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Approach to equilibrium in translation-invariant quantum systems: some structural results

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Dedicated to the memory of Krzysztof Gawędzki

Abstract. We formulate the problem of approach to equilibrium in algebraic quantum statistical mechanics and study some of its structural aspects, focusing on the relation between the zeroth law of thermodynamics (approach to equilibrium) and the second law (increase of entropy). Our main result is that approach to equilibrium is necessarily accompanied by a *strict* increase of the specific (mean) energy and entropy. In the course of our analysis, we introduce the concept of quantum weak Gibbs state which is of independent interest.

1 Introduction

Algebraic quantum statistical mechanics provides a general framework for studying dynamical aspects of infinitely extended quantum systems. Lattice spins and fermions are examples of such systems which, in the translation invariant setting, are also the main focus of this work. Adapting the algebraic framework, in this paper we initiate a research program dealing with the fundamental problem of Boltzmann¹ which is succinctly summarized in [Sim93, Appendix I.1] as follows:

Approach to equilibrium: heuristic description.

“As for the laws of thermodynamics, most textbooks primarily discuss the first and the second law. Actually, there is a fundamental experimental fact basic to all thermodynamic descriptions that is usually implicitly assumed: It is occasionally called the zeroth law² [...]. The zeroth law deals with the observed fact that a large system seem to normally have ‘states’ described by a few macroscopic parameters like a temperature and density, and that any system not in one of these states, left alone, rapidly approaches one of these states. When Boltzmann and Gibbs tried to find a macroscopic basis for thermodynamics, they realized that the approach to equilibrium was the most puzzling and deepest problem in such a formalism.”

¹For additional information and references about this problem see for example [Leb93, UF63]

²This terminology is unfortunate; see [BU01]

Previous works on this topic in the algebraic formalism are scarce. Approach to equilibrium was discussed in [HKK73, LR72, Suk83] in the context of quasi-free fermionic dynamics, and more generally for interacting fermionic systems in [ESY04, Hug83, Hug87]. The quantum Ising model was analyzed in [Rad70].

The goal of this work is to investigate some structural properties of the quantum dynamical systems associated to interacting, infinitely extended lattice spin systems and lattice Fermi gases. Besides setting the program, we examine one important special case where the system, initially in thermal equilibrium w.r.t. an interaction Ψ , evolves according to the dynamics generated by some other interaction Φ , focusing on the relation between the zeroth and the second law of thermodynamics. Our main result states that, in this setting, approach to equilibrium is accompanied by a *strict* increase of the specific entropy and of the specific energy of the original interaction Ψ . Let us emphasize the *strict* increase aspect of our result. That the entropy can't decrease is an easy consequence of the upper-semicontinuity of the specific entropy and of the classical result of Lanford and Robinson [LR68] that this specific entropy remain constant along the state trajectory. That the specific energy of Ψ cannot decrease is a consequence of the Gibbs variational principle and a general estimate of Hiai and Petz [HP93, Lemma 2.3]; see Theorem 2.18. One compelling aspect of our results is their generality.

Our analysis builds on the foundational works on statistical mechanics of quantum spin systems that go back to 1970's (summarized in the monographs [Rue69, BR81, Isr79, Sim93]), and their extensions to fermionic systems [AM03]. The two additional ingredients are:

- (a) The notion of weak Gibbs states.
- (b) The set of ideas that emerged during the last twenty years in the studies of entropy production in the algebraic framework of non-equilibrium quantum statistical mechanics; see [JP01b, Rue00].

The notion of weak Gibbs states was implicit in the early works on thermodynamic formalism of classical spin systems, but surprisingly it was formalized only relatively late [Yur02]; see also [BFV19, FP97, KLN04, JR11, MRVML99, PS20, Var12, vEV04]. Similarly, the notion of quantum weak Gibbs state has been implicit in a number of works in quantum statistical mechanics [AI74, Ara76, HP93, HMO07, ORB11] but, to the best of our knowledge, it has not been formalized before. Besides our work, the study of quantum weak Gibbs states is of independent interest, and most of foundational questions remain open.

Regarding (b), and more generally in order to put the results of this paper and the research program it initiates in a proper perspective, the next section provides a short account of dynamical aspects of algebraic quantum statistical mechanics, assuming that the reader has had a previous exposure to the subject. The problem of approach to equilibrium in algebraic quantum statistical mechanics is also formulated in this section.

1.1 The algebraic approach to nonequilibrium quantum statistical mechanics

Our starting point is a C^* -dynamical system (\mathcal{O}, α) , where \mathcal{O} is the unital³ C^* -algebra of observables of the quantum mechanical system under consideration. The Heisenberg dynamics of this system is described by a strongly continuous one-parameter subgroup $\alpha = \{\alpha^t \mid t \in \mathbb{R}\}$ of the group $\text{Aut}(\mathcal{O})$ of $*$ -automorphisms of \mathcal{O} —we will often refer to such α as a C^* -dynamics. States of the system are normalized positive linear functionals on \mathcal{O} . The set $\mathcal{S}(\mathcal{O})$ of all states

³The unit will be denoted by $\mathbb{1}$.

is a convex weak*-compact subset of the dual Banach space \mathcal{O}^* . In the specific case of a system of spins or fermions on a lattice, we will denote the algebra of observables by \mathfrak{A} ; see Section 2.1. For some models the natural starting point is rather a W^* -dynamical system; we will comment on such models in Section 2.4.

The seminal work [HHW67] introduced the KMS-condition as a characterization of thermal equilibrium states of (\mathcal{O}, α) at inverse temperature $\beta > 0$. A state $\omega \in \mathcal{S}(\mathcal{O})$ is (α, β) -KMS if, for all $A, B \in \mathcal{O}$, the function defined by

$$\mathbb{R} \ni t \mapsto F_{A,B}(t) = \omega(A\alpha^t(B)),$$

has an analytic continuation to the strip $0 < \text{Im } z < \beta$, that is bounded and continuous on its closure, and satisfies the KMS-boundary condition

$$F_{A,B}(t + i\beta) = \omega(\alpha^t(B)A).$$

Any (α, β) -KMS state is α -invariant. A quantum dynamical system $(\mathcal{O}, \alpha, \omega)$, where ω is a (α, β) -KMS state, describes a physical system in thermal equilibrium at temperature $1/\beta$.

It is mathematically convenient to extend, in the obvious way, the definition of KMS-states to all $\beta \in \mathbb{R}$. Of particular interest is the value $\beta = -1$ which links the KMS-condition to the Tomita–Takesaki modular theory of operator algebras.

The general theory of KMS states, developed in the early days of algebraic quantum statistical mechanics, is summarized in [BR81, Sections 5.3 and 5.4]. To set up the notation to be used below, let us mention the following remarkable stability property of a (α, β) -KMS state $\omega \in \mathcal{S}(\mathcal{O})$. Denoting by δ the generating derivation $\alpha^t = e^{t\delta}$, there is a norm-continuous map $\mathcal{O} \ni V = V^* \mapsto \omega_V \in \mathcal{S}(\mathcal{O})$, such that $\omega_0 = \omega$ and ω_V is (α_V, β) -KMS, where α_V is generated by $\delta + i[V, \cdot]$. We shall say that the C^* -dynamics α_V is a local perturbation of α .

Dynamical characterizations of KMS states are of particular relevance in the context of the present work; see [BR81, Section 5.4.2]. Indeed, the problem of approach to equilibrium can be viewed as an ultimate step in such characterizations. More generally, the foundations of algebraic quantum statistical mechanics are described in the classical monographs [BR87, BR81, Haa96, Isr79, Sim93, Rue69, Thi02]; for a more modern perspective see [DJP03, JOPP10, Pil06]. From those foundations stem the two directions of research that were actively pursued over the last twenty-five years.

1. Return to Equilibrium. The formulation of this property of quantum dynamical systems and the first basic results go back to the seminal works of Robinson [Rob73, Rob76]; [BM83, AM03, JP96, JP97, BFS00, JP01a, BF02, DJ03, FMSU03, FM04, DRK11] is an incomplete list of references of the follow-up works on the subject. Among several equivalent formulations of return to equilibrium we choose here the following one. The quantum dynamical system $(\mathcal{O}, \alpha, \omega)$, in thermal equilibrium at inverse temperature β , is said to have the property of return to equilibrium if, for all $V = V^* \in \mathcal{O}$ and all $A \in \mathcal{O}$,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \omega_V \circ \alpha^t(A) dt = \omega(A).$$

In the setting of classical dynamical systems, the property of return to equilibrium is equivalent to ergodicity, and its importance/relevance in quantum statistical mechanics parallels the classical one.

2. *Non-Equilibrium Steady States and Entropy Production.* This topic was implicit in some early works in algebraic quantum statistical mechanics; see in particular [PW78]. Its modern formulation goes back to [Rue00, Rue01, JP01b] and builds on the notions of non-equilibrium steady states and entropy production in classical statistical mechanics introduced in early 1990's; see [Rue99] for references and additional information. To describe this topic, consider a quantum dynamical system $(\mathcal{O}, \alpha, \omega)$ where ω is α -invariant but *not* (α, β) -KMS for any $\beta \in \mathbb{R}$. The Non-Equilibrium Steady States (NESS) of $(\mathcal{O}, \alpha, \omega)$ associated to $V = V^* \in \mathcal{O}$ are the weak*-limit points of the net

$$\left\{ \frac{1}{T} \int_0^T \omega \circ \alpha_V^t dt \right\}_{T>0}$$

as $T \uparrow \infty$. The set of NESS is non-empty and its elements are α_V -invariant. To define the entropy production of a NESS, we suppose that there exists a reference C^* -dynamics ζ_ω such that ω is a $(\zeta_\omega, -1)$ -KMS state. Let δ_ω be the generator of ζ_ω , and suppose that V is in the domain of δ_ω . The associated entropy production observable is $\sigma_V = \delta_\omega(V)$. The entropy production rate of a NESS ω_+ is the real number $\omega_+(\sigma_V)$. The pertinence of this definition stems from the entropy balance equation of [PW78, Rue78, JP01b]:

$$S(\omega \circ \alpha_V^T | \omega) = \int_0^T \omega \circ \alpha_V^t(\sigma_V) dt, \quad (1)$$

where $S : \mathcal{S}(\mathcal{O}) \times \mathcal{S}(\mathcal{O}) \rightarrow [0, \infty]$ is Araki's relative entropy functional.⁴ In particular, the sign of S and the definition of NESS immediately give that $\omega_+(\sigma_V) \geq 0$. The works [HA00, Pil01, JP01b, JP02a, JP02b, FMU03, JP03, MO03, TM03, Oga04, AJPP06, JOP06a, JOP06c, JOP06b, Pil06, AJPP07, JOP07, MMS07a, MMS07b, DR09, JOPP10, JOPS12] build on these starting points and develop the structural theory of NESS and entropy production, including studies of several classes of concrete physically relevant models.

In this paper we initiate a third direction of research that also originates in the early foundations of algebraic quantum statistical mechanics, and closes the circle of ideas and techniques introduced in the study of the above two directions.

