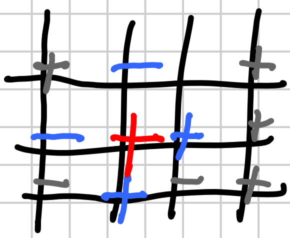
The Ising Model

2-state spin system with nearest neighbor interaction

Ernst Ising, Beitrag zur Theorie des Ferromagnetismus, Z. Physik 31, 253 (1925), suggested by Wilhelm Lenz as PhD topic

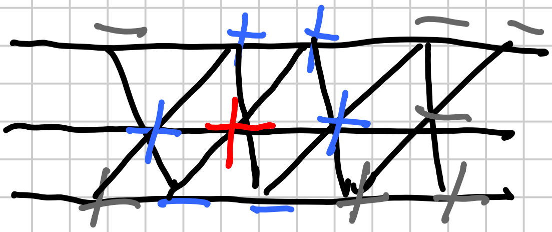
1D: − + − − + + − + − ...

2D:



nearest neighbors

also possible: triangular lattice



3D: bcc lattice with 50% copper and zinc as in beta brass

Hamiltonian depends on classical spin variable s_i at site i

$$s_i \in \{-1, +1\}$$

$$\boxed{\mathcal{H} = -\underbrace{J}_{\text{exchange energy}} \sum_{\langle ij \rangle} s_i s_j - \underbrace{H}_{\text{external magnetic field}} \sum_i s_i}$$

$J = 0$: paramagnet,
only external field leads to magnetic ordering

$J \neq 0$: Spin interact with each other
↳ phase transition possible even for $H = 0$

Why should we look at simple lattice models?

1. description for actual magnet, e.g. MnF_2
2. already simple models have very rich mathematical structure
3. universality of phase transitions allows conclusions for much more complicated (molecular) systems

Statistical mechanics for Spin System
- a refresher -

canonical partition function

$$Z(T, H) = \sum_n e^{-\beta E_n}$$

sum over all n states with energy E_n
with $\beta = 1/k_B T$

free energy for magnet

$$\mathcal{F}(T,H) = -k_B T \ln \mathcal{Z}(T,H)$$

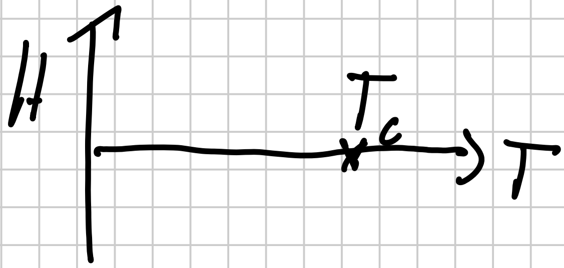
similar: free energy for fluid

$$\mathcal{F}(T,V) = -k_B T \ln \mathcal{Z}(T,V)$$

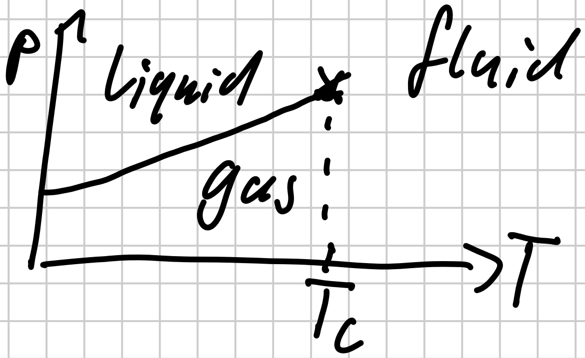
all macroscopic thermodynamic properties follow from free energy by differentiation

	magnet	fluid
energy	$dU = TdS - MdH$	$dU = TdS - pdV$
	1st law of thermodynamics	
internal energy	$U = -\partial_\beta \ln \mathcal{Z}$	
entropy	$S = -\partial_T \mathcal{F}\vert_H$	$S = -\partial_T \mathcal{F}\vert_V$
specific heat	$c_H = \partial_T U\vert_H = T\partial_T S\vert_H$	$c_V = \partial_T U\vert_V = T\partial_T S\vert_V$
	$c_M = T\partial_T S\vert_M$	$c_p = T\partial_T S\vert_p$
	$M = -\partial_H \mathcal{F}\vert_T$ magnetization	$p = -\partial_V \mathcal{F}\vert_T$ pressure
isothermal ...	$\chi_T = \partial_H M\vert_T$ susceptibility	$\kappa_T = -\frac{1}{V}\partial_p V\vert_T$ compressibility

