The Quantum Statistical Free Energy Minimum Principle for Multi-Lattice Mean Field Theories

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The quantum statistical frame for infinite multi-lattice spin systems is introduced. The thermodynamic functionals specific internal energy, entropy and free energy are shown to exist on the set of permutation invariant states for polynomial mean field interactions by direct estimation methods. Their dependence on the relative sizes of the sublattice systems is made explicit. The set of homogeneous minimal free energy states is shown to be a Bauer simplex which contains all limiting Gibbs states. For the extremal minimal free energy states the self-consistency equations are derived.

1. Introduction

The idea of the present work is to provide the quantum statistical frame for infinite multi-lattice mean field models and to use it for the foundation of the thermodynamic variational formalism. For this purpose we emphasize those operator algebraic notions which are relevant for the macroscopic aspects of the considered theory.

The restriction to lattice systems circumvents many technical difficulties inherent in the rigorous theory of continuous systems but has, nevertheless, a large variety of physical applications. The set of possible applications is even considerably enlarged by admitting a sublattice structure, that is, the set of lattice indices decomposes into a finite union of subsets, each of which becomes infinite in the thermodynamic limit. The relative sizes of the sublattices, which should assume well-defined limiting values, are then additional thermodynamic parameters. They cause non-trivial complications in calculating the thermodynamic functions and seem not to have been considered previously within a rigorous discussion in the published literature. Our approach goes back to the unpublished thesis of Fleig [1], where as an illustrative example is elaborated a BCS-superconductor with paramagnetic impurities. Another class of multi-lattice systems is worked out in terms of the present formalism in [2], where also more references to the usual literature of multi-lattice mean field theories are provided. (For rigorous discussions of one-lattice mean field theories see also [3, 4].) Quite generally it is obvious, that composite macroscopic systems are basic for thermodynamics and are of even increasing interest with respect to their quantum mechanical features.

Concerning the mean field character of the considered model class, a systematic foundation may be given by admitting only a restricted class of (quantum statistical) states. For the thermodynamic point of view only those states seem to be relevant, which are not too irregular in their spatial properties. We satisfy in the present formalism this requirement in the strongest possible way: the selected set of states, which is considered as a representative of the thermodynamic state space consists of those, which are completely homogeneous in each sublattice. This sublattice permutation invariance should be considered only as the starting point of the discussion of long range interacting systems. (For some prospective generalizations see below.) It does not exclude, however, global non-equilibrium states. Here it motivates the crucial role played by a certain kind of intensive observables. These are called here "density observables" (and should not be confused with the density matrices of the states). They have to be discriminated from the other set of intensive variables, the so-called "contact variables", [5, 6] as e.g. temperature and chemical potential, which have no microscopic counterparts. The density observables are always norm-bounded but are elements of the basic C^*-algebra of observables only, if the space average is carried out over a finite lattice region. (Their infinite volume limits have to be performed in a representation-dependent weak topology.)

Now, any interaction in a finite lattice region is for homogeneous states equivalent to a permutation in-

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variant one and by this automatically a polynomial of the density observables corresponding to the selected region. This polynomial may in principle depend for itself on the (cardinality of the) finite lattice region. Here we consider, however, only models with fixed maximal degree of the polynomial interaction.

In order to locate the origin of the macroscopic-classical features of the considered models we present in Sect. 2 the quantum statistical set up in some detail. For the operator algebraic notions we refer to [7–9], and [10]. We try to elucidate the physical meaning of some of the mathematical concepts. The sublattice structure allows for the introduction of concentration vectors by restricting the family of local lattice regions to certain directed absorbing sub-families (which are called "funnels"). In this connection some care is required to formulate the notion of a (unique) limiting Gibbs state. The whole elaboration gives various arguments for considering the set of all permutation invariant states $\mathscr{S}^{\mathfrak{P}}$ as the representative of a fundamental macroscopic-classical structure which is inherent in the state space of the quasi-local algebra and should be taken into account, also if larger sets of states are used. The extremal boundary $\partial_e \mathscr{S}^{\mathfrak{P}}$ of $\mathscr{S}^{\mathfrak{P}}$ leads to the definition of general (not necessarily equilibrium) pure phase states.

The specific thermodynamic potentials are introduced in Sect. 3 as functionals on $\mathscr{S}^{\mathfrak{P}}$. To prove their existence in the thermodynamic limit we use the most direct estimation techniques. The sublattice structure makes the discussion of the limiting entropy density rather involved. The fact that we use the absolute (and not the relative) entropy density has some advantages in future studies of the low temperature asymptotics.

In Sect. 4 it is established that the limiting Gibbs states minimize the free energy. The total set of equilibrium states for a given temperature and concentration vector – consisting of the minimal free energy states – is proven to be a stable face of $\mathscr{S}^{\mathfrak{P}}$ and to constitute a classical sub-structure being for itself a Bauer simplex. The extremal boundary of this Bauer simplex is seen to be the intersection of the simplex with $\partial_e \mathscr{S}^{\mathfrak{P}}$, so that the notion of an equilibrium pure phase state is consistent with the general pure phase concept.

In Sect. 5 the necessary self-consistency equations for the equilibrium pure phase states are obtained by forming the Frechet derivative of the free energy functional (augmented by Lagrange parameter terms). Only here the effective mean field Hamiltonians may be recognized in the local density matrices of the pure phase states.

Altogether we obtain in this way a foundation of the quantum statistical variational formalism by straightforward and typical thermodynamic methods, where an arbitrary finite set of concentration parameters is incorporated. In the way the concentrations are treated here, they describe a preparation of the macroscopic subsystems in fixed relative amounts. By varying the concentrations as external parameters complicated phase diagrams may show up, which often give a qualitatively correct picture of the phases of real substances, e.g. for metallic alloys. It is of course also possible to vary over some (or all) concentration parameters in calculating the minimal free energy, what, would e.g., be useful in the case of hydrogenium dissolved in metal. If the sub-systems are not really macroscopic but mesoscopic (think of the granules of a high T_c superconductor) the values of the concentration parameters may be subjected to an additional statistical distribution.

There are already developments in the rigorous literature which transcend the here treated models in two decisive respects: on the one hand the polynomial interactions for one-lattice systems are generalized to continuous functions of the density observables [11], which requires completely new mathematical concepts for their definition, but many of the here presented techniques seem still to be applicable. On the other hand the limit to an infinite number of subsystems has been worked out for specific models [12]. These are very interesting limiting cases of the present model class and add to the motivation to clarify the structure of the latter as much as possible. These further structural questions concern, e.g., the following: since one has by the mentioned Bauer simplices of equilibrium states a concise notion of the classical equilibrium properties of a quantum system (also expressible by a Boolean lattice) one may analyze their changes in the course of phase transitions. Another point is the connection to dynamical concepts already being made available for subclasses of the present models in [13–15].

2. Quantumstatistical Frame for Multi-Lattice Mean Field Theories

2.1. Quasi-local Algebra

We treat here the general case of a composite lattice system with $r \in \mathbb{N}$ components. Since every lattice vec-

tor has integer coordinates, each lattice may be described by $\mathbb{Z}^d$, where $d \in \mathbb{N}$ is the dimension of the space, or – after a renumbering – by $\mathbb{N}$ itself. The multi-lattice is then represented by $\mathscr{R} = \mathscr{I} \times \{1, \ldots, r\}$, where $\mathscr{I}$ equals $\mathbb{Z}^d$ or $\mathbb{N}$ and $\{1, \ldots, r\}$, is the index set to identify the sublattices. With each lattice site $(i, p) \in \mathscr{R}$, $i \in \mathscr{I}$, $p \in \{1, \ldots, r\}$, is attached a finite-dimensional quantum system with the observable algebra $\mathscr{A}_{ip}$, which is isomorphic to the full matrix algebra $\mathscr{B}_p := \mathscr{M}_{m(p)}(\mathbb{C})$ in the Hilbert space $\mathbb{C}^{m(p)}$. As we are going to describe, the $m(p) \in \mathbb{N}$, $p \in \{1, \ldots, r\}$ characterize the observable algebras of the local and the infinite lattices and this may be called "type" of the multi-lattice system. In algebraic terms the type may be expressed by the tupel

$$\mathscr{B} := \mathscr{B}_1 \times \ldots \times \mathscr{B}_r . \tag{2.1}$$

For a thorough elaboration it is useful to recall the construction of the quasi-local lattice algebra. One introduces first of all the set $\mathscr{L}$ of all finite multi-lattice subregions $\Lambda \subset \mathscr{R}$, the cardinalities of which are denoted by $|\Lambda|$. $\mathscr{L}$ is then directed by inclusion with the inclusion relation $\Lambda \subset \Lambda'$, $\Lambda, \Lambda' \in \mathscr{L}$, and constitutes a partial order in $\mathscr{L}$ such that for every pair $\Lambda, \Lambda' \in \mathscr{L}$ there is a $\Lambda'' \in \mathscr{L}$ with $\Lambda \subset \Lambda''$ and $\Lambda' \subset \Lambda''$. For every $\Lambda \in \mathscr{L}$ one has the corresponding observable algebra

$$\mathscr{A}_\Lambda := \bigotimes_{(i,p) \in \Lambda} \mathscr{A}_{ip} . \tag{2.2}$$

In order to exhibit the sublattice structure let us write $\Lambda_p := \{(i, p') \in \Lambda \mid p' = p\}$. Since then $\Lambda = \bigcup_{p=1}^{r} \Lambda_p$, $\Lambda_p \cap \Lambda_{p'} = \emptyset$, for $p \neq p'$, we find $|\Lambda| = \sum_{p=1}^{r} |\Lambda_p|$. With this, one has

$$\mathscr{A}_\Lambda = \bigotimes_{p=1}^{r} \mathscr{A}_{\Lambda_p} . \tag{2.3}$$

For every pair $\Lambda, \Lambda' \in \mathscr{L}$ with $\Lambda \subset \Lambda'$, one has the natural embedding $*$-isomorphism

$$\eta_{\Lambda', \Lambda} : \mathscr{A}_\Lambda \to \mathscr{A}_{\Lambda'}, \quad A \to \eta_{\Lambda', \Lambda}(A) = A \otimes \mathbb{1}_{\Lambda' \setminus \Lambda}, \quad A \in \mathscr{A}_\Lambda, \tag{2.4}$$

where $\mathbb{1}_\Lambda$ is the unit in $\mathscr{A}_\Lambda$. It clearly holds for $\Lambda \subset \Lambda' \subset \Lambda''$:

$$\eta_{\Lambda'', \Lambda} = \eta_{\Lambda'', \Lambda'} \circ \eta_{\Lambda', \Lambda} \quad \text{and} \quad \eta_{\Lambda', \Lambda}(\mathbb{1}_\Lambda) = \mathbb{1}_{\Lambda'} . \tag{2.5}$$

The properties in (2.5) give rise to the C^*-inductive limit algebra $\mathscr{A}$ (cf. [9, 10]), for the infinite system, which is an abstract C^*-algebra. From the general mathematical theory one knows the basic properties of $\mathscr{A}$, where most of them are relevant for the quantum statistical formalism and its physical interpretation. The quasi-local algebra $\mathscr{A}$ is a minimal form of an observable algebra in the thermodynamic limit in the following sense. For every $\Lambda \in \mathscr{L}$ the set-up of the C^*-inductive limit leads to an embedding $*$-isomorphism of the original local algebras

$$\eta_\Lambda : \mathscr{A}_\Lambda \to \mathscr{A} \quad \text{with} \quad \eta_\Lambda(\mathbb{1}_\Lambda) = \mathbb{1} \in \mathscr{A} \tag{2.6}$$

and $\Lambda \subset \Lambda'$ implying

$$\eta_\Lambda(\mathscr{A}_\Lambda) = \eta_{\Lambda'} \circ \eta_{\Lambda', \Lambda}(\mathscr{A}_\Lambda) \subset \eta_{\Lambda'}(\mathscr{A}_{\Lambda'}) . \tag{2.7}$$

The minimality of $\mathscr{A}$ is now expressed by

$$\mathscr{A} = \overline{\bigcup_{\Lambda \in \mathscr{L}} \eta_\Lambda(\mathscr{A}_\Lambda)}^{\|\cdot\|} , \tag{2.8}$$

i.e., the local observables are dense in $\mathscr{A}$ in the strongest possible topology, the $\|.\|$-topology of $\mathscr{A}$. Furtheron $\mathscr{A}$ is a separable so-called UHF-algebra, which is simple and thus has a trivial center. The "type" ("invariant" in [16]) of $\mathscr{A}$ is given by the prime number decomposition of the $m(p)$, $p \in \{1, \ldots, r\}$. Thus quite different multi-lattice systems may lead to $*$-isomorphic quasi-local algebras. The multi-lattice structure is, however, basic for the definition of the Hamiltonians and the limiting equilibrium states, and will be made explicit throughout the discussion.

