## Mathematical Statistical Physics 2020

Classical part 1 The Ising model.

1.2 Existence of the thermodynamic limit

April 15, 2021

Friedli-Velenik Sections 3.1 and 3.2.1, 3.2.2



### Overview

- Some additional vocabulary and notation.
- ▶ Van Hove sequence—how do we let  $\Lambda \nearrow \mathbb{Z}^d$ ?
- Existence of the thermodynamic limit. Bulk free energy does not depend:
  - shape of the container (limit along growing cubes or balls?)
  - boundary conditions.

## Notation: some minor changes

Previously:

$$\mathscr{H}_{\Lambda;h}(\omega) = -\sum_{\substack{i,j \in \Lambda: \\ i \sim j}} \omega_i \omega_j - h \sum_{i \in \Lambda} \omega_i,$$

Boltzmann weight  $\exp(-\beta \mathscr{H}_{\Lambda;h}(\omega))$ .

From now on, instead:

$$\mathscr{H}_{\Lambda;\beta,h}^{\varnothing}(\omega) = -\beta \sum_{\{i,j\} \in \mathscr{E}_{\Lambda}} \sigma_i(\omega) \sigma_j(\omega) - h \sum_{i \in \Lambda} \sigma_i(\omega),$$

Boltzmann weight  $\exp(-\mathcal{H}_{\Lambda;\beta,h}(\omega))$ . New notation  $\sigma_i(\omega) = \omega_i$ ,

$$\mathscr{E}_{\Lambda} = \{\{i, j\} : i, j \in \Lambda, i \sim j\}$$

set of nearest neighbor edges within  $\Lambda$ . Superscript  $\varnothing = \text{empty}/\text{free boundary conditions} = \text{no interactions with the outside } \Lambda^c$ .

## Boundary conditions

Configuration space for infinite lattice  $\mathbb{Z}^d$ :

$$\Omega = \{+1, -1\}^{\mathbb{Z}^d} = \{\omega = (\omega_i)_{i \in \mathbb{Z}^d} : \omega_i = \pm 1\}.$$

Fix a configuration  $\eta \in \Omega$ , e.g.  $\eta_i \equiv +1$ . Look at configurations  $\omega$  that can be anything they want inside  $\Lambda$  but with frozen degrees of freedom  $\omega_i = \eta_i$  outside  $\Lambda$ 

$$\Omega_{\Lambda}^{\eta} = \big\{ \omega \in \Omega : \ \omega_i = \eta_i \text{ for all } i \in \mathbb{Z}^d \setminus \Lambda \big\}.$$

## Boundary conditions

Configuration space for infinite lattice  $\mathbb{Z}^d$ :

$$\Omega = \{+1, -1\}^{\mathbb{Z}^d} = \{\omega = (\omega_i)_{i \in \mathbb{Z}^d} : \omega_i = \pm 1\}.$$

Fix a configuration  $\eta \in \Omega$ , e.g.  $\eta_i \equiv +1$ . Look at configurations  $\omega$  that can be anything they want inside  $\Lambda$  but with frozen degrees of freedom  $\omega_i = \eta_i$  outside  $\Lambda$ 

$$\Omega_{\Lambda}^{\eta} = \big\{ \omega \in \Omega : \ \omega_i = \eta_i \text{ for all } i \in \mathbb{Z}^d \setminus \Lambda \big\}.$$

Include nearest neighbor edges that cross the border of  $\Lambda$ 

$$\mathscr{E}^{\mathrm{b}}_{\Lambda} = \big\{ \{i, j\} \subset \mathbb{Z}^d : \{i, j\} \cap \Lambda \neq \emptyset, \big\}$$

## Boundary conditions

Configuration space for infinite lattice  $\mathbb{Z}^d$ :

$$\Omega = \{+1, -1\}^{\mathbb{Z}^d} = \{\omega = (\omega_i)_{i \in \mathbb{Z}^d} : \omega_i = \pm 1\}.$$

Fix a configuration  $\eta \in \Omega$ , e.g.  $\eta_i \equiv +1$ . Look at configurations  $\omega$  that can be anything they want inside  $\Lambda$  but with frozen degrees of freedom  $\omega_i = \eta_i$  outside  $\Lambda$ 

$$\Omega_{\Lambda}^{\eta} = \big\{ \omega \in \Omega : \ \omega_i = \eta_i \text{ for all } i \in \mathbb{Z}^d \setminus \Lambda \big\}.$$

