$$N \longrightarrow N' = \lambda N \longrightarrow N'' = \mu N' = \lambda\mu N$$

$$N \longrightarrow N'' = (\lambda\mu) N$$

$$b \longrightarrow b' = \phi(\lambda) b \longrightarrow b'' = \phi(\mu) b' = \phi(\mu)\phi(\lambda) b$$

$$b \longrightarrow b'' = \phi(\lambda\mu) b$$

$$\phi(\lambda\mu) = \phi(\lambda)\,\phi(\mu)$$

fractal dimension:

$$N \propto R^{d_f}$$

"mass" — "size"

d_f : fractal dimension

compact: $N \propto R^{d}$

d spatial dimension

non-compact $d_f < d$

polymer:

$$R \propto N^{\nu} \quad \begin{cases} \nu = 1/2 & \text{RW} \\ \nu > 1/2 & \text{SAW} \end{cases}$$

$$N \propto R^{1/\nu} \longrightarrow \boxed{d_f = 1/\nu}$$

polymer is a random fractal

Structure factor ⟷ density-density correlation function:

$$\rho(\vec{r}) = \sum_n \delta(\vec{r}_n - \vec{r}) \qquad \int d^3\vec{r}\, \rho(\vec{r}) = N$$

$$\rho(\vec{r})\, \rho(\vec{r}\,') = \sum_{mn} \delta(\vec{r}_m - \vec{r})\, \delta(\vec{r}_n - \vec{r}\,')$$

$$\exp\left[i \vec{q} \cdot (\vec{r} - \vec{r}\,') \right] \rho(\vec{r})\, \rho(\vec{r}\,') =$$

$$= \sum_{mn} \exp\left[i\vec{q} \cdot (\vec{r} - \vec{r}\,') \right] \delta(\vec{r}_m - \vec{r})\, \delta(\vec{r}_n - \vec{r}\,') =$$

$$= \sum_{mn} \exp\left[i\vec{q} \cdot (\vec{r}_m - \vec{r}_n) \right] \delta(\vec{r}_m - \vec{r})\, \delta(\vec{r}_n - \vec{r}\,')$$

$$\int d^3\vec{r} \int d^3\vec{r}\,' \; \rho(\vec{r})\, \rho(\vec{r}\,')\, \exp\left[i\vec{q}\cdot(\vec{r}-\vec{r}\,') \right] =$$

$$= \sum_{mn} \exp\left(i\vec{q}\cdot(\vec{r}_m - \vec{r}_n) \right) \qquad \Big| \; \langle \ldots \rangle$$

$$\int d^3\vec{r} \int d^3\vec{r}\,' \; \langle \rho(\vec{r})\, \rho(\vec{r}\,') \rangle \, \exp\left[i\vec{q}\cdot(\vec{r}-\vec{r}\,') \right]$$

$$= \sum_{mn} \langle \exp(i\vec{q}\cdot\vec{r}_{mn}) \rangle = N\, S(q)$$

translational invariance:

$$\langle \rho(\vec{r})\, \rho(\vec{r}\,') \rangle = \langle \rho(\vec{r}-\vec{r}\,')\, \rho(0) \rangle$$

$$\underbrace{V \int d^3\vec{r}\, \langle \rho(\vec{r})\, \rho(0) \rangle \exp\left[i\vec{q}\cdot\vec{r} \right] = N\, S(q)}$$

intermezzo:

$$\langle A \rangle = \frac{1}{Z} \int d^3\bar{r}_1 \int d^3\bar{r}_2 \ldots \int d^3\bar{r}_N \; \exp(-\beta \mathcal{H})\, A$$

