4.5) The Ferromagnetic transition & the mean field Ising model

Ising model: accont for exchange interactions* between electrons in a solid, which favors aligned spins.

Lattice with $N = L^d$ sites, where spin $S_i \in \{\pm 1\}$ are located.

Hamiltonian $H = -J \sum_{i \sim j} S_i S_j - h \sum_i S_i$

J: coupling constant (exchange energy)

$h = \mu \hat{h}$ is the potential energy of the spin with magnetic moment μ in a magnetic field $\hat{h}$. (We refer to h as the field, for simplicity)

$\sum_{i \sim j}$ is a sum over nearest neighbors.

Configurations $\{S_i\} \Rightarrow 2^N$ configurations

* $J = 0 \Rightarrow 2^N$ non interacting two-level systems.

* $M = \sum_{i=1}^{N} S_i$ is the total magnetization of the system.

$m = \frac{M}{N}$ is the magnetization per spin.

* Electrons are fermions $\Rightarrow$ antisymmetric wave function. If spins are aligned, the spin part is symmetric $\Rightarrow$ spatial part is antisymmetric $\Rightarrow$ "pushed" away from each other $\Rightarrow$ lower the Coulomb energy $\frac{e^2}{r_{12}}$ $\Rightarrow$ favored.

* The spins tend to align with the magnetic field. This is called paramagnetism.

* Here we want to understand ferromagnetism, which is the emergence of non-zero magnetization in the absence of magnetic field.

* Ferromagnets correspond to $J>0$, which favors $\uparrow\uparrow$ & $\downarrow\downarrow$.

  Antiferromagnets ——— $J<0$, ——— $\uparrow\downarrow$ & $\downarrow\uparrow$

Canonical ensemble:

$T=\infty$, $P(\{S_i\}) = \frac{1}{Z}$ since $\beta = \frac{1}{k_B T} = 0 \Rightarrow$ all configurations equiprobable

$\Rightarrow \langle m \rangle = 0$

$T=0$, $P(\{S_i\}) = 0$ if $\{S_i\} \neq (1,1,\dots,1)$ or $(-1,\dots,-1) \Rightarrow m = \pm 1$.

Q: What happens in between?

Partition function: Keep h finite for now

$$Z = \sum_{\{S_i\}} e^{\beta\left[J\sum_{i\sim j} S_i S_j + h\sum_i S_i\right]}$$

such that $\langle M \rangle = \frac{1}{\beta}\frac{\partial}{\partial h}\ln Z \Rightarrow \boxed{\langle m \rangle\Big|_{h=0} = \frac{kT}{N}\frac{\partial}{\partial h}\ln Z\Big|_{h=0}}$

"Just" need to compute Z:

$d=1 \to$ can be done exactly using transfer matrix

$d=2 \to$ Yes, at $h=0$. Onsager 1942 (Pain & suffering)

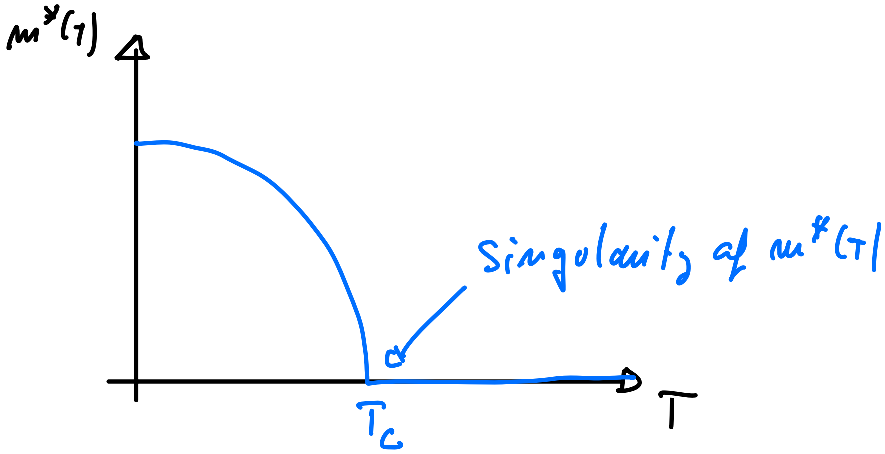
· Wigner – Jordan transform

$d=3 \to$ No exact result but progress thanks to extension of conformal field theory & lots of numerics $\Rightarrow$ well understood

