Mathematical aspects of phase transitions

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Chapter 1: Introduction

The aim of this course is to cover some mathematical issues, together with the corresponding techniques, arising in the study of phase transitions.

1 Some definitions

In the context of statistical mechanics a physical system can be modeled (in the most simple version) by a *field*

$$\begin{aligned} \varphi: \quad & \Lambda \to \Omega \\ & x \to \varphi(x) \end{aligned}$$

where $\Lambda \subset \mathbb{Z}^d$ is a finite set of lattice points (you may think of them as equilibrium positions of atoms in a cristal), and $\varphi(x)$ describes the *state* or *configuration* of our system at the position x (for example the displacement of the atom from its equilibrium position, or the orientation of the local magnetic moment).

According to the physical problem we want to model, the set of possible local states (or configurations) Ω may be

$$\Omega = \mathbb{R}^N, \quad \mathbb{C}^N, \quad \mathcal{S}_N, \quad N \geq 1,$$

where $\mathcal{S}_N = \{x \in \mathbb{R}^N | \|x\| = 1\}$ is the N-dimensional sphere. When $N = 1$ this reduces to $\mathcal{S}_1 = \{+1, -1\}$ (the Ising model), when $N = 2$ $\varphi(x)$ in on a circle (the $XY-$model, or classical rotator), when $N = 3$ we $\varphi(x)$ in on the 3-dimensional sphere (the classical Heisenberg model).

The set of possible states (configurations) for the system is then

$$\Omega_\Lambda = (\Omega)^\Lambda = \{\varphi : \Lambda \to \Omega\}.$$

The price paid by the system to take a configuration far from its equilibrium is encoded in the energy functional

$$\begin{aligned} H_\Lambda: \quad & (\Omega)^\Lambda & \to \mathbb{R} \\ & \varphi & \to H(\varphi) \end{aligned} \tag{1.1}$$

We will consider the probability distribution on Ω_Λ defined by

$$d\mu_\Lambda(\varphi) = \frac{e^{-\beta H(\varphi)}}{Z_\Lambda} d\varphi$$

where $\beta = 1/T^1$, T is the temperature, Z_Λ (the *partition function*) is the normalization constant

$$Z_\Lambda = \int e^{-\beta H(\varphi)} d\varphi.$$

Finally $d\varphi$ is a product measure

$$d\varphi = \prod_{j\in\Lambda} d\varphi_j.$$

When $\Omega = \mathbb{R}^n$, $d\varphi_j$ is a product Lebesgue measure $d\varphi_j = \prod_{\alpha=1}^n d\varphi_{j,\alpha}$. When $\Omega = \mathcal{S}_n$, $d\varphi_j$ is the invariant measure on the sphere (Haar measure) normalized so that

$$\int_{\mathcal{S}_n} d\varphi_j = 1.$$

The probability measure $d\mu_\Lambda$ is called *Gibbs measure* for the system with energy functional H.

Remark For very low temperature $T \ll 1$ the parameter β is large and the measure is concentrated around the configurations minimizing the energy. On the contrary for very hight temperature $T \gg 1$ the parameter β is small and the measure is uniformly distributed on the whole set of configurations. This is consistent with the physical intuition that at low temperature the system is ordered (the probability is concentrated near a fixed configuration) and for high temperature it is disordered (any configuration is possible).

2 Ferromagnetic order: the O(N) model

As a precise example let us consider the $O(N)$ model, $N \geq 1$. In this case the configuration set is

$$\Omega_\Lambda = \mathcal{S}_N^\Lambda = \{\mathbf{S} : \Lambda \to \mathcal{S}_N\}, \qquad \mathbf{S}(x) = S_x \in \mathcal{S}_N = \{S \in \mathbb{R}^N \,|\, \|S\| = 1\}.$$

One may think of S_x as a "spin" (local magnetic moment) associated to the atom at position x. The energy functional is

$$H_\Lambda(\mathbf{S}) = -\tfrac{1}{2} \sum_{x,y\in\Lambda} J_{xy}(S_x, S_y) - \frac{1}{\beta} \sum_{x\in\Lambda} (\mathbf{h}_x, S_x)$$

[1] The true relation is $\beta = (Tk_B)^{-1}$, where k_B is the Boltzman constant. Here we use the (often applied) convention $k_B = 1$ to simplify the notations.

where $J_{xy} = J_{yx} \geq 0$, $(v, v') = \sum_{\alpha=1}^{n} v_\alpha v'_\alpha$ is the standard Euclidean scalar product, $\beta = 1/T$, and $\mathbf{h}_x \in \mathbb{R}^N$ plays the role of a local magnetic field. The corresponding finite volume Gibbs measure is

$$d\mu_{\Lambda,N}^{\beta,\mathbf{h}_\Lambda}(\mathbf{S}) = \frac{d\mathbf{S}}{Z_{\Lambda,N}(\beta,\mathbf{h}_\Lambda)} e^{\frac{\beta}{2}\sum_{x,y\in\Lambda} J_{xy}(S_x,S_y)} e^{\sum_{x\in\Lambda}(\mathbf{h}_x,S_x)} \tag{2.2}$$

where $\mathbf{h}_\Lambda = \{\mathbf{h}_x\}_{x\in\Lambda}$ and

$$Z_{\Lambda,N}(\beta,\mathbf{h}_\Lambda) = \int d\mathbf{S}\ e^{\frac{\beta}{2}\sum_{x,y\in\Lambda} J_{xy}(S_x,S_y)} e^{\sum_{x\in\Lambda}(\mathbf{h}_x,S_x)}.$$

In the following we use the notation

$$\mathbb{E}_{\Lambda,N}^{\beta,\mathbf{h}_\Lambda}[f] = \int f(\mathbf{S}) d\mu_{\Lambda,N}^{\beta,\mathbf{h}_\Lambda}(\mathbf{S})$$

for any function $f : \mathcal{S}_N^\Lambda \to \mathbb{R}$.