2.5. Scaling of the Structure Factor for the SAW

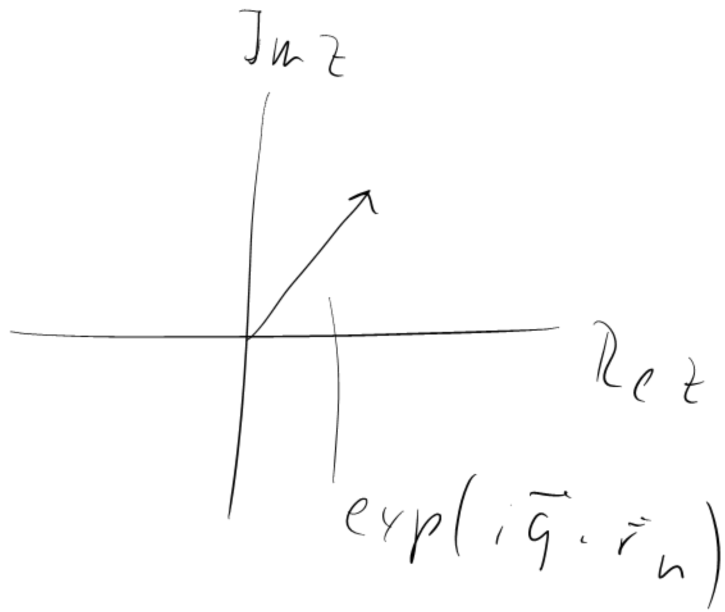
$$S(q) = \frac{1}{N} \left\langle \left| \sum_n \exp(i \vec{q} \cdot \vec{r}_n) \right|^2 \right\rangle$$

$$q \to 0 : \; S(q) \simeq N \left[1 - \frac{1}{3} q^2 \langle R_G^2 \rangle + O(q^4) \right]$$

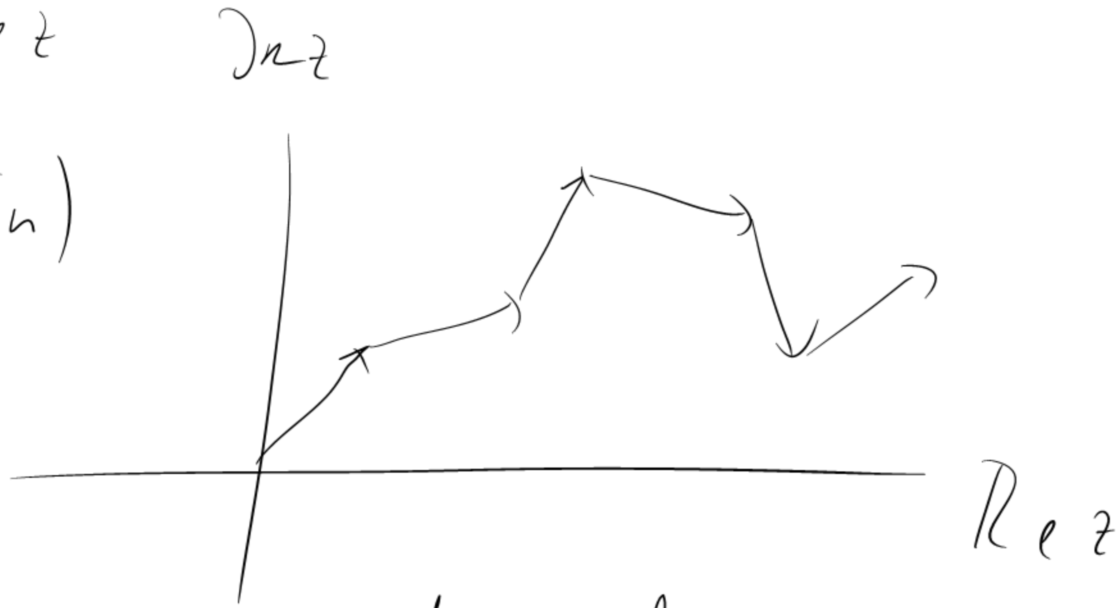
<u>regimes:</u>

- $q \ll \frac{1}{R_G}$ $\quad S(q) \simeq N$
- $\frac{1}{R_G} \ll q \ll \frac{1}{b}$ $\quad$ scaling
- $\frac{1}{b} \ll q$ $\quad$ non-universal regime

$\exp(i\vec{q}\cdot\vec{r}_n)$ is a complex number of absolute value <u>one</u>.



