Notes on the thermodynamic limit ($N \to \infty$)

Why do we need the thermodynamic limit to have a phase transition?
There are many different reasons. Some are complementary, some are the same under different angles.
The dynamic reasons have been evoked previously. But the "ensembles" view of statistical mechanics does not use dynamics. How do we understand the need for the thermodynamic limit?

Let's recall the definition of m:

$$m(h) = -\frac{1}{N}\frac{\partial F_N}{\partial h}$$

so that the spontaneous magnetization, that is m if $h=0$, is

$$m = -\lim_{h \to 0} \frac{1}{N}\frac{\partial F_N}{\partial h}$$

But $F_N(h) = -k_B T \ln Z_N(h)$, and

$$Z_N(h) = \sum_{\{S_i\}} e^{-\beta H_N(h)}$$

The partition function is thus the sum over all possible spin configurations (2^N of them) of exponentials.
The exponential is an analytic function, and the sum of a finite (no matter how large) number of analytic functions is also analytic.

Thus $Z_N(h)$ is analytic $\forall h$. Since $Z_N(h) > 0$, $\ln Z_N(h)$ is also analytic.

Thus $F_N(h)$ is analytic. Moreover, since $Z_N(h)$ is an even function of h (by flip-symmetry of all spins, rigorously called $\mathbb{Z}_2$ symmetry), its derivative with respect to h is odd.

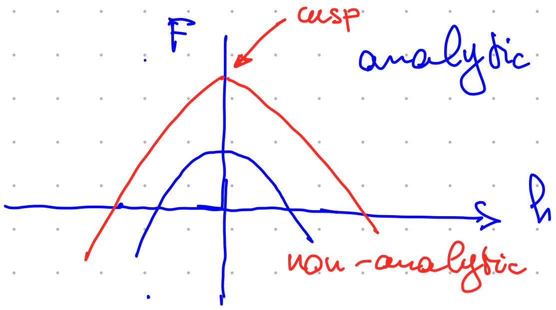
Since $F_N(h)$ is analytic, it is C^∞, and an odd function $\left(\frac{\partial F_N(h)}{\partial h}\right)$ vanishes at the origin.

As a consequence

$$m = \lim_{h \to 0} \left[-\frac{1}{N} \frac{\partial F_N}{\partial h} \right] = 0$$

There is only one way out: F must be non-analytic.

Graphically:



$$m_+ = \lim_{h \to 0^+} \left(-\frac{1}{N} \frac{\partial F}{\partial h} \right) = - \lim_{h \to 0^-} \left(-\frac{1}{N} \frac{\partial F}{\partial h} \right) = -m_- \qquad m_+ = -m_- \neq 0$$

the $\mathbb{Z}_2$ symmetry must be respected

We thus need a non-analytic behavior: not the first time we meet it.

But (there is always a "but"): we said that $Z_N(h)$ is analytic $\forall N$. The only way to get non-analytic behavior is to let $N \to \infty$ so that $Z_\infty(h)$ is the sum of an infinite number of analytic functions, that can be non-analytic

Think $f_M(x) = \sum_{k=0}^{M} x^k = \dfrac{1 - x^{M+1}}{1 - x}$

is analytic for any N, but

$$\lim_{M\to\infty} f(x) = \frac{1}{1-x}$$ is non-analytic.

Since for N spins there are 2^N terms in $Z_N(h)$ [maybe very large but finite], the only way to have an infinite number of terms is $N \to \infty$.

There is one more note:

$$m = \begin{cases} \overset{?}{\nearrow} \lim_{N\to\infty}\left[\lim_{h\to 0^+}\left(-\frac{1}{N}\frac{\partial F_N}{\partial h}\right)\right] = \lim_{N\to\infty} 0 = 0 \\ \overset{?}{\searrow} \lim_{h\to 0^+}\left[\lim_{N\to\infty}\left(-\frac{1}{N}\frac{\partial F_N}{\partial h}\right)\right] = \lim_{h\to 0^+} m(h) = m^+ \end{cases}$$

spontaneous magnetisation

The two limits do not commute. First $N \to \infty$ and then $h \to 0$.

Physically we understand it: dynamically the system switches from + to − with a probability per unit time (rate) that behaves as $e^{-\beta(F_N(0) - F_N(m^*))}$

The argument is extensive, so that it does not flip anymore if $N \to \infty$

Thus a small h makes the system prefer $m^* > 0$. If we send $h \to 0$ before $N \to \infty$, the system will flip-flop and $\langle s_i \rangle = 0$.

