:

$$F^{MF} = -kT \ln\left(Z_1^{MF}\right)^N = -NkT \ln Z_1^{MF} = -NkT \ln\left(2\cosh(\beta H_{eff})\right)$$

$$H_{eff} = J\left\langle s_i \right\rangle + H$$

Consistency condition :

$$\left\langle s_i \right\rangle = \frac{1}{Z_1}\sum_{s_i} s_i e^{-\beta H_{eff} s_i} = \tanh\left[\beta\left(J\left\langle s_i \right\rangle + H\right)\right]$$

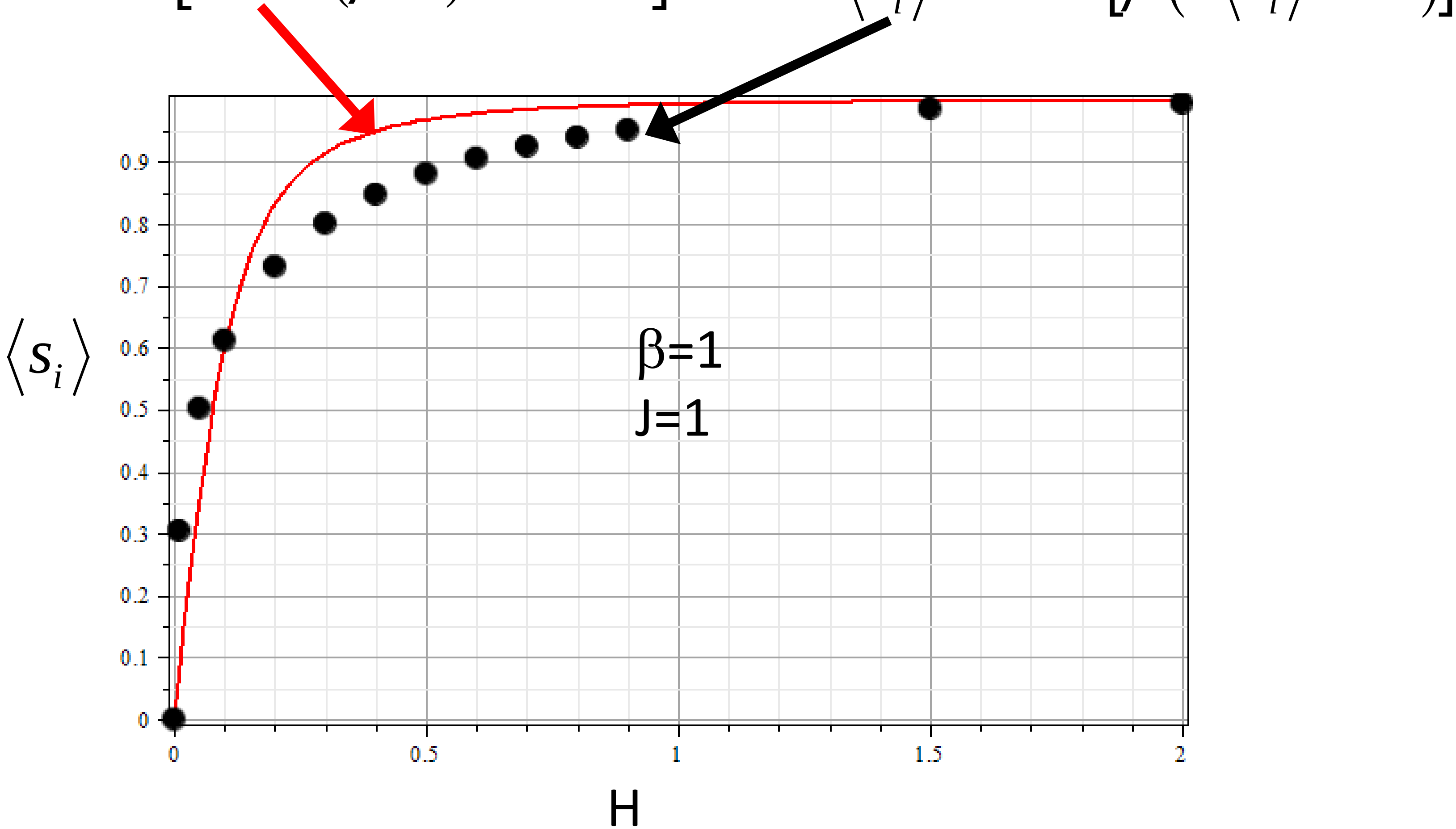
One dimensional Ising model with periodic boundary conditions:

