

PHY 341/641 Thermodynamics and Statistical Physics

Lecture 18

Methodologies of statistical mechanics. (Chapter 5 in STP)

Ising model systems

- Definition
- Exact solution for 1-dimension
- Mean field solution

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

1

5	1/27/2012	Entropy	2.10-2.19	HW 5	1/30/2012
6	1/30/2012	Thermodynamic Potentials	2.20-2.21	HW 6	2/1/2012
7	2/1/2012	Thermodynamic Potentials	2.22-2.24	HW 7	2/3/2012
8	2/3/2012	Introduction to probability theory	3.1-3.3	HW 8	2/6/2012
9	2/6/2012	Probability distributions	3.4-3.5	HW 9	2/8/2012
10	2/8/2012	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			
	3/2/2012	APS -- no class; take-home exam			
18	3/5/2012	Exam due -- Ising model	5.5	HW 17	03/05/2012
	3/8/2012				
	3/9/2012				
	3/12/2012	Spring Break			
	3/14/2012	Spring Break			
	3/16/2012	Spring Break			

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

2

Statistical mechanics of spin $\frac{1}{2}$ systems

Microstate s :

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

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

Partition function for N non-interacting spins:

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

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

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 16

3

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:

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

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

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

3/5/2012

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4

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 :

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

3/5/2012

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5

Ising model for $H = 0$ and $N=2$

Microstate s :

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

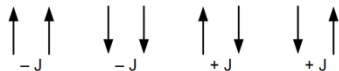


Figure 5.3: The four possible microstates of the $N = 2$ Ising chain.

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

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

3/5/2012

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6

Ising model for $H \neq 0$ and $N=2$

Microstate s :

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

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

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

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

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

3/5/2012

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7

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

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

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

where :

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

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

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

8

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

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

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

where :

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

$$Z_N = \text{Tr}(\mathbf{T}^N)$$

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

9

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. $\mathbf{T}\mathbf{T}\mathbf{T}\cdots\mathbf{T} = \mathbf{T}\mathbf{U}\mathbf{U}^{-1}\mathbf{T}\mathbf{U}\mathbf{U}^{-1}\mathbf{T}\mathbf{U}\cdots\mathbf{U}^{-1}\mathbf{T}$

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

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

3/5/2012

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10

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

In this case :

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

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

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

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

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

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

11

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

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

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

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

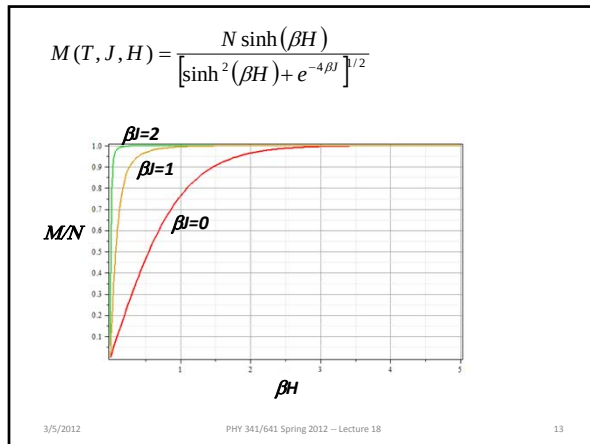
$$= -NJ - kT \ln \left[\cosh(\beta H) + \left[\sinh^2(\beta H) + e^{-4\beta J} \right]^{1/2} \right]$$

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

3/5/2012

PHY 341/641 Spring 2012 -- Lecture 18

12



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 :

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

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

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

3/5/2012 PHY 341/641 Spring 2012 -- Lecture 18 14

Mean field partition function and Free energy:

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

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

Consistency condition :

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

3/5/2012 PHY 341/641 Spring 2012 -- Lecture 18 15
