Lecture 23

19.04.2019

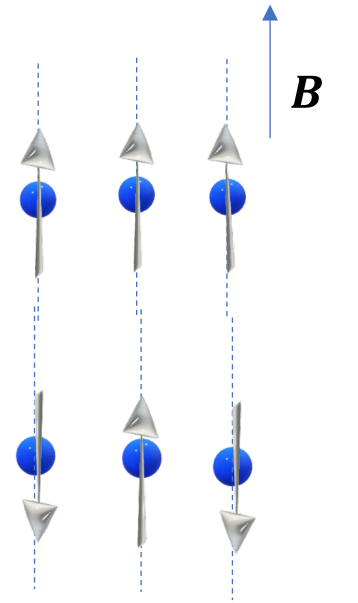
Weiss mean-field theory

Ferromagnetic phase transition

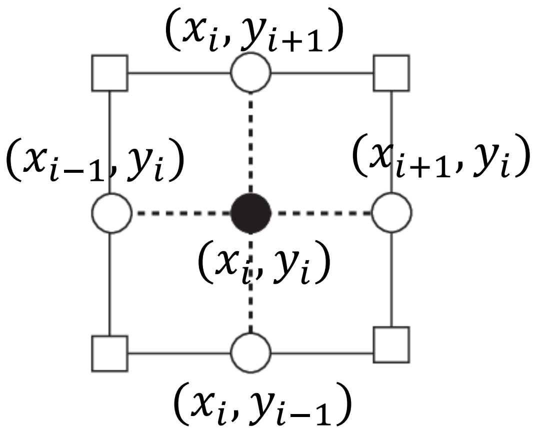
Ising model for ferromagnets

A system of N spins $s_i = \pm 1$ on a periodic lattice and in a uniform magnetic field B. Spins interact with their nearest neighbor on the lattice

$$H_N = -J \sum_{i} \sum_{\substack{j= \\ n.n.\, of\, i}} s_i s_j - \sum_i s_i B\,, \qquad (\mu_B = 1)$$

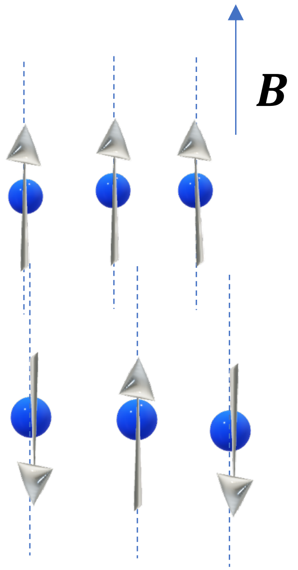


- $\mathrm{J} > 0$ is the coupling constant, such that the energy is minimized when neighboring spins point in the same direction
- Summation over the nearest neighbors (n.n.) j atoms that are coupled to the ith atom on a crystal lattice (short hand notation used sometime $\equiv \langle \mathrm{ij} \rangle$)
- The form of the spin-spin interaction as $-J s_i s_j$ originates the Coulomb interactions between the electrons (spin carriers); magnetic dipole interactions are too weak.



Ising model for ferromagnets

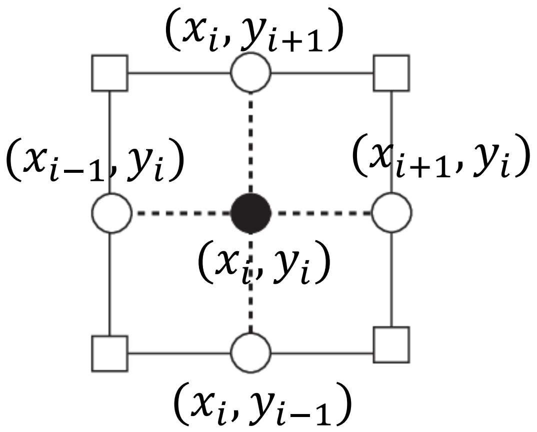
A system of N spins $s_i = \pm 1$ *on a periodic lattice and in a uniform magnetic field* B. *Spins interact with their nearest neighbor on the lattice*



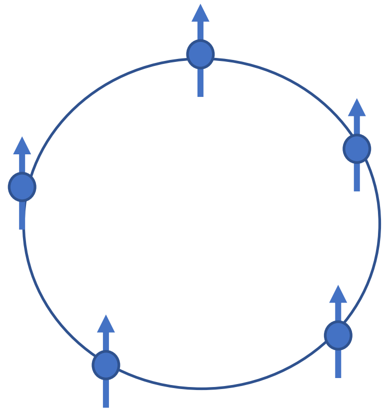
$$H_N = -J \sum_{i} \sum_{\substack{j= \\ n.n.\,of\,i}} s_i s_j - \sum_i s_i B\,, \qquad (\mu_B = 1)$$

- Ising model exhibits a **critical phase transition** at a finite tempeture T_c and applied field $B = 0$

- The properties of this ferromagnetic phase transition can be studied within the mean-field approximation



1D Ising model: No phase transition



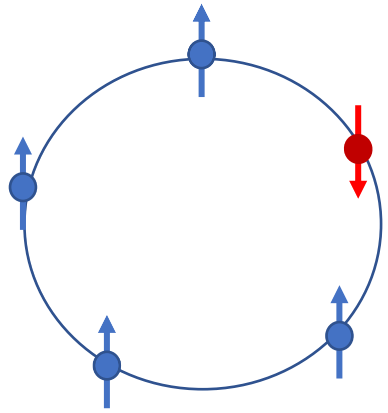
At any nonzero temperature, it is energetically favorable to create defects (kinks) due to thermal fluctuations

Change in energy for flipping a spin (kink in the ordered state)

$$U_0 = -NJ\ (order), \qquad U_1 = -(N-2)J + 2J\ (with\ a\ kink) \rightarrow \Delta U = 4J$$

Change in entropy for flipping a spin anywhere in the 1D chain (N sites)

$$\Delta S = k \log N$$

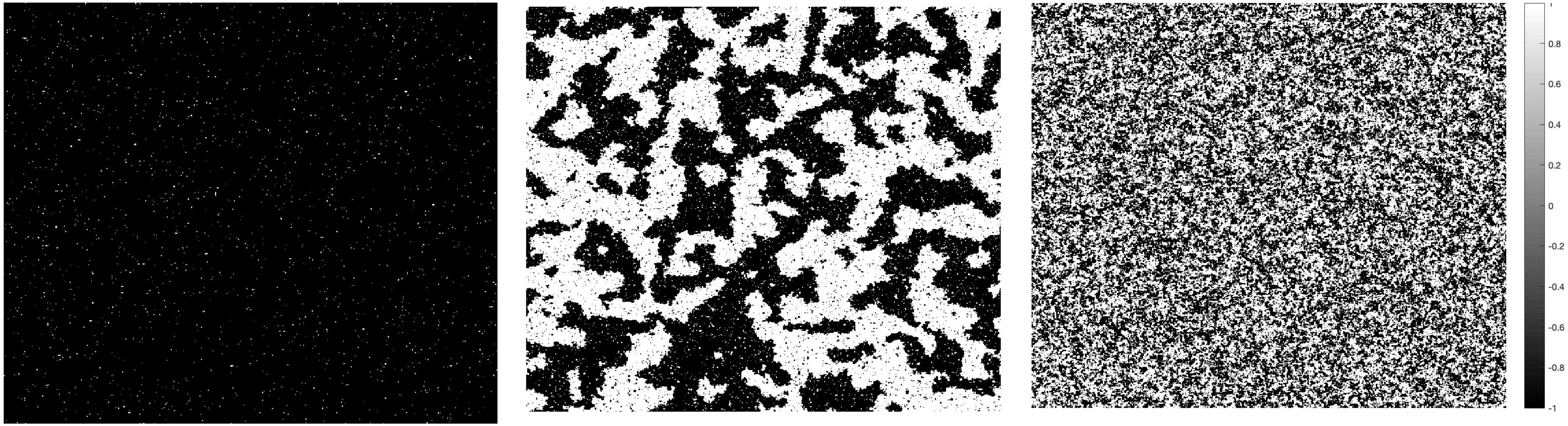


The spin flipping due to thermal fluctuations is favored when it lowers the **Helmholtz free energy**

