

# Notes for Mathematical Statistical Physics (LMU, SS 2020)

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# Chapter 1

## Introduction

### On the physics side:

1. This course is about systems with very many or even *infinitely many degrees of freedom*.
2. The initial physical motivation is statistical physics and a mathematically rigorous understanding of phase transitions.
3. We will cover systems in thermal equilibrium, classical and quantum.

### On the maths side, we will go through

1. Classical: probability theory, Gibbs measures, DLR conditions.  
Reference: Friedli, S. and Velenik, Y., *Statistical Mechanics of Lattice Systems: A Concrete Mathematical Introduction*.
2. Quantum:  $C^*$ -algebras, KMS states.  
Reference: Bratteli, Ola and Robinson, Derek William, *Operator Algebras and Quantum Statistical Mechanics II*

# Chapter 2

## Classical Part I: The Ising model

### 2.1 The model

$\Lambda \subseteq \mathbb{Z}^d$  is a finite non empty subset. For each lattice site  $i \in \Lambda$ , there is a spin  $\omega_i \in \{+1, -1\}$ . The configuration space is

$$\Omega_\Lambda = \{+1, -1\}^\Lambda = \{(\omega_i)_{i \in \Lambda} : \omega_i = \pm 1\} \quad (2.1)$$

and the energy with inverse temperature  $\beta$ , external field  $h \in \mathbb{R}$  and *empty boundary condition* is

$$\mathcal{H}_{\Lambda, \beta, h}^\emptyset(\omega) = -\beta \sum_{\{i, j\} \in \mathcal{E}_\Lambda^\emptyset} \omega_i \omega_j - h \sum_{i \in \Lambda} \omega_i, \quad (2.2)$$

where

$$\mathcal{E}_\Lambda^\emptyset = \{\{i, j\} : i, j \in \Lambda, i \sim j\} \quad (2.3)$$

is the set of nearest neighbor edges within  $\Lambda$ .

Another type of boundary condition will include nearest neighbor edges crossing the border of  $\Lambda$ . Fix a configuration  $\eta \in \Omega$ . Freeze the degrees of freedom outside  $\Lambda$  with  $\eta$  and the configuration space is

$$\Omega_\Lambda^\eta = \{\omega \in \{+1, -1\}^{\mathbb{Z}^d} : \omega_i = \eta_i, \forall i \in \mathbb{Z}^d \setminus \Lambda\}. \quad (2.4)$$

The set of nearest neighbor edges is now

$$\mathcal{E}_\Lambda^\eta = \{\{i, j\} \subset \mathbb{Z}^d : \{i, j\} \cap \Lambda \neq \emptyset, i \sim j\} \quad (2.5)$$

and the energy with *boundary condition*  $\eta$  is

$$\mathcal{H}_{\Lambda;\beta,h}^\eta(\omega) = -\beta \sum_{\{i,j\} \in \mathcal{E}_\Lambda^\eta} \omega_i \omega_j - h \sum_{i \in \Lambda} \omega_i. \quad (2.6)$$

We use superscript  $\# = \emptyset, \eta, \dots$  to cover all boundary conditions.

## 2.2 Thermodynamic limit

**Question:** Is there a phase transition as  $\beta$  and  $h$  vary? What is a phase transition? In physics, the answer could be: jump discontinuity of physical quantities; or coexistence of two phases. We will discuss the first aspect.

Given the *partition function*

$$Z_{\Lambda;\beta,h}^\# = \sum_{\omega \in \Omega_\Lambda^\#} e^{-\mathcal{H}_{\Lambda;\beta,h}^\#(\omega)}, \quad (2.7)$$

the *Gibbs measure*, or the probability measure on configuration space, is

$$\mu_{\Lambda;\beta,h}^\#(\omega) = e^{-\mathcal{H}_{\Lambda;\beta,h}^\#(\omega)} / Z_{\Lambda;\beta,h}^\#. \quad (2.8)$$

The *free energy density* is defined as

$$\psi_\Lambda^\#(\beta, h) = \frac{1}{|\Lambda|} \log Z_{\Lambda;\beta,h}^\# \quad (2.9)$$

such that the expectation value of average magnetism writes

$$\begin{aligned} \frac{\partial}{\partial h} \psi_\Lambda^\# &= \frac{1}{|\Lambda|} \frac{1}{Z_{\Lambda;\beta,h}^\#} \sum_{\omega \in \Omega_\Lambda^\#} \sum_{i \in \Lambda} \omega_i e^{-\mathcal{H}_{\Lambda;\beta,h}^\#(\omega)} \\ &= \sum_{\omega \in \Omega_\Lambda^\#} \frac{\sum_{i \in \Lambda} \omega_i}{|\Lambda|} \mu_{\Lambda;\beta,h}^\#(\omega) \\ &= \frac{\langle M \rangle_{\Lambda;\beta,h}}{|\Lambda|}. \end{aligned} \quad (2.10)$$

However, there is no discontinuity of magnetism in *finite volume*! All functions are analytic. In order to see phase transition, we have to take the limit  $\Lambda \nearrow \mathbb{Z}^d$ . We want a notion of convergence such that the boundaries  $\partial\Lambda$  become irrelevant.

**Definition 2.1.** Given a sequence  $(\Lambda_n)_{n \in \mathbb{N}}$  of domains  $\Lambda_n \Subset \mathbb{Z}^d$ , it converges to  $\mathbb{Z}^d$  in the sense of **van Hove**  $(\Lambda_n \uparrow \mathbb{Z}^d)$  if

1.  $\Lambda_n \subset \Lambda_{n+1}, \forall n$ .
2.  $\bigcup_{n \in \mathbb{N}} \Lambda_n = \mathbb{Z}^d$ .
3.  $\lim_{n \rightarrow \infty} |\partial \Lambda_n|/|\Lambda_n| = 0$ , where  $\partial \Lambda = \{i \in \Lambda : \exists j \notin \Lambda, i \sim j\}$ .

**Theorem 2.2.** (FV Theorem 3.6) *Existence of the thermodynamic limit.*

1. *The limit*

$$\psi(\beta, h) = \lim_{n \rightarrow \infty} \frac{1}{|\Lambda_n|} \log Z_{\Lambda_n; \beta, h}^{\#} \quad (2.11)$$

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

2. *The limit does not depend on the choice of boundary condition.*
3. *The function  $\mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}, (\beta, h) \mapsto \psi(\beta, h)$  is convex.*
4. *The function  $h \mapsto \psi(\beta, h)$  is even:  $\psi(\beta, -h) = \psi(\beta, h)$*

*Proof.* 1. Start from free boundary condition and choose  $\Lambda_n = D_n$ , where  $D_n := \{-2^n + 1, \dots, 2^n - 1, 2^n\}^d$ . As the partition of  $D_{n+1}$  is  $2^d$  translates of  $D_n$ , the energy of  $\omega$  in  $D_{n+1}$  can be written as

$$\mathcal{H}_{D_{n+1}}^{\emptyset} = \sum_{i=1}^{2^d} \mathcal{H}_{D_n^{(i)}}^{\emptyset} + R_n, \quad (2.12)$$

where  $R_n$  represents the interactions between the boundaries of the sub-boxes. Since each face of  $D_{n+1}$  has  $(2^{n+2})^{d-1}$  points, we have  $|R_n(\omega)| \leq \beta d (2^{n+2})^{d-1}$ . Therefore

$$\begin{aligned} Z_{D_{n+1}}^{\emptyset} &\leq e^{\beta d 2^{(n+2)(d-1)}} \sum_{\omega \in \Omega_{D_{n+1}}} \prod_{i=1}^{2^d} \exp(-\mathcal{H}_{D_n^{(i)}}^{\emptyset}(\omega)) \\ &= e^{\beta d 2^{(n+2)(d-1)}} (Z_{D_n}^{\emptyset})^{2^d}. \end{aligned} \quad (2.13)$$

Similarly,

$$Z_{D_{n+1}}^{\emptyset} \geq e^{-\beta d 2^{(n+2)(d-1)}} (Z_{D_n}^{\emptyset})^{2^d}. \quad (2.14)$$

Take logarithms and divide by  $|D_{n+1}| = 2^{d(n+2)}$ , and we get

$$|\psi_{D_{n+1}}^{\emptyset} - \psi_{D_n}^{\emptyset}| \leq \beta d 2^{-(n+2)}, \quad (2.15)$$



which implies  $\psi_{D_n}$  is a Cauchy sequence:  $\forall n \leq m$ ,

$$|\psi_{D_m}^\varnothing - \psi_{D_n}^\varnothing| \leq \beta(2^{-n} - 2^{-m}). \quad (2.16)$$

Therefore,  $\lim_{n \rightarrow \infty} \psi_{D_n}^\varnothing$  exists. Denote it by  $\psi$ .

Now consider an arbitrary sequence  $\Lambda_n \uparrow \mathbb{Z}^d$ . Fix some integer  $k$  and  $\mathbb{Z}^d$  can be divided into adjacent disjoint translates of  $D_k$ . For each  $n$ , consider a minimal covering of  $\Lambda_n$  by elements  $D_k^{(j)}$  and let  $[\Lambda_n] := \bigcup_j D_k^{(j)}$ . The following estimate holds:

$$|\psi_{\Lambda_n}^\varnothing - \psi| \leq |\psi_{\Lambda_n}^\varnothing - \psi_{[\Lambda_n]}^\varnothing| + |\psi_{[\Lambda_n]}^\varnothing - \psi_{D_k}^\varnothing| + |\psi_{D_k}^\varnothing - \psi|. \quad (2.17)$$

For any  $\epsilon > 0$ , there exists  $k_0$  such that  $|\psi_{D_k}^\varnothing - \psi| < \epsilon/3$ ,  $\forall k > k_0$ .

In the same spirit as in part 1, write

$$\mathcal{H}_{[\Lambda_n]}^\varnothing = \sum_j \mathcal{H}_{D_k^{(j)}}^\varnothing + W_n, \quad (2.18)$$

where  $|W_n| \leq \beta d(2^{k+1})^{d-1} |[\Lambda_n]| / |D_k| = \beta d 2^{-(k+1)} |[\Lambda_n]|$ . Therefore there exists  $k_1$  such that  $|\psi_{[\Lambda_n]}^\varnothing - \psi_{D_k}^\varnothing| < \epsilon/3$ ,  $\forall k > k_1$ .

Finally, let  $\Delta_n := [\Lambda_n] \setminus \Lambda_n$ . It can be observed that

$$|\mathcal{H}_{[\Lambda_n]}^\varnothing - \mathcal{H}_{\Lambda_n}^\varnothing| \leq (2d\beta + |h|) |\Delta_n| \quad (2.19)$$

and hence

$$\begin{aligned} Z_{[\Lambda_n]}^\varnothing &= \sum_{\omega \in \Omega_{[\Lambda_n]}} e^{-\mathcal{H}_{[\Lambda_n]}(\omega)} \leq \sum_{\omega \in \Omega_{\Lambda_n}} \sum_{\omega \in \Omega_{\Delta_n}} e^{-\mathcal{H}_{\Lambda_n}(\omega)} e^{(2d\beta + |h|) |\Delta_n|} \\ &\leq e^{(2d\beta + |h| + \log 2) |\Delta_n|} Z_{\Lambda_n}^\varnothing. \end{aligned} \quad (2.20)$$

We can similarly achieve the lower bound and

$$\begin{aligned} |\log Z_{\Lambda_n}^\varnothing - \log Z_{[\Lambda_n]}^\varnothing| &\leq (2d\beta + |h| + \log 2) |\Delta_n| \\ &\leq (2d\beta + |h| + \log 2) |\partial \Lambda_n| |D_k|. \end{aligned} \quad (2.21)$$

As

$$1 \leq \frac{|[\Lambda_n]|}{|\Lambda_n|} \leq 1 + \frac{|\Lambda_n| |D_k|}{|\Lambda_n|}, \quad (2.22)$$

and  $|\partial \Lambda_n| / |\Lambda_n| \rightarrow 0$  as  $n \rightarrow \infty$ , for sufficiently large  $n$ ,

$$|\psi_{\Lambda_n}^\varnothing - \psi_{[\Lambda_n]}^\varnothing| < \epsilon/3. \quad (2.23)$$

Put everything together, for  $k \geq \max(k_0, k_1)$  and large enough  $n$ ,

$$|\psi_{\Lambda_n}^\varnothing - \psi| < \epsilon \quad (2.24)$$

holds.

2. Independence of the boundary condition. It can be observed that

$$|\mathcal{H}_{\Lambda_n}^\eta(\omega) - \mathcal{H}_{\Lambda_n}^\emptyset(\omega)| \leq 2d\beta|\partial\Lambda_n|, \quad (2.25)$$

so

$$|\psi_{\Lambda_n}^\eta - \psi| \leq 2d\beta \frac{|\partial\Lambda_n|}{|\Lambda_n|} \rightarrow 0 \quad (2.26)$$

as  $n \rightarrow \infty$ .

3. Convexity.

#### Notes

(FV Theorem B.12) Convexity is good because

- Every local minimizer or critical point is automatically a global minimizer.
- A convex function is continuous in the interior, with left and right derivatives everywhere, which can be different for at most countable points.
- Pointwise limits of convex functions are convex.
- The derivative is monotone increasing. Physically reasonable models often have built-in monotonicities, such as magnetization increases with external field.

First apply the Hölder's inequality in finite volume:

$$\sum_{\omega} |f(\omega)g(\omega)| \leq \left(\sum_{\omega} g(\omega)^p\right)^{1/p} \left(\sum_{\omega} f(\omega)^q\right)^{1/q} \quad (2.27)$$

for  $p, q \geq 1$ ,  $1/p + 1/q = 1$ . Choose  $t = 1/p$ ,

$$f(\omega) = e^{-(1-t)\beta_1 \mathcal{H}(\omega)}, \quad g(\omega) = e^{-t\beta_2 \mathcal{H}(\omega)} \quad (2.28)$$

and the convexity of free energy density quickly follows. Since it pointwise converges to  $\psi(\beta, h)$ , the convexity can also be passed on to infinite case.

4.  $\mathbb{Z}_2$  Symmetry. The Gibbs measures

$$\mu_{\Lambda; \beta, h}^\emptyset(\omega) = \mu_{\Lambda; \beta, -h}^\emptyset(-\omega) \quad (2.29)$$

and hence  $\psi$  is even with regard to  $h$ .

□

**Magnetization per unit volume** Remember in finite volume,

$$\langle m \rangle_{\Lambda; \beta, h}^{\#} = \frac{\partial}{\partial h} \psi_{\Lambda; \beta, h}^{\#}. \quad (2.30)$$

Can we pass this also to the infinite volume limit? The problems are

1. Is the limit function differentiable?
2. Can we exchange the limit and differentiation?

According to convexity, the set of jump discontinuities of  $\partial_h \psi$

$$\mathcal{B}_{\beta} = \{ h \in \mathbb{R} : \psi(\beta, \cdot) \text{ not differentiable at } h \} \quad (2.31)$$

is at most countable.

**Corollary 2.3.** *For all  $h \notin \mathcal{B}_{\beta}$ , the average magnetization density*

$$m(\beta, h) = \lim_{\Lambda_n \uparrow \mathbb{Z}^d} m_{\Lambda_n}^{\#}(\beta, h) \quad (2.32)$$

*is well defined, independent of the choice of sequence and the boundary condition and*

$$m(\beta, h) = \frac{\partial \psi}{\partial h}(\beta, h). \quad (2.33)$$

*It is also non-decreasing and continuous on  $\mathbb{R} \setminus \mathcal{B}_{\beta}$ . It is however not continuous at each  $h \in \mathcal{B}_{\beta}$ , while the left and right limits still exist. In particular, the spontaneous magnetization*

$$m^*(\beta) := \lim_{h \rightarrow 0^+} m(\beta, h) \quad (2.34)$$

*is always well defined.*

## 2.3 Peierls' argument

**Definition 2.4.** *The free energy density  $\psi(\beta, h)$  exhibits a **first order phase transition** at  $(\beta, h)$  if  $h \mapsto \psi(\beta, h)$  fails to be differentiable at that point.*

In the following we will work at external field  $h = 0$  and dimension  $d = 2$ . Write  $\# = +$  for plus *plus boundary condition*  $\eta_i = +1$

### Key inequality

**Theorem 2.5.** *There exists a function  $\delta(\beta)$  with*

$$\lim_{\beta \rightarrow \infty} \delta(\beta) = 0 \quad (2.35)$$

(and actually decays exponentially fast) such that for all  $\Lambda \Subset \mathbb{Z}^d$  and  $i \in \Lambda$ ,

$$\mu_{\Lambda; \beta, h}^+(\sigma_i = -1) \leq \delta(\beta). \quad (2.36)$$

Note that here  $\delta(\beta)$  does not depend on  $\Lambda$  or points  $i \in \Lambda$ .

#### Notes

To fix ideas, take  $i = 0$  and  $\Lambda = B(n) = \{-n, \dots, n\}^2$ . The key inequality implies that for large  $\beta$ ,

$$\mu_{\Lambda; \beta, h}^+(\sigma_0 = -1) \leq \delta(\beta) < 1 - \delta(\beta) \leq \mu_{\Lambda; \beta, h}^+(\sigma_0 = +1). \quad (2.37)$$

1. The plus boundary condition induces a + preference everywhere.
2. The preference survives in infinite volume limit  $\Lambda \uparrow \mathbb{Z}^d$ . (Non trivial!)

It is not true for small  $\beta$ , where instead

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \mu_{\Lambda; \beta, h}^\#(\sigma_0 = -1) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \mu_{\Lambda; \beta, h}^\#(\sigma_0 = +1) = \frac{1}{2} \quad (2.38)$$

regardless of the boundary condition.

*Proof.* 1. Change the variable from configurations ( $\omega$ ) to contours that move along borders of regions with minus spins (set  $\Gamma(\omega)$ ). Observe that the energy function can be written as

$$\mathcal{H}_{\Lambda; \beta, 0}^+ = -\beta |\mathcal{E}_\Lambda^+| + 2\beta \sum_{\gamma \in \Gamma(\omega)} |\gamma|. \quad (2.39)$$

2. Long contours are unlikely. For all  $\beta > 0$  and fixed contour  $\gamma_*$ ,

$$\begin{aligned} \mu_{\Lambda; \beta, 0}^+(\Gamma \ni \gamma_*) &= \sum_{\omega: \Gamma(\omega) \ni \gamma_*} \mu_{\Lambda; \beta, 0}^+(\omega) \\ &= e^{-2\beta |\gamma_*|} \frac{\sum_{\omega: \Gamma(\omega) \ni \gamma_*} \prod_{\gamma \in \Gamma(\omega) \setminus \{\gamma_*\}} e^{-2\beta |\gamma|}}{\sum_{\omega} \prod_{\gamma \in \Gamma(\omega)} e^{-2\beta |\gamma|}}. \end{aligned} \quad (2.40)$$

The right hand side can be upper bounded by 1, since the numerator represents configurations that flip all spins within  $\gamma_*$ . Therefore

$$\mu_{\Lambda;\beta,0}^+(\Gamma \ni \gamma_*) \leq e^{-2\beta|\gamma_*|}. \quad (2.41)$$

3. The number of the contours can be bounded by

$$|\{ \gamma_* : \text{Int}(\gamma_*) \ni i, |\gamma_*| = k \}| \leq \frac{k}{2} \cdot 4 \cdot 3^{k-1}. \quad (2.42)$$

A contour that surrounds a certain point  $i = (x, y)$  necessarily contains vertices from the set  $\{ (u + x - 1/2, y + 1/2) : u = 1, 2, \dots, [k/2] \}$ , while the number of contours of length  $k$  starting from a certain vertex is at most  $4 \cdot 3^{k-1}$ , while

4. Gathering the estimates, and we get

$$\mu_{\Lambda;\beta,0}^+(\sigma_i = -1) \leq \frac{2}{3} \sum_{k \geq 4} k(3e^{-2\beta})^k = \frac{54e^{-8\beta}(4 - 9e^{-2\beta})}{(1 - 3e^{-2\beta})^2} = \delta(\beta). \quad (2.43)$$

□

**From key inequality to phase transition** According to key inequality,

$$\begin{aligned} m_{\Lambda}^+(\beta, 0) &= \frac{1}{|\Lambda|} \sum_{i \in \Lambda} \langle \sigma_i \rangle_{\Lambda;\beta,0}^+ \\ &\geq \frac{1}{|\Lambda|} \sum_{i \in \Lambda} (-1 \cdot \delta(\beta) + 1 \cdot (1 - \delta(\beta))) \\ &= 1 - 2\delta(\beta), \end{aligned} \quad (2.44)$$

Repeat the same thing for the minus boundary condition, and

$$m_{\Lambda}^-(\beta, 0) \leq -1 + 2\delta(\beta). \quad (2.45)$$

We can find  $\beta_* < \infty$  such that  $\delta(\beta) < 1/2$ ,  $\forall \beta > \beta_*$ . Then we have

$$\liminf_{\Lambda \uparrow \mathbb{Z}^d} m_{\Lambda}^+(\beta, 0) \neq \limsup_{\Lambda \uparrow \mathbb{Z}^d} m_{\Lambda}^-(\beta, 0). \quad (2.46)$$

Therefore  $h \mapsto \psi(\beta, h)$  is not differentiable at  $h = 0$ .

# Chapter 3

## Classical Part II: Infinite-volume Gibbs Measures

We have shown the discontinuity of the magnetization with regard to external field  $h$  in Ising model. In this chapter we will discuss two more aspects of the Ising phase transition:

1. Non-uniqueness of equilibrium measures: coexistence of  $(+)$  and  $(-)$  phases at  $h = 0$ ?
2. Spontaneous breaking of the spin flip symmetry at  $h = 0$ ?

### 3.1 DLR approach

Let's start in a finite volume  $\Lambda \Subset \mathbb{Z}^d$  with free boundary conditions. The configuration space is  $\Omega_\Lambda = \{-1, 1\}^\Lambda$  and we are interested in energy functions of the form

$$\mathcal{H}_\Lambda(\omega) = \sum_{B \in \Lambda} J_B \prod_{s \in B} \omega_s \quad (3.1)$$

with  $(J_B)_{B \in \mathbb{Z}^d}$  a family of coupling constants  $J_B \in \mathbb{R}$ . The key idea is to look at the behavior of system in a small window  $\Delta \Subset \Lambda$  when degrees of freedom in  $\Lambda \setminus \Delta$  are frozen.

Some new notations:

- *Projection:* if  $\omega \in \Omega_\Lambda$ , write  $\omega_\Delta = (\omega_x)_{x \in \Delta}$ .
- *Concatenation:* If  $\omega_\Delta \in \Omega_\Delta$  and  $\eta_{\Lambda \setminus \Delta} \in \Omega_{\Lambda \setminus \Delta}$ , then their union  $\omega_\Delta \eta_{\Lambda \setminus \Delta}$  is an element in  $\Omega_\Lambda$ .

