PHY 341/641 Thermodynamics and Statistical Mechanics
MWF: Online at 12 PM & FTF at 2 PM

Record!!!

Discussion for Lecture 35:

Treatment of particle interactions in statistical mechanics; electron spin effects

Reading: Sections 8.2

1. **Effects of spin interactions – Ising model**
2. **Mean field solution**
3. **Exact solution for special cases**

28	Fri: 04/09/2021	Chap. 7.3 & 7.4	Bose and Fermi statistics	#23	04/12/2021
29	Mon: 04/12/2021	Chap. 7.3	Fermi examples	#24	04/16/2021
30	Wed: 04/14/2021	Chap. 7.5	Bose examples and lattice vibrations		
31	Fri: 04/16/2021	Chap. 7.6	Bose condensation		
32	Mon: 04/19/2021	Chap. 7.6 & 8.1	Interacting particles	#25	04/21/2021
33	Wed: 04/21/2021	Chap. 8.1	Interacting particles	#26	04/23/2021
34	Fri: 04/23/2021	Chap. 8.2	Spin magnetism		
35	Mon: 04/26/2021	Chap. 8.2	Spin magnetism		
36	Wed: 04/28/2021		Review		
37	Fri: 04/30/2021		Review		
37	Mon: 05/03/2021		Review		
38	Wed: 05/05/2021		Review		

Instead of a HW set, please send me your thoughts on topics, examples, etc. that you would like to see in our review starting on Wed. 4/28/2021.

Important dates: Final exams available < May 6; due May 14
Outstanding work due May 14

Comment on homework (generally and also #26)

➔It is important to check your units when you are doing numerical evaluations.

Specifically for #26, you need to evaluate B(T) which modifies the ideal gas equation of state..

$$P = \frac{NkT}{V}\left(1 + \frac{B(T)}{V/N}\right)$$

What are the units of B?

Your questions –

From Mike -- I'm assuming the Ising model is only an accurate approximation for ferromagnets. In this case, how do we deal with antiferromagnets?

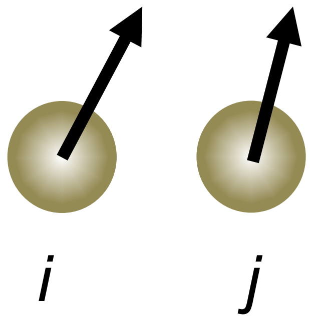
From Kristen -- 1. How is it that the system discussed can become more ordered as the temperature gets higher, doesn't this violate entropy?
2. Could you go over how we get the average expected spin values (equation 8.49) from the partition function, just in this case especially?

Some results from Friday   focusing on multi-electron atoms with net composite spin *S* (half integer or integer values) in the presence of a magnetic field **B** and nearest neighbor spin interactions (*J*) modeled according to the Heisenberg model:

$$\mathcal{H} = -\mu_a \sum_i \mathbf{S}_i \cdot \mathbf{B} - J \sum_{ij(neighbors)} \mathbf{S}_i \cdot \mathbf{S}_j$$

assuming that B is in the z-direction and also assuming that the z component of spin dominates the dot product --

$$\mathcal{H} \approx -\mu_a \sum_i S_{iz} B - J \sum_{ij(neighbors)} S_{iz} S_{jz}$$



Review from Friday, continued --

$$\mathcal{H} \approx -\mu_a \sum_i S_{iz} B - 2J \sum_{ij(neighbors)} S_{iz} S_{jz}$$

$$= -\sum_i S_{iz} \left(\mu_a B + 2J \sum_{\substack{j \\ \text{(neighbors of i)}}} S_{jz} \right)$$

Note that in some equations presented Friday, *J* should have been written *2J*. Apologies.

Approximation using mean field approach --

$S_{jz} \rightarrow \langle S_{jz} \rangle$ (canonical average)

Mean field Hamiltonian --

$$\mathcal{H}_{MF} = -\mu_a \sum_i S_{iz} \left(B + B_{neigh} \right) \quad \text{where} \quad B_{neigh} \equiv \frac{2J}{\mu_a} \sum_{\substack{j \\ \text{(neighbors of i)}}} \langle S_{jz} \rangle$$

Evaluating the canonical partition function for N atoms in mean field approximation:

$$Z(T,N)=\left(\frac{\sinh\left(\left(S+\frac{1}{2}\right)\beta\mu_a B_{tot}\right)}{\sinh\left(\frac{1}{2}\beta\mu_a B_{tot}\right)}\right)^N \qquad \text{where } B_{tot}\equiv B+B_{neigh}$$