At first sight it seems disappointing that the center of $\mathscr{A}$ is trivial, i.e. that only $\mathbb{C}$-numbers commute with all other elements of $\mathscr{A}$. Observe that this property is shared with the algebra of all bounded operators in a Hilbert space, which characterizes traditional quantum mechanics for systems with finitely many degrees of freedom. The essential new features of the quasi-local observable algebras are expressed by the technical term "anti-liminarity" [9] and are connected with the existence of overcountably many disjoint (irreducible) representations. The disjointness is a notion which is connected with the closures of the represented observable algebra in the weak operator topologies of the respective representation Hilbert spaces. The in this way extended representation algebras may exhibit non-isomorphic structures and especially non-isomorphic centers. We illustrate this by the following observables, which are basic for mean field models.

Let for every $p \in \{1, \ldots, r\}$ be $\{e_p^n \mid 1 \leq n \leq n(p)\}$ with $n(p) := m^2(p)$, a selfadjoint basis in $\mathscr{B}_p$. If these spin observables are placed onto the i-th lattice point and considered as part of the total lattice algebra $\mathscr{A}$ they are denoted by $e_{ip}^n := \eta_{\{(i,p)\}}(e_p^n) \in \eta_{\{(i,p)\}}(\mathscr{A}_{ip}) \subset \mathscr{A}$.

For a macroscopic observer the density observables for every $\Lambda \in \mathscr{L}$

$$m_\Lambda(e_p^n) := \frac{1}{|\Lambda|} \sum_{i \in \Lambda_p} e_{ip}^n \tag{2.9}$$

are important. Since every $x \in \mathscr{B}_p$ is a linear combination of the e_p^n, $1 \leq n \leq n(p)$, we obtain $m_\Lambda(x)$ by a linear combination of (2.9). Especially we find

$$m_\Lambda(\mathbb{1}_p) = \frac{|\Lambda_p|}{|\Lambda|} \mathbb{1} \in \mathscr{A}. \tag{2.10}$$

In a thermodynamic description Λ has to tend to infinity in a way that the values of (2.10) tend to a number $c_p \in (0, 1)$. In spite of being norm bounded the net $(m_\Lambda(x);\ \Lambda \in \mathscr{L})$ does not converge in the norm topology. It may however converge in many representations in the weak operator topologies, and the limits may then indicate disjoint representations. Or, turning the argument around: The fact that the quasi-local algebra $\mathscr{A}$ has overcountably many disjoint representations is the prerequisite for the density observables becoming thermodynamic state variables with a continuum of values in the thermodynamic limit.

2.2. *Local Hamiltonians and Symmetries*

A physical interaction of a (multi-)lattice system would not be strictly of a finite range, but would decrease with large distances. The reasonable potentials are described in [8, 17, 18]. From a strict thermodynamic point of view such an interaction is considered in homogeneous states only. The maximal degree of homogeneity is permutation invariance.

Definition 2.1. (i) *The group of permutations $\mathscr{P}$ is given by all bijections P of $\mathscr{R}$ of the form*

$$P(i, p) = (P_p(i), p), \quad i \in \mathscr{I}, p \in \{1, \ldots, r\} \tag{2.11}$$

with the subsidiary condition, that they are equal to the identity map outside a region $\Lambda \in \mathscr{L}$, which depends on P.

(ii) *A representation of $\mathscr{P}$ by $*$-automorphisms of $\mathscr{A}$ is given by the following prescription: Let be $\bigotimes_{(i,p) \in \Lambda} x_{ip}$ with $x_{ip} \in \mathscr{A}_{ip}$ a product operator in $\mathscr{A}_\Lambda$; then define for $P \in \mathscr{P}$ the set*

$$P\Lambda := \{P(i, p) \mid (i, p) \in \Lambda\} \tag{2.12}$$

and the transformation of the embedded product operators

$$\Theta_P\Big(\eta_\Lambda\Big(\bigotimes_{(i,p) \in \Lambda} x_{ip}\Big)\Big) := \eta_{P\Lambda}\Big(\bigotimes_{(i,p) \in \Lambda} x_{P(i,p)}\Big). \tag{2.13}$$

After having verified the well-definedness of (2.13), linear extension and norm-closure gives the action of Θ_P on an arbitrary element of $\mathscr{A}$.

The assumption that in homogeneous states the potential looks as being permutation invariant leads to mean field models. The local Hamiltonians are then simple permutation covariant expressions satisfying

$$\Theta_P(H_\Lambda) = H_{\Lambda'}, \qquad \Lambda' = P\Lambda, \ \forall P \in \mathscr{P}, \ \forall \Lambda \in \mathscr{L}. \tag{2.14}$$

We restrict our discussion to the case that we have m-body interactions with finite $m \in \mathbb{N}$. We are thus led to polynomials in the density observables $m_\Lambda(e_p^n)$, $1 \leq p \leq r$, $1 \leq n \leq n(p)$, of (2.9). The local Hamiltonian H_Λ is in general a sum of different m-body interactions, say for $m \in \{1, \ldots, q\}$, $q \in \mathbb{N}$ fixed. According to the number of the basis elements in all of the $\mathscr{B}_p$, $1 \leq p \leq r$, we have for every $\Lambda \in \mathscr{L}$ the set of $\sum_{p=1}^{r} n(p)$ density observables

$$\hat{m}_\Lambda := (m_\Lambda(e_1^1), m_\Lambda(e_1^2), \ldots, m_\Lambda(e_r^{n(r)})), \tag{2.15}$$

for which we employ the indicated vector notation. Then a homogeneous polynomial of degree m is defined as

$$Q^m(\hat{m}_\Lambda) := \sum_{p_1=1}^{r} \sum_{n_1=1}^{n(p_1)} \cdots \sum_{p_m=1}^{r} \sum_{n_m=1}^{n(p_m)} {}^mC_{p_1 \ldots p_m}^{n_1 \ldots n_m}(\Lambda)\, m_\Lambda(e_{p_1}^{n_1}) \ldots m_\Lambda(e_{p_m}^{n_m}). \tag{2.16}$$

In view of the great number of indices, the notation will be made more transparent by using multiindices $\pi_m = (p_1, \ldots, p_m)$ and $\nu_m = (n_1, \ldots, n_m)$, where we even neglect the index m, if the degree of the homogeneous polynomial is known.

Further we have to choose the local coupling constants ${}^mC_\pi^\nu(\Lambda)$ in a way, such that $Q^m(\hat{m}_\Lambda)$ be a selfadjoint operator in $\eta_\Lambda(\mathscr{A}_\Lambda)$, e.g.

$${}^mC_{p_1 \ldots p_m}^{n_1 \ldots n_m}(\Lambda) = {}^mC_{p_{s(1)} \ldots p_{s(m)}}^{n_{s(1)} \ldots n_{s(m)}}(\Lambda) \in \mathbb{R}, \quad \forall s \in \mathscr{S}_m, \tag{2.17}$$

$\mathscr{S}_m$ being the symmetric group of m elements.

The thermodynamic limit is performed over certain subsets of $\mathscr{L}$. Let us call a subset $\mathscr{N} \subset \mathscr{L}$, which is again directed by inclusion and absorbing – i.e. every $\Lambda \in \mathscr{L}$ is dominated by a $\Lambda' \in \mathscr{N}$ – a funnel. A funnel

is then indexed by a so-called concentration vector $c:=(c_1,\dots,c_r)$ with each $c_p\in(0,1)$, $\sum_{p_1=1}^{r} c_p=1$, and written $\mathcal{N}(c)$, if for all $\varepsilon>0$ exists a $k\in\mathbb{N}$ such that for all $\Lambda\in\mathcal{N}(c)$ with $|\Lambda|>k$:

$$\left|\frac{|\Lambda_p|}{|\Lambda|}-c_p\right|<\varepsilon,\quad 1\le p\le r. \tag{2.18}$$

It is clear, that for a given c there exist many funnels $\mathcal{N}(c)$. Let us specify the dependence of the coupling constants on $\Lambda\in\mathcal{L}$ and demand that the ${}^{m}C_{\pi}^{\nu}(\Lambda)$ be only dependent on the relative sizes of the sublattices in a continuous way, that means in abuse of notation ${}^{m}C_{\pi}^{\nu}(\Lambda)={}^{m}C_{\pi}^{\nu}\left(\frac{|\Lambda_1|}{|\Lambda|},\dots,\frac{|\Lambda_r|}{|\Lambda|}\right)$ and that the limit

$$\lim_{\Lambda\in\mathcal{N}(c)} {}^{m}C_{\pi}^{\nu}(\Lambda)={}^{m}C_{\pi}^{\nu}(c) \tag{2.19}$$

exists for all concentrations c, all funnels $\mathcal{N}(c)$ and all m, ν, π.

Now we can introduce the Hamiltonian of the system as a sum of the m-body interactions, which may be physically of different type but here are combined to one homogeneous polynomial for every m.

Definition 2.2. (i) *Let be $Q^m(\hat{m}_\Lambda)$ as defined above. Then the considered local Hamiltonians are of the form*

$$H_\Lambda:=|\Lambda|\sum_{m=1}^{q} Q^m(\hat{m}_\Lambda),\quad \forall\Lambda\in\mathcal{L}. \tag{2.20}$$

(ii) *If $\hat{m}\in\times_{p=1}^{r}\mathbb{R}^{n(p)}$ with components m_p^m, $1\le p\le r$, $1\le n\le n(p)$ and c a concentration vector, we define*

$$\begin{aligned} Q(c,\hat{m})&=\sum_{m=1}^{q} Q^m(c_1 m_1^1,\dots,c_r m_r^{n(r)}) \qquad (2.21)\\ &=\sum_{m=1}^{q}\sum_{\pi_m}\sum_{\nu_m} {}^{m}C_{\pi_m}^{\nu_m}(c)\, c_{p1} m_{p_1}^{n_1}\dots c_{p_m} m_{p_m}^{n_m}, \end{aligned}$$

where the homogeneous polynomials on the right hand side are of the type (2.16) with the $m_\Lambda(e_p^n)$ replaced by $c_p m_p^n\mathbb{1}$ and the coupling constants in the limit are used. We consider (2.21) as a real polynomial, which later will appear in expressions for the energy density.

