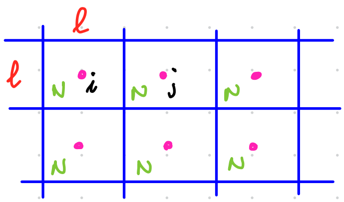
The Ginzburg - Landau theory

We want to address a system which is extended in space $\longrightarrow$ going toward field theory

Let' divide space in (hyper-) cubic parcels of side ℓ, each containing N spins.



"i" (and "j") indicate the positions of the centers of the cubes.

The Hamiltonian of the system is

$$H = -\frac{J}{N} \sum_{\langle i,j \rangle} \left(\sum_{\alpha \in i} s_\alpha \right) \left(\sum_{\beta \in j} s_\beta \right) - h \sum_i \left(\sum_{\alpha \in i} s_i \right)$$

Observation: here we take all possible interactions between two blocks. As we will see later in the course, this has no consequences.

We can now write the partition function

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} =$$

$$= \sum_{\{s\}} e^{\beta \frac{J}{N} \sum_{\langle i,j \rangle} \left(\sum_{\alpha \in i} s_\alpha \right) \left(\sum_{\beta \in j} s_\beta \right) + \beta h \sum_i \sum_{\alpha \in i} s_\alpha}$$

Now we introduce a concept/procedure that we are going to encounter also later on: COARSE GRAINING

For every block, we introduce a variable $M_i \in [-N, N]$, and

$$\sum_{M_i=-N}^{+N} \underbrace{\delta_{M_i, \sum_{\alpha\in i} s_\alpha}} = 1$$

Kroenecker's delta that ensures $M_i = \sum_{\alpha\in i} s_\alpha$

because for any choice of $\{s_\alpha\}$ there will be only one value of m_i that matches it

Since the left-hand-side is equal to 1, we can safely insert it in the expression of the partition function

$$Z = \sum_{\{s_\alpha\}} e^{-\beta H} \underbrace{\prod_i \left[\sum_{M_i=-N}^{N} \delta_{M_i, \sum_{\alpha\in i} s_\alpha}\right]}_{\text{This is a product of 1's}} =$$

$$= \underbrace{\sum_{M_1=-N}^{N} \sum_{M_2=-N}^{N} \cdots}_{\text{sum for all blocks}} \sum_{\{s_\alpha\}} e^{\beta \frac{J}{N} \sum_{\langle i,j\rangle} \left[\sum_{\alpha\in i} s_\alpha\right]\left[\sum_{\beta\in j} s_\beta\right] + \beta h \sum_i \sum_{\alpha\in i} s_i} \cdot \prod_i \delta_{M_i, \sum_{\alpha\in i} s_\alpha}$$

exchange the sums

Now we can use the Kroenecker's delta and substitute m_i in place of $\sum_{\alpha \in i} s_\alpha$.

Careful: in summing on $\sum_{\{s_\alpha\}}$ we perform this substitution each time $\sum_{\alpha \in i} s_\alpha = m_i$, for a given m_i (we perform the sum over m_i only later). We must thus take into account all the times this happens. It is a sort of local entropy, as we will see.

Can we compute this multiplicity?

Out of the N spins in a block, N_+ are positive and N_- are negative. Thus

$$\begin{cases} N_+ - N_- = M \\ N_+ + N_- = N \end{cases} \Rightarrow \begin{cases} N_+ = \dfrac{N+M}{2} \\ N_- = \dfrac{N-M}{2} \end{cases}$$

The number of ways we can thus get M out of N is

$$\binom{N}{N_+} = \binom{N}{\frac{N+M}{2}}$$

We can thus go back to the partition function

$$Z = \sum_{M_1=-N}^{+N} \sum_{M_2=-N}^{+N} \cdots \prod_i \binom{N}{\frac{N+M_i}{2}} e^{\beta \frac{J}{N} \sum_{\langle i,j \rangle} M_i M_j + \beta \frac{h}{N} \sum_i M_i} =$$

$$= \sum_{M_1} \sum_{M_2} \cdots e^{\beta \frac{J}{N} \sum_{\langle i,j \rangle} M_i M_j + \beta \frac{h}{N} \sum_i M_i + \sum_i \ln \binom{N}{\frac{N+M_i}{2}}}$$

How do we deal with $\ln \binom{N}{\frac{N+M}{2}}$?