Properties of the finite volume Gibbs measure. Physically, the two most interesting situations are:

(a) When $\mathbf{h}_x = 0\ \forall x \in \Lambda$ the measure is invariant under *flip*

$$d\mu_{\Lambda,N}^{\beta,0}(\mathbf{S}) = d\mu_{\Lambda,N}^{\beta,0}(-\mathbf{S})$$

where $-\mathbf{S}(x) = -S_x\ \forall x$. This is a discrete symmetry. Moreover, for $N \geq 2$ the measure has also a *continuous symmetry*

$$d\mu_{\Lambda,N}^{\beta,0}(\mathbf{S}) = d\mu_{\Lambda,N}^{\beta,0}(U\mathbf{S})$$

where $U\mathbf{S}(x) = US_x$ and U is any rotation in $\mathbb{R}^n$.

Since $J_{xy} \geq 0$ the density of the measure is maximal on *constant spin configurations* where

$$S_x = S\ \forall x \in \Lambda.$$

For $N = 1$ this selects two possible configurations: $S_x = +1\ \forall x$, or $S_x = -1\ \forall x$. For $N \geq 2$ the maximal is on a compact manifold $S_x = S\ \forall x$, with $\|S\| = 1$. In analogy with ferromagnetic materials we say that $J_{xy} \geq 0$ is a *ferromagnetic interaction.*

(b) When a *constant* magnetic field is present

$$\mathbf{h}_\Lambda = \mathbf{h}, \qquad \text{i.e. } \mathbf{h}_x = \mathbf{h} = h\mathbf{n} \quad \|\mathbf{n}\| = 1\ \forall x \in \Lambda$$

the corresponding term in the measure density breaks the symmetries and favors *one* configuration among the set of all constant configurations, namely

$$S_x = \mathbf{n} \quad \forall x \in \Lambda,$$

where all spins are aligned with the constant magnetic field.

In the following, we will consider always **(a)** or **(b)**. Nevertheless, we will often use the more general formula (2.2) as a computational tool.

3 Thermodynamic limit

The typical number of particles in a physics system is 10^{23}, so we are interested in the properties of the measure $d\mu^{\beta,\mathbf{h}}_{\Lambda,N}(\mathbf{S})$ as the volume $\Lambda \to \mathbb{Z}^d$. This is the so called *thermodynamic limit*.

Definition 1 We say that the sequence of measures $\mu^{\beta,\mathbf{h}}_{\Lambda,N}$ converges weakly to some limit measure $\mu^{\beta,\mathbf{h}}_{N}$ as $\Lambda \to \mathbb{Z}^d$ if

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[f] = \int f(\mathbf{S}) d\mu^{\beta,\mathbf{h}}_{\Lambda,N}(\mathbf{S}) \to \int f(\mathbf{S}) d\mu^{\beta,\mathbf{h}}_{N}(\mathbf{S}) = \mathbb{E}^{\beta,\mathbf{h}}_{N}[f]$$

for any *local function* $f : \mathcal{S}_N^{\mathbb{Z}^d} \to \mathbb{R}$.

Definition 2 A function $f : \mathcal{S}_N^{\mathbb{Z}^d} \to \mathbb{R}$ is local if there exist some set $X \subset \mathbb{Z}^d$ with $|X| < \infty$ such that f depends only on $\mathbf{S}_{|X} = \{S_x\}_{x\in\Lambda}$ (it depends only on the value of S_x for points x in a finite set.)

Correlation functions It is is enough to study the limit as $\Lambda \to \mathbb{Z}^d$ for the moments (correlation functions) of the measure

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[\prod_{j=1}^{m} S^{\alpha_j}_{x_j}\right]$$

where S^{α}_{x} is the α-th component ($\alpha = 1, \ldots d$) of the vector S_x. In the product above the same position x or component α may appear several times. By a straightforward computation one gets

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[\prod_{j=1}^{m} S^{\alpha_j}_{x_j}\right] = \tfrac{1}{Z_{\Lambda,N}(\beta,\mathbf{h})} \prod_{j=1}^{m} \partial_{h^{\alpha_j}_{x_j}} \left[Z_{\Lambda,N}(\beta, \mathbf{h}_\Lambda)\right]_{|\mathbf{h}_\Lambda=\mathbf{h}} .$$

Actually, for any $m \geq 2$ it is better to study the so called *connected correlation function* (or cumulants) defined by

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\Big[\prod_{j=1}^{m} S^{\alpha_j}_{x_j}\Big]_C = \sum_{P\in\mathcal{P}[I_m]} (-1)^{|P|-1}(|P|-1)! \prod_{J\in P} \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\Big[\prod_{j\in J} S^{\alpha_j}_{x_j}\Big]$$

where $I_m = \{1, 2, \ldots, m\}$, $\mathcal{P}[I_m]$ is the set of all partitions of I_m into subsets (not necessarily connected). In particular for $m = 2$ we get

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[S^{\alpha_1}_{x_1} S^{\alpha_2}_{x_2}\right]_C = \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[S^{\alpha_1}_{x_1} S^{\alpha_2}_{x_2}\right] - \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[S^{\alpha_1}_{x_1}\right] \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\left[S^{\alpha_2}_{x_2}\right].$$

The function $\ln Z_{\Lambda,N}(\beta, \mathbf{h}_\Lambda)$ is called the *generating functional* for connected correlation functions. Indeed

$$\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}\Big[\prod_{j=1}^{m} S^{\alpha_j}_{x_j}\Big]_C = \prod_{j=1}^{m} \partial_{h^{\alpha_j}_{x_j}} \left[\ln Z_{\Lambda,N}(\beta, \mathbf{h}_\Lambda)\right]_{|\mathbf{h}_\Lambda=\mathbf{h}} .$$

4 Definition of a phase transition.

A large class of physically interesting functions can be obtained as derivatives with respect to β or h_α ($\alpha = 1, \ldots n$) of $\ln Z_{\Lambda,N}(\beta, \mathbf{h})$. We define the *finite volume free energy* as

$$\Phi_{\Lambda,N}(\beta, \mathbf{h}) = -\frac{1}{|\Lambda|} \ln Z_{\Lambda,N}(\beta, \mathbf{h})$$

This function is analytic in h and β for any finite volume Λ.

