

Lecture 2

Continue MFT of the Ising model.

Mean-field free energy:

$$F = \frac{N\beta M^2}{2} - NT \ln \left[2 \cosh \left(\frac{M\beta}{T} \right) \right]$$

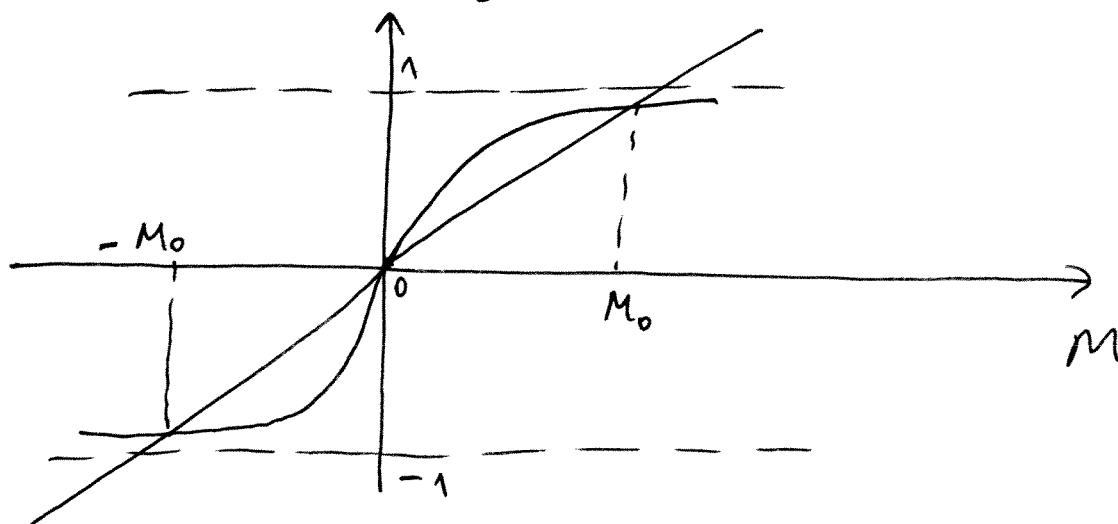
Find M by minimizing the free energy:

$$\frac{\partial F}{\partial M} = N\beta M - N\beta \tanh \left(\frac{M\beta}{T} \right) = 0$$

Thus we obtain a nonlinear equation for M :

$$M = \tanh \left(\frac{M\beta}{T} \right)$$

Solve graphically.



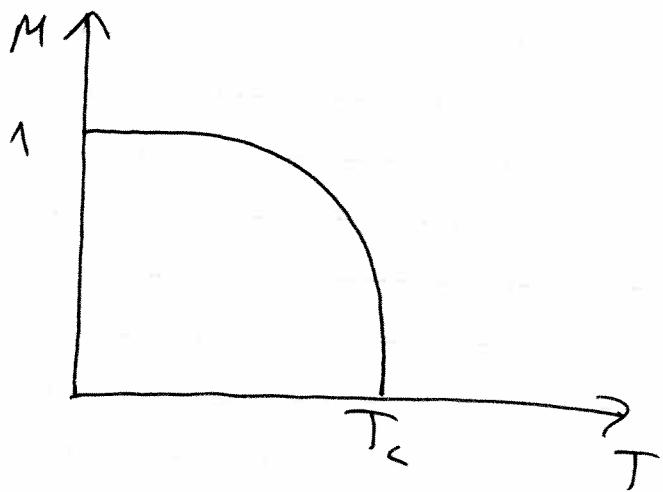
The slope of $\tanh\left(\frac{M\gamma}{T}\right)$ ~~is proportional to~~ is equal to $\frac{\gamma}{T}$ at small M . The transition happens when the slope becomes equal to 1.

Thus $T_c = \gamma$ in MFT.

$T > T_c$ — the only solution is $M=0$.

~~$T < T_c$~~ $T < T_c$ — two nontrivial solutions $M = \pm M_0$. The system will spontaneously pick one of the solutions — spontaneously broken symmetry.

The full numerical solution has the following form:



M vanishes continuously at $T=T_c$ — second order transition.

Important observation: since M vanishes at T_c continuously near T_c it will be small \Rightarrow we can expand the free energy in Taylor series in powers of M .