Recall the Stirling approximation for the factorial

$$n! \simeq n^{n+\frac{1}{2}} e^{-n} \sqrt{2\pi}$$

which is very good already for $n \simeq 4$ and gets better and better:

	Exact	Stirling	
$n=4$	24	23.5	2%
$n=7$	5040	4980	1.2%
	⋮	⋮	

Then

$$\binom{N}{\frac{N+M}{2}} = \frac{N!}{\left(\frac{N+M}{2}\right)! \left(\frac{N-M}{2}\right)!} =$$

$$\simeq \frac{N^{N+\frac{1}{2}} e^{-N} \sqrt{2\pi}}{\left(\frac{N+M}{2}\right)^{\frac{N+M+1}{2}} e^{-\frac{N+M}{2}} \sqrt{2\pi} \left(\frac{N-M}{2}\right)^{\frac{N-M+1}{2}} e^{-\frac{N-M}{2}} \sqrt{2\pi}} =$$

$$= \frac{N^{N+1/2}}{\sqrt{2\pi}\left(\frac{N+M}{2}\right)^{\frac{N+M+1}{2}}\left(\frac{N-M}{2}\right)^{\frac{N-M+1}{2}}} =$$

$$= \frac{N^{N+1/2}\, 2^{N+1}}{\sqrt{2\pi}\,(N+M)^{\frac{N+M+1}{2}}\,(N-M)^{\frac{N-M+1}{2}}}$$

Then

$$\ln\binom{N}{\frac{N+M}{2}} \simeq \ln\left(\frac{N^{N+1/2}\,2^{N+1}}{\sqrt{2\pi}}\right) - \left(\frac{N+M+1}{2}\right)\ln(N+M) - \left(\frac{N-M+1}{2}\right)\ln(N-M)$$

$$= \text{const} - (N+1)\ln N - \frac{N+M+1}{2}\ln\left(1+\frac{M}{N}\right) - \frac{N-M+1}{2}\ln\left(1-\frac{M}{N}\right)$$

Remember that

$$\ln\left(1+\frac{M}{N}\right) \simeq x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots$$

$$\ln\left(1-\frac{M}{N}\right) \simeq -\left(x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4} + \dots\right)$$

Then

$$\ln\binom{N}{\frac{N+M}{2}} \simeq \text{const} - \frac{N+M-1}{2}\left(\frac{M}{N} - \frac{1}{2}\frac{M^2}{N^2} + \frac{1}{3}\frac{M^3}{N^3} - \frac{1}{4}\frac{M^4}{N^4}\right) +$$

$$+ \frac{N-M+1}{2}\left(\frac{M}{N} + \frac{1}{2}\frac{M^2}{N^2} + \frac{1}{3}\frac{M^3}{N^3} + \frac{1}{4}\frac{M^4}{N^4}\right) =$$

$$= \text{const} - \frac{N+1}{2}\left(-\frac{M^2}{N^2} - \frac{1}{2}\frac{M^4}{N^4}\right) - \frac{M}{2}\left(2\frac{M}{N} + \frac{2}{3}\frac{M^3}{N^3}\right) \underset{\substack{N+1 \simeq N \\ \text{if } N \gg 1}}{\simeq}$$

$$= \text{const} + \frac{M^2}{2N} + \frac{M^4}{4N^3} - \frac{M^2}{N} - \frac{1}{3}\frac{M^4}{N^3} =$$

$$= \text{const} - \frac{M^2}{2N} - \frac{1}{12}\frac{M^4}{N^3}$$

At last we can write

$$Z = \sum_{M_1}\sum_{M_2} \dots e^{\beta \frac{J}{N} \sum_{\langle i,j \rangle} M_i M_j + \beta h \sum_i M_i - \frac{1}{2N}\sum_i M_i^2 - \frac{1}{12N^3}\sum_i M_i^4}$$

