Thermodynamic Formalism and Phase Transitions of Generalized Mean–Field Quantum Lattice Models

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The general structure of thermodynamic equilibrium states for a class of quantum mechanical (multi–lattice) systems is elaborated, combining quantum statistical and thermodynamical methods. The quantum statistical formulation is performed in terms of recent operator algebraic concepts emphasizing the role of the permutation symmetry due to homogeneous coarse graining and employing the internal symmetries. The variational principle of the free energy functional is derived, which determines together with the symmetries the general form of the limiting Gibbs states in terms of their central decomposition. The limiting minimal free energy density and its possible equilibrium states are analyzed on various levels of the description by means of convex analysis, where the Fenchel transforms of the free energies provide entropy like potentials. On the thermodynamic level a modified entropy surface is obtained, which specifies only in combination with its concave envelope the regions of pure and mixed phase states. The symmetry properties of a certain model allow to specify the (non–) differentiability of the minimal free energy density. A characterization and classification of phase transitions in terms of quantum statistical equilibrium states is proposed, and the connection to the Landau theory is established demonstrating that the latter implies a (continuous) deformation of the sets of equilibrium states along a canonically given curve.

1. Introduction

The thermodynamical systems which are investigated here consist each of a finite set of sublattices of equal size, the points of which are combined to certain cells. The observables of each cell constitute finite dimensional algebras, which together tensorize to a Glimm algebra [1] in the thermodynamic limit as the quasi–local algebra $\mathcal{A}$. This type of algebra has a state space which contains overcountably many classes of macroscopically different (i.e., disjoint) states and is thus rich enough to frame a thermodynamical theory, in contrast to ordinary Hilbert space quantum statistics [2].

In order to derive a thermodynamic formalism from the microscopic set up a coarse graining procedure has to be introduced in some way or the other. For our quantum lattice systems we assume as the macroscopically accessible data the averages of the spin resp. particle number observables over the lattice. The expectations of these averaged one–cell quantities, called *mean–field observables* here, exist only in sufficiently homogeneous states. States with too large fluctuations "at infinity", that is at the asymptotic lattice boundary, may produce oscillating values for the mean–field observables preventing convergence in the infinite–lattice limit. Since these observables have not well–defined expectations on the whole of the state space they cannot belong to the quasi–local algebra $\mathcal{A}$. In fact, they belong to the weak closures of the basic lattice algebra in certain representations.

Independently from any representation the values of the mean–field observables induce classes within the set of sufficiently homogeneous states. These classes are then candidates for the concept of *macro–states*, a concept which is not confined to the equilibrium situation. For a simple analytical treatment we choose the completely homogeneous states, which are invariant against all finite permutations of the set of lattice cells, as the distinguished representatives of the macro–states. The following formalism is developed from the point of view of the homogeneous states, the set of which is denoted by $\mathcal{S}^{\mathrm{P}}(\mathcal{A})$.

For the selfconsistency of our theoretical frame the interaction between the lattice particles, tested in

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states from $\mathcal{S}^{\mathrm{P}}(\mathcal{A})$, must also be considered as homogeneous on each sublattice, i.e., as invariant under the permutation of finitely many cells. The generalization of the concept of homogenous n–body potentials leads then to the notion of *approximately symmetric nets* for the family of local Hamiltonians per volume [3]. The described permutation group represents the basic spatial symmetry of our model class. It replaces in some sense the translation group of the more common lattice systems with decreasing interactions, subsumed here under the notion of *short–range interacting systems*.

For short–range quantum lattice systems the operator algebraic quantum statistics is well developed (cf., e.g., [4 - 6] and the references therein). Their equilibrium states can be equivalently characterized as KMS–states of a C^*–automorphic dynamics in the quasi–local (Glimm) algebra or as tangent functionals on the convex surface formed by the so–called pressure (negative free energy) in dependence on the interaction potentials.

Our model class, however, requires many technical modifications and is less treated in the operator–algebraic literature (c.f., e.g., [7 - 10]). The proofs for the existence of the specific free energy (and the more for the equilibrium states [11 - 13], and dynamics [14]) in the thermodynamic limit [15, 16], were originally very involved. A unifying treatment making systematic use of the permutation invariance and the variational principle of the free energy functional seems to have been first rigorously elaborated in the unpublished thesis of Fleig [17]. Further developments in [3, 18, 19] have enlarged the model class enormously.