$$\Delta F = \Delta U - T\Delta S < 0 \rightarrow J - kT \log N < 0$$

This is always satisfied at any $\mathrm{T} > 0$, hence the spin order is spontaneously broken by kinks due thermal fluctuations.

Ising model for ferromagnetism



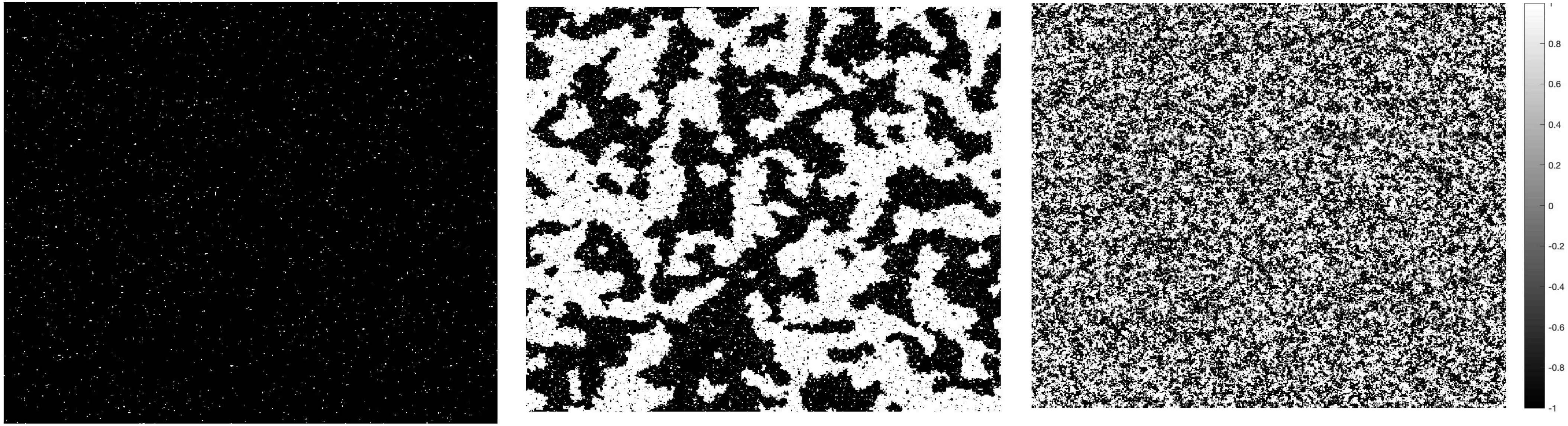
$T < T_C$ $\qquad$ $T \lesssim T_C$ $\qquad$ $T > T_C$

Critical phase transition occurs at a unique point in the $B - T$ diagram: $(B_c = 0, T_c)$

Q: How do we *theoretically* predict this critical point and the behavior near it?

A: Mean-field approximation, Landau field theory, renormalization group techniques

Ising model for ferromagnetism



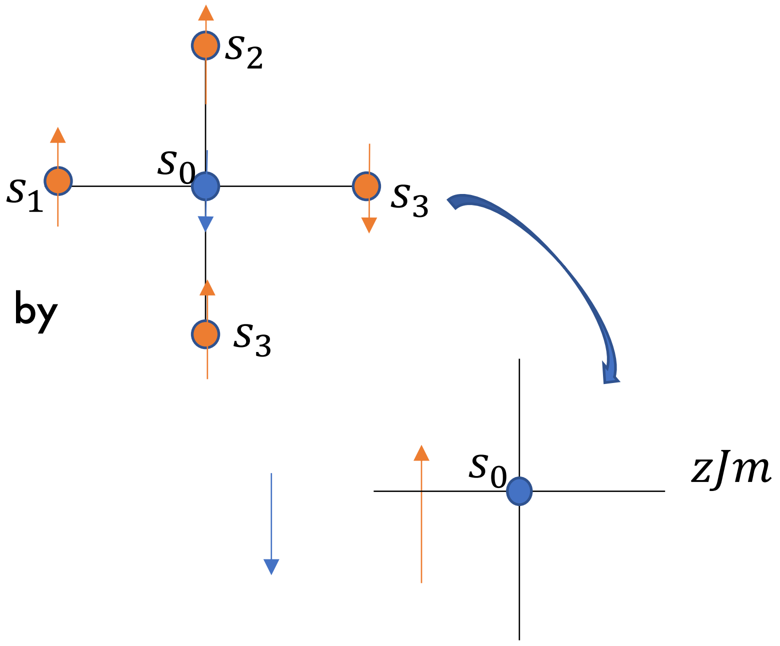
$T < T_C$ $\qquad$ $T \lesssim T_C$ $\qquad$ $T > T_C$

The critical temperature T_C can be estimated in the **mean-field approximation**

2D Exact solution given by Onsager (tour de force!)

Weiss mean-field theory

$$H_N = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i s_i B = -\sum_i s_i \left(J \sum_{j=n.n.(i)}^{z=2d} s_j + B \right)$$



- We assume that each spin interacts on average in the same with its neighbors regardless of its spin value. This means that we can replace the neighboring spin s_j by some mean magnetization + small fluctuations around it

$$s_j = m + (s_j - m) = m + \delta s_j, \qquad m \equiv \frac{1}{N}\left\langle \sum_i s_i \right\rangle \equiv \langle s \rangle$$

- Such that the Hamiltonian reads now as

$$H_N = -\sum_i s_i \left(J \sum_{j=n.n.(i)}^{z} m + B \right) - \sum_i s_i \left[J \sum_j^{z} \delta s_j \right]$$

z is the coordination number; $z = 2d$ for a square lattice ($z = 4$ in 2D, $z = 6$ in 3D)

- ***Mean-field approximation: Ignore the effect of fluctuations around the mean field***

$H = -\sum_i s_i B_{eff}$, where $B_{eff} = B + zJm, \quad z = 2d$

Self-consistent equation: the mean field m must the same as the average magnetization per spin $m \equiv \langle s \rangle$

Self-consistent equation

Mean-field Hamiltonian looks like that for a paramagnetic system, except that the effective magnetic field has a contribution from the mean field

$$H_N = -\sum_i s_i B_{eff}\,, \qquad B_{eff} = B + zJm, \qquad s_i = \pm 1$$

- One-spin partition function

$$Z_1 = e^{\beta(B+zJm)} + e^{-\beta(B+zJm)} = 2\cosh[\beta(B+zJm)]$$

- Mean magnetization per spin must be the same as the mean field

$$m = \langle s \rangle = \frac{1}{\beta}\frac{\partial \ln Z_1}{\partial B_{eff}} \rightarrow m = \tanh[\beta(B+zJm)]$$