Note : we can take the argument of the exponential and write it as

$$-\beta \left\{ -\frac{J}{N}\sum_{\langle i,j \rangle} M_i M_j - h \sum_i M_i + k_B T \left[\sum_i \left(\frac{1}{2N} M_i^2 + \frac{1}{12N^3} M_i^4 \right) \right] \right\}$$

Since Boltzmann tells

$$e^{-\beta H} \implies \text{we can define an "effective" } H:$$

$$H_{eff} = \underbrace{-\frac{J}{N}\sum_{\langle i,j \rangle} M_i M_j - h \sum_i M_i}_{U} + \underbrace{k_B T \left[\sum_i \left(\frac{1}{2N} M_i^2 + \frac{1}{12N^3} M_i^4 \right) \right]}_{-TS}$$

Upon close inspection we see that this is a free-energy

$$U - TS$$

We now focus on $\sum_{\langle i,j \rangle} M_i M_j$: we can rewrite it as

$$\sum_{\langle i,j \rangle} M_i M_j = -\frac{1}{2} \sum_{\langle i,j \rangle} (-2 M_i M_j) = -\frac{1}{2} \sum_{\langle i,j \rangle} (M_i - M_j)^2 +$$

$$+ \frac{1}{2} \sum_{\langle i,j \rangle} (M_i^2 + M_j^2) =$$

coordination number

$$= -\frac{1}{2} \sum_{\langle i,j \rangle} (M_i - M_j)^2 + z \sum_i M_i^2$$

We can now rewrite H_{eff} :

$$H_{eff} = \frac{J}{2N} \sum_{\langle i,j \rangle} (M_i - M_j)^2 + \sum_i \left[-\frac{Jz}{N^2} M_i^2 + k_B T \left(\frac{M_i^2}{2N} + \frac{M_i^4}{12N^3} \right) \right] - h \sum_i M_i$$

$$= \frac{J}{2N} \sum_{\langle i,j \rangle} (M_i - M_j)^2 + \sum_i \left[\left(\frac{k_B T}{2N} - \frac{Jz}{N} \right) M_i^2 + \frac{k_B T}{12 N^3} M_i^4 \right] - h \sum_i M_i$$

$$= \frac{J}{2N} \sum_{\langle i,j \rangle} (M_i - M_j)^2 + N \sum_i \left[\left(\frac{k_B T}{2} - Jz \right) m_i^2 + \frac{k_B T}{12} m_i^4 - h\, m_i \right]$$

$$= N \left\{ \frac{J}{2} \sum_{\langle i,j \rangle} (m_i - m_j)^2 + \sum_i \left[\left(\frac{k_B T}{2} - Jz \right) m_i^2 + \frac{k_B T}{12} m_i^4 - h\, m_i \right] \right\}$$

The choice of the interactions ensures extensivity once we move to the magnetization per spin

$$m_i = \frac{M_i}{N}$$

We now focus on

distance between two blocks

$$\sum_{\langle i,j\rangle} (m_i - m_j)^2 = \ell^2 \sum_{\langle i,j\rangle} \left(\frac{m_i - m_j}{\ell}\right)^2$$

We take now the continuum limit

$$\lim_{\ell \to 0} \sum_{\langle i,j\rangle} \left(\frac{m_i - m_j}{\ell}\right)^2 = \int (\vec{\nabla} m)^2 \, dV$$

Let's take now

$$\sum_i \left[\left(\frac{k_B T}{2} - J\gamma\right) m_i^2 + \frac{k_B T}{12} m_i^4 - h m_i \right] \longrightarrow \int dV \left[\left(\frac{k_B T}{2} - J\gamma\right) m^2(x) + \right.$$
$$\left. + \frac{k_B T}{12} m^4(x) - h\, m(x) \right]$$

At last

$$T_c = \frac{2J\gamma}{k_B}$$

$$H_{eff} = k_B T \int dV \left[\underbrace{\frac{1}{2}\left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 - h\, m}_{\text{We have already seen this! It's the Landau expansion}} + \underbrace{\frac{J'}{2 k_B T} (\vec{\nabla} m)^2}_{\text{This term penalizes fluctuations}} \right]$$

We have already seen this!