Observation: let  $\eta_{\Lambda \setminus \Delta} = \omega_{\Lambda \setminus \Delta}$ , and

$$\mathcal{H}_{\Lambda}(\omega) = \mathcal{H}_{\Delta}^{\eta}(\Omega_{\Delta}) + \mathcal{H}_{\Lambda \setminus \Delta}^{\varnothing}(\eta_{\Lambda \setminus \Delta}). \quad (3.2)$$

Prescribe configurations inside or outside  $\Delta$ : given  $\gamma_{\Delta}$  and  $\eta_{\Lambda \setminus \Delta}$ , set

$$A := \{ \omega \in \Omega_{\Lambda} : \omega_{\Delta} = \gamma_{\Delta} \}, \quad B := \{ \omega \in \Omega_{\Lambda} : \omega_{\Lambda \setminus \Delta} = \eta_{\Lambda \setminus \Delta} \}. \quad (3.3)$$

The conditional probability with respect to Gibbs measure  $\mu_{\Lambda}$  is

$$\begin{aligned} \mu_{\Lambda}(A|B) &= \frac{\mu_{\Lambda}(A \cap B)}{\mu_{\Lambda}(B)} \\ &= \frac{\mu_{\Lambda}(\gamma_{\Delta} \eta_{\Lambda \setminus \Delta})}{\sum_{\omega_{\Delta} \in \Omega_{\Delta}} \mu_{\Lambda}(\omega_{\Delta} \eta_{\Lambda \setminus \Delta})} \\ &= \frac{\exp(-\mathcal{H}_{\Delta}^{\eta}(\gamma_{\Delta} \eta_{\Lambda \setminus \Delta}) - \mathcal{H}_{\Lambda \setminus \Delta}(\eta_{\Lambda \setminus \Delta}))}{\sum_{\omega_{\Delta} \in \Omega_{\Delta}} \exp(-\mathcal{H}_{\Delta}^{\eta}(\omega_{\Delta} \eta_{\Lambda \setminus \Delta}) - \mathcal{H}_{\Lambda \setminus \Delta}(\eta_{\Lambda \setminus \Delta}))} \\ &= \mu_{\Delta}^{\eta}(\gamma_{\Delta}). \end{aligned} \quad (3.4)$$

That is,

$$\mu_{\Lambda}(\omega_{\Delta} = \gamma_{\Delta} | \omega_{\Lambda \setminus \Delta} = \eta_{\Lambda \setminus \Delta}) = \mu_{\Delta}^{\eta}(\gamma_{\Delta}). \quad (3.5)$$

As a consequence,

$$\mu_{\Lambda}(\gamma_{\Delta} \eta_{\Lambda \setminus \Delta}) = \mu_{\Delta}^{\eta}(\gamma_{\Delta}) \mu_{\Lambda}(\omega_{\Lambda \setminus \Delta} = \eta_{\Lambda \setminus \Delta}) \quad (3.6)$$

and

$$\begin{aligned} \langle f \rangle_{\Lambda} &= \sum_{\omega \in \Omega_{\Lambda}} f(\omega) \mu_{\Lambda}(\omega) \\ &= \sum_{\eta_{\Lambda \setminus \Delta} \in \Omega_{\Lambda \setminus \Delta}} \sum_{\gamma_{\Delta} \in \Omega_{\Delta}} f(\gamma_{\Delta} \eta_{\Lambda \setminus \Delta}) \mu_{\Delta}^{\eta}(\gamma_{\Delta}) \mu_{\Lambda}(\omega_{\Lambda \setminus \Delta} = \eta_{\Lambda \setminus \Delta}) \\ &= \sum_{\eta_{\Lambda \setminus \Delta} \in \Omega_{\Lambda \setminus \Delta}} \langle f \rangle_{\Delta}^{\eta} \left( \sum_{\eta_{\Delta} \in \Omega_{\Delta}} \mu_{\Lambda}(\eta_{\Delta} \eta_{\Lambda \setminus \Delta}) \right) \\ &= \sum_{\eta \in \Omega_{\Lambda}} \langle f \rangle_{\Delta}^{\eta} \mu_{\Lambda}(\eta). \end{aligned} \quad (3.7)$$

The latter one is called *the DLR equation* (Dobrushin, Lanford, Ruelle, 1960s). The DLR equation says that, instead of computing averages directly, one can do it in two steps:

1. Average out degrees of freedom inside  $\Delta \Subset \Lambda$  while freezing the degrees of freedom outside, which gives  $\langle f \rangle_\Delta^\eta$ .
2. Average out degree of freedom outside  $\Delta$  with respect to full Gibbs measure.

It is this structural property that we will adopt as a definition of infinite-volume Gibbs measure, which reads

$$\langle f \rangle = \int_{\Omega} \langle f \rangle_\Delta^\eta \mu(d\eta). \quad (3.8)$$

## 3.2 Probability measures for infinite systems

Given the power set  $\mathcal{P}(\Omega) = \{ A : A \subset \Omega \}$ , what is a probability measure on  $\Omega$ ?

**Definition 3.1.** A collection  $\mathcal{F} \subset \mathcal{P}(\Omega)$  is a  $\sigma$ -algebra if

1.  $\emptyset \in \mathcal{F}$ ;
2.  $A \in \mathcal{F}$  implies  $A^c \in \mathcal{F}$ ;
3.  $(A_n)_{n \in \mathbb{N}} \subset \mathcal{F}$  implies  $\bigcup_{n \in \mathbb{N}} A_n \in \mathcal{F}$ .

**Definition 3.2.** A **measurable space** is a pair  $(\Omega, \mathcal{F})$  consisting of a set  $\Omega$  and a  $\sigma$ -algebra  $\mathcal{F} \subset \mathcal{P}(\Omega)$ .

**Definition 3.3. (Kolmogorov axioms)** A **probability measure** on  $(\Omega, \mathcal{F})$  is a map  $\mu : \mathcal{F} \rightarrow [0, 1]$  such that

1.  $\mu(\Omega) = 1$ ;
2. for every sequence  $(A_n)_{n \in \mathbb{N}}$  of disjoint sets  $A_n \in \mathcal{F}$ ,

$$\mu\left(\bigcup_{n \in \mathbb{N}} A_n\right) = \sum_{n=1}^{\infty} \mu(A_n). \quad (3.9)$$

### Notes

Why do we use  $\sigma$ -algebra instead of the total power set?

1. Consider an infinite system with free spins and no external field. Such a system should be described by a probability measure  $\mu$  such that

$$\mu(\{\omega : \omega_x = \pm 1\}) = \frac{1}{2} \quad (3.10)$$



for all sites and

$$\mu(\{\omega : \omega_\Lambda = \eta_\Lambda\}) = \frac{1}{2^{|\Lambda|}} \quad (3.11)$$

for all  $\Lambda \in \mathbb{Z}^d$  and every  $\eta_\Lambda \in \Omega_\Lambda$ . But it is *impossible*!

2. To get an idea, suppose there exists a map  $\lambda : \mathcal{P}(\mathbb{R}) \rightarrow [0, \infty)$  such that it satisfies the properties of a measure, that  $\lambda([a, b]) = b - a$  and that  $\lambda$  is transitionally invariant. It is helpful due to Dyadic expansion (See Appendix B.1).

Define the equivalence relation  $x \sim y \Leftrightarrow y - x \in \mathbb{Q}$ . For each equivalent class in  $[0, 1]$ , pick one representative element  $v$  and call the set of representatives  $V$ . Thus

$$[0, 1] = \bigcup_{v \in V} [v] \quad (3.12)$$

and

$$[0, 1] \subset \bigcup_{q \in \mathbb{Q} \cap [-1, 1]} (q + V) \subset [-1, 2]. \quad (3.13)$$

Use monotonicity and  $\sigma$ -additivity,

$$1 \leq \sum_{q \in \mathbb{Q} \cap [-1, 1]} \lambda(q + V) = \sum_{q \in \mathbb{Q} \cap [-1, 1]} \lambda(V) \leq 3. \quad (3.14)$$

Contradiction!

3. A  $\sigma$ -algebra also encodes information. Let  $\mathcal{E} \subset \mathcal{F}$  be two  $\sigma$ -algebras. For a  $\mathcal{F}$ -measurable function  $f$ , it is also  $\mathcal{E}$ -measurable if and only if  $f$  is dependent only on a  $\mathcal{E}$ -measurable function  $g$ , i.e.,

$$f(\omega) = \tilde{f}(g(\omega)). \quad (3.15)$$

Now what's left is to choose the  $\sigma$ -algebra. The minimum requirement is to be able to ask what is the probability that all spins in some finite window obey a certain behavior.

**Definition 3.4.** A set  $C \subset \Omega$  is a **cylinder set** if

$$\exists \Lambda \in \mathbb{Z}^d, A \subset \Omega_\Lambda : C = \{\omega \in \Omega : \omega_\Lambda \in A\}. \quad (3.16)$$

**Definition 3.5.** *The smallest  $\sigma$ -algebra that contains all cylinder sets is called **product  $\sigma$ -algebra**.*

We choose  $\mathcal{F}$  to be the product  $\sigma$ -algebra, which contains all Cartesian products

$$C = \times_{x \in \mathbb{Z}^d} A_x \quad (3.17)$$

where all but finitely many  $A_x$  equal to  $\{-1, 1\}$ .

### 3.3 Infinite-volume Gibbs measures

**More definitions.** Before we start this section, some more definitions and lemmas are needed.

**Definition 3.6.** *A function  $f : \Omega \rightarrow \mathbb{R}$  is **local** if there exists  $\Lambda \in \mathbb{Z}^d$  and  $g : \Omega_\Lambda \rightarrow \mathbb{R}$  such that*

$$f(\omega) = g(\omega_\Lambda). \quad (3.18)$$

*$C$  is a cylinder set if and only if its **indicator function***

$$\mathbb{1}_C(\omega) = \begin{cases} 1, & \omega \in C; \\ 0, & \omega \in \Omega \setminus C \end{cases} \quad (3.19)$$

*is local.*

*A function  $f : \Omega \rightarrow [0, 1]$  is **quasilocal** if and only if there exists a sequence  $(g_n)_{n \in \mathbb{N}}$  of local functions such that  $\lim_{n \rightarrow \infty} \|g_n - f\|_\infty \rightarrow 0$ .*

**Definition 3.7. (Convergence of probability measures.)** *Let  $(\Omega, \mathcal{F})$  be a measurable space and*

$$\mathcal{M}_1(\Omega) := \{ \mu : \mu \text{ is a probability measure on } (\Omega, \mathcal{F}) \}. \quad (3.20)$$

*We say a sequence  $(\mu_n)_{n \in \mathbb{N}}$  in  $\mathcal{M}_1(\Omega)$  **converges to**  $\mu \in \mathcal{M}_1(\Omega)$ , or  $\mu_n \Rightarrow \mu$ , if*

$$\lim_{n \rightarrow \infty} \mu_n(C) = \mu(C) \quad (3.21)$$

*for all cylinder sets  $C$ . Equivalently, if*

$$\lim_{n \rightarrow \infty} \int_\Omega f d\mu_n = \int_\Omega f d\mu \quad (3.22)$$

*for all local functions. This is also automatically true for all quasilocal functions.*

**Lemma 3.8.** (*Compactness of  $\mathcal{M}_1(\Omega)$ , FV Theorem 6.24*) With the above notion of convergence,  $\mathcal{M}_1(\Omega)$  is sequentially compact: every sequence has a convergent subsequence.

The proof is omitted here.

**Definition 3.9.** Let  $(\Omega, \mathcal{F})$  and  $(\Gamma, \mathcal{E})$  be two measurable spaces. A function  $f : \Omega \rightarrow \Gamma$  is **measurable** if for any  $A \in \mathcal{E}$ ,

$$f^{-1}(A) = \{\omega \in \Omega : f(\omega) \in A\} \in \mathcal{F}. \quad (3.23)$$

**Definition 3.10.** A **potential** is a family  $(\Phi_B)_{B \in \mathbb{Z}^d}$  of maps  $\Phi_B : \Omega \rightarrow \mathbb{R}$  that are local in  $B$ , for instance

$$\Phi_B(\omega) = J(B) \prod_{x \in B} \omega_x. \quad (3.24)$$

The potential is **absolutely summable** if for all  $i \in \mathbb{Z}^d$ ,

$$\sum_{B: i \in B \in \mathbb{Z}^d} \|\Phi_B\|_\infty < \infty. \quad (3.25)$$

Finite range potentials are summable, while the converse is not true. Let

$$\Phi_B := \begin{cases} \omega_i \omega_j / \|i - j\|^\alpha, & B = \{i, j\}; \\ 0, & |B| \neq 2. \end{cases} \quad (3.26)$$

Then for large enough  $\alpha$ ,  $\Phi_B$  is absolutely summable. Absolutely summability ensures the energy functions to be well defined, which is especially important for infinite-range potentials.

**Lemma 3.11.** Assume  $\Phi$  is absolutely summable. For  $\Lambda \in \mathbb{Z}^d$ ,  $\omega_\Lambda \in \Omega_\Lambda$ ,

$$\mu_{\Lambda; \Phi}^{(\cdot)}(\omega_\Lambda) : \eta \mapsto \exp(-\mathcal{H}_{\Lambda; \Phi}(\omega_\Lambda \eta_{\mathbb{Z}^d \setminus \Lambda})) / Z_{\Lambda; \Phi}^\eta \quad (3.27)$$

if *quasilocal*.

*Proof.* Fix  $\eta$  and choose  $\tilde{\eta}$  to be another configuration that coincides with  $\eta$  on  $\Delta \supset \Lambda$ . Let

$$h_t(\omega_\Lambda) := t \mathcal{H}_{\Lambda; \Phi}^\eta(\omega_\Lambda) + (1 - t) \mathcal{H}_{\Lambda; \Phi}^{\tilde{\eta}}(\omega_\Lambda) \quad (3.28)$$

and

$$Z_t = \sum_{\tau_\Lambda \in \Omega_\Lambda} e^{-h_t(\tau_\Lambda)}. \quad (3.29)$$

The difference of Gibbs measure can be written in the form of an integral:

$$|\mu_{\Lambda;\Phi}^\eta(\omega_\Lambda) - \mu_{\Lambda;\Phi}^{\tilde{\eta}}(\omega_\Lambda)| = \left| \int_0^1 \left( \frac{d}{dt} \frac{e^{-h_t(\omega_\Lambda)}}{Z_t} \right) dt \right|. \quad (3.30)$$

The right hand side is bounded by

$$\begin{aligned} \left| \frac{d}{dt} \frac{e^{-h_t(\omega_\Lambda)}}{Z_t} \right| &\leq \max_{\tau_\Lambda \in \Omega_\Lambda} \left| \mathcal{H}_{\Lambda;\Phi}^\eta(\tau_\Lambda) - \mathcal{H}_{\Lambda;\Phi}^{\tilde{\eta}}(\tau_\Lambda) \right| \frac{e^{-h_t(\omega_\Lambda)}}{Z_t} \\ &\leq 2|\Lambda| \max_{i \in \Lambda} \left( \sum_{B: i \in B \subseteq \mathbb{Z}^d, \text{diam}(B) \geq D} \|\Phi_B\|_\infty \right), \end{aligned} \quad (3.31)$$

where  $D$  is the distance between  $\Lambda$  and  $\Delta$ . As  $\Phi$  is absolutely summable, when  $D \rightarrow \infty$ , Eq.(3.31) goes to zero.  $\square$

### Infinite volume Gibbs measures

**Definition 3.12.** Let  $\Phi = (\Phi_B)_{B \in \mathbb{Z}^d}$  be an absolutely summable potential and  $\mu$  a probability measure on  $(\Omega, \mathcal{F})$ . Then  $\mu$  is a **Gibbs measure in infinite volume** if it satisfies DLR equation, i.e., for all  $\Delta \in \mathbb{Z}^d$  and all bounded, measurable local functions  $f : \Omega \rightarrow \mathbb{R}$ ,

$$\int_\Omega f d\mu = \int_\Omega \langle f \rangle_{\Delta;\Phi}^\eta \mu(d\eta). \quad (3.32)$$

The set of Gibbs measures of potential  $\Phi$  is denoted  $\mathcal{G}(\Phi)$ .

**Theorem 3.13.** (Existence.)  $\mathcal{G}(\Phi) \neq \emptyset$ .

*Proof.* 1. Similar to what we have done in 3.1, show the DLR equation for finite volume Gibbs measure, but with arbitrary boundary condition  $\gamma \in \Omega_\Lambda$ :

$$\langle f \rangle_{\Lambda;\Phi}^\gamma = \sum_{\eta \in \Omega_\Lambda^\gamma} \langle f \rangle_{\Delta;\Phi}^\eta \mu_{\Lambda;\Phi}^\gamma(\eta), \quad \Delta \subset \Lambda \in \mathbb{Z}^d, \quad (3.33)$$

where  $f : \Omega \rightarrow \mathbb{R}$  is local.

2. Let  $(\Lambda_n)_{n \in \mathbb{N}}$  be an increasing sequence of bounded domains  $\Lambda_n \subset \Lambda_{n+1} \in \mathbb{Z}^d$  such that  $\forall \Delta \in \mathbb{Z}^d, \exists n_0 \in \mathbb{N}, \forall n \geq n_0, \Delta \subset \Lambda_n$ . Define the finite volume Gibbs measures with boundary condition  $\gamma$ :

$$\mu_n = \mu_{\Lambda_n;\Phi}^\gamma. \quad (3.34)$$

According to sequential compactness, there exists a convergent subsequence

$$\mu_{n_k} \Rightarrow \mu. \quad (3.35)$$

3. For any fixed  $\Delta \Subset \mathbb{Z}^d$ , there exists large enough  $k_0$  such that  $\forall k > k_0$ ,  $\Delta \subset \Lambda_{n_k}$ . Now we have that for a local function  $f$ ,

$$\int f d\mu_{\Lambda_{n_k};\Phi}^\gamma = \int \langle f \rangle_{\Delta;\Phi}^\eta d\mu_{\Lambda_{n_k};\Phi}^\gamma(\eta). \quad (3.36)$$

On the left hand side, by the definition of local convergence, as  $\mu_{n_k} \Rightarrow \mu$ ,

$$\int f d\mu_{\Lambda_{n_k};\Phi}^\gamma \rightarrow \int f d\mu. \quad (3.37)$$

On the right hand side,

$$\langle f \rangle_{\Delta;\Phi}^\eta = \sum_{\omega_\Delta \in \Omega_\Delta} f(\omega_\Delta \eta_{\mathbb{Z}^d \setminus \Delta}) \mu_{\Delta;\Phi}^\eta(\omega_\Delta). \quad (3.38)$$

The product of a local and a quasilocal function is quasilocal, and a finite sum of quasilocal functions is still quasilocal. Thus  $\langle f \rangle_{\Delta;\Phi}^\eta$  is quasilocal, and

$$\int \langle f \rangle_{\Delta;\Phi}^\eta d\mu_{\Lambda_{n_k};\Phi}^\gamma(\eta) \rightarrow \int \langle f \rangle_{\Delta;\Phi}^\eta d\mu^\gamma(\eta). \quad (3.39)$$

Therefore  $\mu \in \mathcal{G}(\Phi)$  satisfies the DLR equation and is an infinite volume Gibbs measurable. □

### 3.4 Spontaneous symmetry breaking

We have shown that there exists a sequence  $\mu_{\Lambda_{n_k};\Phi}^\gamma \Rightarrow \mu \in \mathcal{G}(\Phi)$ .

- Is it possible that the limit  $\mu$  depends on the choice of subsequence?
- Is it possible that the limit  $\mu$  depends on the choice of boundary condition  $\gamma$ ?

If  $|\mathcal{G}(\Phi)| = 1$  (*uniqueness*), the answer is no!

**Theorem 3.14.** (FV Lemma 6.30) *The following are equivalent:*

- (i)  $\mathcal{G}(\Phi) = \{\mu\}$ .
- (ii) For all sequences  $(\Lambda_n)_{n \in \mathbb{N}}$  with  $\Lambda_n \Subset \mathbb{Z}^d$  and  $\Lambda_n \uparrow \mathbb{Z}^d$ , and all boundary conditions  $\gamma$ ,

$$\mu_{\Lambda_n;\Phi}^\gamma \Rightarrow \mu. \quad (3.40)$$

*Proof.* 1. (i)  $\rightarrow$  (ii) follows from the proof of Theorem 3.13.

2. (ii)  $\rightarrow$  (i). Let  $f : \Omega \rightarrow \mathbb{R}$  be a local function and  $\mu, \nu \in \mathcal{G}(\Phi)$ . Due to the DLR equations for  $\mu$  and  $\nu$ , we have

$$\left| \int_{\Omega} f d\mu - \int_{\Omega} f d\nu \right| = \left| \int_{\Omega} \langle f \rangle_{\Lambda; \Phi}^{\gamma} \mu(d\gamma) - \int_{\Omega} \langle f \rangle_{\Lambda; \Phi}^{\eta} \nu(d\eta) \right|. \quad (3.41)$$

Use the fact that  $\int_{\Omega} \mu(d\gamma) = \int_{\Omega} \nu(d\eta) = 1$ , we can write the right hand side as a double integral:

$$\left| \int_{\Omega^2} (\langle f \rangle_{\Lambda; \Phi}^{\gamma} - \langle f \rangle_{\Lambda; \Phi}^{\eta}) \mu(d\gamma) \nu(d\eta) \right|. \quad (3.42)$$

By condition (ii), it goes to 0 as  $\Lambda \uparrow \mathbb{Z}^d$ . We can use dominated convergence to conclude that

$$\int_{\Omega} f d\mu = \int_{\Omega} f d\nu \quad (3.43)$$

for all local functions  $f$ , which indicates

$$\mu = \nu. \quad (3.44)$$

□

**Non-uniqueness of infinite volume Gibbs measure for the Ising model** The potential of Ising model is

$$\Phi_B^{\beta, h}(\omega) = \begin{cases} -h\omega_i, & B = \{i\}; \\ -\beta\omega_i\omega_j, & B = \{i, j\}, i \sim j; \\ 0, & \text{else.} \end{cases} \quad (3.45)$$

Write  $\mathcal{G}(\beta, h) = \mathcal{G}(\Phi^{\beta, h})$ .