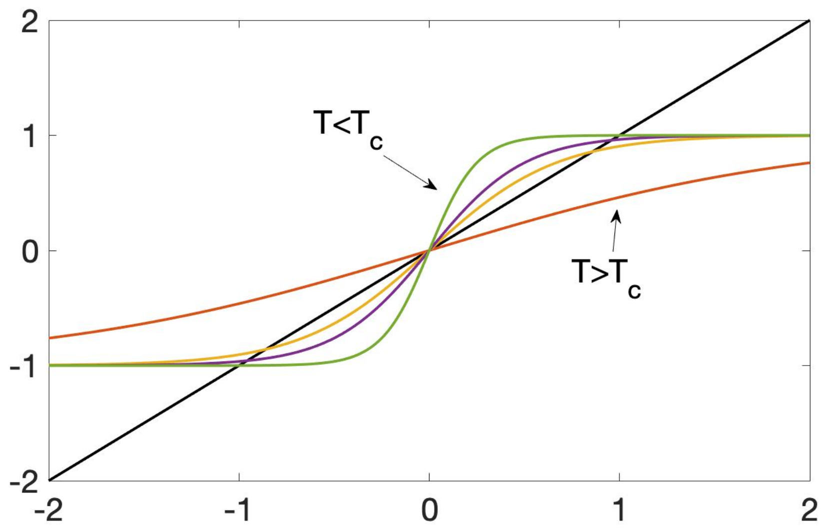
(transcendental equation, not easy to solve analytically; so we look for asymptotic solutions)

Self-consistent equation

- Limit of $B = 0$

$$\boldsymbol{m} = \boldsymbol{tanh}\left[\frac{\boldsymbol{zJm}}{\boldsymbol{kT}}\right]$$

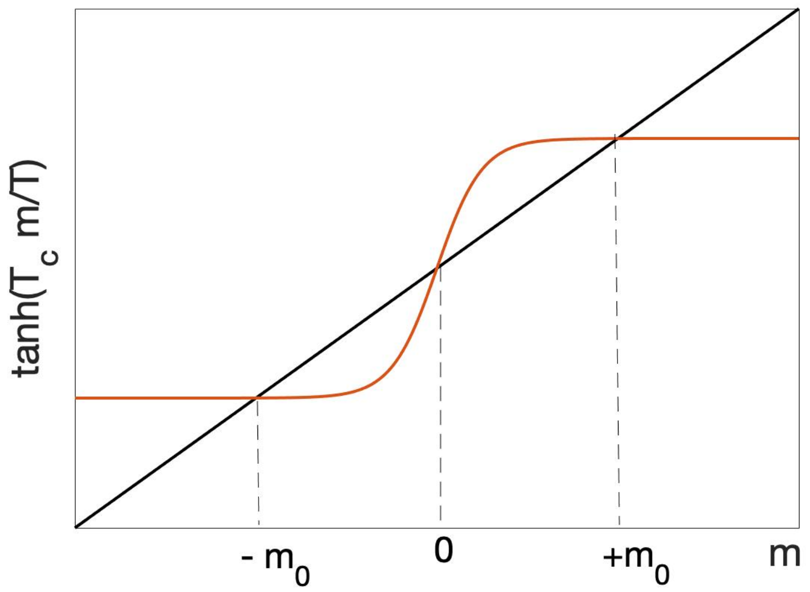
  - solved graphically by looking at the intersection points between the diagonal curve and the $\tanh(x)$



Critical temperature: $\boldsymbol{T_c} = \frac{\boldsymbol{zJ}}{\boldsymbol{k}}$

$$\boldsymbol{m} = \boldsymbol{tanh}\left[\frac{\boldsymbol{T_c}}{\boldsymbol{T}}\boldsymbol{m}\right]$$

- For $T > T_c$, there is only one root at $m = 0$
- For $T < T_c$, there are three roots at $m = 0, \pm m_0(T)$
- The non-zero solutions depend on the temperature below T_c



Self-consistent equation

- Low temperature near $\mathrm{T_c}$, $T \leq T_c$, $m\ small$

$$\boldsymbol{m} = \boldsymbol{tanh}\left[\frac{\boldsymbol{T_c}}{\boldsymbol{T}}\boldsymbol{m}\right] \qquad (\mathbf{1})$$

- For small m, use the Taylor expansion of $\boldsymbol{tanh}(\boldsymbol{x})$

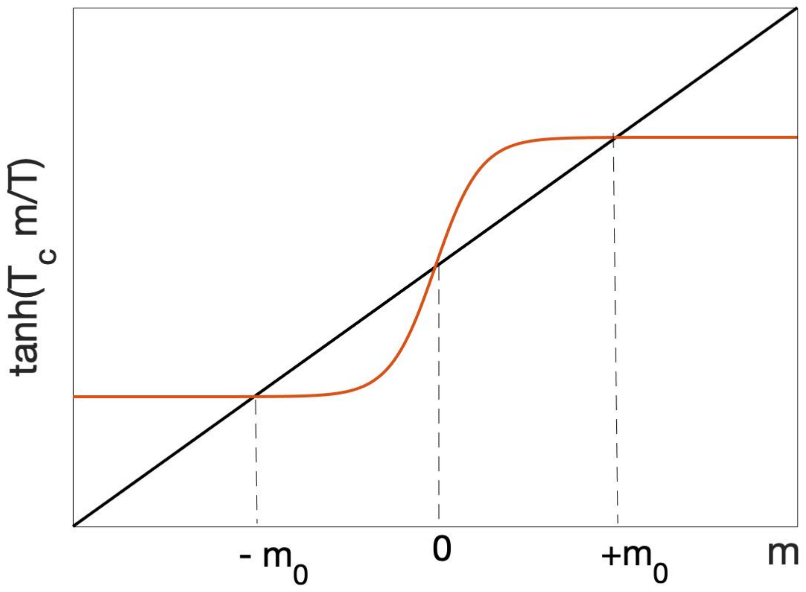
$$\boldsymbol{m} \approx \frac{\boldsymbol{T_c}}{\boldsymbol{T}}\boldsymbol{m} - \frac{\mathbf{1}}{\mathbf{3}}\left(\frac{\boldsymbol{T_c}}{\boldsymbol{T}}\right)^{\mathbf{3}}\boldsymbol{m}^{\mathbf{3}}$$

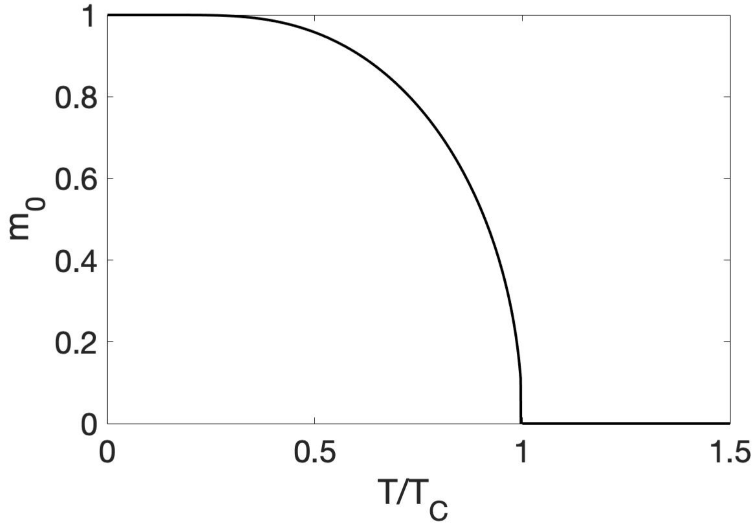
To find the dependence of the roots $m_0(T)$ on temperature

$$m_0(T) = \pm\sqrt{3}\frac{T}{T_c}\left(1 - \frac{T}{T_c}\right)^{\frac{1}{2}}$$

