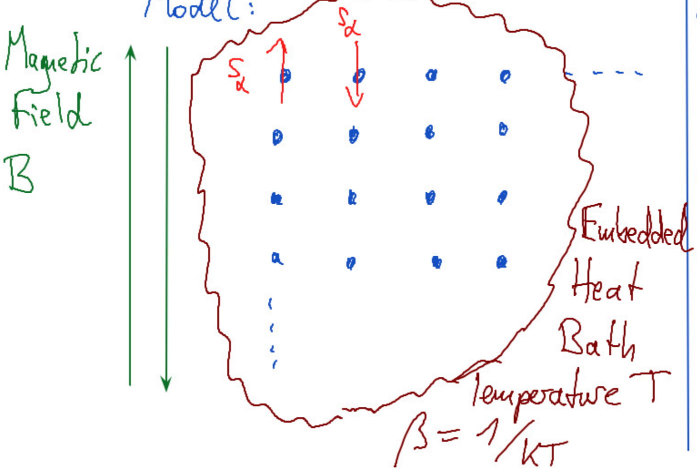
9.1.3. Ising Model

Ernst Ising, 1900 – 1998 Germany / UK / USA

Simple model of ferromagnetism $\Longleftrightarrow$ spontaneous ordering processes

Model:



- 2D mesh of Fe atoms $S_\alpha = \pm 1$
  $\alpha = 1, \ldots$ number of atoms N
  $N = n \times n$ (in Tutorial: $n = 30$, $N = 900$)
- (method of scaling $\Longleftrightarrow$ dimensionless numbers)
- Every spin creates a magnetic moment
  $m = \pm 1 = S_\alpha$

We have in our tutorial $30 \times 30 = 900$ atoms

A spin state: $S = \{ s_1, \dots s_N \}$ describes the physical state of our system.

All possible states of the system: S_i; $i = 1, \dots\dots 2^N \sim 2^{900}$
(forms an ensemble) $\sim 8 \cdot 10^{270}$ states

2^{900} is a <u>really</u> <u>crazy</u> amount of states!

- Number of elementary particles in universe: $\sim 10^{80}$
- Number of Planck time (10^{-44} s) since „Big Bang" $\sim 10^{60}$

Fundamental Quantities:

- Energy of the system H (Hamilton function)

$$H(S_i) = -B \sum_{\alpha} s_\alpha - J \sum_{\langle\alpha\beta\rangle} s_\alpha s_\beta$$

$S_i = \{s_1, \dots s_N\}_i$

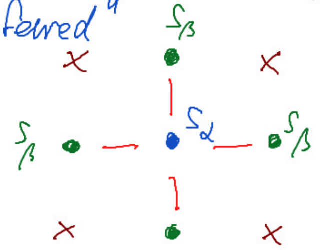
$\alpha = 1 \dots N$

J: spin-spin interaction energy

$J > 0$: ferromagnetic material, parallel spins are „preferred" (smaller energy)

$B > 0$: spins parallel to B „preferred"

$$\sum_{\langle\alpha\beta\rangle} s_\alpha s_\beta = \sum_{\alpha} s_\alpha \Big(\underbrace{\sum_{\beta} s_\beta}_{\text{4 nearest neighbours}} \Big)$$



only consider interactions of s_α with four nearest neighbours

- Magnetic Moment of the system:

$$M(S_i) = \sum_\alpha S_\alpha$$ (remember: every spin $S_\alpha = \pm 1$ corresponds to a magn. mom. $m = \pm 1$)

Note: $-N \le M \le N$ $M=0$: equal number of spin-up and -down

$M=N$: all spins $+1$; $M=-N$ all spins -1

- Magnetic moment per Fe atom (per spin):

$$m(S_i) = \frac{1}{N} M(S_i) \quad ; \quad -1 \le m(S_i) \le +1$$

Note: $m(S_i)$ can take any real value between $-1 \dots +1$

- Energy per Fe atom (per spin):

$$e(S_i) = \frac{1}{N} H(S_i)$$

Thermodynamic Quantities | Statistical Mechanics

- grand canonical ensemble (heat bath, not isolated)
- probability of state S, S_i; $w(S)$, probability density function PDF $p(x)$
- $w(S) = \exp(-\beta H(S)) / Z$

if $H(S)$ is „very" negative $\longleftrightarrow$ probability is high („preferred")
is „very" positive $\longleftrightarrow$ " is small