Definition 3. We say the model has a phase transition if some derivative in β or $\mathbf{h}$ has a discontinuity (or some divergence point) in the thermodynamic limit. The order of this derivative determines the order of the transition. The most frequent cases arising are:

- first order transition (a first derivative has a jump)
- second order transition (a second derivative has a jump)
- Kosterlitz-Thouless transition (all derivatives are continuous, but the free energy is not real analytic).

Universality. Second order phase transitions are particularly interesting because they have some universality properties. This means that the behaviour of a system near a second order phase transition (after some appropriate rescaling) does not depend on the precise details of the physical model behind. The study of a simplified model (as the ones we consider here) can then give information on realistic (but more complicated) physical models.

Some important thermodynamical quantities. We will consider the following derivatives:

- finite volume average magnetization (in direction $\alpha = 1, \ldots n$):

$$M^\alpha_{\Lambda,N}(\beta, \mathbf{h}) = \tfrac{1}{|\Lambda|} \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[\sum_{x\in\Lambda} S^\alpha_x] = -\partial_{h^\alpha} \Phi_{\Lambda,N}(\beta, \mathbf{h}),$$

- finite volume entropy:

$$S_{\Lambda,N}(\beta, \mathbf{h}) = \tfrac{\beta^2}{|\Lambda|} \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[H^{\beta,0}_{\Lambda,N}(\mathbf{S})] = -\beta^2 \partial_\beta \Phi_{\Lambda,N}(\beta, \mathbf{h}),$$

where $H^{\beta,0}_{\Lambda,N}(\mathbf{S}) = -\frac{1}{2} \sum_{xy} J_{xy}(S_x, S_y)$ is the energy at $\mathbf{h} = 0$,

- finite volume magnetic susceptibility:

$$\begin{aligned}\chi^{\alpha,\alpha'}_{\Lambda,N}(\beta,\mathbf{h}) &= \partial_{h_{\alpha'}} M^{\alpha}_{\Lambda,N}(\beta,\mathbf{h}) \\ &= \tfrac{1}{|\Lambda|}\sum_{xy\in\Lambda}\left\{\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[S^{\alpha}_x S^{\alpha'}_y] - \mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[S^{\alpha}_x]\,\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[S^{\alpha'}_y]\right\} \\ &= \tfrac{1}{|\Lambda|}\sum_{xy\in\Lambda}\mathbb{E}^{\beta,\mathbf{h}}_{\Lambda,N}[S^{\alpha}_x S^{\alpha'}_y]_C = -\partial^2_{h^{\alpha}h^{\alpha'}}\Phi_{\Lambda,N}(\beta,\mathbf{h}).\end{aligned}$$

5 Example: Ising model in the mean field case

Let $\Lambda_L = [-L,\dots,L]^d$ a cube in $\mathbb{Z}^d$ centered at the origin. The space of local states is $\Omega = \mathcal{S}_1 = \{-1,+1\}$. A state of the system is described by the function

$$\begin{aligned}\sigma:\quad \Lambda &\to \{1,-1\} \\ x &\to \sigma_x,\end{aligned}$$

assigning spin $\sigma_x \pm 1$ to each lattice site x. The energy functional is given by $H_\Lambda : \Omega^\Lambda \to \mathbb{R}$

$$H_\Lambda(\sigma) = -\frac{1}{2}\sum_{jk\in\Lambda} J_{jk}\sigma_j\sigma_k - \frac{h}{\beta}\sum_{j\in\Lambda}\sigma_j,$$

where $J_{jk} = J_{kj} \geq 0$ is the interaction parameter between σ_j and σ_k. In the mean field regime we set

$$J_{jk} = \frac{1}{|\Lambda|} \quad \forall j,k\in\Lambda.$$

Finally $h\in\mathbb{R}$ is the magnetic field breaking the discrete symmetry $\sigma\to-\sigma$, and $\beta>0$ is the inverse temperature. The probability for a configuration σ is given by the (discrete) Gibbs measure

$$P^{\beta,h}_\Lambda(\sigma) = \frac{e^{-\beta H_\Lambda(\sigma)}}{Z_\Lambda(\beta,h)}$$

where the partition function $Z_\Lambda(\beta,h)$ is

$$\begin{aligned}Z_\Lambda(\beta,h) &= \sum_\sigma e^{-\beta H_\Lambda(\sigma)} = \sum_\sigma e^{\frac{\beta}{2|\Lambda|}\sum_{jk\in\Lambda}\sigma_j\sigma_k} e^{h\sum_{j\in\Lambda}\sigma_j} \\ &= \sum_\sigma e^{\frac{\beta}{2|\Lambda|}\left[\sum_{j\in\Lambda}\sigma_j\right]^2} e^{h\left[\sum_{j\in\Lambda}\sigma_j\right]}.\end{aligned}$$

Theorem 1. The mean field Ising model has a phase transition in any $d\geq 1$. The behavior of the system depends on the temperature.

- At low temperature ($T<1$ ($\equiv \beta>1$) there is a first order phase transition: the magnetization is discontinuous at $h=0$:

$$\lim_{h\to 0+}\lim_{\Lambda\to\mathbb{Z}^d} M_\Lambda(\beta,h) = M(\beta) = -\lim_{h\to 0-}\lim_{\Lambda\to\mathbb{Z}^d} M_\Lambda(\beta,h),$$

where

$$M(\beta) > 0 \qquad \forall \beta > 1$$

is the size of the jump.

- At the critical temperature $T = 1$ ($\beta = 1$) there is a second order phase transition: all first derivatives are continuous in β and h, but the second derivative in h is divergent as $h \to 0$ and $\beta \to 1$:

$$\lim_{\beta\to 1} M(\beta) = 0, \qquad \lim_{\beta\to 1, h\to 0} \chi(\beta, h) = \lim_{\Lambda\to\mathbb{Z}^d} \chi_\Lambda(\beta, h) = +\infty.$$

- At hight temperature ($T > 1$ ($\equiv \beta < 1$) there is no phase transition: $\lim_{\Lambda\to\mathbb{Z}^d} \Phi_\Lambda(\beta, h)$ is analytic in β and h. In particular the magnetization at $h = 0$ vanishes

$$\lim_{h\to 0} \lim_{\Lambda\to\mathbb{Z}^d} M_\Lambda(\beta, h) = 0 = \lim_{\Lambda\to\mathbb{Z}^d} \lim_{h\to 0} M_\Lambda(\beta, h).$$

Moreover, near the critical point ($T = 1$, $h = 0$) the behavior of $M(\beta)$ and $\chi(\beta, 0)$ is given by

$$M(\beta) \sim (1-T)^{\hat\beta} \quad T \leq 1, (1-T) \ll 1, \qquad \hat\beta = \tfrac{1}{2}$$
$$\chi(\beta, 0) \sim \frac{1}{|1-T|^\gamma} \quad |1-T| \ll 1, \qquad \gamma = 1.$$

Remark 1. The exponents $\hat\beta$ and γ are called *critical exponents* and are *universal*. This means that any physical model in the same *universality class* as mean field Ising will have the same exponents, even though the critical temperature will not be $T = 1$ in general and the prefactors will be different.