$\sum_n \exp(i\vec{q}\cdot\vec{r}_n)$



corresponds to a polymer chain in the complex plane random walk with stiffness,

stiffness depends on q

extreme limit $q \gg 1/b$

$\rightarrow$ freely jointed chain, no stiffness left

$$\underline{\underline{S(q)}} = \frac{1}{N} \cdot 1^2 \cdot N = \underline{\underline{1}}$$

what is $S(q)$ for $1/R_g \ll q \ll 1/b$?

$$S(q) = \frac{1}{N} C_\infty \lambda^2 \cdot N = C_\infty \qquad C_\infty = C_\infty(q)$$

INDEPENDENT OF N !

rescaling:

$$N \longrightarrow \lambda N$$

$$R_h \longrightarrow \lambda^\nu R_h$$

$$S(q) \longrightarrow S(q)$$

<u>ansatz</u>: $S(q) = N f(q R_h)$ cf. $q \to 0$ behavior

$$= \lambda N f(q \lambda^\nu R_h) \Rightarrow f(x) = \lambda f(\lambda^\nu x)$$

$$S(x) = \lambda f(\lambda^{\nu} x)$$

$$\lambda = x^{-1/\nu}$$

$$\Rightarrow \lambda^{\nu} = x^{-1}$$

$$f(x) = x^{-1/\nu} \; f(1)$$

$$\lambda^{\nu} x = 1$$

$$S(q) \sim N (q R_G)^{-1/\nu} = q^{-1/\nu} \underbrace{N R_G^{-1/\nu}}$$

independent of N

" " R_G

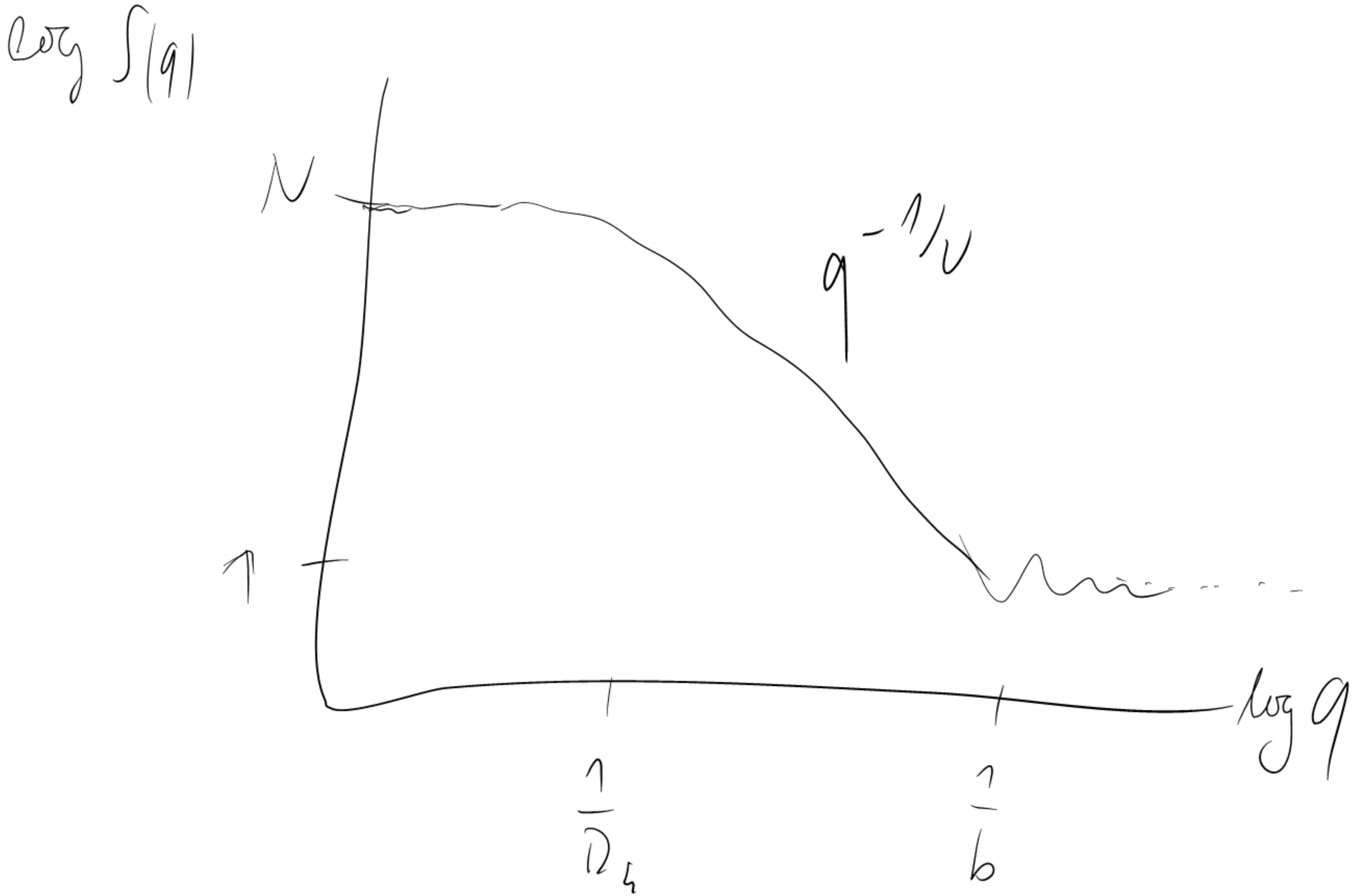
$$R_G \propto N^{\nu}$$

