Statistical Mechanics

List of results and definitions

Function of state		Statistical mechanical expression
U		$-\frac{\mathrm{d}\ln Z}{\mathrm{d}\beta}$
F		$-k_\mathrm{B}T\ln Z$
S	$= -\left(\frac{\partial F}{\partial T}\right)_V = \frac{U-F}{T}$	$k_\mathrm{B}\ln Z + k_\mathrm{B}T\left(\frac{\partial \ln Z}{\partial T}\right)_V$
p	$= -\left(\frac{\partial F}{\partial V}\right)_T$	$k_\mathrm{B}T\left(\frac{\partial \ln Z}{\partial V}\right)_T$
H	$= U + pV$	$k_\mathrm{B}T\left[T\left(\frac{\partial \ln Z}{\partial T}\right)_V + V\left(\frac{\partial \ln Z}{\partial V}\right)_T\right]$
G	$= F + pV = H - TS$	$k_\mathrm{B}T\left[-\ln Z + V\left(\frac{\partial \ln Z}{\partial V}\right)_T\right]$
C_V	$= \left(\frac{\partial U}{\partial T}\right)_V$	$k_\mathrm{B}T\left[2\left(\frac{\partial \ln Z}{\partial T}\right)_V + T\left(\frac{\partial^2 \ln Z}{\partial T^2}\right)_V\right]$

Table 20.1 Thermodynamic quantities derived from the partition function Z.