**Theorem 3.15.** *There exists  $\beta_c < \infty$  such that for all  $\beta \geq \beta_c$ ,*

$$|\mathcal{G}(\beta, 0)| \geq 2. \quad (3.46)$$

*Proof.* In the Peierls' argument,

$$\mu_{\Lambda_n; \beta, 0}^+(\sigma_0 = -1) \leq \delta(\beta), \quad \mu_{\Lambda_n; \beta, 0}^-(\sigma_0 = -1) \geq 1 - \delta(\beta). \quad (3.47)$$

Along the subsequence, measures converge to Gibbs measures  $\mu^{\pm} \in \mathcal{G}(\beta, 0)$ . Since  $C = \{\omega \in \Omega : \omega_0 = -1\}$  is a cylinder set, we can pass the inequalities to the limit and obtain

$$\mu^+(C) \leq \delta(\beta) \quad \mu^-(C) \geq 1 - \delta(\beta). \quad (3.48)$$

For sufficiently large  $\beta$ ,  $\mu^+(C) \neq \mu^-(C)$ . Thus we have found two distinct infinite volume Gibbs measures. □

**Symmetry breaking** The symmetry group of Ising model at  $h = 0$  is  $G = \{-1, 1\}$  with multiplication. An action on  $\Omega$  is the map

$$G \times \Omega \rightarrow \Omega, \quad (g, \omega) \mapsto \tau_g \omega = g\omega \quad (3.49)$$

The finite volume Gibbs measures satisfy

$$\mu_{\Lambda; \beta, 0}^\eta(A) = \mu_{\Lambda; \beta, 0}^{\tau_g^{-1}\eta}(\tau_g^{-1}A) \quad (A \subset \Omega_\Lambda^\eta \subset \Omega). \quad (3.50)$$

**Theorem 3.16.** *There exists  $\beta_c < \infty$  such that for all  $\beta \geq \beta_c$ , there is at least one infinite volume Gibbs measure  $\mu \in \mathcal{G}(\beta, 0)$  with  $\tau_g \mu \neq \mu$ .*

*Proof.* Check  $\tau_g \mu^+ \neq \mu^+$  for large  $\beta$ . □

# Chapter 4

## Classical Part III: Mermin-Wagner Theorem

### 4.1 Settings and the theorem

The local degrees of freedom are *spins* in  $\mathbb{R}^N$ ,  $N \geq 2$ :

$$\mathbf{S}_i \in \mathbb{S}^{N-1} = \{ \mathbf{u} \in \mathbb{R}^N : |\mathbf{u}| = 1 \}, \quad i \in \mathbb{Z}^d \quad (4.1)$$

that can rotate.

**Definition 4.1.** Let  $W : [-1, 1] \rightarrow \mathbb{R}$ . The Hamiltonian of an  $O(N)$ -symmetric model in  $\Lambda \in \mathbb{Z}^d$  is

$$\mathcal{H}_{\Lambda; \beta}^{\#} = \beta \sum_{\{i, j\} \in \mathcal{E}_{\Lambda}^{\#}} W(\mathbf{S}_i \cdot \mathbf{S}_j). \quad (4.2)$$

For instance, when  $W(x) = -x$ , it is the *classical XY model* when  $N = 2$  and *classical Heisenberg model* when  $N = 3$ :

$$\mathcal{H}_{\Lambda; \beta}^{\#} = -\beta \sum_{\{i, j\} \in \mathcal{E}_{\Lambda}^{\#}} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (4.3)$$

**Question** Do there exist infinite volume Gibbs measures that break the rotational symmetry?

**Theorem 4.2. (Mermin-Wagner)** Assume that  $W$  is twice continuously differentiable. If the dimension of the system  $d = 1$  or  $d = 2$ , there are no such infinite volume Gibbs measures that break the rotational symmetry: for all  $\mu \in \mathcal{G}(\beta, N)$ ,  $r \in \text{SO}(N)$ ,

$$r(\mu) = \mu. \quad (4.4)$$



In the following section, we will introduce ingredients for the proof of Mermin-Wagner theorem.

## 4.2 Proof of Mermin-Wagner theorem

### 4.2.1 Spin waves

Choose  $\Lambda$  to be boxes  $B(n) = \{-n, \dots, n\}^d$ . Remember that for the Ising model, which is a discrete case, with plus boundary condition  $\eta_i = 1$ , the minimum energy cost to flip a spin is

$$\min \{ \mathcal{H}_{B(n);\beta}^\eta(\omega) - \mathcal{H}_{B(n);\beta}^\eta(\eta) : \omega \in \Omega_{B(n)}^+, \omega_0 = -1 \} = 8\beta > 0, \quad (4.5)$$

regardless of  $n$ . However, the situation is very different for continuous spins.

**Proposition 4.3.** *For an  $O(2)$ -symmetric model with boundary condition is  $\mathbf{S}_i(\eta) = \mathbf{e}_1 \Rightarrow$ , the minimum cost of flipping a spin*

$$\min \{ \mathcal{H}_{B(n);\beta}^\eta(\omega) - \mathcal{H}_{B(n);\beta}^\eta(\eta) : \omega \in \Omega_{B(n)}^+, \mathbf{S}_0(\omega) = -\mathbf{e}_1 = \leftarrow \} \quad (4.6)$$

goes to 0 as  $n \rightarrow \infty$  when  $d = 1$  or  $d = 2$ .

*Proof.* Take for each site  $\theta_i \in (-\pi, \pi]$  such that  $\mathbf{S}_i = (\cos \theta_i, \sin \theta_i)$ . Also write  $V(\beta) = W(\cos \theta)$  so that

$$\mathcal{H}_{B(n);\beta}^\eta = \beta \sum_{\{i,j\} \in \mathcal{E}_{B(n)}^\eta} W(\mathbf{S}_i \cdot \mathbf{S}_j) = \beta \sum_{\{i,j\} \in \mathcal{E}_{B(n)}^\eta} V(\theta_j - \theta_i). \quad (4.7)$$

Note that  $V'(0) = 0$ . Consider the *spin wave configuration*:  $\omega_i^{\text{SW}} = (\cos \theta_i^{\text{SW}}, \sin \theta_i^{\text{SW}})$  where

$$\theta_i^{\text{SW}} := \left( 1 - \frac{\log(1 + \|i\|_\infty)}{\log(1 + n)} \right) \pi, \quad i \in B(n), \quad (4.8)$$

and  $\theta_i^{\text{SW}} = 0$  for  $i \notin B(n)$ . The nonzero contribution of  $\mathcal{H}_{B(n);\beta}^\eta$  comes from pairs of neighboring  $i, j$  pairs such that  $\|i\|_\infty = \|j\|_\infty - 1$ , and

$$\theta_i^{\text{SW}} - \theta_j^{\text{SW}} = \pi \frac{\log \left( 1 + \frac{1}{\|j\|_\infty} \right)}{\log(1 + n)} \leq \frac{\pi}{\|j\|_\infty \log(1 + n)}. \quad (4.9)$$

Since  $V$  is twice continuously differentiable, there exists a constant  $C$  such that

$$\sup_{\theta \in (-\pi, \pi]} |V''(\theta)| \leq C. \quad (4.10)$$

For large  $n$ , we can Taylor expanding  $V$  as

$$|V(\theta_i^{\text{SW}} - \theta_j^{\text{SW}}) - V(0)| \leq \frac{1}{2} C (\theta_i^{\text{SW}} - \theta_j^{\text{SW}})^2 \leq \frac{C\pi^2}{2\log^2(1+n)} \cdot \frac{1}{\|j\|_\infty^2}. \quad (4.11)$$

Summing over all the contributions of neighboring pairs, and we get

$$\begin{aligned} 0 &\leq \mathcal{H}_{B(n);\beta}^n(\omega^{\text{SW}}) - \mathcal{H}_{B(n);\beta}^n(\eta) \\ &\leq \frac{C\beta\pi^2}{2\log^2(1+n)} \sum_{l=1}^{n+1} 2^d (2l-1)^{d-1} \frac{1}{l^2} \\ &\leq \begin{cases} \frac{C\beta\pi^4}{12\log^2(1+n)}, & d=1; \\ \frac{4C\beta\pi^2}{\log(1+n)}, & d=2; \\ \text{diverges}, & d \geq 3. \end{cases} \end{aligned} \quad (4.12)$$

When  $n \rightarrow \infty$  and  $d \leq 2$ , the energy cost of flipping a spin indeed goes to 0.  $\square$

The spin waves represent collective excitations of arbitrarily low energy, which renders impossible the application of Peierls' argument.

### 4.2.2 Total variation distance and relative entropy

Now we want to measure the distance between two (infinite-volume) Gibbs measures. Naively we want that for close enough Hamiltonians, the Gibbs measures should also be close. Namely if we have for two Hamiltonians  $H, U$

$$\|H_\Lambda - U_\Lambda\|_\infty \leq \epsilon_\Lambda, \quad (4.13)$$

what about the distance between their Gibbs measures? We need to introduce total variation distance and relative entropy for a quantitative discussion.

**Definition 4.4.** *Given two probability measures  $\mu$  and  $\nu$  on measurable space  $(\Omega, \mathcal{F})$ . Their **total variation distance** is*

$$\|\mu - \nu\|_{\text{TV}} := 2 \sup_{A \in \mathcal{F}} |\mu(A) - \nu(A)|. \quad (4.14)$$

**Notes**

The factor 2 is such that

$$2|\mu(A) - \nu(A)| = |\mu(A) - \nu(A)| + |\mu(A^c) - \nu(A^c)|. \quad (4.15)$$

Actually

$$\|\mu - \nu\|_{\text{TV}} = \sup_{n, \{A_1, \dots, A_n\}} \sum_{i=1}^n |\mu(A_i) - \nu(A_i)|. \quad (4.16)$$

**Definition 4.5.** Let  $p_1, \dots, p_n, q_1, \dots, q_n \geq 0$  with  $\sum_i p_i = \sum_i q_i = 1$ . The **relative entropy** (in the finite case) is

$$h(p|q) := \sum_{i=1}^n p_i \log \frac{p_i}{q_i}. \quad (4.17)$$

If there exists  $i$  so that  $p_i > 0$  but  $q_i = 0$ , then  $h(p|q) = \infty$ . When  $p_i = q_i = 0$ , the  $i$ -th contribution is given by 0.

**Notes**

If the reference measure  $q$  is a uniform distribution:  $q_i = 1/n$ , then

$$h(p|q) = \sum_i p_i \ln(np_i) = \ln n - \underbrace{S(p)}_{\text{the Shannon entropy}}. \quad (4.18)$$

**Proposition 4.6.** The relative entropy is non-negative. In particular,  $h(p|q) = 0$  if and only if  $p = q$ .

*Proof.* The strict convexity of exponential function gives that

$$e^x \geq e^a + e^a(x - a) \quad (4.19)$$

for any  $a, x \in \mathbb{R}$  and the equal sign can be taken only when  $x = a$ . Let  $a = \ln p_i$  and  $x = \ln q_i$  and we get

$$q_i \geq p_i + p_i \ln \frac{q_i}{p_i}, \quad (4.20)$$

or equivalently,

$$p_i \ln \frac{p_i}{q_i} \geq p_i - q_i. \quad (4.21)$$

Take a sum over  $i$ , and we get the positivity.  $\square$

**Definition 4.7.** Let  $\mu, \nu$  be two probability measures on  $(\Omega, \mathcal{F})$ . The **relative entropy** is given by

1. If  $\mu$  is absolutely continuous with respect to  $\nu$  with Radon-Nikodym derivative  $\rho = d\mu/d\nu$ , then

$$h(\mu|\nu) = \int_{\Omega} (\rho \ln \rho) d\nu = \int_{\Omega} \left( \ln \frac{d\mu}{d\nu} \right) d\mu. \quad (4.22)$$

2. If  $\mu$  is not absolutely continuous with respect to  $\nu$ , then  $h(\mu|\nu) = \infty$ .

**Proposition 4.8.** 1.  $h(\mu|\nu) \geq 0$  and the equal sign can be taken if and only if  $\mu = \nu$ . Note that  $h$  is not a metric, since it is general not symmetric.

2. (**Pinsker's inequality**) If  $\mu$  is absolutely continuous with regard to  $\nu$ , then

$$\|\mu - \nu\|_{\text{TV}} \leq \sqrt{2h(\mu|\nu)}. \quad (4.23)$$

*Proof.* Since  $1/(1+x)$  is a convex function, we can apply the Jensen's inequality

$$\begin{aligned} (1+x) \ln(1+x) - x &= x^2 \int_0^1 dt \int_0^t ds \frac{1}{1+xs} \\ &\geq \frac{x^2}{2} \cdot \frac{1}{1+x \int_0^1 dt \int_0^t ds 2s} \\ &= \frac{x^2}{2(1+x/3)}. \end{aligned} \quad (4.24)$$

Let  $m = d\mu/d\nu - 1$ . Then  $\langle m \rangle_{\nu} = 0$  and

$$h(\mu|\nu) = \langle (1+m) \ln(1+m) - m \rangle_{\nu} \geq \left\langle \frac{m^2}{2(1+m/3)} \right\rangle_{\nu}. \quad (4.25)$$

While

$$\begin{aligned} \|\mu - \nu\|_{\text{TV}}^2 &= \langle |m| \rangle_{\nu}^2 = \left\langle \frac{|m|}{\sqrt{1+m/3}} \cdot \sqrt{1+m/3} \right\rangle_{\nu}^2 \\ &\leq \left\langle \frac{m^2}{1+m/3} \right\rangle_{\nu} \left\langle 1 + \frac{m}{3} \right\rangle_{\nu} \\ &\leq 2h(\mu|\nu). \end{aligned} \quad (4.26)$$

□

Now for given Gibbs measures

$$\mu_\Lambda(\omega) = \frac{1}{Z_{\Lambda;H}} e^{-H_\Lambda(\omega)}, \quad \nu_\Lambda(\omega) = \frac{1}{Z_{\Lambda;U}} e^{-U_\Lambda(\omega)}, \quad (4.27)$$

the relative entropy is upper bounded by the maximum energy difference:

$$\begin{aligned} h(\mu_\Lambda | \nu_\Lambda) &= \sum_{\omega \in \Omega_\Lambda} \mu_\Lambda(\omega) \ln \frac{\mu_\Lambda(\omega)}{\nu_\Lambda(\omega)} \\ &= \sum_{\omega \in \Omega_\Lambda} \mu_\Lambda(\omega) (U_\Lambda(\omega) - H_\Lambda(\omega)) + \ln \frac{Z_{\Lambda;U}}{Z_{\Lambda;H}} \\ &\leq 2 \|H_\Lambda - U_\Lambda\|_\infty. \end{aligned} \quad (4.28)$$

Therefore the Pinsker's inequality yields

$$\|\mu_\Lambda - \nu_\Lambda\|_{\text{TV}} \leq \sqrt{4 \|H_\Lambda - U_\Lambda\|_\infty}. \quad (4.29)$$

### 4.2.3 Proof for the $N = 2$ case

**Proposition 4.9.** *Under the assumptions of Mermin-Wagner theorem and when  $N = 2$ , there exist constants  $c_1, c_2$  such that for any boundary condition  $\eta \in \Omega$ , any inverse temperature  $\beta < \infty$ , any angle  $\psi \in (-\pi, \pi]$ , any  $l \in \mathbb{Z}_0^+$  and  $n > l$ ,*

$$|\langle f \rangle_{B(n);\beta}^\eta - \langle r_\psi f \rangle_{B(n);\beta}^\eta| \leq \beta^{\frac{1}{2}} |\psi| \|f\|_\infty \begin{cases} \frac{c_1}{\sqrt{n-l}}, & d = 1, \\ \frac{c_2 \sqrt{l}}{\sqrt{\ln(n-l)}}, & d = 2, \end{cases} \quad (4.30)$$

assuming that  $\text{supp}(f) \subset B(l)$ .

*Proof.* 1. Let  $\psi$  be a local rotation inside  $B(l)$ . Choose a spin-wave like field of angles  $\Psi : \mathbb{Z}^d \rightarrow (-\pi, \pi]$ ,  $i \mapsto \Psi_i$  that agrees with  $\psi$  on  $B(l)$  and vanishes outside  $\Lambda \supset B(l)$ . Define the twist map  $t_\Psi : \Omega \rightarrow \Omega$ ,

$$\theta_i(t_\Psi \omega) = \theta_i(\omega) + \Psi_i \quad (4.31)$$

and the twisted energy

$$\mathcal{H}_{\Lambda;\beta}^{\eta;\Psi} := \mathcal{H}_{\Lambda;\beta}^{t_\Psi \eta}(t_\Psi \omega). \quad (4.32)$$

Then

$$\begin{aligned}
 \langle r_{-\Psi} f \rangle_{\Lambda; \beta}^{\eta} &= \frac{1}{Z_{\Lambda; \beta}^{\eta}} \int f(r_{-\Psi} \omega) e^{-\mathcal{H}_{\Lambda; \beta}^{\eta}(\omega_{\Lambda \eta_{\Lambda^c}})} \prod_{i \in \Lambda} d\omega_i \\
 &= \frac{1}{Z_{\Lambda; \beta}^{\eta; \Psi}} \int f(\omega) e^{-\mathcal{H}_{\Lambda; \beta}^{\eta; \Psi}(t_{\Psi}(\omega_{\Lambda \eta_{\Lambda^c}}))} \prod_{i \in \Lambda} d\omega_i \\
 &= \langle f \rangle_{\Lambda; \beta}^{\Psi; \eta}.
 \end{aligned} \tag{4.33}$$

2. Using the relative entropy and follow the same calculations as we did in 4.2.1, we get

$$\begin{aligned}
 |\langle r_{-\Psi} f \rangle_{\Lambda; \beta}^{\eta} - \langle f \rangle_{\Lambda; \beta}^{\Psi; \eta}| &\leq \|f\|_{\infty} \|\mu_{\Lambda} - \nu_{\Lambda}\|_{\text{TV}} \\
 &\leq \|f\|_{\infty} \sqrt{2|h(\mu_{\Lambda; \beta}^{\eta} = \mu_{\Lambda; \beta}^{\Psi; \eta})|} \\
 &\leq \|f\|_{\infty} \sqrt{2C\beta \sum_{\{i,j\} \in \mathcal{E}_{\Lambda}^{\eta}} (\Psi_j - \Psi_i)^2}.
 \end{aligned} \tag{4.34}$$

3. Now we need to choose angles  $\Psi_i$  on  $\Lambda \setminus B(l)$  by minimizing

$$\sum_{\{i,j\} \in \mathcal{E}_{\Lambda}^{\eta}} (\Psi_j - \Psi_i)^2 \tag{4.35}$$

under the constraints  $\Psi_i = \psi, \forall i \in B(l)$  and  $\Psi_i = 0, \forall i \in \Lambda^c$ . By applying the spin wave configuration, it is easy to get the result for  $d = 2$  case. To be more general, let

$$\mathcal{E}(u) = \frac{1}{2} \sum_{\{i,j\} \in \mathcal{E}_{\Lambda \setminus B(l)}^{\eta}} (\nabla u)_{ij}^2, \tag{4.36}$$

where  $(\nabla f)_{ij} := f_i - f_j$  is the discrete gradient, and the discrete Laplacian is defined as  $(\Delta f)_i := \sum_{j \sim i} (\nabla f)_{ij}$ . Now introduce without proof a discrete Green identity:

$$\sum_{\{i,j\} \in \mathcal{E}_{\Lambda}^{\eta}} (\nabla f)_{ij} (\nabla g)_{ij} = - \sum_{i \in \Lambda} g_i (\Delta f)_i + \sum_{i \in \Lambda, j \in \Lambda^c, i \sim j} g_j (\nabla f)_{ij}. \tag{4.37}$$

We want

$$\frac{d}{ds} \mathcal{E}(\Psi + s\delta)|_{s=0} = 0 \tag{4.38}$$

for all perturbations  $\delta : \mathbb{Z}^d \rightarrow \mathbb{R}$  such that  $\delta_i = 0, \forall i \ni \Lambda \setminus B(l)$ . Calculation follows that

$$\begin{aligned} \frac{d}{ds} \mathcal{E}(\Psi + s\delta)|_{s=0} &= \sum_{\{i,j\} \in \mathcal{E}_{\Lambda \setminus B(l)}^\eta} (\nabla \Psi)_{ij} (\nabla \delta)_{ij} \\ &= - \sum_{i \in \Lambda \setminus B(l)} \delta_i (\Delta \Psi)_i + \sum_{i \in \Lambda \setminus B(l), j \ni \Lambda \setminus B(l), j \sim i} \delta_j (\nabla \Psi)_{ij}. \end{aligned} \quad (4.39)$$

The second term is zero since  $\delta_j$  vanishes outside  $\Lambda \setminus B(l)$ . Hence  $(\Delta \Psi)_i$  has to be 0 everywhere in  $\Lambda \setminus B(l)$  and  $\Psi$  is "harmonic". The solution is given by

$$\Psi_i = \psi P(X^i \text{ enters } B(l) \text{ before exiting } \Lambda), \quad (4.40)$$

where  $X^i = (X_k^i)$  is a symmetric simple random walk on  $\mathbb{Z}^d$  starting from  $P(X_0^i = i) = 1$  and moreover, if replacing  $\Lambda$  with  $B(n)$  for any  $n > l$ ,

$$\begin{aligned} \mathcal{E}(\Psi) &= \psi^2 d \sum_{j \in \partial^{\text{int}} B(l)} P(X^j \text{ exits } B(n) \text{ before returning to } B(l)). \\ &\leq \psi^2 d |\partial^{\text{int}} B(l)| P(X^0 \text{ exits } B(n-l) \text{ before returning to } 0). \end{aligned} \quad (4.41)$$

The returning probability is  $O(1/(n-l))$  for  $d = 1$  and  $O(1/\ln(n-l))$  for  $d = 2$  and we conclude the final result as stated.  $\square$

Now we can complete the proof for our version of Mermin-Wagner theorem. Recall the DLR equation:

$$\langle f \rangle_\mu - \langle r_\psi f \rangle_\mu = \int (\langle f \rangle_{\Lambda; \mu}^\eta - \langle r_\psi f \rangle_{\Lambda; \mu}^\eta) \mu(d\eta). \quad (4.42)$$

According to Proposition 4.9, the integrand on the right hand side goes to zero as  $\Lambda \uparrow \mathbb{Z}^d$  for any local function  $f$ . By dominated convergence, the limit and integral on right hand side can be exchanged and the expression on both sides altogether goes to 0. Therefore

$$\langle f \rangle_\mu - \langle f \rangle_{r_{-\psi}(\mu)} = \langle f \rangle_\mu - \langle r_\psi f \rangle_\mu = 0. \quad (4.43)$$

Conclude.