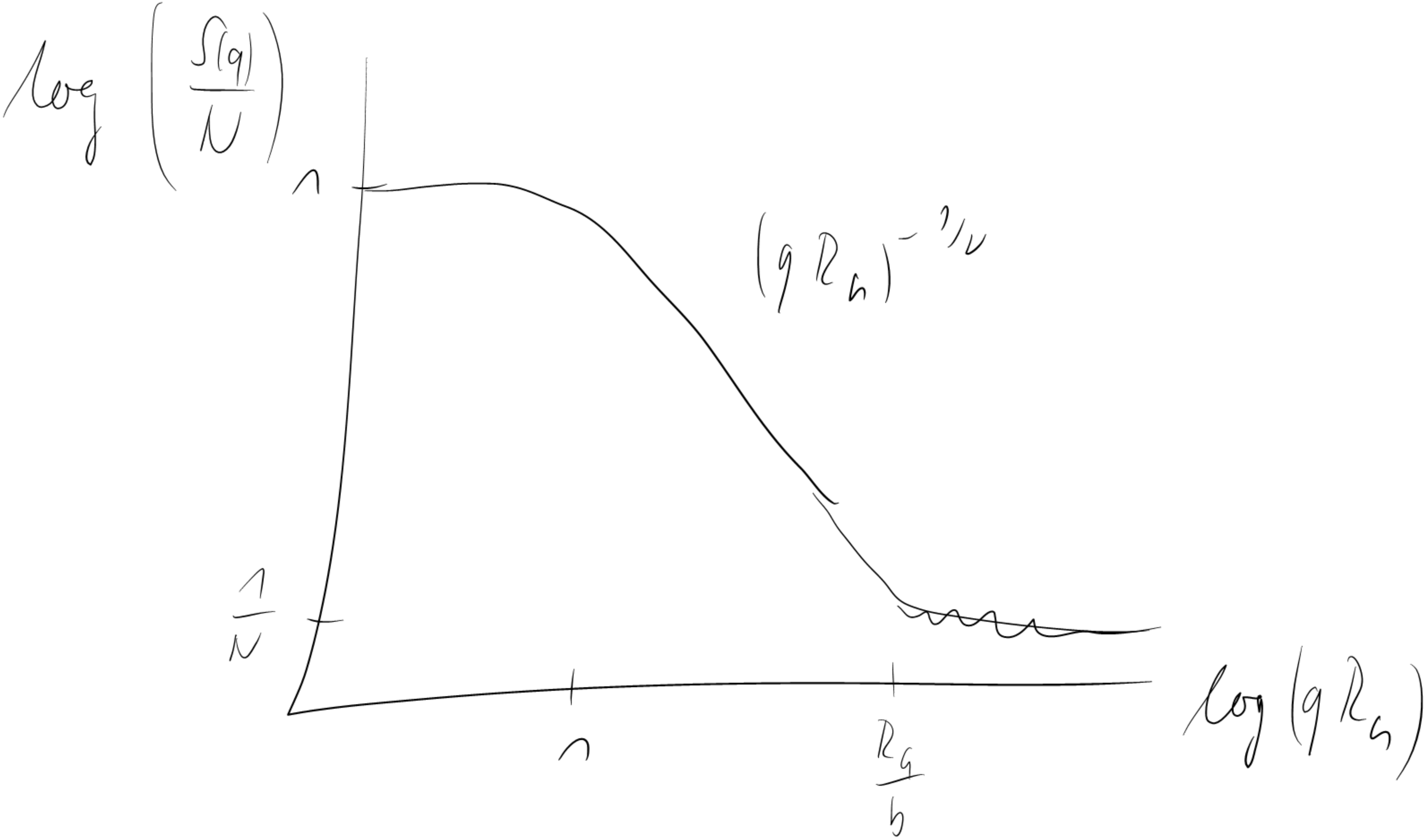
$$R_G^{-1/\nu} \propto N^{-1}$$

$$N R_G^{-1/\nu} \propto N^{0}$$

$$\boxed{S(q) \propto q^{-1/\nu}}$$

fractal scattering law


$\log S(q)$
N
$q^{-1/\nu}$
1
$\log q$
$\frac{1}{R_g}$
$\frac{1}{b}$



$\log\left(\frac{S(q)}{N}\right)$
1
$\frac{1}{N}$
$(qR_n)^{-1/\nu}$
1
$\frac{R_g}{b}$
$\log(qR_n)$

Excursion: Ising Model

Set of spin variables $S_i = \pm 1$

$\uparrow \quad S_i = +1$ spin up

$\downarrow \quad S_i = -1$ spin down

Each Spin is subjed to an external magnetic field H, no interaction between spins.