2.3. States

The mathematical states of $\mathcal{A}$ are the positive, normalized linear functionals on $\mathcal{A}$ (cf., e.g., [7]). They constitute a convex set $\mathcal{S}\equiv\mathcal{S}(\mathcal{A})$, which is w^*-compact (where the w^*-topology is defined by the convergence of the expectation values). That this set is also appropriate for the quantum statistical state concept may be demonstrated by considering the local restrictions

$$\begin{aligned} &\langle\eta_\Lambda^*(\varphi);A\rangle:=\langle\varphi;\eta_\Lambda(A)\rangle,\\ &\varphi\in\mathcal{S},\ A\in\mathcal{A}_\Lambda,\ \Lambda\in\mathcal{L}. \end{aligned} \tag{2.22}$$

Here η_Λ^* maps $\mathcal{S}$ w^*-continuously onto $\mathcal{S}(\mathcal{A}_\Lambda)$. In the same way one defines for $\Lambda\subset\Lambda'$ the mapping $\eta_{\Lambda,\Lambda'}^*$ by

$$\begin{aligned} &\langle\eta_{\Lambda,\Lambda'}^*(\varphi_{\Lambda'});A\rangle:=\langle\varphi_{\Lambda'};\eta_{\Lambda',\Lambda}(A)\rangle,\\ &A\in\mathcal{A}_\Lambda,\ \varphi_{\Lambda'}\in\mathcal{S}(\mathcal{A}_{\Lambda'}) \end{aligned} \tag{2.23}$$

which maps $\mathcal{S}(\mathcal{A}_{\Lambda'})$ w^*-continuously onto $\mathcal{S}(\mathcal{A}_\Lambda)$. From (2.7) it follows

$$\begin{aligned} &\eta_{\Lambda,\Lambda'}^*\circ\eta_{\Lambda'}^*(\varphi)=\eta_\Lambda^*(\varphi),\\ &\forall\varphi\in\mathcal{S}\text{ and }\forall\Lambda,\Lambda'\in\mathcal{L}\text{ with }\Lambda\subset\Lambda'. \end{aligned} \tag{2.24}$$

Since $\mathcal{A}_\Lambda$ is a matrix algebra every $\eta_\Lambda^*(\varphi)$ is associated with a density matrix $\varrho_\Lambda\in\mathcal{A}_\Lambda$. Now there is a bijection between $\mathcal{S}$ and the families $\{\varphi_\Lambda\in\mathcal{S}(\mathcal{A}_\Lambda);\Lambda\in\mathcal{L}\}$ which satisfy the compatibility condition (2.24), where $\eta_\Lambda^*(\varphi)$ corresponds to φ_Λ, for all $\Lambda\in\mathcal{L}$. In other words: Every $\varphi\in\mathcal{S}$ is uniquely given by a compatible family of local density matrices, and thus has a quantum statistical meaning.

Since $\mathcal{A}$ is separable the w^*-topology on $\mathcal{S}$ is metrizable. The σ-algebra of the Borel sets of $\mathcal{S}$ (generated by the w^*-open sets) is therefore equal to the σ-algebra of Baire sets (generated by the w^*-closed G_δ sets). Hence every Borel probability measure μ on $\mathcal{S}$ is regular in the sense that for every Borel set B

$$\begin{aligned} \mu(B)&=\sup\{\mu(F)\,|\,F\subset B,\ F\ w^*\text{-closed}\}\\ &=\inf\{\mu(U)\,|\,B\subset U,\ U\ w^*\text{-open}\}, \end{aligned}$$

where the first relation will be used in the proof of Theorem 4.4.

If for $\omega\in\mathcal{S}$ there is a Borel probability measure μ on $\mathcal{S}$ such that $\omega=\int_{\mathcal{S}}\varphi\,d\mu(\varphi)$ (in the w^*-topology), then we have a statistical decomposition of ω into states, which are in $\operatorname{supp}\mu$, the support of μ. If $\operatorname{supp}\mu\subseteq\delta_e\mathcal{S}$, ω is decomposed into pure states, which is typically non-unique in a quantum theory. In traditional quantum theory $\operatorname{supp}\mu$ is usually a countable set, whereas in macroscopic many body theory continuous measures are important.

The richness of the state space of our quasi-local algebra manifests itself by the existence of many dis-

joint states. Formally two states are disjoint, if their GNS-representations are disjoint in the sense indicated in Section 2.1. Physically disjoint states are globally different from each other, so that the one is not obtained by local perturbations from the other. A state is called factorial, if it is not decomposable into disjoint states in a non-trivial manner, which amounts to being macroscopically pure. For every state there is a canonical decomposition into pair-wise disjoint factorial states, the so-called central decomposition. In traditional Hilbert space quantum theory all states are factorial and the central decompositions are, therefore, trivial. In the case of a quasi-local algebra the central decomposition indicates, which macroscopic properties of the system fluctuate in the considered state.

As mentioned before the states of thermodynamic significance should have a certain spatial homogeneity property. For our present investigation we consider the most homogeneous ones, the permutation invariant states.

Definition 2.3. *A state $\varphi \in \mathcal{S}$ is called permutation invariant, if*

$$\langle \varphi ; \Theta_P(A)\rangle = \langle \varphi ; A\rangle , \quad \forall A \in \mathcal{A}, \forall P \in \mathcal{P}. \tag{2.25}$$

The set of permutation invariant states is denoted by $\mathcal{S}^{\mathcal{P}}$.

From the definition it is easily seen, that $\mathcal{S}^{\mathcal{P}}$ is convex and w^*-closed, hence w^*-compact.

Proposition 2.4. (i) *$\mathcal{S}^{\mathcal{P}}$ is a Bauer simplex. More precisely it holds that every $\omega \in \mathcal{S}^{\mathcal{P}}$ has a unique decomposition*

$$\omega = \int_{\partial_e \mathcal{S}^{\mathcal{P}}} \varphi \, d\mu(\varphi) \tag{2.26}$$

where μ is a probability measure on $\mathcal{S}$ with support in $\partial_e \mathcal{S}^{\mathcal{P}}$, and $\partial_e \mathcal{S}^{\mathcal{P}}$ is w^*-compact. The correspondence (2.26) defines an affine w^*-vague-continuous mapping between $\mathcal{S}$ and the set of probability measures on $\partial_e \mathcal{S}^{\mathcal{P}}$ (the latter being denoted by $\mathcal{M}^1_+(\partial_e \mathcal{S}^{\mathcal{P}})$).

(ii) *The extremal measure μ of (2.26) coincides with the central measure of ω.*

(iii) *A state $\omega \in \mathcal{S}^{\mathcal{P}}$ is in $\partial_e \mathcal{S}^{\mathcal{P}}$ iff it is a product state. That is, iff it satisfies*

$$\left\langle \omega ; \eta_\Lambda \Big(\bigotimes_{(i,p)\in\Lambda} x_{ip} \Big) \right\rangle = \prod_{(i,p)\in\Lambda} \langle \omega ; \eta_{\{(i,p)\}}(x_{ip})\rangle \tag{2.27}$$

for all product operators in $\mathcal{A}_\Lambda$ and all $\Lambda \in \mathcal{L}$. Because of permutation invariance the density matrices corresponding to $\eta^*_{\{(i,p)\}}(\omega)$ depend on p only.

Proof: For one lattice ($r=1$) the assertions (ii), (iii) and the simplex property of $\mathcal{S}^{\mathcal{P}}$ follow from [23]. That this simplex has a w^*-compact extreme boundary $\partial_e \mathcal{S}^{\mathcal{P}}$ is obtained by parametrizing it by the state space of the one lattice point algebra.

If $r \in \mathbb{N}$ is greater than 1, the group of permutations $\mathcal{P}$ is slightly smaller than the group of all finite permutations of the multilattice $\mathcal{R}$. Nevertheless, one can show that $\mathcal{P}$ acts via the automorphisms Θ_P, $P \in \mathcal{P}$, in a norm asymptotically abelian manner on $\mathcal{A}$. Then Størmer's proof can be taken over with only minor modifications. □

From Proposition 2.4 it follows that $\mathcal{S}^{\mathcal{P}}$ is affinely isomorphic to the classical state space $M^1_+(\partial_e \mathcal{S}^{\mathcal{P}})$ which belongs to the commutative C^*-algebra $\mathcal{C}(\partial_e \mathcal{S}^{\mathcal{P}})$ of all continuous complex functions on $\partial_e \mathcal{S}^{\mathcal{P}}$ (equipped with the induced w^*-topology). The radical procedure of making the states spatially homogeneous discloses this classical structure – typified by the Boolean lattice of all subsets on $\partial_e \mathcal{S}^{\mathcal{P}}$ – in the easiest manner. A more subtle analysis reveals that also the set of all local perturbations of $\mathcal{S}^{\mathcal{P}}$, which is mathematically the smallest norm-closed split face $\mathcal{F}^{\mathcal{P}}$ containing $\mathcal{S}^{\mathcal{P}}$, represents the same classical structure. Most of the following considerations could be extended to $\mathcal{F}^{\mathcal{P}}$, but we stick for simplicity to $\mathcal{S}^{\mathcal{P}}$.

In this sense $\mathcal{S}^{\mathcal{P}}$ is considered as set of those quantum statistical states which are of relevance for the thermodynamic point of view. The elements of $\partial_e \mathcal{S}^{\mathcal{P}}$ are then to be interpreted as the pure phases (not necessarily in equilibrium) of the system. The equilibrium states are singled out in the following by the variational principle to be established.

Of special importance are the canonical equilibrium states.

Definition 2.5. (i) *For $\Lambda \in \mathcal{L}$ and for given local Hamiltonian H_Λ of (2.20) the local Gibbs state $\omega^\beta_\Lambda \in \mathcal{S}(\mathcal{A}_\Lambda)$ is defined by*

$$\langle \omega^\beta_\Lambda ; A\rangle := \mathrm{tr}_\Lambda (e^{-\xi_\Lambda - \beta H_\Lambda} A), \quad A \in \mathcal{A}_\Lambda , \tag{2.28}$$

where $\xi_\Lambda \in \mathbb{R}$ is determined by the normalization condition.

