2. The thermodynamic limit for thermodynamic functions: lattice systems

This section follows Ruelle, Statistical mechanics, Chapter 2.

2.1. Limit of an infinite volume

So far we have always considered systems in the boxes $[0,L]^d \subset \mathbb{R}^d$ and $[0,L]^d \cap \mathbb{Z}^d$. To take the thermodynamic limit we have to let $L \to \infty$ in such a way that $\frac{N}{L^d}$ = fixed, where N denotes our degrees of freedom (e.g. particles or spins). In a grand canonical setting N will denote the expected number of particles. In a more satisfactory theory of taking the thermodynamic limit we can choose more general sets Λ than boxes, but then we need to define a notion what it means to let Λ tend to $\mathbb{R}^d$ or $\mathbb{Z}^d$. In the following we describe three such limiting procedures.

Let $a = (a_1, \dots a_d) \in \mathbb{R}^d$ (resp. $\in \mathbb{Z}^d$) with $a_1, \dots, a_d > 0$ and define

$$\Lambda_a = \{ x \in \mathbb{R}^d \ (\text{resp. } \in \mathbb{Z}^d) \mid 0 \le x_i < a_i \text{ for } i = 1 \dots d \}. \quad (1)$$

The volume of Λ_a is

$$|\Lambda_a| = \prod_{i=1}^{d} a_i . \tag{2}$$

We write $a \to \infty$ if $a_1 \to +\infty$, $a_2 \to +\infty$, ..., $a_d \to +\infty$. When $a \to \infty$, Λ_a tends to infinity in a manner suitable for the thermodynamic limit. Nevertheless, there are two more general and physically more satisfactory notions that we introduce now.

We say that a sequence of set $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ with $\Lambda_\alpha \subset \mathbb{R}^d$ (resp. $\mathbb{Z}^d$) converges to $\mathbb{R}^d$ (resp. $\mathbb{Z}^d$) denoted by $\Lambda_\alpha \uparrow \mathbb{R}^d$ or $\Lambda_\alpha \uparrow \mathbb{Z}^d$ if

a) Λ_α is increasing in the sense that $\Lambda_\alpha \subset \Lambda_{\alpha+1}$

b) Λ_α invades $\mathbb{R}^d$ (resp. $\mathbb{Z}^d$): $\bigcup_{\alpha=1}^{\infty} \Lambda_\alpha = \mathbb{R}^d$ (resp. $\mathbb{Z}^d$).

In order to control the influence of the boundary conditions we need to put more regularity on the sets.

For $n \in \mathbb{Z}^d$ let $na = (n_1 a_1, \dots, n_d a_d)$ and define the set

$$\Lambda_a(n) = \Lambda_a + na. \tag{3}$$

The family $\{\Lambda_a(n)\}_{n \in \mathbb{Z}^d}$ forms a partition of $\mathbb{R}^d$ or $\mathbb{Z}^d$.

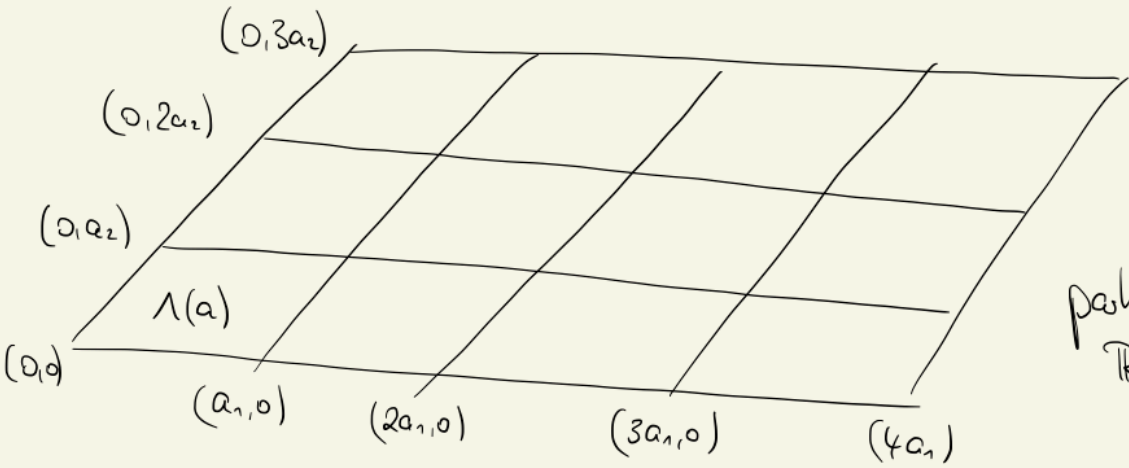

fig 1

partition of $\mathbb{R}^2$

For any $\Lambda \subset \mathbb{R}^d$ (resp. $\mathbb{Z}^d$) we define

$$N_a^+(\Lambda) = \#\{\Lambda_a(n) \mid \Lambda_a(n) \cap \Lambda \neq \emptyset\}, \tag{4}$$

$$N_a^-(\Lambda) = \#\{\Lambda_a(n) \mid \Lambda_a(n) \subset \Lambda\}.$$

An illustration can be found on the next page.

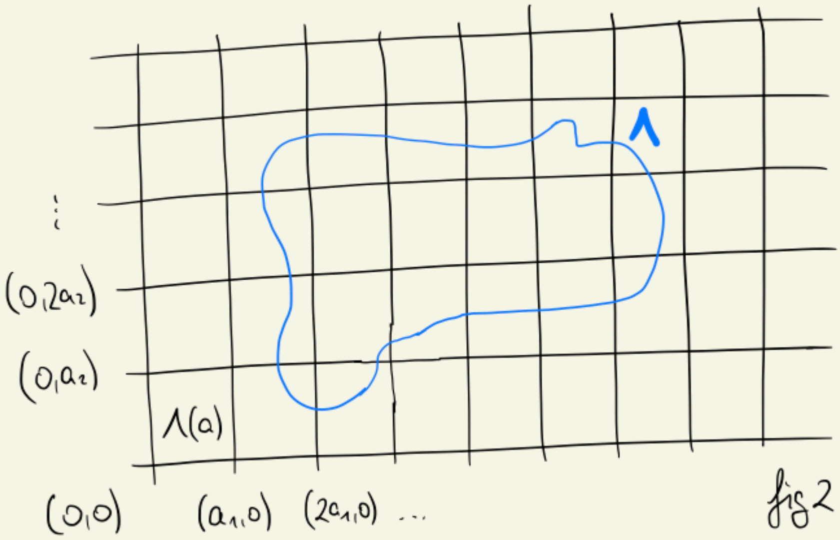

fig 2

$N_a^+(\Lambda) = 20$

$N_a^-(\Lambda) = 4$

Example N_a^+ and N_a^-.

2.1.1. Definition (Van Hove limit): The sets $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ tend to $\mathbb{R}^d$ (resp. $\mathbb{Z}^d$) in the sense of Van Hove if $\Lambda_\alpha \uparrow \mathbb{R}^d$ (resp. $\mathbb{Z}^d$) and

$$\lim_{\alpha\to\infty} N_a^-(\Lambda_\alpha) = +\infty \quad \text{and} \quad \lim_{\alpha\to\infty} \frac{N_a^-(\Lambda_\alpha)}{N_a^+(\Lambda_\alpha)} = 1 \tag{5}$$

for all $a \in \mathbb{R}^d$ resp. $\mathbb{Z}^d$.

We note that this notion is invariant under inhomogeneous linear transformations.

Suppose that the set $\Lambda \subset \mathbb{R}^d$ is Lebesgue measurable and denote its measure by $|\Lambda|$. For $h>0$ we also define

$$V_h(\Lambda) = \left| \{ x \in \mathbb{R}^d \mid \operatorname{dist}(x, \partial\Lambda) \leq h \} \right|. \qquad (6)$$

Claim: The notion of Van Hove convergence to $\mathbb{R}^d$ is equivalent to $\Lambda_\alpha \uparrow \mathbb{R}^d$ such that

$$\lim_{\alpha\to\infty} |\Lambda_\alpha| = +\infty \quad \text{and} \quad \lim_{\alpha\to\infty} \frac{V_h(\Lambda_\alpha)}{|\Lambda_\alpha|} = 0 \qquad (7)$$

holds for all $h > 0$.

The proof of the claim is left as an exercise to the reader.

Examples: $\boxed{\cdot}$ The sequence of sets $\Lambda_\alpha = \{-\alpha, \dots, \alpha\}^d \subset \mathbb{Z}^d$ converges to $\mathbb{Z}^d$ in the sense of Van Hove.