### 4.3 Corollaries of Mermin-Wagner theorem

Clearly in infinite volume, the distribution of a single spin is uniform:

$$\begin{aligned}
 \langle \mathbf{S}_0 \rangle &= \int \omega_0 \mu(d\omega) \\
 &= \int \omega_0 r_\psi(\mu(d\omega)) \\
 &= \int r_{-\psi}(\omega_0) \mu(d\omega) \\
 &= \int \mu(d\omega) \frac{1}{2\pi} \int_{-\pi}^{\pi} d\psi r_{-\psi}(\omega_0) = 0.
 \end{aligned} \tag{4.44}$$

What's more important is below:

**Corollary 4.10.** *There is absence of long-range order under the conditions of Theorem 4.2, namely*

$$\lim_{\|i-j\| \rightarrow \infty} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = 0. \tag{4.45}$$

#### Notes

1. In the finite volume case, the average of spin at origin for a box  $B(n)$  is bounded by Proposition 4.9. For instance, when  $d = 2$ ,

$$\sup_{\eta \in \mathbb{Z}^d} \left\| \langle \mathbf{S}_0 \rangle_{B(n); \beta}^\eta \right\| = O\left(\sqrt{\beta / \ln n}\right) \xrightarrow{n \rightarrow \infty} 0. \tag{4.46}$$

2. The absence of long-range order can be rephrased as

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \langle \mathbf{S}_j \rangle \rightarrow 0, \tag{4.47}$$

which means spins far away are independent.

*Proof.* Take  $i = 0$ ,  $j \neq 0$  and  $n = \|i - j\|_\infty - 1$  so that  $j \in \mathbb{Z}^d \setminus B(n)$ . Use



the DLR equation:

$$\begin{aligned}
 |\langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle| &= \left| \int_{\mathbb{Z}^d} \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle_{B(n);\beta}^\eta \mu(d\eta) \right| \\
 &= \left| \int_{\mathbb{Z}^d} \langle \mathbf{S}_0 \rangle_{B(n);\beta}^\eta \cdot \mathbf{S}_j \mu(d\eta) \right| \quad (j \in \mathbb{Z}^d \setminus B(n)) \\
 &\leq \int_{\mathbb{Z}^d} |\langle \mathbf{S}_0 \rangle_{B(n);\beta}^\eta \cdot \mathbf{S}_j| \mu(d\eta) \\
 &\leq \int_{\mathbb{Z}^d} |\langle \mathbf{S}_0 \rangle_{B(n);\beta}^\eta| \mu(d\eta) \quad (\text{triangle inequality}) \\
 &\xrightarrow{n \rightarrow \infty} 0.
 \end{aligned} \tag{4.48}$$

□

**Corollary 4.11.** *The magnetization  $m_\Lambda(\omega) = \sum_{i \in \Lambda} \mathbf{S}_i(\omega)/|\Lambda|$  also vanishes in the thermodynamic limit:*

$$\lim_{n \rightarrow \infty} \langle ||m_{B(n)}||^2 \rangle_\mu = 0. \tag{4.49}$$

*Proof.* In  $d = 2$  case,

$$\begin{aligned}
 \langle ||m_{B(n)}||^2 \rangle_\mu &= \frac{1}{|B(n)|^2} \sum_{i,j \in B(n)} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_\mu \\
 &\leq \frac{\text{const}}{|B(n)|^2} \sum_{i,j \in B(n)} \frac{1}{\sqrt{\ln(||i-j||_\infty)}} \quad (\text{if } ||i-j||_\infty \leq 1, \text{ replace } \ln \text{ with } 1) \\
 &\leq \frac{\text{const}}{|B(n)|} \sum_{j \in B(n)} \frac{1}{\sqrt{\ln(||j||_\infty)}} \\
 &= \frac{\text{const}}{(2n+1)^2} \left( 9 + \sum_{l=2}^n \frac{8l}{\sqrt{\ln l}} \right) \\
 &\leq \frac{\text{const}}{(2n+1)^2} \left( 9 + \int_2^{n+1} \frac{8x}{\sqrt{\ln x}} dx \right) \\
 &\leq \frac{\text{const}}{(2n+1)^2} \left( 9 + 8\sqrt{2}(n+1)^2 \underbrace{F\left(\sqrt{2\ln(n+1)}\right)}_{\substack{\text{Dawson integral, } \lim_{x \rightarrow \infty} F(x)=0}} \right) \\
 &\xrightarrow{n \rightarrow \infty} 0.
 \end{aligned} \tag{4.50}$$

The  $d = 1$  case is similar and is omitted here.

□

# Chapter 5

## Classical Part IV: Reflection Positivity

### 5.1 Settings and discrete Fourier transforms

In this section we will work on periodic boundary conditions, or the torus (of side length  $L$ ):

$$\mathbb{T}_L = (\mathbb{Z}/L\mathbb{Z})^d. \quad (5.1)$$

Every function  $f : \mathbb{T}_L \rightarrow \mathbb{R}$  can be identified with periodic function  $f : \mathbb{Z}^d \rightarrow \mathbb{R}$ ,

$$f(\mathbf{a} + L\mathbf{e}_k) = f(\mathbf{a}), \quad k = 1, \dots, d. \quad (5.2)$$

The *set of nearest neighbors* in  $\mathbb{T}_L$  is denoted by  $\mathcal{E}_L$ .

As in the last chapter, the configuration space for a single spin is  $\Omega_0 = \mathbb{S}^{N-1}$ ,  $N \geq 2$  with reference measure  $\mu_0$  to be uniform distribution on  $\mathbb{S}^{N-1}$ . The total configuration space is

$$\Omega_L = \Omega_0^{\mathbb{T}_L}. \quad (5.3)$$

Our Hamiltonian will be  $\mathcal{H}_{L;\beta} : \Omega_L \rightarrow \mathbb{R}$ ,

$$\begin{aligned} \mathcal{H}_{L;\beta}(\omega) &= \beta \sum_{\{i,j\} \in \mathcal{E}_L} \|\mathbf{S}_i(\omega) - \mathbf{S}_j(\omega)\|^2 \\ &= -2\beta \sum_{\{i,j\} \in \mathcal{E}_L} \mathbf{S}_i(\omega) \cdot \mathbf{S}_j(\omega) + \text{const}_{L;\beta}. \end{aligned} \quad (5.4)$$

Slightly different writing chosen here is in order to conjure up memories of Gaussian measures. The questions, as usual, are: how do the magnetization and long-range order behave?

To study magnetization, we should first introduce the reciprocal torus and discrete Fourier transform.

**Definition 5.1.** *The reciprocal torus is*

$$\mathbb{T}_L^* := \left\{ \frac{2\pi}{L}(n_1, \dots, n_d) : 0 \leq n_i < L \right\}. \quad (5.5)$$

The **discrete Fourier transform** of  $\mathbf{S} \in \Omega_L$  is  $\hat{\mathbf{S}} \in \Omega_0^{\mathbb{T}_L^*}$ , defined by

$$\hat{\mathbf{S}}_p := \frac{1}{\sqrt{|\mathbb{T}_L|}} \sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \mathbf{S}_j. \quad (5.6)$$

Now the magnetization becomes

$$\mathbf{m}_L = \frac{1}{|\mathbb{T}_L|} \sum_{i \in \mathbb{T}_L} \mathbf{S}_i = \frac{1}{|\mathbb{T}_L|^{1/2}} \hat{\mathbf{S}}_0. \quad (5.7)$$

Plancherel identity gives that

$$|\mathbb{T}_L| = \sum_{i \in \mathbb{T}_L} \|\mathbf{S}_i\|^2 = \sum_{p \in \mathbb{T}_L^*} \|\hat{\mathbf{S}}_p\|^2 \quad (5.8)$$

and hence

$$\|\mathbf{m}_L\|^2 = \frac{1}{|\mathbb{T}_L|} \|\hat{\mathbf{S}}_0\|^2 = 1 - \frac{1}{|\mathbb{T}_L|} \sum_{p \in \mathbb{T}_L^* \setminus \{0\}} \|\hat{\mathbf{S}}_p\|^2. \quad (5.9)$$

Since the finite-volume Gibbs measure on torus is translationally invariant,

$$\begin{aligned} \langle \|\hat{\mathbf{S}}_p\|^2 \rangle_{L;\beta} &= \frac{1}{|\mathbb{T}_L|} \sum_{i,j \in \mathbb{T}_L} e^{ip \cdot (j-i)} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{L;\beta} \\ &= \sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle_{L;\beta}. \end{aligned} \quad (5.10)$$

Gather everything, and we get

$$\langle \|\mathbf{m}_L\|^2 \rangle_{L;\beta} = 1 - \frac{1}{|\mathbb{T}_L|} \sum_{p \in \mathbb{T}_L^*} \sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle_{L;\beta}. \quad (5.11)$$

This form allows us to apply

**Theorem 5.2. (Infrared bound.)** *For all non-zero  $p \in \mathbb{T}_L^*$ ,*

$$\sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle_{L;\beta} \leq \frac{N}{4\beta d} \left( 1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) \right)^{-1}. \quad (5.12)$$

We will finish the proof later. As a consequence of the infrared bound, there will be spontaneously symmetry breaking only for  $d \geq 3$ .

**Theorem 5.3.** *When  $d \geq 3$ , let*

$$\beta_0 := \frac{N}{4d(2\pi)^d} \int_{[-\pi, \pi]^d} \left( 1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) \right)^{-1} dp < \infty. \quad (5.13)$$

*Then for  $\beta > \beta_0$ , we have*

$$\liminf_{L \rightarrow \infty} \langle ||\mathbf{m}_L||^2 \rangle_{L; \beta} \geq 1 - \frac{\beta_0}{\beta}. \quad (5.14)$$

*Proof.* Notice that  $\beta_0$  is viewing the right hand side of Eq.(5.11) as a Riemann sum. However, in the integrand there is singularity at  $p = 0$ . Since

$$1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) = O(p^2), \quad (5.15)$$

when  $d \leq 2$  the integral does not converge.  $\square$

## 5.2 Reflection positivity

**Warm up computation on  $\mathbb{Z}$ .** Consider configuration space  $\Omega = \Omega_0^{\mathbb{Z}}$  with reference measure  $\rho$  on  $\Omega_0$  and product measure  $\mu_0 := \otimes_{i \in \mathbb{Z}} \rho$ . Define reflection at the origin:

$$\Theta : \Omega \rightarrow \Omega, \quad (\Theta \omega)_i = \omega_{-i}. \quad (5.16)$$

Let  $F : \Omega \rightarrow \mathbb{R}$  be local, bounded, measurable and depending only on spins on right half axis  $i \geq 0$ . We may write

$$F(\omega) = f(\omega_0, \dots, \omega_n). \quad (5.17)$$

Then

$$\begin{aligned} \langle F(\Theta)F \rangle_{\mu_0} &= \int_{\Omega_0^{2n+1}} f(\omega_0, \dots, \omega_n) f(\omega_0, \dots, \omega_{-n}) \rho(d\omega_{-n}) \cdots \rho(d\omega_n) \\ &= \int_{\Omega_0} \left( \int_{\Omega_0^n} f(\omega_0, \dots, \omega_n) \rho(d\omega_1) \cdots \rho(d\omega_n) \right)^2 \rho(d\omega_0) \\ &\geq 0. \end{aligned} \quad (5.18)$$

Reflections at half integers are also non-negative. Such kind of product measures are called *reflection positive*.

**Definition 5.4.** Let  $k \in \{1, \dots, d\}$  denote one dimension and  $0 \leq n \leq (L-1)/2$  be an integer. **A reflection on torus through vertices** associated to  $k$  and  $n$  is  $\Theta : \mathbb{T}_L \rightarrow \mathbb{T}_L$ ,

$$\Theta(i)_l = \begin{cases} (2n - i_k) \bmod L, & l = k; \\ i_l, & l \neq k. \end{cases} \quad (5.19)$$

$\Theta$  is a reflection of the torus through a plane  $\Pi$  which is orthogonal to  $\mathbf{e}_k$ :

$$\Pi \cap \mathbb{T}_L = \{i \in \mathbb{T}_L : i_k = n \text{ or } i_k = n + L/2\}. \quad (5.20)$$

This leads to a natural decomposition of the torus into two overlapping halves  $\mathbb{T}_L = \mathbb{T}_{L,+} \cup \mathbb{T}_{L,-}$ , where

$$\begin{aligned} \mathbb{T}_{L,+} &= \{i_L \in \mathbb{T}_L : n \leq i_k \leq n + L/2\}, \\ \mathbb{T}_{L,0} &= \{i_L \in \mathbb{T}_L : 0 \leq i_k \leq n \text{ or } n + L/2 \leq i_k \leq L-1\}. \end{aligned} \quad (5.21)$$

We can similarly define reflection through *edges* by choosing  $n$  to be half integers and the decomposition will be disjoint. We denote by  $\mathcal{A}_+(\Theta)$  (respectively  $\mathcal{A}_-(\Theta)$ ) the algebra of all bounded measurable functions on  $\Omega_L$  whose support is inside  $\mathbb{T}_{L,+}(\Theta)$  (respectively  $\mathbb{T}_{L,-}(\Theta)$ ).

**Definition 5.5.** Let  $\Theta$  be a reflection. A measure  $\mu \in \mathcal{M}(\Omega_L, \mathcal{F}_L)$  is **reflection positivity with respect to  $\Theta$**  if

1.  $\langle f\Theta(g) \rangle_\mu = \langle g\Theta(f) \rangle_\mu$ , for all  $f, g \in \mathcal{A}_+(\Theta)$ ;
2.  $\langle f\Theta(f) \rangle_\mu \geq 0$ , for all  $f \in \mathcal{A}_+(\Theta)$ .

**Lemma 5.6.** The product measure  $\mu_0$  is reflection positive with respect to all reflections  $\Theta$ .

*Proof.* Notice that  $\Theta(\mu_0) = \mu_0$  and  $\Theta(fg) = \Theta(f)\Theta(g)$ . Thus for  $f \in \mathcal{A}_+(\Theta)$ ,

$$\langle f\Theta(f) \rangle_{\mu_0} = \langle f \rangle_{\mu_0} \langle \Theta(f) \rangle_{\mu_0} = \langle f \rangle_{\mu_0}^2 \geq 0. \quad (5.22)$$

□

#### Remark

For Hamiltonian Eq.(5.4), the corresponding Gibbs measure is reflection positive. It does not enter the proof of infrared bound directly and hence its proof is skipped here. See FV Lemma 10.8 and Example 10.10.

### 5.3 Gaussian domination and proof of infrared bound

**Proposition 5.7. (Gaussian domination.)** For  $h \in \Omega_L$ , let

$$Z_{L;\beta}(h) := \left\langle \exp \left( -\beta \sum_{\{i,j\} \in \mathcal{E}_L} \|\mathbf{S}_i - \mathbf{S}_j + h_i - h_j\|_2^2 \right) \right\rangle_{\mu_0}. \quad (5.23)$$

Then we have

$$Z_{L;\beta}(h) \leq Z_{L;\beta}(0). \quad (5.24)$$

*Proof.* First notice that as  $\|h\|_2^2 \rightarrow \infty$ ,  $Z_{L;\beta}(h) \rightarrow 0$ , and hence the maximizer of  $Z_{L;\beta}(h)$  exists. Without losing generality, let  $h_0 = 0$ . Denote by  $h^*$  a maximizer that minimizes

$$N(h) = |\{ \{i, j\} \in \mathcal{E}_L : h_i \neq h_j \}|. \quad (5.25)$$

Suppose that  $N(h^*) > 0$ , so that we can find a pair  $\{i_0, j_0\} \in \mathcal{E}_L$  such that  $h_{i_0}^* \neq h_{j_0}^*$ . Let  $\Theta$  be the reflection through the edge between  $\{i_0, j_0\}$ . Let  $D_+ := \{i : i \in \mathbb{T}_{L,+}, \exists j \in \mathbb{T}_{L,-} \text{ such that } \{i, j\} \in \mathcal{E}_L\}$  and  $r_i \in \mathbb{T}_{L,-}$  be the corresponding  $j$ . For  $i \in D_+$ ,

$$\|\mathbf{S}_i - \mathbf{S}_{r_i} + h_i - h_{r_i}\|_2^2 = \|\mathbf{S}_i + h_i\|_2^2 + \|\mathbf{S}_{r_i} + h_{r_i}\|_2^2 - 2(\mathbf{S}_i + h_i)(\mathbf{S}_{r_i} + h_{r_i}), \quad (5.26)$$

and hence we can decompose

$$\sum_{\{i,j\} \in \mathcal{E}_L} \|\mathbf{S}_i - \mathbf{S}_j + h_i - h_j\|_2^2 = A + \Theta(B) + \sum_{i \in D} U_i \Theta(V_i), \quad (5.27)$$

where  $A, B, U_i, V_i \in \mathcal{A}_+(\Theta)$  and

$$\begin{aligned} A &= \sum_{\{i,j\} \in \mathcal{E}_L; i,j \in \mathbb{T}_{L,+}} \|\mathbf{S}_i - \mathbf{S}_j + h_i - h_j\|_2^2 - \beta \sum_{i \in D_+} \|\mathbf{S}_i + h_i\|_2^2, \\ \Theta(B) &= \sum_{\{i,j\} \in \mathcal{E}_L; i,j \in \mathbb{T}_{L,-}} \|\mathbf{S}_i - \mathbf{S}_j + h_i - h_j\|_2^2 - \beta \sum_{i \in D_+} \|\mathbf{S}_{r_i} + h_{r_i}\|_2^2, \\ U_i &= \sqrt{2}(\mathbf{S}_i + h_i), \quad \Theta(V_i) = \sqrt{2}(\mathbf{S}_{r_i} + h_{r_i}). \end{aligned} \quad (5.28)$$

Using a varied Cauchy-Schwartz inequality: for reflection positive measure  $\mu$  and  $A, B, U_i, V_i \in \mathcal{A}_+(\Theta)$ ,

$$\langle e^{A+\Theta(B)+\sum_i U_i \Theta(V_i)} \rangle_\mu^2 \leq \langle e^{A+\Theta(A)+\sum_i U_i \Theta(U_i)} \rangle_\mu \langle e^{B+\Theta(B)+\sum_i V_i \Theta(V_i)} \rangle_\mu, \quad (5.29)$$

we get

$$Z_{L;\beta}(h^*)^2 \leq Z_{L;\beta}(h_+^*)Z_{L;\beta}(h_-^*), \quad (5.30)$$

where

$$h_\pm^* = \begin{cases} h_i^*, & i \in \mathbb{T}_{L,\pm}; \\ h_{\Theta(i)}^*, & i \in \mathbb{T}_{L,\mp}. \end{cases} \quad (5.31)$$

By assumption,  $h_\pm^*$  are both maximizers of  $Z_{L;\beta}(h)$ . But our choice guarantees that  $\min \{N(h_\pm^*)\} < N(h^*)$ . Contradiction! Therefore  $N(h^*) = 0$  and  $h^* = 0$ .  $\square$

#### Remarks

This inequality is equivalent to the following form:

$$\left\langle \exp \left( \sum_{i \in \mathbb{T}_L} (2\beta \Delta h)_i \cdot \mathbf{S}_i \right) \right\rangle_{L;\beta} \leq \exp \left( -\frac{1}{2} \sum_{i \in \mathbb{T}_L} (2\beta \Delta h)_i \cdot h_i \right). \quad (5.32)$$

It resembles the form of integral of Gaussian measure  $\nu$  on  $\mathbb{R}^d$  with covariance matrix  $C$ :

$$\int_{\mathbb{R}^d} \exp(a \cdot x) \nu(dx) = \exp\left(\frac{1}{2} \langle a, Ca \rangle\right). \quad (5.33)$$

Here  $a = 2\beta \Delta h$  and  $C = (-2\beta \Delta)^{-1}$ . The upper bound is saturated by the Gaussian measure.

Now we come to the proof of infrared bound.

*Proof. (Infrared bound.)* As a consequence of Proposition 5.7, for any fixed  $h$ ,

$$\frac{\partial}{\partial \lambda} Z_{L;\beta}(\lambda h)|_{\lambda=0} = 0, \quad \frac{\partial^2}{\partial \lambda^2} Z_{L;\beta}(\lambda h)|_{\lambda=0} \leq 0. \quad (5.34)$$

Computation follows that the second inequality gives

$$\left\langle \left| \sum_{\{i,j\} \in \mathcal{E}_L} (\mathbf{S}_i - \mathbf{S}_j)(h_i - h_j) \right|^2 \right\rangle_{L;\beta} \leq \frac{1}{2\beta} \sum_{\{i,j\} \in \mathcal{E}_L} \|h_i - h_j\|_2^2. \quad (5.35)$$

Now fix  $p \in \mathbb{T}_L^* \setminus \{0\}$ ,  $l \in \{1, \dots, N\}$  and define  $\alpha_j = e^{ip \cdot j}$ ,  $h_j = \alpha_j \mathbf{e}_l$ . The right hand side is

$$\begin{aligned}
 \sum_{\{i,j\} \in \mathcal{E}_L} \|h_i - h_j\|_2^2 &= \sum_{\{i,j\} \in \mathcal{E}_L} (\nabla \bar{\alpha})_{ij} (\nabla \alpha)_{ij} \\
 &= \sum_{i \in \mathbb{T}_L} \bar{\alpha}_i (-\Delta \alpha)_i \\
 &= \sum_{i \in \mathbb{T}_L} \bar{\alpha}_i \alpha_i \sum_{j \sim i} (1 - e^{ip \cdot (j-i)}) \\
 &= 2d |\mathbb{T}_L| \left\{ 1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) \right\}.
 \end{aligned} \tag{5.36}$$

While the left hand side is

$$\begin{aligned}
 \sum_{\{i,j\} \in \mathcal{E}_L} (\mathbf{S}_i - \mathbf{S}_j)(h_i - h_j) &= \sum_{\{i,j\} \in \mathcal{E}_L} (\nabla S^l)_{ij} (\nabla \alpha)_{ij} \\
 &= \sum_{i \in \mathbb{T}_L} S_i^l (-\Delta \alpha)_i \\
 &= 2d \left\{ 1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) \right\} \sum_{i \in \mathbb{T}_L} S_i^l e^{ip \cdot i}.
 \end{aligned} \tag{5.37}$$

By translational invariance of  $\mu_{L;\beta}$ ,

$$\left\langle \left| \sum_{i \in \mathbb{T}_L} S_i^l e^{ip \cdot i} \right|^2 \right\rangle = \sum_{i,j \in \mathbb{T}_L} e^{ip \cdot (j-i)} \langle S_i^l S_j^l \rangle_{L;\beta} = |\mathbb{T}_L| \sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \langle S_0^l S_j^l \rangle_{L;\beta}. \tag{5.38}$$

Combining the two parts and taking a sum over  $l$ , we arrive at

$$\sum_{j \in \mathbb{T}_L} e^{ip \cdot j} \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle_{L;\beta} \leq \frac{N}{4\beta d} \left( 1 - \frac{1}{2d} \sum_{j \sim 0} \cos(p \cdot j) \right)^{-1}. \tag{5.39}$$

□



# Chapter 6

## Quantum Part I: $C^*$ -algebras and States

### 6.1 Set of observables: $C^*$ -algebras

We will try to give an algebraic formalism for quantum physics. Rather than wavefunctions, we want to start focussing on observables, which live in a  $C^*$ -algebra  $\mathcal{A}$

**Definition 6.1.** A  $C^*$ -*algebra* is a complex algebra with

1. commutative and associative addition
2. complex scalar multiplication
3. associative multiplication
4. ( $*$ -algebra) involution  $*$  :  $\mathcal{A} \rightarrow \mathcal{A}$  such that for any  $a, b \in \mathcal{A}, \lambda \in \mathbb{C}$ 
  - $(a^*)^* = a$
  - $(\lambda a)^* = \bar{\lambda} a^*$
  - $(a + b)^* = a^* + b^*$
  - $(ab)^* = b^* a^*$

elements such that  $a^* = a$  are called self-adjoint.

