Outline for the next couple of lectures

-Magnetism and the Ising Model (today's lecture)

-Liquid-vapor transitions and polymer demixing (Monday's lecture)

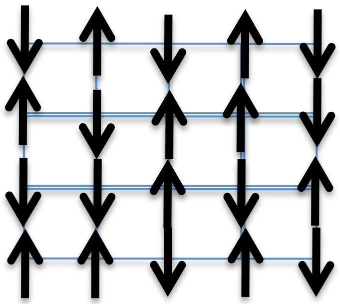
Important concepts to be learnt from these lectures

-How to build a molecular theory and solve it using different (mean-field) approximations. Develop conceptual frameworks on how to solve a given problem.

-Regular solution theory for ordering transitions and the mean-field solution to magnetism are equivalent.

-Thermodynamic results in magnetism, such as the critical (or Curie) temperature below which spontaneous magnetization occurs.

Magnetism: The Ising Model



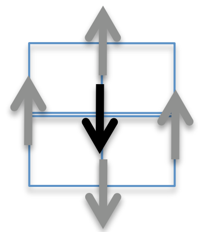
Consider N spins arranged in a lattice,
Q: what is the net magnetization of this material?

Rules for the Ising Model:

1) Spins can be *only* in two states: UP or DOWN

↑ ↓

2) The spin-spin interactions are only with the nearest neighbors (nn):



The spin-spin interaction strength is characterized by the coupling constant J

The energy per spin is then: $\epsilon_i = -J \sum_{j=\{nn\}} \sigma_i \sigma_j - h\sigma_i$

The spins variable takes the values $\sigma = +1(\uparrow), -1(\downarrow)$

Magnetism: The Ising Model (contd.)

Consider first the case of *T*=0 (where entropy vanishes)

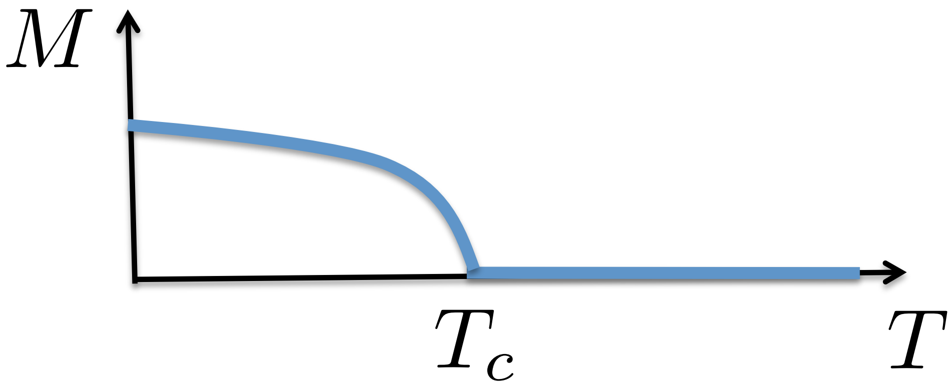
$$J = \begin{cases} > 0 & \text{ferromagnetic} \\ < 0 & \text{antiferromagnetic} \end{cases}$$

ferromagnetic: ↑ ↑ ↑ ↑ ↑ ↑

antiferromagnetic: ↓ ↑ ↓ ↑ ↓ ↑

This implies that for *T*≠0, but sufficiently low, we expect materials with a positive coupling constant to display ferromagnetic behavior!

We expect the system to exhibit the following behavior if *J*>0.



Magnetism: The Ising Model (contd.)

To obtain the thermodynamic properties of this system lets go brute force and calculate the partition function:

$$Q = \sum_{\nu} e^{-\beta E_\nu}$$

In terms of the spin variables, we find

$$Q = \sum_{\sigma_1=+1,-1} \sum_{\sigma_2=+1,-1} \cdots \sum_{\sigma_N=+1,-1} e^{-\beta \sum_i \epsilon_i}$$

$$= \sum_{\sigma_1=+1,-1} \sum_{\sigma_2=+1,-1} \cdots \sum_{\sigma_N=+1,-1} \exp\left(\beta \frac{J}{2} \sum_i \sum_{j=\{nn\}} \sigma_i \sigma_j + \beta h \sum_i \sigma_i\right)$$

Somebody knows how to solve this?

