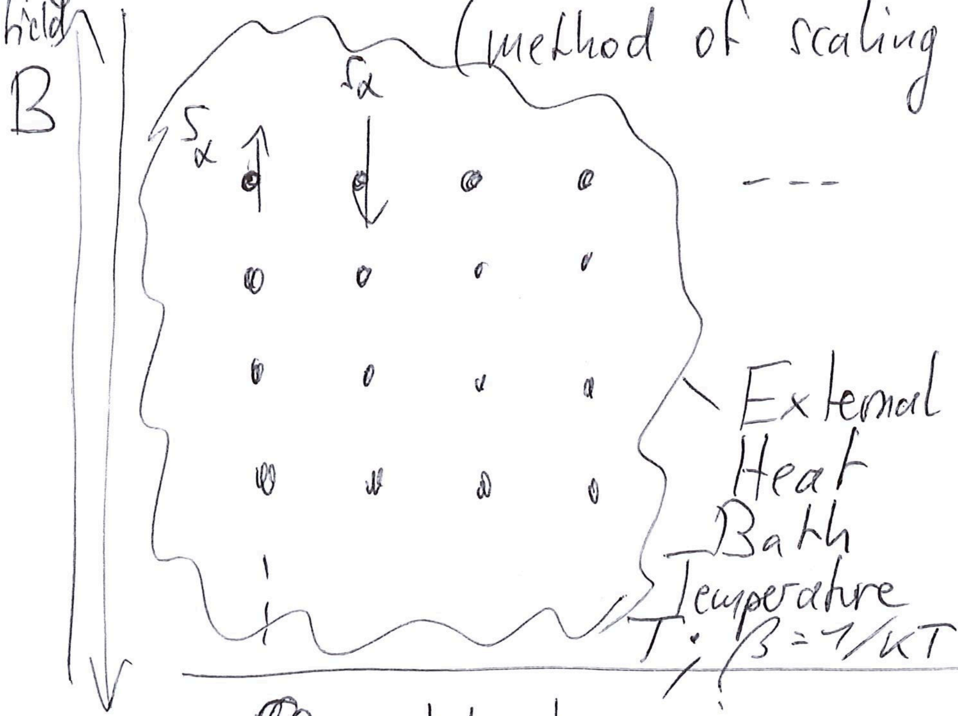
9.1.3. Ising Model

Ernst Ising 1900 – 1998 Germany / UK / USA

Simple model of ferromagnetism $\Longleftrightarrow$ spontaneous ordering processes

External magnetic field

Model: Fe atoms with spin $s_\alpha = \pm 1$ (method of scaling $\Leftrightarrow$ dimensionless number)



Every spin has a magnetic moment, also scaling – dimensionless:

$m = s_\alpha = \pm 1$

We have in exercise $30 \times 30 = 900$ atoms!

A spin state $S = \{s_1, \dots s_N\}$ describes state of the system, all states S_i, $i = 1, \dots N$

There are $\sim 2^N$ states $\sim 8 \cdot 10^{270}$ states

It is a <u>really</u> <u>crazy</u> amount!

Number of elementary particles in universe: $\sim 10^{80}$!

Number of Planck times 10^{-44} s since Big Bang $\sim 10^{60}$!

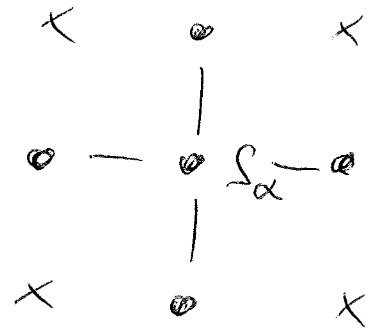
Fundamental Quantities:

- Energy of the System H (Hamilton Function)

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

J: spin-spin interaction energy
$J > 0$: ferromagnetic, parallel spins "preferred" (smaller energy)
$B > 0$: spins parallel to B "preferred")

Special Sum:



$$\sum_{\langle\alpha\beta\rangle} = \sum_\alpha \sum_{4 \text{ neighbours}} S_\alpha S_\beta$$

Only Interaction with 4 nearest neighbours!