Remark 2. At finite volume $M_\Lambda(\beta, 0) = 0$ by the symmetry $\sigma \to -\sigma$ for any temperature $T \geq 0$. At high temperature this remains true also after taking the theormodynamic limit, thus suggesting that the limit measure is still invariant under the symmetry $\sigma \to -\sigma$ when $h = 0$. At low temperature $T < 1$ this is no longer true. We say there is a *spontaneous symmetry breaking.*

Proof of Theorem 1. The rest of this section is devoted to the proof of these results. The main steps are the following.

1. Duality transformation: the free energy and its derivatives can be reexpressed as integrals (or ratios of integrals) of the form

$$\int_{\mathbb{R}} g(x) e^{-Nf(x)} dx,$$

where $N = |\Lambda| \gg 1$.

2. Asymptotic analysis (Laplace method, saddle analysis): as $N = |\Lambda| \to \infty$ the integral above concentrates near the minimum of the function f. In order to make this statement exact we have to perform some asymptotic analysis.

5.1 Duality

The partition function can be reformulated as an integral over one real variable

Lemma 1 *For any dimension $d \geq 1$ we have*

$$Z_\Lambda(\beta,h) = \tfrac{1}{\mathcal{N}_{\Lambda,\beta}} \int_{\mathbb{R}} dx\ e^{-|\Lambda| F(x,\beta,h)}, \qquad \textit{with } \mathcal{N}_{\Lambda,\beta} = \sqrt{\tfrac{2\pi\beta}{|\Lambda|}}\tfrac{1}{2^{|\Lambda|}}$$

$$\begin{array}{lll} F: & \mathbb{R}\times\mathbb{R}_+\times\mathbb{R} & \to \mathbb{R} \\ & (x,\beta,h) & \to F(x,\beta,h) = \tfrac{(x-h)^2}{2\beta} - \ln\cosh x \end{array}$$

Proof Using the formula

$$\int e^{-\frac{\lambda}{2}x^2} e^{yx} dx = \sqrt{\frac{2\pi}{\lambda}} e^{+\frac{1}{2\lambda}y^2} \qquad \forall\lambda>0,\ y\in\mathbb{R}$$

we have

$$e^{\frac{\beta}{2|\Lambda|}\left[\sum_{j\in\Lambda}\sigma_j\right]^2} = \sqrt{\tfrac{|\Lambda|}{2\pi\beta}} \int e^{-\frac{|\Lambda|}{2\beta}x^2} e^{x\left[\sum_{j\in\Lambda}\sigma_j\right]} dx.$$

Then

$$\begin{aligned} Z_\Lambda(\beta,h) &= \sqrt{\tfrac{|\Lambda|}{2\pi\beta}} \sum_\sigma e^{h\left[\sum_{j\in\Lambda}\sigma_j\right]} \int e^{-\frac{|\Lambda|}{2\beta}x^2} e^{x\left[\sum_{j\in\Lambda}\sigma_j\right]} dx \\ &= \sqrt{\tfrac{|\Lambda|}{2\pi\beta}} \int e^{-\frac{|\Lambda|}{2\beta}x^2} \sum_\sigma e^{(h+x)\left[\sum_{j\in\Lambda}\sigma_j\right]} dx \\ &= \sqrt{\tfrac{|\Lambda|}{2\pi\beta}} \int e^{-\frac{|\Lambda|}{2\beta}x^2} \left[2\cosh(x+h)\right]^{|\Lambda|} dx \end{aligned}$$

□

Remarks. The duality reduces the problem to the study of a one variable integral (compared to $2^{|\Lambda|}$ variables in the initial representation). Moreover, for large $|\Lambda|$ the integral will be concentrated around the minimal with respect to x of the function $F(x,\beta,h)$, therefore a saddle point analysis is possible.

5.1.1 Free energy and derivatives in the dual representation.

Using the dual representation above the finite volume free energy can be written as

$$\Phi_\Lambda(\beta,h) = -\frac{1}{|\Lambda|}\ln Z_\Lambda(\beta,h) = -\frac{1}{|\Lambda|}\ln\int e^{-|\Lambda|F(x,\beta,h)}dx + \frac{1}{|\Lambda|}\ln\mathcal{N}_{\Lambda,\beta}. \quad (5.3)$$

The corresponding first order derivatives (magnetization and entropy), and the second derivative in h (magnetic susceptibility) are written as

$$
\begin{aligned}
M_\Lambda(\beta,h) &= \tfrac{1}{\beta}\langle (x-h)\rangle_\Lambda && (5.4)\\
S_\Lambda(\beta,h) &= -\tfrac{1}{2}\langle (x-h)^2\rangle_\Lambda + \tfrac{\beta}{2|\Lambda|}\\
\chi_\Lambda(\beta,h) &= -\frac{1}{\beta} + \frac{|\Lambda|}{\beta^2}\langle (x-\langle x\rangle_\Lambda)^2\rangle_\Lambda && (5.5)\\
&= -\frac{1}{\beta} + \frac{|\Lambda|}{\beta^2}\left[\langle x^2\rangle_\Lambda - \langle x\rangle_\Lambda^2\right],
\end{aligned}
$$

where we defined

$$\langle g(x)\rangle_{|\Lambda|} = \frac{\int_{\mathbb{R}} g(x)e^{-|\Lambda|F(x,\beta,h)}dx}{\int_{\mathbb{R}} e^{-|\Lambda|F(x,\beta,h)}dx}.$$

5.2 Asymptotic analysis

We want to study the asymptotic behaviour as $N\to\infty$ of the integral

$$I_N = \int_{\mathbb{R}} g(x)e^{-Nf(x)}dx,$$

where $f,g:\mathbb{R}\to\mathbb{R}$ are two smooth functions. We define

$$\langle g(x)\rangle_N = \frac{\int_{\mathbb{R}} g(x)e^{-Nf(x)}dx}{\int_{\mathbb{R}} e^{-Nf(x)}dx}.$$

5.2.1 A general result

We will use the following lemma.