In this up to now largest class of homogeneous models given by the above mentioned approximately symmetric nets of Hamiltonian densities, we elaborate in the present work a unified treatment of quantum statistical and thermodynamical aspects of equilibrium states. Note that, e.g., pure phase states and phase transitions are to be introduced in different manners on the quantum statisitical and the thermodynamical level, and that their logical interrelations are not without fine points. Since the thermodynamic equilibrium states constitute in general no simplex, it is not so trivial to decide by thermodynamic measurements over the statistical pure phase components. Analogously, it is not so obvious how to consolidate the thermodynamic differentiability properties of the free energy at a phase transition of the second kind with the nondifferentiability of the statistical free energy functional at any phase transition.

In order to make the formalism, covering several levels of desciption, not even more involved we have renounced of extending our considerations to weak perturbations of homogeneous interactions and states, what would have been possible without basically new ideas.

In detail we proceed as follows.

After having established in Sect. 3 the existence of the specific entropy and free energy in the thermodynamic limit as functionals of the permutation invariant states, some care is invested to introduce a finite dimensional parametrization of the extreme boundary of this w^*–closed compact set in the state space because it is the direct link between micro– and macro–physics. The variational principle of the free energy functional, the self–consistency equations, and the symmetry properties can now be investigated in terms of these macroscopic parameters. The minimal problem for the mean–field free energy gives valuable information on the central decomposition of the limiting Gibbs states. In contrast to [17] and to all investigations known to us, we include into our analysis the case, where the absolute minima of the free energy constitute more than one orbit of the broken internal symmetries. This gives us the tools for treating later on also phase transitions of the first kind.

Section 4 contains four stages of the thermodynamic formalism:

The first stage is based on a free energy functional which depends on the temperature, the model interaction, and the (possibly non–equilibrium) state. In accordance with our coarse graining strategy we vary the interactions over all approximately symmetric nets of Hamiltonian densities. That means, that we are outside of the largest Banach space of interactions used in [6]. The states are taken from the Bauer simplex $\mathcal{S}^{\mathrm{P}}(\mathcal{A})$ which is only a small part of the Poulsen simplex of all translation invariant states. The equilibrium values of the free energy are given by the minimum over the admissible states for fixed temperature and interaction. This is nothing else but the Fenchel transform [20, 21] of the absolute entropy density as an affine functional of the homogeneous states. Entropy and minimal free energy are equivalent in the sense of convex duality. We have tried hard to visualize in Figure 4.1, how an affine – and thus unstructured looking – entropy functional is capable of describing in terms of the extreme boundary of its graph the whole thermodynamics of a model class.

The second stage is only a slight coarsening of the first one, but leads to a completely classical statistical formalism. The basic linear duality is that of the continuous functions on the pure phase states of the homogeneous quantum lattice system, here parametrized by $\mathcal{S}(\mathcal{B})$ — the state space of a unit cell with observable algebra $\mathcal{B}$ — and the (signed) measures on $\mathcal{S}(\mathcal{B})$. The entropy as an affine functional of the measures is the Fenchel transform of the minimal free energy as a functional of the (continuous) energy function on $\mathcal{S}(\mathcal{B})$, associated with the approximately symmetric net of Hamiltonian densities. Beside other things this helps to clarify, in how far a homogeneous mean–field model (also often used in quantum field theory) is "classical" in spite of having a non–trivial quantum dynamics.

The third stage is reached by the straightforward idea to reduce the variation of the interaction to that of the external fields. In spite of this quite natural ansatz for deriving the thermodynamic level, in which the states are now the tupels of the numerical densities, the role of the entropy is drastically modified. Since now only the linear field part of the interaction enters the basic linear duality with the density parameters, the Fenchel transform of the (minimal) free energy (as a function of the fields) is here the entropy minus the internal interaction, both as functions of the density parameters. This modified "entropy" is not concave, and one has need also for its concave envelope to characterize the pure and mixed equilibrium phases. This reminds us of the primitive and derived surface of the geometric van der Waals–Gibbs formalism.

The fourth stage arises from the third by restricting the field parameters to certain subspaces, which are invariant under selected internal symmetries. This reduced thermodynamic formalism provides the basis for a refined analysis of the (non–) differentiability of the free energy function.