3. *The problem of approach to equilibrium in quantum statistical mechanics.* Consider a quantum dynamical system $(\mathfrak{A}, \alpha_\Phi, \omega)$, where \mathfrak{A} is the C^* -algebra of a system of lattice spins or fermions, α_Φ is the C^* -dynamics generated by a sufficiently regular translation invariant interaction Φ , and ω is a translation invariant state. The Equilibrium Steady States (ESS) of $(\mathfrak{A}, \alpha_\Phi, \omega)$ are the weak*-limit points of the net

$$\left\{ \frac{1}{T} \int_0^T \omega \circ \alpha_\Phi^t dt \right\}_{T>0}$$

as $T \uparrow \infty$. The set of ESS is non-empty and its elements are α_Φ -invariant. The aim is to develop the structural theory of ESS and eventually determine the conditions under which ESS are KMS-states for α_Φ .

⁴Our sign and ordering conventions are such that, for density matrices ρ_1, ρ_2 , $S(\rho_1 | \rho_2) = \text{tr}(\rho_1(\log \rho_1 - \log \rho_2))$. We refer the reader to [OP93] for an in depth discussion of relative entropy.

In this work we examine the structural aspects of the problem of approach to equilibrium in the special case where ω is a KMS state for some interaction Ψ . We show that, except in trivial cases, the process of approach to equilibrium is accompanied by a strict increase of the specific energy and entropy. To establish that, we introduce the concept of weak Gibbsianity in quantum statistical mechanics and adapt the idea of entropy balance to the approach to equilibrium setting.

The remaining parts of this article are organized as follows. In Section 2.1, we give a telegraphic review of quantum spin and fermion systems. Weak Gibbs states and the related entropy balance equation are discussed in Section 2.2. Our main results are stated in Section 2.3 and discussed in Section 2.4.

The proofs are given in Section 3.

In the follow-up work [JPT23], we use the same general ingredients (a) and (b) above to examine the status of the adiabatic theorem in the translation invariant setting of infinitely extended lattice quantum spin and fermionic systems.

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2 Setting and main results

2.1 Quantum spin and fermion systems

The spin C^* -algebra. Let \mathcal{H} be the finite dimensional Hilbert space of a single spin and consider the lattice \mathbb{Z}^d equipped with the norm $|x| = \sum_{j=1}^d |x_j|$. Let \mathcal{F} be the collection of all finite subsets of \mathbb{Z}^d . We denote by $\text{diam}(X) = \max\{|x - y| \mid x, y \in X\}$ the diameter of $X \in \mathcal{F}$, and write $\mathcal{H}_X = \otimes_{x \in X} \mathcal{H}_x$, where $\mathcal{H}_x = \mathcal{H}$, and $\mathfrak{A}_X = \mathcal{B}(\mathcal{H}_X)$.⁵ If $Y \subset X$, we identify in a natural way \mathfrak{A}_Y with a subalgebra of \mathfrak{A}_X . For $X \subset \mathbb{Z}^d$, we denote by \mathfrak{A}_X the inductive limit C^* -algebra over the family $\{\mathfrak{A}_Y\}_{Y \supset X \in \mathcal{F}}$. The kinematical algebra of the spin system is $\mathfrak{A}_{\mathbb{Z}^d}$ and in the sequel we will omit the subscript \mathbb{Z}^d . The algebra \mathfrak{A} is simple, which implies in particular that any KMS state on \mathfrak{A} is faithful; see [Isr79, Lemma III.3.3].

For any $X \subset \mathbb{Z}^d$, $X^c = \mathbb{Z}^d \setminus X$, we have the identification $\mathfrak{A} = \mathfrak{A}_X \otimes \mathfrak{A}_{X^c}$, and $\text{tr}_X : \mathfrak{A} \rightarrow \mathfrak{A}_{X^c}$ denotes the usual normalized partial trace. An element $A \in \mathfrak{A}$ is called *local* if $A \in \mathfrak{A}_X$ for some $X \in \mathcal{F}$. The minimal X for which this hold is called the support of A and is denoted by $\text{supp}(A)$. The set $\mathfrak{A}_{\text{loc}}$ of local elements is a dense $*$ -subalgebra of \mathfrak{A} .

In the following Λ will always denote a cube in \mathbb{Z}^d centered at the origin and $\Lambda \uparrow \mathbb{Z}^d$ denotes the limit over an increasing family of such cubes.

⁵ $\mathcal{B}(\mathcal{H})$ denotes the C^* -algebra of all linear operators on the Hilbert space \mathcal{H} .

Translation invariant states. The spin algebra \mathfrak{A} is uniformly asymptotically Abelian w.r.t. the natural group action $\varphi : \mathbb{Z}^d \ni x \mapsto \varphi^x \in \text{Aut}(\mathfrak{A})$, i.e.,

$$\lim_{|x| \rightarrow \infty} \|[\varphi^x(A), B]\| = 0$$

for all $A, B \in \mathfrak{A}$. We denote by $\mathcal{S}_1(\mathfrak{A})$ the set of all translation invariant, i.e., φ -invariant states on \mathfrak{A} . $\mathcal{S}_1(\mathfrak{A})$ is a weak*-compact convex subset of $\mathcal{S}(\mathfrak{A})$ and a Choquet simplex.

Specific entropies. The restriction ν_Λ of a state $\nu \in \mathcal{S}_1(\mathfrak{A})$ to \mathfrak{A}_Λ is represented by a density matrix in \mathfrak{A}_Λ which we denote by the same letter: For any $A \in \mathfrak{A}_\Lambda$,

$$\nu(A) = \nu_\Lambda(A) = \text{tr}(\nu_\Lambda A).$$

The von Neumann entropy of ν_Λ is defined by $S(\nu_\Lambda) = -\text{tr}(\nu_\Lambda \log \nu_\Lambda)$ and is non-negative. The *specific entropy* of ν is given by the limit

$$s(\nu) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\nu_\Lambda)}{|\Lambda|}, \quad (2)$$

which exists and defines an affine, weak*-upper-semicontinuous map $\mathcal{S}_1(\mathfrak{A}) \ni \nu \mapsto s(\nu)$, taking its values in $[0, \log \dim \mathcal{H}]$; see [BR81, Proposition 6.2.38].

The *specific relative entropy* of ν w.r.t. $\omega \in \mathcal{S}_1(\mathfrak{A})$ is defined by

$$s(\nu|\omega) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\nu_\Lambda|\omega_\Lambda)}{|\Lambda|},$$

whenever the limit exists, in which case we have $s(\nu|\omega) \geq 0$.

Interactions. An *interaction* is a family $\Phi = \{\Phi(X)\}_{X \in \mathcal{F}}$, where $\Phi(X) \in \mathfrak{A}_X$ is self-adjoint. The interaction Φ is translation invariant if

$$\varphi^x(\Phi(X)) = \Phi(X+x)$$

holds for all $X \in \mathcal{F}$ and $x \in \mathbb{Z}^d$. In what follows we consider only translation invariant interactions. The *local Hamiltonians* associated to Φ are defined by

$$H_\Lambda(\Phi) = \sum_{X \subset \Lambda} \Phi(X).$$

For $r > 0$ we denote by \mathcal{B}^r the set of all translation invariant interactions such that

$$\|\Phi\|_r = \sum_{X \ni 0} e^{r(|X|-1)} \|\Phi(X)\| < \infty, \quad (3)$$

where $|X|$ denotes the cardinality of $X \in \mathcal{F}$. The pair $(\mathcal{B}^r, \|\cdot\|_r)$ is a Banach space. An interaction Φ is called *finite range* whenever, for some $m \in \mathbb{N}$, $\text{diam}(X) > m$ implies $\Phi(X) = 0$. The set \mathcal{B}_f of all finite range interactions is a dense subspace of \mathcal{B}^r .

In what follows we restrict ourselves to interactions in \mathcal{B}^r although many of the stated results hold in more general settings.

The Gibbs variational principle. [BR81, Proposition 6.2.39 and Theorem 6.2.40] For any interaction $\Phi \in \mathcal{B}^r$ the limit

$$P(\Phi) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \text{tr}(e^{-H_\Lambda(\Phi)}) \quad (4)$$

exists and is finite. The function P defined in this way is called the *pressure*. Setting

$$E_\Phi = \sum_{X \ni 0} \frac{\Phi(X)}{|X|} \in \mathfrak{A},$$

one has

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \left\| H_\Lambda(\Phi) - \sum_{x \in \Lambda} \varphi^x(E_\Phi) \right\| = 0, \quad (5)$$

and in particular

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \omega(H_\Lambda(\Phi)) = \omega(E_\Phi), \quad (6)$$

for any $\omega \in \mathcal{S}_1(\mathfrak{A})$. Thus, E_Φ can be considered as the *specific energy* observable of the interaction Φ .

Theorem 2.1 (Gibbs variational principle). *For any $\beta \in \mathbb{R}$ and $\Phi \in \mathcal{B}^r$,*

$$P(\beta\Phi) = \sup_{\nu \in \mathcal{S}_1(\mathfrak{A})} (s(\nu) - \beta\nu(E_\Phi)).$$

Moreover,

$$\mathcal{S}_{\text{eq}}(\beta\Phi) = \{\nu \in \mathcal{S}_1(\mathfrak{A}) \mid P(\beta\Phi) = s(\nu) - \beta\nu(E_\Phi)\}$$

is a non-empty convex compact subset of $\mathcal{S}_1(\mathfrak{A})$.

The elements of $\mathcal{S}_{\text{eq}}(\beta\Phi)$ are called *equilibrium states* for the interaction $\beta\Phi$.

Dynamics. [Rue67, Theorem 7.6.2] For an interaction $\Phi \in \mathcal{B}^r$ and a finite cube Λ , set

$$\alpha_{\Phi, \Lambda}^t(A) = e^{itH_\Lambda(\Phi)} A e^{-itH_\Lambda(\Phi)}$$

with $t \in \mathbb{R}$ and $A \in \mathfrak{A}_{\text{loc}}$. Then, the limit

$$\alpha_\Phi^t(A) = \lim_{\Lambda \uparrow \mathbb{Z}^d} \alpha_{\Phi, \Lambda}^t(A)$$

exists and is uniform for t in compact sets. Moreover, the family of maps $\alpha_\Phi = \{\alpha_\Phi^t \mid t \in \mathbb{R}\}$, originally defined on $\mathfrak{A}_{\text{loc}}$, extends uniquely to a C^* -dynamics on \mathfrak{A} . The group actions α_Φ and φ commute.

We recall the following basic result [BR81, Theorem 6.2.42].

Theorem 2.2. *Suppose that $\Phi \in \mathcal{B}^r$. Then, for any $\beta \in \mathbb{R}$, $\mathcal{S}_{\text{eq}}(\beta\Phi)$ coincides with the set of all translation invariant (α_Φ, β) -KMS states.*

The proofs of the above results give additional information. In particular, the following result follows from the proofs of [Rue69, Lemma 7.6.1 and Theorem 7.6.2] or [BR81, Theorem 6.2.4]:

Theorem 2.3. *Suppose that $\Phi \in \mathcal{B}^r$. Then, for all $A \in \mathfrak{A}_{\text{loc}}$, the map*

$$\mathbb{R} \ni t \mapsto \alpha_\Phi^t(A) \in \mathfrak{A}$$

has an analytic extension to the strip

$$|\text{Im } z| < \frac{r}{2\|\Phi\|_r},$$

and for z in this strip

$$\|\alpha_\Phi^z(A)\| \leq \|A\| e^{r|\text{supp}(A)|} \frac{r}{r - 2\|\Phi\|_r |\text{Im } z|}.$$

Remark. According to [BR81, Theorem 6.2.4], the conclusions of Theorem 2.3 still hold for interactions Φ which lack translation invariance, provided the norm (3) is replaced by

$$\|\Phi\|_r = \sum_{N \geq 1} \sup_{x \in \mathbb{Z}^d} \sum_{\substack{X \ni x \\ |X|=N}} \|\Phi(X)\| e^{r(|X|-1)} < \infty.$$

Setting $\beta = 1$. To reduce the number of parameters, it is convenient to absorb β into the interaction Φ . With this convention small interactions correspond to high temperatures. We will comment further on this point at the end of Section 2.3.