Result: As $L \to \infty$, $P(m) \sim \frac{1}{2}\delta(m+m^*) + \frac{1}{2}\delta(m-m^*)$

$T > T_c$, $m^* = 0$

$T < T_c$, $m^* \sim \mathcal{O}(1) \neq 0$



Q: Can we understand this behaviour?

Mean-field theory $\quad H = -J \sum_{i \sim j} S_i S_j - h \sum_i S_i$

Contributions involving spin i: $\boxed{H_i = -h S_i - J\left(\sum_{j \sim i} S_j\right) S_i}$

$J \sum_{j \sim i} S_j \leftrightarrow$ effective magnetic field exerted by $\{S_j\}$ on S_i

If system is homogeneous & fluctuations are small $\boxed{\sum_{j \sim i} S_j \simeq q\, m}$

where q is the number of neighbors ($q = 2d$ on a square lattice in dimension d)

$\Rightarrow H_i = -(h + q m J) S_i \Rightarrow$ single spin with field $\boxed{h_{eff} = h + q m J}$

$\Rightarrow$ Solve that problem to compute $\langle m \rangle (h_{eff}) \equiv \bar{m}(h_{eff})$ and check that $\bar{m}(h_{eff}) = m$ so that the hypothesis is self consistent.

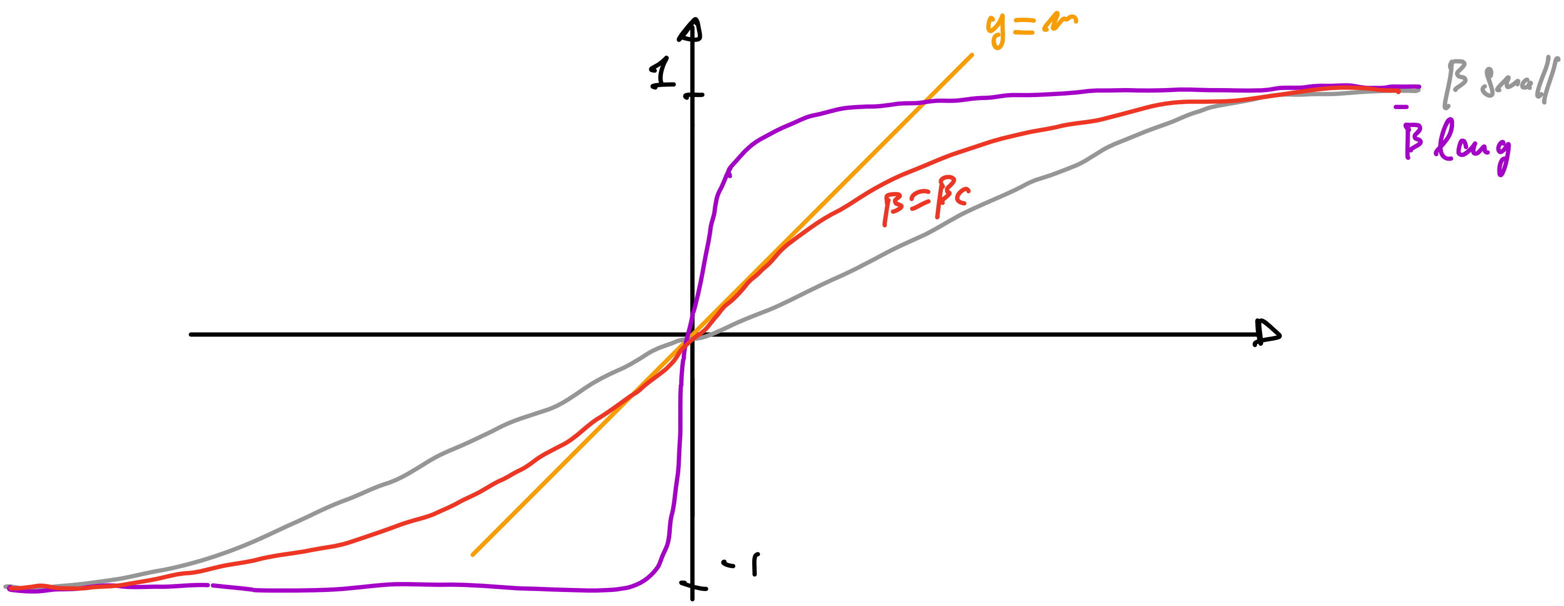
Self consistency condition $\quad Z'(h_{eff}) = e^{-\beta(h+qmJ)} + e^{\beta(h+qmJ)}$