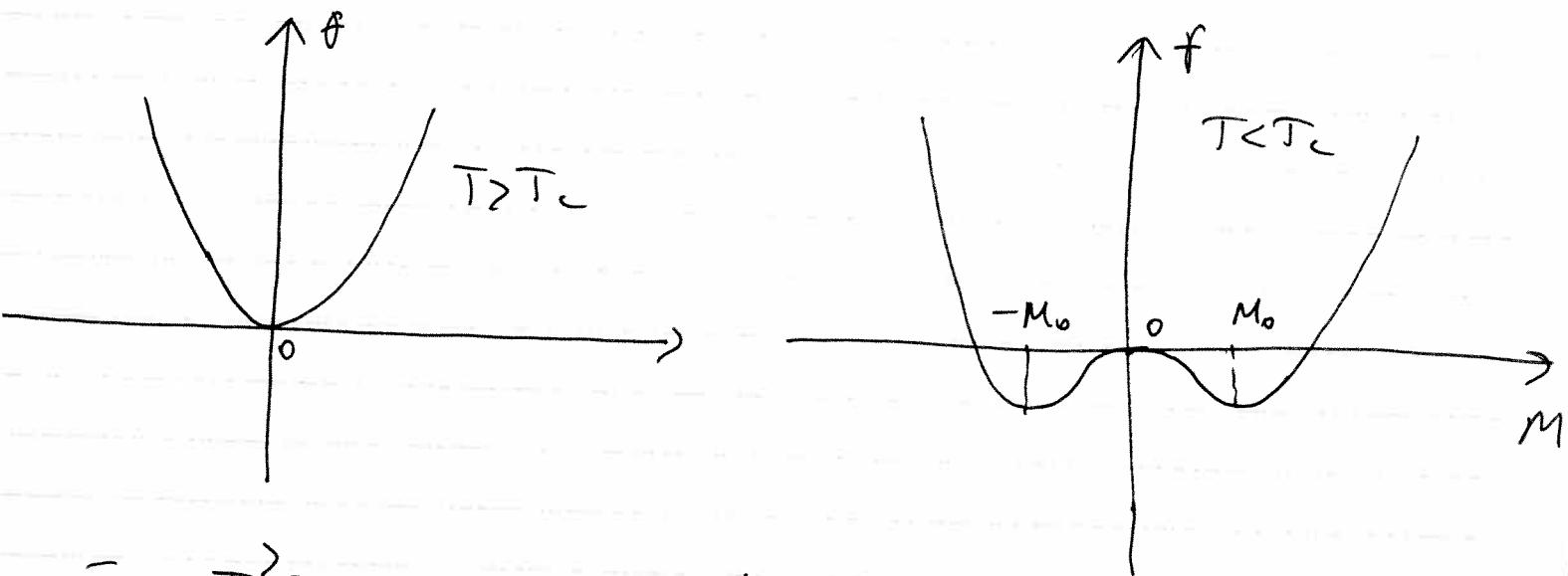
Convenient to define free energy per site:

$$f = \frac{F}{N} = \frac{\gamma M^2}{2} - T \ln \left[2 \cosh \left(\frac{M\gamma}{T} \right) \right]$$

Expanding in powers of M and neglecting an unimportant constant, we obtain:

$$\begin{aligned} f &= \frac{\gamma M^2}{2} - \frac{1}{2} T \left(\frac{M\gamma}{T} \right)^2 + \frac{1}{12} T \left(\frac{M\gamma}{T} \right)^4 = \\ &= \frac{T_c}{2} M^2 \left(1 - \frac{T_c}{T} \right) + \frac{T_c^4}{12 T^3} M^4 \end{aligned}$$

Here I've used $T_c = \gamma$.



For $T > T_c$, the coefficient of the M^2 term in f is positive \Rightarrow minimum of f is at $M=0$.

For $T < T_c$, the coefficient becomes negative \Rightarrow minimum at $M=0$ becomes a maximum and two nontrivial minima at $M = \pm M_0$ develop.

Near T_c , the coefficient of the M^2 term behaves as $\sim (T - T_c)$.

The coefficient of the M^4 term is positive and roughly constant.

Find $M(T)$ explicitly for T near T_c .

$$f = \frac{T_c}{2} \left(1 - \frac{T_c}{T}\right) M^2 + \frac{T_c^4}{12T^3} M^4$$

$$\frac{\partial f}{\partial M} = 0$$

$$T_c \left(1 - \frac{T_c}{T}\right) M + \frac{T_c^4}{3T^3} M^3 = 0.$$

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

Thus we obtain:

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

Thus near T_c M behaves as:

$$M \sim \left(\frac{T_c - T}{T_c}\right)^\beta = (-t)^\beta,$$

where $t = \frac{T - T_c}{T_c}$ - reduced temperature

$\beta = \frac{1}{2}$ - magnetization critical exponent.