Helmholtz free energy:

$$F(T,N)=-NkT\left(\ln\left(\sinh\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a B_{tot}\right)\right)-\ln\left(\sinh\left(\tfrac{1}{2}\beta\mu_a B_{tot}\right)\right)\right)$$

Average magnetic moment along the magnetic field direction:

$$\langle\mu\rangle=-\left(\frac{\partial F}{\partial B}\right)_N=N\mu_a\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a B_{tot}\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}\beta\mu_a B_{tot}\right)\right)$$

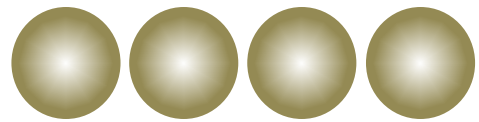
Note that in this approximation the average spin is the same at all sites:

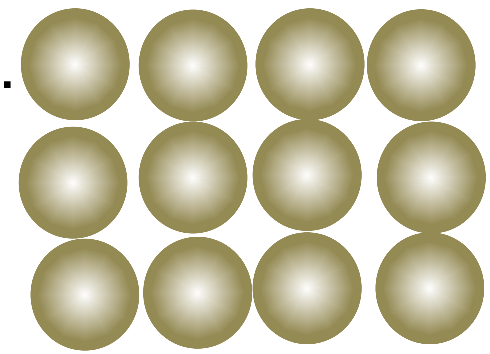
$$\langle S_{jz}\rangle=\frac{\langle\mu\rangle}{N\mu_a}=\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a B_{tot}\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}\beta\mu_a B_{tot}\right)\right)$$

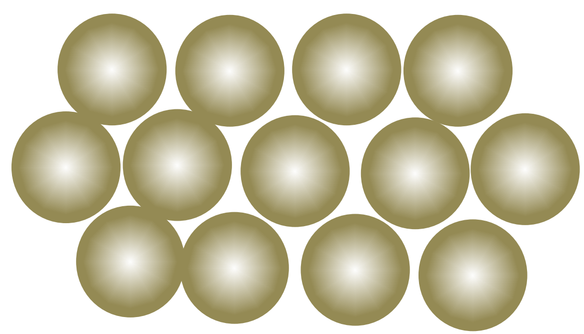
For *n* neighbors, this can be written

$$\Rightarrow B_{neigh}=\frac{2nJ}{\mu_a}\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a B_{tot}\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}\beta\mu_a B_{tot}\right)\right)$$

Comment on *n* neighbors --

Atoms in a line -- …  …… n=2

Atoms in a plane -- …  …… n=4



n=6

Solving the self-consistent mean field equations --

$$B_{neigh} = \frac{2nJ}{\mu_a}\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a\left(B+B_{neigh}\right)\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}\beta\mu_a\left(B+B_{neigh}\right)\right)\right)$$

Transcendental equation that can be solved numerically at each B and T.

Note, that for some materials it is possible to find solutions for zero external magnetic field.

$$\Rightarrow B_{neigh} = \frac{2nJ}{\mu_a}\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)\beta\mu_a B_{neigh}\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}\beta\mu_a B_{neigh}\right)\right)$$

Let $x = \beta\mu_a B_{neigh}$

Equation to solve:

$$x = 2\beta nJ\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)x\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}x\right)\right)$$

In this case, we found that solutions can be found for

$T \le T_c$ where the Curie temperature is:

$$kT_c = 2nJ\left(\frac{S(S+1)}{3}\right)$$

For $T \le T_c$ the material is in a ferromagnetic phase.

The Ising model is a special case of this treatment with $S = 1/2$ --

Self-consistent equation: for $x = \beta\mu_a B_{neigh} = 2\beta nJ\left\langle S_{iz}\right\rangle$

$$x = 2\beta nJ\left(\left(S+\tfrac{1}{2}\right)\coth\left(\left(S+\tfrac{1}{2}\right)x\right)-\tfrac{1}{2}\coth\left(\tfrac{1}{2}x\right)\right)$$

becomes

$$x = \beta nJ\tanh\left(\tfrac{1}{2}x\right) \quad \text{or} \quad \left\langle S_{iz}\right\rangle = \tfrac{1}{2}\tanh\left(\beta nJ\left\langle S_{iz}\right\rangle\right)$$

Notation	Here	Schroeder
	$\left\langle S_{iz}\right\rangle$	$\tfrac{1}{2}\overline{s}$
	J	2ϵ

Critical temperature for this case

Using Schroeder's notation $\overline{s} = \tanh\left(\beta n\epsilon\overline{s}\right)$