If instead we send $N \to \infty$ first, then even if $h \to 0$ afterwards, the system remains frozen.

Back to the Ising model

Exact solution of the 1D Ising model by transfer matrix

$$H = -J \sum_{i=1}^{N} s_i s_{i+1} - h \sum_i s_i$$

periodic boundary conditions : $s_{N+1} = s_1$

$$Z_N = \sum_{\{s_i\}} e^{\beta J \sum_{i=1}^{N} s_i s_{i+1} + \frac{\beta h}{2} \underbrace{\sum_i (s_i + s_{i+1})}}$$

symmetrization of the expression

$$Z_N = \sum_{s_1 = \pm 1} \cdots \sum_{s_N = \pm 1} \prod_{i=1}^{N} e^{\beta J s_i s_{i+1} + \frac{\beta h}{2}(s_i + s_{i+1})}$$

Let's call

$$T(s_i, s_{i+1}) = e^{\beta J s_i s_{i+1} + \frac{\beta h}{2}(s_i + s_{i+1})}$$

Then

$$Z_N = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \cdots \sum_{s_N = \pm 1} T(s_1, s_2)\, T(s_2, s_3) \cdots T(s_N, s_{N+1})$$

This looks like a product of matrices :

$$Z_N = \sum_{s_1 = \pm 1} \sum_{s_3 = \pm 1} \cdots \sum_{s_N = \pm 1} \underbrace{\left[\sum_{s_2 = \pm 1} T(s_1, s_2)\, T(s_2, s_3) \right]}_{T^2(s_1, s_3)} T(s_3, s_4) \cdots T(s_N, s_{N+1})$$

Iteratively applying this procedure we have

$$Z_N = \sum_{s_1 = \pm 1} T^N(s_1, \underbrace{s_{N+1}}_{= s_1}) = \sum_{s_1 = \pm 1} T^N(s_1, s_1) =$$

$$= \mathrm{Tr}\, \underline{T}^N \qquad \underline{T} = \begin{pmatrix} e^{\beta J + \beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta h} \end{pmatrix}$$

transfer matrix

$$\underline{\underline{T}} = \begin{pmatrix} e^{\beta J + \beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta h} \end{pmatrix}$$

Then we recall that $\quad \mathrm{Tr}\, \underline{\underline{T}}^N = \lambda_1^N + \lambda_2^N$

eigenvalues of $\underline{\underline{T}}$

$$F_N = -k_B T \ln Z_N = -k_B T \ln \left(\lambda_{max}^N + \lambda_{min}^N \right) =$$

$$= -k_B T N \ln \lambda_{max} - k_B T \ln \left[1 + \left(\frac{\lambda_{min}}{\lambda_{max}} \right)^N \right]$$

In the thermodynamic limit

$$f = \lim_{N \to \infty} \frac{1}{N} F_N = -k_B T \ln \lambda_{max}$$

Let's compute λ_{MAX}

$$\left(-\lambda + e^{\beta(J+h)} \right) \left(-\lambda + e^{\beta(J-h)} \right) - e^{-2\beta J} = 0$$

$$\lambda^2 - 2\lambda e^{\beta J} \cosh(\beta h) + 2 \sinh(2\beta J) = 0$$

$$\lambda = e^{\beta J} \cosh(\beta h) \pm \sqrt{e^{2\beta J} \cosh^2(\beta h) - 2 \sinh(2\beta J)} =$$

$$= e^{\beta J} \cosh(\beta h) \pm \sqrt{e^{2\beta J} (1 + \sinh^2(\beta h)) - e^{2\beta J} + e^{-2\beta J}}$$

$$= e^{\beta J} \cosh(\beta h) \pm \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}$$

The argument of the square root is always positive

$$\Longrightarrow \quad \lambda_{MAX} = e^{\beta J} \cosh(\beta h) + \sqrt{e^{2\beta J} \sinh^2(\beta h) + e^{-2\beta J}}$$

and

$$f = -k_B T \ln\left[e^{\beta J}\cosh(\beta h) + \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}} \right]$$

Sanity check : $h=0 \Rightarrow f = -k_B T \ln[2\cosh(\beta J)]$

cf. with result from exercise session.