Exact solution:

$$\langle s_i \rangle \equiv \frac{M}{N} = \frac{\sinh(\beta H)}{\left[\sinh^2(\beta H) + e^{-4\beta J}\right]^{1/2}}$$

Mean field solution:

$$\langle s_i \rangle = \tanh\left[\beta\left(J\langle s_i \rangle + H\right)\right]$$



Two-dimensional Ising model – paramagnetic ←→ ferromagnetic phase transition

Onsager's solution for square lattice for $H = 0$:

$$\frac{E}{NJ} = -2\tanh(2\beta J) - \frac{\sinh^2(2\beta J) - 1}{\sinh(2\beta J)\cosh(2\beta J)}\left[\frac{2}{\pi}K_1(\kappa) - 1\right]$$

$$\kappa \equiv 2\frac{\sinh(2\beta J)}{\cosh^2(2\beta J)}$$

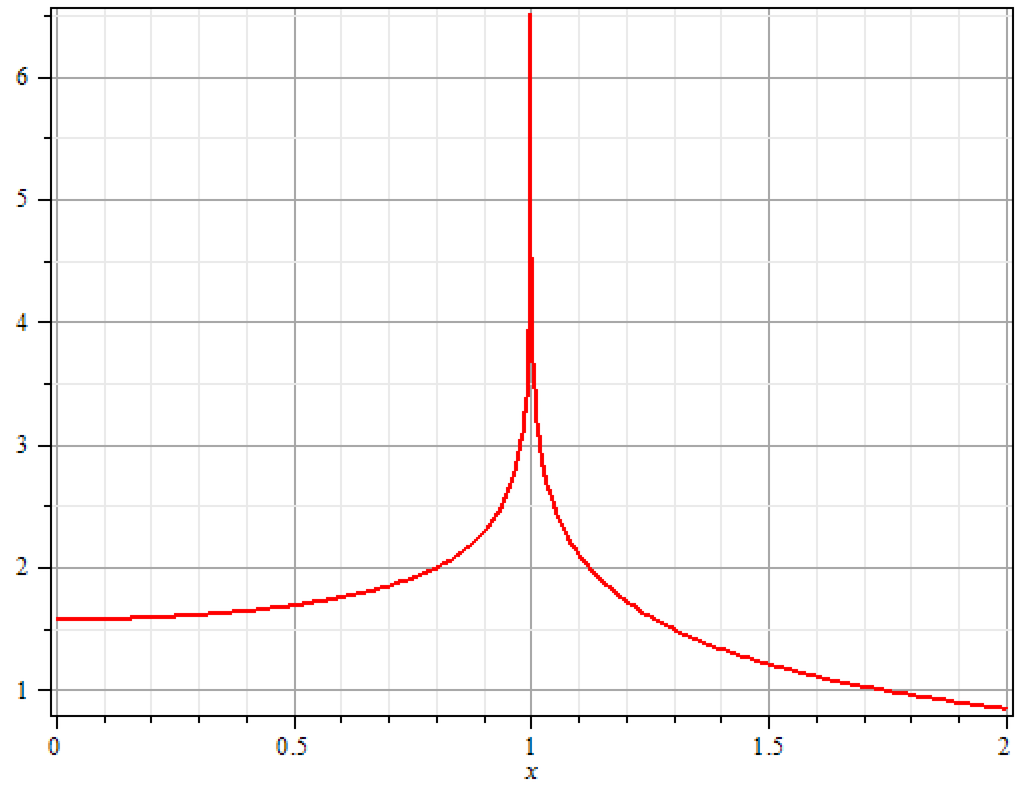
Elliptic integrals:

$$K_1(\kappa) \equiv \int_0^{\pi/2} \frac{d\phi}{\sqrt{1-\kappa^2\sin^2\phi}}$$

$$E_1(\kappa) \equiv \int_0^{\pi/2} d\phi\sqrt{1-\kappa^2\sin^2\phi}$$

Behavior of Elliptic integral function $K_1(x)$

$Re[K_1(x)]$



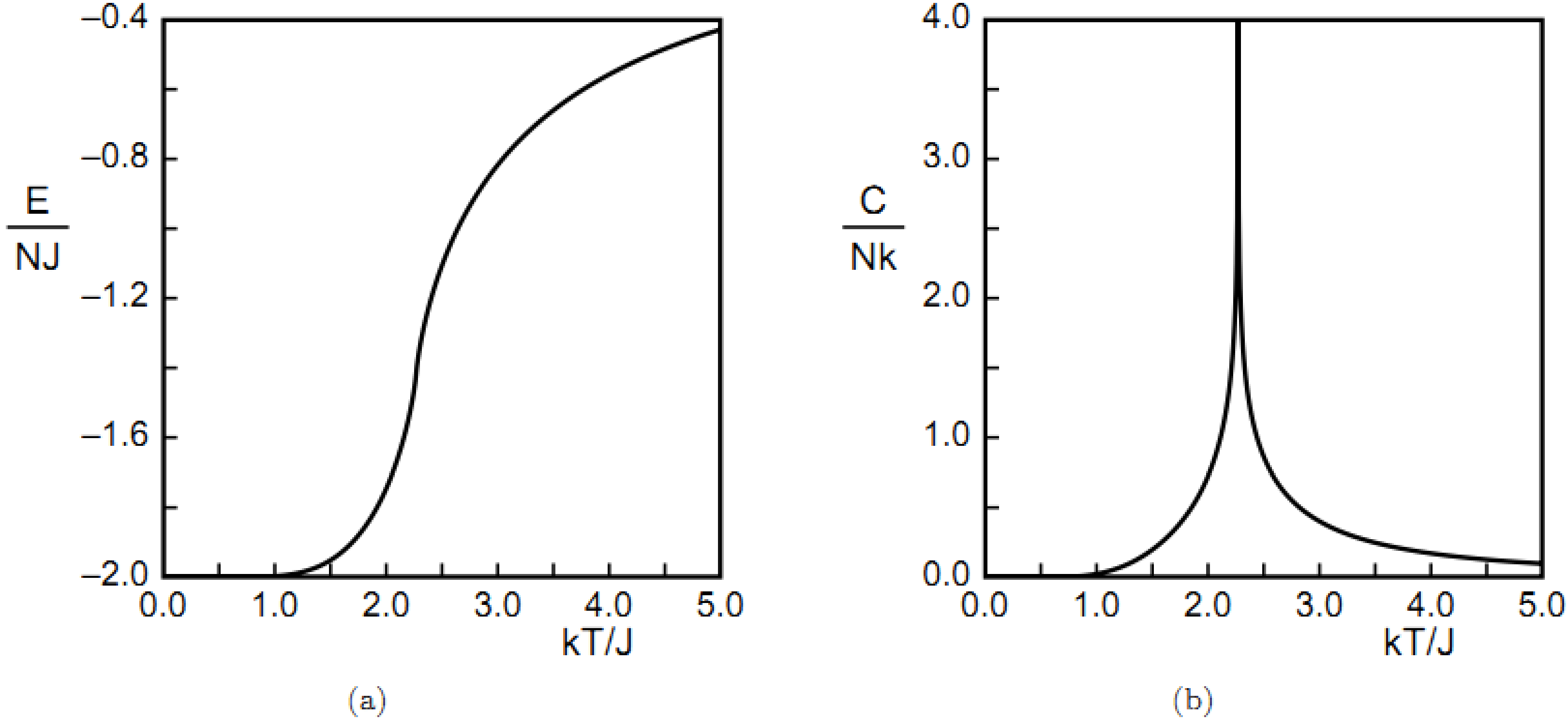


Figure 5.9: (a) Temperature dependence of the energy of the Ising model on the square lattice according to (5.88). Note that $E(T)$ is a continuous function of kT/J. (b) Temperature dependence of the specific heat of the Ising model on the square lattice according to (5.90). Note the divergence of the specific heat at the critical temperature.