For small values of the argument of the tanh, the condition becomes

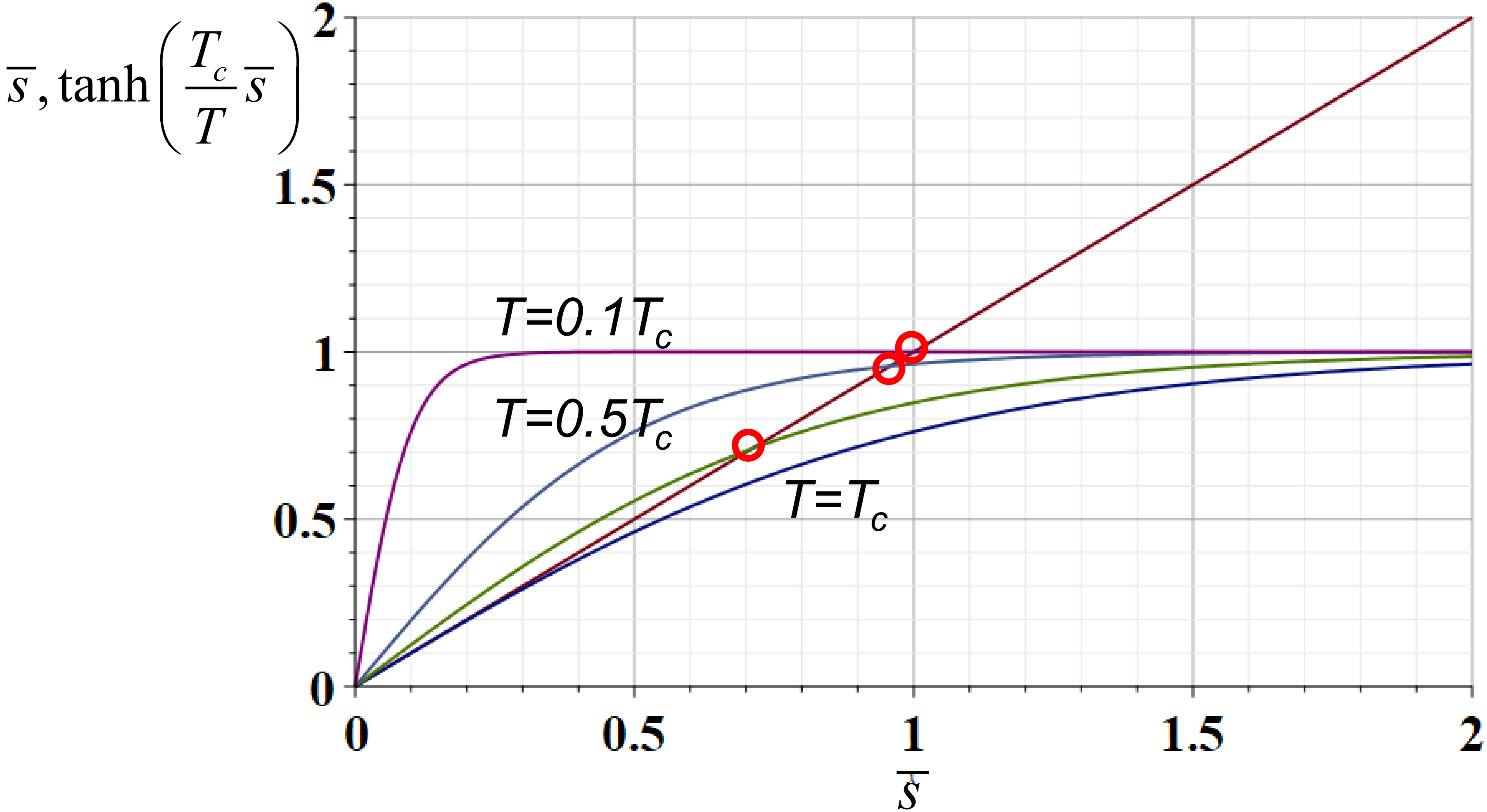
$\overline{s} = \beta_c n\epsilon\overline{s}$ which defines the critical temperature