Solution valid only very close to the critical temperature

$m_0(T)$ is otherwise the numerical solution of eq. (1)





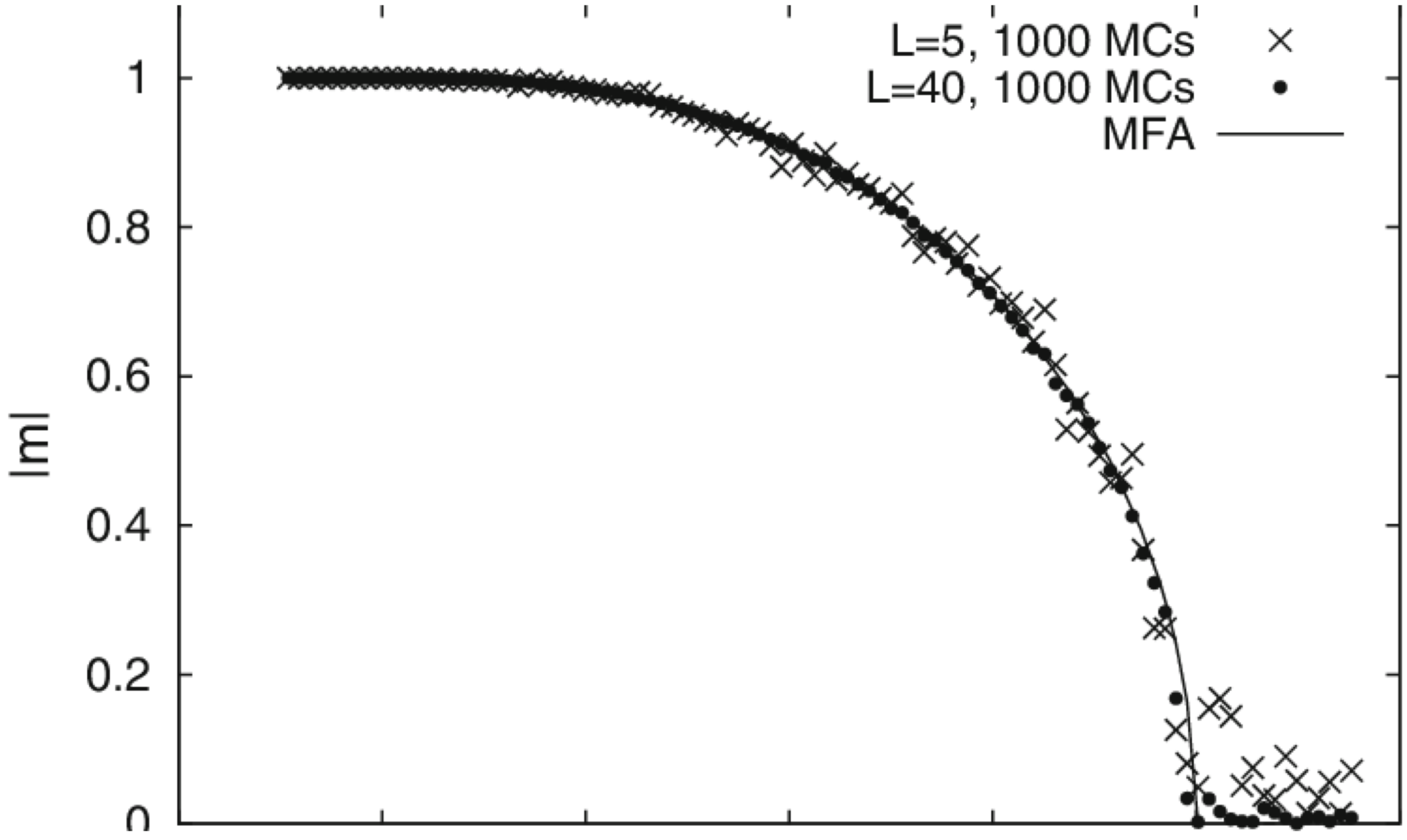
Self-consisten equation

$$|m_0| = \sqrt{3}\left(\frac{T}{T_c}\right)^{\frac{3}{2}}\left(1-\frac{T}{T_c}\right)^{1/2}$$

Critical exponent β:

$$|\boldsymbol{m_0}| \sim (\boldsymbol{T_c} - \boldsymbol{T})^{\boldsymbol{\beta}}$$

$$\boldsymbol{\beta_{MF}} = \frac{\mathbf{1}}{\mathbf{2}}$$



Mean magnetization for $B \neq 0$

$$m = \tanh[\beta(B + zJm)] \qquad (1)$$

- $T \leq T_c,\ m\ small;\ Weak\ applied\ field, B$ such that we Taylor expand the tanh

$$m \approx \beta(B + zJm) - \frac{1}{3}\beta^3(B + zJm)^3$$

$$m \approx \frac{B}{kT} + \frac{T_c}{T}m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3$$

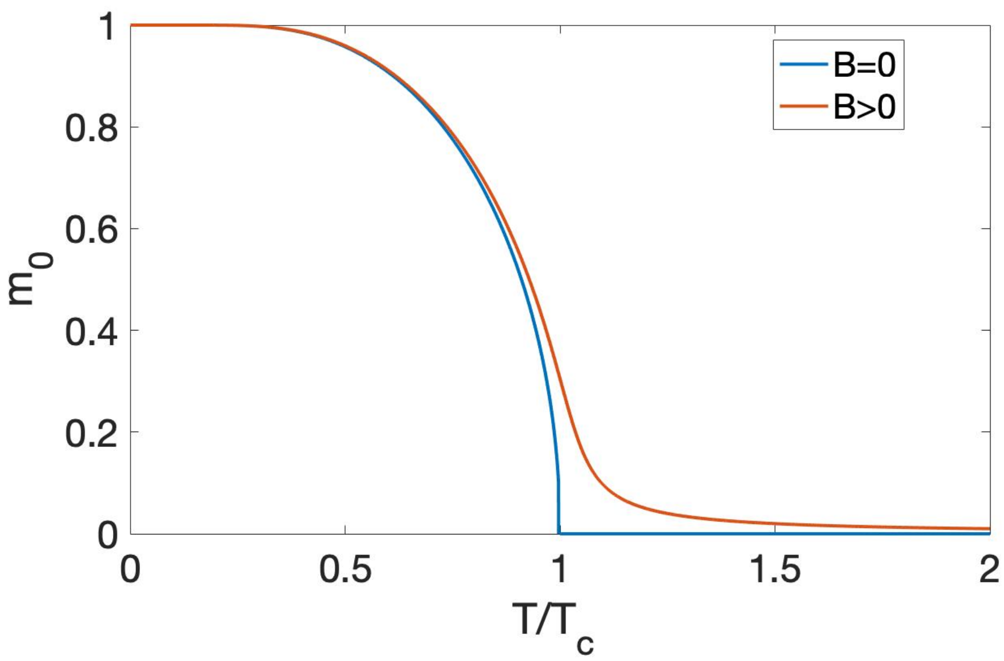
$$\frac{B}{kT} \approx \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 + \left(1 - \frac{T_c}{T}\right)m$$