In the remaining part of the paper we set $\beta = 1$. $(\alpha_\Phi, 1)$ -KMS state will be abbreviated as α_Φ -KMS state.

Uniqueness of equilibrium state.

Theorem 2.4. *Suppose that $\Phi \in \mathcal{B}^r$ and that either:*

- (1) $d = 1$ and $\sum_{X \ni 0} \text{diam}(X) \|\Phi(X)\| < \infty$.
- (2) $d \geq 1$, $r > \log \dim \mathcal{H}$, and $\|\Phi\|_r < \frac{1}{2 \dim \mathcal{H}}$.

Then $\mathcal{S}_{\text{eq}}(\Phi)$ is a singleton.

Part (1) is the classical result of Araki; see [Sim93, Theorem IV.6.1]. Regarding Part (2), among the many results in the literature that establish the uniqueness of the equilibrium state in the high temperature regime, we have quoted here the one obtained relatively recently in [FU15].

The Gibbs condition. [BR81, Proposition 6.2.17] We will only introduce the part of the Gibbs condition that will be needed in the sequel. For an interaction $\Phi \in \mathcal{B}^r$, the *surface energies*

$$W_\Lambda(\Phi) = \sum_{\substack{X \cap \Lambda \neq \emptyset \\ X \cap \Lambda^c \neq \emptyset}} \Phi(X) \tag{7}$$

are well defined and satisfy

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{\|W_\Lambda(\Phi)\|}{|\Lambda|} = 0. \tag{8}$$

Theorem 2.5. *Let ω be a α_Φ -KMS state, and ω_{-W} the perturbed KMS-state with $W = W_\Lambda(\Phi)$. Then for any Λ and any $A \in \mathfrak{A}_\Lambda$ one has*

$$\omega_{-W}(A) = \frac{\text{tr}(e^{-H_\Lambda(\Phi)} A)}{\text{tr}(e^{-H_\Lambda(\Phi)})}.$$

Physical equivalence. The concept of physical equivalence was first introduced in [Roo74] as a physical interpretation of a technical assumption from [GR71], and was further developed in [Isr79]. Our definition below differs from the original one and is based on [Rue78, Section 4.7]; for additional information see [vEFS93, Section 2.4.6].

Definition 2.6. Two interactions $\Phi, \Psi \in \mathcal{B}^r$ are called *physically equivalent*, denoted $\Phi \sim \Psi$, if

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \varphi^x(E_{\Phi-\Psi}) = \text{tr}(E_{\Phi-\Psi}) \mathbb{1}.$$

Notice that $E_{\Phi-\Psi} = E_\Phi - E_\Psi$. Physical equivalence is obviously an equivalence relation on \mathcal{B}^r . Moreover, if $\Phi_1 \sim \Psi_1$ and $\Phi_2 \sim \Psi_2$, then $a\Phi_1 + b\Phi_2 \sim a\Psi_1 + b\Psi_2$ for any $a, b \in \mathbb{R}$.

Theorem 2.7. *Let $\Phi, \Psi \in \mathcal{B}^r$. The following statements are equivalent:*

- (a) $\Phi \sim \Psi$.
- (b) $\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} (H_\Lambda(\Phi) - H_\Lambda(\Psi)) = \text{tr}(E_{\Phi-\Psi}) \mathbb{1}$.
- (c) *The pressure P is linear on the line segment connecting Φ and Ψ .*
- (d) $\mathcal{S}_{\text{eq}}(\Phi) \cap \mathcal{S}_{\text{eq}}(\Psi) \neq \emptyset$.
- (e) $\mathcal{S}_{\text{eq}}(\Phi) = \mathcal{S}_{\text{eq}}(\Psi)$.
- (f) $\alpha_\Phi = \alpha_\Psi$.
- (g) $\sum_{X \in \mathcal{F}} [\Phi(X) - \Psi(X), A] = 0$ for all $A \in \mathfrak{A}_{\text{loc}}$.

The equivalence between (c), (d), (e), and (f) is proved in [Isr79, Theorem III.4.2]. We prove the remaining parts in Section 3.1 below.

The case of fermions. We denote by $\mathcal{A} = \text{CAR}(\mathfrak{h})$ the CAR algebra over the Hilbert space \mathfrak{h} . As usual, $a^*(f)/a(f)$ are the creation/annihilation operators associated to $f \in \mathfrak{h}$, and $a^\#$ stands for either a or a^* . Given a unitary operator u on \mathfrak{h} , the map $a^\#(f) \mapsto a^\#(uf)$ uniquely extends to a $*$ -automorphism α_u of \mathcal{A} , the *Bogoliubov automorphism* generated by u . A strongly continuous one-parameter group of unitaries $t \mapsto u^t$ on \mathfrak{h} generates a strongly continuous one-parameter subgroup of $\text{Aut}(\mathcal{A})$. The gauge group of \mathcal{A} is the group of Bogoliubov automorphisms $\theta \mapsto \vartheta^\theta$ generated by $e^{i\theta \mathbb{1}}$. Physical observables are gauge invariant, *i.e.*, elements of

$$\mathfrak{A}(\mathfrak{h}) = \{A \in \mathcal{A} \mid \vartheta^\theta(A) = A \text{ for all } \theta \in \mathbb{R}\},$$

which coincides with the C^* -algebra generated by $\{a^*(f)a(g) \mid f, g \in \mathfrak{h}\} \cup \{\mathbb{1}\}$. We will only consider the case $\mathfrak{h} = \ell^2(\mathbb{Z}^d)$ and write \mathfrak{A} for $\mathfrak{A}(\ell^2(\mathbb{Z}^d))$. For $X \subset \mathbb{Z}^d$ we set $\mathfrak{A}_X = \mathfrak{A}(\ell^2(X))$ and identify \mathfrak{A}_X with the C^* -subalgebra of \mathfrak{A} generated by

$$\{a^*(f)a(g) \mid f, g \in \ell^2(\mathbb{Z}^d), \text{supp}(f) \cup \text{supp}(g) \subset X\} \cup \{\mathbb{1}\}.$$

Note that if $X \cap Y = \emptyset$, then \mathfrak{A}_X and \mathfrak{A}_Y commute. The natural unitary group action of \mathbb{Z}^d on $\ell^2(\mathbb{Z}^d)$ gives rise to a group of Bogoliubov automorphisms φ^x such that $\varphi^x(\mathfrak{A}_X) = \mathfrak{A}_{X+x}$.

For $X \in \mathcal{F}$, $\mathcal{A}_X = \text{CAR}(\ell^2(X))$ is isomorphic to the full matrix-algebra $\mathcal{B}(\mathbb{C}^{2^{|X|}})$, so that $\mathcal{A} = \text{CAR}(\ell^2(\mathbb{Z}^d))$ has a unique tracial state tr as the extension of the unique tracial states of \mathcal{A}_X , $X \in \mathcal{F}$. \mathcal{A} is isomorphic to the spin algebra, with the main difference that the identification of \mathcal{A} with $\mathcal{A}_X \otimes \mathcal{A}_{X^c}$ does not hold anymore. Nevertheless, there exists an analogue of partial trace for fermions called conditional expectation in [AM03, Theorem 4.7]: for $X \subset \mathbb{Z}^d$, there exists a projection $\mathcal{T}_X : \mathcal{A} \rightarrow \mathcal{A}_X$ such that $\text{tr}(AB) = \text{tr}(\mathcal{T}_X(A)B)$ for any $B \in \mathcal{A}_X$.

All the above definitions and results stated for the spin algebra extend to the gauge-invariant sector \mathfrak{A} of the fermionic algebra \mathcal{A} . Most, but not all, of these extensions are straightforward: for the Gibbs variational principle and the Gibbs condition see [AM03, Theorems 11.4 and 7.5]. In the fermionic case there is also a special one-body interaction $N \in \mathcal{B}_f$, related to gauge invariance, and given by

$$N(X) = \begin{cases} a_x^* a_x & \text{if } X = \{x\}; \\ 0 & \text{otherwise.} \end{cases}$$

We denote $N_\Lambda = \sum_{X \subset \Lambda} N(X)$ the local Hamiltonians associated to N .⁶ For $\omega \in S_I(\mathfrak{A})$,

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \omega(N_\Lambda) = \omega(E_N),$$

where $E_N = a_0^* a_0$. The perturbed interactions $\Phi - \mu N$ introduces a chemical potential μ .

To summarize, all results of this paper apply to both spin and fermions, and so in the following \mathfrak{A} refers equivalently to the spin or the gauge-invariant sector of the CAR algebra, unless stated explicitly.

We finish this section with:

Conservation laws.

Theorem 2.8. *For any $\omega \in \mathcal{S}_1(\mathfrak{A})$ and any $\Phi \in \mathcal{B}^r$ the following hold for all $t \in \mathbb{R}$:*

- (1) $s(\omega) = s(\omega \circ \alpha_\Phi^t)$.
- (2) $\omega(E_\Phi) = \omega \circ \alpha_\Phi^t(E_\Phi)$.
- (3) *In the fermionic case, $\omega(E_N) = \omega \circ \alpha_\Phi^t(E_N)$.*

Part (1) is due to [LR68]. The proofs of the remaining statements are given in Section 3.2.

2.2 Weak Gibbs states and regularity

We set

$$\omega_{\Phi, \Lambda}^c = e^{-H_\Lambda(\Phi) - P_\Lambda(\Phi)}, \quad P_\Lambda(\Phi) = \log \text{tr}(e^{-H_\Lambda(\Phi)}).$$

Definition 2.9. A state $\omega \in \mathcal{S}_1(\mathfrak{A})$ is called *weak Gibbs* for the interaction $\Phi \in \mathcal{B}^r$ if there exist constants $c_\Lambda > 0$ satisfying

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} c_\Lambda = 0, \tag{9}$$

⁶The interaction N generates the gauge group, $\vartheta^\theta = \alpha_N^\theta$.

and such that, for all Λ ,

$$e^{-c_\Lambda} \omega_{\Phi, \Lambda}^c \leq \omega_\Lambda \leq e^{c_\Lambda} \omega_{\Phi, \Lambda}^c. \quad (10)$$

ω is called *log weak Gibbs* for Φ if there exist constants $c_\Lambda > 0$ satisfying (9) and such that, for all Λ ,

$$-c_\Lambda + \log \omega_{\Phi, \Lambda}^c \leq \log \omega_\Lambda \leq c_\Lambda + \log \omega_{\Phi, \Lambda}^c. \quad (11)$$

We denote by $\text{WG}(\Phi)$ the set of all weak Gibbs states for Φ , and by $\text{LWG}(\Phi)$ the set of all log weak Gibbs states.