$\boxed{\cdot}$ Any sequence $\Lambda_\alpha \uparrow \mathbb{Z}^d$ whose boundary grows as fast as its volume will not converge in the sense of Van Hove. A concrete example is provided by
$\Lambda_\alpha = \{-\alpha, \dots, \alpha\}^d \cup \{ (i, 0, \dots, 0) \in \mathbb{Z}^d \mid 0 \leq i \leq e^\alpha \}$.

In some cases when $\Lambda_\alpha \uparrow \mathbb{R}^d$ it is necessary to use a stronger notion of convergence that we introduce now in order to prove the existence of the thermodynamic limit.

In the following we denote by $d(\Lambda)$ the diameter of the set $\Lambda \subset \mathbb{R}^d$, that is, $d(\Lambda) = \sup_{x,y\in\Lambda} |x-y|$.

2.1.2. Definition (Fisher limit): The measurable sets $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ tend to $\mathbb{R}^d$ in the sense of Fisher if $\Lambda_\alpha \uparrow \mathbb{R}^d$ s.t. there exists a function $\Pi : \mathbb{R}_+ \to \mathbb{R}_+$ with

$$\lim_{x\to 0} \Pi(x) = 0 \tag{9}$$

and for sufficiently small x and all $\alpha \in \mathbb{N}$ we have

$$\frac{V_{x d(\Lambda_\alpha)}(\Lambda_\alpha)}{|\Lambda_\alpha|} \le \Pi(x) \tag{10}$$

with $V_{x d(\Lambda_\alpha)}$ defined in (6).

The notion of convergence in the sense of Fisher is invariant under inhomogeneous linear transformations.

Example: Let us consider the sequence of sets

$$\Lambda_\alpha = \left\{ (x,y) \in \mathbb{R}^2 \mid 0 \le x \le \alpha^2,\ 0 \le y \le \alpha \right\}. \tag{11}$$

We claim that $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ converges to $\mathbb{R}^d$ in the sense of Van Hove but not in the sense of Fisher.

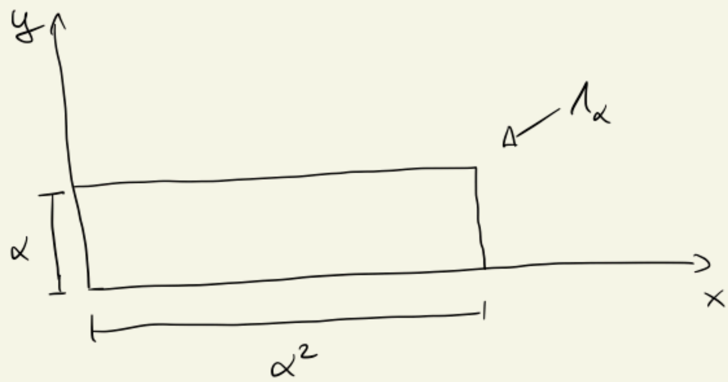

fig 3

To see this, we compute

$$\left.\begin{aligned} &\bullet\ |\Lambda_\alpha| = \alpha^3 \\ &\bullet\ V_h(\Lambda_\alpha) \le 4h(\alpha+\alpha^2) \end{aligned}\right\} \text{ for any fixed } h>0 \text{ we thus have } \quad \frac{V_h(\Lambda_\alpha)}{|\Lambda_\alpha|} \le \frac{8h}{\alpha} \xrightarrow{\alpha\to\infty} 0 \tag{12}$$

$\Rightarrow$ Convergence to $\mathbb{R}^d$ in the sense of Van Hove.

- $d(\Lambda_\alpha) = \sqrt{\alpha^2+\alpha^4}$

OK for x small enough

- $$V_{x d(\Lambda_\alpha)}(\Lambda_\alpha) \geqslant 4x\sqrt{\alpha^2+\alpha^4}\left(\alpha+\alpha^2\right) - 8x^2\left(\alpha^2+\alpha^4\right) \qquad (13)$$

- $|\Lambda_\alpha| = \alpha^3$

- $$\frac{V_{x d(\Lambda_\alpha)}(\Lambda_\alpha)}{|\Lambda_\alpha|} \geqslant \frac{4x\alpha^4\sqrt{\alpha^{-2}+1}\left(\alpha^{-1}+1\right) - 8x^2\alpha^4\left(1+\alpha^{-2}\right)}{\alpha^3}$$

Since the r.h.s. grows as α there can be no function $\Pi(x)$ bounding this expression independently of α. Note that this would be possible in case of $\Lambda_\alpha = [0,\alpha]^2$.

2.2. Interactions of quantum lattice systems

We start our study of the thermodynamic limit with quantum lattice systems and introduce the set-up.

Let $\Lambda \subset \mathbb{Z}^d$ be finite. To each such set we associate the Hilbert space

$$\mathcal{H}(\Lambda) = \bigotimes_{x \in \Lambda} \mathcal{H}_x \tag{14}$$

unitary equivalence.

with n-dimensional Hilbert spaces $\mathcal{H}_x \simeq \mathbb{C}^n$ at each site. The Hilbert spaces at each point are describing the local degrees of freedom as e.g. spins or particles.

To every finite $\Lambda \subset \mathbb{Z}^d$ we also associate a Hamiltonian $H(\Lambda)$, that is, a self-adjoint operator (aka hermitian matrix) acting on $\mathcal{H}(\Lambda)$. If $\Lambda = \emptyset$ we define $H(\Lambda) = 0$.

If $\Lambda_1 \cap \Lambda_2 = \emptyset$ we can naturally identify

$$\mathcal{H}(\Lambda_1 \cup \Lambda_2) \simeq \mathcal{H}(\Lambda_1) \otimes \mathcal{H}(\Lambda_2). \tag{15}$$

We will also identify any operator A_1 on $\mathcal{H}(\Lambda_1)$ with the operator $A_1 \otimes \mathbb{1}_{\mathcal{H}(\Lambda_2)}$ on $\mathcal{H}(\Lambda_1) \otimes \mathcal{H}(\Lambda_2)$. In particular, for any $\Lambda \supset \Lambda_1$, $H(\Lambda_1)$ will be identified with an operator on $\mathcal{H}(\Lambda)$.

In order to introduce translation invariant Hamiltonians, we define for each $a \in \mathbb{Z}^d$ and each $x \in \mathbb{Z}^d$ a unitary mapping (translation operator)

$$V_x(a) : \mathcal{H}_x \to \mathcal{H}_{x+a} \tag{16}$$

such that (a) $V_x(0) = \mathbb{1}_{\mathcal{H}_x}$, (17)

(b) $V_x(a_1 + a_2) = V_{x+a_2}(a_1) V_x(a_2)$.

We also define

$$V_\Lambda(a) = \bigotimes_{x \in \Lambda} V_x(a). \tag{18}$$

We will consider Hamiltonians H that are translation-invariant in the sense that

$$H(\Lambda+a) = V_\Lambda(a)\, H(\Lambda)\, V_{a+\Lambda}(-a) \tag{19}$$

holds. If no confusion about the indices can appear we also write this as

$$H(\Lambda+a) = V(a)\, H(\Lambda)\, V(a)^{-1}. \tag{20}$$

It will be convenient to write $H(\Lambda)$ as

$$H(\Lambda) = \sum_{X\subset\Lambda} \Phi(X) \tag{21}$$

with the interaction potential Φ describing the interactions of the subsystems in the theory (compare with the concrete examples in Section 1.7.). The operator-valued set function Φ obeys

$$\Phi(X+a) = V(a)\, \Phi(X)\, V(a)^{-1}. \tag{22}$$

Let us describe the classes of translation-invariant interaction potentials in the sense of (21) that we will use in the sequel.

2.2.1. Definition (finite range interactions):

We say that Φ has finite range if there are only finitely many bounded sets $X \subset \mathbb{Z}^d$ with $0 \in X$ and $\Phi(X) \neq 0$. The bounded set

$$\Delta = \left\{ x \in \mathbb{Z}^d \mid \exists\, X \in \mathbb{Z}^d \text{ with } 0, x \in X \text{ and } \Phi(X) \neq 0 \right\} \qquad (23)$$

is called the range of Φ.

Claim: We have $\Delta = -\Delta$. Moreover, if $x, y \in X$ and $x - y \notin \Delta$, then $\Phi(X) = 0$.