As far as we know, there has been made no attempt to give a quite general definition of a phase transition in the framework of operator algebraic quantum statistics but only examples are treated [22]. We are incautious enough to propose such a definition in Section 5, which seems at least appropriate for all model discussions we have encountered so far. For this and for the subdivision in phase transitions of the first and second kind we use the sets of equilibrium states as such. The non–differentiability of the minimal free energy function is related to a discontinuous change of the set of equilibrium states. These subtle implications are treated here in terms of the sub–formalism of the above mentioned fourth stage. This allows us, to discriminate between symmetric and non–symmetric subgradients. We finally show that Landau's scenario for phase transitions of the second kind may be subsumed under our general definition. Especially, this type of phase transition retains differentiability properties in symmetric subspaces of the field parameters. That in fact our greater generality is required by physics has been illustrated in terms of specific multi–lattice models [23, 24] and will be recalled shortly in Section 6.

Having emphasized the thermodynamical merits of long–range interacting models in the thermodynamic limit let us say a word to the other extreme, to the short–range interacting lattice models. That are in many cases models with nearest and next–nearest neighbour interaction only, the thermodynamic properties of which seem to be calculable mostly with sophisticated numerical methods [25 - 28]. Since in the latter case just the typical thermodynamical concepts are hard to obtain, the here elaborated thermodynamics of the long–range models may serve as guiding lines. Just the method of the thermodynamic variational principles may be used to clarify further the connections between the equilibrium states and phase transitions of short– and long–range models, where the latter often are intended to approximate the former ones [6].

2. Homogeneous Interactions and Symmetries of Quantum Lattice Systems

2.1. *The Algebraic Structure of the Lattice System*

The thermo–statistical concepts to be developed in the following refer in principle to a multi–partite quantum lattice system. Its geometric structure enters our general considerations, however, merely in terms of the symmetry group. Thus we consider a lattice in a *d*–dimensional real vector space indicating every lattice point by a *d*–tupel of integers according to a chosen basis. The set of all lattice points is denoted by $\mathcal{R} := \mathbb{Z}^d$ and all finite subsets $\Lambda \subset \mathcal{R}$ are elements of $\mathcal{L} := \{\Lambda \subset \mathcal{R} \mid |\Lambda| < \infty\}$, where $|\Lambda|$ denotes the number of sites in Λ. $\mathcal{L}$ is a directed set by means of the inclusion relation. On each site of the lattice, there is a finite dimensional quantum system with

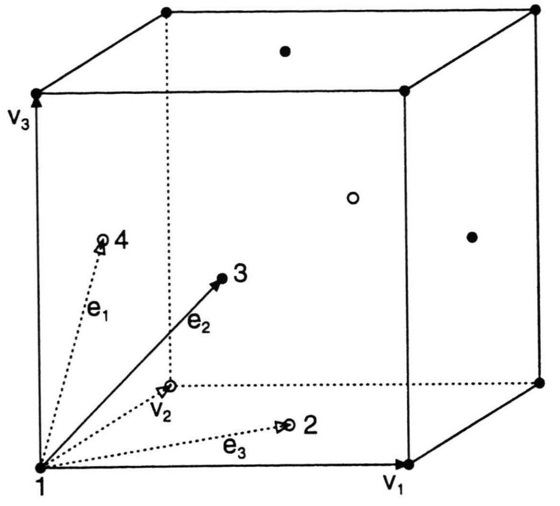

Fig. 2.1. Conventional unit cell of the face centered cubic (FCC) lattice (cf. e.g. [64]) with the primitive translation vectors e_1, e_2, e_3 and the four simple cubic sublattices (the FCC lattice is the infinite periodic extension of the above cell in the directions of v_1, v_2, v_3).

Hilbert space $\mathcal{H} = \mathbb{C}^n$ for some fixed $n \in \mathbb{N}$ and the corresponding observable algebra $\mathcal{B}$ is given by $\mathbb{M}^n$, the $n \times n$ matrices. If we consider e.g. a simple lattice of spin particles with spin $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots$ we have $\mathcal{H} = \mathbb{C}^{2s+1}$ and if we discuss a system of n–level atoms, we have $\mathcal{H} = \mathbb{C}^n$.