- Magnetic Moment of the System:

$$M(S_i) = \sum_\alpha S_\alpha$$

(remember both spin and magn. mom. ± 1!)

- Energy per spin:

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

- Magnetic moment per spin:

$$m(S_i) = \frac{1}{N} M(S_i)$$

Thermodynamic Quantities / Statistical Mechan

- grand canonical ensemble (heat bath, not isolated) $\sum_{S_i} w(S_i) = 1$ Here!
- probability of state S:
  $w(S) = \exp(-\beta H(S)) / Z$; $\beta = \frac{1}{kT}$
- partition sum (Zustandssumme)
  $Z = \sum_{S_i} \exp(-\beta H(S_i))$ $\quad 2^N$ summands

  log = ln = log
- Free Energy $F = -kT \log Z = -\frac{1}{\beta} \log Z$
- Internal Energy $U = kT^2 \frac{\partial \log Z}{\partial T} = -\frac{\partial \log Z}{\partial \beta}$
- Mean Magnetization $M = -\frac{\partial F}{\partial B} = \frac{1}{\beta} \frac{\partial}{\partial B} \log Z$

Compute M and U:

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

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

$$= \sum_{S_i} w(S_i) M_i \quad \text{with } M_i = \left(\sum_{\alpha=1}^{N} S_\alpha \right)_i \checkmark$$

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

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

$$= \sum_{S_i} w(S_i) H(S_i) \quad \text{with } H(S_i) = U_i$$

internal energy of state.

dimensionless values:

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

$$h = -b \sum_{\alpha} s_\alpha - j \sum_{\alpha<\beta} s_\alpha s_\beta$$

Varying in our experiment:

b: magnetic field

j: temperature (indirect via $j = \frac{J}{kT}$)

For $j < j_{crit}$: no order

$j > j_{crit}$: spontaneous order

Approximate Model (mean field): $j_{crit} = 0.25$

Real, our experiment: $j_{crit} = 0.4406868\ldots$

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

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

$$j_{crit} = \frac{\ln(1+\sqrt{2})}{2}$$

$$\sinh^{-1}(x) = \ln\left(x + \sqrt{x^2+1}\right)$$

Ising Model Mean Field Approx.

First: $J = 0$:

$$w(S) \cdot Z = \exp(-\beta H(S)) = \exp\left(+\beta B \sum_\alpha s_\alpha\right)$$
$$= \prod_\alpha \exp(\beta B s_\alpha)$$

$$Z = \sum_{S_i} \exp(-\beta H(S_i)) = \sum_{S_i} \prod_\alpha \exp(\beta B s_\alpha)$$

$$= \left(\exp(\beta B) + \exp(-\beta B)\right)^N$$

Proof by induction: N = 1: trivial

N -> N + 1:

$$Z_{N+1} = \sum_{S_{i,N+1}} \exp(-\beta H(S_i)) = Z_N \exp(-\beta B) + Z_N \exp(+\beta B)$$

$$= \left(\exp(\beta B) + \exp(-\beta B)\right)^{N+1} \checkmark$$

x x

x x

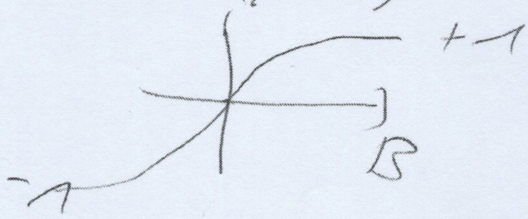
x

$$\log \mathcal{Z} = N \cdot \log\left(e^{\beta B} + e^{-\beta B}\right)$$

$$M_{mf} = \frac{1}{\beta}\,\frac{\partial}{\partial B}\log \mathcal{Z} = N \cdot \frac{e^{\beta B} - e^{-\beta B}}{e^{\beta B} + e^{-\beta B}}$$

$$= N \cdot \tanh(\beta B)$$

$$m_{mf} = \tanh(\beta B)$$



Now assume:

$$H = -\sum_{\alpha} s_\alpha \underbrace{\left(B + J \sum_{\langle\beta\rangle} s_\beta\right)} = -B_{mf} \sum_{\alpha} s_\alpha$$

with $\underline{B_{mf}} = B + 4J\langle s\rangle \Rightarrow m_{mf} = \tanh(\beta B_{mf}) = \langle s\rangle!$

$$= B + 4J \tanh(\beta \underline{B_{mf}})$$

dimensionless

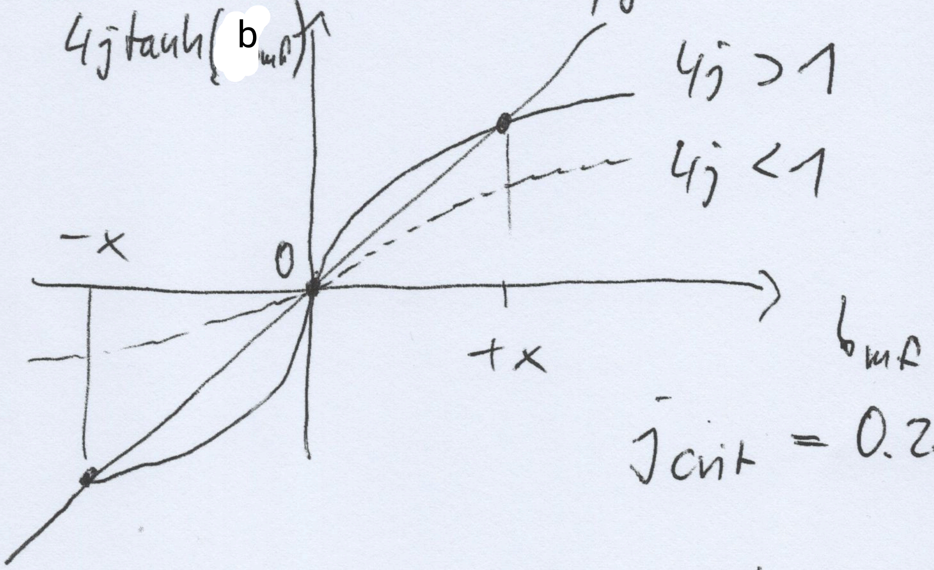
$$\underline{b_{mf}} = b + 4j \tanh(\underline{b_{mf}})$$

For each pair of values b, j we get:

1, 3 solutions for b_{mf} (and m_{mf})

Step 1: Find solutions for b_{mf}, m_{mf} as functions of b, j:

Case (a): $b = 0$:



$J_{crit} = 0.25$

$4j < 1$: only one solution, $b_{mf} = 0$

$\Rightarrow m_{mf} = 0$

$4j > 1$: three solutions, $b_{mf} = 0, +x, -x$

$m_{mf} = 0, \tanh(x), \tanh(-x)$

spontaneous magnetization!