Proof: Assume that $a \in \Delta$. Then there exists $X \subset \mathbb{Z}^d$ with

$$\begin{aligned}
&(a) \quad 0 \in X \Leftrightarrow -a \in X - a \\
&(b) \quad a \in X \Leftrightarrow 0 \in X - a \\
&(c) \quad \Phi(X) \neq 0.
\end{aligned} \qquad (24)$$

By translation-invariance we have $\Phi(X-a) = V(a)^{-1}\Phi(X)V(a)$. Since $V(a)$ is unitary and $\Phi(X) \neq 0$ we conclude that $\Phi(X-a) \neq 0$. In combination with (a) and (b) this proves the first claim.

To prove the second claim we note that

$$\text{(c)} \quad 0 \in X-y, \tag{25}$$

$$\text{(d)} \quad x-y \in X-y.$$

Assume that $\Phi(X) \neq 0$. Then we know that $\Phi(X-y) \neq 0$ by the argument above. In combination with (c) and (d) this implies $x-y \in \Delta$, which contradicts the assumption $x-y \notin \Delta$. We conclude $\Phi(X) = 0$.

$\blacksquare$

Claim: Let Φ be a (translation-invariant) finite range interaction, let $\Lambda_1, \Lambda_2 \subset \mathbb{Z}^d$ be two bounded sets and let $a \in \mathbb{Z}^d$ be such that

$$a \notin \Lambda_1 - \Lambda_2 + \Delta. \tag{26}$$

Then the Hamiltonian H in (21) obeys

$$H(\Lambda_1 \cup (\Lambda_2 + a)) = H(\Lambda_1) + H(\Lambda_2 + a). \tag{27}$$

Remark: The claim shows that the regions Λ_1 and $\Lambda_2 + a$ "do not interact" if Φ has finite range and if $|a| = \left(\sum_{i=1}^{d} a_i^2\right)^{1/2}$ is chosen large enough.

Proof: By definition

$$H(\Lambda_1 \cup (\Lambda_2 + a)) = \sum_{X \subset \Lambda_1 \cup (\Lambda_2 + a)} \Phi(X). \tag{28}$$

We check that (26) is equivalent to $[\Lambda_1 - (\Lambda_2 + a)] \cap \Delta = \phi$. Accordingly, if $x \in \Lambda_1$ and $y \in \Lambda_2 + a$ then we have $x - y \notin \Delta$. This, in particular, implies $\Phi(X) = 0$ if $x, y \in X$

by the previous claim on p. 12, as well as

$$\sum_{X\subset \Lambda_1 \cup (\Lambda_2+a)} \Phi(X) = \sum_{X\subset\Lambda_1} \Phi(X) + \sum_{X\subset \Lambda_2+a} \Phi(X) \qquad (29)$$

$$= H(\Lambda_1) + H(\Lambda_2+a).$$

$\boxtimes$

Next we define the space of interaction potentials, for which we are going to prove the existence of the thermodynamic limit.

2.2.2. Definition (The Banach space $\mathcal{B}$): By $N(\Lambda)$ we denote the number of points in the set $\Lambda\subset\mathbb{R}^d$. The real vector space $\mathcal{B}$ consists of all translation-invariant interaction potentials Φ that obey

$$\|\Phi\| = \sum_{X \subset \mathbb{Z}^d \,:\, 0 \in X} \frac{\|\Phi(X)\|}{N(X)} < +\infty, \tag{30}$$

where $\|\Phi(X)\|$ denotes the operator norm of the matrix $\Phi(X)$, that is,

norm in $\mathcal{H}(X)$

$$\|\Phi(X)\| = \sup_{\substack{\psi \in \mathcal{H}(X) \\ \psi \neq 0}} \frac{\|\Phi(X)\psi\|}{\|\psi\|}. \tag{31}$$

Remark: The vector space $\mathcal{B}$ together with the norm in (30) is a Banach space. The linear subspace $\mathcal{B}_0$ of finite range interactions is a dense subset of $\mathcal{B}$.

Remark: A Banach space is a complete normed vector space, that is, any Cauchy sequence has a limit in the space.

Remark: Let A be a hermitian matrix and let $\lambda_1 \dots \lambda_n$ be its eigenvalues. The operator norm of A equals

$$\|A\| = \sup_{i=1\dots n} |\lambda_i|. \tag{32}$$

Using the definition of H in (21) as well as (30), we see that the operator norm of $H(\Lambda)$ obeys the bound

$$\|H(\Lambda)\| = \Big\| \sum_{x\in\Lambda} \sum_{\substack{X\subset\Lambda:\\ x\in X}} \frac{\Phi(X)}{N(X)} \Big\| \leq \sum_{x\in\Lambda} \sum_{\substack{X\subset\mathbb{Z}^d:\\ x\in X}} \frac{\|\Phi(X)\|}{N(X)}$$

$$= N(\Lambda)\,\|\Phi\|. \tag{33}$$

The partition function related to the Hamiltonian $H(\Lambda)$ is given by

$$Z_\Lambda = \mathrm{tr}_{\mathcal{H}(\Lambda)} \exp\big(-\beta H(\Lambda)\big), \tag{34}$$

where β denotes the inverse temperature. The corresponding thermodynamic function in finite volume is given by

$$\mathcal{P}_\Lambda = \frac{\ln(Z_\Lambda)}{N(\Lambda)} . \tag{35}$$

In the particle interpretation (see lattice fermions in Section 1.7.) $\mathcal{P}_\Lambda$ equals $-\beta$ times the pressure of the system.

In the spin system interpretation of the model, where we assume that $\mathcal{H}_x$ is a Hilbert space describing a spin and H describes the interaction between the spins, $\mathcal{P}_\Lambda$ would be $-\beta$ times the specific free energy of the system. Quantum spin systems will be introduced later in more detail when we discuss the Mermin-Wagner theorem. During the discussion of the thermodynamic limit we will absorb β in the interaction potential, which is equivalent to setting $\beta = 1$. This is also the reason why we have omitted β in the notation in (34) and (35).

By translation-invariance we have

$$Z_{\Lambda+a} = Z_\Lambda \quad \text{and} \quad P_{\Lambda+a} = P_\Lambda . \tag{36}$$

Before we start with the proof of the existence of the thermodynamic limit for $P(\Lambda)$ we prove some preparatory statements that will be needed during that proof. The first is the following Lemma.

2.2.3. Lemma (Duhamel's formula):

Let $A: \mathbb{R} \to \mathbb{R}^{n\times n}$ be a C^2 matrix-valued function in the sense that every matrix element is C^2. Then

$$\frac{d}{dt} e^{A(t)} = \int_0^1 e^{sA(t)} A'(t)\, e^{(1-s)A(t)}\, ds . \tag{37}$$

Proof: When we use Taylor's formula with remainder for each matrix element separately, we see that

$$A(t+h) = A(t) + A'(t)h + h^2 \underbrace{\int_0^1 (1-x) A''(t+hx)\,dx}_{B(t,h)}. \qquad (38)$$

By assumption A'' is continuous, and hence B is jointly continuous in t and h.

Next, we define the function $E(s) = e^{sA(t+h)} e^{(1-s)A(t)}$ and note that

$$e^{A(t+h)} - e^{A(t)} = E(1) - E(0) = \int_0^1 E'(s)\,ds \qquad (39)$$

$$= \int_0^1 \left(e^{sA(t+h)} A(t+h)\, e^{(1-s)A(t)} - e^{sA(t+h)} A(t)\, e^{(1-s)A(t)} \right) ds.$$

To come to the last line, we used $\frac{d}{ds} e^{sC} = C e^{sC} = e^{sC} C$ for a $n \times n$ matrix C. This can easily be proved by expanding the exponential in a power series. Eq. (39) implies

$$\lim_{h\to 0} \frac{e^{A(t+h)} - e^{A(t)}}{h} = \lim_{h\to 0} \int_0^1 e^{sA(t+h)} \underbrace{\frac{A(t+h)-A(t)}{h}}_{= A'(t) + h\, B(t,h)} e^{(1-s)A(t)}\, ds \tag{40}$$

$$= \int_0^1 e^{sA(t)} A'(t)\, e^{(1-s)A(t)}\, ds.$$

$\blacksquare$

Lemma 2.2.1 can be used to prove the following statement.

2.2.4. Lemma: If A and B are self-adjoint operators on $\mathbb{C}^n$, then

$$\left| \ln \mathrm{tr}[e^A] - \ln \mathrm{tr}[e^B] \right| \le \|A-B\|. \tag{41}$$

(As before $\|\cdot\|$ denotes the operator norm.)