Normalization factor Z partition sum
- $\sum_{S_i} w(S_i) = 1$

$$Z = \sum_{S_i} \exp(-\beta H(S_i)) \Longrightarrow$$

$$\sum_{S_i} w(S_i) = \frac{1}{Z} \underbrace{\sum_{S_i} \exp(-\beta H(S_i))}_{Z} = 1$$

- Free Energy $F = -kT \log Z = -\frac{1}{\beta} \log Z$
- Internal Energy (equivalent to H) $\beta = 1/kT$ $U = kT^2 \frac{\partial \log Z}{\partial T} = -\underline{\frac{\partial \log Z}{\partial \beta}}$
- Mean Magnetization $M = -\frac{\partial F}{\partial B} = \underline{\frac{1}{\beta} \frac{\partial \log Z}{\partial B}}$

$$M = \frac{1}{\beta Z} \cdot \frac{\partial Z}{\partial B} = \frac{1}{\beta Z} \frac{\partial}{\partial B} \sum_{S_i} \exp(-\beta H(S_i))$$

$$= \underline{\frac{1}{Z}} \sum_{S_i} \underline{\left(\sum_\alpha S_\alpha\right)} \underline{\exp(-\beta H(S_i))} = \sum_{S_i} \underline{w(S_i)} \underline{M_i} =$$

Reminder: $H(S_i) = -B \overline{\sum_\alpha S_\alpha} - J \sum_{\langle\alpha\beta\rangle} S_\alpha S_\beta$ | $M_i = \sum_\alpha S_\alpha$

Average over ensemble!

$$M = \sum_{S_i} w(S_i)\, M_i \qquad M_i = \sum_{\alpha} s_\alpha$$

One state!

mean magnetization
average over all possible spin states
weighted with known prob. $w(S_i)$

M_i is magnetization of one single spin state

$$U = -\frac{1}{Z}\frac{\partial}{\partial\beta} Z = -\frac{1}{Z}\frac{\partial}{\partial\beta}\sum_{S_i} \exp(-\beta H(S_i))$$

$$= \frac{1}{Z}\sum_{S_i} H(S_i)\exp(-\beta H(S_i))$$

$$= \sum_{S_i} w(S_i) H(S_i) \qquad \text{with } H(S_i) = U(S_i)$$

weighted average of $H(S_i)$ over our ensemble!

$$M = \sum_{S_i} w(S_i)\, \underline{M_i} \quad ; \quad U = \sum_{S_i} w(S_i)\, \underline{H(S_i)}$$

Tutorial: • start with random spin state $S_i \rightarrow w(S_i)\cdot Z$

• choose a new state by flipping one spin $\longrightarrow$ accept or reject Metropolis algorithm

in Metropolis we need: $w(S_{i+1}) \,/\, w(S_i)$

• sweeps : N_{spin} times spin flipping

$$\frac{H}{kT} = \beta H \; ; \; h = \beta H \; ; \; b = \beta B \; ; \; j = \beta J$$

$$h = -b \sum_{\alpha} s_\alpha - j \sum_{\langle \alpha\beta \rangle} s_\alpha s_\beta \qquad w(S_i) = \frac{1}{Z} \exp(-h(S_i))$$

Varying in experiment: • b magnetic field • j temperature ($j = J/kT$)

For $j < j_{crit}$ no order

For $j > j_{crit}$ spontaneous order $\rightarrow$ ferromagnetism

- Approximate Model: mean field model $j_{crit} = 0.25$ not real!
- Real case, our experiment: $j_{crit} = 0.4406868\ldots$

Onsager 1944, $\sinh(2 j_{crit}) = 1$

$$\sinh^{-1}(1) = 2 j_{crit} = \ln(1+\sqrt{2})$$

$$\sinh^{-1}(x) = \ln\left(x + \sqrt{x^2+1}\right) \quad \Rightarrow j_{crit} = \frac{\ln(1+\sqrt{2})}{2}$$

$$\sim 0.4406868\ldots$$