$$\bar{m}(h_{eff}) = \frac{1}{\beta} \frac{\partial}{\partial h} \ln \left[e^{\beta(h+qmJ)} + e^{-\beta(h+qmJ)} \right]$$

$$\bar{m} = \tanh\left[\beta(h + q m J)\right]$$

To find the spontaneous magnetization at $h = 0$, we thus want

$$\boxed{m = \tanh(q \beta J m)}$$



$T > T_c \to$ only one solution, $m = 0$

$T < T_c \to$ three solutions, $m = \pm m_0$ & $m = 0$

Critical temperature: $\tanh(q\beta J m) \simeq q\beta J m$ as $m \to 0$

$$T < T_c \iff q\beta J > 1 \iff \boxed{T < \frac{qJ}{k_B} \equiv T_c}$$

Q: Why don't we see the $m=0$ solution?

Landau free energy: why solution is selected?

$$H = -J \sum_{\langle ij \rangle} S_i S_j - h \sum_i S_i = -J \frac{1}{2} \sum_i S_i \underbrace{\sum_{j \text{ near } i} S_j}_{qm} - N h m = -J \frac{N q m^2}{2} - h m N$$

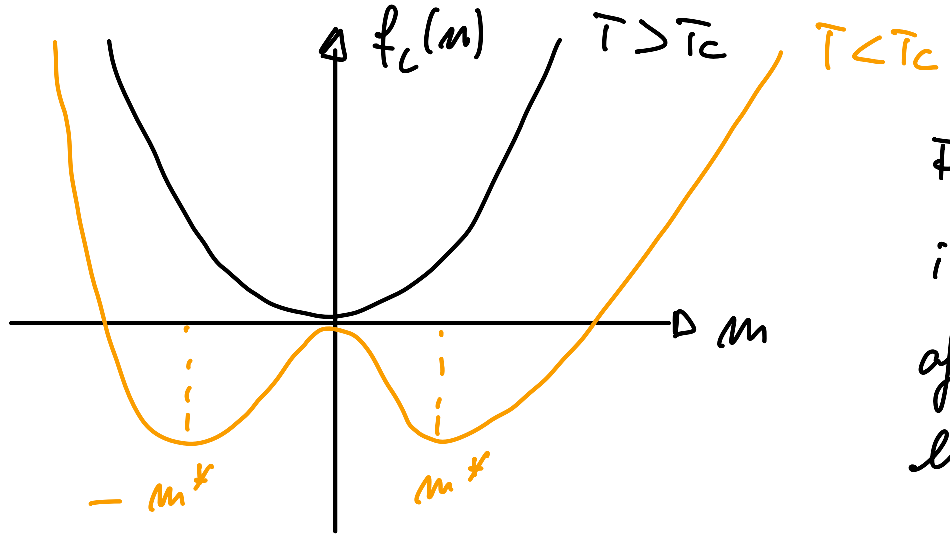
$$P(m) = \frac{1}{Z} \Omega(m) \, e^{+J \frac{Nqm^2}{2} + hmN}$$ where $\Omega(m) = \#$ of configurations with magnetization m