The next proposition, whose proof is given in Section 3.3, collects a few elementary properties of the sets $\text{WG}(\Phi)$ and $\text{LWG}(\Phi)$.

Proposition 2.10. *For $\Phi, \Psi \in \mathcal{B}^r$, the following hold:*

- (1) $\omega \in \text{LWG}(\Phi) \iff \limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_\Lambda - \log \omega_{\Phi, \Lambda}^c\| = 0$.
- (2) $\text{WG}(\Phi) \subset \text{LWG}(\Phi) \subset \mathcal{S}_{\text{eq}}(\Phi)$.
- (3) *Either $\text{LWG}(\Phi) = \text{LWG}(\Psi)$ or $\text{LWG}(\Phi) \cap \text{LWG}(\Psi) = \emptyset$.*
- (4) $\Phi \sim \Psi \implies \text{LWG}(\Phi) = \text{LWG}(\Psi)$. *Moreover, if $\text{LWG}(\Phi) = \text{LWG}(\Psi) \neq \emptyset$, then $\Phi \sim \Psi$.*

Regarding possible equalities in Part (2), one has the following results.

Theorem 2.11. *Suppose that either:*

- (a) $d = 1$ and $\Phi \in \mathcal{B}_f$;
- (b) $d \geq 1$, $\Phi \in \mathcal{B}^r$, and $\|\Phi\|_r < r$.

Then $\text{WG}(\Phi) = \text{LWG}(\Phi) = \mathcal{S}_{\text{eq}}(\Phi)$.

Section 3.4 is devoted to the proof which is based on general results from [Ara69] and [AI74, Section 3.1 and proof of Theorem 2], see also [Ara76] and [LRB05].

The following characterization of $\text{WG}(\Phi)$, based on the Gibbs condition, is proved in Section 3.5.

Proposition 2.12. *Suppose that $\Phi \in \mathcal{B}^r$ and let $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$. Set*

$$\underline{d}_\Lambda = \inf_{\substack{A \in \mathfrak{A}_\Lambda \\ A > 0}} \frac{\omega(A)}{\omega_{-W_\Lambda(\Phi)}(A)}, \quad \bar{d}_\Lambda = \sup_{\substack{A \in \mathfrak{A}_\Lambda \\ A > 0}} \frac{\omega(A)}{\omega_{-W_\Lambda(\Phi)}(A)}.$$

Then $\omega \in \text{WG}(\Phi)$ iff

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \underline{d}_\Lambda = \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \log \bar{d}_\Lambda = 0. \quad (12)$$

We finish this brief discussion of quantum weak Gibbs states with a characterization of $\text{LWG}(\Phi)$.

Proposition 2.13. *Suppose that $\Phi \in \mathcal{B}^r$ and let $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$.*

- (1) *For any $\nu \in \mathcal{S}(\mathfrak{A})$ and all $\Lambda \in \mathcal{F}$,*

$$S(\nu_\Lambda | \omega_\Lambda) - S(\nu_\Lambda | \omega_{\Phi, \Lambda}^c) \leq 2 \|W_\Lambda(\Phi)\|.$$

(2) For $\Lambda \in \mathcal{F}$, set

$$D_\Lambda = \inf_{\nu \in \mathcal{S}(\mathfrak{A})} (S(\nu_\Lambda | \omega_\Lambda) - S(\nu_\Lambda | \omega_{\Phi, \Lambda}^c)).$$

Then $\omega \in \text{LWG}(\Phi)$ iff

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{D_\Lambda}{|\Lambda|} = 0. \quad (13)$$

Part (1) is easily seen to be equivalent to the statement that for all $\Lambda \in \mathcal{F}$,

$$\log \omega_{\Phi, \Lambda}^c - \log \omega_\Lambda \leq 2 \|W_\Lambda(\Phi)\|,$$

which is proven in [HP93, Lemma 2.3]. With D_Λ as defined in Part (2), one has

$$D_\Lambda \leq \log \omega_{\Phi, \Lambda}^c - \log \omega_\Lambda,$$

so that Part (2) is an immediate consequence of Part (1), Relation (8) and the definition of log weak Gibbs states.

For our purposes, the importance of weak Gibbs states stems from the following result that is an immediate consequence of Definition 2.9.

Proposition 2.14. *Let $\Phi \in \mathcal{B}^r$ and $\omega \in \text{LWG}(\Phi)$. Then for any $\nu \in \mathcal{S}_1(\mathfrak{A})$,*

$$s(\nu | \omega) = -s(\nu) + \nu(E_\Phi) + P(\Phi). \quad (14)$$

In particular, $s(\nu | \omega) = 0$ iff $\nu \in \mathcal{S}_{\text{eq}}(\Phi)$.

We will comment further on weak Gibbsianity and regularity in Section 2.4.

Since the validity of (14) plays a central role in our arguments, we single it out in:

Definition 2.15. A pair $(\omega, \Phi) \in \mathcal{S}_1(\mathfrak{A}) \times \mathcal{B}^r$ is called regular whenever Relation (14) holds for any $\nu \in \mathcal{S}_1(\mathfrak{A})$.

Remarks. 1. Obviously, if the pair (ω, Φ) is regular, then $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$. If, in addition, $\mathcal{S}_{\text{eq}}(\Phi) = \{\omega\}$, then ω is φ -ergodic since it is extreme point of the simplex $\mathcal{S}_1(\mathfrak{A})$ (see [BR81, Theorem 6.2.44] and its proof). Using the regularity assumption, one can also argue in the following way. Suppose that $\omega = \alpha\mu + (1-\alpha)\nu$ for some $\mu, \nu \in \mathcal{S}_1(\mathfrak{A})$ and $\alpha \in]0, 1[$. The joint convexity of the relative entropy [OP93, Theorem 1.4] yields

$$\begin{aligned} 0 = s(\omega | \omega) &\leq \alpha s(\mu | \omega) + (1-\alpha)s(\nu | \omega) \\ &= \alpha(-s(\mu) + \mu(E_\Phi) + P(\Phi)) + (1-\alpha)(-s(\nu) + \nu(E_\Phi) + P(\Phi)) \\ &= -s(\alpha\mu + (1-\alpha)\nu) + (\alpha\mu + (1-\alpha)\nu)(E_\Phi) + P(\Phi) = s(\omega | \omega) = 0, \end{aligned}$$

from which we conclude that $s(\mu | \omega) = s(\nu | \omega) = 0$ and hence $\mu, \nu \in \mathcal{S}_{\text{eq}}(\Phi) = \{\omega\}$.

2. For $\nu \in \mathcal{S}_1(\mathfrak{A})$ and $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$, $\Phi \in \mathcal{B}^r$, we set

$$\bar{s}(\nu | \omega) = \limsup_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\nu_\Lambda | \omega_\Lambda)}{|\Lambda|}.$$

By Part (1) of Proposition 2.13 and Relations (2), (4) and (6),

$$\bar{s}(\nu | \omega) \leq -s(\nu) + \nu(E_\Phi) + P(\Phi). \quad (15)$$

Hence, proving regularity reduces to establishing the lower bound

$$\liminf_{\Lambda \uparrow \mathbb{Z}^d} \frac{S(\nu_\Lambda | \omega_\Lambda)}{|\Lambda|} \geq -s(\nu) + \nu(E_\Phi) + P(\Phi).$$

Remarkably, Theorem 2.11 remains the best existing result about this estimate.

3. In [HMO07, ORB11], the authors consider *asymptotically decoupled* states $\omega \in \mathcal{S}(\mathfrak{A})$ defined by the property

$$e^{-c_\Lambda} \omega_\Lambda \otimes \omega_{\Lambda^c} \leq \omega \leq e^{c_\Lambda} \omega_\Lambda \otimes \omega_{\Lambda^c},$$

where the c_Λ satisfy (9). If in addition $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$, $\Phi \in \mathcal{B}^r$, the proof of [HP93, Lemma 2.3] gives that $\omega \in \text{LWG}(\Phi)$.

2.3 Main results

For $\omega \in \mathcal{S}_1(\mathfrak{A})$ and $\Phi \in \mathcal{B}^r$, we set

$$\bar{\omega}_T = \frac{1}{T} \int_0^T \omega \circ \alpha_\Phi^t dt, \quad (16)$$

and denote by $\mathcal{S}_+(\omega, \Phi)$ the set of weak*-limit points of the net $\{\bar{\omega}_T\}_{T>0}$ as $T \rightarrow \infty$. We will call the elements of $\mathcal{S}_+(\omega, \Phi)$ *Equilibrium Steady States* (ESS) of $(\mathfrak{A}, \alpha_\Phi, \omega)$. The set $\mathcal{S}_+(\omega, \Phi)$ is obviously non-empty. Since \mathfrak{A} is separable, $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$ iff there exists sequence $T_n \uparrow \infty$ such that $\omega_+ = \lim_{n \rightarrow \infty} \bar{\omega}_{T_n}$. The invariance properties stated in Theorem 2.8 survive time-averaging, see Section 3.6.

Proposition 2.16. *For any $\omega \in \mathcal{S}_1(\mathfrak{A})$ and any $\Phi \in \mathcal{B}^r$ the following hold for all $T \in \mathbb{R}$:*

- (1) $s(\omega) = s(\bar{\omega}_T)$.
- (2) $\omega(E_\Phi) = \bar{\omega}_T(E_\Phi)$.
- (3) *In the fermionic case, $\omega(E_N) = \bar{\omega}_T(E_N)$.*

The elements of $\mathcal{S}_+(\omega, \Phi)$ have the following basic properties:

Proposition 2.17. *Let $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$. Then:*

- (1) $\omega_+ \in \mathcal{S}_1(\mathfrak{A})$ and $\omega_+ \circ \alpha_\Phi^t = \omega_+$ for all $t \in \mathbb{R}$.
- (2) $s(\omega) \leq s(\omega_+)$.
- (3) $\omega(E_\Phi) = \omega_+(E_\Phi)$.
- (4) *In the fermionic case, $\omega(E_N) = \omega_+(E_N)$.*

Part (1) follows from the translation invariance of the time averaged states $\bar{\omega}_T$ and a well known property on Cesàro averages. Part (2) follows from Proposition 2.16-(2) and the upper semi-continuity of the specific entropy. Parts (3) and (4) follows from Parts (2) and (3) of Proposition 2.16.

We now turn to our main results.

Theorem 2.18. *Let $\Phi, \Psi \in \mathcal{B}^r$, $\omega \in \mathcal{S}_{\text{eq}}(\Psi)$, and $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$. Then $\omega(E_\Psi) \leq \omega_+(E_\Psi)$.*

The remaining results depend critically on the regularity assumption.

Theorem 2.19. *Let $\Phi, \Psi \in \mathcal{B}^r$. Suppose that (ω, Ψ) is a regular pair and that $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$. Then the following statements are equivalent:*

- (a) $\omega(E_\Psi) = \omega_+(E_\Psi)$.
- (b) $\omega_+ \in \mathcal{S}_{\text{eq}}(\Psi)$ and $s(\omega) = s(\omega_+)$.

Suppose in addition that $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$. Then (a) and (b) are further equivalent to:

- (c) $\Phi \sim \Psi$.
- (d) $\omega = \omega_+$.