Lemma 2 *Let $f,g:\mathbb{R}\to\mathbb{R}$ be two smooth functions satisfying*

- *f has a unique global minimum at the point x_0 and $f''(x_0)>0$;*
- *all other minima are at a finite distance from $f(x_0)$. Precisely there exists $\epsilon_0>0$ such that $\forall\epsilon\le\epsilon_0$ we have*

$$\inf_{B^c(x_0,\epsilon)} f(x) = \max\{f(x_0+\epsilon), f(x_0-\epsilon)\}$$

- *there exists $N_0>0$ such that $\forall N\ge N_0$*

$$\int_{\mathbb{R}} e^{-Nf(x)}dx<\infty, \qquad \int_{\mathbb{R}} e^{-Nf(x)}|g(x)|dx<\infty.$$

Then we have

$$\int_{\mathbb{R}} e^{-Nf(x)}dx = e^{-Nf(x_0)}\sqrt{\frac{2\pi}{Nf''(x_0)}}\left[1+o\left(\frac{1}{N^{1/2}}\right)\right] \tag{5.6}$$

$$\langle g(x)\rangle_N = g(x_0) + \frac{1}{2N}\left[\frac{g''(x_0)}{f''(x_0)} - \frac{g'(x_0)f'''(x_0)}{f''(x_0)^2}\right] + o(N^{-1}). \tag{5.7}$$

Proof By the assumptions above there exists an $\epsilon_0 \ll 1$ (independent of N) such that

$$f(x) \geq \inf\{f(x_0+\epsilon), f(x_0-\epsilon)\} \qquad \forall x \in B(x_0,\epsilon)^c, \quad \forall \epsilon \leq \epsilon_0.$$

This means the local minima do not play a role here. Since $\epsilon \ll 1$ we can expand around x_0

$$f(x_0 \pm \epsilon) - f(x_0) = \frac{f''(x_0)}{2}\epsilon^2 + O(\epsilon^3) \geq \frac{f''(x_0)\epsilon^2}{4}$$

for ϵ small enough. Then we can break the integral as follows

$$\begin{aligned}
&\int_{\mathbb{R}} e^{-N[f(x)-f(x_0)]} g(x)dx \\
&= \int_{B(x_0,\epsilon)} e^{-N[f(x)-f(x_0)]} g(x)dx + \int_{B(x_0,\epsilon)^c} e^{-N[f(x)-f(x_0)]} g(x)dx
\end{aligned}$$

where $f(x) - f(x_0) \geq 0$ hence for any $N \geq 2N_0$ we have

$$\begin{aligned}
&\int_{B(x_0,\epsilon)^c} |g(x)| e^{-N[f(x)-f(x_0)]} dx \\
&\leq [\sup_{x \in B(x_0,\epsilon)^c} e^{-N/2[f(x)-f(x_0)]}] \int_{B(x_0,\epsilon)^c} |g(x)| e^{-N/2[f(x)-f(x_0)]} dx \\
&\leq e^{-\frac{Nf''(x_0)\epsilon^2}{8}} \int_{B(x_0,\epsilon)^c} |g(x)| e^{-N_0[f(x)-f(x_0)]} dx \\
&\leq e^{-\frac{Nf''(x_0)\epsilon^2}{8}} \int_{\mathbb{R}} |g(x)| e^{-N_0[f(x)-f(x_0)]} dx \leq \ C \ e^{-\frac{Nf''(x_0)\epsilon^2}{8}}
\end{aligned}$$

where $C > 0$ is a constant independent of N and ϵ. The contribution from $B(x_0,\epsilon)^c$ is exponentially small even if we let ϵ go to zero as $N \to \infty$. Precisely let

$$\epsilon_N = \frac{N^\alpha}{N^{1/2}}.$$

Then for any $1/2 > \alpha > 0$

$$\epsilon_N \to_{N\to\infty} 0, \qquad N\epsilon_N^2 = N^{2\alpha} \to_{N\to\infty} \infty.$$

The main contribution to the integral comes then from the ball $B(x_0,\epsilon_N) \to_{N\to\infty} \{x_0\}$. Since $\epsilon_N \ll 1$ we can expand in powers around x_0:

$$N[f(x) - f(x_0)] = \frac{f''(x_0)}{2}N(x-x_0)^2 + \frac{f'''(x_0)}{3!}N(x-x_0)^3 + o(N^{-1/2})$$

where we chose α such that

$$N\epsilon_N^4 = o(N^{-1/2}).$$

Inserting these estimates in the integral we obtain

$$\int_{B(x_0,\epsilon_N)} e^{-N[f(x)-f(x_0)]}dx = \int_{B(x_0,\epsilon_N)} e^{-\frac{f''(x_0)}{2}N(x-x_0)^2}\left[1-\frac{f'''(x_0)}{3!}(x-x_0)^3+o(N^{-1/2})\right]dx$$
$$= \frac{1}{\sqrt{N}}\int_{B(0,\epsilon_N\sqrt{N})} e^{-\frac{f''(x_0)}{2}y^2}\left[1-\frac{f'''(x_0)}{3!}\frac{y^3}{\sqrt{N}}+o(N^{-1/2})\right]dy = \left[1+o(N^{-1/2})\right]\sqrt{\frac{2\pi}{Nf''(x_0)}}$$

where we chose α such that

$$N\epsilon_N^4 = o(N^{-1/2}), \quad (N\epsilon_N^3)^2 = o(N^{-1/2}),$$

and

$$\int_{B(x_0,\epsilon_N)} \cdot dy = \int_{\mathbb{R}} \cdot dy + e^{-O(N\epsilon^2)} \to_{N\to\infty} \int_{\mathbb{R}} \cdot dy$$

since $N\epsilon_N^2 \to_{N\to\infty} \infty$. This concludes the proof of (5.6). To prove (5.7) take α in the definition of ϵ_N very small $\alpha = 1/10$ such that

$$\epsilon_N^4 N = o(N^{-1/2}), \quad (\epsilon_N^3 N)^2 = o(N^{-1/2}), \quad \epsilon^3 = o(N^{-1/2}).$$