$$\beta_c n\epsilon = 1 \quad \text{or} \quad T_c = \frac{n\epsilon}{k}$$

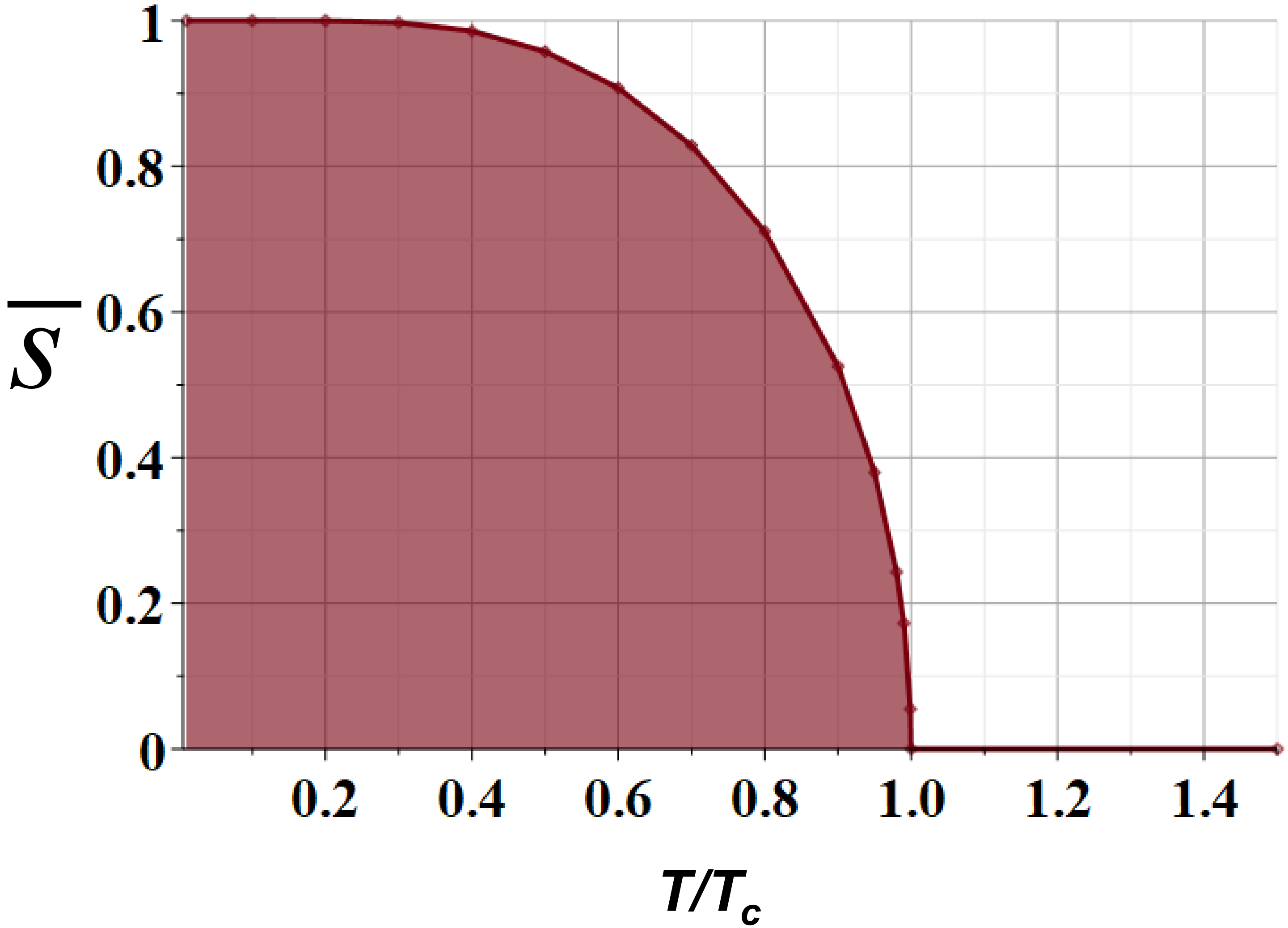
Alternate form of self-consistency condition: $\overline{s} = \tanh\left(\frac{T_c}{T}\overline{s}\right)$

Summary -- $\overline{s} = \begin{cases} \tanh\left(\frac{T_c}{T}\overline{s}\right) & \text{for } T \le T_c \\ 0 & \text{for } T > T_c \end{cases}$

$$\bar{s} = \tanh\left(\frac{T_c}{T}\bar{s}\right)$$



Self-consistent solutions to the mean field approximation to the Ising model in the absence of an external magnetic field.



How accurate is the mean field approximation?

The Ising model can be solved exactly in some cases and used to access the accuracy of the mean field approximation.