Theorem 2.20. *Let $\omega \in \mathcal{S}_1(\mathcal{Q})$, $\Phi \in \mathcal{B}^r$. For any $\omega_+ \in \mathcal{S}_+(\omega, \Phi) \cap \mathcal{S}_{\text{eq}}(\Phi)$ one has*

$$s(\omega) = s(\omega_+) \iff \omega = \omega_+.$$

An immediate consequence of these two theorems is:

Corollary 2.21. *Let $\omega \in \mathcal{S}_1(\mathcal{Q})$, $\Phi, \Psi \in \mathcal{B}^r$, $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$, and suppose that ω is not α_Φ -invariant.*

- (1) *If the pair (ω, Ψ) is regular and $\mathcal{S}_{\text{eq}}(\Psi) = \{\omega\}$, then $\omega(E_\Psi) < \omega_+(E_\Psi)$.*
- (2) *If $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$, then $s(\omega) < s(\omega_+)$.*

The proofs of Theorems 2.18, 2.19, and 2.20 are given in Sections 3.7, 3.8 and 3.9. Although they are technically not difficult, to the best of our knowledge they are the first general results about the strict increase of specific energy/entropy in quantum statistical mechanics. Central to the proof of the inequality $\omega(E_\Psi) < \omega_+(E_\Psi)$ is the properly identified concept of regularity. We emphasize that the latter property is quite universal: recall that according to Theorem 2.11, every equilibrium state at high temperature is weak Gibbs and hence is regular. The inequality $s(\omega) < s(\omega_+)$ is an immediate consequence of energy conservation $\omega(E_\Phi) = \omega_+(E_\Phi)$ and the Gibbs variational principle applied to $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$.

Remark. Fixing $\beta = 1$ arises differently in the contexts of the initial state $\omega \in \mathcal{S}_{\text{eq}}(\Psi)$ and the EES $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$. In the case of ω , β is simply absorbed in Ψ . On the other hand, rescaling Φ as $\gamma\Phi$, $\gamma > 0$, does not change EES, and instead gives a free parameter γ . Since ω_+ can be in at most one of the sets $\mathcal{S}_{\text{eq}}(\gamma\Phi)$, $\gamma > 0$,⁷ if it happens that we have approach to equilibrium and that $\omega_+ \in \mathcal{S}_{\text{eq}}(\tilde{\gamma}\Phi)$ for some $\tilde{\gamma} > 0$, rescaling Φ as $\tilde{\gamma}\Phi$ sets the inverse temperature of ω_+ to 1. In the next section we will comment on the choice of sign $\gamma > 0$ in this remark.

2.4 Remarks

Approach to equilibrium in algebraic quantum statistical mechanics. As we have already remarked, algebraic quantum statistical mechanics provides a natural mathematical framework for the study of dynamical aspects of important classes of infinitely extended quantum systems. In spite of its many successes, it remains unknown whether this framework, even in principle, can account for the zeroth law of thermodynamics. To the best of our knowledge,

⁷These sets are disjoint

the works [LR68, Hug83, Hug87] are the only attempts at a formulation of the problem. Guided by more recent works on foundations of non-equilibrium quantum statistical mechanics in the algebraic framework, we have presented here what we believe to be the minimal formulation of the problem of approach to equilibrium, and have obtained several structural results that are physically natural. Much remains to be done in developing a general structural theory and studying concrete physically relevant models in the context of this proposal.

We emphasize that Theorem 2.20 and the second parts of Theorem 2.19 and Corollary 2.21 are conditional results. The basic questions when the set $\mathcal{S}_+(\omega, \Phi)$ of ESS contains ω_+ such that $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$ remains open; no non-trivial example is known.

Theorem 2.18 and the first part of Theorem 2.19 and Corollary 2.21 are unconditional results. Their basic consequence is the inherent irreversibility of approach to equilibrium. To elucidate this point, let $\Phi, \Psi \in \mathcal{B}^r$, and suppose that (ω, Ψ) is a regular pair satisfying $\mathcal{S}_{\text{eq}}(\Psi) = \{\omega\}$. Let $\omega_+ \in \mathcal{S}_+(\omega, \Phi)$ and assume reversibility in the sense that $\omega \in \mathcal{S}_+(\omega_+, \Psi)$. Then, by Part (3) of Proposition 2.17, $\omega(E_\Psi) = \omega_+(E_\Psi)$, and the implication (a) \Rightarrow (b) of Theorem 2.19 gives that $\omega_+ \in \mathcal{S}_{\text{eq}}(\Psi) = \{\omega\}$. Hence, $\omega = \omega_+$, and the setting is trivial in the sense that ω is α_Φ -invariant. This irreversibility is in sharp contrast with the reversibility of return to equilibrium which we discuss below.

Direction of time. Changing the direction of time amounts to replacing the average (16) with

$$\bar{\omega}_T = \frac{1}{T} \int_0^T \omega \circ \alpha_\Phi^{-t} dt.$$

We denote by $\mathcal{S}_-(\omega, \Phi)$ the corresponding set of ESS. Since $\mathcal{S}_-(\omega, \Phi) = \mathcal{S}_+(\omega, -\Phi)$, none of results discussed in this paper is affected by such a change, as expected; see [Pei79, Section 3.8] for a lucid discussion of this point. If the quantum dynamical system $(\mathfrak{A}, \alpha_\Phi, \omega)$ is time-reversal invariant with time-reversal Θ^8 , then $\nu \in \mathcal{S}_-(\omega, \Phi)$ iff $\overline{\nu \circ \Theta} \in \mathcal{S}_+(\omega, \Phi)$ and $\mathcal{S}_-(\omega, \Phi) \cap \mathcal{S}_{\text{eq}}(\Phi) = \mathcal{S}_+(\omega, \Phi) \cap \mathcal{S}_{\text{eq}}(\Phi)$.

Question of Ruelle. To the best of our knowledge, the question about the increase of specific entropy with time was first raised in 1967 by David Ruelle. In [Rue67, p. 1666] Ruelle writes:

It is unclear to the author whether the evolution of an infinite system should increase its entropy per unit volume. Another possibility is that, when the time tends to $+\infty$, a state has a limit with strictly larger entropy.

In the context of quantum spin systems, the first part of the question was answered a year later by Lanford and Robinson [LR68]—the specific entropy remains constant for finite times. One of our main results sheds a light on the second part of Ruelle’s question by establishing the conditional result: if $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$ and $\omega \neq \omega_+$, then $s(\omega_+) > s(\omega)$. As discussed above, a parallel to Ruelle’s question and another signature of irreversibility is the inequality $\omega_+(E_\Psi) > \omega(E_\Psi)$. Our other main result is that this inequality unconditionally holds in the high temperature regime and that its general validity is linked to the concept of regularity.

Comparison with return to equilibrium. In spite of a formal similarity, it is important to emphasize that the properties of return to equilibrium and approach to equilibrium are very different. Return to equilibrium is an ergodic property asserting that thermal equilibrium states

⁸ Θ is an anti-linear $*$ -automorphism of \mathfrak{A} satisfying $\Theta \circ \alpha_\Phi^t = \alpha_\Phi^{-t} \circ \Theta$ for all $t \in \mathbb{R}$ and $\omega(\Theta(A)) = \omega(A^*)$ for all $A \in \mathfrak{A}$.

are stable under *local perturbations*. Approach to equilibrium asserts that, under a *global perturbation*, the system approaches a new equilibrium state. The mechanisms leading to the respective phenomena are completely different. In return to equilibrium, a local perturbation V disperses to spatial infinity while the specific entropy remains constant in the large time limit. It is perfectly possible, and in fact quite common, that $\omega \neq \omega_V$ and that both dynamical systems $(\mathcal{O}, \alpha, \omega)$ and $(\mathcal{O}, \alpha_V, \omega_V)$ have the property of return to equilibrium, in which case return to equilibrium is non-trivially reversible in the sense that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \omega \circ \alpha_V^t dt = \omega_V \quad \text{and} \quad \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \omega_V \circ \alpha^t dt = \omega.$$

In comparison, approach to equilibrium is inherently irreversible, as discussed in the previous remark.

The formal similarity between the return and approach to equilibrium requires a further comment. Consider a triple $(\mathfrak{A}, \alpha_\Psi, \omega)$, where $\Psi \in \mathcal{B}^r$ and ω is a α_Ψ -KMS state. Let $\Phi \in \mathcal{B}^r$ and consider the local perturbation

$$V_\Lambda = \sum_{X \subset \Lambda} (\Phi(X) - \Psi(X)).$$

Denoting by α_Λ the perturbed C^* -dynamics, and by ω_Λ the perturbed KMS-state, and assuming that $(\mathfrak{A}, \alpha_\Lambda, \omega_\Lambda)$ has the property of return to equilibrium, one has

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \omega \circ \alpha_\Lambda^t dt = \omega_\Lambda.$$

It is not difficult to show that $\lim_{\Lambda \uparrow \mathbb{Z}^d} \alpha_\Lambda^t = \alpha_\Phi^t$ strongly, and that for sufficiently small interactions $\lim_{\Lambda \uparrow \mathbb{Z}^d} \omega_\Lambda = \omega_+$, where ω_+ is the unique α_Φ -KMS state. Under these circumstances⁹ one has

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \omega \circ \alpha_\Lambda^t dt = \omega_+. \quad (17)$$

If the two limits in (17) can be interchanged, then approach to equilibrium holds. Our main results imply that this strategy cannot be reduced to technical improvements of the existing spectral/scattering estimates used in the literature to establish return to equilibrium and that novel ideas are needed.

Comparison with the non-equilibrium theory. The mathematical theory of non-equilibrium quantum statistical mechanics developed over the last twenty years has played an important role in the genesis of this work. In fact, a strong similarity exists between the conceptual framework of the present paper and the one developed in [JP01b, Rue99], in the context of a now mature non-equilibrium quantum statistical program.

The entropy balance equation, Identity (1), is the central starting point of the non-equilibrium theory. The regularity condition (14) plays a similar role in the structural theory of approach to equilibrium developed in this work.

In the construction of Non-Equilibrium Steady States (NESS) proposed in the above mentioned program, the state of the system at time t , given by $\omega \circ \alpha_V^t$, is normal with respect to the initial state ω . The NESS, however, are typically singular with respect to ω , and in fact under suitable regularity assumptions, the strict positivity of entropy production—a signature of non-equilibrium—is equivalent to this singularity. These regularity assumptions can be either verified generically or by a detailed study of concrete models; for discussion of these points we refer

⁹The principal of which is that $(\mathfrak{A}, \alpha_\Lambda, \omega_\Lambda)$ has the property of return to equilibrium for all large enough Λ .

the reader to [AJPP06,JP02a,JP07]. On the other hand, in the context of Theorems 2.19 and 2.20, and recalling the remark after Definition 2.15, if (ω, Ψ) is a regular pair such that $\mathcal{S}_{\text{eq}}(\Psi) = \{\omega\}$, then, for any t , the state $\omega \circ \alpha_{\Phi}^t$ is φ -ergodic, and so either $\omega \circ \alpha_{\Phi}^t = \omega$ or the states $\omega \circ \alpha_{\Phi}^t$ and ω are mutually singular. The same holds for the ESS $\omega_+ \in \mathcal{S}_+(\omega, \Phi) \cap \mathcal{S}_{\text{eq}}(\Phi)$: either $\omega = \omega_+$ or the states ω and ω_+ are mutually singular, and in the later case $s(\omega_+) > s(\omega)$. To summarize, the singularity of the NESS in the non-equilibrium setting is an essential and non-trivial dynamical problem. The singularity of ESS in the approach of equilibrium setting is a direct consequence of the translation invariance and the general structure of algebraic quantum statistical mechanics. The generality of our results, in comparison with related results in non-equilibrium statistical mechanics, can be understood in these terms.