The average of g can be written as

$$\langle g(x)\rangle_N = g(x_0) + \langle g(x) - g(x_0)\rangle_N$$

where

$$\langle g(x) - g(x_0)\rangle_N = \frac{\int_{B(x_0,\epsilon_N)}[g(x)-g(x_0)]\ e^{-N[f(x)-f(x_0)]}dx}{\int_{\mathbb{R}} e^{-N[f(x)-f(x_0)]}dx}$$
$$+ \frac{\int_{B(x_0,\epsilon_N)^c}[g(x)-g(x_0)]\ e^{-N[f(x)-f(x_0)]}dx}{\int_{\mathbb{R}} e^{-N[f(x)-f(x_0)]}dx}$$

By the same arguments as above, the second integral is exponentially small (true as long as $\alpha > 0$). Then we are reduced to study the integral restricted to the region $B(x_0, \epsilon_N)$. For all $x \in B(x_0, \epsilon_N)$

$$\sqrt{N}[g(x)-g(x_0)] = g'(x_0)\sqrt{N}(x-x_0) + \frac{g''(x_0)}{2}\sqrt{N}(x-x_0)^2 + O(\sqrt{N}\epsilon^3),$$
$$N[f(x)-f(x_0)] = \frac{f''(x_0)}{2}N(x-x_0)^2 + \frac{f'''(x_0)}{3!}N(x-x_0)^3 + O(N\epsilon_N^4).$$

Inserting these expansions and rescaling $y = \sqrt{N}(x - x_0)$

$$\int_{B(x_0,\epsilon_N)} [g(x)-g(x_0)]\ e^{-N[f(x)-f(x_0)]}dx$$
$$= \int_{B(x_0,\epsilon_N\sqrt{N})} \frac{dy}{\sqrt{N}} e^{-\frac{f''(x_0)}{2}y^2}$$
$$\frac{1}{\sqrt{N}}\left[g'(x_0)y + \frac{g''(x_0)}{2}\frac{y^2}{\sqrt{N}} + o(N^{-1/2})\right]\ \left[1 - \frac{f'''(x_0)}{3!}\frac{y^3}{\sqrt{N}} + o(N^{-1/2})\right]$$
$$= \frac{1}{\sqrt{N}}\left[\frac{A}{\sqrt{N}} + o(N^{-1/2})\right]\sqrt{\frac{2\pi}{Nf''(x_0)}}\left[1 + e^{-O(\sqrt{N})}\right]$$

where we defined

$$A = \frac{g''(x_0)}{2f''(x_0)} - \frac{g'(x_0)f'''(x_0)}{2f''(x_0)^2},$$

we chose α such that

$$\sqrt{N}\epsilon^3 = o(N^{-1/2}), \qquad N\epsilon_N^4 = o(N^{-1/2}), \qquad (N\epsilon_N^3)^2 = o(N^{-1/2}).$$

and we used

$$\frac{\int e^{-\lambda\frac{x^2}{2}}x^2dx}{\int e^{-\lambda\frac{x^2}{2}}dx} = \frac{1}{\lambda} \qquad \frac{\int e^{-\lambda\frac{x^2}{2}}x^4dx}{\int e^{-\lambda\frac{x^2}{2}}dx} = \frac{3}{\lambda^2}.$$

Finally inserting

$$\int_{\mathbb{R}} e^{-N[f(x)-f(x_0)]}dx = \sqrt{\tfrac{2\pi}{Nf''(x_0)}}\left[1 + o(N^{-1/2})\right]$$

the result follows. □

5.2.2 Application to the Ising model

In order to check if we can apply the lemma above we have to study the minima of the function F.

Lemma 3 *Let*

$$F(x,\beta,h) = \frac{(x-h)^2}{2\beta} - \ln\cosh x, \qquad x \in \mathbb{R}, \beta > 0, h \in \mathbb{R}.$$

There are three regimes.

1. *When $h \neq 0$ (for any β) or when $h = 0$ and $\beta < 1$ (high temperature) F has one global minimum at $x_0(\beta,h)$ and one local minimum, for any β. Moreover $\partial_x^2 F(x_0,\beta,h) > 0$.*

2. *When $\beta = 1$ and $h = 0$ (critical point). F has one global minimum at $x_0 = 0$ and one local minimum. But $\partial_x^2 F(0,1,0) = 0$.*

3. *When $h = 0$ and $\beta > 1$ (low temperature) F has two minima at the same height, at symmetric positions $\pm x_1(\beta)$ and $\partial_x^2 F(\pm x_1,\beta,0) > 0$.*

Proof The first three derivatives of F are

$$\partial_x F = \tfrac{(x-h)}{\beta} - \tanh x, \quad \partial_x^2 F = \tfrac{1}{\beta} - \tfrac{1}{(\cosh x)^2}, \quad \partial_x^3 F = \tfrac{2\sinh x}{(\cosh x)^3}$$

Note that $\partial_x^3 F$ does not depend on h of β, it is an odd function satisfying $\partial_x^3 F(x) > 0$ $\forall x > 0$. Then the behaviour of F depends on the sign of the hessian $\partial_x^2 F(0,\beta)$ at the origin.

Non negative hessian: $\partial_x^2 F(0,\beta) \geq 0$. This corresponds to

$$\tfrac{1}{\beta} - 1 \geq 0 \quad \Leftrightarrow \quad \beta \leq 1 \quad \Leftrightarrow \quad T \geq 1.$$

In this case $\partial_x^3 F(x) > 0 \ \forall x > 0$ implies $\partial_x^2 F(x,\beta) > 0$ for all $x \neq 0$. Then F has only one minimum at position $x_0(\beta,h)$. From $\partial_x F(0,\beta,h) = -h/\beta$ we deduce that

$$x_0(\beta,h) \begin{cases} > 0 & h > 0 \\ < 0 & h < 0 \\ = 0 & h = 0. \end{cases}$$

Moreover, since $\partial_x^2 F(x,\beta) > 0$ for all $x \neq 0$ we have $\partial_x^2 F(x_0(\beta,h),\beta) \geq 0 \ \forall h$ and equality holds only when $h = 0$.