Case (b): $b > 0$: $-x$ and „0" approach each other

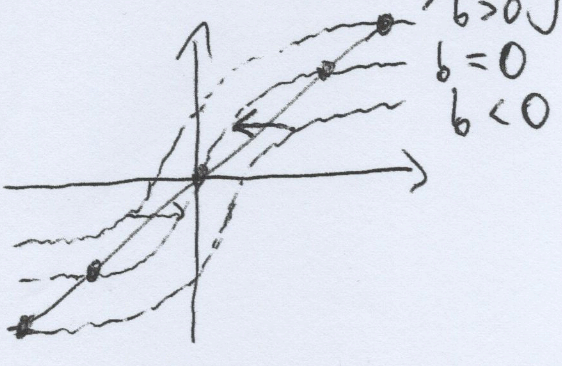
$+x \to \infty$

Case (c): $b < 0$ $+x$ and „0" approach each other

$-x \to -\infty$

If $b > 0$ very large: only one solution $b_{mf} > 0$

$b < 0$ very negative: " " " $b_{mf} < 0$

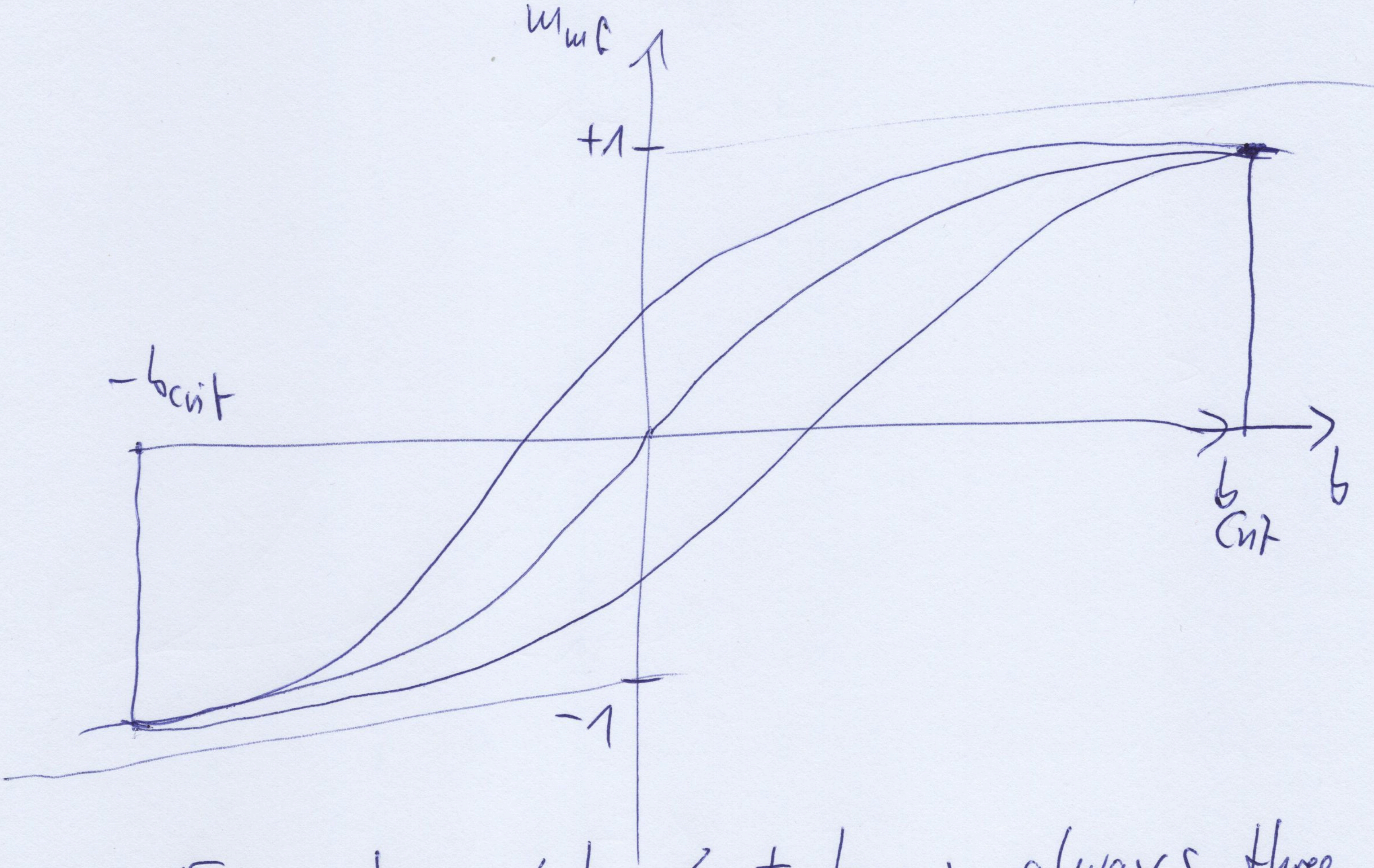


$b > b_{crit}$

$b < -b_{crit}$

Step 2:

Collect all results and plot m_{mf} against b (for some j):
Hysteresis (case $j > j_{crit}$)



For $-b_{crit} < b < +b_{crit}$: always three solutions for m_{mf}

For $j < j_{crit}$: only one curve
only one solution for m_{mf}