(ii) *A state $\omega^\beta \in \mathcal{S}$ is called a limiting Gibbs state (of temperature β and concentration vector c) if there is a*

funnel $\mathcal{N}(c)$ such that

$$\eta_\Lambda^*(\omega^\beta) = \lim_{\Lambda' \in \mathcal{N}(c)} \eta_{\Lambda,\Lambda'}^*(\omega_\Lambda^\beta), \quad \forall \Lambda \in \mathcal{L}. \tag{2.29}$$

(iii) *The system (specified by $(H_\Lambda; \Lambda \in \mathcal{L})$) is said to have a unique limiting Gibbs state for given β and c if every $\mathcal{N}(c)$ leads to a limiting Gibbs state in the sense of (ii) and all these limiting Gibbs states coincide.*

One can show that for a given family of local Hamiltonians there always exist limiting Gibbs states for all $\beta \in (0, +\infty)$ and all concentration vectors c due to the compactness of $\mathcal{S}$ and that these are elements of $\mathcal{S}^\mathcal{P}$. The limit on the right hand side of (2.29) – if it exists – defines by the w^*-continuity of the restriction map and by (2.24) automatically a compatible family of local states and thus is a constructive method for finding the limiting Gibbs states. The question, which of the considered mean field interactions lead to unique limiting Gibbs states is far from being solved.

Let us end here our sketch of the quantum statistical frame for multi-lattice mean field theories, which has indicated that the following attributes are intimately connected with each other: the anti-liminarity property of the quasi-local algebra $\mathcal{A}$, overcountably many disjoint representations of $\mathcal{A}$, overcountably many values of the limiting density observables $m_\Lambda(x)$, $x \in \mathcal{B}$, and a non-trivial classical structure of the set of homogeneous states $\mathcal{S}^\mathcal{P}$, which will be taken as the quantum statistical representative of the thermodynamic state space. Thus, the choice of the algebra of observables decides already over the triviality of the thermodynamic aspects. Consider, e.g., the case $m(p)=2$ for $1 \le p \le r$, so that $\mathcal{A}$ is isomorphic to the CAR-algebra, and represent it in the Fock space. If one would incautiously choose the weak closure of this operator algebra as algebra of observables, one would arrive at a post-liminary algebra (in an irreducible representation). Then all other irreducible representations of it would be unitary equivalent to each other [9].

3. Thermodynamic Functionals

In this section the fundamental thermodynamic functionals entropy, energy, and free energy are introduced. These quantities are first defined on a finite region of the lattice; then the infinite volume limits of the specific quantities are calculated and some fundamental properties discussed. The thermodynamic limit shows an essential dependence of the funnel $\mathcal{N}(c)$.

3.1. Internal Energy

Definition 3.1. (Local Internal Energy). *Let $\omega \in \mathcal{S}$ and $\Lambda \in \mathcal{L}$. Then the local internal energy of the lattice is defined as*

$$U_\Lambda(\omega) := \langle \omega; H_\Lambda \rangle.$$

Proposition 3.2. (Specific Internal Energy). *Let c be a concentration vector with the funnel $\mathcal{N}(c)$, $(\omega_\Lambda \in \mathcal{S}^{\mathcal{P}(\Lambda)}; \Lambda \in \mathcal{N}(c))$ with $\omega_\Lambda \xrightarrow{w^*} \omega \in \mathcal{S}^\mathcal{P}$. Then the following limit exists:*

$$u(c, \omega) := \lim_{\Lambda \in \mathcal{N}(c)} \frac{U_\Lambda(\omega_\Lambda)}{|\Lambda|}. \tag{3.1}$$

This limit is called the specific internal energy and is a w^*-continuous affine functional on $\mathcal{S}^\mathcal{P}$.

Proof: We may reduce our calculation to a monomial, since U_Λ is linear. Further we will assume that the set $\{1, \dots, m\}$ is part of each Λ_p if $|\Lambda|$ is large enough. If this is not fulfilled, one can choose a new enumeration of the lattice points. Now we calculate

$$\langle \omega_\Lambda; m_\Lambda(e_{p_1}^{n_1}) \dots m_\Lambda(e_{p_m}^{n_m}) \rangle = \frac{1}{|\Lambda|^m} \sum_{i_1 \in \Lambda_{p_1}} \dots \sum_{i_m \in \Lambda_{p_m}} \langle \omega_\Lambda; e_{i_1 p_1}^{n_1} \dots e_{i_m p_m}^{n_m} \rangle.$$

By permutation invariance and an easy combinatoric calculation one can check, that

$$\lim_{\Lambda \in \mathcal{N}(c)} \langle \omega_\Lambda; m_\Lambda(e_{p_1}^{n_1}) \dots m_\Lambda(e_{p_m}^{n_m}) \rangle = \lim_{\Lambda \in \mathcal{N}(c)} \frac{1}{|\Lambda|^m} \sum_{i_1 \in \Lambda_{p_1}} \dots \sum_{i_m \in \Lambda_{p_m}} \langle \omega_\Lambda; e_{i_1 p_1}^{n_1} \dots e_{i_m p_m}^{n_m} \rangle = \langle \omega; c_{p_1} e_{1 p_1}^{n_1} \dots c_{p_m} e_{m p_m}^{n_m} \rangle.$$

In general the desired limit is

$$\lim_{\Lambda \in \mathcal{N}(c)} \frac{U_\Lambda(\omega_\Lambda)}{|\Lambda|} = \sum_{m=1}^{q} \sum_{\pi_m, \nu_m} {}^m C_{\pi_m}^{\nu_m}(c) \langle \omega; c_{p_1} e_{1 p_1}^{n_1} \dots c_{p_m} e_{m p_m}^{n_m} \rangle.$$

The continuity and affinity in $\omega \in \mathcal{S}^\mathcal{P}$ is clear by inspection. □

Observation 3.3. *Use the notation of the last proposition. If $\omega \in \partial_e \mathcal{S}^\mathcal{P}$, set $m_p^n := \langle \omega; e_{1p}^n \rangle$ and find by the product property:*

$$u(c, \omega) = \sum_{m=1}^{q} Q^m(c_1 m_1^1, \dots, c_r m_r^{n(r)}) = Q(c, \hat{m}).$$

3.2. Entropy

For quantum spin systems the connection of states of the infinite system with a family of local density matrices as described in Sect. 2.3 leads to a natural definition of an absolute thermodynamic entropy density (and not only to a relative one).

Definition 3.4. (Local Entropy). *Let $\omega \in \mathscr{S}$. Then the restriction $\eta_\Lambda^*(\omega)$ of ω to $\mathscr{A}_\Lambda$ is a state on $\mathscr{A}_\Lambda$ with a density matrix $\varrho_\Lambda \in \mathscr{A}_\Lambda$, such that for all $A \in \mathscr{A}_\Lambda$*

$$\langle \eta_\Lambda^*(\omega); A\rangle = \mathrm{tr}_\Lambda(\varrho_\Lambda A).$$

Now, we can define the entropy functional S_Λ on $\mathscr{A}$:

$$S_\Lambda : \mathscr{S} \to \mathbb{R} : \omega \to S_\Lambda(\omega) := -\mathrm{tr}_\Lambda(\varrho_\Lambda \ln \varrho_\Lambda).$$

In the case, that there exists an eigenvalue $\lambda = 0$ of ϱ_Λ, one uses the continuity of $t \to -t \ln t$ at $t = 0$.

A consequence of this definition is the subadditivity of the local entropies, (cf., e.g. (6.2.24) in [8]). That is, we have for all $\Lambda, \Omega \in \mathscr{L}$ with $\Lambda \cap \Omega = \emptyset$ and arbitrary $\omega \in \mathscr{S}$:

$$S_{\Lambda\cup\Omega}(\omega) \leq S_\Lambda(\omega) + S_\Omega(\omega).$$

Lemma 3.5. *Let c be a concentration vector with funnel $\mathscr{N}(c)$. For all $\varepsilon > 0$, there exists a number $k \in \mathbb{N}$, such that for all $\Omega \in \mathscr{N}(c)$ with $|\Omega| \geq k$ holds: there is a $\tilde{\Lambda} \in \mathscr{N}(c)$, such that for all $\Lambda \in \mathscr{N}(c)$ with $\tilde{\Lambda} \subseteq \Lambda$ and arbitrary $\omega \in \mathscr{S}^{\mathscr{P}(\Lambda)}$ the following estimation is valid:*

$$\frac{1}{|\Lambda|} S_\Lambda(\omega) \leq \frac{1}{|\Omega|} S_\Omega(\omega) + \varepsilon.$$

Proof: The main task is an estimation of the size of regions in a funnel $\mathscr{N}(c)$. The proof, therefore, is a very complicated juggling with the sizes of Λ, $\Lambda_p, \ldots$ and is elaborated in the appendix A.1.

Proposition 3.6 (Specific Entropy). *Let c be a concentration vector with funnel $\mathscr{N}(c)$. For all $\omega \in \mathscr{S}^{\mathscr{P}}$, the limit*

$$s(c, \omega) := \lim_{\Lambda \in \mathscr{N}(c)} \frac{S_\Lambda(\omega)}{|\Lambda|} \tag{3.2}$$

exists. This limit (the specific entropy) is a w-continuous, affine functional on $\mathscr{S}^{\mathscr{P}}$.*

Proof: (i) Let $\Lambda \in \mathscr{L}$. If there is another finite region $\Omega \in \mathscr{L}$, with the same size of the subregions Ω_p, as that of the Λ_p for $P \in \{1, \ldots, r\}$, then there exists a permutation $P \in \mathscr{P}$ with $P(\Omega) = \Lambda$. By invariance of the entropy under a permutation, if $\omega \in \mathscr{S}^{\mathscr{P}}$, we have $S_\Lambda(\omega) = S_\Omega(\omega)$. By the subadditivity of the entropy one calculates for $\omega \in \mathscr{S}^{\mathscr{P}(\Lambda)}$ (and therefore for all $\omega \in \mathscr{S}^{\mathscr{P}}$), that

$$0 \leq S_\Lambda(\omega) \leq \sum_{p=1}^{r} \sum_{i \in \Lambda_p} S_{\{(i,p)\}}(\omega) = \sum_{p=1}^{r} |\Lambda_p| \, S_{\{(p,p)\}}(\omega).$$

Since the entropy is bounded on a lattice point, we have the relation:

$$0 \leq \frac{S_\Lambda(\omega)}{|\Lambda|} \leq S_{\max} \quad \forall \omega \in \mathscr{S}^{\mathscr{P}(\Lambda)}. \tag{3.3}$$

(ii) Now it is possible to define the following properties, since $\dfrac{S_\Lambda(\omega)}{|\Lambda|}$ is bounded:

$$\underline{s_\Lambda(c, \omega)} := \inf\left\{\frac{S_{\Lambda'}(\omega)}{|\Lambda'|} \,|\, \Lambda \subseteq \Lambda' \in \mathscr{N}(c)\right\}$$

$$\overline{s_\Lambda(c, \omega)} := \sup\left\{\frac{S_{\Lambda'}(\omega)}{|\Lambda'|} \,|\, \Lambda \subseteq \Lambda' \in \mathscr{N}(c)\right\}$$

and

$$\underline{s(c, \omega)} := \lim_{\Lambda \in \mathscr{N}(c)} \underline{s_\Lambda(c, \omega)} \leq \lim_{\Lambda \in \mathscr{N}(c)} \overline{s_\Lambda(c, \omega)} =: \overline{s(c, \omega)},$$

(iii) With given $\varepsilon > 0$, use Lemma 3.5 for all $\Lambda \supseteq \tilde{\Lambda}$; we conclude:

$$\overline{s_\Lambda(c, \omega)} \leq \frac{1}{|\Omega|} S_\Omega(\omega) + \varepsilon \quad \forall \Lambda, \Omega \in \mathscr{N}(c)$$
$$\text{with } \tilde{\Lambda} \subseteq \Lambda \text{ and } |\Omega| \geq k.$$

Now let us take that limit for $\Lambda \in \mathscr{N}(c)$, which exists, and we obtain

$$\overline{s(c, \omega)} \leq \frac{1}{|\Omega|} S_\Omega(\omega) + \varepsilon.$$

The same procedure can be carried through with the right hand side, since there is only the condition that $\Omega \in \mathscr{N}(c)$ with $|\Omega| \geq k$.

$$\overline{s(c, \omega)} \leq \underline{s_\Omega(c, \omega)} + \varepsilon \quad \forall \Omega \in \mathscr{N}(c) \text{ with } |\Omega| \geq k$$

and

$$\overline{s(c, \omega)} \leq \underline{s(c, \omega)} + \varepsilon.$$

Since $\varepsilon > 0$ is arbitrarily small, the existence of the limit (3.2) is proved.