$$\mathcal{H} = -H \sum_i S_i$$

$H > 0 \rightarrow S_i$ likes to be positive

$H < 0 \rightarrow$ " " " " negative

$T = 0 \rightarrow$ perfect alignment

$T = \infty \rightarrow$ random orientation

$$m = \frac{1}{N} \sum_i \langle S_i \rangle = \langle S \rangle$$

magnetization

# of spins

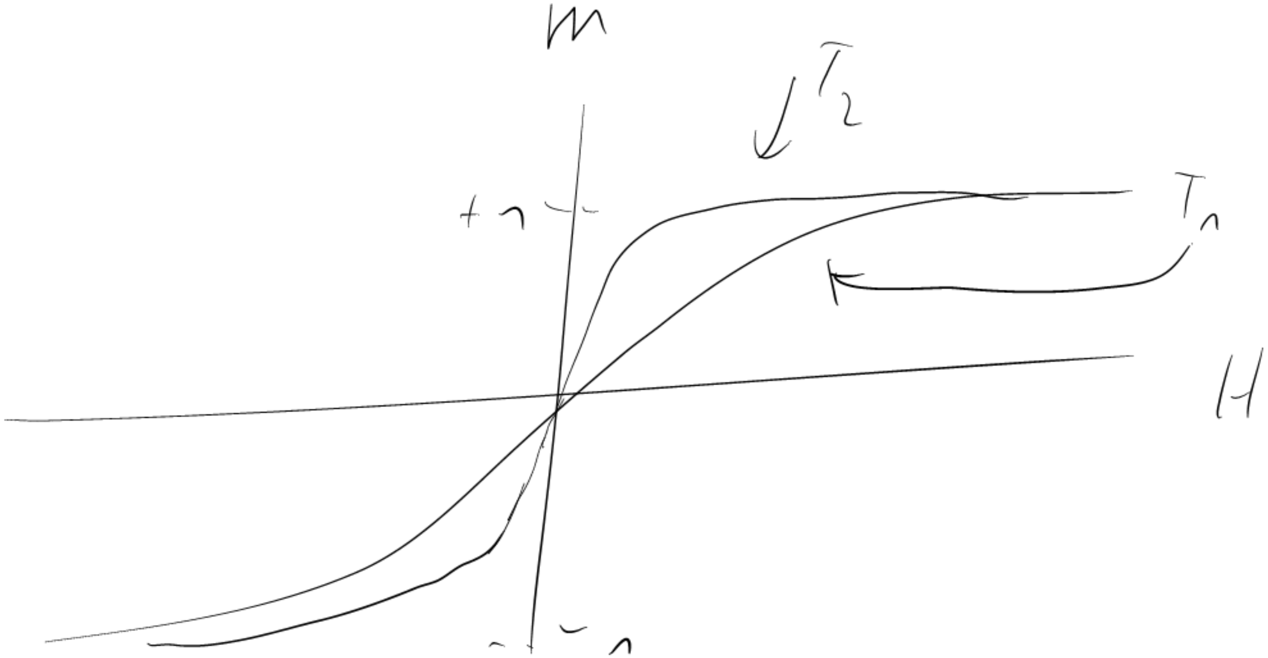
no interaction $\rightarrow$ sufficient to just look at one single spin single spin: $\mathcal{H} = -HS \qquad S = \pm 1$

$$\langle S \rangle = \frac{(+1)\, e^{-\beta \mathcal{H}_+} + (-1)\, e^{-\beta \mathcal{H}_-}}{e^{-\beta \mathcal{H}_+} + e^{-\beta \mathcal{H}_-}} \qquad \beta = \frac{1}{k_B T}$$

$$\mathcal{H}_+ = -H \qquad \mathcal{H}_- = +H$$

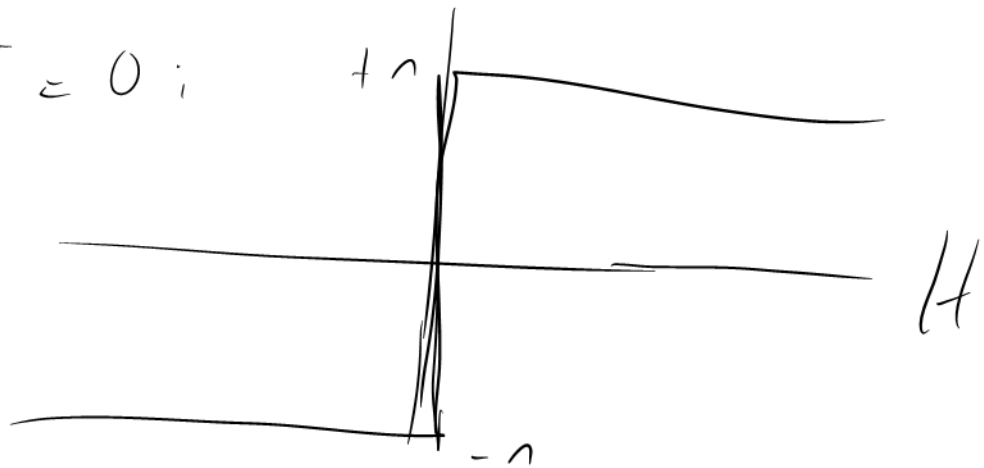
$$\langle S \rangle = \frac{e^{+\beta H} - e^{-\beta H}}{e^{+\beta H} + e^{-\beta H}} = \frac{2 \sinh(\beta H)}{2 \cosh(\beta H)} = \tanh(\beta H)$$