5. (Banach algebra) norm
  - $\|a + b\| \leq \|a\| + \|b\|$
  - $\|a\| = 0 \Rightarrow a = 0$

- $\|ab\| = \|a\| \|b\|$
  - $\|a^*\| = \|a\|$
6.  $\|a^*a\| = \|a\|^2$  ( $C^*$ -property)

**Examples 6.2.** 1. Let  $\mathcal{H}$  be a Hilbert space. For linear operators  $a : \mathcal{H} \rightarrow \mathcal{H}$  with operator norm

$$\|a\| = \sup_{0 \neq \psi \in \mathcal{H}} \frac{\|a\psi\|}{\|\psi\|}, \quad (6.1)$$

the set of bounded operators

$$\mathcal{B}(\mathcal{H}) = \{a : \mathcal{H} \rightarrow \mathcal{H} \text{ linear} \mid \|a\| < \infty\} \quad (6.2)$$

Unfortunately, at least one of the usual canonical operators  $x$  and  $p$  on  $L^2(\mathbb{R})$  with  $[x, p] = i\hbar$  is not in  $\mathcal{B}(\mathcal{H})$ . A trick is, rather than studying  $x$  and  $p$ , looking at operators  $U(a) = e^{iax}$  and  $V(b) = e^{ibp}$  for  $a, b \in \mathbb{R}$ .

Note that one can show, for every  $C^*$ -algebra  $\mathcal{A}$ , there is a Hilbert space  $\mathcal{H}$  such that  $\mathcal{A}$  is a closed sub-algebra of  $\mathcal{B}(\mathcal{H})$ . While this  $\mathcal{H}$  is constructed by Hahn-Banach theorem and is usually really, really big.

2. Again on Hilbert space  $\mathcal{H}$ . A sub-algebra  $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$  such that  $a \in \mathcal{A} \Rightarrow a^* \in \mathcal{A}$  and closed in  $\|\cdot\|$ -topology is also a  $C^*$ -algebra.
3. In the special case  $\dim \mathcal{H} = n < \infty$  (quantum information case),

$$\mathcal{B}(\mathcal{H}) = \text{Mat}(n \times n, \mathbb{C}). \quad (6.3)$$

A finite dimensional  $C^*$ -algebra  $\mathcal{A}$  is always a direct sum of  $\text{Mat}(n \times n, \mathbb{C})$  algebras.

4. Let  $X$  be a locally compact Hausdorff space. Let

$$C_0(X) = \{f : X \rightarrow \mathbb{C} : f \text{ is continuous and vanishes at } \infty\}. \quad (6.4)$$

That  $f$  vanishes at  $\infty$  means that for all  $\epsilon > 0$ , there exists compact subset  $K \subset X$  such that

$$\|f\|_{X \setminus K} < \epsilon. \quad (6.5)$$

If moreover for  $f, g \in C_0(X)$ ,  $\lambda \in \mathbb{C}$

- $(f + g)(x) = f(x) + g(x)$

- $(\lambda f)(x) = \lambda f(x)$
- $(f \cdot g)(x) = f(x) \cdot g(x)$
- $(f^*)(x) = \overline{f(x)}$
- $\|f\| = \sup_{x \in X} |f(x)| (< \infty),$

then  $C_0(X)$  is a commutative  $C^*$ -algebra, which is the classical case.

If  $\mathcal{A}$  is a commutative  $C^*$ -algebra, according to Gelfand-Naimark, there is a local compact Hausdorff space  $X(\mathcal{A})$  such that

$$\mathcal{A} \cong C_0(X(\mathcal{A})). \quad (6.6)$$

*Sketch of proof (of Gelfand-Naimark):*

- (a) For a locally compact Hausdorff space  $X$  and  $x \in X$ , let  $f \in C_0(X)$  and

$$\begin{aligned} \pi_x : C_0(X) &\rightarrow \mathbb{C}, \quad f \mapsto f(x) \\ \pi_x(f + g) &= \pi_x(f) + \pi_x(g) \\ \pi_x(f^*) &= \overline{f(x)}, \end{aligned} \quad (6.7)$$

which defines a  $*$ -homomorphism from  $C_0(X)$  to  $\mathbb{C}$ . This suggests that

$$X(\mathcal{A}) = \{ \pi : \mathcal{A} \rightarrow \mathbb{C} : \pi \text{ is a } * \text{-homomorphism.} \} \quad (6.8)$$

- (b) Topology for  $X(\mathcal{A})$  is given in terms of closure operation: for  $S \subset X(\mathcal{A})$ ,  $\bar{\cdot} : S \mapsto \bar{S}$  such that

- i.  $S \subset \bar{S}$
- ii.  $\bar{\bar{S}} = \bar{S}$
- iii.  $\bar{\emptyset} = \emptyset$
- iv.  $\bar{S}_1 \cup \bar{S}_2 = \overline{S_1 \cup S_2}$ .

Choose  $S$  to be the interval where all functions vanish:

$$\bar{S} = \bigcap \{ f^{-1}(0) : f \in C_0(X), f|_S = 0 \}. \quad (6.9)$$

Algebraically,

$$S = \{ \pi_x : \mathcal{A} \rightarrow \mathbb{C} : \pi \text{ is a } * \text{-homomorphism.} \} \quad (6.10)$$

**Remarks**

1. Unit. A  $C^*$ -algebra  $\mathcal{A}$  is not required to have a unit element  $\mathbb{1}$  such that  $\mathbb{1}a = a\mathbb{1} = a$  for all  $a$ . For example, let  $\mathcal{A} \subset C_0(X)$ . A unit function in  $\mathcal{A}$  is  $f : X \rightarrow \mathbb{C}$  such that  $f(x) = 1$  for all  $x \in X$ . While if  $X$  is compact, all functions should vanish at infinity.

But in general, if a  $C^*$ -algebra does not have a unit, you can add one through

$$\tilde{\mathcal{A}} = \mathcal{A} \oplus \mathbb{C}\mathbb{1}. \quad (6.11)$$

In the  $C_0(X)$  case, this corresponds to a 1-point compactification

$$\widetilde{C_0(X)} \ni f + \mu\mathbb{1}, \quad \pi_\infty(f + \mu\mathbb{1}) = \mu \quad (6.12)$$

and  $X = X \cup \{\infty\}$ . So when not specified, we assume a unit in our  $C^*$ -algebra.

2. Spectrum.

**Definition 6.3.** Let  $\mathcal{A}$  be a  $C^*$ -algebra and  $a \in \mathcal{A}$ . Its **spectrum** is

$$\text{spec}(a) = \{ \lambda \in \mathbb{C} : (a - \lambda\mathbb{1}) \text{ is not invertible.} \} \quad (6.13)$$

$$\text{spec}(a) \subset \overline{B_0(\|a\|)}.$$

**Definition 6.4.**  $a \in \mathcal{A}$  is **normal** if and only if  $a^*a = aa^*$ .

For  $a$  normal,

$$\|a\| = \sup \{ |\lambda| : \lambda \in \text{spec}(a) \}. \quad (6.14)$$

In general

$$\|a\| = \sqrt{\|a\|^2} = \sqrt{\|aa^*\|} \quad (6.15)$$

$aa^*$  is not only normal, but also self-adjoint. Thus all norms are determined by the spectrums. Thus there cannot be two different  $C^*$ -norms on the same  $C^*$ -algebra. For  $C_0(X) \ni f : X \rightarrow \mathbb{C}$ ,  $(f - \lambda)^{-1}(x) = 1/(f(x) - \lambda)$  exists if  $f(x) \neq \lambda$ .

## 3. Positivity.

**Definition 6.5.**  $a \in \mathcal{A}$  is **positive** if and only if  $\text{spec}(a) \in \mathbb{R}_{\geq 0}$ .

**Proposition 6.6.**  $a$  is positive if and only if  $\exists b \in \mathcal{A}$  such that  $a = b^*b$ .

 4. For a general  $\mathcal{A} \ni a$  normal, there is a sub  $C^*$ -algebra generated by polynomials of  $a$  and  $a^*$ :

$$N := \overline{\{\text{poly}(a, a^*)\}} \subset \mathcal{A}. \quad (6.16)$$

This sub-algebra is now commutative. Thus elements of  $N$  are functions  $\mathcal{A} \supset N \ni f : X(N) \rightarrow \mathbb{C}$ . Let  $g : \text{spec}(f) \rightarrow \mathbb{C}$ , then

$$\mathcal{A} \supset N \ni g \circ f : X(N) \xrightarrow{f} \text{spec}(f) \xrightarrow{g} \mathbb{C}, \quad (6.17)$$

which is usually denoted by  $g(f) \in \mathcal{A}$ , is called *spectral calculus*. For instance,  $\sin(a)$ .

 5.  $C^*$ -homomorphism.

**Definition 6.7.** For two  $C^*$ -algebras  $\mathcal{A}$  and  $\mathcal{B}$ , linear maps  $\Phi : \mathcal{A} \rightarrow \mathcal{B}$  are called  **$C^*$ -homomorphisms** if

$$\begin{aligned} \Phi(ab) &= \Phi(a)\Phi(b) \\ \Phi(a)^* &= \Phi(a^*) \end{aligned} \quad (6.18)$$

for all  $a, b \in \mathcal{A}$ .

**Proposition 6.8.** For every  $C^*$ -homomorphism  $\Phi : \mathcal{A} \rightarrow \mathcal{A}$ ,

$$\|\Phi(a)\| \leq \|a\|. \quad (6.19)$$

*Proof.* Consider  $\text{spec}(a)$  for a normal element  $a \in \mathcal{A}$ . If  $\lambda$  is not in  $\text{spec}(a)$ , then we can map its inverse with  $\Phi$ :

$$\Phi\left(\frac{1}{a - \lambda \mathbb{1}}\right) = \frac{1}{\Phi(a) - \lambda \mathbb{1}}. \quad (6.20)$$

Thus  $\lambda \notin \text{spec}(\Phi(a))$  as well.  $\square$

If  $\Phi$  is invertible as a  $C^*$ -norm, then it has to preserve the norm.

## 6.2 States

A *state*  $\omega$  of a system is determined by the preparation, and should assign an expectation value for each  $a \in \mathcal{A}$ .

**Definition 6.9.** A *state* is a linear map

$$\omega : \mathcal{A} \rightarrow \mathbb{C} \quad (6.21)$$

such that

- $\omega$  is positive:  $\omega(b^*b) \geq 0$  for  $b \neq 0$ ;
- $\omega(\mathbb{1}) = 1$ , or equivalently  $\|\omega\| = \sup_{a \neq 0} |\omega(a)| / \|a\| = 1$ .

### Notes

The variance  $\text{Var}(a) = \omega(a^2) - \omega(a)^2$  is already encoded in  $\omega$  and  $\omega$  gives all moments of the probability distribution.

**Examples 6.10.** 1.  $\mathcal{A} = \text{Mat}(n \times n, \mathbb{C})$ . In general for a state  $\omega$  and  $a \in \mathcal{A} = (a)_{ij}$

- *Linearity:*

$$\omega(a) = \sum_{ij} \rho_{ji} a_{ij} = \text{tr}(\rho a) \quad (6.22)$$

for some  $\rho \in \text{Mat}(n \times n, \mathbb{C})$ .

- *Normalization:*  $1 = \omega(\mathbb{1}) = \text{tr}(\rho \mathbb{1}) \text{tr} \rho$ .
- *Positivity:*

$$\begin{aligned} \omega(b^*b) &= \text{tr}(\rho b^*b) = \text{tr}(b \rho b^*) \\ &= \sum_i \left( \sum_j b_{ij} \rho_{jk} b_{ik}^* \right) \geq 0 \end{aligned} \quad (6.23)$$

for any  $b$ , and hence

$$\langle v, \rho v \rangle \geq 0 \quad (6.24)$$

for any vector  $v \in \mathbb{C}^n$ . That is,  $\rho$  is positive.

So  $\rho$  is a density matrix.

2.  $\mathcal{A} = \mathcal{B}(\mathcal{H})$ . States  $\omega_\rho$  are such that  $\omega_\rho = \text{tr}(\rho a)$  with density operators  $\rho$  of the trace class ( $\rho \in \mathcal{S}^1(\mathcal{H})$ ,  $\text{tr}|\rho| < \infty$ ) and  $\text{tr}\rho = 1$ ,  $\rho \geq 1$ . For instance,  $\rho = |\psi\rangle\langle\psi|$  with  $|\psi\rangle \in \mathcal{H}$ .
3.  $\mathcal{A} = C_0(X)$ . For  $\mathcal{A} \ni f : X \rightarrow \mathbb{C}$ ,  $x \in X$ , we can choose

$$\omega_x(f) = f(x). \quad (6.25)$$

All points (in the phase space) correspond to states.

More generally, we can choose a probability distribution  $d\mu$  on  $X$  (the phase space) and

$$\omega(f) = \int_X f d\mu \quad (6.26)$$

also gives rise to a state.

#### Notes

In the infinite case, almost all states are density operators. The leftovers are hard to illustrate and we pretend density operators to be the whole story.

**Definition 6.11.** The set of all states for a  $C^*$ -algebra is denoted  $\mathcal{E}(\mathcal{A})$ .

For  $\omega_0, \omega_1 \in \mathcal{E}(\mathcal{A})$  and  $0 \leq \lambda \leq 1$ ,

$$\omega_\lambda = (1 - \lambda)\omega_0 + \lambda\omega_1 \quad (6.27)$$

is also in  $\mathcal{E}(\mathcal{A})$ , which is called a *mixture* of  $\omega_0$  and  $\omega_1$ . Therefore  $\mathcal{E}(\mathcal{A})$  is a *convex* space.

**Definition 6.12.** The extremal points  $\omega$  such that

$$\omega = (1 - \lambda)\omega_0 + \lambda\omega_1 \quad (6.28)$$

implies  $\lambda = 0$  or  $\lambda = 1$  or  $\omega_0 = \omega_1$  are called **pure states**.

- In the finite dimensional case,  $\rho$  is a pure state if and only if only one of its eigenvalue is 1, or  $\rho = |\psi\rangle\langle\psi|$  for some  $|\psi\rangle \in \mathcal{H}$ .
- In the classical case, points  $x_0 \in X$ , or  $d\mu = \delta_{x-x_0}$  are pure states.

### Notes

Pure states are on the boundary of  $\mathcal{E}(\mathcal{A})$ . Every state can be written as a mixture of pure states. In general it is not unique.

**Definition 6.13.** A convex set such that the pure state decomposition is always unique is called a **simplex**.

- In the classical case,  $\mathcal{E}(C_0(X))$  is a simplex:

$$\omega(f) = \int f(x)\rho(x)dx = \int \rho(y) \left[ \int f(x)\delta_{x-y}dx \right] dy. \quad (6.29)$$

- In the quantum case,  $\mathcal{E}(\mathcal{B}(\mathcal{H}))$  is not a simplex.

## 6.3 GNS construction

**Definition 6.14.** A **representation** of a  $C^*$ -algebra  $\mathcal{A}$  is a Hilbert space  $\mathcal{H}$  and a  $C^*$ -homomorphism

$$\pi : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H}). \quad (6.30)$$

**Definition 6.15.** Two representations  $\pi_{1,2} : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H}_{1,2})$  are called **unitarily equivalent** if there is a unitary map  $U : \mathcal{H}_1 \rightarrow \mathcal{H}_2$  such that for all  $a \in \mathcal{A}$ ,

$$U \circ \pi_1(a) = \pi_2 \circ U(a). \quad (6.31)$$

The representations can be constructed from states:

**Theorem 6.16. Gelfand–Naimark–Segal (GNS) construction.** Let  $\mathcal{A}$  be a  $C^*$ -algebra and  $\omega$  is a state. Then there is a triple  $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$  of Hilbert space  $\mathcal{H}_\omega$ , representation  $\pi_\omega : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H}_\omega)$  and  $\Omega_\omega \in \mathcal{H}_\omega$  with

$$\|\Omega_\omega\| = 1, \quad \omega(a) = \langle \Omega_\omega, \pi(a)\Omega_\omega \rangle. \quad (6.32)$$

Moreover,  $\Omega_\omega$  is **cyclic**:  $\pi(\mathcal{A})\Omega_\omega$  is dense in  $\mathcal{H}_\omega$ .  
This triple is unique up to unitary equivalence.

*Proof.* The proof is constructive.



1. Let  $J_\omega = \{a \in \mathcal{A} : \omega(a^*a) = 0\}$ . Observe that  $J_\omega$  is a left ideal:

$$a \in \mathcal{A}, j \in J_\omega \Rightarrow aj \in J_\omega \quad (6.33)$$

since

$$\begin{aligned} |\omega((aj)^*(aj))|^2 &= |\omega(\underbrace{j^*}_u \underbrace{a^*aj}_v)|^2 \\ &\leq \underbrace{\omega(u^*u)}_{=\omega(j^*j)=0} \omega(v^*v) \text{ (Cauchy-Schwartz)} \\ &= 0. \end{aligned} \quad (6.34)$$

2. Let  $\mathcal{H}_0 = \mathcal{A}/J_\omega$ . That is, for  $a, b \in \mathcal{A}$ , the equivalent classes  $[a] = [b] \Leftrightarrow a - b \in J_\omega$ . Define the map  $\pi_0 : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H}_0)$  by

$$\pi_0(a)[b] = [ab]. \quad (6.35)$$

It is well defined since

$$\pi_0(a)[b + j] = [ab + aj] = [ab] \quad (6.36)$$

for  $j \in J_\omega$ .

3. Define a scalar product on  $\mathcal{H}_0$ :

$$\langle [a], [b] \rangle = \omega(a^*b). \quad (6.37)$$

It is positive definite as  $\omega$  is positive semi-definite.

4.  $\mathcal{H}_\omega := \overline{\mathcal{H}_0}$  equipped with the norm above is a Hilbert space.  $\pi_\omega$  can be extended from  $\pi_0$  by continuity since  $\mathcal{H}_0$  is a dense subset of  $\mathcal{H}_\omega$ .

5. Take  $\Omega_\omega = [\mathbb{1}]$ . We can check that

$$\langle \Omega_\omega, \pi_\omega(a)\Omega_\omega \rangle = \langle [\mathbb{1}], [a\mathbb{1}] \rangle = \omega(\mathbb{1}^*a\mathbb{1}) = \omega(a) \quad (6.38)$$

and

$$\pi_\omega(\mathcal{A})[\mathbb{1}] = [\mathcal{A}] = \mathcal{H}_0 \quad (6.39)$$

is dense in  $\mathcal{H}_\omega$ .

6. The uniqueness of the triple is essentially determined by

$$\omega(a) = \langle \Omega_\omega, \pi(a)\Omega_\omega \rangle. \quad (6.40)$$

Thus any two representations are related by a unitary map.

□

**Definition 6.17.** An  $\omega$ -**normal** state is such that it can be written as a density operator in the GNS Hilbert space of  $\omega$ .

**How much does the GNS triple  $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$  depend on the state?**

- Start from a state  $\omega$  and do the GNS representation. Then take  $\psi \in \mathcal{H}_\omega$  with  $\psi \neq 0$ . Define a new state

$$\omega_\psi(a) = \frac{\langle \psi, \pi_\omega(a)\psi \rangle}{\|\psi\|^2}. \quad (6.41)$$

The corresponding GNS representation is unitarily equivalent to the first!

- If we take instead a density operator  $\rho \in \mathcal{S}^1(\mathcal{H}_\omega)$  and choose

$$\omega_\rho = \text{tr}_{\mathcal{H}_\omega}(\rho \pi(a)), \quad (6.42)$$

this yields a direct sum of several copies of  $\mathcal{H}_\omega$ . Note that if  $\rho$  is a mixed state, the GNS construction gives rise to a vector state  $\Omega_{\omega_\rho}$ , but

$$\pi_{\omega_\rho}(\mathcal{A}) \subsetneq \mathcal{B}(\mathcal{H}_{\omega_\rho}). \quad (6.43)$$

- Recall that in quantum mechanics we write the *Weyl* operators instead of the position and moment operators:

$$U(a) = e^{iax}, \quad V(b) = e^{ibp} \quad (6.44)$$

such that

$$\begin{aligned} U(a)U(b) &= U(a+b) \\ V(a)V(b) &= V(a+b) \\ U(a)V(b) &= V(b)U(a)e^{iab} \end{aligned} \quad (6.45)$$

**Theorem 6.18. Stone-von Neumann.** *There is a unique (up to unitary equivalence) representation for which*

$$\mathbb{R} \rightarrow \mathcal{H}, \quad a \mapsto \pi(U(a))\psi \quad (6.46)$$

*is continuous for every  $\psi$  and similarly for  $b \mapsto \pi(V(b))\psi$ .*

- In general the state does matter in the GNS construction. See B.4 in appendix.

## 6.4 Symmetries

The symmetries of a  $C^*$ -algebra  $\mathcal{A}$  are its automorphisms  $\alpha \in \text{Aut}(\mathcal{A})$ . In particular for  $a, b \in \mathcal{A}$ ,

$$\alpha(ab) = \alpha(a)\alpha(b), \quad \alpha(a^*) = \alpha(a)^*. \quad (6.47)$$

In a representation, there should be a unitary operator  $U_\alpha \in U(\mathcal{H})$  that implements  $\alpha$ :

$$U_\alpha \pi(a) U_\alpha^* = \pi(\alpha(a)). \quad (6.48)$$

### Notes

1. In general,  $U_\alpha$  does not necessarily exist. If it exists, the choice is still not unique; adding an additional phase  $e^{i\phi}$ ,  $\phi \in \mathbb{R}$  will still do the job.
2. Now the group law fails at most by a phase:

$$U_{\alpha_1} U_{\alpha_2} = U_{\alpha_1 \alpha_2} e^{i\phi_{\alpha_1 \alpha_2}}. \quad (6.49)$$

Can we choose the phases such that  $\phi_{\alpha_1 \alpha_2} = 0$  for all  $\alpha_{1,2}$ ? The answer is still no. It's measured by the second group cohomology of the automorphism group. Physicists call this *anomaly*.