$$\beta = \frac{1}{k_B T}$$

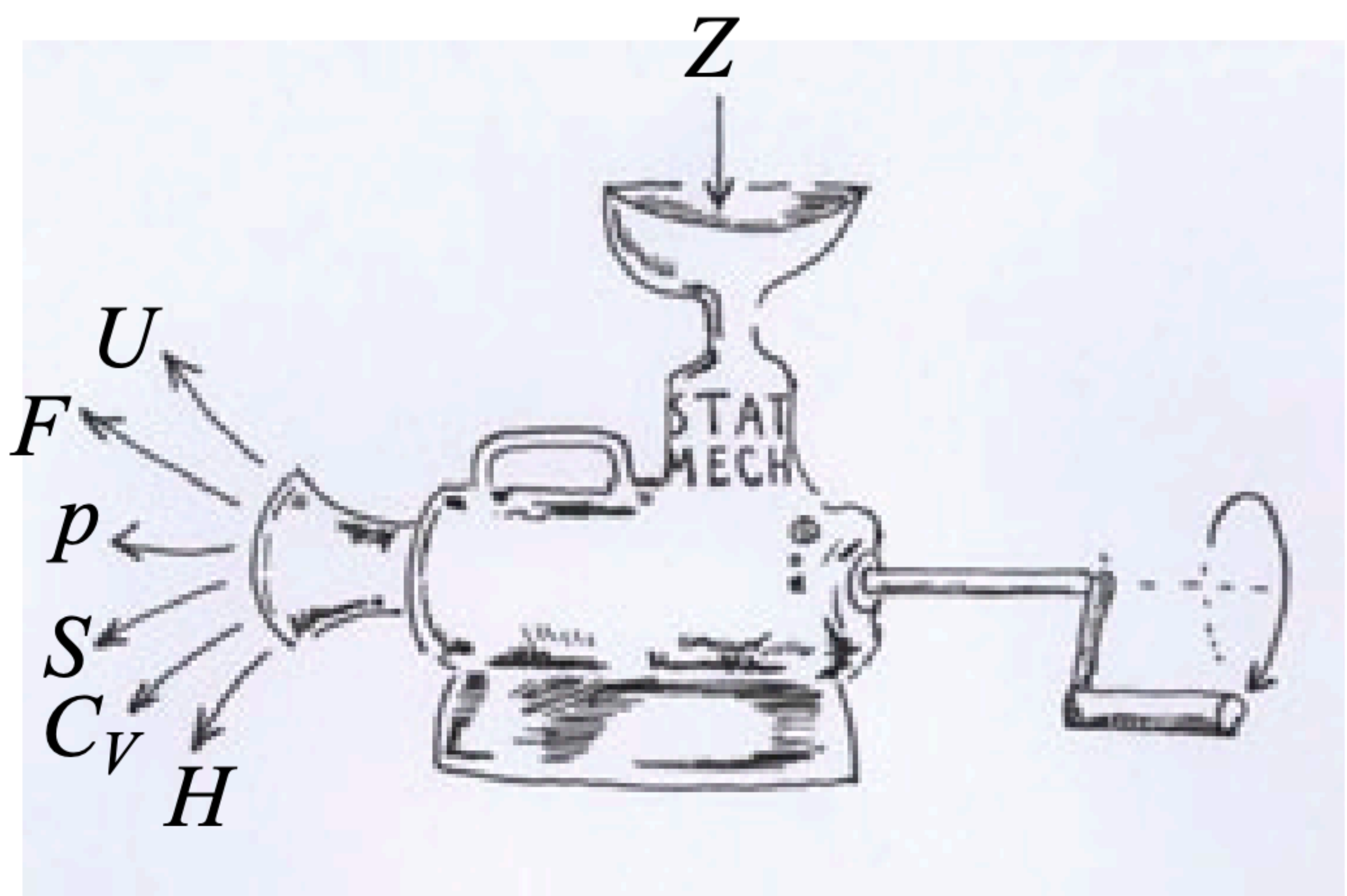


Fig. 20.3 Given Z, it takes only a turn of the handle on our 'sausage machine' to produce other functions of state.