The Ising Model: Macroscopic Observables

Imagine that we knew how to calculate Q !!!

The magnetization of the system can then be calculated by

$$\langle M \rangle = \langle \sum_i \sigma_i \rangle = \frac{1}{\beta} \frac{\partial}{\partial h} \log Q$$

And the magnetization per spin is simply

$$m = \frac{\langle M \rangle}{N} = \langle \sigma \rangle$$

The Ising Model

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The Ising Model: Mean-Field Theory

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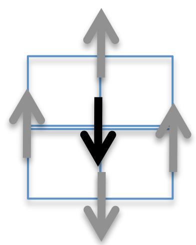
A collection of <u>independent</u> non-interacting spins!!!

Q: how can we convert the Ising Model to something we can solve?

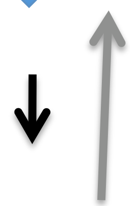
Solution: consider the average (or mean) field from the neighboring spins.

$$\epsilon_i = -J \sum_{j=\{nn\}} \sigma_i \sigma_j - h\sigma_i$$



$$\epsilon_i = -Jz\sigma_i \langle \sigma \rangle - h\sigma_i$$

Lattice coordination $z = 2D$



$$h_{mol} = Jz\langle \sigma \rangle$$

The Ising Model: Mean-Field Theory

By factorization, we can calculate the partition function as

$$Q = q^N$$

where the single spin partition function is

$$q = \sum_{\sigma=+1,-1} e^{\beta\sigma(h_{mol}+h)} = 2\cosh\left(\beta(h_{mol}+h)\right)$$

$$\Downarrow$$

$$q = 2\cosh\left(\beta J z\langle\sigma\rangle + \beta h\right)$$

The Ising Model: Mean-Field Theory

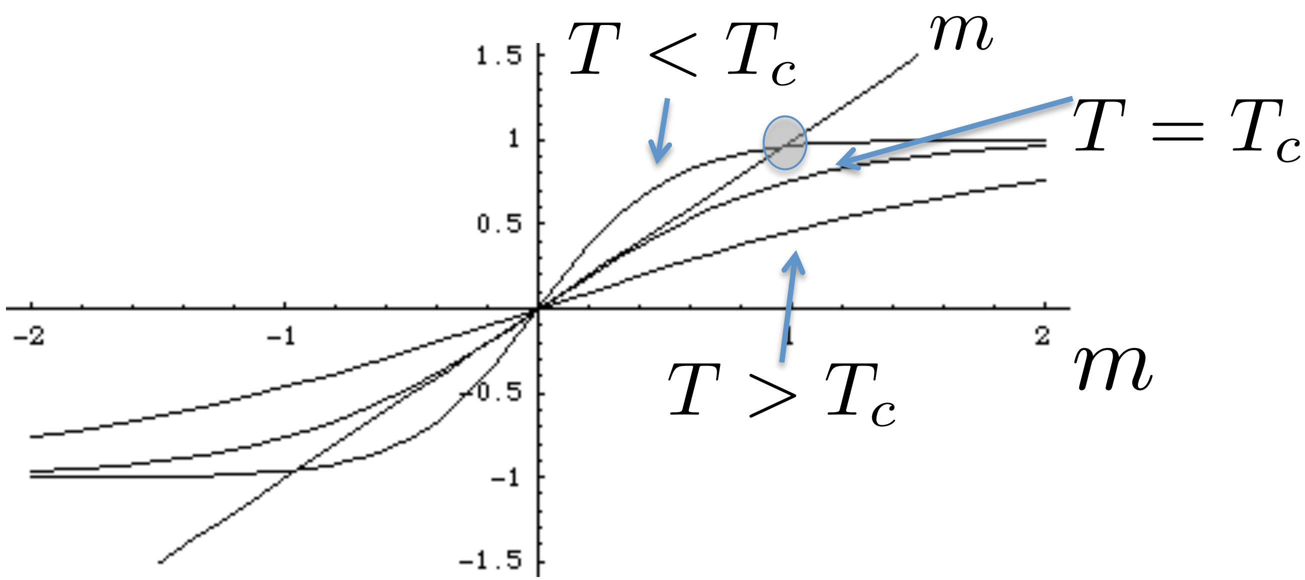
The average magnetization per spin is calculated as

$$m = \langle \sigma \rangle = \frac{1}{\beta} \frac{\partial}{\partial h} \log q$$

$$m = \tanh\left(\beta h + \beta J z m\right)$$

trascendental eq.