Proof: Let $A(h) = hA + (1-h)B$ and note that Lemma 2.2.1 implies

$$\frac{d}{dh} \mathrm{tr}\, e^{A(h)} = \int_0^1 \mathrm{tr}\left[e^{sA(h)}(A-B)\, e^{(1-s)A(h)}\right] ds \tag{42}$$

$$\overset{\text{cyclicity of trace}}{=} \int_0^1 \mathrm{tr}\left[(A-B)\, e^{A(h)}\right] ds = \mathrm{tr}\left[(A-B)\, e^{A(h)}\right].$$

The absolute value of the r.h.s. can be bounded as follows

$$\left| \operatorname{tr}(A-B)\, e^{A(u)} \right| = \left| \operatorname{tr} e^{A(u)/2} (A-B)\, e^{A(u)/2} \right| \tag{43}$$

$$= \left| \sum_{i=1}^{n} \left\langle e^{A(u)/2} \psi_i ,\ (A-B)\, e^{A(u)/2} \underset{\text{ONB}}{\psi_i} \right\rangle \right|$$

$$\leq \sum_{i=1}^{n} \underbrace{\left| \left\langle e^{A(u)/2} \psi_i ,\ (A-B)\, e^{A(u)/2} \psi_i \right\rangle \right|}$$

$$\leq \|A-B\| \ \underbrace{\left\langle e^{A(u)/2} \psi_i ,\ e^{A(u)/2} \psi_i \right\rangle}_{\geq 0}$$

$$\leq \|A-B\| \ \operatorname{tr} e^{A(u)} .$$

In combination, (42) and (43) imply

$$\left| \frac{d}{du} \ln \operatorname{tr} e^{A(u)} \right| = \left| \frac{\frac{d}{du} \operatorname{tr} e^{A(u)}}{\operatorname{tr} e^{A(u)}} \right| \leq \| A-B \| . \tag{44}$$

Eq. (44) allows us to prove the claim because

$$\left| \ln \operatorname{tr} e^{A} - \ln \operatorname{tr} e^{B} \right| = \left| \int_0^1 \left(\frac{d}{du} \ln \left(\operatorname{tr} \left[e^{A(u)} \right] \right) \right) du \right| \leq \|A-B\| . \tag{45}$$

$\blacksquare$

The next two statements are called propositions because they are of independent interest (their proves are quite simple). The main reason for us to prove them is that they are needed in the proof of Proposition 2.4.7. below.

2.2.5. Proposition (Peierls' inequality): Let A be a self-adjoint operator on $\mathbb{C}^n$ and let $\{\varphi_i\}_{i=1}^n$ be an ONB. Then

$$\sum_{i=1}^n \exp\left[-\langle \varphi_i, A\varphi_i\rangle\right] \leq \operatorname{tr} e^{-A}. \qquad (46)$$

Moreover, we have equality if and only if $\{\varphi_i\}_{i=1}^n$ is the eigenbasis of A.

Proof: Let $\{\lambda_i\}_{i=1}^n$ and $\{\psi_i\}_{i=1}^n$ the eigenvalues and eigenvectors of A, respectively. We have

$$\operatorname{tr} e^{-A} = \sum_{i=1}^n \langle \varphi_i, e^{-A}\varphi_i\rangle = \sum_{i,j=1}^n e^{-\lambda_j} |\langle \varphi_i, \psi_j\rangle|^2. \qquad (47)$$

Since $\sum_{j=1}^{n} |\langle \varphi_i, \psi_j \rangle|^2 = 1$ and $x \mapsto e^{-x}$ is convex we can apply Jensen's inequality to the r.h.s. of (47) and find

$$\sum_{i,j=1}^{n} e^{-\lambda_j} |\langle \varphi_i, \psi_j \rangle|^2 \geqslant \sum_{i=1}^{n} e^{-\sum_{j=1}^{n} \lambda_j |\langle \varphi_i, \psi_j \rangle|^2}$$

$$= \sum_{i=1}^{n} e^{-\langle \varphi_i, A\varphi_i \rangle} . \tag{48}$$

We have equality in (48) if and only if $\{\varphi_i\}_{i=1}^{n}$ is the eigenbasis of A. $\blacksquare$

Jensen's inequality: Let $(\Omega, \mathcal{F}, P)$ be a probability space, g a real-valued function in $L^1(P)$ and φ a convex function on the real line. Then we have

$$\varphi\left(\int_{\Omega} g(x)\, dP(x) \right) \leq \int_{\Omega} \varphi(g(x))\, dP(x). \tag{49}$$

Let us denote the complex vector space of self-adjoint operators on $\mathbb{C}^n$ by S. We say that an operator $A \in S$ is nonnegative if all its eigenvalues are nonnegative. In this case we write $A \geq 0$. We also define a partial order on S by saying that $A \geq B$ holds if $A - B \geq 0$. A function $f : S \to \mathbb{R}$ is called monotone increasing if $A \leq B$ implies $f(A) \leq f(B)$.

The next proposition will allow us to show that P_1 is a convex function of the interaction potential. Its proof uses Peierls' inequality.

2.5.6. Proposition: The function $A \mapsto \ln \operatorname{tr} e^A$ is convex and monotone increasing on S.

Proof: To prove the first claim we note that for $0 < \alpha < 1$

$$\operatorname{tr} e^{\alpha A + (1-\alpha) B} \overset{(46)}{=} \sup_{\{\varphi_i\}_{i=1}^n \text{ ONB}} \sum_{i=1}^n \exp\Big(\langle \varphi_i, (\alpha A + (1-\alpha) B) \varphi_i \rangle \Big) \qquad (50)$$

$$= \sup_{\{\varphi_i\}_{i=1}^n \text{ ONB}} \sum_{i=1}^n \left[\exp\left(\langle \varphi_i, A\varphi_i\rangle\right)\right]^\alpha \left[\exp\left(\langle \varphi_i, B\varphi_i\rangle\right)\right]^{1-\alpha}$$

$$\underset{\substack{\uparrow \\ \text{Hölder with } p=\frac{1}{\alpha} \text{ and } q=\frac{1}{1-\alpha}}}{\leq} \sup_{\{\varphi_i\}_{i=1}^n \text{ ONB}} \left[\sum_{i=1}^n \exp\left(\langle \varphi_i, A\varphi_i\rangle\right)\right]^\alpha \Bigg[\underbrace{\sum_{i=1}^n \exp\left(\langle \varphi_i, B\varphi_i\rangle\right)}_{\underset{(46)}{\leq} \operatorname{tr} e^B}\Bigg]^{1-\alpha}$$

$$\underset{(46)}{\leq} \left(\operatorname{tr} e^A\right)^\alpha \left(\operatorname{tr} e^B\right)^{1-\alpha} .$$

Accordingly, we have

$$\ln \operatorname{tr} e^{\alpha A + (1-\alpha)B} \leq \alpha \ln \operatorname{tr} e^A + (1-\alpha) \ln \operatorname{tr} e^B, \tag{51}$$

which proves convexity.

To prove monotonicity we pick $A, B \in S$ with $A \leq B$ and note that (46) implies

$$\operatorname{tr} e^A = \sup_{\{\varphi_i\}_{i=1}^n \text{ ONB}} \sum_{i=1}^n \exp\left(\langle \varphi_i, A\varphi_i\rangle\right) \underset{\substack{\uparrow \\ A\leq B \Rightarrow \langle \psi, A\psi\rangle \leq \langle \psi, B\psi\rangle \text{ for} \\ \text{all } \psi\in\mathbb{C}^n.}}{\leq} \sup_{\{\varphi_i\}_{i=1}^n \text{ ONB}} \sum_{i=1}^n \exp\left(\langle \varphi_i, B\varphi_i\rangle\right)$$

$$= \operatorname{tr} e^B. \tag{52}$$

∎

The next statement provides us with the information of how P_Λ depends on the interaction potential. Its proof uses Proposition 2.5.6.

2.2.7. Proposition: (a) If $\Phi, \Psi \in \mathcal{B}$, then

$$|P_\Lambda(\Phi) - P_\Lambda(\Psi)| \leq \|\Phi - \Psi\|. \tag{53}$$

(b) The function $\Phi \mapsto P_\Lambda(\Phi)$ is convex on $\mathcal{B}$.