What about the magnetization?

$$m(h) = -\frac{\partial f}{\partial h} = \frac{e^{\beta J}\sinh(\beta h) + e^{2\beta J}\sinh(\beta h)\cosh(\beta h)\left(e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}\right)^{-1/2}}{e^{\beta J}\cosh(\beta h) + \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}}} =$$

$$= \sinh(\beta h)\, \frac{e^{\beta J} + e^{2\beta J}\cosh(\beta h)\left(e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}\right)^{-1/2}}{e^{\beta J}\cosh(\beta h) + \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}}}$$

$$= \frac{e^{2\beta J}\sinh(\beta h)}{\sqrt{1 + e^{4\beta J}\sinh^2(\beta J)}}$$ (after some tedious math)

at last the spontaneous magnetization is

$$\boxed{m = \lim_{h\to 0} m(h) = 0}$$

because $\sinh(\beta h) = 0$ if $h=0$

Not only the Ising model does not have a phase transition, it is completely disordered at any $\beta \neq \infty$.

What did the mean field get wrong?

We had that
$$T_c = \frac{J z}{k_B} \qquad \text{with } z=2 \text{ in 1D}$$

What does the mean-field neglect?

Remember:
$$s_i s_j = \underbrace{(s_i - m)(s_j - m)}_{\text{neglects fluctuations}} + m(s_i + s_j) - m^2$$

Could fluctuations be the culprit?

Let's see: the fully ordered state is, say

$$+ + + + + + + + + + \; . \; . \; . \; . \; . \; + + + + + \qquad N \text{ spins}$$

In how many ways can we disorder it with the least increase of energy?

Flip one side of the lattice

$$+ + + + + + + \, \} - - - \; . \; . \; . \; . \; - - - - -$$

This creates a "wall" that costs $2J$ in energy

Let's look at the first two terms of the partition function:

$$Z_N = g_{gs} + g_1 e^{-2\beta J} + \dots$$

g_{GS} is the degeneracy of the ground state $g_{GS} = 1$

g_1 is the degeneracy of the states with 1 wall:

$g_1 \simeq N$ because we can flip it at N bonds

$$\Rightarrow \quad Z_N = 1 + N e^{-2\beta J} + \dots$$

In the thermodinamic limit, if $\beta < \infty$ then the second term dominates.

Given 1 spin, it will be in the + state in as many configurations as in the − state. Thus its average is 0 in the first excited state.

The state with two walls is even more disordered and more degenerate.

Hence, for any $\beta < \infty$ $m = 0$.

The Ising model in 1D is disordered because fluctuations dominate its behavior at any finite temperature ($T > 0 \Leftrightarrow \beta < \infty$).

Mean-field neglects fluctuations!!!

The free-energy approach to mean-field (Exo. Session 2) shows that mean field also neglects correlations.

This is a general principle in physics:

correlations $\Longleftrightarrow$ fluctuations

Think about the magnetic susceptibility:

$$\chi = \frac{dm}{dh} \propto \langle M^2 \rangle - \langle M \rangle^2 \qquad \text{fluctuations}$$

$$\propto \langle \sum_{ij} s_i s_j \rangle - \langle \sum_i s_i \rangle^2 =$$

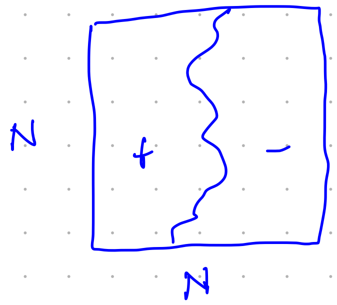
$$= \sum_{ij} \langle s_i s_j \rangle - \left(\sum_i \langle s_i \rangle \right)^2 =$$

$$= \sum_{ij} \left(\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right)$$

correlations!

Before moving on, there is a crucial question: if Ising 1D has no phase transition, how do we know that Ising for $d>1$ instead does?

Let's look again at the problem of building a "wall"



- There are N^2 spins
- there are μ^N ways of building a wall
- Each wall breaks N bonds (flip one side)

Partition function:

energy cost of a wall

$$Z_{N^2} = 1 + \underbrace{g_1}_{\mu^N} e^{-\beta(2JN)} + \ldots =$$

$$= 1 + e^{-\beta[2JN - k_B T N \ln\mu]} + \ldots =$$

$$= 1 + e^{-\beta\underbrace{[2J - k_B T \ln\mu]}N}$$

can see this as the "free energy" of the wall: energy $2J$
entropy $-k_B \ln\mu$

Thus now the wall term in the partition function dominates only if

$$2J - k_B T \ln\mu < 0$$

$$\Rightarrow \quad T > \frac{2J}{k_B \ln\mu}$$

hints at a critical temperature!

this is a crude version of the more rigorous Peierls argument, but morally the same.