Solve graphically (for the case $h = 0$)



The Ising Model: Mean-Field Theory

The critical temperature is simply evaluated by the condition

$$\beta = \frac{1}{Jz} \quad \Rightarrow \quad T_c = \frac{Jz}{k_B}$$

In 3D the critical temperature is

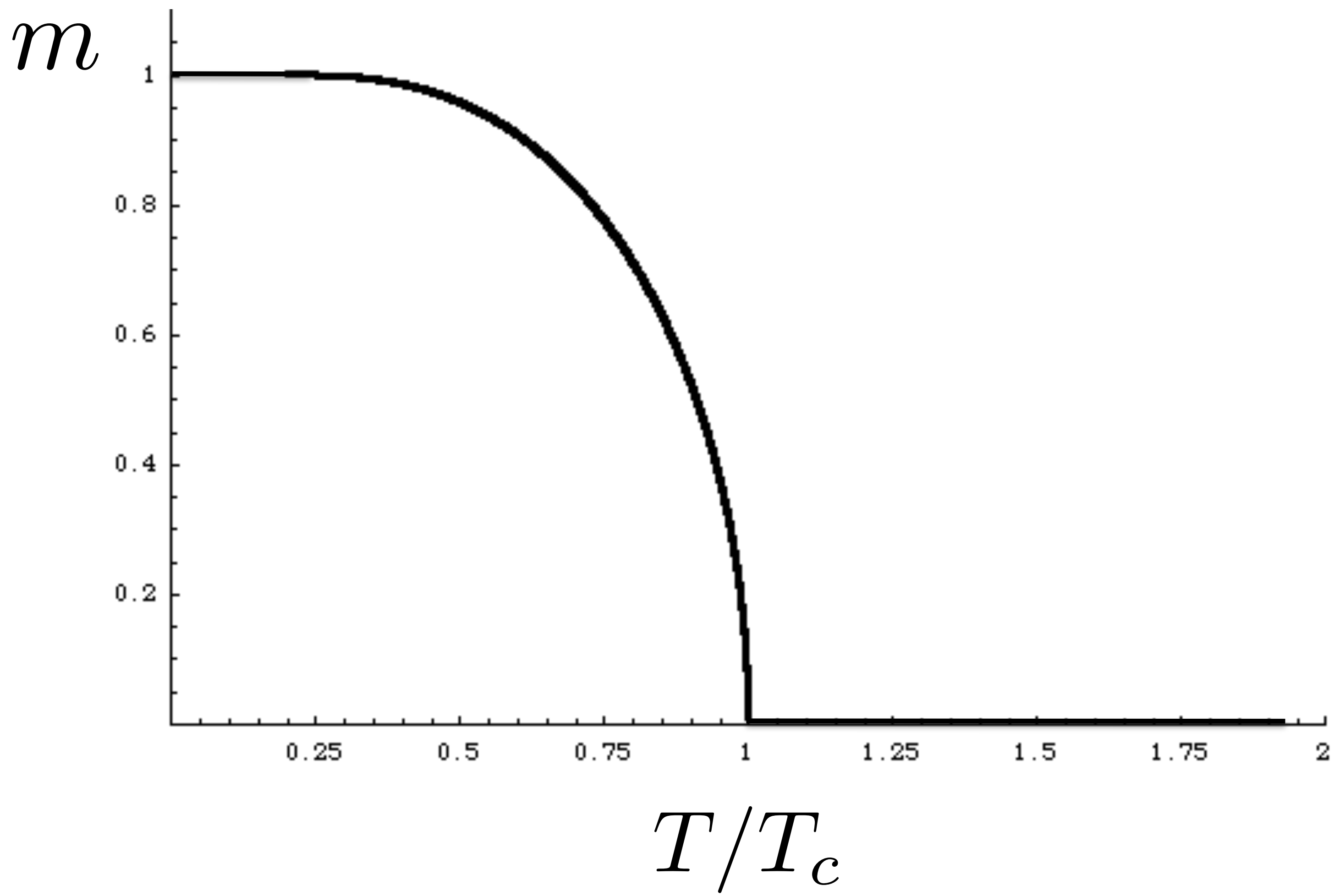
$$T_c^{MF}(3D) = \frac{6J}{k_B} \qquad T_c^{exact}(3D) = \frac{4J}{k_B}$$