Answer – The mean field approximation is generally qualitatively correct except in certain cases

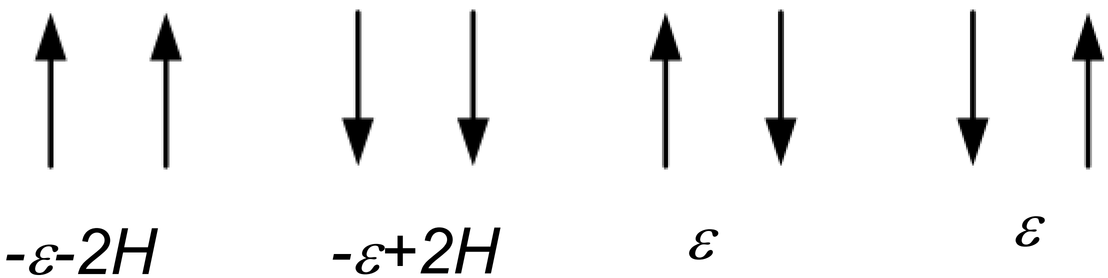
The following slides use material from previous course notes based on the textbook Statistical and Thermal Physics by Gould and Tobochnik

Some exact treatments using the Ising model

Model Hamiltonian with magnetic field $H \equiv \frac{1}{2}\mu_e B$

$$\mathcal{H} = -\epsilon \sum_{i,j(nn)}^{N} s_i s_j - H \sum_{i=1}^{N} s_i \quad \Rightarrow s_i = \pm 1 \text{ respresenting up and down spin}$$

For N=2, $\mathcal{H} = -\epsilon s_1 s_2 - H(s_1 + s_2)$



Canonical partition function

$$Z(T) = e^{\beta(\epsilon+2H)} + e^{\beta(\epsilon-2H)} + 2e^{-\beta\epsilon}$$

Exact solution for 2 particle Ising model -- continued

$$\mathcal{H} = -\epsilon s_1 s_2 - H(s_1 + s_2)$$

Canonical partition function

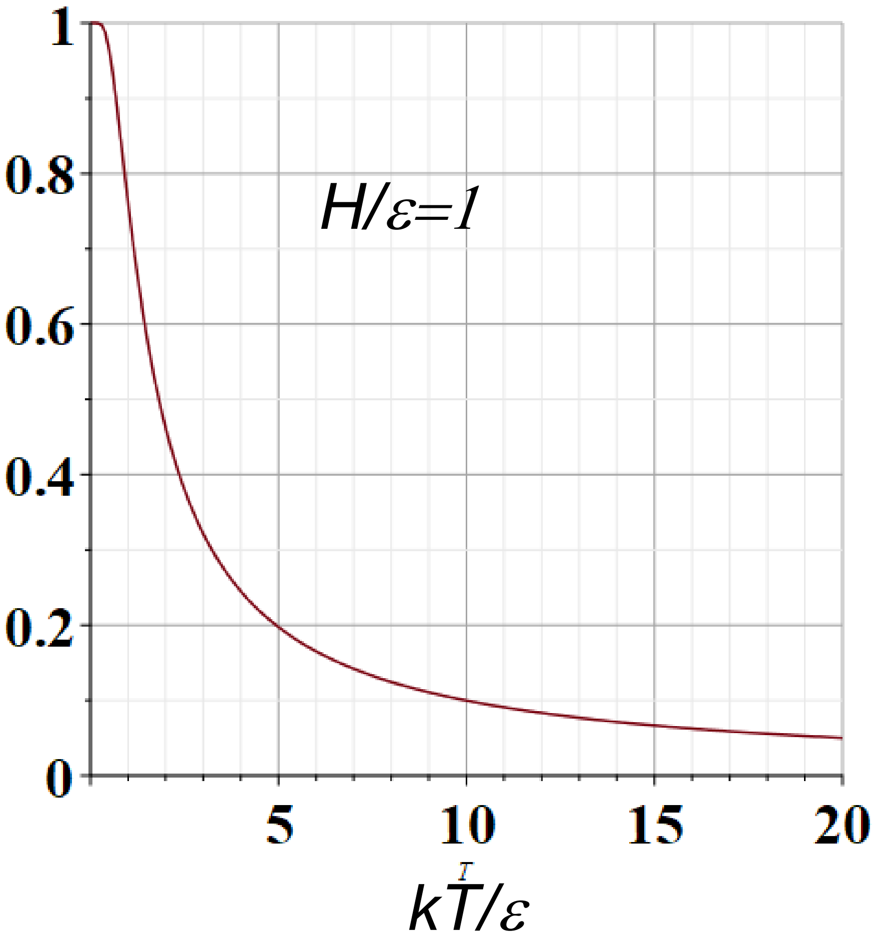
$$Z(T) = e^{\beta(\epsilon+2H)} + e^{\beta(\epsilon-2H)} + 2e^{-\beta\epsilon}$$