Critical temperature:

$$\frac{kT_c}{J} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.269 \qquad \text{Note}: \sinh\left(2\beta_c J\right) = 1 \text{ and } \kappa_c = 1$$

Magnetic properties of 2-dimensional Ising model

Solution by C. N. Yang :

$$\frac{M}{N} = -\frac{1}{N}\left(\frac{\partial F}{\partial H}\right)_{T,H\to 0} \equiv m(T) = \begin{cases} \left(1 - 1/\sinh^4(2\beta J)\right)^{1/8} & T < T_c \\ 0 & T > T_c \end{cases}$$

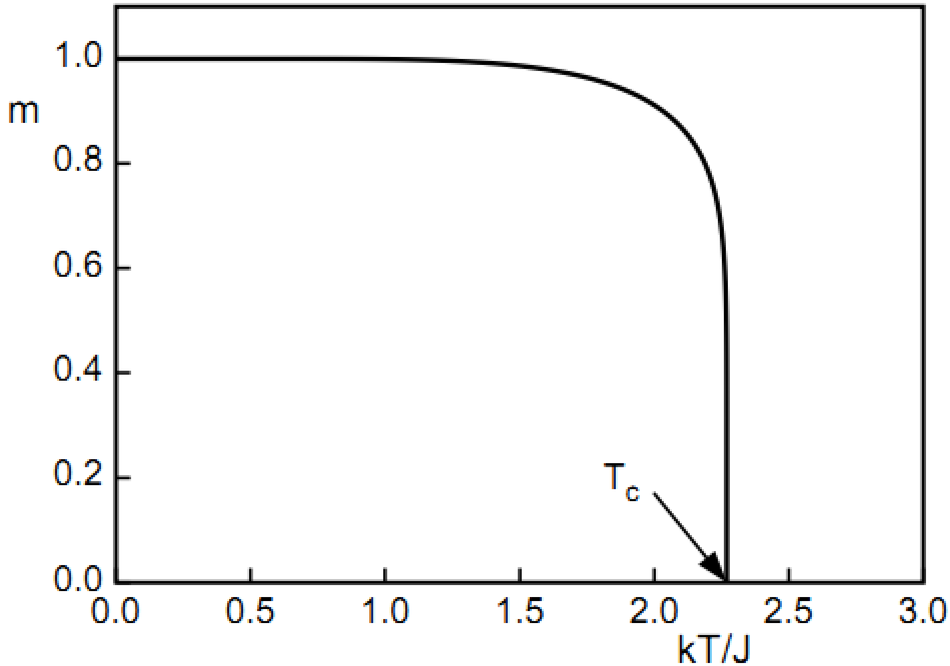
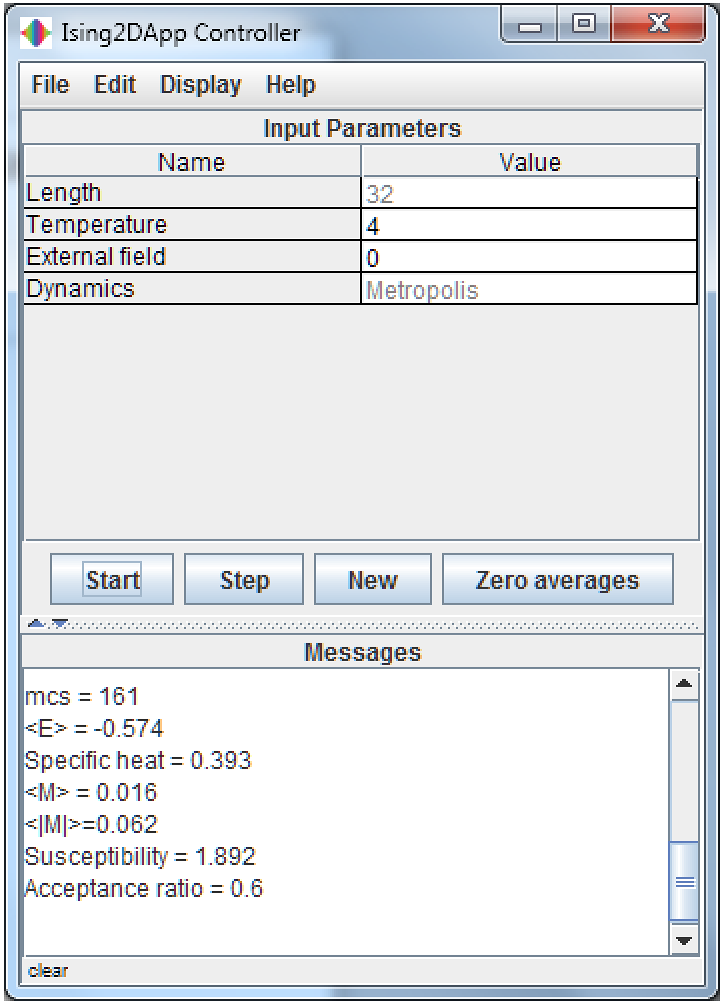
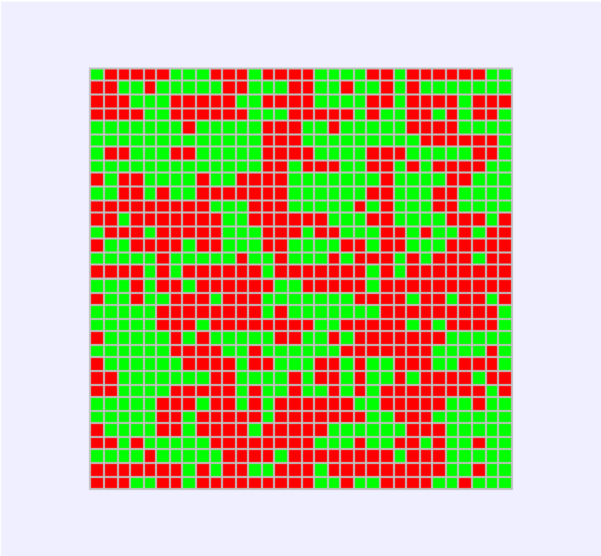


