PHY 341/641
Thermodynamics and Statistical Physics

Lecture 18

Methodologies of statistical mechanics. (Chapter 5 in STP)

Ising model systems

a. Definition
b. Exact solution for 1-dimension
c. Mean field solution

5	1/27/2012	Entropy	2.15-2.19	HW 5	1/30/2012
6	1/30/2012	Thermodynamic Potentials	2.20-2.21	HW 6	2/1/2012
7	2/01/2012	Thermodynamic Potentials	2.22-2.24	HW 7	2/3/2012
8	2/03/2012	Introduction to probability theory	3.1-3.3	HW 8	2/6/2012
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	03/05/2012
	3/07/2012				
	3/09/2012				
	3/12/2012	*Spring Break*			
	3/14/2012	*Spring Break*			
	3/16/2012	*Spring Break*			

Statistical mechanics of spin ½ systems

Microstates:

$$\varepsilon_i = -\mu s_i B \quad \text{where } s_i = \pm 1,\ \mu B \equiv \text{ spin alignment energy}$$

$$\mu \equiv \tfrac{1}{2} g \mu_B = -9.28 \times 10^{-24}\, J/T \quad \text{(for an electron)}$$

Partition function for N non-interacting spins:

$$Z_N = \sum_s e^{\beta E_s} = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{s_3=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta \mu B \left(\sum_{i=1}^{N} s_i \right)}$$

$$= \left(\sum_{s_1=\pm 1} e^{\beta \mu B s_1} \right)^N = \left(Z_1 \right)^N$$

Calculation of Z_1

$$Z_1 = \sum_{s_1=\pm 1} e^{\beta\mu B s_1} = e^{-\beta\mu B} + e^{\beta\mu B} = 2\cosh(\beta\mu B)$$

Thermodynamic functions:

$$F = -kT\ln\left(Z_1\right)^N = -NkT\ln Z_1 = -NkT\ln\left(2\cosh(\beta\mu B)\right)$$

$$\left\langle E\right\rangle = -N\frac{\partial \ln Z_1}{\partial\beta} = -N\mu B\tanh\left(\beta\mu B\right)$$

$$C = \left(\frac{\partial\left\langle E\right\rangle}{\partial T}\right)_B = kN\left(\beta\mu B\right)^2\operatorname{sech}^2\left(\beta\mu B\right)$$

Independent particle system

Microstates :

$$E_s = -\sum_{i=1}^{N} \mu s_i B \equiv -H \sum_{i=1}^{N} s_i$$

Interacting particle system – Ising model

Microstates :

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

Ising model for H = 0 and N=2

Microstates :

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

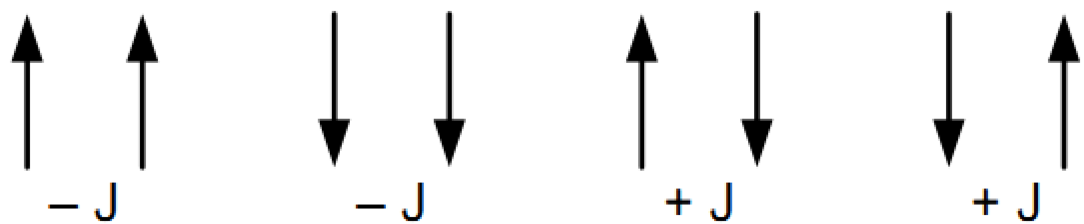


Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

$$Z_2 = e^{\beta J} + e^{\beta J} + e^{-\beta J} + e^{-\beta J} = 4\cosh(\beta J)$$

$$\langle E \rangle = -\frac{\partial \ln Z_2}{\partial \beta} = -J \tanh(\beta J)$$

Ising model for H ≠ 0 and N=2

Microstates:

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

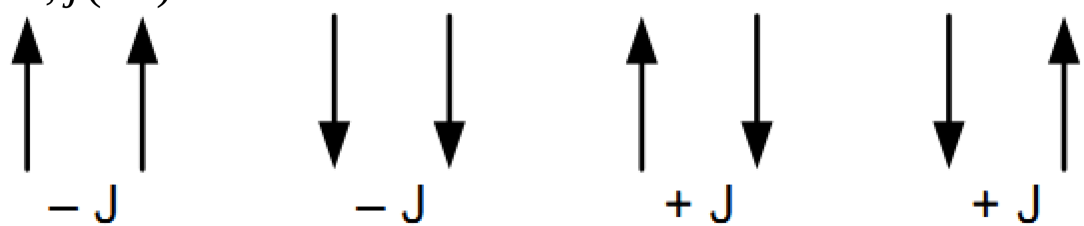


Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

$$Z_2(J,H) = e^{\beta(J+2H)} + e^{\beta(J-2H)} + e^{-\beta J} + e^{-\beta J}$$

$$= 2e^{\beta J}\cosh(2\beta H) + 2e^{-\beta J}$$

$$\text{Note}: Z_2(J=0,H) = 2\cosh(2\beta H) + 2 = (2\cosh(\beta H))^2$$

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

$$Z_N = \sum_s \exp\left[\beta J \sum_{i=1}^{N} s_i s_{i+1} + \frac{\beta H}{2}\left(s_i + s_{i+1}\right)\right]$$

$$\equiv \sum_{s_1, s_2, s_3 \cdots s_N} f(s_1, s_2) f(s_2, s_3) \cdots f(s_{N-1}, s_N) f(s_N, s_{N+1})$$

where:

$$f(s,s') = \begin{pmatrix} f(1,1) & f(1,-1) \\ f(-1,1) & f(-1,-1) \end{pmatrix}$$

$$\equiv \begin{pmatrix} e^{(\beta J + \beta H)} & e^{(-\beta J)} \\ e^{(-\beta J)} & e^{(\beta J - \beta H)} \end{pmatrix} \equiv \mathbf{T}$$

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

$$Z_N = \sum_{s_1, s_2, s_3 \cdots s_N} f(s_1, s_2)\, f(s_2, s_3) \cdots f(s_{N-1}, s_N)\, f(s_N, s_{N+1})$$

$$= \sum_{s_1, s_2, s_3 \cdots s_N} T_{s_1 s_2} T_{s_2 s_3} T_{s_3 s_4} T_{s_4 s_5} \cdots T_{s_N s_{N+1}}$$

where:

$$\mathbf{T} \equiv \begin{pmatrix} e^{(\beta J + \beta H)} & e^{(-\beta J)} \\ e^{(-\beta J)} & e^{(\beta J - \beta H)} \end{pmatrix}$$

$$Z_N = \mathrm{Tr}\left(\mathbf{T}^N\right)$$

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

Some tricks from linear algebra:

1. Any symmetric matrix $\mathbf{T}$ can be diagonalized by a transformation

$$\text{of the type } \mathbf{U}^{-1}\mathbf{T}\mathbf{U} = \mathbf{\Lambda} \equiv \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \lambda_n \end{pmatrix}.$$

2. $\mathbf{TTT}\cdots\mathbf{T} = \mathbf{TUU}^{-1}\mathbf{TUU}^{-1}\mathbf{TU}\cdots\mathbf{U}^{-1}\mathbf{T}$

3. $\mathrm{Tr}(\mathbf{TTT}\cdots\mathbf{T}) = \mathrm{Tr}(\mathbf{U}^{-1}\mathbf{TTT}\cdots\mathbf{TU}) = \mathrm{Tr}(\mathbf{\Lambda\Lambda}\cdots\mathbf{\Lambda})$

$$\Rightarrow \mathrm{Tr}(\mathbf{T}^N) = \lambda_1^N + \lambda_2^N + \lambda_3^N \cdots \lambda_n^N$$

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

In this case:

$$\mathbf{T} \equiv \begin{pmatrix} e^{(\beta J + \beta H)} & e^{(-\beta J)} \\ e^{(-\beta J)} & e^{(\beta J - \beta H)} \end{pmatrix}$$

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

$$\lambda_1 = e^{\beta J} \left\{ \cosh(\beta H) + \left[\sinh^2(\beta H) + e^{-4\beta J} \right]^{1/2} \right\}$$

$$\lambda_2 = e^{\beta J} \left\{ \cosh(\beta H) - \left[\sinh^2(\beta H) + e^{-4\beta J} \right]^{1/2} \right\}$$