Proof: To prove (a) we note that

$$|P_\Lambda(\Phi) - P_\Lambda(\Psi)| \overset{(35)}{=} \frac{|\ln \operatorname{tr} \exp(H_\Phi(\Lambda)) - \ln \operatorname{tr} \exp(H_\Psi(\Lambda))|}{N(\Lambda)} \tag{54}$$

$$\overset{(41)}{\leq} \frac{\|H_\Phi(\Lambda) - H_\Psi(\Lambda)\|}{N(\Lambda)} = \frac{\|H_{\Phi-\Psi}(\Lambda)\|}{N(\Lambda)} \overset{(33)}{\leq} \|\Phi - \Psi\|.$$

The second statement is a direct consequence of Proposition 2.5.6.

The last preparatory statement we prove is the following proposition.

2.2.8. Proposition: If $\Phi \in \mathcal{B}$, then

$$|P_\Lambda(\Phi) - \ln(n)| \leqslant \|\Phi\|. \tag{55}$$

Here n denotes the dimension of the local Hilbert spaces $\mathcal{H}_x$.

Proof: We have

$$P_\Lambda(0) = \frac{\ln \operatorname{tr}_{\mathcal{H}(\Lambda)} \mathbb{1}}{N(\Lambda)} = \frac{\ln\left(n^{N(\Lambda)}\right)}{N(\Lambda)} = \ln(n). \tag{56}$$

In combination with (53) with the choice $\Psi = 0$, this implies

$$|P_\Lambda(\Phi) - \ln(n)| = |P_\Lambda(\Phi) - P_\Lambda(0)| \leq \|\Phi\| \tag{57}$$

and proves the claim. $\square$

2.3. Thermodynamic limit for quantum lattice systems

The goal of this section is to prove the following theorem.

2.3.9. Theorem: Assume that $\Phi \in \mathcal{B}$ and that $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ is a sequence of sets with $\Lambda_\alpha \uparrow \mathbb{Z}^d$ in the sense of Van Hove. Then the limit

$$P(\Phi) = \lim_{\alpha \to \infty} P_{\Lambda_\alpha}(\Phi) \tag{58}$$

exists, is finite and does not depend on the sequence $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$. Furthermore,

(a) If $\Phi, \Psi \in \mathcal{B}$, then $|P(\Phi) - P(\Psi)| \leq \|\Phi - \Psi\|$,

(b) the function $P(\cdot)$ is convex on $\mathcal{B}$.

The proof of the above theorem is based on two lemmata. The first quantifies the effect of interactions between two regions Λ_1 and Λ_2 on $P_{\Lambda_1 \cup \Lambda_2}(\Phi)$ for finite range interactions.

2.3.10. Lemma: Assume that $\Phi \in \mathcal{B}_0$ and let Δ be its range. Let $\Lambda_1, \Lambda_2 \subset \mathbb{Z}^d$ be such that $\Lambda_1 \cap \Lambda_2 = \emptyset$ and denote by $N(\Lambda_1, \Lambda_2)$ the number points $a \in \mathbb{Z}^d$ such that $\Lambda_1 \cap (\Delta + a) \neq \emptyset$ and $\Lambda_2 \cap (\Delta + a) \neq \emptyset$. Then we have

$$\left| N(\Lambda_1 \cup \Lambda_2) P_{\Lambda_1 \cup \Lambda_2}(\Phi) - N(\Lambda_1) P_{\Lambda_1}(\Phi) - N(\Lambda_2) P_{\Lambda_2}(\Phi) \right| \tag{59}$$

$$\leq N(\Lambda_1, \Lambda_2) \, \|\Phi\|.$$

Proof: Using (21) we write

$$\| H(\Lambda_1 \cup \Lambda_2) - H(\Lambda_1) - H(\Lambda_2) \| = \Big\| \sum_{\substack{X \subset \Lambda_1 \cup \Lambda_2 \text{ s.t.} \\ X \cap \Lambda_1 \neq \emptyset \text{ and } X \cap \Lambda_2 \neq \emptyset}} \Phi(X) \Big\| \tag{60}$$

$$= \Big\| \sum_{x \in \Lambda_1 \cup \Lambda_2} \sum_{\substack{X \subset \Lambda_1 \cup \Lambda_2 \text{ s.t. } x \in X \text{ and} \\ X \cap \Lambda_1 \neq \emptyset \text{ and } X \cap \Lambda_2 \neq \emptyset}} \Phi(X) \, N(X)^{-1} \Big\|$$

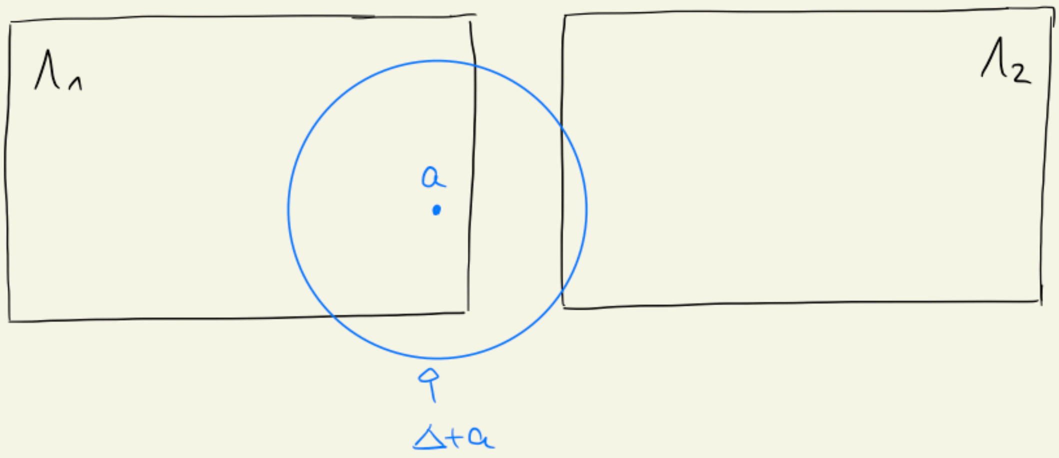

fig. 4

The r.h.s. of (60) is bounded by $\|\Phi\|$ times

$$N\Big(\big\{x \in \Lambda_1 \cup \Lambda_2 \;\big|\; \exists\, X \subset \Lambda_1 \cup \Lambda_2 \text{ with } X \cap \Lambda_1 \neq \phi,\ X \cap \Lambda_2 \neq \phi,\ x \in X \text{ and } \Phi(X) \neq 0\big\}\Big). \tag{61}$$

We have $\Delta = \bigcup_{\substack{0 \in X \\ \Phi(X) \neq 0}} X \Rightarrow \Delta + x = \bigcup_{\substack{x \in X \\ \Phi(X) \neq 0}} X$, and hence

$\Phi(X)$ vanishes unless $X \subset \Delta + x$. Accordingly, $\Phi(X)$ in the requirements in (61) vanishes unless $\Lambda_1 \cap (\Delta + x) \neq \phi$ and $\Lambda_2 \cap (\Delta + x) \neq \phi$. We thus see that the number in (61) is bounded by $N(\Lambda_1, \Lambda_2)$ and that

$$\| H(\Lambda_1 \cup \Lambda_2) - H(\Lambda_1) - H(\Lambda_2) \| \leq N(\Lambda_1, \Lambda_2) \|\Phi\| \tag{62}$$

holds.

Next, we note that the l.h.s. of (59) equals

$$\left| \ln \operatorname{tr} e^{-H(\Lambda_1 \cup \Lambda_2)} - \ln \operatorname{tr} e^{-H(\Lambda_1)} - \ln \operatorname{tr} e^{-H(\Lambda_2)} \right| \tag{63}$$

$$= \Big| \ln \operatorname{tr} e^{-H(\Lambda_1 \cup \Lambda_2)} - \ln \Big(\underbrace{\operatorname{tr} e^{-H(\Lambda_1)} \operatorname{tr} e^{-H(\Lambda_2)}}_{\operatorname{tr} e^{-H(\Lambda_1) - H(\Lambda_2)} \quad (\Lambda_1 \cap \Lambda_2 = \emptyset)} \Big) \Big|$$

$$\overset{(41)}{\leq} \| H(\Lambda_1 \cup \Lambda_2) - H(\Lambda_1) - H(\Lambda_2) \| \underset{(62)}{\leq} N(\Lambda_1, \Lambda_2) \|\Phi\|.$$

This proves the claim. $\blacksquare$

The following lemma establishes the existence of the thermodynamic limit for finite range interactions.

2.3.11. Lemma: Assume that $\Phi \in \mathcal{B}_0$ and that $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$ is a sequence of sets with $\Lambda_\alpha \uparrow \mathbb{Z}^d$ in the sense of Van Hove. Then the limit

$$P(\Phi) = \lim_{\alpha \to \infty} P_{\Lambda_\alpha}(\Phi) \tag{64}$$

exists, is finite and does not depend on the sequence $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$.