This is a very important general feature of all continuous phase transitions - thermodynamic properties, like the order parameter, behave as universal power laws.

The exponents, characterizing these power laws are called critical exponents.

Calculate some other critical exponents in MFT.

Add uniform magnetic field :

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j - B \sum_i \sigma_i$$

The mean-field Hamiltonian is given by :

$$\begin{aligned} H &= -MJ \sum_i \sigma_i - B \sum_i \sigma_i + \frac{1}{2} NJM^2 = \\ &= -(MJ+B) \sum_i \sigma_i + \frac{1}{2} NJM^2 \end{aligned}$$

Sometimes it's convenient to use $B_m = MJ$ - "molecular field" as the order parameter instead of M .

The physical meaning of B_m - effective magnetic field, acting on a given spin due to its interactions with other spins.

The free energy is given by :

$$F = \frac{NJM^2}{2} - NT \ln \left[2 \cosh \left(\frac{MJ+B}{T} \right) \right]$$

$$M = \tanh \left(\frac{MJ+B}{T} \right)$$

Find magnetic susceptibility $\chi = \frac{\partial M}{\partial B}$ for $T > T_c$.

When $T > T_c$ we expect $M \sim B$ for small B since $M=0$ when $B=0$.

Expanding \tanh for small M and B , we obtain:

$$M \approx \frac{M\gamma + B}{T}$$

$$M \left(1 - \frac{T_c}{T}\right) = \frac{B}{T}$$

$$\chi = \frac{1/T}{1 - \frac{T_c}{T}} = \frac{1}{T - T_c}$$

For $T < T_c$ we would find:

$$\chi = \frac{1}{2(T_c - T)}$$

$$\text{Thus } \chi \sim |t|^{-1} = |t|^{-\delta}$$

$\delta = 1$ - susceptibility critical exponent.

Now find how M depends on B at $T = T_c$.

$$\text{Use } \tanh x = x - \frac{x^3}{3}$$

$$M = \frac{M\gamma + B}{T_c} - \frac{1}{3} \left(\frac{M\gamma + B}{T_c} \right)^3 =$$

$$= M + \frac{B}{T_c} - \frac{1}{3} \left(M + \frac{B}{T_c} \right)^3$$

$$\text{This gives } B = \frac{T_c}{3} \left(M + \frac{B}{T_c} \right)^3$$

$$M + \frac{B}{T_c} = \left(3 \frac{B}{T_c}\right)^{1/3}$$

Since $\left(\frac{B}{T_c}\right)^{1/3} \ll \frac{B}{T_c}$ at small $\frac{B}{T_c}$, we obtain:

$$M \sim \left(\frac{B}{T_c}\right)^{1/3} = B^{1/3} = B^{1/8}$$

Here $B = \frac{B}{T_c}$ - reduced field and $\delta = 3$ - field critical exponent.

Finally, calculate the behavior of the specific heat near T_c .

$$C_V = -\frac{1}{N} T \frac{\partial^2 F}{\partial T^2} \quad - \text{specific heat per lattice site.}$$

$$C_V = -T \frac{\partial^2 f}{\partial T^2}$$

$$f = \frac{T_c}{2} \left(1 - \frac{T_c}{T}\right) M^2 + \frac{T_c^4}{12T^3} M^4 =$$

$$= \frac{T_c}{2} \frac{T-T_c}{T} M^2 + \frac{T_c^4}{12T^3} M^4 \approx$$

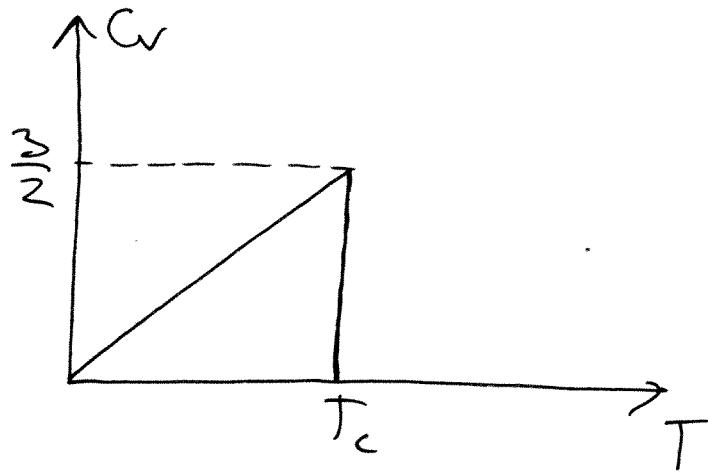
$$= \frac{1}{2} (T-T_c) M^2 + \frac{T_c}{12} M^4$$