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

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

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

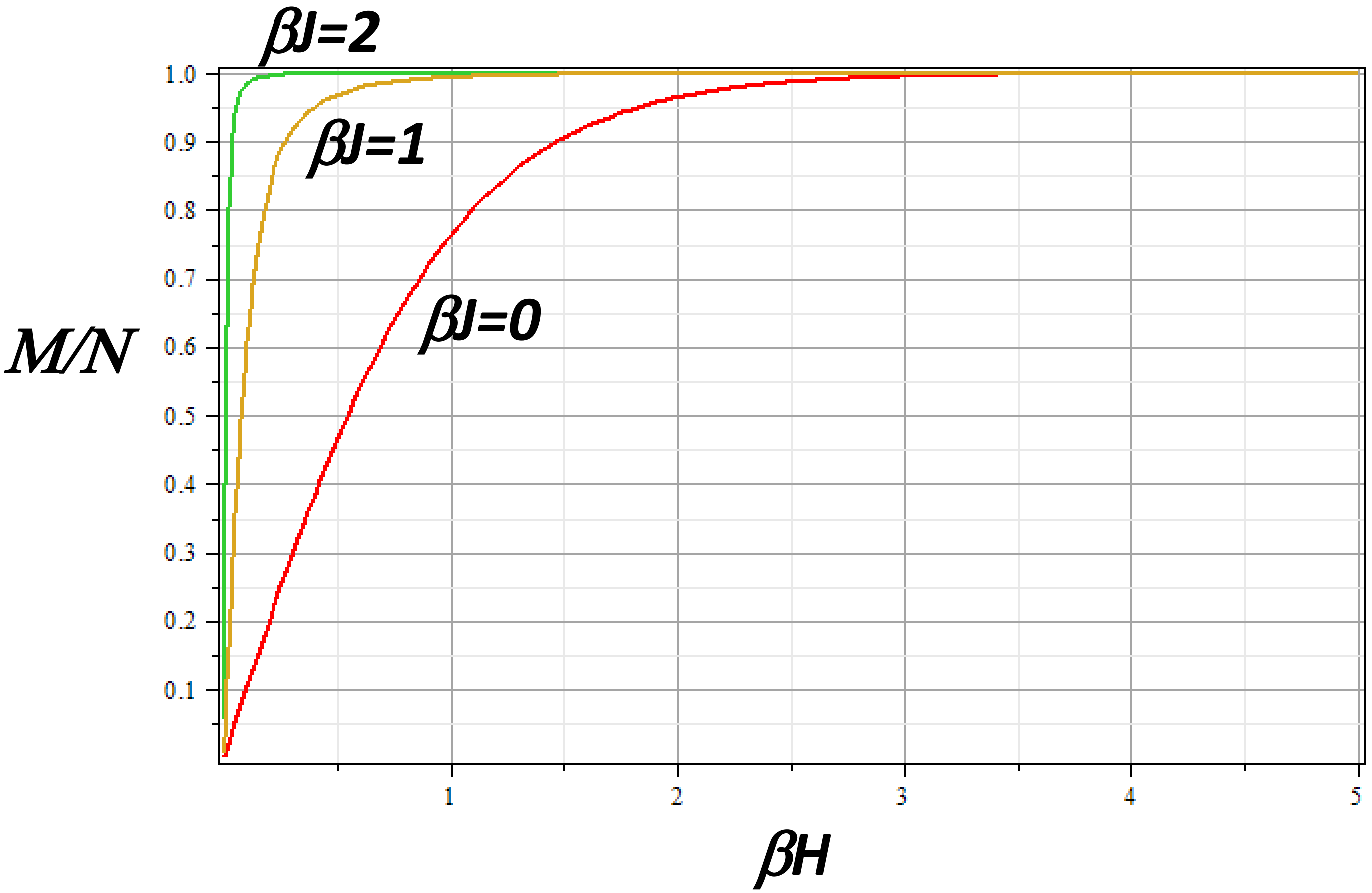
$$F(T,J,H) = -kT\ln Z_N = -NkT\ln\lambda_1 - kT\ln\left[1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right]$$

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

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

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

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



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:

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

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

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

Mean field partition function and Free energy:

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

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

Consistency condition :

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