Depending on a given crystallographic lattice one can introduce additional sublattices in the following way: Add to the given lattice $r - 1$ copies of it and translate the original lattice by

$$e_k = \sum_{i=1}^{d} \lambda_k^i v_i, \; 0 < \lambda_k^i < 1, \; k = 1, \ldots, r-1,$$

where $\{v_i \mid i = 1, \ldots, d\}$ is the chosen basis. Each of the r lattices gained in this way with the same translational properties is called a *sublattice*. A generalized parallelepiped spanned by the d basis vectors $\{v_i \mid i = 1, \ldots, d\}$, called a *cell*, contains then r points each of them belonging to another sublattice. An example with $d = 3$, $r = 4$ and the sublattices having simple cubic structure is shown in Fig. 2.1 and further are treated in [23]. Obviously, the Hilbert space of a cell is given by $\mathcal{H} = \otimes_{q=1}^{r} \mathbb{C}^{n(q)}$, $n(q) \in \mathbb{N}$, and the observables for each cell constitute $\mathcal{B} = \otimes_{q=1}^{r} \mathbb{M}^{n(q)}$.

In the next step we introduce the Hilbert space of a finite subsystem of the lattice. For each $\Lambda \in \mathcal{L}$ we set $\mathcal{H}_\Lambda := \otimes_{i\in\Lambda}\mathcal{H}_i$ with $\mathcal{H}_i \cong \mathcal{H} = \mathbb{C}^n$. Corresponding to these finite dimensional Hilbert spaces we have the local observable algebras

$$\mathcal{A}_\Lambda := \otimes_{i\in\Lambda}\mathcal{B}_i, \text{ with } \mathcal{B}_i \cong \mathcal{B} \cong \mathbb{M}^n.$$

The usual standard construction of the algebra for the infinite lattice is the so–called C^*–inductive limit [29]

$$\mathcal{A} := \lim_{\Lambda}\{\mathcal{A}_\Lambda, \eta_{\Lambda',\Lambda} \mid \Lambda, \Lambda' \in \mathcal{L}, \Lambda \subseteq \Lambda'\},$$

where $\eta_{\Lambda',\Lambda} : \mathcal{A}_\Lambda \longrightarrow \mathcal{A}_{\Lambda'}$ denotes the natural embedding–isomorphism

$$\eta_{\Lambda',\Lambda}(A) := A \otimes \mathbb{1}_{\Lambda'\setminus\Lambda} \, .$$

Here $A \in \mathcal{A}_\Lambda$ and $\mathbb{1}_{\Lambda'}$ is the unit of $\mathcal{A}_{\Lambda'}$ for $\Lambda' \in \mathcal{L}$. Taking the limit $\Lambda' \longrightarrow \infty$ (that is Λ' approaches the whole of $\mathcal{R}$) we obtain the embedding–isomorphisms into the limit algebra

$$\eta_\Lambda : \mathcal{A}_\Lambda \longrightarrow \mathcal{A} \, .$$

$\mathcal{A}$ is commonly also denoted by

$$\mathcal{A} = \overline{\bigcup_{\Lambda\in\mathcal{L}} \mathcal{A}_\Lambda}^{\|\cdot\|} =: \overline{\mathcal{A}_0}^{\|\cdot\|}$$

and called *quasi–local algebra*. Observe that a matrix $A \in \mathcal{A}_\Lambda$ gives after the embedding a bounded algebra element $\eta_\Lambda(A) \in \mathcal{A}$, which corresponds in a representation, however, not to a *compact* operator in virtue of the infinite dimensional unit element, which is tensorized to A. In order to avoid an over–formalization, we neglect the embeddings η_Λ and consider operators $A \in \mathcal{A}_\Lambda$ as elements in $\mathcal{A}$ and $\mathcal{A}_\Lambda$ as a subalgebra of $\mathcal{A}$.

For the type of algebra we are going to consider the C^*–inductive limit is also described in [1] and leads to the infinite C^*–tensor product of the algebra $\mathcal{B}$ of one lattice site (or cell in the case of a multi–lattice).