Include nearest neighbor edges that cross the border of  $\Lambda$ 

$$\mathscr{E}^{\mathbf{b}}_{\Lambda} = \{\{i,j\} \subset \mathbb{Z}^d : \{i,j\} \cap \Lambda \neq \emptyset, \}$$

Energy with boundary condition  $\eta$ 

$$\mathscr{H}^{\eta}_{\Lambda;\beta,h}(\omega) = -\beta \sum_{\{i,j\} \in \mathscr{E}^h_{\Lambda}} \sigma_i(\omega) \sigma_j(\omega) - h \sum_{i \in \Lambda} \sigma_i(\omega)$$

includes some contributions  $\sigma_i(\omega)\eta_i(\omega)$ .



## Gibbs measure with b.c.

$$\mathscr{H}^{\eta}_{\Lambda;\beta,h}(\omega) = -\beta \sum_{\{i,j\} \in \mathscr{E}^{\mathsf{b}}_{\Lambda}} \sigma_i(\omega) \sigma_j(\omega) - h \sum_{i \in \Lambda} \sigma_i(\omega)$$

Partition function

$$\mathbf{Z}^{\eta}_{\Lambda;eta,h} = \sum_{\omega \in \Omega^{\eta}_{\Lambda}} \exp\Bigl(-\mathscr{H}^{\eta}_{\Lambda;eta,h}(\omega)\Bigr)$$

Gibbs measure

$$\mu^{\eta}_{\Lambda;\beta,h}(\omega) = \frac{1}{\mathbf{Z}^{\eta}_{\Lambda;\beta,h}} \exp\Bigl(-\mathscr{H}^{\eta}_{\Lambda;\beta,h}(\omega)\Bigr), \quad \omega \in \Omega^{\eta}_{\Lambda}.$$

Another b.c.: periodic boundary conditions  $\rightarrow$  book.

Notation covering both free boundary conditions and b.c.  $\eta$ : Superscript  $\#=\varnothing$ ,  $\eta$ .



# Van Hove sequences

#### Wanted:

a notion of convergence  $\Lambda \nearrow \mathbb{Z}^d$  that makes boundaries  $\partial \Lambda$  irrelevant.

Why?

#### **Heuristics:**

Each volume  $\Lambda \subseteq \mathbb{Z}^d$  is assigned a free energy  $\Psi_{\Lambda}(\beta, h) = \log \mathbf{Z}_{\Lambda}$ . We would like to say

$$\Psi_{\Lambda}(\beta, h) = |\Lambda| \, \psi(\beta, h) + \mathsf{const}_{\beta, h} \, |\partial \Lambda|$$

i.e. free energy = volume  $\times$  free energy density + a boundary correction.

#### Wanted:

a notion of convergence  $\Lambda \nearrow \mathbb{Z}^d$  that makes boundaries  $\partial \Lambda$  irrelevant.

Why?

#### **Heuristics:**

Each volume  $\Lambda \subseteq \mathbb{Z}^d$  is assigned a free energy  $\Psi_{\Lambda}(\beta, h) = \log \mathbf{Z}_{\Lambda}$ . We would like to say

$$\Psi_{\Lambda}(\beta, h) = |\Lambda| \psi(\beta, h) + \mathsf{const}_{\beta, h} |\partial \Lambda|$$

i.e. free energy = volume  $\times$  free energy density + a boundary correction.

The bulk contribution proportional to the volume should be the dominant term—we want

 $|\partial \Lambda|$  small compared to  $|\Lambda|$ .



Given: sequence  $(\Lambda_n)_{n\in\mathbb{N}}$  of domains  $\Lambda_n \in \mathbb{Z}^d$ .

A weak notion of convergence:  $\Lambda_n \uparrow \mathbb{Z}^d$  if

- 1.  $\Lambda_n \subset \Lambda_{n+1}$  for all n.
- 2.  $\bigcup_{n\in\mathbb{N}} \Lambda_n = \mathbb{Z}^d$ .

We want something stronger.