Proof: To prove the lemma we will show that for given $\varepsilon > 0$, there exist a_0, $\alpha_0(a_0)$ s.t. for $a = (\tilde{a}, \dots \tilde{a}) \in \mathbb{Z}^d$ with $\tilde{a} \geq a_0$ and $\alpha \geq \alpha_0(a_0)$ we have

$$\left| P_{\Lambda_\alpha}(\Phi) - P_{\Lambda_a}(\Phi) \right| < \varepsilon . \tag{65}$$

We recall the definitions of Λ_a and $N_a^-(\Lambda_\alpha)$ in (1) and (4).

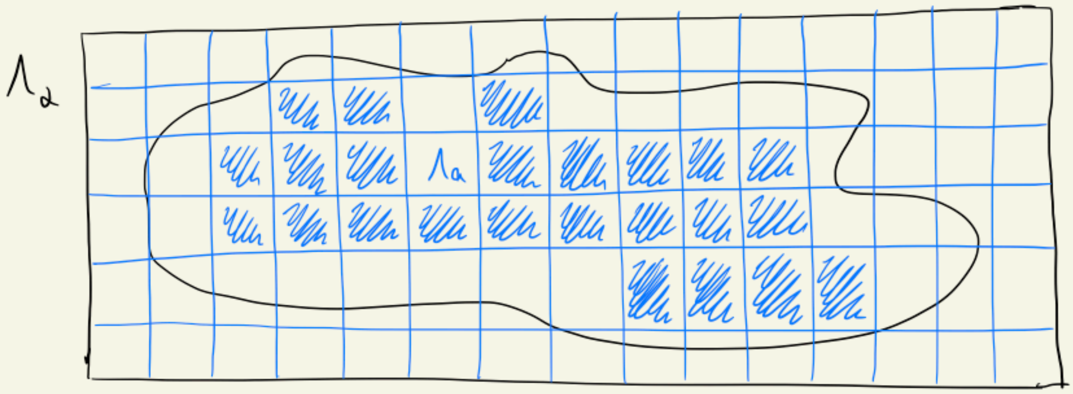

fig. 5

By $\Gamma_a^- \subset \Lambda_\alpha$, see in fig. 5, we denote the union of the $N_a^-(\Lambda)$ translates of Λ_a contained in Λ_α. The single translates are denoted by $\{\Lambda_j(a)\}_{j=1}^{N_a^-(\Lambda)}$ and we also define the set

$$\Gamma(j) = \left(\Lambda_\alpha \setminus \Gamma_a^-\right) \bigcup_{i=1}^{j} \Lambda_i(a). \tag{65}$$

We note that $\Gamma(N_a^-(\Lambda)) = \Lambda_\alpha$.

From Lemma 2.3.10 we know that

$$\left| N(\Gamma(j)) P_{\Gamma(j)}(\Phi) - N(\Gamma(j-1)) P_{\Gamma(j-1)}(\Phi) - N(\Lambda(a)) P_{\Lambda_a}(\Phi) \right| \leq N\left(\Gamma(j-1), \Lambda_j(a)\right) \|\Phi\|. \tag{66}$$

This implies

$$\left| N(\Lambda_\alpha) P_\Lambda(\Phi) - N(\Lambda_\alpha \setminus \Gamma_a^-) P_{\Lambda\setminus\Gamma_a^-}(\Phi) - N_a^-(\Lambda_\alpha) N(\Lambda(a)) P_{\Lambda(a)}(\Phi) \right| \tag{67}$$

$$\leq \sum_{j=1}^{N_a^-(\Lambda_\alpha)} \left| N(\Gamma(j)) P_{\Gamma(j)}(\Phi) - N(\Gamma(j-1)) P_{\Gamma(j-1)}(\Phi) - N(\Lambda(a)) P_{\Lambda(a)}(\Phi) \right|$$

$$\leq \|\Phi\| \sum_{j=1}^{\tilde{N}_a(\Lambda_\alpha)} N\Big(\Gamma(j-1), \Lambda_j(a)\Big).$$

By definition $N\big(\Gamma(j-1), \Lambda_j(a)\big)$ is less than the number of points x such that $\Delta + x$ intersects both $\Lambda_j(a)$ and its complement. These points are located at the boundary of $\Lambda_j(a)$, and hence there exists a constant $C > 0$ s.t. their number is bounded by $C\,\tilde{a}^{d-1}$. Accordingly, we have

$$\frac{N\big(\Gamma(j-1), \Lambda_j(a)\big)}{N(\Lambda_j(a))} \leq \frac{C}{\tilde{a}} < \frac{\varepsilon}{2\|\Phi\|} \tag{68}$$

for $\tilde{a}$ chosen sufficiently large. Insertion into (67) yields

$$\Big| N(\Lambda_\alpha) P_{\Lambda_\alpha}(\Phi) - N(\Lambda_\alpha \setminus \Gamma_a^-) P_{\Lambda \setminus \Gamma_a^-}(\Phi) - \tilde{N}_a(\Lambda_\alpha) N(\Lambda(a)) P_{\Lambda(a)}(\Phi) \Big|$$

$$< \frac{\varepsilon}{2} \tilde{N}_a(\Lambda_\alpha) N(\Lambda_\alpha) \tag{69}$$

This, in particular, implies

$$\left| N(\Lambda_\alpha)\left[P_{\Lambda_\alpha}(\Phi) - P_{\Lambda(a)}(\Phi)\right] - N(\Lambda_\alpha \setminus \Gamma_a^-)\left[P_{\Lambda_\alpha \setminus \Gamma_a^-}(\Phi) - P_{\Lambda_a}(\Phi)\right]\right|$$

$$= \left| N(\Lambda_\alpha) P_{\Lambda_\alpha}(\Phi) - N(\Lambda_\alpha \setminus \Gamma_a^-) P_{\Lambda \setminus \Gamma_a^-}(\Phi) - N_a^-(\Lambda_\alpha) N(\Lambda_a) P_{\Lambda_a}(\Phi) \right|$$

$$\overset{(69)}{\leq} \frac{\varepsilon}{2} N_a^-(\Lambda_\alpha)\, N(\Lambda_a). \tag{70}$$

Using (55), we see that

$$\left| P_{\Lambda_\alpha \setminus \Gamma_a^-}(\Phi) - P_{\Lambda_a}(\Phi) \right| \leq 2\|\Phi\|. \tag{71}$$

We also know that

$$\frac{N(\Lambda_\alpha \setminus \Gamma_a^-)}{N(\Lambda_\alpha)} \leq \frac{N_a^+(\Lambda_\alpha) - N_a^-(\Lambda_\alpha)}{N_a^-(\Lambda_\alpha)} < \frac{\varepsilon}{4\|\Phi\|} \tag{72}$$

holds for α chosen large enough (depending on a) because $\Lambda_\alpha \uparrow \mathbb{Z}^d$ in the sense of Van Hove. When we combine (70), (71) and (72), we find

$$\left|P_{\Lambda_\alpha}(\Phi)-P_{\Lambda_a}(\Phi)\right| \leq \overbrace{\frac{N_a^-(\Lambda)\,N(\Lambda_a)}{N(\Lambda_a)}}^{\leq 1}\,\frac{\varepsilon}{2}$$

$$+\underbrace{\frac{N(\Lambda\setminus\Gamma_a^-)}{N(\Lambda_\alpha)}}_{<\frac{\varepsilon}{4\|\Phi\|}}\underbrace{\left|P_{\Lambda\setminus\Gamma_a^-}(\Phi)-P_{\Lambda_a}(\Phi)\right|}_{\leq 2\|\Phi\|} \qquad (73)$$

$$< \varepsilon .$$

This proves the claim. $\blacksquare$

We are now prepared to prove the main result of this subsection.