Figures taken from Blundell

What about the Ising Model?

What is good/used for?

- Ferromagnetism.
- Widely used in the theory of phase transitions.

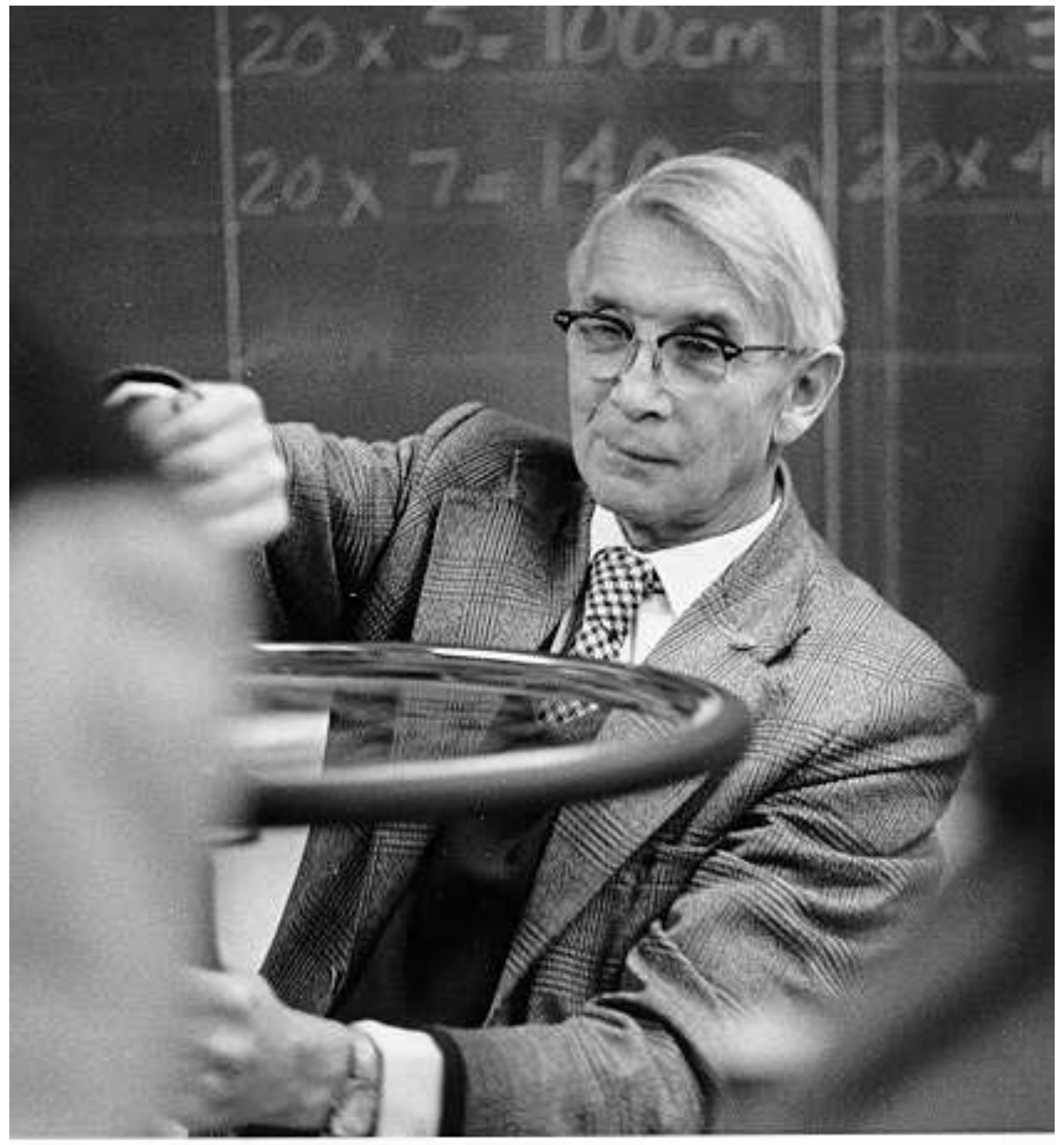
Why is so “famous”?

