Mean-Field Ising Model close to the critical point

Let's redefine $Jz \to J$

Equation of State

$$M = \tanh(\beta J M + \beta H) \qquad (*)$$

fixes Magnetization $M = M(T,H)$ given a temperature T and a field H

Close to critical point $H=0$, $k_B T_c = J$

Magnetization is small $M \ll 1$

Define Reduced Temperature

$$t := \frac{T - T_c}{T_c} = \frac{T}{T_c} - 1$$

Taylor-Expansion of $(*)$ yields

$$M = \beta J M + \beta H - \frac{1}{3}(\beta J M)^3 + \mathcal{O}(H^2, M^4)$$

$$\Rightarrow \quad H = J t M + \frac{J}{3}(\beta J)^2 M^3$$

Emergence of Order Parameter below T_c @ $H=0$:

$$-\mathcal{J}t M_f = \frac{\mathcal{J}}{3}(\beta\mathcal{J})^2 M_f^3 \Rightarrow M_f = \frac{\sqrt{3}}{\beta\mathcal{J}}(-t)^{1/2}$$

Susceptibility around T_c:

$$\chi = \frac{\partial M}{\partial H}\bigg|_{H\to 0} = \frac{1}{\mathcal{J}t + \mathcal{J}(\beta\mathcal{J})^2 M^2}$$

with $M = \begin{cases} 0 & t>0 \\ M_f & t<0 \end{cases}$ for

$$\chi = \begin{cases} \frac{1}{\mathcal{J}t} & t>0 \\ -\frac{1}{2\mathcal{J}t} & t<0 \end{cases} \text{ for}$$

Field-Dependence @ T_c

$$H = \frac{\mathcal{J}}{3}(\beta\mathcal{J})^2 M^3 \Rightarrow M = \frac{1}{\beta\mathcal{J}}(3\beta H)^{1/3}$$

Ising vs. van-der-Waals

	Ising	vdW
Order Parameter:	Magnetization M	Density Difference $\Delta\rho$
Conjugate Field:	Magnetic Field H	Pressure p
Susceptibility:	$\chi = \frac{\partial M}{\partial H}$	$\kappa_T = -\frac{1}{\rho}\frac{\partial \rho}{\partial p}$
Critical Field:	$H_c = 0$	$p_c \neq 0$

Order Parameter continuously grows from zero below T_c

Ising	vdW
$M \sim (-t)^\beta$	$\Delta\rho \sim (-t)^\beta$
$\chi \sim \lvert t \rvert^{-\gamma}$	$\kappa_T \sim \lvert t \rvert^{-\gamma}$
$M \sim H^{1/\delta}$	$\Delta\rho \sim (p-p_c)^{1/\delta}$

(Mean-Field) Critical Exponents

$$\beta = 1/2 \qquad \gamma = 1 \qquad \delta = 3$$

Landau theory

To calculate the partition function

$$Z = \sum_{\{S_i\}} e^{-\beta \mathcal{H}}$$

consider the set of configurations

$\{S_i \mid \sum_i S_i = NM\}$ with a fixed magnetization M

and write

$$Z = \sum_M \sum_{\{S_i \mid \sum_i S_i = NM\}} e^{-\beta \mathcal{H}}$$

now define $\mathcal{F}(M,T,H)$ by

$$e^{-\beta \mathcal{F}} := \sum_{\{S_i \mid \sum_i S_i = NM\}} e^{-\beta \mathcal{H}}$$

then

$$Z = \sum_M e^{-\beta \mathcal{F}} \xrightarrow{N \to \infty} \int_{-1}^{1} dM\, e^{-\beta \mathcal{F}(M,T,H)}$$

The integral will be dominated by the saddle point $\bar{M}$ where

$$\frac{\partial \mathcal{F}}{\partial M}(\bar{M}) \overset{!}{=} 0$$

which yields the

Equation of State $\bar{M} = \bar{M}(T,H)$

with $\bar{M}$ we get the free Energy

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

It is very difficult to (approximately) determine $\mathcal{F}$ from the microscopic Hamiltonian $\mathcal{H}$

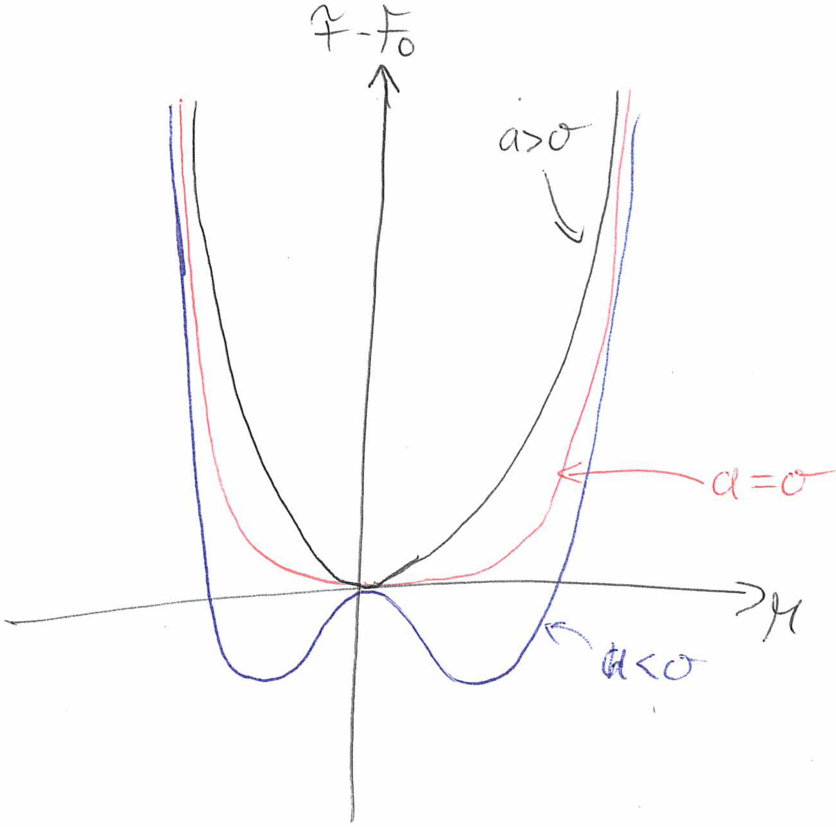
Near the critical point, we can guess, though, how $\mathcal{F}$ should look like:

1. For small M we can expand $\mathcal{F}$ in a Taylor-Series
2. $\mathcal{F}$ must be invariant under $M \to -M$ in zero field $H=0$, i.e. only even powers of M are allowed
3. $\mathcal{F}$ must be bounded from below

To 4th order this is obeyed by

$$\mathcal{F}(M,T) = F_0(T) + a(T)M^2 + b(T)M^4$$

with $b(T) > 0$



To ensure this behavior near the critical point it is enough to assume

$$a(T) = At + O(t^2) \qquad A, B > 0$$
$$b(T) = B + O(t)$$

Together with the external field H we write

$$\boxed{F(M,T,H) = F_0(T) - MH + AtM^2 + BM^4}$$

From $\frac{\partial F}{\partial M}(\bar{M}) = 0$ we get the Equation of State

$$H = 2At\bar{M} + 4B\bar{M}^3$$

At $H=0$ we find

$\bar{M}=0$ for $t>0$

$$\bar{M}^2 = -\frac{At}{2B} \quad \text{for } t<0$$

or $\bar{M} \sim (-t)^{1/2}$

Moreover

$$\chi^{-1} = \frac{\partial H}{\partial \bar{M}} = 2At + 12B\bar{M}^2 = \begin{cases} 2At & \text{for } t>0 \\ -4At & \text{for } t<0 \end{cases}$$

and at $t=0$

$$H = 4B\bar{M}^3$$

The critical exponents are determined by the symmetries of the order parameter alone and are independent of the (unknown) details in F_0, A, B.

The function $\mathcal{F}(M,T,H)$ is called the

Landau Free Energy or the

Free Energy Functional

but beware that it is not the free energy, only $\mathcal{F}(\bar{M}(T,H),T,H)$ is.
Also it is not a functional (yet), as M is just a variable.

For the infinite range Ising model you calculated

$$\mathcal{F} = \frac{N}{2} J M^2 - N k_B T \ln[2 \cosh(\beta J M)]$$

in the exercise

Expanding in M:

$$\mathcal{F} \approx \frac{N}{2} J M^2 - N k_B T \ln 2 - \frac{N}{2} J (\beta J) M^2 + \frac{N}{12} J (\beta J)^3 M^4$$

$$= F_0 + A t M^2 + B M^4$$

with $F_0 = -N k_B T \ln 2$ entropic

$A = NJ/2$ and $B = NJ/12$

Spatial Variations

Assume we divide our system into a large number of subsystems $n = 1, 2, 3, \ldots$ of characteristic size Λ^{-1} such that each subsystem still contains a large number of spins. Each subsystem has its own magnetization M_n such that

$$Z = \int dM e^{-\beta F} \rightarrow \int \prod_n dM_n e^{-\beta F}$$

For large systems L such that $L\Lambda^{-1} \gg 1$ we can think of M_n as a field $M(\underline{r})$ and write the partition function as a functional integral

$$Z = \int \mathcal{D}[M(\underline{r})] e^{-\beta F}$$

We will also use the Fourier representation

$$\tilde{M}(q) = \int d\underline{r}\, M(\underline{r}) e^{-i\underline{k}\cdot\underline{r}}$$

For a finite system, the wave numbers will be discrete and we can write

$$Z = \int \prod_{\substack{q \\ |q|<\Lambda}} d\tilde{M}(q)\, e^{-\beta F}$$

which makes the coarse-graining length scale Λ^{-1} explicit and can serve as a definition for the functional integral

We assume $\langle M(r)\rangle$ to be smoothly varying inspace. If we naively write

$$F[M] = \int d\underline{r}\, \frac{1}{V}\, F(M(\underline{r}))$$

nothing enforces the smoothness if we minimize F. In the spirit of the Landau expansion, we add the lowest order terms in the gradient ∇M that respect the symmetries of the system

For a spatially homogeneous and isotropic system the following terms are allowed

$$(\nabla M)^2, \quad M\nabla^2 M, \text{ and } \nabla\cdot(M\nabla M)$$

For the last one we have

$$\int_V d^d r\, \nabla\cdot(M\nabla M) = \int_{\partial V} d^{d-1} r\, M\nabla M$$

and we assume surface terms to be negligible

We can also rewrite

$$M\nabla^2 M = -(\nabla M)^2 + \nabla\cdot(M\nabla M)$$

such that $(\nabla M)^2$ is the only relevant term, i.e.,

$$\mathcal{F}[M] = F_0 + \int d\underline{r}\left[At M^2(\underline{r}) + BM^4(\underline{r}) + \kappa\left(\nabla M(\underline{r})\right)^2\right]$$

with a new parameter κ