PHY 341/641
Thermodynamics and Statistical Physics

Lecture 17

Methodologies of statistical mechanics. (Chapter 5 in STP)

A. Non-interacting spin systems
B. Ising model systems

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	Magnetic systems	5.5	Exam due	
	3/07/2012				
	3/09/2012				
	3/12/2012	*Spring Break*			
	3/14/2012	*Spring Break*			
	3/16/2012	*Spring Break*			

Examples of ensembles for magnetic interactions
(Chapter 5 in STP)

Microstate s :

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

$$\mu \equiv \tfrac{1}{2} g\mu_B = -9.28\times 10^{-24}\, J/T$$

$$Z_N = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} \cdots \sum_{s_N=\pm1} e^{\beta\mu B\left(\sum_{i=1}^{N} s_i\right)}$$

$$= \left(\sum_{s_1=\pm1} e^{\beta\mu B s_1} \right)^N = (Z_1)^N$$

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:

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

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

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

Magnetic field dependence of Z:

$$Z_N(T,N,B) = (2\cosh(\beta\mu B))^N$$

Magnetization :

$$M = \mu\sum_{i=1}^{N}\langle s_i\rangle$$

$$\langle s_i\rangle = \frac{\sum_{s_1=\pm 1} s_1 e^{\beta\mu B s_1}}{\sum_{s_1=\pm 1} e^{\beta\mu B s_1}} = \frac{1}{\beta\mu}\frac{\partial \ln Z_1}{\partial B}$$

$$\Rightarrow M = N\mu\tanh(\beta\mu B) = -\frac{\partial F}{\partial B}$$

$$\chi \equiv \left(\frac{\partial M}{\partial B}\right)_T = -\left(\frac{\partial^2 F}{\partial B^2}\right)_T = N\mu^2\beta\operatorname{sech}^2(\beta\mu B)$$

Independent particle system

Microstate s :

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

Interacting particle system – Ising model

Microstate s :

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

Ising model for H = 0 and N=2

Microstate s :

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

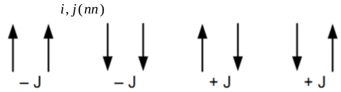

Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

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

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

Ising model for H ≠ 0 and N=2

Microstate s :

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

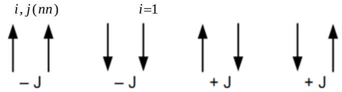

Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

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

Partition function for arbitrary N with periodic boundary conditions ($s_{N+1}=s_1$)

$$Z_N = \sum_s \exp\left[\beta J \sum_{i=1}^{N} s_i s_{i+1} + \frac{\beta H}{2}(s_i + s_{i+1})\right]$$
$$\equiv \sum_s f(s_1,s_2)\, f(s_2,s_3) \cdots f(s_{N-1},s_N)$$

where :

$$f(s,s') = \begin{pmatrix} f(1,1) & f(1,-1) \\ f(-1,1) & f(-1,-1) \end{pmatrix}$$
$$\equiv \begin{pmatrix} e^{\left(\beta J + \frac{1}{2}\beta H\right)} & e^{(-\beta J)} \\ e^{(-\beta J)} & e^{\left(\beta J - \frac{1}{2}\beta H\right)} \end{pmatrix}$$