- Because it’s very simple!

A little bit of history

“Drama”?

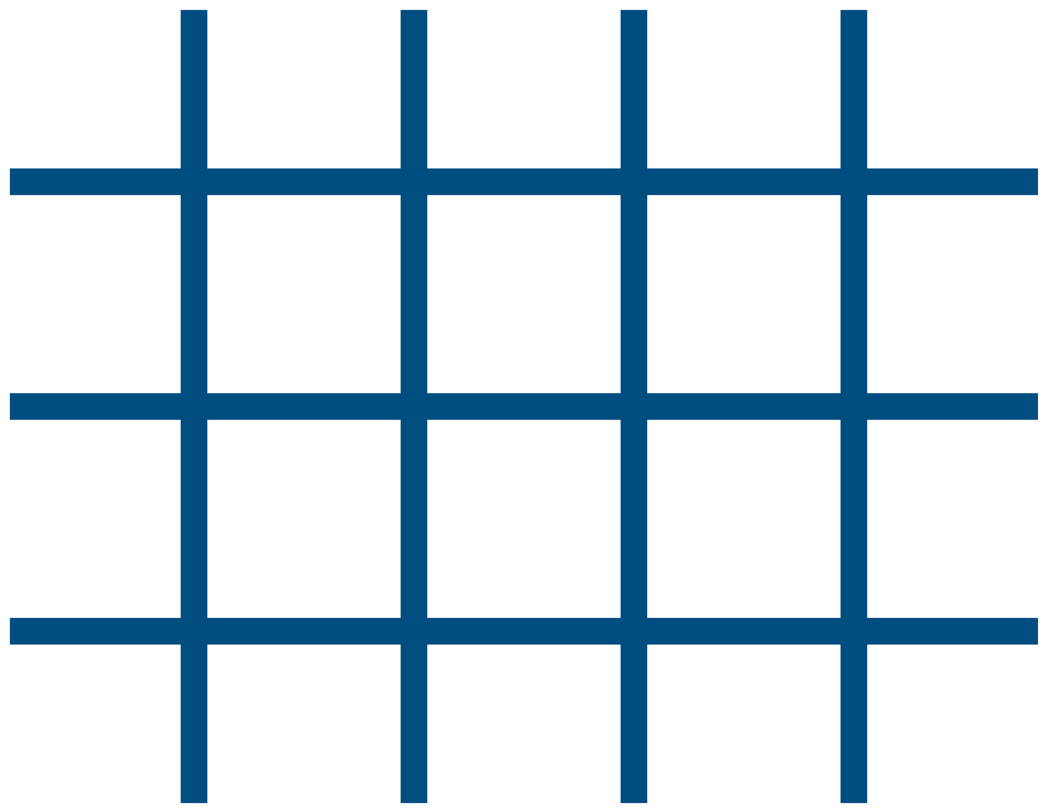
- (1920) Lenz invented the model (PI).
- Lenz: “Hey Ising, I have a cool project for a PhD…”
  - Infinite 1D lattice with coupling and interactions.
- (1925) Ising publish the results (**its only paper btw..**)
  - He didn’t found a phase transition :(
- Exact solutions by Onsager and Kramers in 2D
  - Onsager: “Hey, I have a cool project for a PhD…”
    - 3D extension: **has not yet solved**