(iv) The affinity is a consequence of two well known convexity and concavity relations for the local entropy, see (6.2.25) in [8].

The continuity is calculated with the help of the central decomposition of a state $\omega \in \mathcal{S}^{\mathcal{P}}$ (Theorem 2.4) and the following observation 3.7 (cf. [19], [1]). □

Observation 3.7. *If $\omega \in \partial_e \mathcal{S}^{\mathcal{P}}$, this state is associated with a tupel of density matrices $(\varrho_1, \ldots, \varrho_r) \in \mathcal{B}$ and one calculates immediately*

$$s(c,\omega) = \lim_{\Lambda \in \mathcal{N}(c)} \frac{S_\Lambda(\omega)}{|\Lambda|} = \lim_{\Lambda \in \mathcal{N}(c)} \sum_{p=1}^{r} \sum_{i \in \Lambda_p} \frac{S_{\{(i,p)\}}(\omega)}{|\Lambda|}$$

$$= \lim_{\Lambda \in \mathcal{N}(c)} \sum_{p=1}^{r} \frac{|\Lambda_p|}{|\Lambda|} S_{\{(p,p)\}}(\omega)$$

$$= -\sum_{p=1}^{r} c_p \operatorname{tr}_p(\varrho_p \ln \varrho_p). \tag{3.4}$$

3.3. Free Energy

Definition 3.8. (Local Free Energy). *Let $\omega \in \mathcal{S}$, $\Lambda \in \mathcal{L}$ and $\beta \in (0, +\infty)$. Then the local free energy of the lattice is defined as*

$$F_\Lambda(\beta, \omega) := U_\Lambda(\omega) - \frac{1}{\beta} S_\Lambda(\omega).$$

By means of the forgoing section, the next proposition follows at once:

Proposition 3.9. (Specific Free Energy). *Let c a concentration with funnel $\mathcal{N}(c)$. For all $\omega \in \mathcal{S}^{\mathcal{P}}$, the limit*

$$f(c,\beta,\omega) := \lim_{\Lambda \in \mathcal{N}(c)} \frac{F_\Lambda(\beta,\omega)}{|\Lambda|} = u(c,\omega) - \frac{1}{\beta} s(c,\omega) \tag{3.5}$$

exists and is called the specific free energy. This limit is a w-continuous, affine functional on $\mathcal{S}^{\mathcal{P}}$.*

Observation 3.10. *If $\omega \in \partial_e \mathcal{S}^{\mathcal{P}}$, this state is associated with a tupel of density matrices $\varrho = (\varrho_1, \ldots, \varrho_r) \in \mathcal{B}$ and as specific free energy it results*

$$f(c,\beta,\omega) = Q(c,\hat{m}) + \frac{1}{\beta} \sum_{p=1}^{r} c_p \operatorname{tr}_p(\varrho_p \ln \varrho_p),$$

with $\hat{m} \equiv \hat{m}(\varrho) := (\operatorname{tr}_p(\varrho_p e_p^n))_{1,\ldots,r}^{1,\ldots,n(p)}$. (3.6)

4. Minimum Principle for the Free Energy Density

The minimum principle of the free energy for limiting Gibbs states in our context is based on the minimum principle of the local free energy for local Gibbs states and the convergence of the net $\left(\frac{F_\Lambda(\beta,\omega_\Lambda^\beta)}{|\Lambda|};\ \Lambda \in \mathcal{L}\right)$. This last statement is very specific for the free energy density and is not provable for the two other thermodynamic functionals in general.

Lemma 4.1. *Let $\Lambda \in \mathcal{L}$. Then the following minimum principle is valid:*

$$F_\Lambda(\beta, \omega_\Lambda^\beta) = \inf_{\varphi \in \mathcal{S}} \{F_\Lambda(\beta,\varphi)\}. \tag{4.1}$$

Proof: The proposition is a consequence of well known properties of the free energy in traditional quantum statistics, cf., e.g., (6.2.21) in [8]. □

Lemma 4.2. *We define the density of the local free energy with the corresponding local Gibbs state for an arbitrary finite region $\Lambda \in \mathcal{L}$ as*

$$\xi_\Lambda(\beta) := \frac{F_\Lambda(\beta,\omega_\Lambda^\beta)}{|\Lambda|}. \tag{4.2}$$

Now let c be a concentration vector with funnel $\mathcal{N}(c)$. Then choose a monotone and absorbing sequence $(\Lambda_n)_{n\in\mathbb{N}} \subseteq \mathcal{N}(c)$ with $\lim_{n\to\infty} \xi_{\Lambda_n}(\beta) = \xi(c,\beta)$ and $\lim_{n\to\infty} \omega_{\Lambda_n}^\beta = \omega \in \mathcal{S}^{\mathcal{P}}$. Then it holds

$$f(c,\beta,\omega) \le \xi(c,\beta).$$

Proof: We will give the proof in three steps, dividing the specific free energy in the parts of internal energy and entropy:

(i) By convergence, calculated as in Theorem 3.2, we have for a fixed $\varepsilon > 0$, the existence of a $n_0 \in \mathbb{N}$ such that for all $n \ge n_0$ holds

$$u(c,\omega) \le \frac{U_{\Lambda_n}(\omega_{\Lambda_n}^\beta)}{|\Lambda_n|} + \varepsilon. \tag{4.3}$$

(ii) In order to treat the entropy, we choose for the given ε the k from Lemma 3.5. Then there exists by definition of $S(c,\omega)$ a $n_1 \in \mathbb{N}$ and $|\Lambda_{n_1}| \ge k$ such that

$$s(c,\omega) \ge \frac{S_{\Lambda_{n_1}}(\omega)}{|\Lambda_{n_1}|} - \varepsilon. \tag{4.4}$$

Since $S_{\Lambda_{n_1}}$ is w*-continuous and $\omega_{\Lambda_n}^\beta \to \omega$, there exists a $n_2 \ge n_1$, such that for all $n \ge n_2$ it holds

$$\frac{S_{\Lambda_{n_1}}(\omega)}{|\Lambda_{n_1}|} \ge \frac{S_{\Lambda_{n_1}}(\omega_{\Lambda_n}^\beta)}{|\Lambda_{n_1}|} - \varepsilon. \tag{4.5}$$

That this holds for all $n \geq n_2$ follows from the monotony of the sequence $(\Lambda_n)_{n \in N}$. Now use Lemma 3.5. This is possible, since we have chosen $n \geq k$ with k from this lemma. Therefore, it exists a $n_3 \geq n_2$, such that for all $n \geq n_3$

$$\frac{S_{\Lambda_n}(\varphi)}{|\Lambda_n|} \leq \frac{S_{\Lambda_{n_1}}(\varphi)}{|\Lambda_{n_1}|} + \varepsilon \tag{4.6}$$

holds, if $\varphi \in \mathscr{S}^{\mathscr{P}(\Lambda_n)}$. Remember, that $\omega^{\beta}_{\Lambda_n} \in \mathscr{S}^{\mathscr{P}(\Lambda_n)}$. Therefore, it results from (4.4), (4.5), (4.6) for all $n \geq n_3$:

$$\begin{aligned} s(c, \omega) &\geq \frac{S_{\Lambda_{n_1}}(\omega)}{|\Lambda_{n_1}|} - \varepsilon \geq \frac{S_{\Lambda_{n_1}}(\omega^{\beta}_{\Lambda_n})}{|\Lambda_{n_1}|} - 2\varepsilon \\ &\geq \frac{S_{\Lambda_n}(\omega^{\beta}_{\Lambda_n})}{|\Lambda_n|} - 3\varepsilon. \end{aligned} \tag{4.7}$$

(iii) Let us finish the proof with the conclusions from (4.3) and (4.7). It hold's for all $n \geq \max\{n_0, n_3\}$:

$$\begin{aligned} f(c, \beta, \omega) &= u(c, \omega) - \frac{1}{\beta} s(c, \omega) \leq \frac{U_{\Lambda_n}(\omega^{\beta}_{\Lambda_n})}{|\Lambda_n|} \\ &\quad - \frac{1}{\beta} \frac{S_{\Lambda_n}(\omega^{\beta}_{\Lambda_n})}{|\Lambda_n|} + \varepsilon\left(1 + \frac{3}{\beta}\right) = \xi_{\Lambda_n}(\beta) + \varepsilon\left(1 + \frac{3}{\beta}\right). \end{aligned}$$

□

Theorem and Definition 4.3. *Let c be a concentration with funnel $\mathscr{N}(c)$. Then it holds*

$$f(c, \beta) := \lim_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) = \inf_{\varphi \in \mathscr{S}^{\mathscr{P}}} \{f(c, \beta, \varphi)\}. \tag{4.8}$$

$f(\beta, c)$ is the minimal free energy density.

Note, that this theorem gives the minimum of the free energy density with the help of the original local Gibbs states!

Proof: This proof is a consequence of the foregoing propositions. With Lemma 4.1., we know, that for an arbitrary $\varphi \in \mathscr{S}^{\mathscr{P}}$:

$$\begin{aligned} \limsup_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) &\leq \limsup_{\Lambda \in \mathscr{N}(c)} \frac{F_{\Lambda}(\beta, \varphi)}{|\Lambda|} = \lim_{\Lambda \in \mathscr{N}(c)} \frac{F_{\Lambda}(\beta, \varphi)}{|\Lambda|} \\ &= f(c, \beta, \varphi). \end{aligned}$$

Since this is holding for an arbitrary $\varphi \in \mathscr{S}^{\mathscr{P}}$, we conclude

$$\limsup_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) \leq \inf_{\varphi \in \mathscr{S}^{\mathscr{P}}} \{f(c, \beta, \varphi)\}. \tag{4.9}$$

There exists a monotone, absorbing sequence $(\Lambda_n)_{n \in N} \subseteq \mathscr{N}(c)$ with

$$\lim_{n \to \infty} \xi_{\Lambda_n}(\beta) = \liminf_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta).$$

Then choose a subsequence $\Lambda_k := \Lambda_{n_k}$ with the convergence relation $\lim_{k \to \infty} \omega^{\beta}_{\Lambda_k} = \omega$ and use the foregoing Proposition 4.2.:

$$\begin{aligned} \liminf_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) &= \lim_{k \to \infty} \xi_{\Lambda_k}(\beta) \geq f(c, \beta, \omega) \\ &\geq \inf_{\varphi \in \mathscr{S}^{\mathscr{P}}} \{f(c, \beta, \varphi)\}. \end{aligned}$$

Together with (4.9), one concludes

$$\begin{aligned} \inf_{\varphi \in \mathscr{S}^{\mathscr{P}}} \{f(c, \beta, \varphi)\} &\leq \liminf_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) \leq \limsup_{\Lambda \in \mathscr{N}(c)} \xi_{\Lambda}(\beta) \\ &\leq \inf_{\varphi \in \mathscr{S}^{\mathscr{P}}} \{f(c, \beta, \varphi)\}. \end{aligned}$$

□

The foregoing considerations involve direct estimations and rather modest mathematical techniques. They imply, however, results, of principal physical importance and structural interest.