It's the Landau expansion

This term penalizes fluctuations

What happens to the partition function?

$$Z = \sum_{m_1} \dots \sum_{m_2} e^{-\beta H_{eff}} \longrightarrow \int \mathcal{D}m \, e^{-\beta H_{eff}[m]}$$

functional integral over all possible fields

Let's look at all possible homogeneous fields $m(x) = m \;\; \forall x$
$\Rightarrow \vec{\nabla} m = 0$

$$H_{eff}[m] = N \int \left[\frac{1}{2}\left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 - h m\right] dV \;\; k_B T$$

$$= k_B T \, N V \left[\frac{1}{2}\left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 - h m\right]$$

How do we find the average m?

$$\langle m \rangle = \frac{1}{Z} \int_{-\infty}^{+\infty} dm \; e^{-NV\left[\frac{1}{2}\left(1 - \frac{T_c}{T}\right) m^2 + \frac{1}{12} m^4 - h m\right]} \cdot m$$

$-\infty \rightarrow N$, but N very large

How do we solve this?

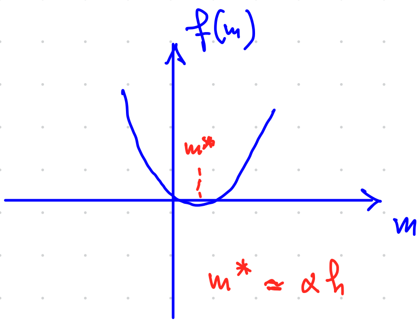
We use the "Gaussian" approximation (a special case of the more general "saddle point" approximation)

Let's take the argument of the exponential :

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

We search the zeroes of $f'(m)$. We have two cases

<u>Case 1</u>: $T > T_c$



if m is small (we are close to T_c) then we expect

$m \propto h$ (h also small)

We then expand $f(m)$ around m^*

$$f(m) \simeq f(m^*) + \frac{1}{2} f''(m^*)(m - m^*)^2 + O\left((m - m^*)^3\right)$$

Let's write Z

$$Z \simeq \int_{-\infty}^{+\infty} e^{-NVf(m^*) - \frac{1}{2} f''(m^*) NV (m - m^*)} \, dm$$

Then

$$\langle m \rangle \simeq \int_{-\infty}^{+\infty} dm \; m \; \frac{e^{\cancel{-NVf(m^*)} - \frac{1}{2} NV f''(m^*)(m-m^*)^2}}{\int_{-\infty}^{+\infty} e^{\cancel{-NVf(m^*)} - \frac{1}{2} NV f''(m^*)(m-m^*)^2}} =$$

$$= \int_{-\infty}^{+\infty} dm \; m \; \underbrace{\frac{e^{-\frac{1}{2} NV f''(m^*)(m-m^*)^2}}{\int_{-\infty}^{+\infty} e^{-\frac{1}{2} NV f''(m^*)(m-m^*)^2}}}$$

This is a Gaussian around m^*, well normalized.

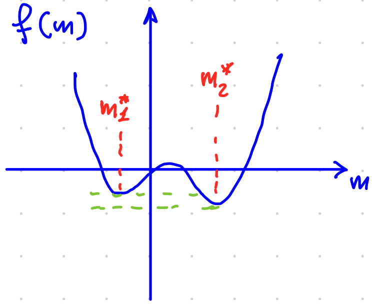
The variance is $\frac{1}{\sqrt{NV f''(m^*)}}$: if $N, V \to \infty$ (thermodynamic limit) the variance goes to 0