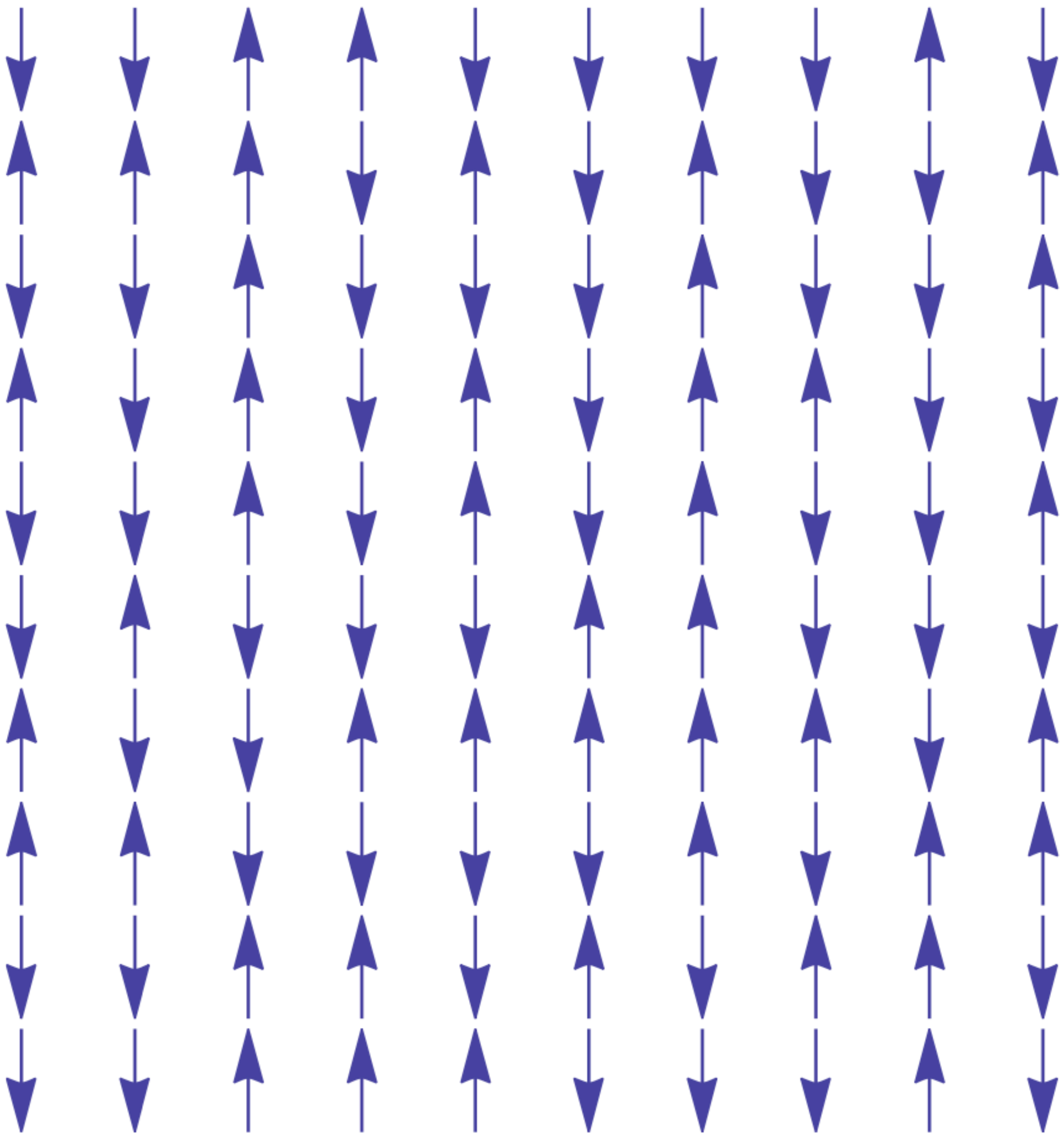
Ernst Ising

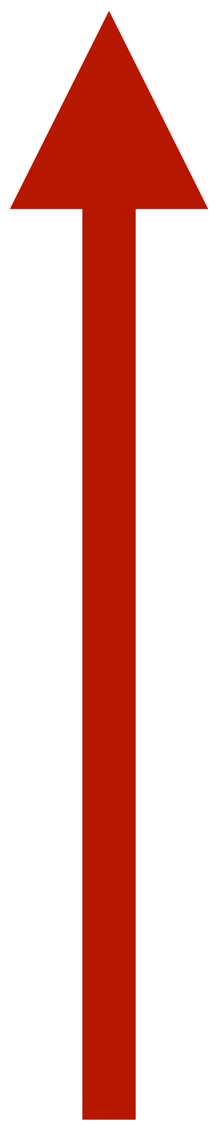
“…it was not until 1949 that he found out from the scientific literature that his model had become widely known…”

(http://theor.jinr.ru/~kuzemsky/isingbio.html)



Lattice of spins





Magnetic Field

What are the "important" things?

Ising-like Hamiltonians

$$E = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i$$

Total Energy

Neighbors **interaction**

Strength of the **B** field

Let's define an order parameter…

$$M = \left\langle \frac{N_\uparrow - N_\downarrow}{N} \right\rangle$$

Compute M as function of:
the **interaction strength**, the **magnetic field**, and the **temperature**

First Case: Non-Interacting Spins

Non-Interacting Spins: Entropy

What do we need?

$$N = N_\uparrow + N_\downarrow \qquad M = \frac{N_\uparrow - N_\downarrow}{N} \qquad \Omega = \frac{N!}{N_\uparrow! N_\downarrow!}$$