The solution below T_c for m is given by

$$\beta = \frac{1}{2Jzm} \log\left(\frac{1+m}{1-m}\right)$$

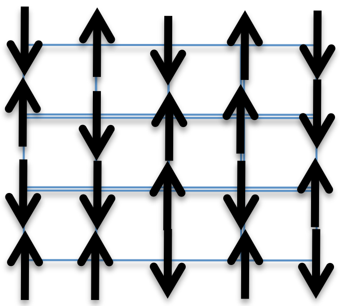
The Ising Model: Mean-Field Theory

The magnetization per spin as a function of T



The Ising Model: The bold approach

Also called the Bragg-Williams Theory



Consider the same problem as before. The magnetization (per spin)can be computed as

$$m = (N_{\uparrow} - N_{\downarrow})/N$$

The Ising Model: The bold approach

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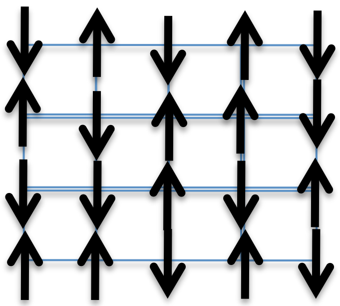

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$$m = (N_{\uparrow} - N_{\downarrow})/N$$

The entropy (per spin) for a fixed *m* is given by

$$\frac{-S}{k_B N} = f_{\uparrow} \log f_{\uparrow} + (1 - f_{\uparrow}) \log(1 - f_{\uparrow})$$

$$= -\log 2 + \frac{1}{2}(1+m)\log(1+m) + \frac{1}{2}(1-m)\log(1-m)$$

The Ising Model: The bold approach

Assume directly that the energy contribution is given by a mean-field

$$\frac{E}{N} = \epsilon = -\frac{1}{2} J z m^2 - hm$$

The free energy (per spin) is then

$$\frac{F}{k_B T N} = f(m) = -\frac{1}{2}\beta J z m^2 - hm - \log 2$$
$$+ \frac{1}{2}(1+m)\log(1+m) + \frac{1}{2}(1-m)\log(1-m)$$

The Ising Model: The bold approach

How does the free energy look like?