Proposition 2.1 (Quasi–local Algebra)

$$\mathcal{A} = \bigotimes_{i\in\mathcal{R}} \mathcal{B}_i =: \overline{\mathcal{A}_0}^{\|\cdot\|}$$

is a Glimm algebra of rank $\{m(i), i \in \mathcal{R}\}$, $m(i) = n$ *for all* $i \in \mathcal{R}$, *with the properties*

(i) $\mathcal{A}$ *is a separable, simple* C^**–algebra with unit and has a unique tracial state* $\tau : \mathcal{A} \longrightarrow \mathbb{C}$,

(ii) $\mathcal{A}$ *is antiliminary,*

(iii) $\mathcal{A}$ *has a trivial center.*

PROOF: The C^*–inductive limit is constructed in [1, Chapt. 6.4]. (i) [1, Prop. 6.4.3]. (ii) [1, Theorem 6.5.7]. (iii) is obvious.

The third statement in Prop. 2.1 indicates that $\mathcal{A}$ as the smallest algebra of the infinite lattice system containing all local (quantum) observables has no nontrivial classical observables. The property (ii) characterizes a C^*–Algebra, which has many inequivalent representations and, in connection with this, many macroscopically different states. Both is a prerequisite to obtain a nontrivial thermodynamics in the state space $\mathcal{S}(\mathcal{A})$ of $\mathcal{A}$. ($\mathcal{S}(\mathcal{A})$ consists of all linear functionals $\varphi \in \mathcal{A}^*$, which give positive expectation values $\langle \varphi\,; A\rangle \geq 0$ for all positive elements $A \in \mathcal{A}$ and which satisfy the normalization condition $\langle \varphi\,; \mathbb{1}\rangle = 1$.)

Let us note that the above restriction to matrix algebras $\mathbb{M}^n$ as observables of one lattice site is not necessary but avoids technical difficulties in the following, comp. [3]. This frame suffices for the treatment of examples like usual spin–lattices or CAR–algebras.

2.2. Local Hamiltonians and their Symmetries

We start this subsection with the introduction of certain symmetry transformations which allow to define the model class in terms of invariant interactions. Two kinds of symmetries are considered: the *permutation of lattice sites* (resp. cells if a multi–lattice is considered) which leads to a homogeneous long range interaction and the so–called *internal symmetries* acting on each lattice site (cell) independently. Because the main property of our model class will be the homogeneity of the interactions, we start with the definition of the permutation transformations.

Definition 2.2 (Permutation Symmetry)

For all $\Lambda \in \mathcal{L}$, set $\mathsf{P}(\Lambda) := \{\sigma : \mathcal{R} \to \mathcal{R} \mid \sigma$ bijective with $\sigma(i) = i$ for all $i \notin \Lambda\}$. Then the permutation group P is given by $\mathsf{P} := \cup_{\Lambda\in\mathcal{L}} \mathsf{P}(\Lambda)$. P is implemented on $\mathcal{A}$ as a group of automorphisms $\Theta_{\mathsf{P}} \subset \mathrm{Aut}(\mathcal{A})$ by linear and continuous extension of

$$\Theta_\sigma(\bigotimes_{i\in\mathcal{R}} x_i) := \bigotimes_{i\in\mathcal{R}} x_{\sigma(i)},$$

for all $\sigma \in \mathsf{P}$, and $\bigotimes_{i\in\mathcal{R}} x_i \in \mathcal{A}_0$.

The model class will be introduced in terms of Hamiltonians H_Λ for each finite subsystem $\Lambda \in \mathcal{L}$ which are invariant with respect to $\mathsf{P}(\Lambda)$. In order to treat the thermodynamic limit it is necessary that these local Hamiltonians have "good" asymptotic properties for large local regions Λ. In [3] there were introduced conditions on the local Hamiltonians, such that n–particle interactions with arbitrary $n \in \mathbb{N}$ are included as are those interactions, which are approximated in norm by the the former ones in the following sense:

Definition 2.3 ((Approximately) Symmetric Nets [3])

Let $\Omega, \Lambda \in \mathcal{L}$ with $\Omega \subseteq \Lambda$ and $j_{\Lambda\Omega} := \frac{1}{|\Lambda|!}\sum \Theta_\sigma$, where the summation runs over all $\sigma \in \mathsf{P}(\Lambda)$. Let $\mathcal{L} \ni \Lambda \to x_\Lambda$ be a net x with $x_\Lambda \in \mathcal{A}_\Lambda$ and $x_\Lambda = j_{\Lambda\Lambda} x_\Lambda$ for all $\Lambda \in \mathcal{L}$. Moreover, x_Λ and $x_{\Lambda'}$ satisfy $\Theta_\sigma(x_\Lambda) = x_{\Lambda'}$ for $\Lambda, \Lambda' \in \mathcal{L}$ with $|\Lambda| = |\Lambda'|$ and all $\sigma \in \mathsf{P}$ with $\sigma(\Lambda) = \Lambda'$. x is called