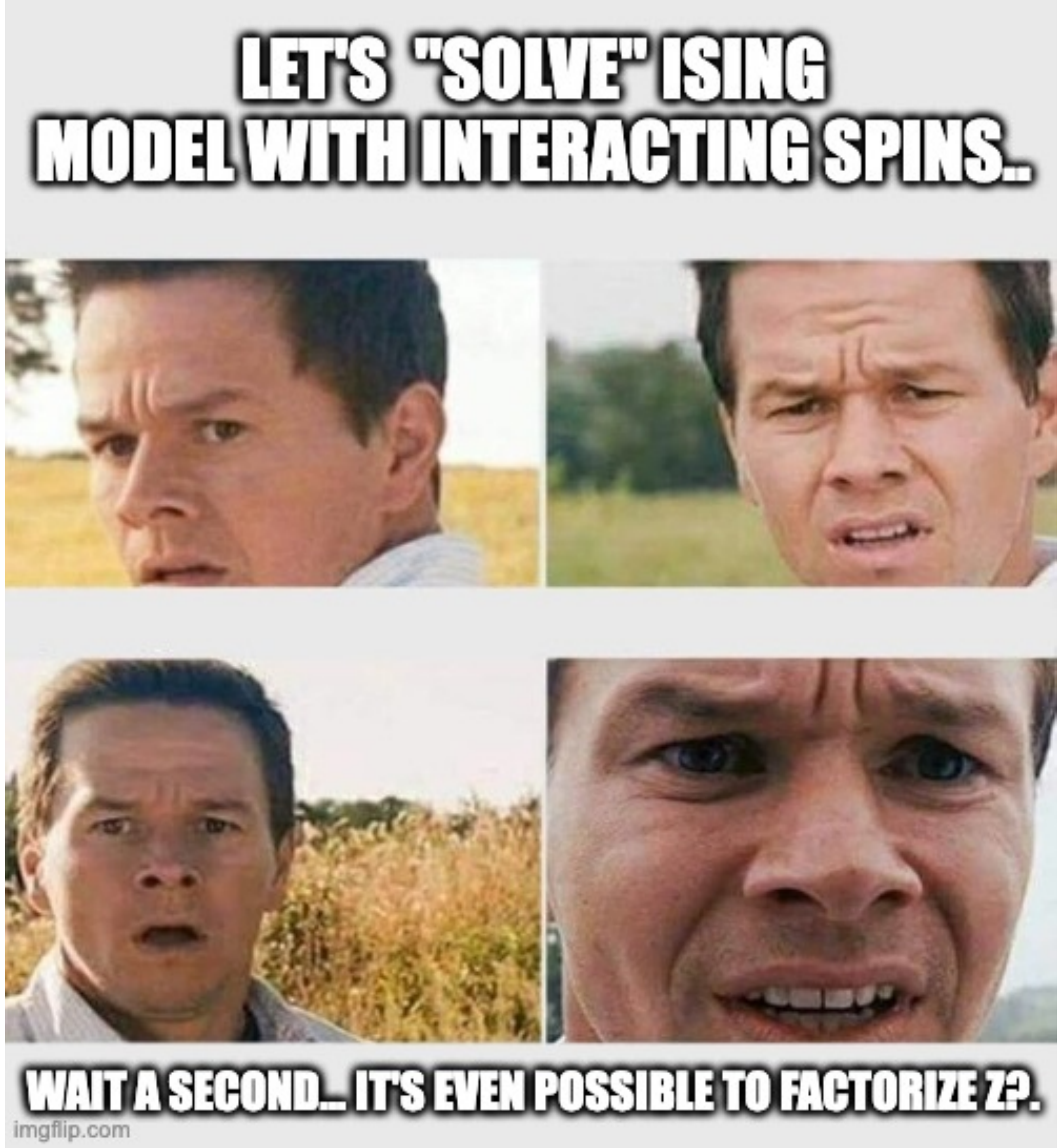
$$\downarrow$$

$$S = -k_B T \left[\left(\frac{1+M}{2} \right) \ln \left(\frac{1+M}{2} \right) + \left(\frac{1-M}{2} \right) \ln \left(\frac{1-M}{2} \right) \right]$$

Second Case: Interacting Spins

Ok, let's do the same!

Wait, something is wrong…



What is the “problem”?

$$Z = \sum_{\sigma_1} \sum_{\sigma_2} \cdots \sum_{\sigma_N} \exp \left[\frac{J}{k_B T} \sum_{<i,j>} \sigma_i \sigma_j + \frac{h}{k_B T} \sum_i \sigma_i \right]$$

All spins are coupled between each other

Issues with Interacting Spins

- “Unfortunately, this problem is much harder than the non-interacting spins. It is not just harder in the sense that I need to look up a tricky integral, or that I have to get Mathematica to calculate something numerically. It is harder in the sense that it consists of a huge number of variables that are all coupled together.” (Selinger)

So, what to do now?

Mean Field Theory Approximation

- We **neglect the correlations** between neighboring spins.
- Assume that they are each **fluctuating independently** with the same statistical distribution.

Let's make mathematicians cry!

$$E_{int} = -J \sum_{<i,j>} \sigma_i \sigma_j$$

$$\langle E_{int} \rangle = -J \sum_{<i,j>} \langle \sigma_i \sigma_j \rangle$$

Let's make mathematicians cry!

$$\langle \sigma_i \sigma_j \rangle \approx \langle \sigma_i \rangle \langle \sigma_j \rangle$$

$$\langle E_{int} \rangle \approx -J \sum_{<i,j>} \langle \sigma_i \rangle \langle \sigma_j \rangle$$

$$\langle E_{int} \rangle \approx -\frac{1}{2} N J q M^2$$

coordination number

$$F = \langle E \rangle - TS$$

We have everything we need to compute the free energy!

The Free Energy:

$$\frac{F}{Nk_BT} = -\left(\frac{Jq}{2k_BT}\right)M^2 - \left(\frac{h}{k_BT}\right)M + \left(\frac{1+M}{2}\right)\ln\left(\frac{1+M}{2}\right) + \left(\frac{1-M}{2}\right)\ln\left(\frac{1-M}{2}\right)$$

Let’s explore the behavior of this function!

Last but not least

What to do next?