- At the critical temperature $T \approx T_c$,

$$\frac{B}{kT_c} \approx \frac{1}{3}m^3 \rightarrow |\boldsymbol{m}| \approx \boldsymbol{B}^{\frac{1}{\delta}}$$

- Critical exponent: $\delta_{MF} = 3$

Numerical solution of eq. (1)



Mean magnetization for $B \neq 0$

$$m = \tanh[\beta(B + zJm)]$$

- $T \leq T_c$, m *small*; *Weak applied field,* B such that we Taylor expand the tanh

$$m \approx \beta(B + zJm) - \frac{1}{3}\beta^3(B + zJm)^3$$

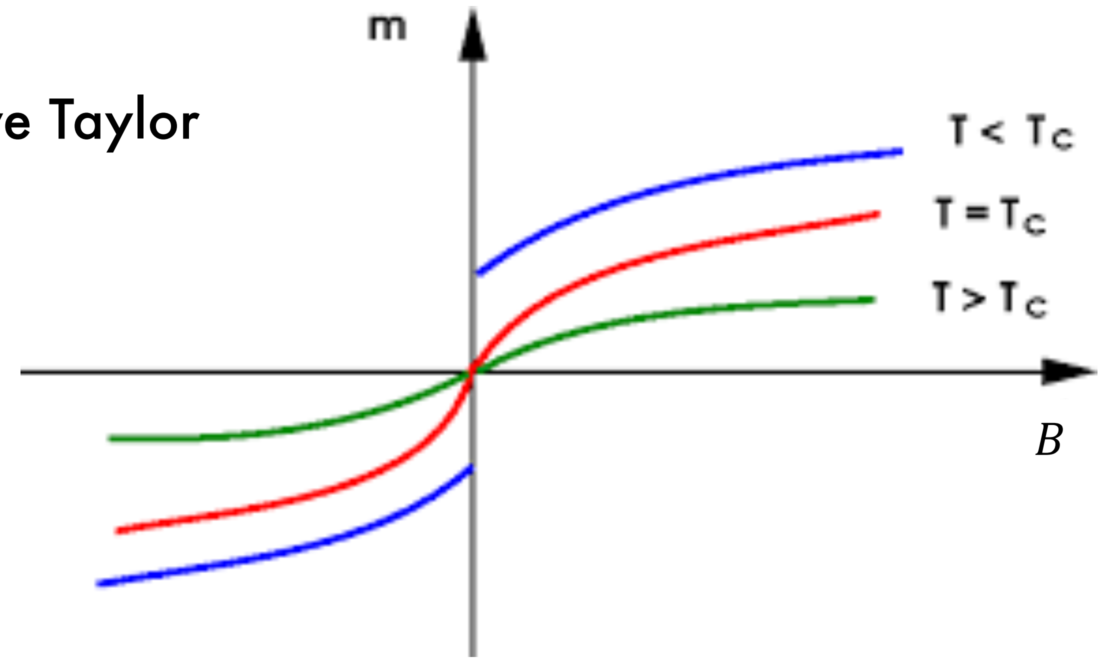
$$m \approx \frac{B}{kT} + \frac{T_c}{T}m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3$$

$$\frac{B}{kT} \approx \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 + \left(1 - \frac{T_c}{T}\right)m$$

- At the critical temperature $T \approx T_c$,

$$\frac{B}{kT_c} \approx \frac{1}{3}m^3 \rightarrow |\boldsymbol{m}| \approx \boldsymbol{B}^{\frac{1}{\delta}}$$

- Critical exponent: $\delta_{MF} = 3$



Inflection point at $T = T_c$ and $B = 0$, where $\chi = \frac{\partial m}{\partial B} \rightarrow \infty$

Susceptibility near critical point

- Near the critical point $T \approx T_c$

$$\frac{B}{kT} \approx \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 + \left(1 - \frac{T_c}{T}\right) m,$$

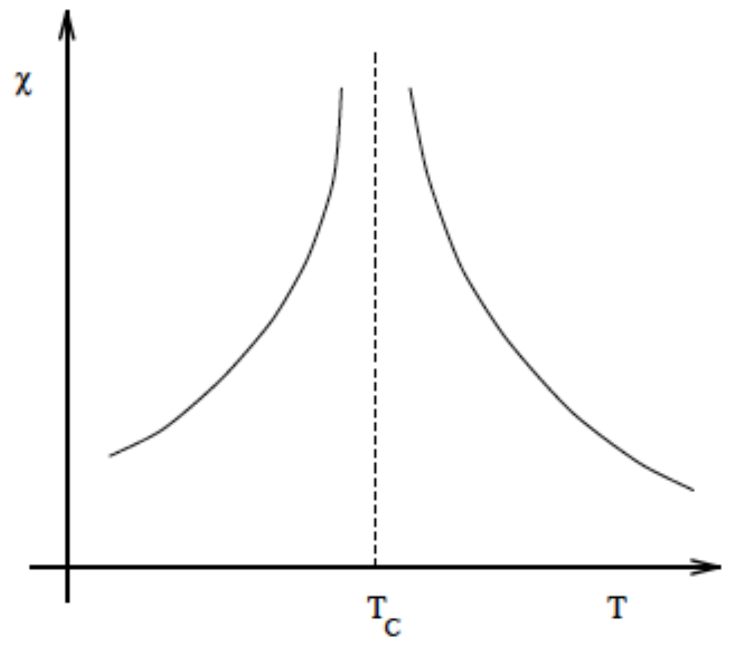
$$\chi(T) = \left(\frac{\partial B}{\partial m}\right)_T^{-1} = \left[kT\left(\frac{T_c}{T}\right)^3 m_0^2 + kT\left(1 - \frac{T_c}{T}\right)\right]^{-1}$$

$$m_0^2 = \begin{cases} 0, & T \gtrsim T_c \\ 3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T} - 1\right), & T \lesssim T_c \end{cases}$$

Critical exponent γ *near the phase transition*

$$\chi = \begin{cases} k\,(T_c - T)^{-1}, & T \gtrsim T_c \\ 2k(T - T_c)^{-1}, & T \lesssim T_c \end{cases}$$

$$\chi \sim |T_c - T|^{-\gamma}, \qquad \gamma_{MF} = 1$$



Curie-Weiss law

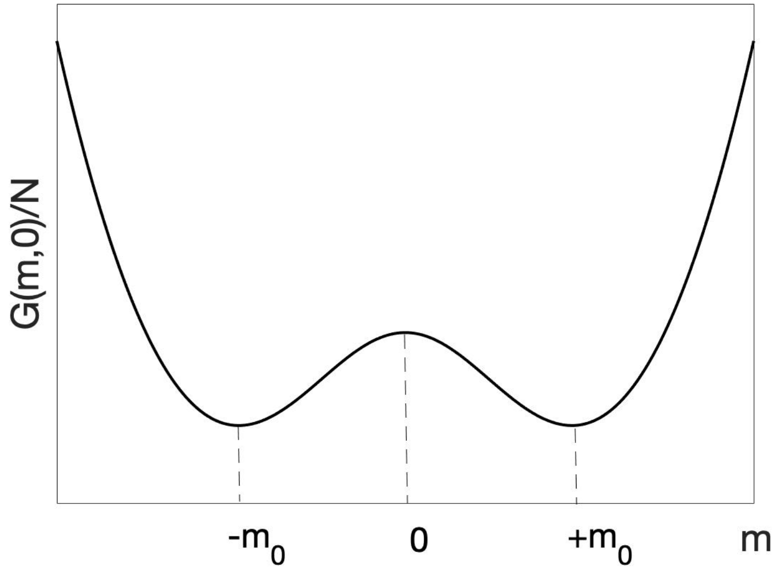
Gibbs free energy minimized by $\pm m_0$