3. If  $\omega$  is symmetric, i.e.,

$$\omega(a) = \omega(\alpha(a)), \quad \forall a \in \mathcal{A}, \quad (6.50)$$

or  $\omega = \omega \circ \alpha$ , the situation is better.

$$U_\alpha[a] = [\alpha(a)] \quad (6.51)$$

defines an operator on  $\mathcal{H}_\omega$ . It is unitary since

$$\begin{aligned} \langle U_\alpha[a], U_\alpha[b] \rangle &= \langle [\alpha(a)], [\alpha(b)] \rangle \\ &= \omega(\alpha(a)^* \alpha(b)) \\ &= \omega(\alpha(a^* b)) \\ &= \omega(a^* b) = \langle [a], [b] \rangle. \end{aligned} \quad (6.52)$$

In this definition, the group law is automatically satisfied.

# Chapter 7

## Quantum Part II: Equilibrium: KMS States

In this chapter, we discuss thermal equilibrium states, namely the *Kubo–Martin–Schwinger (KMS) states*.

### 7.1 Definition

**Definition 7.1.**  $(\mathcal{A}, \tau)$  is called a  *$C^*$ -dynamical system* if  $\mathcal{A}$  is a  $C^*$ -algebra and  $\tau : \mathbb{R} \rightarrow \text{Aut}(\mathcal{A})$  is a group homomorphism that is strongly continuous:

$$\tau_{t+\epsilon}(a) \xrightarrow{\epsilon \rightarrow 0} \tau_t(a), \quad \forall a \in \mathcal{A}. \quad (7.1)$$

**Examples 7.2.** Let  $\mathcal{A} = \text{Mat}(n \times n, \mathbb{C})$ ,  $\mathcal{H} \in \mathcal{A}$  that is self-adjoint and

$$\tau_t(a) = e^{it\mathcal{H}} a e^{-it\mathcal{H}}. \quad (7.2)$$

Then  $(\mathcal{A}, \tau)$  is a  $C^*$ -dynamical system. In this case, we know that the thermal states are Gibbs states

$$\omega_\beta(a) = \frac{\text{tr}(e^{-\beta\mathcal{H}} a)}{\text{tr}(e^{-\beta\mathcal{H}})}. \quad (7.3)$$

#### Notes

Our goal is to generalize this to more  $C^*$ -algebras. There are several obstacles:

- $\mathcal{H}$  does not exist in general for infinite systems.
- $e^{-\beta\mathcal{H}}$  may not be in the trace class.

- The trace requires a Hilbert space.

Here we can do a quick calculation:

$$\begin{aligned}
 \omega_\beta(ab) &= \frac{1}{\text{tr}(e^{-\beta H})} \text{tr}(e^{-\beta H} ab) \\
 &= \frac{1}{\text{tr}(e^{-\beta H})} \text{tr}(e^{-\beta H} a e^{\beta H} e^{-\beta H} b) \\
 &= \frac{1}{\text{tr}(e^{-\beta H})} \text{tr}(e^{-\beta H} b e^{-\beta H} e^{\beta H} a e^{\beta H}) \\
 &= \frac{1}{\text{tr}(e^{-\beta H})} \text{tr}(e^{-\beta H} b \tau_{i\beta}(a)) \\
 &= \omega_\beta(b \tau_{i\beta}(a)).
 \end{aligned} \tag{7.4}$$

This will be our defining equation.

We need a technical step. Let  $(\mathcal{A}, \tau)$  be a  $C^*$ -dynamical system and define

$$\delta_t : \mathcal{A} \rightarrow \mathcal{A}, \quad \delta_t(a) = \frac{\tau_t(a) - a}{t}. \tag{7.5}$$

Let

$$D(\delta) = \{ a \in \mathcal{A} : \lim_{\epsilon \rightarrow 0^+} \delta_\epsilon(a) \text{ exists} \}. \tag{7.6}$$

Finally

$$\delta : D(\delta) \rightarrow \mathcal{A}, \quad \delta(a) = \lim_{\epsilon \rightarrow 0^+} \delta_\epsilon(a). \tag{7.7}$$

**Proposition 7.3.**  *$\delta$  is a closed densely defined map such that*

- $\mathbb{1} \in D(\delta)$  and  $\delta(\mathbb{1}) = 0$ .
- $\delta(ab) = \delta(a)b + a\delta(b)$ .
- $\delta(a^*) = \delta(a)^*$ .

This is functional analysis stuff and will not be proved here.

There is also an opposite direction. Starting from the derivation  $\delta$ ,  $a \in \mathcal{A}$  is called *analytic* if  $a \in D(\delta^n)$  for all  $n \in \mathbb{N}$  and

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} \|\delta^n(a)\| < \infty, \quad \forall 0 \leq t < t_a. \tag{7.8}$$

**Theorem 7.4.** *Let  $\mathcal{A}$  be a  $C^*$ -algebra with a unit. A densely defined, closed operator  $\delta$  on  $\mathcal{A}$  generates a strongly continuous group of  $*$ -automorphisms if and only if*

- $\delta$  is a  $*$ -automorphism.
- $\delta$  has a dense set of analytic elements.
- $\|a + \lambda\delta(a)\| \geq \|a\|$ ,  $\forall \lambda \in \mathbb{R}$ ,  $A \in D(\delta)$ .

Again this will not be proved. Before we move on to KMS states, we need to first do analytic continuation of  $\tau$ .

**Definition 7.5.**  *$a \in \mathcal{A}$  is called an **analytic element** if and only if  $t \mapsto \tau_t(a)$  can be analytically continued to all  $t \in \mathbb{C}$ .*

**Theorem 7.6.** *The analytic elements are dense in  $\mathcal{A}$ .*

*Proof.* For  $a \in \mathcal{A}$  and  $n \in \mathbb{N}$ , let

$$a_n = \sqrt{\frac{n}{\pi}} \int_{\mathbb{R}} \tau_t(a) e^{-nt^2} dt. \quad (7.9)$$

1.  $\tau_z(a_n)$  is analytic in  $z \in \mathbb{C}$ :

$$\begin{aligned} \|\tau_z(a_n)\| &= \left\| \sqrt{\frac{n}{\pi}} \int_{\mathbb{R}} \tau_t(a) e^{-n(t-z)^2} dt \right\| \\ &\leq \|a\| e^{-n(\Im z)^2}. \end{aligned} \quad (7.10)$$

2. By dominated convergence, it is also easy to check  $a_n \in D(\delta^n)$ , and that  $a_n$  is analytic for  $\delta$ .
3.  $\lim_{n \rightarrow \infty} a_n = a$  and hence the analytic elements are dense.

□

**Definition 7.7.** *Let  $(\mathcal{A}, \tau)$  be a  $C^*$ -dynamical system. A state  $\omega : \mathcal{A} \rightarrow \mathbb{C}$  is called a  $(\tau, \beta)$ -**KMS state** if for all  $a, b \in \mathcal{A}$  there is a function  $F(a, b, z)$  that is analytic in*

$$S_\beta = \{ z \in \mathbb{C} : 0 \leq \Im z < \beta \}, \quad (7.11)$$

*continuous on  $\overline{S_\beta}$  and*

$$\begin{aligned} F(a, b, t) &= \omega(a\tau_t(b)), \quad t \in \mathbb{R} \\ F(a, b, t + i\beta) &= \omega(\tau_t(b), a). \end{aligned} \quad (7.12)$$

We have shown that in the finite dimensional case, the Gibbs state is a KMS state and they are indeed equivalent. Moreover, KMS state is a good generalization when the Gibbs states is not available.

### Properties of KMS states

**Theorem 7.8.** *Let  $(\mathcal{A}, \tau)$  be a  $C^*$ -dynamical system.  $\omega : \mathcal{A} \rightarrow \mathbb{C}$  is  $(\beta, \tau)$ -KMS if and only if*

$$\omega(ab) = \omega(b\tau_{i\beta}(a)) \quad (7.13)$$

for all  $a, b \in \mathcal{A}$  and  $a$  being analytic.

**Proposition 7.9.** *KMS states are **stationary**, i.e.,*

$$\omega = \omega \circ \tau_t, \quad \forall t \in \mathbb{R}. \quad (7.14)$$

*Proof.* For an analytic element  $a \in \mathcal{A}$ , consider  $g : z \mapsto \omega(\tau_z(a))$ . Then

$$g(z + i\beta) = \omega(\mathbb{1}\tau_{z+i\beta}(a)) = \omega(\tau_z(a)\mathbb{1}) = g(z). \quad (7.15)$$

Hence  $g$  is periodic in  $\mathbb{C}$  with period  $i\beta$ . Decompose  $z = x + iy$ , where  $x, y \in \mathbb{R}$ , and

$$\begin{aligned} |g(z)| &= |\omega(\tau_x \circ \tau_{iy}(a))| \\ &\leq \|\tau_x \circ \tau_{iy}(a)\| \\ &= \|\tau_{iy}(a)\| \\ &\leq \sum_{y \in [0, \beta]} \|\tau_{iy}(a)\| < \infty. \end{aligned} \quad (7.16)$$

$g$  is a bounded, holomorphic complex function, and therefore it is a constant. As a result,

$$\omega(\tau_z(a)) = g(z) = g(0) = \omega(a). \quad (7.17)$$

□

#### Notes

In the GNS construction,  $\tau_t$  is implemented by  $U_t \in U(\mathcal{H}_\omega)$ , where  $U_t = e^{it\mathcal{H}_\omega}$  for a Hamiltonian in GNS representation such that

$$\mathcal{H}_\omega \Omega_\omega = 0. \quad (7.18)$$

## 7.2 Energy entropy balance inequality

### Preparations

- (*Jensen's inequality.*) Let  $\mu$  be a probability measure on  $\Omega$ ,  $g : \Omega \rightarrow \mathbb{R}$  be a measurable function and  $f : \mathbb{R} \rightarrow \mathbb{R}$  a convex function. Then

$$\int_{\Omega} f \circ g d\mu \geq f\left(\int_{\Omega} g d\mu\right). \quad (7.19)$$

- (*Spectral theorem for self-adjoint operators.*) For a self-adjoint operator  $a$ ,

$$a = \int \lambda dP(\lambda), \quad (7.20)$$

where  $P(\lambda)$  is a projection valued measure. Moreover,

$$f(a) = \int f(\lambda) dP(\lambda) \quad (7.21)$$

for a smooth function  $f$ .

**Theorem 7.10.** (*Energy entropy balance (EEB) inequality.*) A state  $\omega$  is a KMS state if and only if for all  $a \in D(\delta)$

$$-i\beta\omega(a^*\delta(a)) \geq \omega(a^*a) \ln \frac{\omega(a^*a)}{\omega(aa^*)}. \quad (7.22)$$

### Remarks

- In the matrix case and in GNS representation, the left hand side is

$$-i\beta \langle \Omega_{\omega} | a^* i[H_{\omega}, a] \Omega_{\omega} \rangle = \beta \langle \Omega_{\omega}, a^* H_{\omega} a \Omega_{\omega} \rangle = \beta \langle H_{\omega} \rangle_{a\Omega_{\omega}}. \quad (7.23)$$

While the right hand side looks like a (relative) entropy.

- The inequality survives in limits.

**Corollary 7.11.** Let  $\tau^n$  be a family of time evolutions and for all  $a \in \mathcal{A}$ ,

$$\lim_{n \rightarrow \infty} \tau_t^n(a) = \tau_t(a) \quad (7.24)$$

for some time evolution  $\tau$ . There is also a family of KMS states  $\omega^n$  for  $\tau^n$ . Due to Banach-Alaoglu, the set of states is weak\*-compact.



*There are accumulation points of the  $\omega^n$  and let  $\omega$  be one of them. Then  $\omega$  is a KMS state.*

*Proof.* We only prove  $\text{KMS} \Rightarrow \text{EEB}$  inequality here.

1. Let  $f$  be the Fourier transformation of  $\check{f} \in C_0^\infty(\mathbb{R})$  (a test function in  $\mathbb{R}$  with particularly a compact support). Then  $f$  is analytic and

$$|f(z)| \leq c_n \frac{e^{R|\Im z|}}{1 + |z|^n} \quad (7.25)$$

for constants  $R, c_n$ .

For analytic  $a$ , define

$$\tau_f(a) := \int f(t) \tau_t(a) dt \in D(\delta). \quad (7.26)$$

Then (use the notations in GNS representation, omit the subscripts  $\omega$ )

$$\begin{aligned} \omega(a^* \tau_f(a)) &= \int f(t) \langle \pi(a) \Omega, e^{iHt} \pi(a) \Omega \rangle dt \\ &= \int \int f(t) e^{i\lambda t} \underbrace{\langle \pi(a) \Omega, dP(\lambda) \pi(a) \Omega \rangle}_{d\mu_a(\lambda)} dt \\ &= \int \check{f}(\lambda) d\mu_a(\lambda). \end{aligned} \quad (7.27)$$

Similarly  $\omega(\tau_f(a) a^*) = \int \check{f}(\lambda) d\nu_a(\lambda)$ , where

$$d\nu_a(\lambda) = \langle \pi(a^*) \Omega, dP(-\lambda) \pi(a^*) \Omega \rangle. \quad (7.28)$$

Apply the KMS condition:

$$\begin{aligned} \omega(a^* \tau_f(a)) &= \int f(t + i\beta) \omega(\tau_t(a) a^*) dt \\ &= \int \check{f}(\lambda) e^{\beta\lambda} d\nu_a(\lambda). \end{aligned} \quad (7.29)$$

Since this holds for all  $\check{f}$ , the measures should be the same:

$$d\mu_a(\lambda) = e^{\beta\lambda} d\nu_a(\lambda). \quad (7.30)$$

2. Now

$$\begin{aligned}
 \exp\left(\beta \frac{\langle \pi(a)\Omega, H\pi(a)\Omega \rangle}{\langle \pi(a)\Omega, \pi(a)\Omega \rangle}\right) &= \exp\left(\frac{\int \beta \lambda d\mu_a(\lambda)}{\int d\mu_a(\lambda)}\right) \\
 &\leq \frac{\int \exp(-\lambda\beta) d\mu_a(\lambda)}{\int d\mu_a(\lambda)} \quad (\text{Jensen's inequality}) \\
 &= \frac{\int d\nu_a(\lambda)}{\int d\mu_a(\lambda)} = \frac{\omega(a^*a)}{\omega(aa^*)}.
 \end{aligned} \tag{7.31}$$

Take a logarithm on both sides and we get the EEB inequality.

□

**Second law of thermodynamics.** For unitary elements  $U$  such that  $UU^* = \mathbb{1}$ , EEB says

$$-i\beta\omega(U^*\delta(U)) \geq 0. \tag{7.32}$$

Consider that we start from a KMS state  $|\Omega\rangle$  and move to a new state with a unitary operator  $U$ . Then the energy difference is

$$\begin{aligned}
 \langle U\Omega, HU\Omega \rangle - \langle \Omega, H\Omega \rangle &= \langle \Omega, U^*HU\Omega \rangle - \langle \Omega, H\Omega \rangle \\
 &= \langle \Omega, U^*[H, U]\Omega \rangle \\
 &= -i\omega(U^*\delta(U)) \geq 0.
 \end{aligned} \tag{7.33}$$

So we cannot extract energy from an equilibrium state with unitary (cyclic) operations.

**Carnot process.** A Carnot machine contains two parts: a hot reservoir 1 and a cold reservoir 2. Initially the combined the time evolution is  $\tau^1 \otimes \tau^2$  and its generators are

$$\delta_1 \otimes \mathbb{1}_2 \text{ and } \mathbb{1}_1 \otimes \delta_2. \tag{7.34}$$

Define

$$\delta = \beta_1 \delta_1 \otimes \mathbb{1}_2 + \beta_2 \mathbb{1}_1 \otimes \delta_2. \tag{7.35}$$

This generates a time evolution and let  $\omega$  be the corresponding KMS state with  $\beta = 1$ . After a process, the energy differences are

$$\begin{aligned}
 Q_1 &= -i\omega(U^*(\delta_1 \otimes \mathbb{1}_2)U), \\
 Q_2 &= -i\omega(U^*(\mathbb{1}_1 \otimes \delta_2)U).
 \end{aligned} \tag{7.36}$$

Since  $\omega$  is passive,

$$0 \leq -i\omega(U^*\delta U) = \beta_1 Q_1 + \beta_2 Q_2 = \frac{Q_1}{T_1} + \frac{Q_2}{T_2}. \quad (7.37)$$

For  $W = Q_1 + Q_2$ , where  $Q_1 > 0$ ,  $Q_2 < 0$ , we get

$$\frac{W}{Q_1} \leq 1 - \frac{T_2}{T_1}, \quad (7.38)$$

which is the efficiency of a Carnot engine.

### 7.3 Passivity and stability

**Passivity.** Passivity is defined from above.

**Definition 7.12.** A state for which for all unitaries  $U$  Eq.(7.32) holds is called *passive*.

Note that passive states are not necessarily KMS states (there is no temperature in the definition). Now start from a state  $\omega$ . Look at  $\pi_\omega(\mathcal{A}) \subset \mathcal{B}(\mathcal{H}_\omega)$ . Its commutant is

$$\pi_\omega(\mathcal{A})' = \{a \in \mathcal{B}(\mathcal{H}) : [a, \pi_\omega(\mathcal{A})] = 0\} \quad (7.39)$$

and  $\pi_\omega(\mathcal{A})'' \supset \pi_\omega(\mathcal{A})$ . In fact  $\pi_\omega(\mathcal{A})''$  is the weak closure of  $\pi_\omega(\mathcal{A})$ ; a really close sub-algebra of  $\mathcal{B}(\mathcal{H})$  is called a von Neumann algebra. The *center*

$$Z(\pi_\omega(\mathcal{A})) := \pi_\omega(\mathcal{A})' \cap \pi_\omega(\mathcal{A})'' \quad (7.40)$$

contains elements in the von Neumann algebra that commute with everything. They are also called *sharp observables*.

**Definition 7.13.** A von Neumann algebra for which  $Z = \mathbb{C}\mathbf{1}$  is called a **factor**. A state  $\omega$  for which  $\pi_\omega(\mathcal{A})''$  is a factor is called a **factor state** or a **primary state**.

**Theorem 7.14.** A factor state which is completely passive ( $\otimes^n \omega$  is passive for  $\otimes^n \mathcal{A}$ ) for all  $n$  is a KMS state.

**Stability.** We want to perturb our system by a (local) perturbation  $V = V^* \in \mathcal{A}$ . The new generator of perturbed time evolution is

$$\delta^V = \delta^0 + i[V, \cdot] \quad (7.41)$$

and  $D(\delta^V) = D(\delta^0)$ . We can integrate the time evolution by the *Duhamel's formula*:

$$\tau_t^V(a) = \tau_t^0(a) + \int_0^t \tau_{t-s}(i[V, a])ds \quad (7.42)$$

**Theorem 7.15. (*Structural stability.*)** *Let  $\omega$  be a  $\tau^0$ -KMS state. For every self-adjoint perturbation  $V \in \mathcal{A}$  there is a  $\tau^V$ -KMS state  $\omega^V$  with*

1.  $\omega \mapsto \omega^V$  is a bijection.
2.  $\omega^V$  is  $\omega$ -normal.
3.  $\exists c > 0$  such that  $\|\omega - \omega^V\| \leq c\|V\|$ .

The proof is not given, but essentially we need

$$\omega^V(a) = \omega(e^{-\beta V} A). \quad (7.43)$$

**Corollary 7.16.** *We cannot induce a **phase transition** by a local perturbation.*

**Theorem 7.17. (*Dynamical stability.*)** *For a self-adjoint  $V$  and  $\tau^V$ -KMS state  $\omega^V$ , consider the state  $\omega^V \circ \tau_t^0$  for every  $t$ . By Banach-Alaoglu, there is an accumulation point  $\tilde{\omega}$  for  $t \rightarrow \infty$ . If*

$$\lim_{t \rightarrow \infty} \|[V, \tau_t^0(a)]\| = 0 \quad \forall a \in \mathcal{A}, \quad (7.44)$$

*then  $\tilde{\omega}$  is a  $\tau^0$ -KMS state.*

*Proof.*

$$\begin{aligned} \tilde{\omega}(a^*a) \ln \frac{\tilde{\omega}(a^*a)}{\tilde{\omega}(aa^*)} &\leq \liminf_{t \rightarrow \infty} \omega \circ \tau_t^0(a^*a) \ln \frac{\omega \circ \tau_t^0(a^*a)}{\omega \circ \tau_t^0(aa^*)} \\ &= \liminf_{t \rightarrow \infty} \omega^V(\tau_t^0(a)^* \tau_t^0(a)) \ln \frac{\omega^V(\tau_t^0(a)^* \tau_t^0(a))}{\omega^V(\tau_t^0(a) \tau_t^0(a)^*)} \\ &\leq \liminf_{t \rightarrow \infty} -i\beta \omega^V(\tau_t^0(a)^* \delta^V(\tau_t^0(a))) \\ &= \liminf_{t \rightarrow \infty} -i\beta \omega^V \left( \tau_t^0(a)^* (\delta^0(\tau_t^0(a)) + \underbrace{i[V, \tau_t^0(a)]}_{=0}) \right) \\ &= -i\beta \tilde{\omega} \tau_t^0(a^* \delta(a)). \end{aligned} \quad (7.45)$$

The first  $\leq$  sign comes from the lower semi-continuity of  $u, v \mapsto u \log(u/v)$  and the second one is EEB inequality.  $\square$

### Notes

We did not show the existence of the limit (only the accumulation point instead). It can be shown that if, for example,  $t \mapsto \omega([V, \tau_t^0(a)])$  is integrable:

$$\int_{\mathbb{R}} dt |\omega([V, \tau_t^0(a)])| < \infty, \quad (7.46)$$

there will be a unique limit.

## 7.4 On the set of KMS states

Fix the  $C^*$ -dynamical system  $(\mathcal{A}, \tau)$  and denote the set of KMS states at temperature  $\beta$  by  $S_\beta(\mathcal{A})$ .

**Theorem 7.18.** *For  $\beta > 0$ ,*

1.  $S_\beta(\mathcal{A})$  is convex and weak  $*$ -compact.
2. For  $\omega \in S_\beta(\mathcal{A})$ , in the GNS construction,  $\omega$  can be extended to  $\pi_\omega(\mathcal{A})''$  (by continuity) and is still KMS.
3.  $\omega \in S_\beta(\mathcal{A})$  is an extremal point if and only if it is a factor state. And if  $\omega'$  is an  $\omega$ -normal, extremal KMS state, then  $\omega = \omega'$ .
4. The center  $\pi_\omega(\mathcal{A})' \cap \pi_\omega(\mathcal{A})''$  consists of time invariant elements.
5.  $S_\beta(\mathcal{A})$  is a simplex: IF  $\omega \in S_\beta(\mathcal{A})$  such that the GNS Hilbert space is separable, there is a unique probability measure  $\mu$  on  $S_\beta(\mathcal{A})$ , which is concentrated on the extremal points such that  $\omega = \int_{S_\beta(\mathcal{A})} \nu d\mu(\nu)$ .