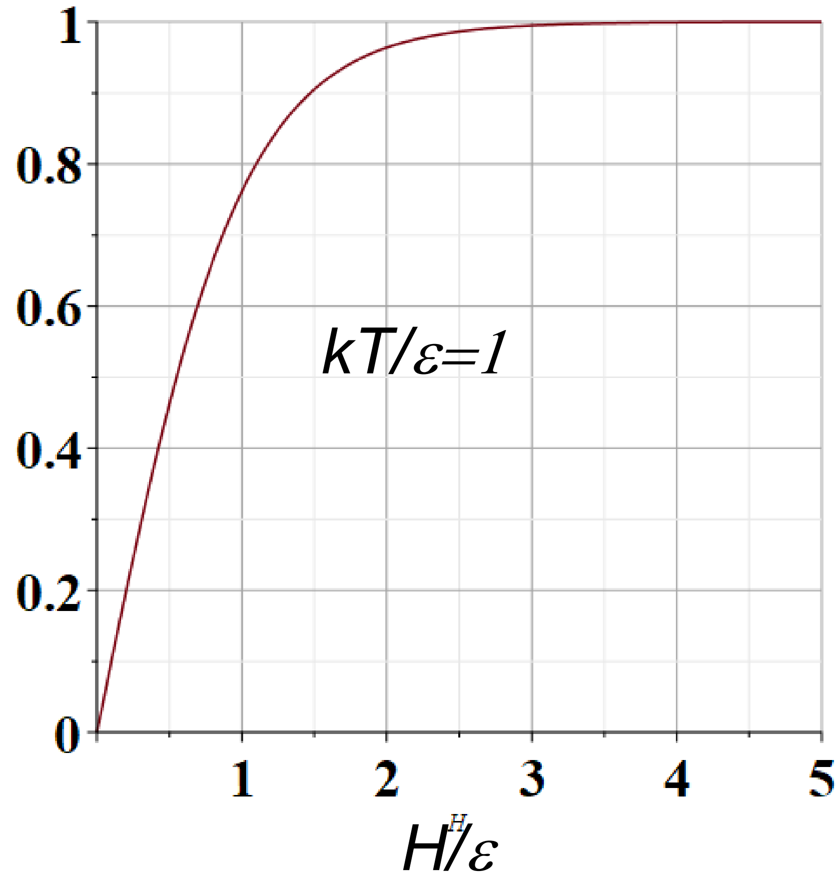
Calculation of the average spin for this system

$$\langle s \rangle = \frac{1}{2}\langle s_1 + s_2 \rangle = \frac{1}{2Z(T)}\left(2e^{\beta(\epsilon+2H)} - 2e^{\beta(\epsilon-2H)}\right)$$

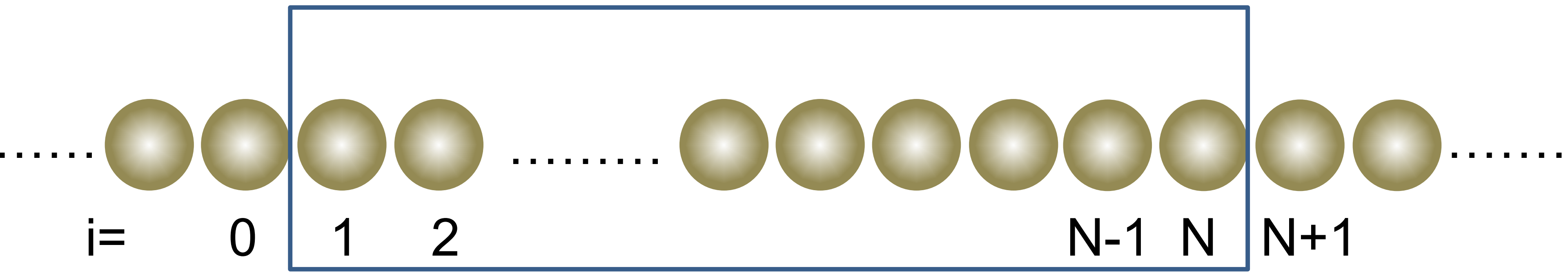
Exact solution for 2 particle Ising model -- continued

Plots of $\langle s \rangle$





Now consider an infinite system where we treat N particles with periodic boundary conditions



The index i ranges between 1 and N; N+1 maps to 1

0 maps to N

One dimensional Ising model

One-dimensional system with periodic boundary conditions:

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$$

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

$$Z(T,N) = \sum_{\{s\}} \exp\left[\sum_{i=1}^{N}\left(\beta\varepsilon s_i s_{i+1} + \frac{\beta H}{2}\left(s_i + s_{i+1}\right)\right)\right]$$