Proof of Theorem 2.3.8.: Let $\Phi \in \mathcal{B}$ and choose $\Psi \in \mathcal{B}_0$ with $\|\Phi-\Psi\| < \varepsilon/3$. We estimate

$$\left|P_{\Lambda_\alpha}(\Phi)-P_{\Lambda_a}(\Phi)\right| \leq \left|P_{\Lambda_\alpha}(\Phi)-P_{\Lambda_\alpha}(\Psi)\right|^{①}+\left|P_{\Lambda_a}(\Phi)-P_{\Lambda_a}(\Psi)\right|^{②}$$

$$+\left|P_{\Lambda_\alpha}(\Psi)-P_{\Lambda_a}(\Psi)\right|^{③}, \qquad (74)$$

with Λ_a defined as in the proof of Lemma 2.3.11. From (53) we know that

$$① + ② \leq 2 \|\Psi - \Phi\| < \frac{2\varepsilon}{3}. \tag{75}$$

Moreover, using Lemma 2.3.11 we see that $③ < \varepsilon/3$ if $\tilde{a} \geq a_0$ and $\alpha \geq \alpha_0(a_0)$ for some $a_0, \alpha_0(a_0)$. This proves the first claim.

The second claim follows from the first and (53). The last claim follows from the first and Proposition 2.2.7. (b).

$\boxtimes$

Remark: In practice it is often convenient to consider systems with periodic boundary conditions, that is, a periodic box obtained by "glueing together opposite faces" of Λ_a. In some applications it is also relevant to introduce other boundary conditions as e.g. described in Section 1.7. The systems we studied so far have open boundary conditions (all degrees of freedom inside a set $\Lambda \subset \mathbb{Z}^d$ interact but there is nothing special happening at the boundary). As we have seen in the proof of Theorem 2.3.9., boundary effects do not affect $P(\Phi)$. Using the techniques we used to prove the Theorem, it is therefore straightforward to show that $P(\Phi)$ does not depend on typical boundary conditions (as e.g. spins in a fixed quantum state at the boundary).

We conclude our discussion of quantum lattice systems with the concrete example of a spin system and introduce the spin $\frac{1}{2}$ quantum Heisenberg model.

2.3.12. Example (Spin ½ quantum Heisenberg model):

Let Λ be a bounded subset of the lattice $\mathbb{Z}^d$ with $d \geq 1$. As local Hilbert space we choose $\mathcal{H}_x = \mathbb{C}^2$. Spins in quantum mechanics should be thought of as the quantum version of angular momentum vectors. As usual in quantum mechanics, observables are given by operators. In case of spin ½ the relevant operator is the spin operator

$$S = (S_1, S_2, S_3) \quad \text{with}$$

$$S_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; S_2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; S_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The components of the spin operator S satisfy the $\underbrace{su(2)}_{\text{Lie algebra}}$ commutation relations

$$[S_i, S_j] = i \underbrace{\varepsilon_{ijk}}_{\text{Levy-Cevita tensor:}} S_k .$$

Since $SU(2)$ is a double cover of $SO(3)$ these commutation relations provide a link to the rotation group.

Levy-Cevita tensor:

$\varepsilon_{123} = 1$ | $\varepsilon_{ijk} = 0$ if not all indices are distinct

$\varepsilon_{213} = -1$

$\varepsilon_{ijk} = \varepsilon_{kij}$

In the following we denote $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Since $S_3|\uparrow\rangle = \frac{1}{2}|\uparrow\rangle$ and $S_3|\downarrow\rangle = -\frac{1}{2}|\downarrow\rangle$ the physical interpretation of these states is that the projection of a spin in the state $|\uparrow\rangle$ onto the z-axis is $1/2$ while it is $-1/2$ in the case of $|\downarrow\rangle$ (recall that our spins have length $1/2$).

As Hamiltonian we choose

$$H_\Lambda = -J \sum_{\substack{i,j\in\Lambda \\ \underbrace{i\sim j}_{\text{nearest neighbors}}}} S_i \cdot S_j + h \cdot \sum_{i\in\Lambda} S_i$$

$J>0$; $h \in \mathbb{R}^3$, models magnetic field

where $S_i = (S_{i1}, S_{i2}, S_{i3})$ is the spin operator at lattice point i. To be more precise one would need to write

$S_i \otimes \mathbb{1}_{\bigotimes_{j\neq i} \mathbb{C}^2_j}$ ← HS at site j.

That is,

$$\Phi(X) = \Phi^{(1)}(X) + \Phi^{(2)}(X)$$

with

$$\Phi^{(1)}(X) = \begin{cases} 0 & \text{if } N(X) \neq 1 \\ hS_i & \text{if } X = \{i\}, \end{cases}$$

and

$$\Phi^{(2)}(X) = \begin{cases} 0 & \text{if } N(X) \neq 2 \\ -J S_i \cdot S_j \underbrace{\mathbb{1}(i\sim j)}_{\substack{=1 \text{ if } i \text{ and } j \text{ are nearest neighbors} \\ =0 \text{ instead}}} & \text{if } X = \{i,j\}. \end{cases}$$

In order to get to know this model a little better I recommend the following exercise.

<u>Exercise</u>: Compute the lowest eigenvalue and the corresponding eigenvector of H_Λ for $\Lambda = [0,L]^2 \cap \mathbb{Z}^2$ and $k = (0,0,1)$.

2.4. Thermodynamic limit for classical lattice systems

We consider systems on the lattice $\mathbb{Z}^d$ and assume that the states of the subsystem at point $x \in \mathbb{Z}^d$ are numbered by $n_x \in \{0, 1, \dots, N\}$. The numbers n_x could be interpreted as describing the species of particles present at x (describing an alloy), as an occupation number (lattice gas interpretation, see Section 1.7.) or we may interpret $S_x = n_x - \frac{1}{2}N$ as a spin component (spin interpretation, see the Ising model in Section 1.7.).

An ensemble of classical mechanics is a measure on the set of all possible configurations of the system within a region $\Lambda \subset \mathbb{Z}^d$. There are $(N+1)^{N(\Lambda)}$ such configurations parametrized by the $N(\Lambda)$-tuples $(n_{x_1} \dots n_{x_{N(\Lambda)}})$, where

$x_1 \dots x_{|\Lambda|}$ denote the points in Λ, and an ensemble will attribute a certain weight to each of them. Here we introduce only a grand canonical ensemble for which the weight is

$$\frac{\exp\left(\beta \sum_{i=1}^{N(\Lambda)} \mu\left(n_{x_i}\right)\right) \exp\left(-\beta \mathcal{U}\left(n_{x_1} \dots n_{N(\Lambda)}\right)\right)}{\sum\limits_{n_{x_1} \dots n_{N(\Lambda)}=0}^{N} \exp\left(\beta \sum_{i=1}^{N(\Lambda)} \mu\left(n_{x_i}\right)\right) \exp\left(-\beta \mathcal{U}\left(n_{x_1} \dots n_{N(\Lambda)}\right)\right)} . \quad (76)$$

The function $\mathcal{U}(x_1 \dots x_{N(\Lambda)})$ gives the potential energy corresponding to the configuration $(n_{x_1} \dots n_{x_{N(\Lambda)}})$. In the alloy interpretation $\mu(n_x)$ is the chemical potential for the species n_x. In the lattice gas interpretation we would take $\mu(n_x) = \mu n_x$ and the numerator of (76) equals

$$z^n \exp\left(-\beta \mathcal{U}(x_1 \dots x_{N(\Lambda)})\right) \quad (77)$$

with $z = e^{\beta\mu}$ and $n = \sum_{i=1}^{N(\Lambda)} n_{x_i}$. The expression in in (77) is clearly analogous to (26) in Section 1 defining the configurational grand canonical ensemble in the continuous case.

In the spin interpretation the spins may interact with a magnetic field h and we choose $\mu(n_x)$ to be minus the relevant interaction energy, that is, $\mu(n_x) = S_x h = (n_x - \frac{1}{2}N)h$. In this case the numerator in (76) is given by

$$\exp\left(\left(n - \tfrac{1}{2}N\, N(\Lambda)\right)\beta h - \beta\, \mathcal{U}(x_1 \dots x_{N(\Lambda)})\right). \tag{78}$$

Irrespective of the interpretation, the thermodynamic function related to the measure in (76) is given by

$$P_\Lambda = \ln(Z_\Lambda) \tag{79}$$

with

$$Z_\Lambda = \sum_{n_{x_1} \dots n_{N(\Lambda)} = 0}^{N} \exp\left(\beta \sum_{i=1}^{N(\Lambda)} \mu(n_{x_i})\right) \exp\left(-\beta\, \mathcal{U}(n_{x_1} \dots n_{N(\Lambda)})\right). \tag{80}$$

In the following we will absorb the term with the chemical potential in the definition of $\mathcal{U}$.

To prove the existence of the thermodynamic limit for P_Λ, we will map the problem to the quantum case we have already established.