### Remarks

The extremal points of  $S_\beta(\mathcal{A})$  can be interpreted as the *phases* of the system.

# Chapter 8

## Quantum Part III: Free Quantum Gases

In this chapter, we will discuss Fermi-Dirac and Bose-Einstein distributions as KMS states.

### 8.1 Fermions

Traditionally, let  $|\Omega\rangle$  be the vacuum and creation and annihilation operators are  $a^*(\mathbf{k})$  and  $a(\mathbf{k})$  such that

$$\{a^*(\mathbf{k}), a(\mathbf{p})\} = \delta^{d-1}(\mathbf{k} - \mathbf{p}). \quad (8.1)$$

A typical state in the Fock space is

$$f \ni a^*(\mathbf{k}_1) \cdots a^*(\mathbf{k}_n) |\Omega\rangle. \quad (8.2)$$

There are however several concerns:

1.  $\mathbf{k}$  assumes translational invariance.
2.  $\delta(\mathbf{k} - \mathbf{p})$  as a distribution is singular.
3. Fock space is the Hilbert space and we want things abstract to algebras.

The first two can be addressed by reality and we pretend that  $\{e^{i\mathbf{k}\cdot\mathbf{x}} : \mathbf{k} \in \mathbb{R}^{d-1}\}$  is a basis of  $L^2(\mathbb{R}^{d-1})$ . Rather than doing so, we can just take an abstract Hilbert space  $h$  of one particle states (e.g.,  $L^2(\mathbb{R}^{d-1})$ ) and define ladder operators for  $f \in h$ :  $a(f)$  and  $a^*(f)$  with anti-commutation relations

$$\begin{aligned} \{a(f), a(g)\} &= 0 \\ \{a^*(f), a^*(g)\} &= 0 \\ \{a(f), a^*(g)\} &= \langle f, g \rangle \end{aligned} \quad (8.3)$$

where  $\langle \cdot, \cdot \rangle$  is the scalar product in  $h$  and  $f \mapsto a(f)$  is anti-linear:

$$\lambda f + g \mapsto a(\lambda f + g) = \bar{\lambda}a(f) + a(g), \quad a(f^*) = a(f)^*. \quad (8.4)$$

The norm is given by

$$\begin{aligned} \|a(f)\|^4 &= \|(a^*(f)a(f))^2\| \\ &= \|a^*(f)a(f)a^*(f)a(f)\| \\ &= \|a^*(f)(\{a(f), a^*(f)\} - a^*(f)a(f))a(f)\| \\ &= \|f\|^2 \|a^*(f)a(f)\| \\ &\Rightarrow \|a(f)\| = \|a^*(f)\| = \|f\|. \end{aligned} \quad (8.5)$$

The  $C^*$ -algebra generated by all these  $a(f)$  is unique and called  $\text{CAR}(h)$  (*canonical anti-commutation relations*).

**Proposition 8.1.** 1. For  $\dim h = n < \infty$ ,  $\text{CAR}(h) = \text{Mat}(2^n \times 2^n, \mathbb{C})$ .

2.  $\text{CAR}(h)$  is separable if and only if  $h$  is separable.

3. If we have two bounded operators  $U, V : h \rightarrow h$  such that  $U$  is linear,  $V$  is anti-linear and

$$\begin{aligned} V^*U + U^*V &= UV^* + VU^* = 0 \\ U^*U + V^*V &= UU^* + VV^* = \mathbb{1}, \end{aligned} \quad (8.6)$$

then there exists a unique  $*$ -automorphism  $\gamma$ :

$$\gamma(a(f)) = a(U(f)) + a^*(V(f)), \quad (8.7)$$

which is the Bogoliubov transformation.

We will not really prove it, but will construct a Bogoliubov transformation by doing a change of variables. Define the *field* operators

$$B(f) = \frac{1}{\sqrt{2}}(a(f) + a^*(f)). \quad (8.8)$$

Using linearity, it can be inverted as

$$a(f) = \frac{1}{\sqrt{2}}(B(f) + iB(if)). \quad (8.9)$$

The anti-commutation relation turns into

$$\{B(f), B(g)\} = \frac{1}{2}(\langle f, g \rangle + \langle g, f \rangle) = \Re \langle f, g \rangle. \quad (8.10)$$

This algebra uses only half of the scalar product. We can rewrite the algebra with a real positive definite bilinear form  $s : h \times h \rightarrow \mathbb{R}$ . The transition from  $B$  to  $a$  needs a complex structure on  $h$   $J : h \rightarrow h$  that is  $\mathbb{R}$ -linear and  $J^2 = -\mathbb{1}_h$ . It would be compatible with that

$$s(Jf, g) = -s(f, Jg) \quad (8.11)$$

and

$$a_J(f) = \frac{1}{\sqrt{2}}(B(f) + iB(Jf)). \quad (8.12)$$

$J$  determines what is a particle and what is an anti-particle. Since the algebra of  $B$  is dependent only on  $s$  (and not on  $J$ ), symmetries of  $s$  induce automorphisms of the algebra:

$$\begin{aligned} \exists \mathcal{O} \in O_s(h), \quad s(\mathcal{O}(f), \mathcal{O}(g)) &= s(f, g) \\ \Rightarrow \gamma : \quad \gamma(B(f)) &:= B(\mathcal{O}(f)) \text{ is an automorphism.} \end{aligned} \quad (8.13)$$

In gneral,  $\mathcal{O}J \neq J\mathcal{O}$  and thus

$$\gamma(a(f)) = \frac{1}{\sqrt{2}}(\gamma(B(f)) + i \underbrace{\gamma(B(Jf))}_{\neq B(J\mathcal{O}f)}). \quad (8.14)$$

But  $J$  can split  $\mathcal{O} = \mathcal{O}_1 + \mathcal{O}_2$ :

$$\begin{aligned} \mathcal{O}_{1,2} &= \frac{1}{2}(\mathcal{O} \pm J\mathcal{O}J) \\ \mathcal{O}_{1,2}J &= \frac{1}{2}(\mathcal{O}J \pm J\mathcal{O}J^2) \\ &= \frac{1}{2}(-J^2\mathcal{O}J \mp J\mathcal{O}) \\ &= \mp J\mathcal{O}_{1,2}. \end{aligned} \quad (8.15)$$

So  $\mathcal{O}_1$  anti-commutes while  $\mathcal{O}_2$  commutes with  $J$ . Therefore

$$\gamma(a(f)) = a(\mathcal{O}_2f) + a^*(\mathcal{O}_1f). \quad (8.16)$$

This is the Bogoliubov transformation.

#### Notes

When  $V$  is a unitary and  $U = 0$ , and this could be the dynamics in the 1-particle Hilbert space  $h$ . Given the Hamiltonian  $H : h \rightarrow h$ , there is a  $C^*$ -dynamical system given by  $(\text{CAR}(h), \tau)$  with

$$\tau_t(a^*(f)) := a^*(e^{iHt}f). \quad (8.17)$$



This is the free time evolution.

**Quasi-free states of CAR**  $a \in \text{CAR}(h)$  is a linear combination of products of  $a$ 's and  $a^*$ 's. We can use the anti-commutation relations to bring everything to normal ordering ( $a$ 's to the right and  $a^*$ 's to the left).

**Definition 8.2.** A state  $\omega : \text{CAR}(h) \rightarrow \mathbb{C}$  is called **quasi-free**, if it can be written as

$$\omega(a^*(f_1) \cdots a^*(f_n) a(g_1) \cdots a(g_m)) = \delta_{nm} \det(\langle g_i, \rho f_j \rangle) \quad (8.18)$$

for some  $\rho \in \mathcal{B}(h)$  such that  $0 \leq \rho = \rho^* \leq \mathbb{1}$ .

Such a state is already determined by two-point functions  $\omega(a^*(f)a(g))$  and there is no higher correlations between the  $a$ 's and  $a^*$ 's.

**Proposition 8.3.** For every  $\rho \in \mathcal{B}(h)$  such that  $\rho = \rho^* \leq \mathbb{1}$ , there is a unique quasi-free state.

**Examples 8.4.** •  $\rho = 0$ . Then  $\omega(a^*(f)a(g)) = 0$ , but

$$\omega(a(g)a^*(f)) = \omega(\langle g, f \rangle \mathbb{1} - a^*(f)a(g)) = \langle g, f \rangle. \quad (8.19)$$

We can build a GNS Hilbert space on this state, and what we get is the Fock state:

$$\|\pi_\omega(a^*(f))|\Omega_\omega\rangle\| = \|f\|. \quad (8.20)$$

- $\rho$  is a projector. Then for  $f \in \ker \rho$ ,  $\pi(a(f))$  acts as the annihilation operator as above; while for  $f \in (\ker \rho)^\perp$ ,  $\pi(a(f))$  acts as a creation operator.

**Theorem 8.5.** For  $0 \leq \rho = \rho^* \leq \mathbb{1}$ , the state  $\omega_\rho$  is a density state in the Fock state, i.e., its GNS representation is quasi-equivalent to the Fock state, if and only if  $\rho \in \mathcal{S}^1(h)$ . If  $\text{tr} \rho = \infty$ , then the two representations are inequivalent.

In physics, let  $e_i$  be an orthonormal basis of  $h$ . The expected number of particles of type  $i$  in a state  $\omega$  is

$$N_i = \omega(a^*(e_i)a(e_i)) = \langle e_i, \rho e_i \rangle \quad (8.21)$$

and hence the total particle number is

$$N = \sum_i N_i = \sum_i \langle e_i, \rho e_i \rangle = \text{tr} \rho. \quad (8.22)$$

The states with infinite particle numbers are not in the Fock space. Note that in  $\mathbb{R}^n$ , states with finite constant particle density have infinite many particles.

## 8.2 Bosons

You might have the idea of repeating the same story with the commutation relation:

$$[a(f), a^*(g)] = \langle f, g \rangle \quad (8.23)$$

and

$$\Phi(f) = \frac{1}{\sqrt{2}}(a(f) + a^*(f)). \quad (8.24)$$

Then

$$\underbrace{[\Phi(f), \Phi(if)]}_{\text{"}x\text{"}} = \frac{1}{2}(\langle f, if \rangle - \langle if, f \rangle) = i \|f\|^2. \quad (8.25)$$

But we know that  $x$  and  $p$  cannot be realized with bounded operators. Instead, we can use the Weyl operators

$$W(f) = e^{i\Phi(f)} \quad (8.26)$$

with commutation relation

$$[\Phi(f), \Phi(g)] = i \underbrace{\Im \langle f, g \rangle}_{\sigma(f,g)}. \quad (8.27)$$

Therefore

$$W(f)W(g) = W(f+g)e^{\frac{i}{2}\Im \langle f, g \rangle}. \quad (8.28)$$

### Remarks

$\Im \langle f, g \rangle$  is a real, symplectic and non-degenerate form on  $h$  if viewing  $h$  as a  $\mathbb{R}$ -vector space.

**Definition 8.6.** Let  $(h, \sigma)$  be a symplectic space. Then there is a unique  $C^*$ -algebra  $\text{CCR}(h)$  (**canonical commutation relations**) generated by elements  $W(f)$  of **Weyl algebra** with commutation relation

$$W(f)W(g) = W(f+g)e^{\frac{i}{2}\sigma(f,g)}. \quad (8.29)$$

This is the quantization of the phase space  $(h, \sigma)$ .

Indeed  $\text{CCR}(h) = \overline{\{\sum_{i=1}^N \lambda_i W(f_i)\}}^{\|\cdot\|}$ .

**Proposition 8.7.** 1.  $W(-f) = W(f)^* = W(f)^{-1}$ .  $W(f)$  is a unitary and in particular  $W(0) = \mathbb{1}$ .

2.  $\text{CCR}(h)$  is non-separable if  $h \neq 0$ .

3.  $\|W(f)\mathbb{1}\| = 0$  if  $f = 0$  and otherwise 2.

4. If  $T : h \rightarrow h$  is a symplectomorphism, that is,

$$\forall f, g \in h : \sigma(Tf, Tg) = \sigma(f, g), \quad (8.30)$$

there is an automorphism  $\gamma$ :

$$\gamma(W(f)) = W(Tf). \quad (8.31)$$

5. Alternatively,  $h$  is a pre-Hilbert space (complex vector space with non-degenerate scalar product) and  $\sigma(f, g) = \Im \langle f, g \rangle$ .

*Proof.* 3.  $W(f)$  can be changed by a phase with unitary transformations if  $f \neq 0$ :

$$W(g)W(f)W(-g) = W(f)e^{i\sigma(g,f)}. \quad (8.32)$$

As  $W(f)$  is unitary,  $\text{spec}(W(f)) \subset \{z \in \mathbb{C} : |z| = 1\}$ . Since the spectrum is invariant under unitary transformations,

$$\text{spec}(W(f)) = \{z \in \mathbb{C} : |z| = 1\}. \quad (8.33)$$

2. Notice that the map  $f \mapsto W(f)$  is not continuous.

□

### Notes

You might think

$$\Phi(f) = \lim_{\epsilon \rightarrow 0} \frac{W(\epsilon f) - W(f)}{i\epsilon}, \quad (8.34)$$

but this limit never exists as

$$\left\| \frac{W(\epsilon f) - W(f)}{i\epsilon} \right\| = \frac{2}{\epsilon} \quad (8.35)$$

for  $f \neq 0$  and  $\epsilon \neq 0$ .

But if you have a representation  $\pi : \text{CCR}(h) \rightarrow \mathcal{B}(\mathcal{H})$  with

$$f \mapsto \pi(W(f))\psi \quad (8.36)$$

which is continuous for all  $\psi \in \mathcal{H}$ .  $\pi$  is called a *regular representation*. Then for those  $\psi \in \mathcal{H}$ , there is an operator  $\Phi(f)$  defined by

$$\Phi(f)\psi = \lim_{\epsilon \rightarrow 0} \pi \left( \frac{W(\epsilon f) - W(0)}{i\epsilon} \right) \psi \quad (8.37)$$

on a dense but not bounded subset of  $\mathcal{H}$ .

**Examples 8.8.** Take  $h = \mathbb{R}^{2n} = \mathbb{C}^n$  and  $\sigma(f, g) = \Im \langle f, g \rangle$ . Take an orthonormal basis of  $\mathbb{C}^n$   $e_1, \dots, e_n$ , which also functions as a basis of  $\mathbb{R}^{2n}$   $e_1, ie_1, \dots, e_n, ie_n$ . Then

$$\begin{aligned} [\Phi(e_i), \Phi(e_j)] &= 0 \\ [\Phi(e_i), \Phi(ie_j)] &= i\delta_{ij}. \end{aligned} \quad (8.38)$$

Thus

$$\Phi(e_i) = \hat{x}_i, \quad \Phi(ie_i) = \hat{p}_i. \quad (8.39)$$

It is the canonical commutation relation for  $n$  degrees of freedom and  $\text{CCR}(h)$  for finite dimensional  $h$  is just quantum mechanics.

**Theorem 8.9. (Stone-von Neumann)** For  $\dim h = n < \infty$ , there is a unique (up to unitary equivalence) regular representation, namely the **Schrödinger representation** on  $\mathcal{H} = L^2(\mathbb{R}^n)$ :

$$\begin{aligned} (\hat{x}_i \psi)(x) &= x_i \psi(x), \\ (\hat{p}_i \psi)(x) &= -i \frac{\partial}{\partial x_i} \psi(x). \end{aligned} \quad (8.40)$$

For  $\dim h = \infty$ , there are infinitely many inequivalent representations.

### 8.3 Thermal states of free quantum gases

**Fermions** For free time evolution given in terms of (not necessarily bounded) Hamiltonian  $H$  on  $h$ :

$$\tau_t \in \text{Aut}(\text{CAR}(h)), \quad \tau_t(a^*(f)) := a^*(e^{iHt}f), \quad (8.41)$$

what are the  $(\tau, \beta)$ -KMS states?

Assume  $\omega$  is a  $(\tau, \beta)$ -KMS state. Then

$$\begin{aligned} \omega(a^*(f)a(g)) &\stackrel{\text{KMS}}{=} \omega(a(g)\tau_{i\beta}(a^*(f))) \\ &= \omega(a(g)a^*(e^{-\beta H}f)) \\ &\stackrel{\text{CAR}}{=} \omega(\langle g, e^{-\beta H}f \rangle - a^*(e^{-\beta H}f)a(g)), \end{aligned} \quad (8.42)$$

which gives

$$\begin{aligned}\langle g, e^{-\beta H} f \rangle &= \omega(a^*(f)a(g)) + \omega(a^*(e^{-\beta H} f)a(g)) \\ &= \omega(a^*((\mathbb{1} + e^{-\beta H})f)a(g)) \\ \Rightarrow \langle g, \frac{e^{-\beta H}}{\mathbb{1} + e^{-\beta H}} f \rangle &= \omega(a^*(f)a(g)).\end{aligned}\tag{8.43}$$

This is the *Fermi-Dirac distribution*. Repeat the calculation and we get

$$\omega(a^*(f_1) \cdots a^*(f_n)a(g_1) \cdots a(g_m)) = \delta_{nm} \det_{ij} \langle g_i, \frac{e^{-\beta H}}{\mathbb{1} + e^{-\beta H}} f_j \rangle.\tag{8.44}$$

So  $\omega$  is a quasi-free state with  $\rho = \frac{e^{-\beta H}}{\mathbb{1} + e^{-\beta H}}$ .

**Theorem 8.10.**  $(\text{CAR}(h), \tau_t)$  has a unique  $\beta$ -KMS state, which is quasi-free and given by

$$\rho = \frac{e^{-\beta H}}{\mathbb{1} + e^{-\beta H}} \in \mathcal{B}(h).\tag{8.45}$$

In particular, there is no phase transition for the free Fermi gas.

**Bosons** Assume there is a regular representation and thus we have  $\Phi(f)$  which defines  $a^*(f)$  and  $a(f)$ . Assume  $\omega$  is  $\beta$ -KMS state for chemical potential  $\mu \in \mathbb{R}$ :

$$\tau_t(a^*(f)) = a^*(e^{i(H-\mu)t} f)\tag{8.46}$$

in terms of a self-adjoint  $H$  acting on  $h$ . Then

$$\begin{aligned}\omega(a^*(f)a(g)) &\stackrel{\text{KMS}}{=} \omega(a(g)\tau_{i\beta}(a^*(f))) \\ &= \omega(a(g)a^*(e^{-\beta(H-\mu)} f)) \\ &\stackrel{\text{CCR}}{=} \omega(\langle g, e^{-\beta(H-\mu)} f \rangle + a^*(e^{-\beta(H-\mu)} f)a(g)).\end{aligned}\tag{8.47}$$

If we repeat the lines for the fermions, we would get  $\mathbb{1} - e^{-\beta(H-\mu)}$ , which is not invertible for  $\mu \in \text{spec}(H)$ . We can iterate for  $N$  times and get

$$\omega(a^*(f)a(g)) = \omega(a^*(e^{-N\beta(H-\mu)} f)a(g)) + \sum_{k=1}^N \langle g, e^{-N\beta(H-\mu)} f \rangle.\tag{8.48}$$

If  $H - \mu > C\mathbb{1}$  for some  $C > 0$ , i.e.,  $\mu < \inf \text{spec}(H)$ , then  $\lim_{N \rightarrow \infty} (e^{-N\beta(H-\mu)} f) = 0$  and

$$\omega(a^*(f)a(g)) = \langle g, \frac{e^{-\beta(H-\mu)}}{\mathbb{1} - e^{-\beta(H-\mu)}} f \rangle,\tag{8.49}$$

which is the *Bose-Einstein distribution*.

What happens as  $\mu \rightarrow \inf \text{spec}(H)$ ?  $e^{-N\beta(H-\mu)}$  will approach the projector to the 0 mode of Hamiltonian. Let's look at this in an example.  $\Lambda \in \mathbb{R}^n$  is a compact set and  $h = L^2(\Lambda)$ . Let  $H = -\Delta = -\nabla^2$  with Dirichlet boundary condition  $\psi|_{\partial\Lambda} = 0$ . Then we automatically get  $\inf \text{spec}(H) > C$  for some constant  $C > 0$ . The total density of particles is

$$\begin{aligned} \rho(\beta, \mu) &= \frac{N}{|\Lambda|} \\ &= \frac{\sum_n \omega(a^*(f_n)a(f_n))}{|\Lambda|} \\ &= \frac{1}{|\Lambda|} \text{tr} \frac{e^{-\beta(H-\mu)}}{\mathbb{1} - e^{-\beta(H-\mu)}} \\ &\xrightarrow{\mu \rightarrow \inf \text{spec}(H)} \infty. \end{aligned} \tag{8.50}$$

Furthermore, a simple calculation shows  $\partial\rho/\partial\mu > 0$  and  $\lim_{\mu \rightarrow \infty} \rho(\beta, \mu) = 0$  and hence

$$(-\infty, \inf \text{spec}(H)) \rightarrow \mathbb{R}_+, \quad \mu \mapsto \rho(\beta, \mu) \tag{8.51}$$

is a bijection. Thus we can solve  $\rho_0 = \rho(\beta, \mu)$  for any  $\rho_0 > 0$ .

For infinite volume, however, we can compute the trace in momentum space. Let  $z = e^{\beta\mu}$  (*activity*,  $z < 1$ ).

$$\begin{aligned} \rho(\beta, \mu) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} d^d p \frac{ze^{-\beta p^2}}{1 - ze^{-\beta p^2}} \\ &\stackrel{z < 1}{\leq} \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} d^d p \frac{e^{-\beta p^2}}{1 - e^{-\beta p^2}} \\ &= \frac{1}{(2\pi\sqrt{\beta})^d} \int_{\mathbb{R}^d} d^d p \frac{e^{-p^2}}{1 - e^{-p^2}} =: \rho_c \end{aligned} \tag{8.52}$$

It is finite for  $d > 2$ . Thus  $\rho_0 = \rho(\beta, \mu)$  can be solved only for  $\rho_0 < \rho_c$ ; there is a maximum density that we can achieve by tuning  $\mu$ .

What happens when we pass on the finite case to infinity? If  $\gamma_\Lambda$  is the smallest eigenvalue of  $-\Delta$  on  $\Lambda$ , the occupation of the lowest energy level is

$$\lim_{\Lambda \rightarrow \mathbb{R}^n} \frac{1}{|\Lambda|} \frac{z_\Lambda e^{-\beta\gamma_\Lambda}}{1 - z_\Lambda e^{-\beta\gamma_\Lambda}} = \rho_0 - \rho_c(\beta) \tag{8.53}$$

for  $\rho_0 > \rho_c$ .