$$M \approx \sqrt{3 \left(1 - \frac{T}{T_c}\right)} \quad \text{- plug this in } f:$$

$$f = \frac{-3}{2T_c} (T - T_c)^2 + \frac{3}{4T_c} (T - T_c)^4 = \\ = -\frac{3}{4T_c} (T - T_c)^2$$

$$C_V = -T \frac{\partial^2 f}{\partial T^2} = \bullet \frac{3}{2} \frac{T}{T_c} \quad \text{for } T < T_c.$$

$C_V = 0$ for $T > T_c$.



Can write this as $C_V \sim |t|^{-\alpha} + \text{const}$ as $T \rightarrow T_c$.

In MFT $\alpha = 0$. α - specific heat critical exponent.

The set of critical exponents fully characterizes a continuous phase transition.

Landau's idea: The general form of the free energy near a continuous phase transition can be written down without referring to any specific microscopic Hamiltonian and doing an explicit mean-field theory calculation.

All we need to know is the order parameter and the symmetry of the Hamiltonian.

In our case the order parameter is $M = \langle \sigma_i \cdot \rangle$.

The Hamiltonian is invariant under the $\sigma_i \rightarrow -\sigma_i$ transformation. This means that the free energy as a function of M must also be invariant under $M \rightarrow -M$ transformation. It immediately follows that the Taylor expansion of f in powers of M must have the form,

$$f = \gamma M^2 + u M^4$$

f can't depend on odd powers of M .

Postulating that $\Gamma_0 \sim T - T_c$ and $u > 0$ is constant, we will obtain the same result for the critical exponents as from microscopic mean-field theory above.

Landau's idea then suggests that all continuous transitions are characterized by the same critical exponents:

$$\beta = \frac{1}{2}, \alpha = 0, \gamma = 1, \delta = 3.$$

This is to ~~be considered~~ simple to be true.

In reality, phase transitions observed in nature can be classified in ~~essentially~~ a number of different universality classes.

Universality class is characterized by a particular set of critical exponents.

If two microscopically distinct systems exhibit phase transitions with the same set of critical exponents, these transitions are said to belong to the same universality class.

For example, ferromagnet-paramagnet transition in a uniaxial magnet, described by the 3D Ising model is observed to be in the same universality class as the liquid-gas transition in a liquid if we identify $\rho_{\text{liquid}} - \rho_{\text{gas}}$ as the order parameter.

Identification of different universality classes and calculation of the corresponding critical exponents is the main goal of the modern theory of phase transitions.

Mean-field theory, and its generalized version due to Landau gives us the correct general idea about what happens near continuous phase transitions, i.e. power law behavior of thermodynamic properties. But MFT is too naive - it predicts that all transitions are in one universality class - this is not what is observed experimentally. Mean-field values of the critical exponents are almost never observed.

Critical exponents turn out to depend on dimensionality, nature of the order parameter (e.g. scalar M versus vector \vec{M}), etc.

The reason MFT fails is that it neglects fluctuations of the order parameter - it treats M as simply a parameter, with respect to which the free energy is

minimized. Instead it should be treated as a mesodynamic variable, which can be nonuniform in space and which has thermal fluctuations.

In the next few lectures we will develop a theory of a fluctuating order parameter.

Start again from the Ising model Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j.$$

The partition function is given by:

$$Z = \sum_{\{\sigma\}} e^{-\frac{\mathcal{H}}{T}} = \sum_{\{\sigma\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j}$$

To proceed let us prove the following identity:

$$\begin{aligned} & \frac{1}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_n e^{-\frac{1}{2} \varphi_i A_{ij} \varphi_j + \varphi_i \delta_i} \\ &= \frac{1}{\sqrt{\det A}} e^{\frac{1}{2} \delta_i A_{ij}^{-1} \delta_j} \end{aligned}$$

Here A is a positive-definite real symmetric matrix summation over repeated indices is implied (Einstein summation convention) and φ_i are real variables.
 δ_i are arbitrary real numbers.