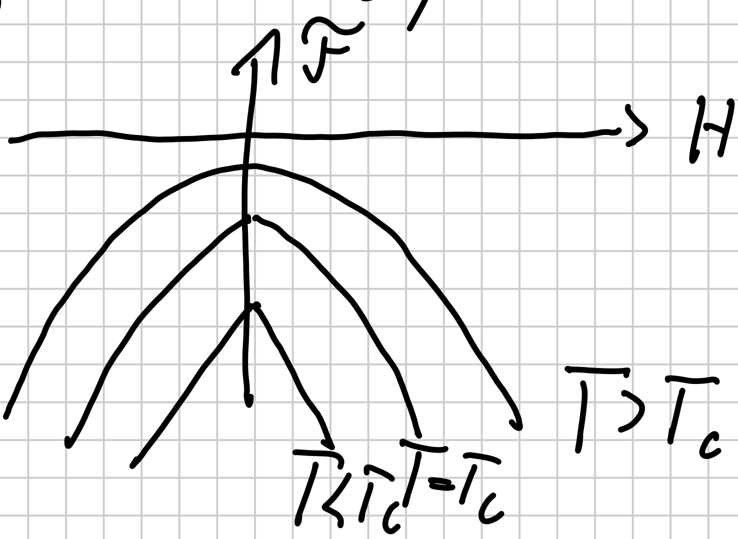
phase diagram of a ferromagnet



cf.



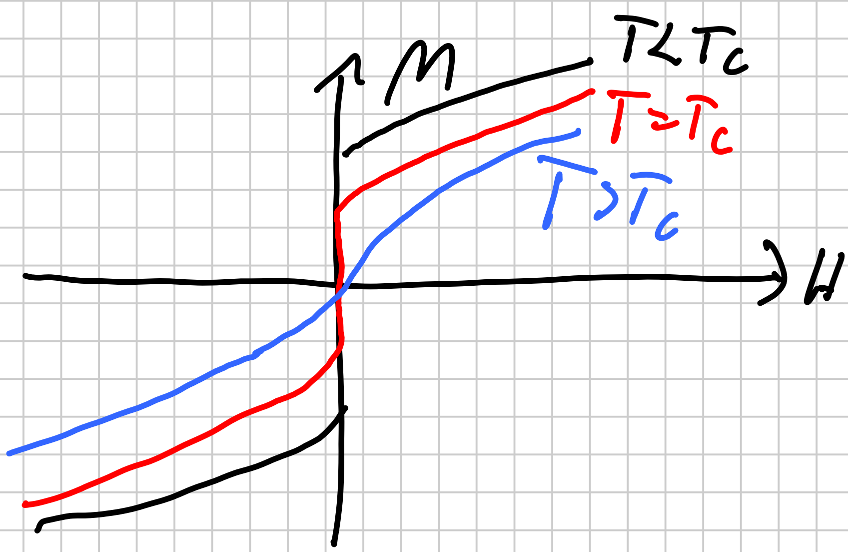
free energy



- symmetric for $\pm H$
- smooth for $T > T_c$
- discontinuous 1st derivative for $T < T_c$
  $\hookrightarrow$ 1st order phase transition
- at $T = T_c$, $H = 0$ discontinuity in 2nd derivative
  (Ehrenfest: "2nd order phase transition", should not be used → "continuous phase transition")