Weak coupling limit. The weak coupling (or van Hove) limit sheds further light on the above remarks. In the context of return to equilibrium, NESS, and Entropy Production, open quantum systems consisting of small quantum system with finite dimensional Hilbert space locally coupled to finitely many free fermionic or bosonic reservoirs—such models are often called Pauli–Fierz systems—play a privileged role. The weak coupling limit of such models is described by Pauli’s master equation and the respective theory was developed in seminal works [Dav74,SL78]; for modern expositions of this theory see [DF06,JPW14]. The weak coupling limit theory played a very important role in more recent studies of return of equilibrium. In a similar spirit, the interacting fermion systems of [ESY04,Hug83,Hug87] play a privileged role in study of approach to equilibrium. The weak coupling limit of such models is formally described by the quantum Boltzmann equation whose mathematically rigorous derivation remains an outstanding open problem; see [BCEP07,LS11,HLP21] for a review and important progresses in this direction.

Weak Gibbsianity and regularity. In spite of its relative late appearance, the concept of weak Gibbs state plays an important role in the study of invariant measures of classical dynamical systems, as a natural boundary for the validity of the thermodynamic formalism. In the framework of statistical mechanics it is known that, under very general conditions, the equilibrium states of classical spin systems with summable interactions are weak Gibbs¹⁰ [PS20]. Theorem 2.11 is a much weaker result. Its proof relies on the Gibbs condition (see Proposition 2.12) and Theorem 3.1, the restrictions coming from the latter result. Regarding these restrictions, we mention the article [Mor20] where the proof of regularity of any pair $(\omega, \Phi) \in \mathcal{S}_{\text{eq}}(\Phi) \times \mathcal{B}^r$ is announced. Unfortunately, this proof is incomplete and cannot be fixed along the proposed lines.¹¹

A better understanding of the status of weak Gibbs states in equilibrium quantum statistical mechanics, and more generally quantum spin dynamics, is central to the success of the proposed research program. We also believe that, similarly to the classical setting, quantum weak Gibbs states will find many other applications in quantum statistical mechanics.

W^* -dynamical systems. In many important physical examples, and in particular those involving bosons, it may be more convenient to work in a W^* -framework. Similar to the non-equilibrium quantum statistical mechanics¹², it appears difficult to develop a general struc-

¹⁰The converse does not hold.

¹¹The error concerns the identity (32) in [Mor20], which implies that the KMS vector representative constructed by Ejima and Ogata in [EO19] is in the natural cone. Unfortunately, a simple argument shows that this is so only in the commutative case.

¹²See [MMS07a,MMS07b].

tural theory of approach to equilibrium in the W^* -setting. In this case one is naturally limited to the study of concrete models.

3 Proofs

3.1 Proof of Theorem 2.7

In this section we prove the parts of Theorem 2.7 that are not in [Isr79, Theorem III.4.2].

(a) \Leftrightarrow (b). This equivalence is a direct consequence of Relation (5) and the fact that

$$H_\Lambda(\Phi) - H_\Lambda(\Psi) = H_\Lambda(\Phi - \Psi).$$

(f) \Leftrightarrow (g). By [BR81, Theorem 6.2.4], if $\Phi \in \mathcal{B}^r$, then $\alpha_\Phi^t = e^{t\delta}$, where the generating derivation δ is the closure of the map

$$\mathfrak{A}_{\text{loc}} \ni A \mapsto \sum_{Y \cap \text{supp}(A) \neq \emptyset} i[\Phi(Y), A].$$

Thus, $\alpha_\Phi = \alpha_\Psi$ iff, for any $A \in \mathfrak{A}_{\text{loc}}$,

$$\sum_{Y \cap \text{supp}(A) \neq \emptyset} i[\Phi(Y) - \Psi(Y), A] = 0.$$

Since $i[\Phi(Y) - \Psi(Y), A] = 0$ whenever $Y \cap \text{supp}(A) = \emptyset$, this condition is equivalent to (g).

(g) \Rightarrow (b). By the simplicity of \mathfrak{A} , (g) implies that for any Λ there exists $C_\Lambda \in \mathbb{R}$ such that

$$\sum_{X \cap \Lambda \neq \emptyset} (\Phi(X) - \Psi(X)) = C_\Lambda \mathbb{1}.$$

Recalling (7), we deduce

$$\frac{1}{|\Lambda|} (H_\Lambda(\Phi) - H_\Lambda(\Psi)) = \frac{C_\Lambda}{|\Lambda|} \mathbb{1} - \frac{1}{|\Lambda|} W_\Lambda(\Phi - \Psi), \quad (18)$$

while (5) further yields

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \text{tr}(H_\Lambda(\Phi) - H_\Lambda(\Psi)) = \text{tr}(E_{\Phi - \Psi}).$$

Taking the trace on both sides of (18) and taking (8) into account yields

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{C_\Lambda}{|\Lambda|} = \text{tr}(E_{\Phi - \Psi}).$$

Finally, letting $\Lambda \uparrow \mathbb{Z}^d$ in (18) gives (b).

(b) \Rightarrow (c). For $t \in [0, 1]$ set $\Phi_t = (1 - t)\Psi + t\Phi$ and note that

$$H_\Lambda(\Phi_t) - H_\Lambda(\Psi) = H_\Lambda(\Phi_t - \Psi) = t(H_\Lambda(\Phi) - H_\Lambda(\Psi))$$

and (b) imply

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} (H_\Lambda(\Phi_t) - H_\Lambda(\Psi)) = t \text{tr}(E_{\Phi - \Psi}) \mathbb{1}.$$

Thus, given $\delta > 0$, and for large enough Λ ,

$$H_\Lambda(\Psi) + |\Lambda|(t \text{tr}(E_{\Phi - \Psi}) - \delta) \mathbb{1} \leq H_\Lambda(\Phi_t) \leq H_\Lambda(\Psi) + |\Lambda|(t \text{tr}(E_{\Phi - \Psi}) + \delta) \mathbb{1}.$$

Invoking the finite-volume Gibbs variational principle [OP93, Proposition 1.10]

$$P_\Lambda(\Phi) = \log \operatorname{tr} e^{-H_\Lambda(\Phi)} = \max_{\rho \in \mathcal{S}(\mathfrak{A}_\Lambda)} (S(\rho) - \rho(H_\Lambda(\Phi))), \quad (19)$$

the previous inequalities yield

$$|P_\Lambda(\Phi_t) - P_\Lambda(\Psi) + |\Lambda| t \operatorname{tr}(E_{\Phi-\Psi})| \leq \delta |\Lambda|.$$

In view of (4), dividing both sides of this estimate by $|\Lambda|$, taking the thermodynamic limit $\Lambda \uparrow \mathbb{Z}^d$, and finally letting $\delta \downarrow 0$, we deduce

$$P(\Phi_t) = P(\Psi) - t \operatorname{tr}(E_{\Phi-\Psi}),$$

which is (c).

3.2 Proof of Theorem 2.8

(1) Invariance of the specific entropy goes back to [LR68, Theorem 5]. Even though it may look surprising, its proof can be understood as follows. Consider a tiling of \mathbb{Z}^d with a large cube Λ , and perturb the interaction Φ so that all cubes are disconnected. The entropy of ω restricted to Λ is constant under the perturbed dynamics because it is a closed finite system by construction. Finally, the entropy of the perturbed dynamics coincides with the original one up to a $o(|\Lambda|)$ boundary term whose contribution to the specific entropy vanishes in the $\Lambda \uparrow \mathbb{Z}^d$ -limit.

(2) We recall again that, by [BR81, Theorem 6.2.4], $\alpha_\Phi^t = e^{t\delta}$, where the generator δ is the closure of the map

$$\mathfrak{A}_{\text{loc}} \ni A \mapsto \sum_{Y \cap \operatorname{supp}(A) \neq \emptyset} i[\Phi(Y), A].$$

Since $\omega \circ \alpha_\Phi^t \in \mathcal{S}_1(\mathfrak{A})$, it suffices to show that $E_\Phi \in \operatorname{Dom}(\delta)$ and $\omega(\delta(E_\Phi)) = 0$ for all $\omega \in \mathcal{S}_1(\mathfrak{A})$.

For latter reference, we will show that $E_\Psi \in \operatorname{Dom}(\delta)$ holds for all $\Psi \in \mathcal{B}^r$. Setting

$$E_{\Psi,n} = \sum_{\substack{X \ni 0 \\ \operatorname{diam}(X) \leq n}} \frac{\Psi(X)}{|X|} \in \mathfrak{A}_{\text{loc}},$$

and observing that

$$\sum_{n=0}^{\infty} \sum_{\substack{X \ni 0 \\ \operatorname{diam}(X)=n}} \frac{\|\Psi(X)\|}{|X|} \leq \|\Psi\|_r < \infty,$$

we have

$$\lim_{n \rightarrow \infty} \|E_\Psi - E_{\Psi,n}\| \leq \lim_{n \rightarrow \infty} \sum_{\substack{X \ni 0 \\ \operatorname{diam}(X) > n}} \frac{\|\Psi(X)\|}{|X|} = 0.$$

Moreover, for $m \leq n$, the formula

$$\delta(E_{\Psi,n}) - \delta(E_{\Psi,m}) = \sum_{\substack{X \ni 0 \\ m < \operatorname{diam}(X) \leq n}} \frac{1}{|X|} \sum_{Y \cap X \neq \emptyset} i[\Phi(Y), \Psi(X)],$$

gives the estimate

$$\begin{aligned} \|\delta(E_{\Psi,n}) - \delta(E_{\Psi,m})\| &\leq 2 \sum_{\substack{X \ni 0 \\ m < \operatorname{diam}(X) \leq n}} \frac{\|\Psi(X)\|}{|X|} \sum_{Y \cap X \neq \emptyset} \|\Phi(Y)\| \\ &\leq 2 \sum_{\substack{X \ni 0 \\ \operatorname{diam}(X) > m}} \|\Psi(X)\| \frac{1}{|X|} \sum_{x \in X} \sum_{Y \ni x} \|\Phi(Y)\| \leq 2 \|\Phi\|_r \sum_{\substack{X \ni 0 \\ \operatorname{diam}(X) > m}} \|\Psi(X)\|, \end{aligned}$$

which shows that the sequence $(\delta(E_{\Psi,n}))_{n \in \mathbb{N}}$ is Cauchy. It follows that $E_{\Psi} \in \text{Dom}(\delta)$ and

$$\delta(E_{\Psi}) = \sum_{X \ni 0} \frac{1}{|X|} \sum_{Y \cap X \neq \emptyset} i[\Phi(Y), \Psi(X)]. \quad (20)$$