Negative hessian: $\partial_x^2 F(0,\beta) < 0$. This corresponds to

$$\tfrac{1}{\beta} - 1 < 0 \quad \Leftrightarrow \quad \beta > 1 \quad \Leftrightarrow \quad T < 1.$$

Let us restrict to $h \leq 0$. The case $h > 0$ follows in the same way. Then

$$\partial_x F(0,\beta,h) = -h/\beta \geq 0.$$

Equality holds only when $h = 0$. Now, since $\partial_x^2 F(x = 0) < 0$ and $\partial_x^3 F(x) > 0$ $\forall x > 0$ there must be two symmetric points $\pm y$, for some $y > 0$ (remenber that $\partial_x^2 F$ is an even function, independent of h) such that

$$\partial_x^2 F(x) > 0 \ \forall |x| > y, \quad \partial_x^2 F(x) < 0 \ \forall |x| < y.$$

Then in the region $x \leq 0$ the function F has exactly one minimum at position $x_0(\beta,h) < -y < 0$ (true also when $h = 0$). By the relation above $\partial_x^2 F(x_0) > 0$. In the region $x > 0$ there are two possible behaviours.

Large $|h|$. For $|h|$ large enough we have

$$\partial_x F(y,\beta,h) = \frac{y}{\beta} - \tanh y - \frac{h}{\beta} \geq 0,$$

where remember that y is a function of β only. In this case the function F is non decreasing for all $x > 0$, hence there is only one global minimum at $x_0 < 0$.

Small $|h|$. For $|h|$ small enough we have

$$\partial_x F(y,\beta,h) < 0.$$

In this case the function has a minimum at position $x_0'(\beta,h) > y > 0$ and a local maximum at position $0 < x_0''(\beta,h) < y$. The question arises which of the two minima $x_0 < 0$, $x_0' > 0$ is lower. We start with $h = 0$. In this case the function F is even and has two equal minima at symmetric positions $x_0'(\beta,0) = x_1(\beta) > 0$,

$x_0 = -x_0' = -x_1(\beta)$. In order to study the variation of $F(x_0)$ and $F(x_0')$ as a function of h we compute

$$\begin{aligned} d_h F(x_0(\beta,h),\beta,h) &= \partial_x F(x_0,\beta,h)\partial_h(x_0) + \partial_h F(x_0(\beta,h),\beta,h) \\ &= -\frac{(x_0-h)}{\beta} = -\tanh x_0 \end{aligned}$$

where we used $\partial_x F(x_0,\beta,h) = 0$. Repeating for x_0' we get

$$d_h F(x_0(\beta,h),\beta,h) > 0, \qquad d_h F(x_0'(\beta,h),\beta,h) < 0.$$

When h becomes negative the minimum at $x_0 < 0$ become deeper while the minimum at $x_0' > 0$ becomes shallower, so the x_0 is the unique global minimum.

This concludes the proof. □

Lemma 4 *When $h \neq 0$ or $h = 0$ and $\beta < 1$ the finite volume free energy has a limit as $\Lambda \to \mathbb{Z}^d$*

$$\lim_{|\Lambda|\to\infty} \Phi_\Lambda(\beta,h) = \Phi(\beta,h) \tag{5.8}$$

where

$$\Phi(\beta,h) = F(x_0(\beta,h),\beta,h) - \ln 2.$$

and $x_0(\beta,h)$ is the global minimum (with respect to x) of the function $F(x,\beta,h)$. Moreover the first derivatives satisfy

$$\begin{aligned} M(\beta,h) &= -\lim_{|\Lambda|\to\infty} \partial_h \Phi_\Lambda(\beta,h) = \tfrac{x_0-h}{\beta} = -\partial_h \Phi(\beta,h) \\ S(\beta,h) &= -\lim_{|\Lambda|\to\infty} \beta^2 \partial_\beta \Phi_\Lambda(\beta,h) = \tfrac{(x_0-h)^2}{2} = -\beta^2 \partial_\beta \Phi(\beta,h) \end{aligned}$$

Finally the magnetic susceptibility

$$\chi(\beta,h) = -\lim_{|\Lambda|\to\infty} \partial_h^2 \Phi_\Lambda(\beta,h) = -\frac{1}{\beta} + \frac{1}{\beta^2 H} = -\partial_h^2 \Phi(\beta,h)$$

where we defined

$$H = \partial_x^2 F(x_0(\beta,h),\beta,h) = \frac{1}{\beta} - \frac{1}{\cosh x_0(\beta,h)} \tag{5.9}$$

(the Hessian at the minimum).

Proof From Lemma 3 we deduce that Lemma 2 can be applied whenever $h \neq 0$ or $h = 0$ and $\beta < 1$. The (5.8) follows directly from (5.3) and (5.6) applying

$$\begin{aligned} -\tfrac{1}{|\Lambda|} \ln \int e^{-|\Lambda| F(x,\beta,h)} dx &= -\tfrac{1}{|\Lambda|} \ln \left[e^{-|\Lambda| F(x_0,\beta,h)} \sqrt{\tfrac{2\pi}{H|\Lambda|}} (1 + o(|\Lambda|^{-1/2})) \right] \\ &\to_{|\Lambda|\to\infty} F(x_0,\beta,h) \end{aligned}$$

where H was defined in (5.9). Finally

$$\frac{1}{|\Lambda|}\ln\mathcal{N}_{\Lambda,\beta}\rightarrow_{|\Lambda|\rightarrow\infty}=-\ln 2.$$