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

Clever trick for performing sum over s_i – write f factors as 2x2 matrices and perform matrix multiplication

$$Z(T,N) = \sum_{\{s\}} \exp\left[\sum_{i=1}^{N}\left(\beta\varepsilon s_i s_{i+1} + \frac{\beta H}{2}\left(s_i + s_{i+1}\right)\right)\right]$$

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

where:

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

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

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

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

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

where:

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

Because all of the $\mathbf{T}$ matrices are identical:

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

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 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:

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

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

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

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

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

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

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

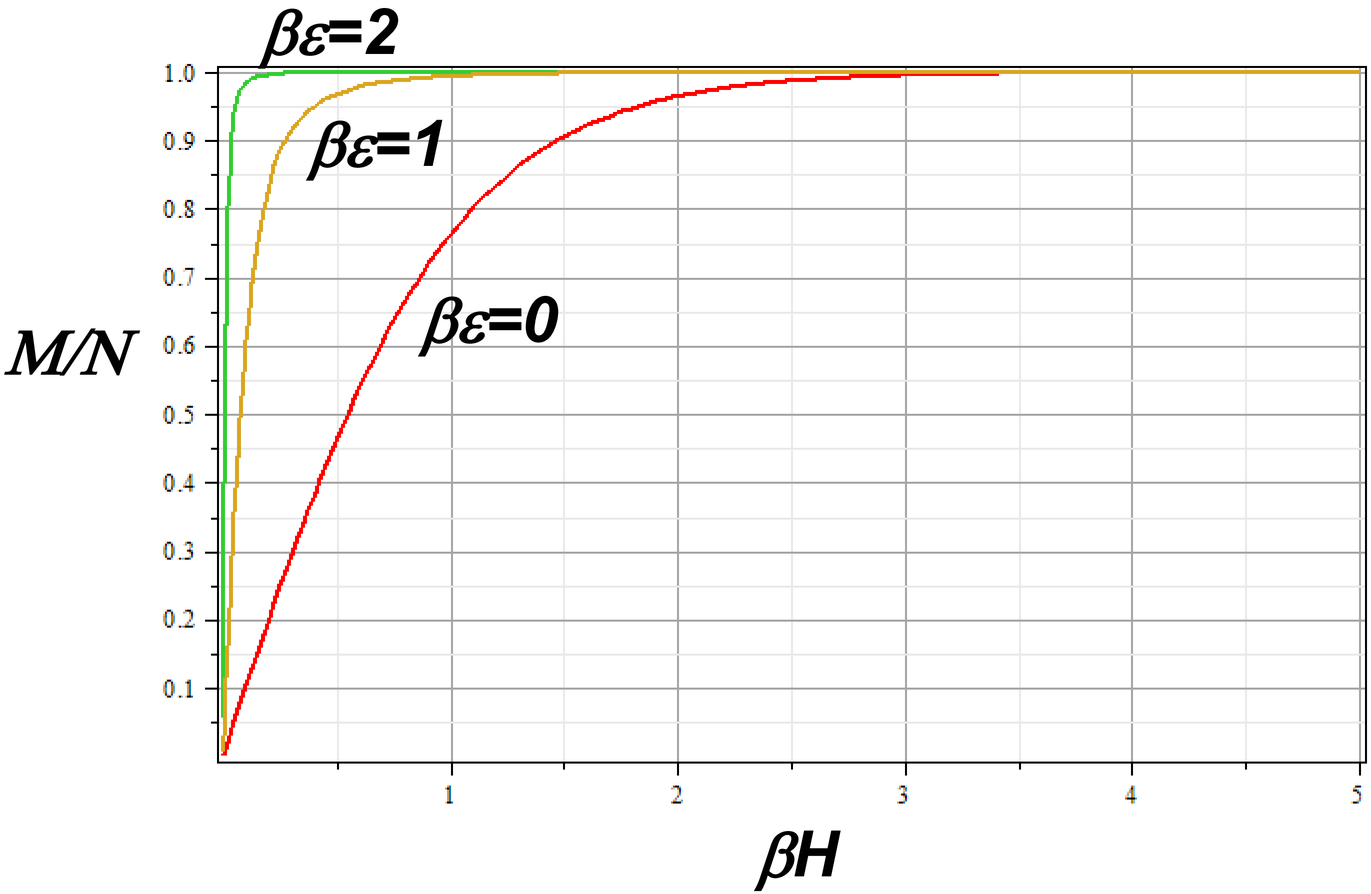
$$F(T,N) = -kT\ln Z(T,N) = -NkT\ln\lambda_1 - kT\ln\left[1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right]$$

$$\approx -NkT\ln\lambda_1 \qquad \text{because } \frac{\lambda_2}{\lambda_1}<1$$