To proceed, we equip $X \in \mathcal{F}$ with the lexicographic order observing that translation invariance implies $\min(X+x) = \min(X) + x$ for any $X \in \mathcal{F}$ and $x \in \mathbb{Z}^d$. Set

$$\mathcal{F}_0 = \{X \in \mathcal{F} \mid \min(X) = 0\},$$

and note that the set of translates of $X \in \mathcal{F}_0$ containing 0 is

$$\mathcal{F}_X = \{X - x \mid x \in X\}.$$

Finally, for $X, Y \in \mathcal{F}_0$, let

$$Z(X, Y) = \{z \in \mathbb{Z}^d \mid X \cap (Y+z) \neq \emptyset\}.$$

Relation (20) thus writes

$$\delta(E_{\Phi}) = \sum_{X \in \mathcal{F}_0} \frac{1}{|X|} \sum_{x \in X} \sum_{Y \cap (X-x) \neq \emptyset} i[\Phi(Y), \varphi^{-x}(\Phi(X))].$$

Now for $Y \in \mathcal{F}$ one has $Y = Y_0 + y$, with $Y_0 \in \mathcal{F}_0$ and $y = \min(Y)$. Moreover,

$$\emptyset \neq Y \cap (X-x) = (Y_0 + y) \cap (X-x) = ((Y_0 + x + y) \cap X) - x$$

iff $x + y \in Z(X, Y_0)$, so that

$$\delta(E_{\Phi}) = \sum_{X \in \mathcal{F}_0} \frac{1}{|X|} \sum_{x \in X} \sum_{Y \in \mathcal{F}_0} \sum_{x+y \in Z(X, Y)} i[\varphi^y(\Phi(Y)), \varphi^{-x}(\Phi(X))].$$

It follows that, for $\omega \in \mathcal{A}_1(\mathfrak{A})$,

$$\begin{aligned} \omega(\delta(E_{\Phi})) &= \sum_{X \in \mathcal{F}_0} \frac{1}{|X|} \sum_{x \in X} \sum_{Y \in \mathcal{F}_0} \sum_{z \in Z(X, Y)} \omega(i[\varphi^z(\Phi(Y)), \Phi(X)]) \\ &= \sum_{X, Y \in \mathcal{F}_0} \sum_{z \in Z(X, Y)} \omega(i[\varphi^z(\Phi(Y)), \Phi(X)]). \end{aligned}$$

Symmetrizing the inner sum and observing that $Z(Y, X) = -Z(X, Y)$ yields

$$\begin{aligned} \omega(\delta(E_{\Phi})) &= \frac{1}{2} \sum_{X, Y \in \mathcal{F}_0} \sum_{z \in Z(X, Y)} \omega(i[\varphi^z(\Phi(Y)), \Phi(X)] + i[\varphi^{-z}(\Phi(X)), \Phi(Y)]) \\ &= \frac{1}{2} \sum_{X, Y \in \mathcal{F}_0} \sum_{z \in Z(X, Y)} \omega(i[\varphi^z(\Phi(Y)), \Phi(X)] - i[\varphi^z(\Phi(Y)), \Phi(X)]) = 0. \end{aligned}$$

(3) In a similar spirit, it suffices to show that $E_N \in \text{Dom}(\delta)$, with $\omega(\delta(E_N)) = 0$ for all $\omega \in \mathcal{A}_1(\mathfrak{A})$.

The generator γ of the gauge group is the closure of the map

$$\mathfrak{A}_{\text{loc}} \ni A \mapsto \sum_{x \in \text{supp}(A)} i[a_x^* a_x, A] = \sum_{x \in \text{supp}(A)} i[\varphi^x(E_N), A].$$

Since any state $\omega \in \mathcal{A}_1(\mathfrak{A})$ is gauge-invariant¹³, one has $\omega(\gamma(A)) = 0$ for any $A \in \text{Dom}(\gamma)$, and in particular

$$0 = \omega(\gamma(\Phi(X))) = \sum_{x \in X} \omega(i[\varphi^x(E_N), \Phi(X)]) = \sum_{x \in X} \omega(i[E_N, \varphi^{-x}(\Phi(X))]) = - \sum_{Y \in \mathcal{F}_X} \omega(i[\Phi(Y), E_N]).$$

for all $X \in \mathcal{F}$. We conclude that

$$\omega(\delta(E_N)) = \sum_{X \ni 0} \omega(i[\Phi(X), E_N]) = \sum_{X \in \mathcal{F}_0} \sum_{Y \in \mathcal{F}_X} \omega(i[\Phi(Y), E_N]) = 0.$$

¹³Any state $\omega \in \mathcal{A}_1(\mathfrak{A})$ restricts to the gauge-invariant state $\tilde{\omega} = \int_0^{2\pi} \omega \circ \vartheta^\theta \frac{d\theta}{2\pi} \in \mathcal{A}_1(\mathfrak{A})$.

3.3 Proof of Proposition 2.10

(1) Is merely a reformulation of the defining relations (11) and (9) which will be convenient in the proofs of the remaining statements.

(2) By the operator monotonicity of the logarithm [Pet08, Example 11.16], the inequalities (11) follow from (10), which proves the first inclusion. To deal with the second one, we note that

$$\log \omega_{\Phi, \Lambda}^c = -H_{\Lambda}(\Phi) - P_{\Lambda}(\Phi),$$

so that any $\omega \in \text{LWG}(\Phi)$ satisfies

$$-c_{\Lambda} \leq \log \omega_{\Lambda} + H_{\Lambda}(\Phi) + P_{\Lambda}(\Phi) \leq c_{\Lambda},$$

where c_{Λ} is such that (9) holds. Multiplying with ω_{Λ} and taking the trace yields

$$|S(\omega_{\Lambda}) - \omega(H_{\Lambda}(\Phi)) - P_{\Lambda}(\Phi)| \leq c_{\Lambda}.$$

Dividing by $|\Lambda|$, letting $\Lambda \uparrow \mathbb{Z}^d$ and invoking (2), (4) and (6) gives

$$P(\Phi) = s(\omega) - \omega(E_{\Phi}),$$

and hence $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$.

(3) If $\omega \in \text{LWG}(\Phi) \cap \text{LWG}(\Psi)$, then

$$\limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_{\Lambda} - \log \omega_{\Phi, \Lambda}^c\| = \limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_{\Lambda} - \log \omega_{\Psi, \Lambda}^c\| = 0.$$

It follows that

$$\limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_{\Phi, \Lambda}^c - \log \omega_{\Psi, \Lambda}^c\| = 0,$$

which, in view of (1), immediately leads to $\text{LWG}(\Phi) = \text{LWG}(\Psi)$.

(4) Let $\omega \in \text{LWG}(\Phi)$, and suppose that $\Psi \sim \Phi$. By definition one has

$$\limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_{\Lambda} - \log \omega_{\Phi, \Lambda}^c\| = 0. \quad (21)$$

Theorem 2.7-(b) further implies that, for any $\delta > 0$,

$$|\Lambda|(\text{tr}(E_{\Phi-\Psi}) - \delta) \mathbb{1} \leq H_{\Lambda}(\Phi) - H_{\Lambda}(\Psi) \leq |\Lambda|(\text{tr}(E_{\Phi-\Psi}) + \delta) \mathbb{1} \quad (22)$$

provided Λ is large enough. Writing the variational formula (19) as

$$P_{\Lambda}(\Psi) = \max_{\rho \in \mathcal{S}(\mathfrak{A}_{\Lambda})} (S(\rho) - \rho(H_{\Lambda}(\Phi)) + \rho(H_{\Lambda}(\Phi) - H_{\Lambda}(\Psi))),$$

the inequalities (22) allow us to deduce

$$|\Lambda|(-\text{tr}(E_{\Phi-\Psi}) - \delta) \leq P_{\Lambda}(\Phi) - P_{\Lambda}(\Psi) \leq |\Lambda|(-\text{tr}(E_{\Phi-\Psi}) + \delta).$$

Adding the last inequalities to (22) gives

$$\|\log \omega_{\Phi, \Lambda}^c - \log \omega_{\Psi, \Lambda}^c\| \leq 2\delta |\Lambda|.$$

Combining this estimate with (21) yields

$$\limsup_{\Lambda \uparrow \mathbb{Z}^d} |\Lambda|^{-1} \|\log \omega_{\Lambda} - \log \omega_{\Psi, \Lambda}^c\| \leq 2\delta,$$

and taking $\delta \downarrow 0$ allows us to conclude that $\omega \in \text{LWG}(\Psi)$.

Reciprocally, if $\omega \in \text{LWG}(\Phi) = \text{LWG}(\Psi)$, then it follows from (1) that $\omega \in \mathcal{S}_{\text{eq}}(\Phi) \cap \mathcal{S}_{\text{eq}}(\Psi)$ and Theorem 2.7-(d) yields $\Phi \sim \Psi$.

3.4 Proof of Theorem 2.11

We will make use of [LRB05, Theorem 3.7], which we state and prove in the general setting of Section 1.1.

Theorem 3.1. *Let ω be a faithful $(\alpha, 1)$ -KMS state and ω_V the perturbed $(\alpha_V, 1)$ -KMS state induced by $V = V^* \in \mathcal{O}$.*

(i) *If the map*

$$\mathbb{R} \ni t \mapsto \alpha^t(V) \in \mathcal{O} \quad (23)$$

has an analytic extension to the strip $0 < \text{Im } z < 1/2$ which is bounded and continuous on its closure, then

$$\omega_V \leq C_V \omega,$$

where $C_V = e^{\|V\| + \|\alpha^{i/2}(V)\|}$.

(ii) *If the map (23) has an analytic extension to the strip $|\text{Im } z| < 1/2$ which is bounded and continuous on its closure, then we also have a lower bound*

$$\omega_V \geq D_V \omega,$$

where $D_V = e^{-\|V\| - \|\alpha_V^{i/2}(V)\|}$.

Proof. For later reference, we give here a proof that is different from the original argument in [LRB05] and emphasizes the role of the modular structure. We will freely use the notation and results of modular theory and perturbation of the KMS-structure discussed in [DJP03]. In particular, E_V^α denotes the Araki–Dyson expansion associated to V ,

$$E_V^\alpha(t) = \sum_{n \geq 0} (it)^n \int_{0 \leq s_n \leq \dots \leq s_1 \leq 1} \alpha^{ts_n}(V) \cdots \alpha^{ts_1}(V) ds_1 \cdots ds_n, \quad (24)$$

see [DJP03, Section 3.1].

(i) Passing to the GNS representation $(\mathcal{H}, \pi, \Omega)$ induced by ω , we need to prove that for any $A > 0$ in \mathcal{O} ,

$$\omega_V(A) = \frac{\langle \Omega_V, \pi(A) \Omega_V \rangle}{\|\Omega_V\|^2} \leq C_V \langle \Omega, \pi(A) \Omega \rangle,$$

where $\Omega_V = \pi(E_V^\alpha(i/2))\Omega$. Since $\|\Omega_V\| \geq e^{-\|V\|/2}$ by the Peierls–Bogoliubov inequality, it suffices to prove that

$$\sup_{\mathcal{O} \ni A > 0} \frac{\langle \Omega_V, \pi(A) \Omega_V \rangle}{\langle \Omega, \pi(A) \Omega \rangle} \leq e^{\|\alpha^{i/2}(V)\|}. \quad (25)$$

From the fact that $J\Omega_V = \Omega_V$ we get

$$\langle \Omega_V, \pi(A) \Omega_V \rangle = \|\pi(A^{1/2}) J \pi(E_V^\alpha(i/2)) \Omega\|^2 = \|\pi(E_V^\alpha(i/2)) J \pi(A^{1/2}) \Omega\|^2,$$

and $\langle \Omega, \pi(A) \Omega \rangle = \|J \pi(A^{1/2}) \Omega\|^2$ yields

$$\sup_{\mathcal{O} \ni A > 0} \frac{\langle \Omega_V, \pi(A) \Omega_V \rangle}{\langle \Omega, \pi(A) \Omega \rangle} = \|\pi(E_V^\alpha(i/2))\|^2,$$

so that (25) easily follows from (24).