$H_N = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i s_i B$, *replace the spins by* $s_i = m + (s_i - m)$

$$H_N = zJN\, m^2 - (B + 2zJm)\sum_i s_i \rightarrow Z_1 = e^{-\beta NzJm^2}\, 2\cosh(\beta(2zJm + B))$$

Gibbs free energy
$G(B,T) = -NkT\ln(Z_1)$

$$\frac{G(B,T)}{N} = \frac{k\,T_c}{2}m^2 - kT\ln\left[2\cosh\left(\frac{T_c}{T}m + \frac{B}{kT}\right)\right]$$



- **Low temperature** $T < T_c, B = 0$

Gibbs free energy per spin at zero applied field

$$\boldsymbol{g(0,m) = \frac{G(0,m)}{N} \approx -kT\,ln(2) + \frac{kT_c}{2}\left(1 - \frac{T_c}{T}\right)m^2 + \frac{kT_c^4}{12T^3}m^4}$$

has two minima corresponding to $\pm m_0(T)$ *for* $T < T_c$

Heat capacity

- Low temperature $T < T_c, \;\; B = 0$

$$G(0, m(T)) \approx -c_0 - c_1 m^2 + c_2 m^4, \qquad m(T) \approx (T_c - T)^{1/2}$$

Heat capacity measured the heat exchange per temperature increase

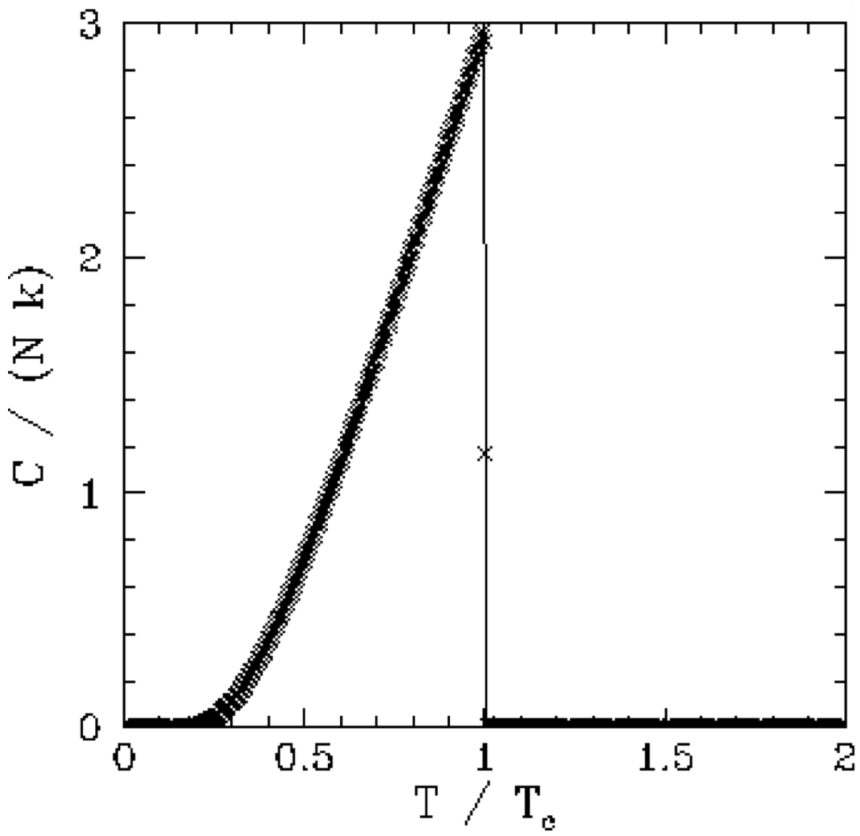
$$C_B = T\left(\frac{\partial S}{\partial T}\right)_B = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_B$$

$$C_B \sim -Tm'\frac{\partial}{\partial m}\left(m'\frac{\partial G}{\partial m}\right) \sim -T\frac{1}{m}\frac{\partial}{\partial m}\left(\frac{1}{m}(-2c_1 m + 4c_2 m^3)\right) \sim \boldsymbol{const}$$

Critical exponent α at $T \approx T_c$ and $B = 0$

$$\boldsymbol{C_B \approx |T - T_c|^{\alpha}}$$

$$\boldsymbol{\alpha_{MF} = 0}$$



Critical exponents for the magnetic phase transition

Mean-field universality class

Order parameter $M(T, B = 0) \sim (T_c - T)^{\beta}, \quad \beta_{MF} = \frac{1}{2}$

Critical isotherm $\mathrm{M}(T_c, B) \sim |B|^{\delta}, \quad \delta_{MF} = 3$

Susceptibility $\chi(T, B = 0) \sim |T_c - T|^{-\gamma}, \quad \gamma_{MF} = 1$

Heat capacity $C_B(T, B = 0) \sim |T_c - T|^{-\alpha}, \quad \alpha_{MF} = 0$

Exponent	2D	3D	Mean field
α	0	0.11	0
β	1/8	0.32	1/2
γ	7/4	1.24	1
δ	15	4.90	3

Universality class of the magnetic phase transition

Universality class is defined by two main parameters:

1. **Spacial dimension, d**
2. **The dimension of the «order parameter», n**

The Ising Hamiltonian $H_N = -J \sum_{\langle i,j \rangle} s_i s_j$ is invariant under spin reflection, $s_i \to -s_i$.
However, the mean magnetization is not invariant under spin transformation = order parameter

$\langle M \rangle \neq 0$ **in the *ferromagnetic* phase**

$\langle M \rangle = 0$ **in the *paramagnetic* phase**

Ising universality class

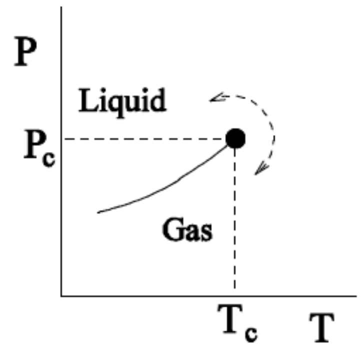
Is characterized by:

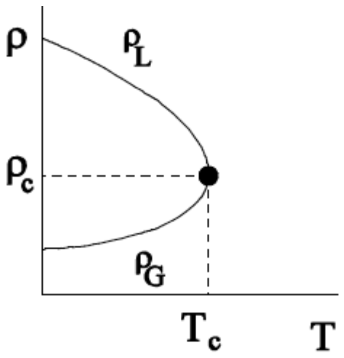
1. **Spacial dimension, $d = 3$**
2. **The dimension of the scalar magnetic field, $n = 1$**

The Ising universality class is characterized by the same critical exponents the van der Waals fluids near the critical gas-liquid phase transition