Figure 5.10: The temperature dependence of the spontaneous magnetization $m(T)$ of the two-dimensional Ising model.

Simulation of 2-dimensional Ising model with Monte Carlo sampling

[stp_Ising2D.jar]

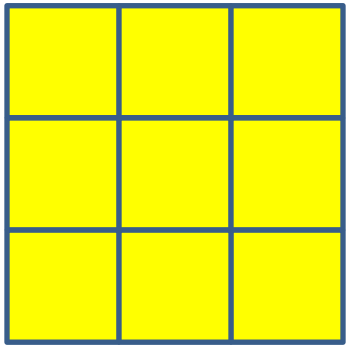




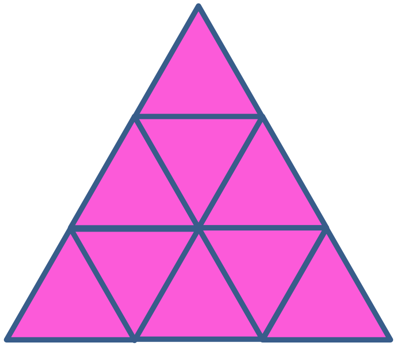
Ising model in various lattices – mean field solutions

$$\text{Microstates :}$$

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



q=4



q=6

$$H_{eff} \equiv J \sum_{j=1}^{q} s_j + H$$

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

Self-consistency condition for mean field treatment

$$H_{eff} \equiv J\sum_{j=1}^{q} s_j + H$$

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

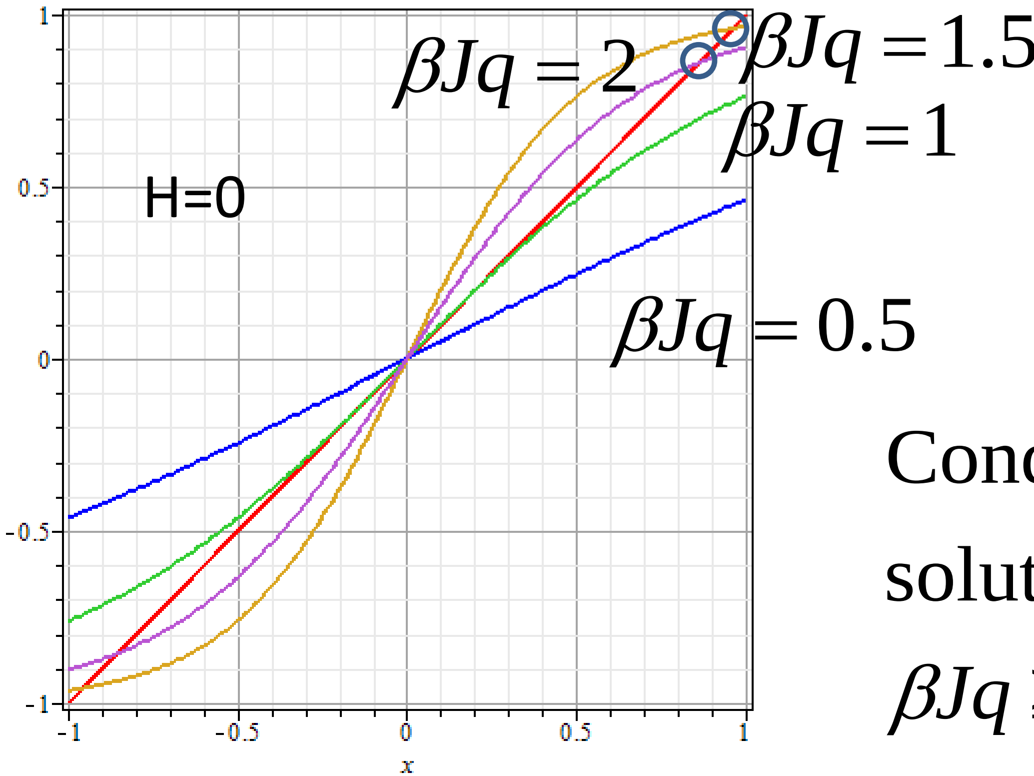