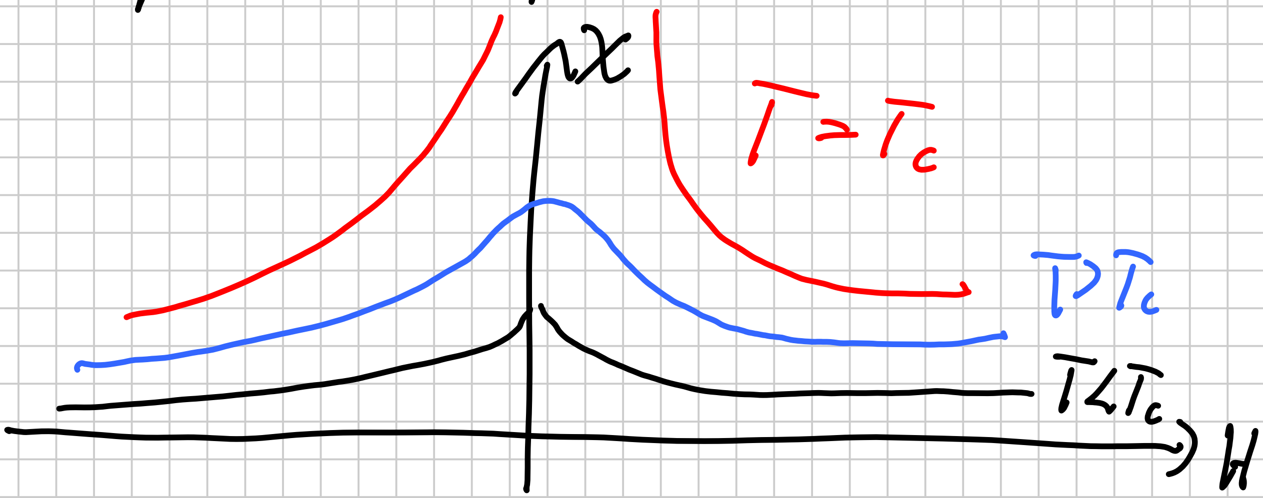
magnetization

$$M = -\partial_H \tilde{F}|_T$$

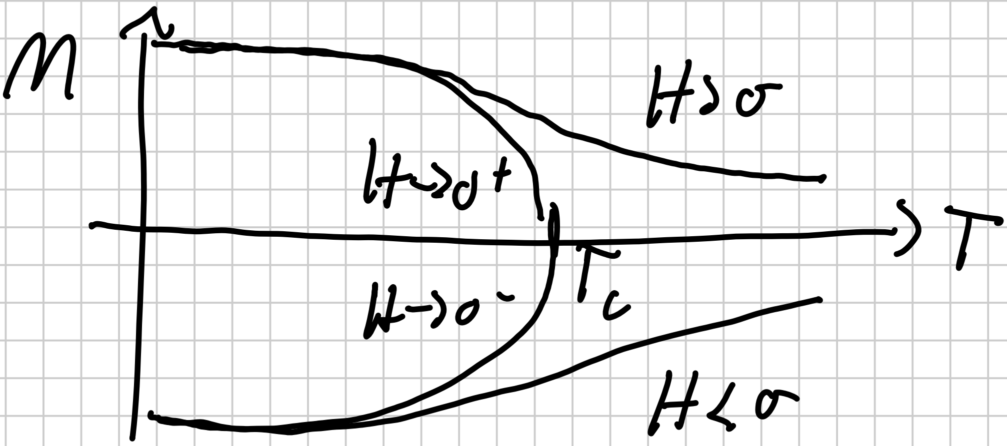


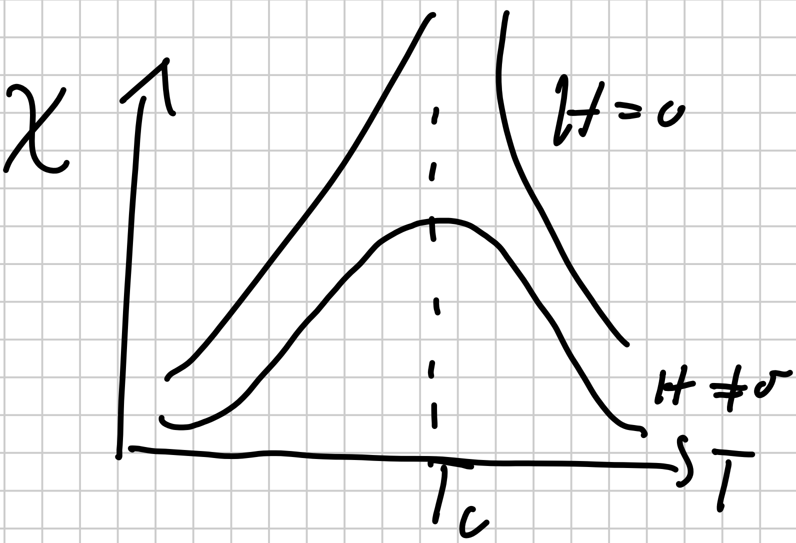
susceptibility

$$\chi_T = -\partial_H^2 F|_T > 0$$



dependence on temperature for finite field





Spatial correlation functions

most important example: pair correlation

$$\Gamma(\vec{r}_i, \vec{r}_j) = \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle$$

translational invariance: $\langle S_i \rangle = \langle S_j \rangle = S$

homogeneity

$$\Gamma(\vec{r}_i, \vec{r}_j) = \Gamma(\vec{r} = \vec{r}_i - \vec{r}_j)$$

isotropy $\Gamma(\vec{r}) = \Gamma(r = |\vec{r}|)$

experimental finding: spins become uncorrelated for $r \to \infty$, also for $T < T_c$ where $\langle S_i \rangle = S \neq 0$

exponential decay of correlations

$$\Gamma(r) \sim r^{-\tau} e^{-r/\xi}$$

with <u>correlation length</u> ξ

experimental evidence close to critical point: $\xi \to \infty$, long-range order develops.

↳ power-law decay of correlations

$$\Gamma(r) \sim 1/r^{d-2+\eta}$$

critical exponent η

Summary of critical exponents -19-

	magnet	fluid
specific heat	$c_H \sim \|t\|^{-\alpha}$	$c_V \sim \|t\|^{-\alpha}$
order parameter	$M \sim (-t)^{\beta}$	$(\rho_{liq} - \rho_{gas}) \sim (-t)^{\beta}$
susceptibility	$\chi_T \sim \|t\|^{-\gamma}$	$\kappa_T \sim \|t\|^{-\gamma}$
critical isotherm	$H \sim \|M\|^{\delta} \operatorname{sgn} M$	$p - p_c \sim \|\Delta\rho\|^{\delta} \operatorname{sgn} \Delta\rho$ $\Delta\rho := \rho_{liq} - \rho_{gas}$
correlation length	$\xi \sim \|t\|^{-\nu}$	
pair correlation at T_c	$G(r) \sim 1/r^{d-2+\eta}$	

ferromagnet
T_c: Curie temperature

antiferromagnet
T_c: Néel temperature

$$M \sim (T_N - T)^{\beta}$$

Heller/Benedek, PRL 8, 428 (1962): $\boxed{\beta \approx 1/3}$