$$m = \tanh(\beta H)$$



$$T_2 < T_1$$

$T = 0$:



now, <u>interacting</u> Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j \qquad \underline{\underline{J > 0}}$$

magnetic coupling constant

i lattice site, S_i site on i

$\langle ij \rangle$ nearest-neighbors

$S_i \cdot S_j > 0 \longrightarrow$ energy is decreased

system wants the spins <u>aligned</u>

$T=0$ all spins up OR all spins down

$T=\infty$ random orientation

$0<T<\infty$: difficult

Mean Field approximation $\rightarrow$ replace many-body problem with an effective single-body " (uncontrolled)

$$m = \langle S \rangle = \frac{1}{N} \sum_i \langle S_i \rangle$$

$$S_i = m + \delta S_i$$

quadratic in fluctuations $\rightarrow$ discard

$$S_i S_j = m^2 + \delta S_i \delta S_j + m \delta S_i + m \delta S_j$$

assumption: fluctuations are small and can be neglected

$$S_i S_j \longrightarrow m^2 + m(\delta S_i + \delta S_j) =$$

$$= m^2 + m(S_i + S_j - 2m) = m(S_i + S_j) - m^2$$

$$\mathcal{H} \to \mathcal{H}_{MF} = -J \sum_{\langle ij \rangle} \left\{ m (S_i + S_j) - m^2 \right\}$$

m does not depend on S_i, view it as just a number

constant energy offsets do not matter $\to$

$$\mathcal{H}_{MF} = -Jm \sum_{\langle ij \rangle} (S_i + S_j)$$

z : coordination # $\equiv$ # of nearest neighbors around a given site e.g. $z = 4$ square lattice

$z = 6$ triangular "

$z = 6$ simple-cubic lattice

$z = 12$ fcc lattice etc.

count # of nearest-neighbor bonds:

$N \cdot z \cdot \frac{1}{2}$ study: $\sum_{\langle ij \rangle} (S_i + S_j)$

# of spins → each spin occurs z times

$$\mathcal{H}_{MF} = -Jmz\sum_i S_i$$

<u>Same</u> Hamiltonian as the paramagnet with effective magnetic field $H_{eff} = Jmz$