As external thermodynamic parameters, we have introduced explicitly the temperature β and the relative concentrations $(c_1, \ldots, c_r)$. Implicitly, certain parameters in the Hamiltonians H_{Λ} may have the same physical status, especially in the linear part of the H_{Λ} may appear external field variables (cf., e.g., [2, 19]). In the present discussion we fix the family of local Hamiltonians and consider as thermodynamic equilibrium states those homogeneous states (in $\mathscr{S}^{\mathscr{P}}$), which minimize the free energy density for given values of c and β, i.e., we introduce

$$\mathscr{S}(c, \beta) := \{\varphi \in \mathscr{S}^{\mathscr{P}} \mid f(c, \beta, \varphi) = f(c, \beta)\}. \tag{4.10}$$

Observe that we are transforming here intuitive thermodynamic notions into rigorous mathematical concepts within a certain class of models, where every interpretational step can and must be thoroughly tested. Thus it is to be investigated if all mathematical states in $\mathscr{S}(c, \beta)$ correspond in fact to physical equilibrium states. A more cautious formulation would be to consider as such only the accumulation points of the net $(\omega^{\beta}_{\Lambda})_{\Lambda \in \mathscr{N}(c)}$ together with the components in their central decomposition, since this structure arises directly from the ω^{β}_{Λ}. In which way both notions are related to each other is partially clarified by the following results.

Theorem 4.4. *Let be c an arbitrary concentration vector and $\beta \in (0, +\infty)$ an arbitrary natural temperature. Then it holds:*

(i) *$\mathscr{S}(c, \beta)$ is a compact stable face of $\mathscr{S}^{\mathscr{P}}$;*

(ii) *$\mathcal{S}(c,\beta)$ is a Bauer simplex with extreme boundary*

$$\partial_e \mathcal{S}(c,\beta) = \partial_e \mathcal{S}^{\mathcal{P}} \cap \mathcal{S}(c,\beta);$$

(iii) *Every accumulation point of $(\omega_\Lambda^\beta)_{\Lambda\in\mathcal{N}(c)}$ lies in $\mathcal{S}(c,\beta)$ and its central decomposition is equal to its unique extremal decomposition in $\mathcal{S}(c,\beta)$.*

Proof: (i) Since $f(c,\beta,.)$ is affine, $\mathcal{S}(c,\beta)$ is convex and since $f(c,\beta,\cdot)$ is w^*-continuous, $\mathcal{S}(c,\beta)$ is w^*-closed, hence (as a subset of the compact set $\mathcal{S}$) w^*-compact. If

$$\mathcal{S}(c,\beta) \ni \omega = \int_{\mathcal{S}^{\mathcal{P}}} \varphi \, d\mu(\varphi)$$

for some probability Borel measure on $\mathcal{S}^{\mathcal{P}}$, one has

$$f(c,\beta) = f(c,\beta,\omega) = \int_{\mathcal{S}^{\mathcal{P}}} f(c,\beta,\varphi)\, d\mu(\varphi). \quad (4.11)$$

If $\mathrm{supp}(\mu)$ would not be contained in $\mathcal{S}(c,\beta)$, there would be a compact set $\mathcal{K} \subset \mathcal{S}^{\mathcal{P}}$ with $\mu(\mathcal{K})>0$ and $\mathcal{K} \cap \mathcal{S}(c,\beta)=\emptyset$. Then it would hold: $\min\{f(c,\beta,\varphi);\ \varphi\in\mathcal{K}\} > f(c,\beta)$, which could not be compensated by the values $f(c,\beta,\varphi)\in\mathcal{S}^{\mathcal{P}}\setminus\mathcal{K}$ and thus would contradict (4.11). Thus we must conclude, that $\mathrm{supp}(\mu)\subset\mathcal{S}(c,\beta)$, which is the characterizing property of a stable face.

(ii) According to section 2.3, there is an affine w^*-vague-continuous bijection between the states $\omega\in\mathcal{S}^{\mathcal{P}}$ and the probability measures $\mu_\omega \in M_+^1(\partial_e\mathcal{S}^{\mathcal{P}})$. If $\omega\in\mathcal{S}(c,\beta)\subset\mathcal{S}^{\mathcal{P}}$, then $\mathrm{supp}(\mu_\omega)\subset\partial_e\mathcal{S}^{\mathcal{P}}\cap\mathcal{S}(c,\beta)$ according to (i). Thus the mentioned bijection reduced to $\mathcal{S}(c,\beta)$ induces an affine, w^*-vague-continuous mapping onto $M_+^1(\partial_e\mathcal{S}^{\mathcal{P}}\cap\mathcal{S}(c,\beta))$, where the latter is a Bauer simplex according to [20], §4. Since the extreme boundary of $M_+^1(\partial_e\mathcal{S}^{\mathcal{P}}\cap\mathcal{S}(c,\beta))$ consists of the point measures on the w^*-compact set $\partial_e\mathcal{S}^{\mathcal{P}}\cap\mathcal{S}(c,\beta)$, the latter constitutes the extreme boundary of $\mathcal{S}(c,\beta)$.

(iii) If ω is an accumulation point of $(\omega_\Lambda^\beta)_{\Lambda\in\mathcal{N}(c)}$, then we have a convergent subnet of $(\omega_\Lambda^\beta)_{\Lambda\in\mathcal{N}(c)}$, which may be chosen as a sequence, since $\mathcal{S}$ is separable in the w^*-topologie. Now, we can employ Lemma 4.2. and Theorem 4.3. to show, that ω has minimal free energy and thus is in $\mathcal{S}(c,\beta)$. According to (ii) and (i) the unique extremal decompositions of ω in $\mathcal{S}(c,\beta)$ and in $\mathcal{S}^{\mathcal{P}}$ coincide, where the latter is just the central decomposition. □

The results of Theorem 4.4. justify to consider the elements of $\partial_e\mathcal{S}(c,\beta)$ as the pure equilibrium phase states: first of all they are factor states and thus macroscopically pure and second every mixed phase state $\omega\in\mathcal{S}(c,\beta)$ decomposes into them in a unique manner. Therefore, in order to know all of $\mathcal{S}(c,\beta)$ it is sufficient to determine $\partial_e\mathcal{S}(c,\beta)$ what will be done in the next section. It is an interesting open problem whether the union of the central components of the accumulation points equals all of $\partial_e\mathcal{S}(c,\beta)$.

In this context it is also important to note that the free energy minimum principle may be restricted to macroscopically pure states only.

Corollary 4.5. (Minimum Principle in $\partial_e\mathcal{S}^{\mathcal{P}}$) *For every choice of c and β it holds*

$$\partial_e\mathcal{S}(c,\beta) = \{\omega\in\partial_e\mathcal{S}^{\mathcal{P}} \mid f(c,\beta,\omega) = f(c,\beta)\}. \quad (4.12)$$

Proof: This follows directly from the fact that $\partial_e\mathcal{S}(c,\beta)\subset\partial_e\mathcal{S}^{\mathcal{P}}$, which holds by Theorem 4.4.(ii). □

Now we have sufficient information to develop a calculation procedure for the pure equilibrium phases.

5. Selfconsistency-Equations

By the results of the last section, we deduce the well known selfconsistency equations as a consequence of the minimum principle of the specific free energy. For this, we need

Lemma 5.1. *Let be $\beta\in(0,\infty)$, c a concentration vector and $\omega\in\partial_e\mathcal{S}(c,\beta)$ a pure phase equilibrium state with the tupel of density matrices $(\varrho_1,\ldots,\varrho_r)\in\mathcal{B}$. Then we have $0\notin\sigma(\varrho_p)$ $\forall p\in 1,\ldots,r$.*

Proof: See Appendix A.2. □

Note that the set of all density matrices in a matrix-algebra with non-zero eigenvalues is an open set in the norm-topology. The minimizing states of Lemma 5.1. are not in the boundary of the states on $\mathcal{B}_p$. This is important for calculating the derivatives of the thermodynamic functionals on the space of extremal permutation invariant states. Let us begin with the specific entropy on the extremal permutation invariant states, which can be reduced to the entropy of a finite dimensional matrix-algebra:

Lemma 5.2. *Let M_n the algebra of $n\times n$-matrices and $U=\{\varrho\in M_n \mid \varrho$ selfadjoint and $\sigma(\varrho)\subset(0,1)\}$. Now take the functional $\tilde{s}: U\to\mathbb{R}$, $\varrho\to\tilde{s}(\varrho)=-$*

$\mathrm{tr}(\varrho \ln(\varrho))$. *Then we have for selfadjoint* $h \in M_n$, *such that* $\varrho + h \in U$:

$$\tilde{s}(\varrho + h) = \tilde{s}(\varrho) + \tilde{s}'_\varrho(h) + o(\|h\|) \tag{5.1}$$

with the rest term $o(\|h\|)$, *vanishing more rapidly than first order in* $\|h\|$ *and the linear functional* $\tilde{s}'_\varrho : \mathcal{M}_n^{sa} \to \mathbb{R}$

$$\tilde{s}'_\varrho(h) = -\mathrm{tr}(h(\mathbb{1} + \ln(\varrho))), \tag{5.2}$$

where the quantity $\tilde{s}'_\varrho$ *is called the total derivative of* $\tilde{s}$ *with respect to* ϱ.

Proof: See Appendix A.3. □

Now we deal with the derivative of the multi lattice specific energy in the following lemma, the proof of which requires only differentiation rules for numerical polynomials $Q : \mathbb{R}^n \to \mathbb{R}$.