Moreover by a direct application of (5.7)

$$M(\beta,h)=\lim_{|\Lambda|\rightarrow\infty}\tfrac{1}{\beta}\langle(x-h)\rangle_\Lambda=\tfrac{x_0(\beta,h)-h}{\beta}=-\partial_h\Phi(\beta,h)$$
$$S(\beta,h)=\lim_{|\Lambda|\rightarrow\infty}[\tfrac{1}{2}\langle(x-h)^2\rangle_\Lambda+\tfrac{\beta}{2|\Lambda|}]=\tfrac{(x_0-h)^2}{2}=-\beta^2\partial_\beta\Phi(\beta,h)$$

where we used

$$\partial_h\Phi(\beta,h)=[\partial_h x_0]\partial_x F(x_0,\beta,h)+\partial_h F(x_0,\beta,h)=\partial_h F(x_0,\beta,h),$$

since $\partial_x F(x_0,\beta,h)=0$. The same arguments apply for ∂_β. It remains to study

$$\chi(\beta,h)=\lim_{|\Lambda|\rightarrow\infty}\chi_\Lambda(\beta,h)=\lim_{|\Lambda|\rightarrow\infty}[-\tfrac{1}{\beta}+\tfrac{|\Lambda|}{\beta^2}\left[\langle x^2\rangle_\Lambda-\langle x\rangle_\Lambda^2\right]].$$

To simplify notations let $F^{(3)}=\partial_x^3 F(x_0(\beta,h),\beta,h)$. Then using (5.7) with $N=|\Lambda|$ and $g(x)=x^2$

$$\langle x^2\rangle_\Lambda=x_0^2+\tfrac{1}{2|\Lambda|}\left[\frac{2}{H}-\tfrac{2x_0F^{(3)}}{H^2}\right]+o(|\Lambda|^{-1}).$$

Using (5.7) with $N=|\Lambda|$ and $g(x)=x$ we get

$$\langle x\rangle_\Lambda^2=\left[x_0+\tfrac{1}{2|\Lambda|}\left[-\frac{F^{(3)}}{H^2}\right]+o(|\Lambda|^{-1})\right]^2=x_0^2-\frac{2x_0}{2|\Lambda|}\frac{F^{(3)}}{H^2}+o(|\Lambda|^{-1}).$$

Putting these together we get

$$\chi(\beta,h)=-\frac{1}{\beta}+\frac{1}{\beta^2H}.$$

Notice that

$$-\partial_h^2\Phi(\beta,h)=\partial_h M(h,\beta)=-\frac{1}{\beta}+\frac{\partial_h x_0}{\beta}$$

and $\partial_h x_0=(\beta H)^{-1}$ from

$$0=\partial_h\left[\frac{x_0-h}{\beta}-\tanh x_0\right]=-\frac{1}{\beta}+H\partial_h x_0.$$

Therefore

$$-\partial_h^2\Phi(\beta,h)=-\frac{1}{\beta}+\frac{1}{\beta^2H}.$$

This concludes the proof of the lemma. □

5.2.3 Proof of the phase transition.

A direct study of the function $\Phi(\beta, h)$ and its derivatives shows that

$$\lim_{h\to 0_\pm} M(\beta,h) = 0 \qquad \forall T \geq 1$$
$$\lim_{h\to 0^+} M(\beta,h) = \frac{x_1(\beta)}{\beta} = -\lim_{h\to 0^-} M(\beta,h) \qquad \forall T < 1,$$

where

$$x_1(\beta) = \lim_{h\to 0^+} x_0(\beta,h) > 0 \qquad \beta > 1.$$

More precisely x_1 is the unique positive solution of the equation $x/\beta - \tanh x = 0$. Therefore the magnetization has a jump of size $2x_1(\beta) > 0$ for all $\beta > 1$. This means there is a first order transition at $h = 0$ for all $T < 1$. When $T > 1$ the magnetization is continuous at $h = 0$. Since $S(\beta, h)$ is continuous everywhere, there is no first order transition for $T \leq 1$. Since $H = \partial_x^2 F(x_0, 1, 0) = 0$ the magnetic susceptibility is divergent as $T \to 1$ and $h \to 0$, but is continuous everywhere else

$$\lim_{\beta\to 1, h\to 0} \chi(\beta,h) = +\infty.$$

Therefore there is a second order transition at $T = 1, h = 0$. This is called the *critical point*. Using similar arguments one can show that also the other second order derivatives are continuous when $T > 1$ so there is no first or second order transition in this region of temperatures. Actually one can prove that there is no phase transition at all in this region, but this will be done later.

Finally, to obtain the critical exponents we need the behaviour of $x_1(\beta)$ near $\beta = 1$. When $x_1 \simeq 0$ the corresponding equation is

$$0 = \frac{x_1}{\beta} - \tanh(x_1) = \frac{x_1}{\beta} - x_1 + \frac{x_1^3}{3} + o(x_1^4)$$

Then

$$x_1\left[x_1^2 - \delta + o(x_1^3)\right] = 0 \quad \Rightarrow \quad x_1^2 = 3\delta + o(x_1^3) = 3\delta[1 + o(\delta^2)]$$
$$\Rightarrow \quad x_1(\beta) = \sqrt{3\delta}[1 + o(\delta^2)] \sim (1 - T)$$

where we defined

$$0 < \delta = 1 - \tfrac{1}{\beta} = 1 - T \ll 1.$$

To study the divergence in $\chi(\beta, h)$ we remark that the Hessian at $h = 0$, $\beta > 1$ satisfies

$$H(\beta,0) = \frac{1}{\beta} - \frac{1}{\cosh x_1(\beta)} = \frac{1}{\beta} - 1 + x_1^2 + o(x_1^3) = 2\delta + o(\delta^{3/2}) \sim (1 - T)$$

where we used

$$(\cosh x_1)^{-2} = (1 + \tfrac{x_1^2}{2} + o(x^3))^{-2} = (1 + x_1^2 + o(x^3))^{-1} = 1 - x_1^2 + o(x^3).$$

On the other hand when $h = 0$, $\beta < 1$, $x_0(\beta, 0) = 1$ hence

$$H(\beta, 0) = \frac{1}{\beta} - 1 = T - 1$$

Therefore

$$\chi(\beta, 0) \sim |1 - T|^{-1} \quad |T - 1| \ll 1.$$

Therefore the critical exponents are $\hat{\beta} = 1/2$ and $\gamma = 1$.