$$N = N^+ + N^- \; ; \; mN = N^+ - N^- \; ; \; N^+ = \frac{N + Nm}{2} \; ; \; N^- = \frac{N - Nm}{2}$$

$$\Omega(m) = \binom{N}{N^+} = \frac{N!}{N^+! \, N^-!} \sim e^{N \ln N - N - \frac{N+Nm}{2} \ln \frac{N+Nm}{2} + \frac{N+Nm}{2} - \frac{N-Nm}{2} \ln \frac{N-Nm}{2} + \frac{N-Nm}{2}}$$

$$\Omega(m) \simeq e^{-N\left[\frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2}\right]}$$

$$P(m) = \frac{1}{Z} e^{-N f_L(m)} \; ; \; f_L(m) = -\frac{Jq}{2} m^2 - hm + \frac{1+m}{2} \ln \frac{1+m}{2} + \frac{1-m}{2} \ln \frac{1-m}{2}$$



For $T<T_c$, $m=0$ is a local maximum of the Landau free energy.

Comment: If you do not like the self consistency approach, compute $Z = \int dm\, e^{-N f_L(m)}$

extrema of f: $\frac{\partial f_L}{\partial m} = 0 \iff m = \tanh(q\beta J m)$

Minimizing the Landau free energy is equivalent to the self consistency condition. Thus,

$$T>T_c \Rightarrow m=0\ ; \ Z \underset{N\to\infty}{\sim} e^{-N f_L(0)} \quad \& \ P \underset{N\to\infty}{\propto} \delta(m)$$

$$T<T_c \Rightarrow m = \pm m^*;\ Z \sim e^{-Nf(m^*)} + e^{-Nf(-m^*)}$$

$$\& \ P(m) \simeq \frac{1}{2}\delta(m-m^*) + \frac{1}{2}\delta(m+m^*)$$

Universality & critical exponents

Expanding $\tanh(x) = x - \frac{x^3}{3}$, we see that

$$m \simeq \beta q m J - \frac{(\beta q m J)^3}{3}$$

$$\Leftrightarrow (\beta - \beta_c) q J m = \frac{1}{3}\beta^3 q^3 m^3 J^3 \Rightarrow m \propto \pm\sqrt{\frac{1}{T} - \frac{1}{T_c}}$$

$$\Rightarrow |m| \propto (T_c - T)^\beta ; \; \beta_{MF} = \frac{1}{2} ; \; \text{exact result } \beta_{2d} = \frac{1}{8}$$

Magnetic field

$$m \simeq \beta h + m\frac{T_c}{T} - \frac{m^3}{3}\frac{T_c^3}{T} \qquad \text{using } k_B T_c = qJ$$

$$T = T_c \Rightarrow m \propto h^{1/3}$$

$$T \neq T_c \Rightarrow m\frac{T - T_c}{T} \underset{m \to 0}{=} \beta h \Rightarrow \chi = \left.\frac{\partial m}{\partial h}\right|_{h=0} \sim \frac{1}{T - T_c}$$

* Again, the MF exponents are quantitatively wrong, but the real ones are universal.

* $n_i = \frac{1 + S_i}{2} \in \{0, 1\}$ is a lattice gas model

$m \propto h^{1/3}$ & $\chi \sim \frac{1}{T - T_c}$ maps onto the LG exponents $v - v_c \propto (p - p_c)^{1/3}$

$$\chi_T \propto \frac{1}{T - T_c}$$

* The world of phase transitions is filled with these unexpected mappings.