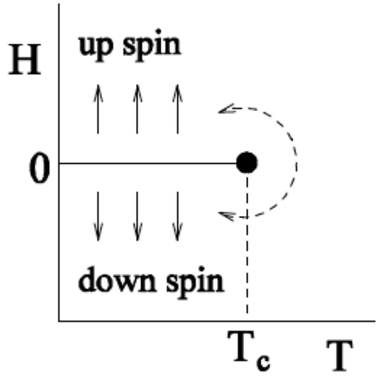
Mean field Ising universality class

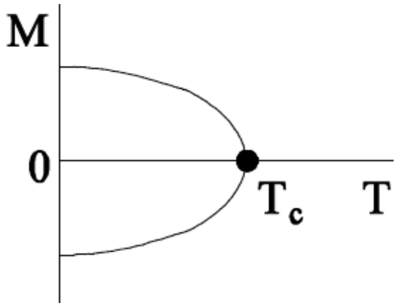
Correspondence between magnetics and fluids





Gas-Liquid	Magnets
Volume, V or density, ρ	Mean magnetization, $-M$
Pressure, P	Magnetic field, B
Gibbs free energy, $G(P,T)$	Gibbs free energy, $G(B,T)$
Compressibility, $\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial P}$	Susceptibility, $\chi = \frac{\partial M}{\partial B}$
Heat capacity, $C_P = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_P$	Heat capacity, $C_B = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_B$





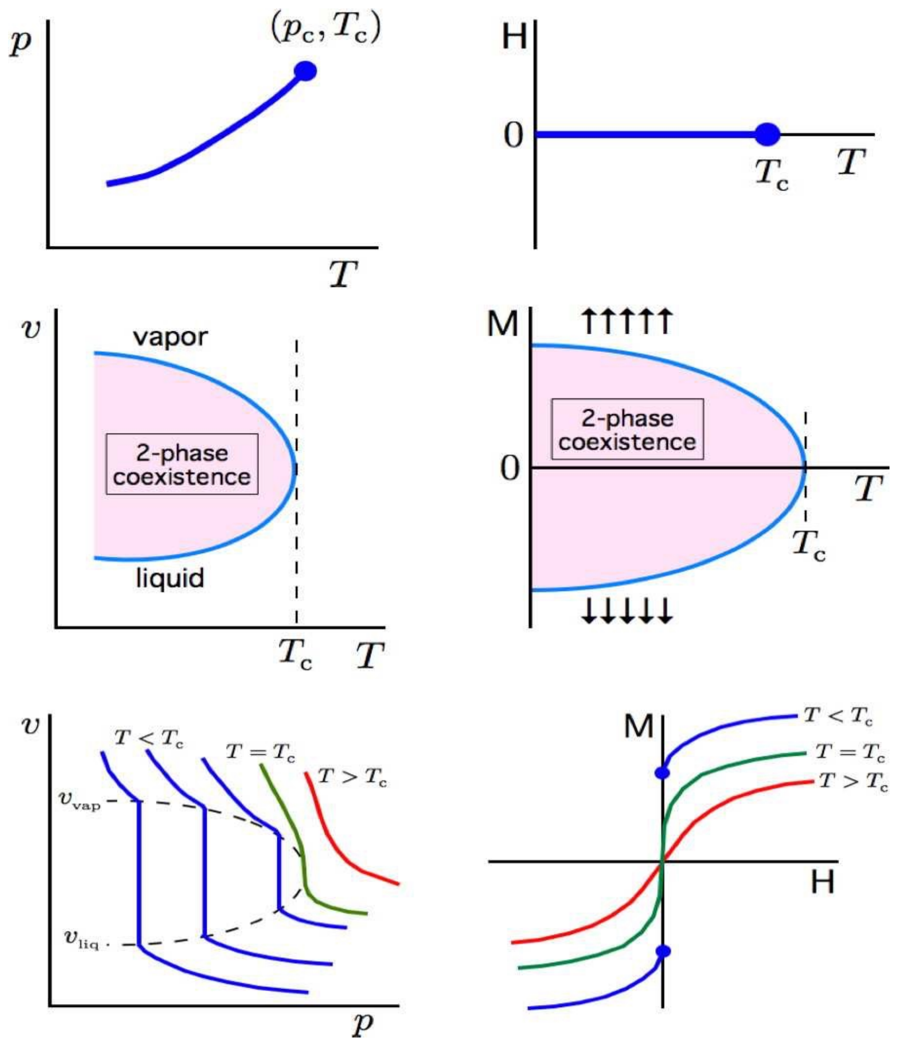
Density (Order parameter) $\rho(T,P_c) \sim (T_c - T)^{\beta}, \quad \beta_{MF} = \frac{1}{2}$

Critical isotherm $V(P,T_c) \sim P^{\delta}, \quad \delta_{MF} = 3$

Compressibility $\kappa_T(T) \sim |T_c - T|^{-\gamma}, \quad \gamma_{MF} = 1$

Heat capacity $C_P(T) \sim |T_c - T|^{-\alpha}, \quad \alpha_{MF} = 0$

Correspondence between magnetics and fluids



Van der Waals fluids and their critical point (reminder…)

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{ij} u(r_{ij}),\, u(r) = \begin{cases} \infty, r \le \sigma \\ u_1(r), r > \sigma \end{cases}$$

Mean-field approximation: $H = \sum_i \frac{p_i^2}{2m} + N\bar{u}$

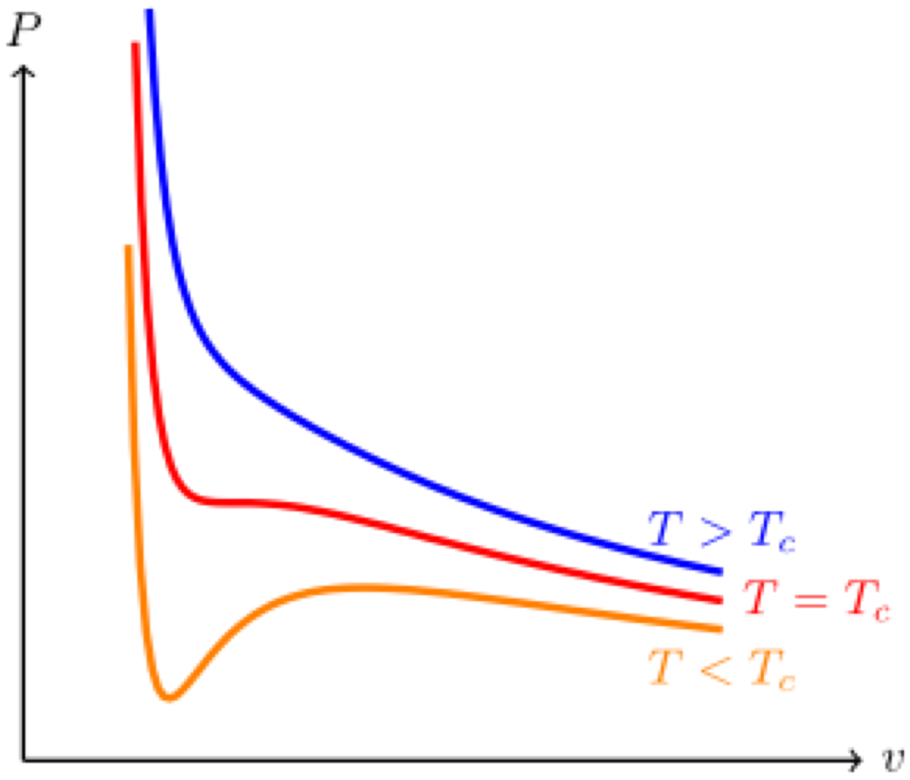
Van-der-Waals equation of state

$$P = \frac{\rho k T}{1-\rho b} - a\rho^2$$

Critical point: inflection point in the $P-V$ diagram:

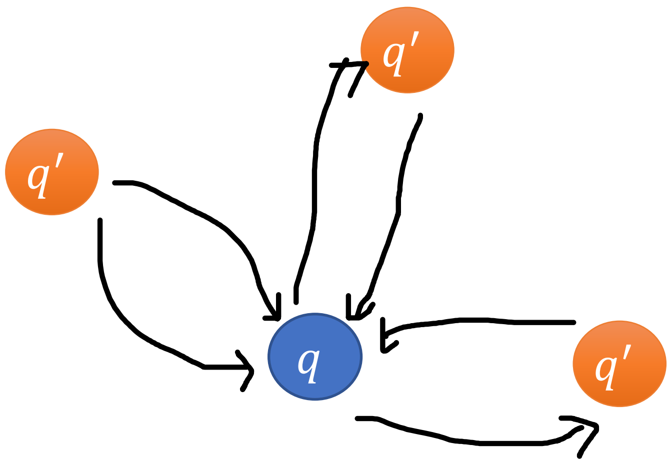
$$\frac{\partial P}{\partial V} = 0, \qquad \frac{\partial^2 P}{\partial V^2} = 0$$

$$P_c = \frac{a}{27b^2}, T_c = \frac{8a}{27b}, \rho_c = \frac{1}{3b}$$



Beyond the mean field approximation: Monte Carlo simulation

- Sampling equilibrium spin configurations in the canonical ensemble through Metropolis algorithm



- Metropolis rule for the transition probability to go from congifuration $q = \{s_i\}$ to another configuration $q' = \{s_i{}'\}$

$$\boldsymbol{W}(\boldsymbol{q} \rightarrow \boldsymbol{q}') = \begin{cases} 1, & \Delta\mathrm{E} \leq 0 \\ e^{-\beta\Delta E}, & \Delta E > 0 \end{cases},$$

Where $E = -\frac{J}{2}\sum_{\langle i,j\rangle} s_i s_j$ is the energy of a N-spins configuration at $B =$

0

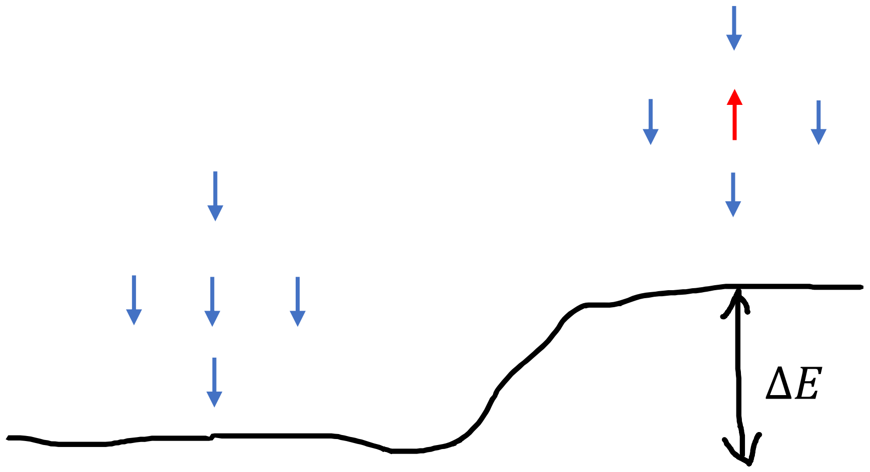
Metropolis Monte Carlo : Ising model

- Detailed balance: $\frac{P_{eq}(s_{k'})}{P_{eq}(s_k)} = \frac{W(s_k \to s'_k)}{W(s'_k \to s_k)} = e^{-\beta\Delta E}, E = -\frac{J}{2}\sum_{\langle i,j\rangle} s_i s_j$,

$s = \pm 1$

Metropolis rule for the transition probability

$$W(s_k \to s'_k) = \begin{cases} 1, & \Delta E \leq 0 \\ e^{-\beta\Delta E}, & \Delta E > 0 \end{cases}$$



- ***Pick a random spin s_k and flip its value***

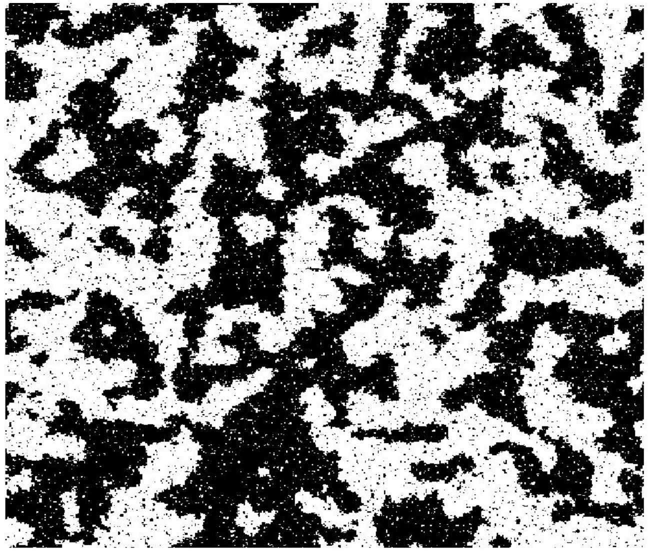
$s_k^{new} = -s_k^{old}$ and calculate the energy cost ΔE

$$\Delta E = -J\,\Delta s_k \sum_{j=n.n.(k)} s_j$$

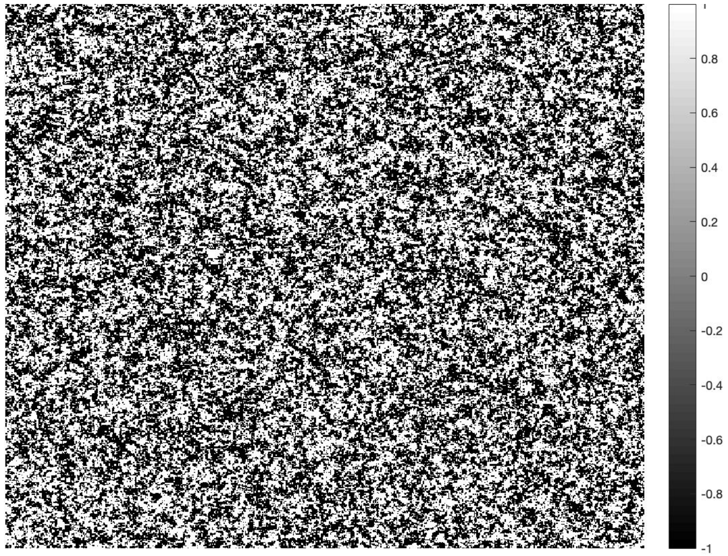
- Accept the spin flit every time $\text{rand} < e^{-\beta\Delta E}$

Metropolis Monte Carlo : Ising model

$T < T_C$



$T \lesssim T_C$



$T > T_C$