(ii) We infer from the relation $\alpha_{-V}^t(V) = E_{-V}^\alpha(t) \alpha^t(V) E_{-V}^\alpha(t)^*$ that $\alpha_{-V}^z(V) = E_{-V}^\alpha(z) \alpha^z(V) E_{-V}^\alpha(\bar{z})^*$ is analytic in the strip $0 < \text{Im } z < 1/2$ and bounded and continuous on its closure. Part (i) and the relation $\omega = (\omega_{-V})_V$ yield the claim. \square

We now proceed with the proof of Theorem 2.11. To simplify the notation, we write α and W_Λ for α_Φ and $W_\Lambda(\Phi)$.

We only need to prove that $\mathcal{S}_{\text{eq}}(\Phi) \subset \text{WG}(\Phi)$. To this end, let $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$. By Theorem 3.1, if the surface energy W_Λ is α -analytic in the strip $|\text{Im } z| < a$ for some $a > 1/2$, then

$$e^{-\|W_\Lambda\| - \|\alpha^{i/2}(W_\Lambda)\|} \leq \frac{\omega(A)}{\omega_{-W_\Lambda}(A)} \leq e^{\|W_\Lambda\| + \|\alpha^{i/2}(W_\Lambda)\|}$$

holds for any $A \in \mathfrak{A}_\Lambda$ such that $A > 0$. By (8) and Proposition 2.12, to prove that $\omega \in \text{WG}(\Phi)$ it is then sufficient to show that

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \|\alpha^{i/2}(W_\Lambda)\| = 0, \quad \lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \|\alpha_{-W_\Lambda}^{i/2}(W_\Lambda)\| = 0. \quad (26)$$

In the case (a), this follows from the celebrated estimate of Araki [Ara69], see also [LRB05, Proposition 3.9] and discussion after it, and [Mat03, Proposition 2.4]. In the case (b) we argue as follows. Let

$$a = \frac{r}{2\|\Phi\|_r} > 1/2.$$

Then, by Theorem 2.3, for any $X \in \mathcal{F}$ the map $\mathbb{R} \ni t \mapsto \alpha^t(\Phi(X))$ has analytic extension to the strip $|\text{Im } z| < a$ such that

$$\|\alpha^{i/2}(\Phi(X))\| \leq \|\Phi(X)\| \frac{e^{r|X|}}{1 - \|\Phi\|_r/r}. \quad (27)$$

This estimate gives that the map $\mathbb{R} \ni t \mapsto \alpha^t(W_\Lambda)$ also has an analytic extension to the strip $|\text{Im } z| < a$ and that

$$\|\alpha^{i/2}(W_\Lambda)\| \leq \sum_{\substack{X \cap \Lambda \neq \emptyset \\ X \cap \Lambda^c \neq \emptyset}} \|\Phi(X)\| \frac{e^{r|X|}}{1 - \|\Phi\|_r/r}.$$

Thus, to establish the first limit in (26) it suffices to show that

$$\lim_{\Lambda \uparrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{\substack{X \cap \Lambda \neq \emptyset \\ X \cap \Lambda^c \neq \emptyset}} \|\Phi(X)\| e^{r|X|} = 0.$$

This relation is immediate for $\Phi \in \mathcal{B}_f$. The general case follows from the density of \mathcal{B}_f in \mathcal{B}^r and the bound

$$\frac{1}{|\Lambda|} \sum_{X \cap \Lambda \neq \emptyset} \|\Psi(X)\| e^{r|X|} \leq e^r \|\Psi\|_r$$

that holds for all $\Psi \in \mathcal{B}^r$.

To deal with the second limit in (26) we observe that the perturbed dynamics α_{-W_Λ} is associated with the non-translation-invariant interaction Φ_Λ given by

$$\Phi_\Lambda(X) = \begin{cases} 0 & \text{if } X \cap \Lambda \neq \emptyset \text{ and } X \cap \Lambda^c \neq \emptyset; \\ \Phi(X) & \text{otherwise.} \end{cases}$$

By the Remark after Theorem 2.3, and in view of the obvious fact that $\|\Phi_\Lambda\|_r \leq \|\Phi\|_r$, the estimate (27) holds with α_{-W_Λ} replacing α . We can then argue as before.

3.5 Proof of Proposition 2.12

Theorem 2.5 gives

$$\omega_{-W_\Lambda(\Phi)} = \omega_{\Phi, \Lambda}^c. \quad (28)$$

If $\omega \in \text{WG}(\Phi)$, then for any $A \in \mathfrak{A}_\Lambda$ satisfying $A > 0$ one has

$$e^{-c_\Lambda} \leq \frac{\omega(A)}{\omega_{-W_\Lambda}(A)} \leq e^{c_\Lambda},$$

and (12) follows.

To prove the converse statement, for $A \in \mathfrak{A}_\Lambda$ satisfying $A > 0$, the definitions of \underline{d}_Λ and \bar{d}_Λ and Relation (28) give

$$\underline{d}_\Lambda \omega_{\Phi, \Lambda}^c(A) \leq \omega(A) \leq \bar{d}_\Lambda \omega_{\Phi, \Lambda}^c(A).$$

Setting $c_\Lambda = \log \max(\bar{d}_\Lambda, 1/\underline{d}_\Lambda)$, one deduces from (12) that $\omega \in \text{WG}(\Phi)$.

3.6 Proof of Proposition 2.16

Parts (2) and (3) are immediate consequences of the corresponding statements of Theorem 2.8.

To prove Part (1), writing the integral (16) as a weak*-limit of Riemann sums and using that the entropy map is affine and upper-semicontinuous, we derive the inequality

$$s(\bar{\omega}_T) \geq \limsup_{N \rightarrow \infty} \sum_{k=0}^{N-1} \frac{1}{N} s(\omega \circ \alpha_\Phi^{kt/N}).$$

Part (1) of Theorem 2.8 further gives $s(\omega \circ \alpha_\Phi^{kt/N}) = s(\omega)$, so that $s(\bar{\omega}_T) \geq s(\omega)$. To prove the reverse inequality, note first that the identity,

$$\bar{\omega}_T = \frac{1}{2} \bar{\omega}_{T/2} + \frac{1}{2} \bar{\omega}_{T/2} \circ \alpha_\Phi^{T/2},$$

the affine property of the specific entropy, and Part (1) of Theorem 2.8 give that $s(\bar{\omega}_T) = s(\bar{\omega}_{T/2})$. Consequently, $s(\bar{\omega}_T) = s(\bar{\omega}_{T/2^n})$ for any $n \in \mathbb{N}$, and invoking again the upper-semicontinuity, we conclude

$$s(\bar{\omega}_T) = \lim_{n \rightarrow \infty} s(\bar{\omega}_{T/2^n}) \leq s(\omega).$$

3.7 Proof of Theorem 2.18

By Part (1) of Proposition 2.16, $s(\bar{\omega}_T) = s(\omega)$. Relation (15) and the non-negativity of relative entropy give

$$\begin{aligned} 0 \leq \bar{s}(\bar{\omega}_T | \omega) &\leq -s(\bar{\omega}_T) + \bar{\omega}_T(E_\Psi) + P(\Psi) \\ &= -s(\omega) + \bar{\omega}_T(E_\Psi) + P(\Psi) \\ &= \bar{\omega}_T(E_\Psi) - \omega(E_\Psi). \end{aligned} \quad (29)$$

Pick a sequence (T_n) such that $\bar{\omega}_{T_n} \rightarrow \omega_+$. Taking the limit along this sequence in (29), we derive that $\omega_+(E_\Psi) \geq \omega(E_\Psi)$.

3.8 Proof of Theorem 2.19

Since our hypothesis implies that $\omega \in \mathcal{S}_{\text{eq}}(\Psi)$, we can write

$$\begin{aligned} 0 &\leq s(\bar{\omega}_T|\omega) = -s(\bar{\omega}_T) + \bar{\omega}_T(E_\Psi) + P(\Psi) \\ &= -s(\omega) + \bar{\omega}_T(E_\Psi) + P(\Psi) \\ &= \bar{\omega}_T(E_\Psi) - \omega(E_\Psi). \end{aligned} \tag{30}$$

Pick again a sequence (T_n) such that $\bar{\omega}_{T_n} \rightarrow \omega_+$ and note that Relation (14) gives that the map $\mathcal{S}_1(\mathfrak{A}) \ni \nu \mapsto s(\nu|\omega)$ is lower-semicontinuous. Hence, Relation (30) further yields

$$0 \leq s(\omega_+|\omega) \leq \liminf_{n \rightarrow \infty} s(\bar{\omega}_{T_n}|\omega) = \omega_+(E_\Psi) - \omega(E_\Psi).$$

Thus, if $\omega_+(E_\Psi) = \omega(E_\Psi)$, then $s(\omega_+|\omega) = 0$ and, in view of the fact that $\omega_+ \in \mathcal{S}_1(\mathfrak{A})$, (14) gives

$$0 = s(\omega_+|\omega) = -s(\omega_+) + \omega_+(E_\Psi) + P(\Psi). \tag{31}$$

This allows us to conclude that $\omega_+ \in \mathcal{S}_{\text{eq}}(\Psi)$. Since $\omega \in \mathcal{S}_{\text{eq}}(\Psi)$, we also have

$$0 = -s(\omega) + \omega(E_\Psi) + P(\Psi) = -s(\omega) + \omega_+(E_\Psi) + P(\Psi)$$

which, upon comparison with (31), shows that $s(\omega) = s(\omega_+)$, and so (a) \Rightarrow (b). The implication (b) \Rightarrow (a) is obvious.

If in addition $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi)$, then (b) gives that $\omega_+ \in \mathcal{S}_{\text{eq}}(\Phi) \cap \mathcal{S}_{\text{eq}}(\Psi)$ and (c) follows from Theorem 2.7-(d).

Finally, if $\Phi \sim \Psi$, then $\alpha_\Phi = \alpha_\Psi$ by Theorem 2.7-(f), and so ω is α_Φ -invariant. Hence, $\omega = \omega_+$, and so (c) \Rightarrow (d). Obviously (d) \Rightarrow (a).

3.9 Proof of Theorem 2.20

Suppose that $s(\omega) = s(\omega_+)$. Then, since $\omega_+(E_\Phi) = \omega(E_\Phi)$,

$$\begin{aligned} 0 &= -s(\omega_+) + \omega_+(E_\Phi) + P(\Phi) \\ &= -s(\omega) + \omega(E_\Phi) + P(\Phi), \end{aligned}$$

and so $\omega \in \mathcal{S}_{\text{eq}}(\Phi)$. This gives that ω is α_Φ -invariant and that $\omega = \omega_+$.

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