Lemma 5.3. *Take an element* $\varrho \in W = W_1 \times \ldots \times W_r$ *with each* W_p *equal to the U from Lemma 5.2. Then define the functional* $\tilde{u}(c, \varrho)$ *on W with a fixed concentration vector c as*

$$\begin{aligned}\tilde{u}(c, \varrho) &:= Q(c, \hat{m}(\varrho)) \\ &= Q(c, \mathrm{tr}_1(\varrho_1 e_1^1), \ldots, \mathrm{tr}_r(\varrho_r e_r^{n(r)}),\end{aligned}$$

where (2.21) and (3.6) has been employed. Then we have for $h := (h_1, \ldots, h_r) \in \mathcal{B}$ *with each* h_p *selfadjoint and* $\varrho_p + h_p \in W_p$

$$\begin{aligned}&\tilde{u}(c, (\varrho_1 + h_1, \ldots, \varrho_r + h_r)) \\ &\qquad = \tilde{u}(c, \varrho) + \tilde{u}'_\varrho(h) + o(\|h\|),\end{aligned} \tag{5.3}$$

where $o(\|h\|)$ *is a remainder term in* $\|h\|$ *and* $\tilde{u}'_\varrho$ *a linear functional on* $\mathcal{B}$ *of the form*

$$\tilde{u}'_\varrho(h) = \sum_{p=1}^{r} \sum_{n=1}^{n(p)} \mathrm{tr}_p(h_p e_p^n) \frac{\partial}{\partial m_p^n} Q|(c, \hat{m})|_{\hat{m}(\varrho)}. \tag{5.4}$$

Note that the two lemmas treat the differentiation of the functionals $\tilde{s}$, $\tilde{u}$ over positive matrices with $\sigma(\varrho) \subset (0, 1)$. If we restrict ourselves to density matrices, we have the usual thermodynamic functionals for extremal permutation invariant states.

Theorem 5.4. *Let* $\varrho = (\varrho_1, \ldots, \varrho_r) \in \mathcal{B}$ *belong to an extremal permutation invariant state in* $\partial_e \mathcal{S}(c, \beta)$. *Then it satisfies the so-called matrix-valued selfconsistency-equations:*

$$\varrho_p = \frac{e^{-\frac{\beta}{c_p} \sum_{n=1}^{n(p)} e_p^n \frac{\partial}{\partial m_p^n} Q(c, \hat{m})|_{\hat{m}(\varrho)}}}{\mathrm{tr}_p\left(e^{-\frac{\beta}{c_p} \sum_{n=1}^{n(p)} e_p^n \frac{\partial}{\partial m_p^n} Q(c, \hat{m})|_{\hat{m}(\varrho)}}\right)}, \qquad \text{for } 1 \le p \le r. \tag{5.5}$$

Proof: The formula is proved with the help of the foregoing lemmas. The variational principle is carried out on the open set W, defined as in Lemma 5.3., on which the functional

$$\tilde{u}(c, \varrho) - \frac{1}{\beta} \sum_{p=1}^{r} c_p \tilde{s}_p(\varrho_p) \tag{5.6}$$

is varied under the subsidiary conditions:

$$g_p(\varrho) := \mathrm{tr}_p(\varrho_p) - 1 = 0, \quad \text{for } 1 \le p \le r. \tag{5.7}$$

Since

$$\begin{aligned}&g'_{p\varrho}(h) = \mathrm{tr}_p(h_p), \\ &\text{for } 1 \le p \le r,\ \varrho \in W \ \text{ and } h = (h_1, \ldots, h_r),\end{aligned} \tag{5.8}$$

we have the linear independence of these r linear functionals in the variable $h \in \mathcal{B}$, and thus every $\varrho \in W$ is a regular point for the subsidiary conditions in the sense of [21]. Thus in order that ϱ belongs to a state in $\partial_e \mathcal{S}(c, \beta)$, it is necessary ([21]), that there are r real constants (the Lagrange parameters) $\lambda_1, \ldots, \lambda_r$ such that it holds for sufficiently small selfadjoint $h_p \in \mathcal{B}_p$:

$$\begin{aligned}0 &= \tilde{u}'_\varrho(h) - \frac{1}{\beta} \sum_{p=1}^{r} \tilde{s}'_{\varrho_p}(h) + \sum_{p=1}^{r} \lambda_p g'_p(h) \\ &= \sum_{p=1}^{r} \mathrm{tr}_p\Bigg[\Bigg(h_p \sum_{n=1}^{n(p)} e_p^n \frac{\partial}{\partial m_p^n} Q(c, \hat{m})|_{\hat{m}(\varrho)} \\ &\qquad + \frac{c_p}{\beta}(\mathbb{1}_p + \ln(\varrho_p)) + \lambda_p \mathbb{1}_p\Bigg)\Bigg].\end{aligned}$$

Since the h_p are arbitrary if $\|h_p\|$ is sufficiently small, one concludes for all p:

$$\begin{aligned}\ln(\varrho_p) = &-\frac{\beta}{c_p} \sum_{n=1}^{n(p)} e_p^n \frac{\partial}{\partial m_p^n} Q(c, \hat{m})|_{\hat{m}(\varrho)} \\ &-\left(1 + \frac{\beta}{c_p} \lambda_p\right) \mathbb{1}_p\end{aligned}$$

At this place we use the conditions $\mathrm{tr}_p(\varrho_p) = 1$ and fix the multipliers λ_p. □

A) Appendix

A.1 Proof of Lemma 3.5.:

(i) Let c a concentration vector with funnel $\mathcal{N}(c)$, $\varepsilon > 0$ and without loss of generality, we consider $\varepsilon \le \frac{1}{2}$. Then we choose the new quantity ε' as

$$\varepsilon' = \min\left(\varepsilon, \frac{c_1^2}{1 + c_1}, \ldots, \frac{c_r^2}{1 + c_r}\right). \tag{A.9}$$

By the definition of concentration dependent funnels $\mathcal{N}(c)$, there exists a $k \in \mathbb{N}$, such that for all $\Lambda \in \mathcal{N}(c)$ with $|\Lambda| \geq k$

$$\left| \frac{|\Lambda_p|}{|\Lambda|} - c_p \right| \leq \frac{\varepsilon'}{2} \quad \forall p = 1, \ldots, r. \tag{A.10}$$

Consequently for all Λ, $\Lambda' \in \mathcal{N}(c)$ with $|\Lambda|$, $|\Lambda'| \geq k$ one has $\left| \frac{|\Lambda_p|}{|\Lambda|} - \frac{|\Lambda'_p|}{|\Lambda'|} \right| \leq \varepsilon'$ and with (A.10), (A.9):

$$\frac{|\Lambda|}{|\Lambda_p|} \leq 1 + \frac{1}{c_p}. \tag{A.11}$$

Now choose this k as the k in the statement of the lemma and take an arbitrary $\Omega \in \mathcal{N}(c)$ with $|\Omega| \geq k$ and choose $\tilde{\Lambda} \in \mathcal{N}(c)$ with $\Omega \subset \tilde{\Lambda}$ and $|\tilde{\Lambda}| \geq \frac{|\Omega|}{\varepsilon}$.

(ii) The aim in the proof and point where the preceding estimations come into play is the decomposition of $\tilde{\Lambda} \subseteq \Lambda \in \mathcal{N}(c)$ into disjoint sets Λ^l, $l = 0, \ldots, \tilde{m}$, such that:

$$\Lambda = \Lambda^0 \cup \left(\bigcup_{l=1}^{\tilde{m}} \Lambda^l \right) \tag{A.12}$$

with $|\Lambda^l_p| = |\Omega_p|$, $l = 1, \ldots, \tilde{m}$ and $p = 1, \ldots, r$.

Then one has to estimate $|\Lambda^0|$ with respect to $|\Lambda^0_p|$.

(iii) Take an arbitrary $\Lambda \in \mathcal{N}(c)$ with $\tilde{\Lambda} \subseteq \Lambda$. Then, one has $|\Lambda| = m|\Omega| + n$ with $m \geq 2$ and $0 \leq n < |\Omega|$. Further we have $|\Lambda_p| \geq |\Omega_p|$, $p = 1, \ldots, r$ and thus there exist maximal numbers $m_p \geq 1$ with $|\Lambda_p| \geq m_p |\Omega_p|$. Finally we define $\tilde{m} := \min(m_1, \ldots, m_r)$. Thus we have:

$$|\Lambda_p| = \tilde{m}|\Omega_p| + k_p \quad p = 1, \ldots, r. \tag{A.13}$$

Note, that we have $\tilde{m} \leq m$, because $\Omega \subset \tilde{\Lambda} \subseteq \Lambda$ and suppose $m < \tilde{m}$.

Now we begin with the estimations of k_p, which can be identified with $|\Lambda^0_p|$ of (ii).

$$k_p = |\Lambda_p| - \tilde{m}|\Omega_p| = |\Lambda_p| - m|\Omega_p| + (m - \tilde{m})|\Omega_p|. \tag{A.14}$$

Therefore, we calculate

$$\begin{aligned} ||\Lambda_p| - m|\Omega_p|| &= \left| |\Lambda| \left(\frac{|\Lambda_p|}{|\Lambda|} - \frac{|\Omega_p|}{|\Omega|} \right) + \frac{|\Omega_p|}{|\Omega|} |\Lambda| - m|\Omega_p| \right| \\ &\leq \varepsilon' |\Lambda| + n \frac{|\Omega_p|}{|\Omega|} \leq \varepsilon' |\Lambda| + |\Omega_p|. \end{aligned} \tag{A.15}$$

Put this into the equation (A.14) and obtain

$$\begin{aligned} k_p &= |\Lambda_p| - m|\Omega_p| + (m - \tilde{m})|\Omega_p| \leq \varepsilon' |\Lambda| \\ &\quad + (m - \tilde{m} + 1)|\Omega_p|. \end{aligned} \tag{A.16}$$

Now, we need an estimation of m and $\tilde{m}$: by definition, there exists one $\tilde{p} \in \{1, \ldots, r\}$ with $|\Lambda_{\tilde{p}}| \leq (\tilde{m} + 1)|\Omega_p|$ and with the estimation (A.15) it results:

$$\begin{aligned} (\tilde{m} + 1)|\Omega_{\tilde{p}}| &\geq (m - 1)|\Omega_{\tilde{p}}| - \varepsilon' |\Lambda|, \\ (m - \tilde{m} + 1) &\leq \varepsilon' \frac{|\Lambda|}{|\Omega_{\tilde{p}}|} + 3. \end{aligned} \tag{A.17}$$

Replacing $(m - \tilde{m} + 1)$ in equation (A.16) by this result, we have

$$k_p \leq \varepsilon' \left(1 + \frac{|\Omega_p|}{|\Omega_{\tilde{p}}|} \right) |\Lambda| + 3|\Omega_p| \leq \varepsilon' \left(2 + \frac{1}{c_{\tilde{p}}} \right) |\Lambda| + 3|\Omega_p| \quad \text{by (A.11).} \tag{A.18}$$

Now there are all equations available for estimating the size of the considered regions. We use the decomposition indicated in Part (ii). Then we have

$$|\Lambda^0| = \sum_{p=1}^{r} k_p \leq \left(2 + \frac{1}{c_{\tilde{p}}} \right) |\Lambda| \, r \, \varepsilon' + 3|\Omega|. \tag{A.19}$$

(iv) In the last step of the proof we can estimate the specific entropy in a finite region for an arbitrary state $\omega \in \mathcal{S}^{\mathcal{P}(\Lambda)}$:

$$\begin{aligned} \frac{S_\Lambda(\omega)}{|\Lambda|} &\leq \frac{1}{|\Lambda|} \left(\sum_{l=1}^{\tilde{m}} S_{\Lambda^l}(\omega) + S_{\Lambda^0}(\omega) \right) \quad \text{(by subadditivity)} \\ &= \frac{1}{|\Lambda|} (\tilde{m} \, S_\Omega(\omega) + S_{\Lambda^0}(\omega)) \quad \text{(by } |\Lambda^l_p| = |\Omega_p|, \ \omega \in \mathcal{S}^{(\Lambda)}) \\ &\overset{(3.3)}{\leq} \frac{\tilde{m}}{|\Lambda|} S_\Omega(\omega) + \frac{|\Lambda^0|}{|\Lambda|} S_{\max} \\ &\leq \frac{S_\Omega(\omega)}{|\Omega|} + \frac{\tilde{m}|\Omega| - |\Lambda| + |\Lambda^0|}{|\Lambda|} S_{\max} \\ &\leq \frac{S_\Omega(\omega)}{|\Omega|} + \frac{(\tilde{m} - m)|\Omega| + |\Lambda^0|}{|\Lambda|} S_{\max} \leq \frac{S_\Omega(\omega)}{|\Omega|} + \frac{|\Lambda^0|}{|\Lambda|} S_{\max} \\ &\leq \frac{S_\Omega(\omega)}{|\Omega|} + \left(\left(2 + \frac{1}{c_{\tilde{p}}} \right) r \, \varepsilon' + 3 \frac{|\Omega|}{|\Lambda|} \right) S_{\max} \quad \text{(by (A.19))} \\ &\leq \frac{S_\Omega(\omega)}{|\Omega|} + \varepsilon \left(\left(2 + \frac{1}{c_{\tilde{p}}} \right) r + 3 \right) S_{\max} \quad \text{(by (i)).} \end{aligned} \tag{A.20}$$

This is the desired estimation, which yields the correct result by using a scaling factor $\left(\left(\left(2 + \frac{1}{c_{\tilde{p}}} \right) r + 3 \right) S_{\max} \right)^{-1}$ in the proof. □

A.2 Proof of Lemma 5.1.