$$\Rightarrow \langle S \rangle = \tanh(\beta H_{eff})$$

$$m = \tanh(\beta J z m)$$

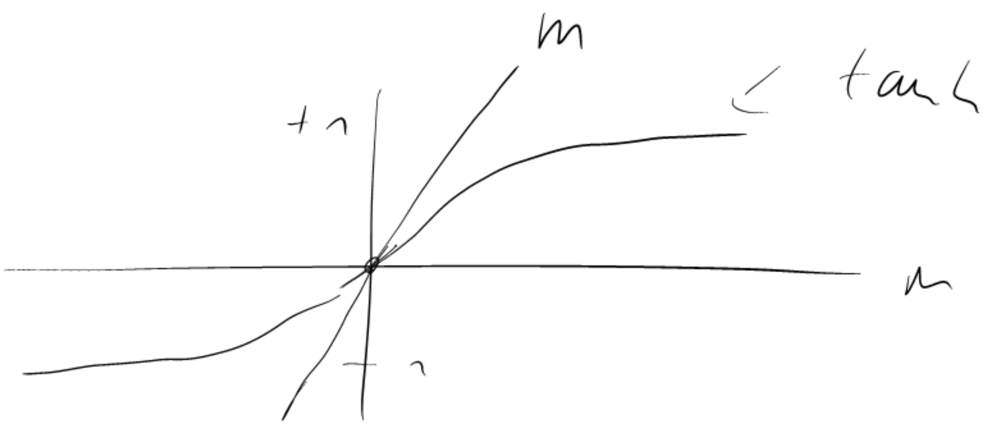
self-consistency condition

$k_B T_c = J z \qquad T_c \equiv$ critical temperature

$$\beta J z = \frac{1}{k_B T} k_B T_c = \frac{T_c}{T}$$

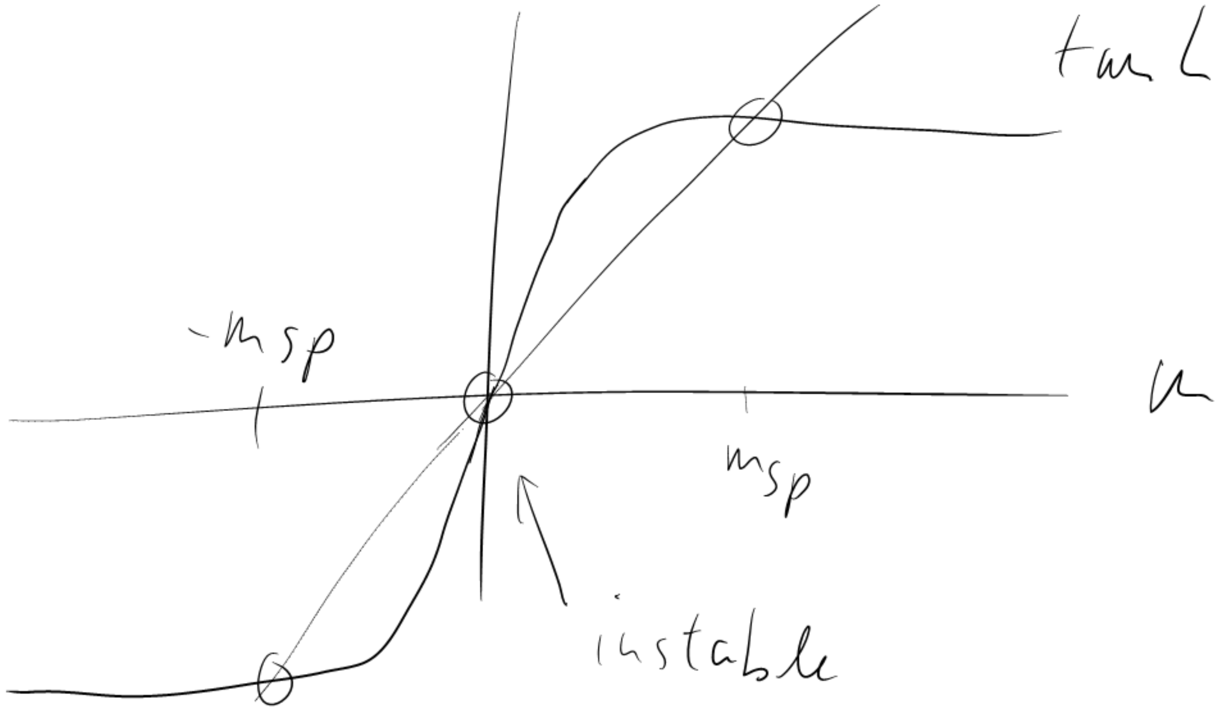
$$m = \tanh\left(\frac{T_c}{T} m\right)$$

$$T > T_c \Rightarrow \frac{T_c}{T} < 1$$



$$\boxed{m = 0}$$

$T < T_c \qquad \frac{T_c}{T} > 1$



m_{sp}: "spontaneous magnetization"

3. Self-Consistent Field Theory of Polymers

Mean Field Theory for polymers

<u>idea:</u> polymer chain = RW + interactions

excluded volume

other intra-molecular interactions

interactions with other chains

replaced by

polymer = RW + interaction with an external field

to be determined self-consistently

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how to treat a RW in an external potential?