**Theorem 8.11.** *For  $h = L^2(\mathbb{R}^d)$ ,  $d > 2$  and  $\rho_0 > 0$ , there is a unique KMS state that arises as thermodynamic limit of the unique KMS states for  $h_L = L^2([-L, L]^d)$  and  $H = -\Delta$  with Dirichlet boundary conditions:*

$$\omega(A) = \lim_{L \rightarrow \infty} \omega_L(A). \quad (8.54)$$

$\omega$  is quasi-free and for  $\rho_0 < \rho_c(\beta)$ ,

$$\omega(a^*(f)a(f)) = \langle f, \frac{z_0 e^{-\beta H}}{1 - z_0 e^{-\beta H}} f \rangle \quad (8.55)$$

and for  $\rho_0 \geq \rho_c$ ,

$$\omega(a^*(f)a(f)) = 2^{d+1}(\rho_0 - \rho_c) \langle 1, f \rangle^2 + \langle f, \frac{e^{-\beta H}}{1 - e^{-\beta H}} f \rangle. \quad (8.56)$$

This is the **Bose-Einstein condensation**.

There are different KMS states for  $\rho_0 > \rho_c$ , which is a phase transition. In the traditional sense (of phase transition), we can instead see how  $\mu$  behaves when we vary the temperature for fixed density  $\rho_0$ . This will correspond to a critical temperature  $T_0$  such that  $\rho_0 = \rho_c(1/T_0)$ . When  $T < T_0$ ,  $\mu = 0$ ; what about when  $T > T_0$ ? Let's take a look at  $d = 3$  case. In the energy space  $\epsilon = (\beta p)^2$ ,  $d^3 p = 2\pi\sqrt{\epsilon}\beta^{-\frac{3}{2}}d\epsilon$ . The particle number is at the critical temperature

$$N_0 = \frac{V}{(2\pi)^2} T_0^{\frac{3}{2}} \underbrace{\int_0^\infty d\epsilon \frac{\sqrt{\epsilon}}{e^\epsilon - 1}}_{=\zeta(\frac{3}{2})\gamma_{\frac{3}{2}}=: \kappa}, \quad (8.57)$$

Or

$$T_0 = \left( \frac{(2\pi)^2 \rho_0}{\kappa} \right)^{\frac{2}{3}}. \quad (8.58)$$

Let  $\tilde{N}(T) = \frac{\kappa V}{(2\pi)^2} T^{\frac{3}{2}} = N_0 (T/T_0)^{\frac{3}{2}}$  and

$$N_0 - \tilde{N}(T) = \frac{V}{(2\pi)^2} T^{\frac{3}{2}} \underbrace{\int_0^\infty d\epsilon \sqrt{\epsilon} \left( \frac{1}{e^{\epsilon - \beta\mu} - 1} - \frac{1}{e^\epsilon - 1} \right)}_{=: I(\bar{\mu} = -\beta\mu > 0)}. \quad (8.59)$$

For small  $\mu$ ,

$$I(\bar{\mu}) = \int_0^\infty d\epsilon \sqrt{\epsilon} \frac{(1 - e^{\bar{\mu}})e^\epsilon}{(e^\epsilon - 1)(e^{\epsilon + \bar{\mu}} - 1)}. \quad (8.60)$$

The integral can be divided into two parts:  $\epsilon$  from 0 to 1 and from 1 to  $\infty$ . Since  $1 - e^{\bar{\mu}}$  is  $O(\bar{\mu})$  and that

$$\int_1^\infty d\epsilon \sqrt{\epsilon} \frac{e^\epsilon}{(e^\epsilon - 1)(e^{\epsilon + \bar{\mu}} - 1)} \leq \int_1^\infty d\epsilon C \frac{\sqrt{\epsilon}}{e^\epsilon} = O(1) \quad (8.61)$$

for some constant  $C$ , the latter part is of order  $O(\bar{\mu})$ . While

$$\int_0^1 d\epsilon \sqrt{\epsilon} \frac{e^\epsilon}{e^\epsilon - 1} \frac{1}{e^{\epsilon + \bar{\mu}} - 1} \quad (8.62)$$

Let  $\epsilon = t\bar{\mu}$ , and the first part of integral becomes

$$\begin{aligned} & (1 - e^{\bar{\mu}}) \sqrt{\bar{\mu}} \int_0^{1/\sqrt{\bar{\mu}}} dt \sqrt{t} \frac{e^{\bar{\mu}t}}{e^{\bar{\mu}t} - 1} \cdot \frac{1}{e^{(t+1)\bar{\mu}} - 1} \\ & \xrightarrow{\bar{\mu} \rightarrow 0} -\sqrt{\bar{\mu}} \int_0^\infty dt \frac{\sqrt{t}}{t+1} (1 + O(\bar{\mu})) \\ & = -\sqrt{\bar{\mu}} \pi (1 + O(\bar{\mu})). \end{aligned} \quad (8.63)$$

Thus

$$N_0 - \tilde{N}(T) = -\frac{V}{(2\pi)^2} T^{\frac{3}{2}} \sqrt{\bar{\mu}} \pi + O(\bar{\mu}^{\frac{3}{2}}), \quad (8.64)$$

or

$$-\mu \simeq \frac{(4\pi\rho_0)^2}{T} \left[ \left( \frac{T}{T_0} \right)^{\frac{3}{2}} - 1 \right]^2. \quad (8.65)$$

Introducing a scaling variable  $\delta = (T - T_0)/T_0$  and finally

$$\mu \simeq -\frac{36\pi^2\rho_0^2}{T_0} \delta^2 = -T_0 \left( \frac{3\kappa}{2\pi} \right)^2 \delta^2. \quad (8.66)$$

The second derivative of  $\mu$  is discontinuous at  $T = T_0$  and hence it is a second order phase transition. Similarly, if we compute the total energy by inserting  $\epsilon$  in the integral, we get

$$E = \text{const.} \left( \frac{T}{T_0} \right)^{\frac{3}{2}} TN + \theta(T - T_0) \frac{3}{2} N \left( \frac{T}{T_0} \right)^{\frac{3}{2}} \mu. \quad (8.67)$$

The second derivative with regard to the energy also jumps.



# Appendices

# Appendix A

## Monte Carlo Computations

Monte Carlo computation is useful for

- spin systems
- lattice gauge theory
- protein folding
- ...

### A.1 Setup

**Goal** compute expectation value  $f$  of observables on configuration space  $\Omega = \{-1, 1\}^\Lambda$  of a spin model:

$$f(\omega) \in \mathbb{C}, \quad \omega \in \Omega. \quad (\text{A.1})$$

Given energy  $\mathcal{H}(\omega)$ ,

$$\langle f \rangle = \frac{\sum_{\omega \in \Omega} f(\omega) e^{-\mathcal{H}(\omega)}}{\sum_{\omega \in \Omega} e^{-\mathcal{H}(\omega)}}. \quad (\text{A.2})$$

**Recipe** Use discrete time average to approximate the result.

$$\begin{aligned} c : \mathbb{N} &\rightarrow \Omega \\ \frac{1}{T} \sum_{t=1}^T f(c(t)) &\xrightarrow{T \rightarrow \infty} \langle f \rangle \end{aligned} \quad (\text{A.3})$$

## A.2 Metropolis algorithm

1. Pick any  $c(1) \in \Omega$ .
2. At time  $t$ , pick a random  $i \in \Lambda$ . Choose  $r \in \Omega$  such that

$$r_j = \begin{cases} c(t-1)_j, & \text{if } j \neq i; \\ -c(t-1)_j, & \text{if } j = i. \end{cases} \quad (\text{A.4})$$

If  $\mathcal{H}(r) < \mathcal{H}(c(t-1))$ , choose  $c(t) = r$ . Otherwise pick a random  $p_t$  uniformly in  $[0, 1]$ , and

$$c(t) = \begin{cases} r, & \text{if } p_t < e^{-[\mathcal{H}(r) - \mathcal{H}(c(t-1))]}, \\ c(t-1), & \text{otherwise.} \end{cases} \quad (\text{A.5})$$

3. Repeat 2.

Metropolis algorithm is valid to calculate Gibbs ensemble expectation.

*Proof.* 1. *Markov model.* Assume  $|\Omega| = N < \infty$ . Probabilistic states are  $x \in \mathbb{R}^N$  such that

$$0 \leq x_a \leq 1, \quad \sum_a x_a = 1. \quad (\text{A.6})$$

The probability of jumping from  $a$  to  $b$  is  $P_{ba}$  such that

$$0 \leq P_{ba} \leq 1, \quad \sum_b P_{ba} = 1. \quad (\text{A.7})$$

Start from  $x(0)$  and after  $k$  time steps, we arrive at

$$x(k) = P^k x(0). \quad (\text{A.8})$$

2. A state of a Markov model is *stationary* if

$$Px = x. \quad (\text{A.9})$$

A state  $x$  of a Markov model is said to *obey detailed balance* if for all configurations  $a$  and  $b$ ,

$$P_{ba}x_a = P_{ab}x_b. \quad (\text{A.10})$$

Apparently detailed balance implies stationarity. Moreover, the Gibbs state

$$x_\omega = \frac{e^{-\mathcal{H}(\omega)}}{\sum_{\tilde{\omega} \in \Omega} e^{-\mathcal{H}(\tilde{\omega})}} \quad (\text{A.11})$$

obeys detailed balance in Metropolis algorithm. If two configurations  $\omega, \nu$  differ in at least two sites, then  $P_{\omega\nu} = P_{\nu\omega} = 0$ . Otherwise they are related by a single spin flip, with  $\Delta E = \mathcal{H}(\nu) - \mathcal{H}(\omega)$ . Assume  $\Delta E > 0$ . Then

$$\frac{1}{|\Lambda|} \frac{e^{-\mathcal{H}(\nu)}}{Z} = P_{\omega\nu} x_\nu = P_{\nu\omega} x_\omega = \frac{e^{-\Delta E}}{|\Lambda|} \frac{e^{-\mathcal{H}(\omega)}}{Z}. \quad (\text{A.12})$$

3. Generally a Markov model does not necessarily converge to a unique stationary state, e.g.,

$$P = \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & 1 & 1/2 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{A.13})$$

A Markov model is called *irreducible* if for all sites  $a$  and  $b$ , there is  $t_{ab} \in \mathbb{N}_0$  such that

$$(P^{t_{ab}})_{ba} \neq 0. \quad (\text{A.14})$$

Another counterexample is

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (\text{A.15})$$

A Markov model is called *acyclic* if

$$\gcd_{\forall a}(t_{aa}) = 1. \quad (\text{A.16})$$

**An irreducible, acyclic Markov model converges to a unique stationary state.**

According to Perron-Frobenius theorem (Appendix B.3), an  $N \times N$  matrix  $A = (a_{ij})$  with all  $a_{ij} > 0$  has a unique positive eigenvalue  $\lambda$  with largest norm and the eigenspace of  $\lambda$  is one dimensional.

In Metropolis algorithm,  $P_{ba}$  by itself is not positive, but there exists  $n > 0$  such that  $P^n$  is element wise strictly positive. Thus there is a *unique* stationary state if the initial state is not orthogonal to the Gibbs state, which is true for arbitrary configurations.

□

**Remarks**

Detailed balance implies *reversibility*. If  $x$  is stationary and strictly positive, then we can define

$$\tilde{P}_{ba} = \frac{P_{ab}x_b}{x_a}, \quad (\text{A.17})$$

which is the reserve transition matrix. For detailed balance,  $\tilde{P} = P$ .

### A.3 Example program for 2-D Ising model (by Robert)

```

1  /* Simple 2D Ising simulation
2   Written by Robert C. Helling <helling@atdotde.de>
3
4   Published under GPL 2.0
5
6   Compile as clang -O4 ising.c -lm -o ising
7  */
8  #include <stdio.h>
9  #include <math.h>
10 #include <stdlib.h>
11 #include <time.h>
12 #include <stdbool.h>
13
14 #define SYS_SIZE 600
15 #define PLOTSIZE 80
16 #define torus(a) (a < 0 ? a + SYS_SIZE : (a >= SYS_SIZE ? a -
17   SYS_SIZE : a))
18 #if defined(WIN32) || defined(_WIN32) || defined(__WIN32__) ||
19   defined(__TOS_WIN__)
20 #include <windows.h>
21
22 /*Turns the cursor on off*/
23 void show_console_cursor(bool showFlag)
24 {
25     HANDLE out = GetStdHandle(STD_OUTPUT_HANDLE);
26
27     CONSOLE_CURSOR_INFO    cursorInfo;
28
29     GetConsoleCursorInfo(out, &cursorInfo);
30     cursorInfo.bVisible = showFlag; // set the cursor
    visibility

```

```

31         SetConsoleCursorInfo(out, &cursorInfo);
32     }
33
34     /*Sets cursor to the top left position to overwrite terminal
        output*/
35
36     void home() {
37         /*Initialise objects for cursor manipulation*/
38         HANDLE hStdout;
39         COORD destCoord;
40         hStdout = GetStdHandle(STD_OUTPUT_HANDLE);
41
42         /*Sets coordinates of cursor to (0,0) */
43         destCoord.X = 0;
44         destCoord.Y = 0;
45         SetConsoleCursorPosition(hStdout, destCoord);
46
47         show_console_cursor(false);
48     }
49
50     void fullscreen(bool bl) {
51         if (bl) {
52             ShowWindow(GetConsoleWindow(), SW_MAXIMIZE);
53         }
54     }
55
56
57     int random() {
58         return rand();
59     }
60
61     void srand(unsigned seed){
62         srand(seed);
63     }
64
65     void system_init() {
66         fullscreen(true);
67         show_console_cursor(false);
68     }
69
70     #else
71
72     void system_init() {
73     }
74
75     void home() {
76         printf("\033[1;1H");
77     }
78     #endif

```

```

79
80 int grid[SYS_SIZE][SYS_SIZE];
81
82 void init(){
83     int x,y;
84     FILE *mag;
85
86     system_init();
87     mag = fopen("magnetization","w");
88     fclose(mag);
89
90     for (x=0; x<SYS_SIZE; x++)
91         for (y=0; y<SYS_SIZE; y++)
92             grid[x][y] = random()/(float)RAND_MAX <
93                 0.3 ? -1 : 1;
94
95     srandom((int) time(NULL) % (1 << 31));
96 }
97 void output(){
98     int x,y;
99     int m=0;
100    FILE *mag;
101
102    /* Cursor home */
103    home();
104    for (x=0; x<PLOTSIZE; x++){
105        for (y=0; y<PLOTSIZE*2; y++){
106            if (grid[x][y] == 1)
107                putchar('*');
108            else
109                putchar('.');
110        }
111        putchar('\n');
112    }
113
114    for (x=0; x<SYS_SIZE; x++)
115        for (y=0; y<SYS_SIZE; y++)
116            m += grid[x][y];
117
118    printf("m=%f\n",m/(float)(SYS_SIZE * SYS_SIZE));
119    mag = fopen("magnetization","a");
120    fprintf(mag, "%f\n",m/(float)(SYS_SIZE * SYS_SIZE));
121    fclose(mag);
122 }
123
124 void update(float J, float H){
125     int x = (int)(random() * SYS_SIZE/RAND_MAX);
126     int y = (int)(random() * SYS_SIZE/RAND_MAX);

```

```
127         int sum = grid[x][torus(y+1)] + grid[x][torus(y - 1)] +
128             grid[torus(x + 1)][y] + grid[torus(x - 1)][y];
129
130         double E = 2.0 * grid[x][y] * (J * sum + H);
131
132         if ((E < 0.0) || (exp(-E) > (random()/(double)RAND_MAX))
133             )
134             grid[x][y] *= -1;
135     }
136
137     int main() {
138
139         float T = 1.0;
140         float J = 0.44;
141         float H = 0.001;
142
143         long t;
144
145         init();
146
147         for (t=0L; 1; t++){
148             update(J / T, H / T);
149             if (!(t % 100000)){
150                 output();
151             }
152         }
153         return(0);
154     }
```



# Appendix B

## Completions

### B.1 Dyadic expansion

The goal is to go back and forth between  $[0, 1)$  and  $\Omega = \{0, 1\}^{\mathbb{N}}$ . Define a map  $\phi : \Omega \rightarrow [0, 1)$ ,

$$\omega \mapsto \phi(\omega) = \sum_{j=1}^{\infty} \frac{\omega_j}{2^j}. \quad (\text{B.1})$$

It is not injective, for instance,  $\phi((0, 1, 1, 1, \dots)) = \phi((1, 0, 0, 0, \dots))$ .

The expansion provides translation from functions  $f : [0, 1) \rightarrow \mathbb{R}$  to  $g = f \circ \phi : \Omega \rightarrow \mathbb{R}$ . Note that if  $g$  is continuous, then  $f$  is quasilocal.

### B.2 Specification

**Definition B.1.** Let  $\Lambda \in \mathbb{Z}^d$ . A **probability kernel** is a map  $\pi_{\Lambda} : \mathcal{F} \times \Omega \rightarrow [0, 1]$  such that

- For each  $\eta \in \Omega$ ,  $\pi_{\Lambda}(\cdot | \eta)$  is a probability measure on  $(\Omega, \mathcal{F})$ .
- For each  $A \in \mathcal{F}$ ,  $\pi_{\Lambda}(A | \cdot)$  is  $\mathcal{F}_{\Lambda^c}$  measurable.

If moreover,

$$\pi_{\Lambda}(B | \eta) = \mathbb{1}_B(\eta), \quad \forall B \in \mathcal{F}_{\Lambda^c} \quad (\text{B.2})$$

for all  $\eta \in \Omega$ ,  $\pi_{\Lambda}$  is said to be **proper**.

**Definition B.2.** A *specification* is a family  $\pi = \{\pi\}_{\Lambda \in \mathbb{Z}^d}$  of proper probability kernels that is consistent:

$$\pi_\Lambda \pi_\Delta = \pi_\Lambda, \quad \forall \Delta \subset \Lambda \in \mathbb{Z}^d. \quad (\text{B.3})$$

To clarify,

$$\pi_\Lambda \pi_\Delta(A|\eta) = \sum_{\tau_\Lambda} \pi_\Lambda(\tau_\Lambda|\eta) \pi_\Delta(A|\tau_\Lambda \eta_{\Lambda^c}). \quad (\text{B.4})$$

As an example, for  $\Lambda \in \mathbb{Z}^d$ , define the map

$$\pi_\Lambda^\Phi : \mathcal{F} \times \Omega \rightarrow [0, 1], \quad (A, \eta) \mapsto \pi_\Lambda^\Phi(A|\eta) \quad (\text{B.5})$$

by

$$\pi_\Lambda^\Phi(A|\eta) := \frac{1}{Z_{\Lambda, \Phi}^\eta} \sum_{\omega_\Lambda \in \Omega_\Lambda} \mathbb{1}_A(\omega_\Lambda \eta_{\mathbb{Z}^d \setminus \Lambda}) \exp(-\mathcal{H}_{\Lambda, \Phi}^\eta(\omega_\Lambda)). \quad (\text{B.6})$$

Specifically,

$$\pi_\Lambda^\Phi(\Omega_\Lambda^\eta|\eta) = 1. \quad (\text{B.7})$$

We will abbreviate the notation for a single configuration in the following way:

$$\Omega_\Lambda \times \Omega \rightarrow [0, 1], \quad (\omega_\Lambda, \eta) \mapsto \pi_\Lambda^\Phi(\omega_\Lambda|\eta) := \pi_\Lambda^\Phi(\omega_\Lambda \eta_{\Lambda^c}|\eta). \quad (\text{B.8})$$

It can be checked that  $\pi^\Phi$  is a specification.

### B.3 Perron-Frobenius theorem

Define the following relation for finite-dimensional matrices

$$(a_{ij}) \geq (>)(b_{ij}) \Leftrightarrow \forall i, j : a_{ij} - b_{ij} \geq (>)0. \quad (\text{B.9})$$

**Theorem B.3. (*Perron-Frobenius.*)** Let  $A \in \text{Mat}(n \times n, \mathbb{C})$  such that  $A > 0$ .

1. There exists  $\lambda_0 > 0$  and  $\mathbb{R}^n \ni x_0 > \mathbf{0}$ , such that  $Ax_0 = \lambda_0 x_0$ .
2. If  $\lambda \neq \lambda_0$  is a complex eigenvalue of  $A$ , then  $|\lambda| < \lambda_0$ .
3. The algebraic multiplicity of  $\lambda_0$  is 1.

A poof can be seen **here**.

## B.4 Construction of inequivalent GNS representations

**Definition B.4. *Spin chain.*** Take a lattice  $\mathbb{Z}^d$ . For each  $x \in \Lambda$ , there is a finite, uniformly bounded dimensional Hilbert space  $\mathcal{H}_x$ . For  $\Lambda \subseteq \mathbb{Z}^d$ , define the local algebra  $\mathcal{A}_\Lambda = \mathcal{B}(\otimes_{x \in \Lambda} \mathcal{H}_x)$ . Finally

$$\mathcal{A} = \overline{\bigcup_{\Lambda \in \mathbb{Z}^d} \mathcal{A}_\Lambda}^{\|\cdot\|}, \quad (\text{B.10})$$

which is called **quasi-local algebra**.

Consider a spin-1/2 spin chain, i.e.,  $\mathcal{H}_x = \mathbb{C}^2$  with a basis  $|\uparrow_x\rangle$  and  $|\downarrow_x\rangle$ . Define two states  $\omega_\pm$  on the quasi-local algebra by setting  $K \subseteq \Lambda$  and  $a \in \mathcal{A}_K$

$$\omega_+(a) = (\otimes_{x \in K} |\uparrow_x\rangle) a (\otimes_{x \in K} |\uparrow_x\rangle) \quad (\text{B.11})$$

and replace  $\uparrow$  with  $\downarrow$  for  $\omega_-$ . Extend this by continuity for all elements of  $\mathcal{A}$ . Let  $(\mathcal{H}_\pm, \pi_\pm, \Omega_\pm)$  be the corresponding GNS representations. The local averaged magnetization is a local operator

$$M_N = \frac{1}{2N+1} \sum_{x=-N}^N \sigma_x^z. \quad (\text{B.12})$$

Then  $\pi_\pm(M_N)$  converges weakly to  $\pm \mathbb{1}_{\mathcal{A}_\pm}$ , i.e., for  $\phi_\pm, \psi_\pm \in \mathcal{H}_\pm$ , we have

$$\lim_{N \rightarrow \infty} \langle \phi_\pm | \pi_\pm(M_N) \psi_\pm \rangle_\pm = \pm \langle \phi_\pm | \psi_\pm \rangle. \quad (\text{B.13})$$

So the two GNS representations cannot be unitarily equivalent.

### Notes

In the GNS representation of the quasi-local algebra, only states with finitely many "excitations" are included. In other words,  $\phi_\pm$  and  $\psi_\pm$  are not too far away from  $[\mathbb{1}_{\mathcal{A}_\Lambda}]$ .