This proof is a slight generalization of the techniques used in [22], Lemma II.2. Suppose $0 \in \sigma(\varrho_{\tilde{p}})$ for

a fixed $\tilde{p}$. We choose $\lambda_1 = 0$ as the first eigenvalue of $\varrho_{\tilde{p}}$. Further we have the projections $P_1, \ldots, P_s$ on the different one dimensional eigensubspaces belonging to the eigenvalues. Thus we have

$$\varrho_{\tilde{p}} = \sum_{k=2}^{s} \lambda_k P_k.$$

Now let us choose a new permutation-invariant state $\varphi(t)$, which is identified with the density matrices

$$\varrho(t) := (\varrho_1, \ldots, (1-t)\,\varrho_{\tilde{p}} + t\,P_1, \ldots, \varrho_r),$$

where $t \in [0, 1]$. Calculating the free energy $f(c, \beta, \varphi(t))$, one obtains

$$\begin{aligned} f(t) &:= f(c, \beta, \varphi(t)) = Q(c, \varphi(t)) - \frac{1}{\beta} s(c, \varphi(t)) \\ &= p_1(t) + \frac{1}{\beta} \sum_{p=1}^{r} c_p \operatorname{tr}_p(\varrho(t)_p \ln(\varrho(t)_p)) \\ &= p_2(t) + \frac{c_{\tilde{p}}}{\beta} (t \ln(t) + \sum_{k=2}^{s} (1-t)\,\lambda_k \ln((1-t)\,\lambda_k)) \end{aligned}$$

with $p_1(t)$, $p_2(t)$ polynomials in t. Thus it is possible to evaluate the derivative with respect to t for $t \neq 0$:

$$\begin{aligned} f'(t) &= p_2'(t) + \frac{c_{\tilde{p}}}{\beta} (1 + \ln(t) + \sum_{k=2}^{s} \lambda_k (\ln((1-t)\,\lambda_k) + 1) \\ &= p_3(t) + \frac{c_{\tilde{p}}}{\beta} \ln\left(t \prod_{k=2}^{s} (1-t)^{-\lambda_k} \right) \end{aligned}$$

with a new polynomial $p_3(t)$. But the argument in the logarithmic part in the derivative becomes arbitrarily small in the neighborhood of $t = 0$. This means, that $f'(t) < 0$ as $t \to 0$ and so one reaches a state $\varrho(t)$ with $f(c, \beta, \varrho(t)) < f(c, \beta, \varrho)$ which contradicts the assumption, that ϱ minimizes the specific free energy.

A.3 Proof of Lemma 5.2.

(i) Let us begin with an estimation of the n'th power of the sum of two elements in $\mathcal{M}_n$. It holds for arbitrary $x, y \in \mathcal{M}_n$ and $k \in \mathbb{N}$:

$$(x+y)^k = x^k + \sum_{n=0}^{k-1} x^n\, y\, x^{k-n-1} + r(x, y, k) \quad \text{(A.21)}$$

with

$$\| r(x, y, k) \| \leq k(k-1)\, \| y \|^2 (\| x \| + \| y \|)^{k-2}. \quad \text{(A.22)}$$

This estimation is obtained straight forwardly by calculating $(x+y)^k$.

(ii) Now take an $x \in U$ ($\Rightarrow \| 1 - x \| < 1$). Since U is open in the norm topology, there exist $\delta > 0$ and $\eta < 1$ such that for all selfadjoint h with $\| h \| \leq \delta$, $y := x + h$ is strictly positive and $\| 1 - x \| + \| h \| \leq \eta < 1$.

To investigate the expansion of the entropy-functional, we use the well known series representation of $\ln(t)$ which converges absolutely and uniformly on the interval $[a, 1]$ with $a > 0$. Using the functional calculus, we have

$$\begin{aligned} y \ln(y) &= -\sum_{k=1}^{\infty} \frac{1}{k} y (1-y)^k = x \ln(x) + h \ln(x) \\ &\quad + \sum_{k=1}^{\infty} \frac{1}{k} x \sum_{n=0}^{k-1} (1-x)^n\, h (1-x)^{k-n-1} + \sum_{k=1}^{\infty} \frac{1}{k} h \sum_{n=0}^{k-1} (1-x)^n\, h (1-x)^{k-n-1} \\ &\quad + \sum_{k=1}^{\infty} \frac{1}{k} (x+h)\, r(1-x, -h, k) \qquad \text{(with (A.21))} \\ &= x \ln(x) + h \ln(x) + \sum_{k=1}^{\infty} \frac{1}{k} x \sum_{n=0}^{k-1} (1-x)^n\, h (1-x)^{k-n-1} + q(x, h) \end{aligned} \quad \text{(A.23)}$$

with

$$\begin{aligned} \| q(x, h) \| &= \left\| \sum_{k=1}^{\infty} \frac{1}{k} h \sum_{n=0}^{k-1} (1-x)^n\, h (1-x)^{k-n-1} + \sum_{k=1}^{\infty} \frac{1}{k} (x+h)\, r(1-x, -h, k) \right\| \\ &\leq \sum_{k=1}^{\infty} \frac{1}{k} (\| x \| + \| h \|) \| r(1-x, -h, k \| + \sum_{k=1}^{\infty} \frac{1}{k} \sum_{n=0}^{k-1} \| h \|^2 \| 1-x \|^{k-1} \\ &\leq (\| x \| + \| h \|) \sum_{k=1}^{\infty} (k-1) \| h \|^2 (\| 1-x \| + \| h \|)^{k-2} + \| h \|^2 \sum_{k=1}^{\infty} \| 1-x \|^{k-1} \qquad \text{(with (A.22))} \\ &\leq \| h \|^2 \left((\| x \| + \| h \|) \sum_{k=1}^{\infty} (k-1)\, \eta^{k-2} + \sum_{k=1}^{\infty} \| 1-x \|^{k-1} \right). \end{aligned} \quad \text{(A.24)}$$

Finally, one gets with the properties of the tr and (A.23), (A.24):

$$\begin{aligned}\mathrm{tr}(y\ln(y)) &= \mathrm{tr}(x\ln(x)) + \mathrm{tr}(h\ln(x)) + \sum_{k=1}^{\infty}\frac{1}{k}\sum_{n=0}^{k-1}\mathrm{tr}(x(1-x)^n h(1-x)^{k-n-1}) + o(\|h\|)\\ &= \mathrm{tr}(x\ln(x)) + \mathrm{tr}(h\ln(x)) + \mathrm{tr}\left(x\sum_{k=1}^{\infty}(1-x)^k h\right) + o(\|h\|)\\ &\quad \text{(with the Neumann-series for } x^{-1})\\ &= \mathrm{tr}(x\ln(x) + \mathrm{tr}(h\ln(x)) + \mathrm{tr}(h) + o(\|h\|).\end{aligned}$$

□

Note, that the lemma holds for an arbitrary C*-algebra with $\mathbb{1}$ and a trace state. The proof is then completely the same as in our case.

[1] W. Fleig, Operatoralgebraische Quantenstatistik von zusammengesetzten, langreichweitigen Gittersystemen, Thesis, Universität Tübingen (1985)
[2] H.-J. Volkert and A. Rieckers, Equilibrium States and Phase Transitions of some FCC-Multi-Lattice Systems, Preprint, Tübingen 1989.
[3] M. Fannes, H. Spohn, A. Verbeure, J. Math. Phys. **21,** (2), 355 (1980).
[4] D. Petz, G. A. Raggio, and A. Verbeure, Comm. Math. Phys. **121,** 271 (1989).
[5] G. Falk, Theoretische Physik II, Springer-Verlag, Berlin 1968.
[6] H. Stumpf and A. Rieckers, Thermodynamik I, Viehweg, Braunschweig 1976.
[7] O. Bratelli and D. W. Robinson, Operator Algebras and Statistical Mechanics I, Springer-Verlag, New York 1987.
[8] O. Bratelli and D. W. Robinson, Operator Algebras and Statistical Mechanics II, Springer-Verlag, New York 1981.
[9] G. K. Pedersen, C*-Algebras and their Automorphism Groups, Academic Press, London 1979.
[10] S. Sakai, C*-Algebras and W*-Algebras, Springer-Verlag, Berlin 1971.
[11] G. A. Raggio and R. F. Werner, Helvetica Physica Acta **62,** 980 (1989).
[12] N. G. Duffield and J. V. Pulé, Commun. Math. Phys. **118,** 475 (1988).
[13] E. Duffner and A. Rieckers, Z. Naturforsch **43a,** 521 (1988).
[14] P. Bóna, J. Math. Phys. **29,** 2223 (1988).
[15] P. Bóna, J. Math. Phys. **30,** 2994 (1989).
[16] R. V. Kadison, J. R. Ringrose, Fundamentals of the Theory of Operator Algebras I, II, Academic Press Inc. London 1983, 1986.
[17] D. Ruelle, Statistical Mechanics, W. A. Benjamin, Inc., Amsterdam 1969.
[18] R. B. Israel, Convexity in the Theory of Lattice Gases, Princeton University Press, Princeton 1979.
[19] A. Rieckers and H.-J. Volkert, Variational Principles and Equilibrium States for a Class of Long-Range Interacting Lattice Systems, Preprint Tübingen 1989.
[20] E. M. Alfsen, Compact Convex Sets and Boundary Integrals, Springer-Verlag, Berlin 1971.
[21] D. G. Luenberger, Optimization by Vector space Methods, J. Wiley & Sons, New York 1969.
[22] J. Quaqebeuer and A. Verbeure, Stability for Mean-Field Models, Ann. Inst. Henri Poincaré XXXII, 343 (1980).
[23] E. Størmer, J. Funct. Anal. **3,** 48 (1969).