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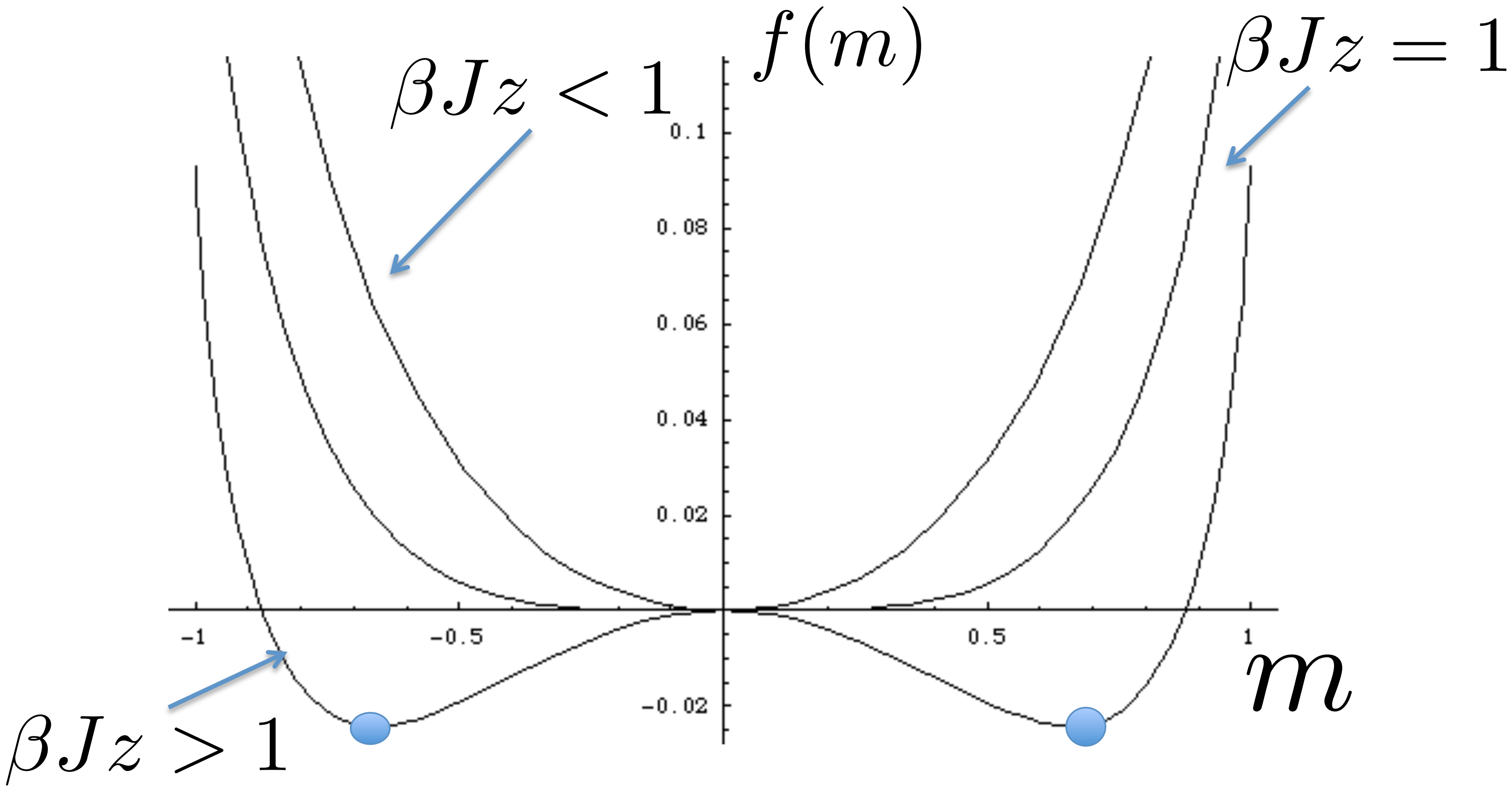

The Ising Model: The bold approach

Near the critical point, the magnetization is small.
What can we do then? Expand in powers of *m*

The free energy (per spin) is then

$$f = \frac{1}{2T}(T - T_c)m^2 + \frac{1}{12}m^4 + \ldots$$

$$T_c = \frac{Jz}{k_B}$$ as before

This is a classical result for system where the symmetry forces the free energy to only have even powers. Landau exploited this idea and constructed a whole field of phase transitions!

The Ising Model: The bold approach

Lets keep on going!

Taking the derivative of the free energy with respect to m and minimizing yields

$$\frac{\partial f}{\partial m} = -\beta J z m - h + \frac{1}{2}\log\left(\frac{1+m}{1-m}\right) = 0$$

$$h = 0$$

$$\beta = \frac{1}{2Jzm}\log\left(\frac{1+m}{1-m}\right)$$

Same result as before!!!

Summary

-The Ising Model can be solved approximately by mean-field methods equivalent to those applied to obtain regular solution theory.

-Provided two independent frameworks on how to think about the Ising Model, and ordering transitions, and how to obtain the observable thermodynamic quantities.

-Showed that using a macorscopic or a microscopic mean field approach yielded the same results.

-The ideas developed for solids and ordering transitions can be directly applied to the case of magnetism.

-The ideas developed for solids and ordering transitions can be directly applied to the case of magnetism and liquid-vapor phase transitions