**Definition**  $(\Lambda_n)$  converges to  $\mathbb{Z}^d$  in the sense of van Hove if  $\Lambda_n \uparrow \mathbb{Z}^d$  and

$$\lim_{n\to\infty}\frac{|\partial^{\mathrm{in}}\Lambda_n|}{|\Lambda_n|}=0$$

where  $\partial^{\text{in}} \Lambda = \{i \in \Lambda : \exists j \notin \Lambda, j \sim i\}$ . Notation:

$$\Lambda_n \uparrow \mathbb{Z}^d$$
.

Call  $(\Lambda_n)_{n\in\mathbb{N}}$  a van Hove sequence.

Existence of the thermodynamic limit

### Theorem (FV Thm 3.6)

(a) The limit

$$\psi(\beta, h) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log \mathbf{Z}_{\Lambda_n; \beta, h}^{\#}$$

exists for every van Hove sequence  $\Lambda_n \uparrow \mathbb{Z}^d$ , and its value does not depend on the precise choice of van Hove sequence.

(b) The limit does not depend on the choice of boundary condition.

## Theorem (FV Thm 3.6)

(a) The limit

$$\psi(\beta, h) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log \mathbf{Z}_{\Lambda_n; \beta, h}^{\#}$$

exists for every van Hove sequence  $\Lambda_n \uparrow \mathbb{Z}^d$ , and its value does not depend on the precise choice of van Hove sequence.

- (b) The limit does not depend on the choice of boundary condition.
- (c) (The function  $\mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$ ,  $(\beta, h) \mapsto \psi(\beta, h)$  is convex.)
- (d) (The function  $h \mapsto \psi(\beta, h)$  is even:  $\psi(\beta, -h) = \psi(\beta, h)$ .)

## Theorem (FV Thm 3.6)

(a) The limit

$$\psi(\beta, h) = \lim_{n \to \infty} \frac{1}{|\Lambda_n|} \log \mathbf{Z}_{\Lambda_n; \beta, h}^{\#}$$

exists for every van Hove sequence  $\Lambda_n \uparrow \mathbb{Z}^d$ , and its value does not depend on the precise choice of van Hove sequence.

- (b) The limit does not depend on the choice of boundary condition.
- (c) (The function  $\mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$ ,  $(\beta, h) \mapsto \psi(\beta, h)$  is convex.)
- (d) (The function  $h \mapsto \psi(\beta, h)$  is even:  $\psi(\beta, -h) = \psi(\beta, h)$ .)

In particular: it doesn't matter whether you take limits along growing sequences cubes, balls, parallelipipeds...

The thermodynamic potential  $\psi(\beta, h)$  does not remember the shape of the container.

(Side remark: clashes with elasticity theory.)



# Proof strategy for (a), (b)

Proof of existence of the limit for free b.c. in two steps:

1. Prove the existence of the limit along sequences of cubes with sidelength  $2^n$ 

$$D_n = \{1, \ldots, 2^n\}^d$$
.

Note: we do not have  $D_n \uparrow \mathbb{Z}^d$  but it is true that  $|\partial^{in} D_n|/|D_n| \to 0$ .

2. Approximate general domains by unions of cubes.



# Proof strategy for (a), (b)

Proof of existence of the limit for free b.c. in two steps:

1. Prove the existence of the limit along sequences of cubes with sidelength  $2^n$ 

$$D_n = \{1, \ldots, 2^n\}^d.$$

Note: we do not have  $D_n \uparrow \mathbb{Z}^d$  but it is true that  $|\partial^{in} D_n|/|D_n| \to 0$ .

2. Approximate general domains by unions of cubes.

Deduce that the limit along every van Hove sequence exists and is equal to the limit along the special sequence of cubes.



# Proof strategy for (a), (b)

Proof of existence of the limit for free b.c. in two steps:

1. Prove the existence of the limit along sequences of cubes with sidelength  $2^n$ 

$$D_n = \{1, \ldots, 2^n\}^d.$$

Note: we do not have  $D_n \uparrow \mathbb{Z}^d$  but it is true that  $|\partial^{in} D_n|/|D_n| \to 0$ .

2. Approximate general domains by unions of cubes.

Deduce that the limit along every van Hove sequence exists and is equal to the limit along the special sequence of cubes.

Then, move over to general b.c.

3. Show that when you change the boundary condition, the energy and the logarithm log  $Z_{\Lambda}^{\#}$  change by a term of order  $|\partial^{\mathrm{in}}\Lambda|$ .



# Coming next

#### Convexity.

What kind of information do we get for free out of the existence of the thermodynamic limit?

Phase transition.