Consider $S[\varphi] = \frac{1}{2} \varphi_i A_{ij} \varphi_j - \varphi_i \delta_i$

First make the following change of variables:

$$\boxed{y_i = \varphi_i - A_{ij}^{-1} \delta_j}$$

It's easy to show that this gives:

$$S[y] = \frac{1}{2} y_i A_{ij} y_j - \frac{1}{2} \delta_i A_{ij}^{-1} \delta_j \quad \text{- we have eliminated terms linear in } \varphi_i.$$

Now let U be the unitary transformation that diagonalizes the matrix A :

$$U^{-1} A U = \Lambda \quad \text{- diagonal matrix of the eigenvalues of } A.$$

Make another variable change:

$$z_i = U_{ij}^{-1} y_j$$

Then it's again straightforward to show that:

$$S[z] = \frac{1}{2} \lambda_i z_i^2 - \frac{1}{2} \delta_i A_{ij}^{-1} \delta_j$$

Here λ_i are the eigenvalues of the matrix A .

Then we obtain:

$$\frac{1}{(2\pi)^{N/2}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2} \sum_i A_{ij} \varphi_i \varphi_j + \varphi_i \sigma_i} = \\ = \frac{1}{(2\pi)^{N/2}} \int_{-\infty}^{\infty} dz_1 \dots dz_N e^{-\frac{1}{2} \lambda_i z_i^2 - \frac{1}{2} \sum_i \sigma_i A_{ij}^{-1} \sigma_j} = *$$

Here we have used the fact that since U is a unitary matrix, i.e. $U^{-1} = U^T$, the Jacobian of the transformation from ' φ to z variables' is equal to 1 since $\det U = 1$.

Now since A is positive-definite by assumption, all eigenvalues λ_i are positive.

Then $\int_{-\infty}^{\infty} dz_i e^{-\frac{1}{2} \lambda_i z_i^2} = \sqrt{\frac{2\pi}{\lambda_i}}$

Then we obtain:

$$* = \frac{1}{(2\pi)^{N/2}} \prod_{i=1}^N \sqrt{\frac{2\pi}{\lambda_i}} e^{\frac{1}{2} \sum_i \sigma_i A_{ij}^{-1} \sigma_j} = \\ = \frac{1}{\sqrt{\det A}} e^{\frac{1}{2} \sum_i \sigma_i A_{ij}^{-1} \sigma_j}$$

Apply this identity to the partition function of the Ising model. We have:

$$e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = (\det \gamma^{-1})^{1/2} T^{N/2} .$$

$$\frac{1}{(2\pi)^{N/2}} \int d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} J_{ij} \varphi_i \varphi_j + \sum_i \sigma_i \varphi_i}$$

Change variables $\varphi_i \rightarrow \frac{\varphi_i}{T}$

$$e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = (\det J)^{-\frac{1}{2}} (2\pi T)^{-\frac{N}{2}}.$$

$$\int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j + \sum_i \frac{\varphi_i \sigma_i}{T}}$$

Here J is an $N \times N$ matrix with matrix elements J_{ij} .

The partition function thus becomes,

$$Z = \sum_{\{\sigma\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} = C \sum_{\{\sigma\}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j}.$$

$$e^{\sum_i \frac{\varphi_i \sigma_i}{T}}$$

$$C = (\det J)^{-1/2} (2\pi T)^{-\frac{N}{2}} - \text{constant which we will ignore henceforth.}$$

Thus we finally obtain:

$$Z = \sum_{\{\sigma\}} e^{\frac{1}{2T} \sum_{ij} J_{ij} \sigma_i \sigma_j} =$$

$$= \sum_{\{\sigma\}} \int_{-\infty}^{\infty} d\varphi_1 \dots d\varphi_N e^{-\frac{1}{2T} \sum_{ij} \varphi_i J_{ij}^{-1} \varphi_j + \sum_i \frac{\varphi_i \sigma_i}{T}}$$

Thus ~~partition function~~ we have transformed a partition function of a system of interacting spins σ_i into a partition function of ~~noninteracting~~ spins, interacting with a fluctuating real field φ_i .

Note that φ_i couples to σ_i as a magnetic field. The physical meaning of φ_i is a fluctuating molecular field.

The above transformation of the partition function is called Hubbard-Stratonovich transformation.