$\Rightarrow$ it becomes $\delta(m - m^*)$

$$\Rightarrow \quad \langle m \rangle \simeq m^* = \alpha h$$

And at last $\quad \lim_{h \to 0} m^* = 0$

Case 2: $T < T_c$



$m_1^* \simeq -m^* + a h$

$m_2^* \simeq m^* + a h$

$f(m_1^*) - f(m_2^*) \simeq b h > 0$

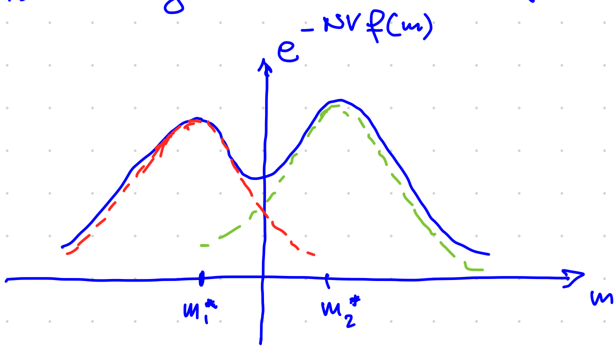
still in the approximation of small h and T close to T_c

Let's define

$$I_\alpha = \int_{-\infty}^{+\infty} dm \; e^{-\frac{1}{2} N V f''(m_\alpha^*)(m - m_\alpha^*)^2}$$

which is the normalization of the Gaussian centered in m_α^* from the second order expansion of $f(m)$.

Essentially, we are taking the original exponential and approximating it as the sum of two Gaussians



Which corresponds to

$$\langle m \rangle = \int_{-\infty}^{+\infty} dm \; m \; \frac{e^{-NVf(m_1^*) - \frac{1}{2}NVf''(m_1^*)(m-m_1^*)^2} + e^{-NVf(m_2^*) - \frac{1}{2}NVf''(m_2^*)(m-m_2^*)^2}}{e^{-NVf(m_1^*)} I_1 + e^{-NVf(m_2^*)} I_2} =$$

$$= \int_{-\infty}^{+\infty} dm \; m \; \frac{e^{-NV(f(m_1^*) - f(m_2^*)) - \frac{1}{2}NVf''(m_1^*)(m-m_1^*)^2} + e^{-\frac{1}{2}NVf''(m_2^*)(m-m_2^*)^2}}{e^{-NV(f(m_1^*) - f(m_2^*))} I_1 + I_2}$$

we recall that $\quad f(m_1^*) - f(m_2^*) = b\,h > 0$

then

$$\lim_{N,V\to\infty} m = \int_{-\infty}^{+\infty} dm \; m \; \underbrace{\frac{e^{-\frac{1}{2}NVf''(m_2^*)(m-m_2^*)}}{I_2}}_{\text{and this becomes } \delta(m - m_2^*)} =$$

$$= m_2^* = +m^* + a\,h$$

At last

$$\lim_{h\to 0} m = +m^*$$

Once again we see the importance of taking the two limits in the correct order

Still, the $m(\vec{x}) = m \ \forall x$ solution is the mean-field one:

$$f(m) = \frac{1}{2} t\, m^2 + \frac{1}{12} a\, m^4 \longrightarrow \frac{\partial f}{\partial m} = 0 \qquad t\,m + \frac{1}{3} a m^3 = 0$$

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

$m = 0$

$m = \sqrt{-\frac{3t}{a}}$

exists if $T < T_c$ $(t<0)$

and then

$m \propto (T_c - T)^{1/2}$

Question: is the Ginzburg-Landau model always mean-field?

No! we have neglected $(\vec{\nabla} m)^2 \Leftarrow$ fluctuations!

Taking the gradient term into account will bring new exponents (using the Renormalization Group: in some lectures)

For the time being we are going to see what happens if we keep $(\vec{\nabla} m)^2$ and drop m^4 (it is a different kind of mean-field)

We are going to look at spatial correlations close to the critical point ($T \sim T_c$, $h = 0$, $m \simeq 0$). We neglect m^4 (I repeat here: it is wrong, at least in some cases, but at least it is solvable).