$$Z_1 = \sum_{s_1=\pm 1} e^{\beta\left\langle H_{eff} \right\rangle s_1} = 2\cosh\left(\beta\left(Jqm + H\right)\right)$$

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

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

Mean field self-consistency condition:

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



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

$$\beta Jq \geq 1$$

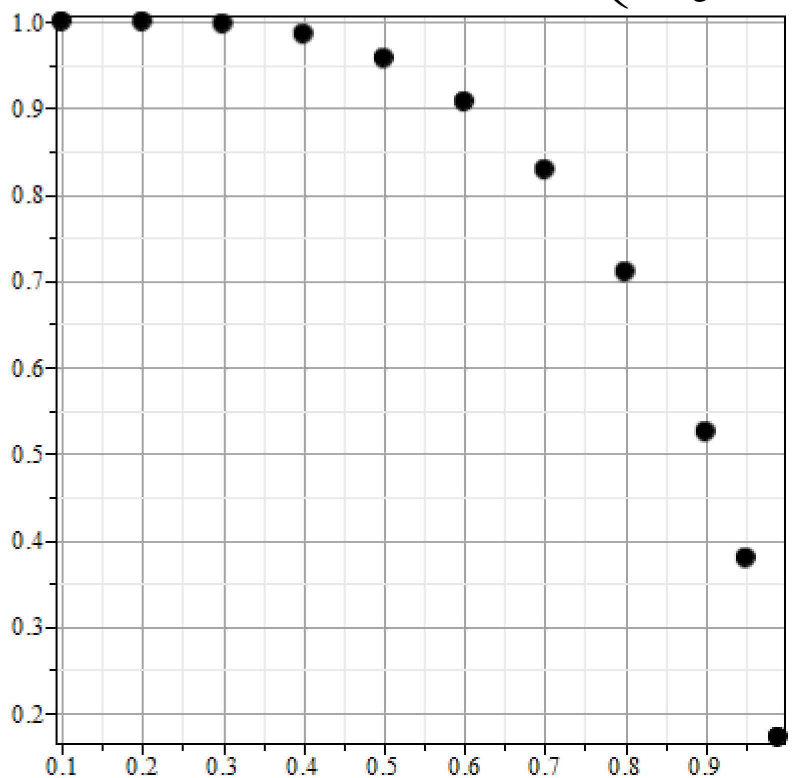
➔Mean field solutions exhibit "critical behavior" (phase transition) at $\beta_c Jq=1$.

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

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

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

m



T/T_c