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

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

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



Mean field approximation for 1-dimensional Ising model

Exact model for Ising model

$$\mathcal{H} = -\varepsilon \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$$

Mean approximate Hamiltonian:

$$\mathcal{H}_{MF} = -\varepsilon \sum_{i=1}^{N} s_i \langle s_i \rangle - H \sum_{i=1}^{N} s_i$$

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

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

Mean field partition function and Free energy:

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

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

Consistency condition:

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

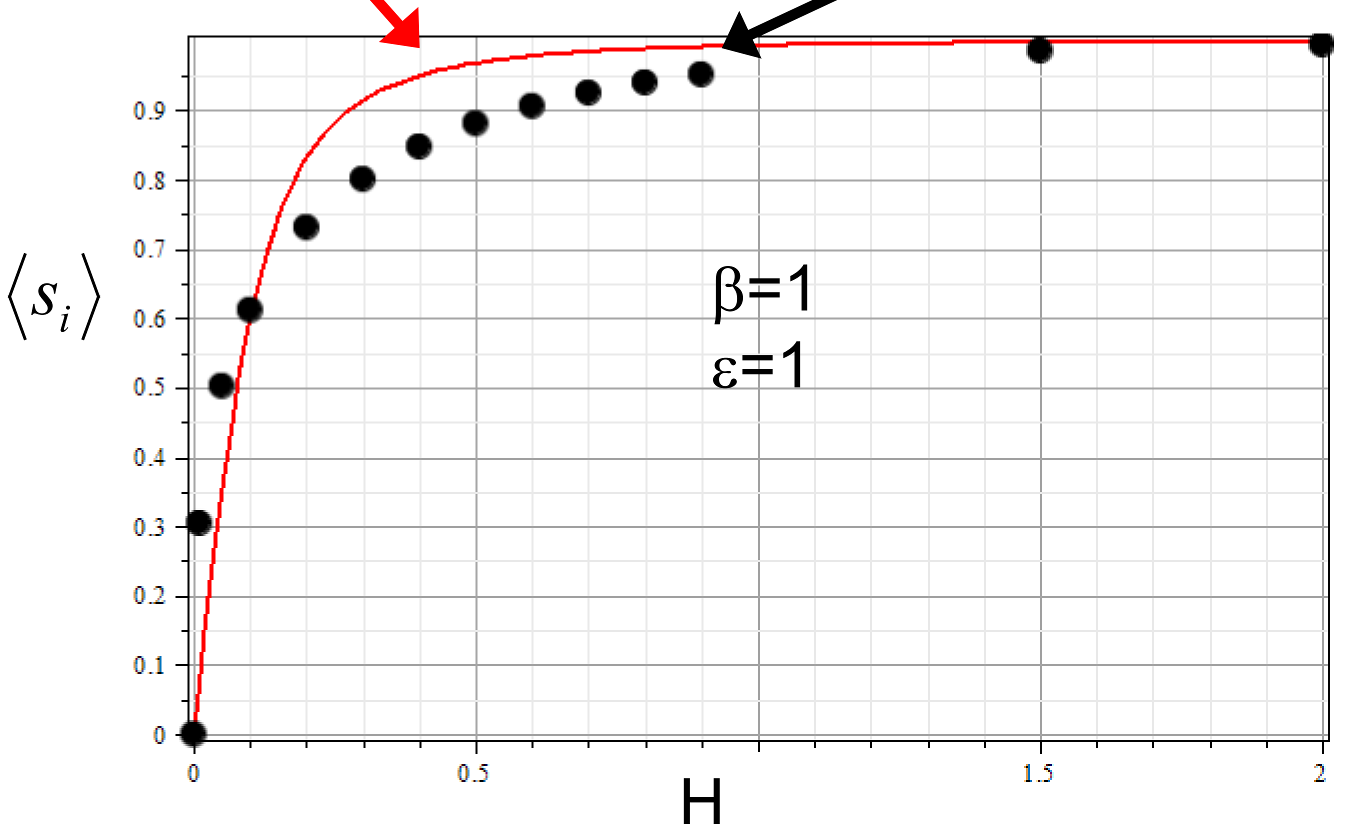
One dimensional Ising model with periodic boundary conditions:

Exact solution:

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

Mean field solution:

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



Comment, while the solution for H>0 is qualitatively similar for the exact and mean field solutions, the solution for H=0 is qualitatively different.

Exact solution in one dimension has no average spin for H=0 while the mean field solution has a finite average spin solution.