For the local Hilbert space $\mathcal{H}_x$ we choose a basis $\{\Psi_{n,x}\}_{n=0}^{N}$, where $N+1 = \dim \mathcal{H}_x$, so that

$$\Psi_{x+a,n} = V_x(a)\,\Psi_{x,n} \tag{81}$$

holds. We introduce number operators n_x and n_Λ via their action on basis vectors by

$$n_{x_k} \bigotimes_{i=1}^{N(\Lambda)} \Psi_{x_i,n_i} = n_k \bigotimes_{i=1}^{N(\Lambda)} \Psi_{x_i,n_i} \quad \text{and} \tag{82}$$

$$n(\Lambda) = \sum_{x\in\Lambda} n_x .$$

Also the Hamiltonian $H(\Lambda)$ is defined via its action on our basis vectors by

$$H(\Lambda) \bigotimes_{i=1}^{N(\Lambda)} \Psi_{x_i, n_i} = \mathcal{U}(n_{x_1}, \dots, n_{x_{N(\Lambda)}}) \bigotimes_{i=1}^{N(\Lambda)} \Psi_{x_i, n_i}. \qquad (83)$$

This is possible because the operators $\{n_x\}_{x \in \Lambda}$ are all diagonal in the same basis. In particular, they all commute.

It remains to choose the interaction potential $\Phi(X)$. For the sake of clarity of the presentation we consider here only the special case of a lattice gas with $N=1$, that is, where each lattice site can be occupied only by either no particle or by one particle. We will also assume that empty sites do not contribute to the energy.

We write

$$\mathcal{U}(n_{x_1}, \dots, n_{x_{N(\Lambda)}}) = \mathcal{U}_\Lambda(X), \qquad (84)$$

where $X = \{x \in \Lambda \mid n_x = 1\}$ and assume that

$$U_\Lambda(X) = \sum_{Y \subset X} \Phi(Y). \tag{85}$$

The function Φ is an operator-valued set function on finite subsets of $\mathbb{Z}^d$. As in the case of the quantum system we need to make assumptions for it. We note that the operator $\Phi(Y)$ is diagonal in the present situation. Its only non-vanishing eigenvalue denoted also by $\Phi(Y)$ in (85) corresponds to the basis vector Ψ, for which $n_y \Psi = \Psi$ holds for all $y \in Y$. We also note that the function $U_\Lambda(X)$ actually only depends on X and not on Λ, and we therefore omit the Λ-index in the following. The invariance relation in (22) translates to

$$U(X+a) = U(X) \tag{86}$$

in the present situation. In the following we will restrict attention to translation-invariant interaction potentials Φ, that is,

$$\Phi(X+a) = \Phi(X) \tag{87}$$

holds for all $a \in \mathbb{Z}^d$, and we assume $\Phi(\overset{\text{empty set}}{\emptyset}) = 0$. We denote by $\tilde{\mathcal{B}}$ the set of those translation-invariant potentials that obey

$$\|\Phi\| = \sum_{X \,:\, 0 \in X} \frac{|\Phi(X)|}{N(X)} < +\infty . \tag{88}$$

By $\tilde{\mathcal{B}}_0$ we denote the subspace of $\tilde{\mathcal{B}}$ of potentials Φ s.t. $\Phi(X) \neq 0$ only for a finite number of sets X with $0 \in X$ (finite range potentials). As in the quantum case, $\tilde{\mathcal{B}}$ is a real Banach space w.r.t. the norm in (88) and $\tilde{\mathcal{B}}_0$ is a dense subset in $\tilde{\mathcal{B}}$. We note that by definition $\tilde{\mathcal{B}} \subset \mathcal{B}$ and $\tilde{\mathcal{B}}_0 \subset \mathcal{B}_0$. If $\Phi \in \tilde{\mathcal{B}}$ and

$$U_\Phi(X) = \sum_{Y \subset X} \Phi(Y), \tag{89}$$

we therefore have

$$|U_\Phi(X)| \leq N(X) \|\Phi\| . \tag{90}$$

Let

$$\mathcal{B}^k = \left\{ \Phi \in \tilde{\mathcal{B}} \mid \Phi(X) = 0 \text{ unless } N(X) = k \right\} \tag{91}$$

denote the space of k-body potentials. Because of (87), $\mathcal{B}^1$ is one-dimensional, and we may write

$$\tilde{\mathcal{B}} = \mathcal{B}^1 \oplus \tilde{\mathcal{B}}', \tag{92}$$

where $\mathcal{B}^1$ is identified with $\mathbb{R}$ and

$$\tilde{\mathcal{B}}' = \left\{ \Phi \in \tilde{\mathcal{B}} \mid \Phi(X) = 0 \text{ if } N(X) = 1 \right\}. \tag{93}$$

Accordingly, we write $\Phi \in \tilde{\mathcal{B}}$ in the following as $\Phi = (\Phi^1, \tilde{\Phi})$ and note that

$$U_\Phi(X) = N(X)\,\Phi^1 + U_{\tilde{\Phi}}(X). \tag{94}$$

This motivates the notation $\Phi^1 = -\mu$ and $z = e^{\beta\mu}$, which allows us to write

$$\exp\left(-\beta U_\Phi(X)\right) = z^{N(X)} \exp\left(-\beta U_{\tilde{\Phi}}(X)\right), \tag{95}$$

which should be compared to (77).

Because all operators are diagonal in the basis $\bigotimes_{i=1}^{N(\Lambda)} \Psi_{x_i, n_i}$,

we can use this basis to evaluate the following trace and see that

$$Z_\Lambda\left(-\beta\left(-\mu, \tilde{\Phi}\right)\right) = \Theta\left(\Lambda, z, \beta\right), \tag{96}$$

where

interpreted as an operator

$$Z_\Lambda\left(\Phi\right) = \mathrm{tr}_{\mathcal{H}(\Lambda)} \exp\left(-\beta \mathcal{U}_\Phi(\Lambda)\right) \tag{97}$$

denotes the quantum partition function and

interpreted as a number

$$\Theta\left(\Lambda, z, \beta\right) = \sum_{n \geq 0} z^n \sum_{X \subset \Lambda,\, N(X) = n} \exp\left(-\beta \mathcal{U}_\Phi(X)\right) \tag{98}$$

the classical one. Eq. (96) is the main result of this subsection because it allows us to map the classical system to a quantum system. We recall that

$$P(\Phi) = \frac{\ln\left(Z_\Lambda(\Phi)\right)}{N(\Lambda)} \tag{99}$$

The following theorem is a direct consequence of Theorem 2.3.9. and establishes the existence of the thermodynamic limit for our classical model.

Theorem 2.4.1.: Let $\Phi \in \tilde{\mathcal{B}}$ and assume that $\Lambda_\alpha \uparrow \mathbb{Z}^d$ as $\alpha \to \infty$ in the sense of Van Hove. Then the limit

$$\mathcal{P}(\Phi) = \lim_{\alpha\to\infty} \mathcal{P}_{\Lambda_\alpha}(\Phi) \tag{100}$$

exists, is finite and does not depend on the sequence $\{\Lambda_\alpha\}_{\alpha=1}^{\infty}$. Furthermore,

(a) If $\Phi, \Psi \in \tilde{\mathcal{B}}$, then

$$\left|\mathcal{P}(\Phi) - \mathcal{P}(\Psi)\right| \leq \|\Phi - \Psi\|, \tag{101}$$

(b) the function $\mathcal{P}(\cdot)$ is convex on $\tilde{\mathcal{B}}$.

Example: We choose $\Phi \in \mathcal{B}^1 \oplus \mathcal{B}^2$, that is, $\Phi(X) = 0$ if $N(X) > 2$ s.t.

$$\Phi^{(1)}(\{x\}) = -\mu \qquad \text{and} \tag{102}$$

$$\Phi^{(2)}(\{x,y\}) = J(x-y).$$

Then

$$U_{\Phi}(X) = -\mu \underbrace{\sum_{x \in X} 1}_{N(X)} + \sum_{x,y \in X} J(x-y) \tag{103}$$

and we obtain the grand canonical version of the classical lattice gas that we introduced in Section 1.7. The different configuration are sets $X \subset \Lambda$ with the interpretation that the points $x \in X$ are those points where a particle sits. In the original representation the configurations have been of the form $(n_1 \ldots n_{N(\Lambda)}) \in \{0,1\}^{N(\Lambda)}$ and the energy function was given by

$$\mathcal{U}(u_1 \ldots u_{N(\Lambda)}) = -\mu \sum_{x \in \Lambda} u_x + \sum_{x,y \in \Lambda} J(x-y)\, u_x u_y . \qquad (104)$$