(i) a symmetric net ($x \in \mathcal{Y}$), if there exists a $k \in \mathbb{N}$, such that for all $\Lambda \in \mathcal{L}$ with $|\Lambda| \geq k$, there is an $\Omega \in \mathcal{L}$, $\Omega \subseteq \Lambda$ with $|\Omega| = k$ and $x_\Lambda = j_{\Lambda\Omega} x_\Omega$.

(ii) an approximately symmetric net ($x \in \widetilde{\mathcal{Y}}$), if for all $\varepsilon > 0$, there exists a $y \in \mathcal{Y}$ and a $n \in \mathbb{N}$, such that for all $\Lambda \in \mathcal{L}$ with $|\Lambda| \geq n$ it holds: $\|x_\Lambda - y_\Lambda\| \leq \varepsilon$.

Definition 2.4 (Local Hamiltonians of the Model Class)

A net of local Hamiltonians $\mathcal{L} \ni \Lambda \to H_\Lambda = H_\Lambda^*$ defines a model of the considered model class, if $\mathcal{L} \ni \Lambda \to h_\Lambda := H_\Lambda/|\Lambda|$ is an approximately symmetric net.

The intuitive meaning of a symmetric net of Hamiltonian densities is that for large Λ the Hamiltonians are obtained by symmetric embedding of a fixed k–particle Hamiltonian. Let us have a look on two–particle interactions in more detail: Let be $n_{\mathcal{B}} := \dim \mathcal{B} = n^2$ the dimension of $\mathcal{B}$ considered as a vector space. With a corresponding basis $\hat{e} := (\hat{e}^1, \ldots, \hat{e}^{n_{\mathcal{B}}})$ of self–adjoint elements of $\mathcal{B}$, $\varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}$, $w = (w_{pq}) \in \mathcal{B}(\mathbb{R}^{n_{\mathcal{B}}})$ symmetric we set:

$$H_\Lambda := \sum_{i\in\Lambda} \varepsilon \bullet \hat{e}_i + \frac{1}{|\Lambda| - 1} \sum_{i\neq k\in\Lambda} \hat{e}_i \bullet w\hat{e}_k, \tag{2.1}$$

where we use the notation

$$\varepsilon \bullet \hat{e}_i := \sum_{p=1}^{n_{\mathcal{B}}} \varepsilon_p \hat{e}_i^p \text{ and } \hat{e}_i \bullet w\hat{e}_k := \sum_{p,q=1}^{n_{\mathcal{B}}} \hat{e}_i^p w_{pq} \hat{e}_k^q \tag{2.2}$$

with $\hat{e}_i^p$ as the embedding of $\hat{e}^p$ at site $i \in \mathcal{R}$. It is easy to check that $\mathcal{L} \ni \Lambda \to H_\Lambda/|\Lambda|$ is a symmetric net in $\mathcal{Y}$. The main feature of this kind of

Hamiltonian is the site independent interaction which is also fulfilled for all Hamiltonians in the model class. Sometimes it is useful to express H_Λ in terms of density observables $m_\Lambda(x)$ for some $x \in \mathcal{B}$ given by $m_\Lambda(x) := j_{\Lambda\{k\}}(x_k) = \frac{1}{|\Lambda|}\sum_{i\in\Lambda} x_i$ for arbitrary $k \in \Lambda$. Up to a deviation which is bounded in norm for large Λ, H_Λ may be replaced by $\widetilde{H}_\Lambda$

$$\widetilde{H}_\Lambda := |\Lambda|\,(\varepsilon \bullet m_\Lambda(\hat{e}) + m_\Lambda(\hat{e}) \bullet w m_\Lambda(\hat{e}))\,. \tag{2.3}$$

Due to the deviation $\widetilde{H}_\Lambda - H_\Lambda$, $\Lambda \longrightarrow \widetilde{H}_\Lambda/|\Lambda|$ no longer defines a symmetric net. Nevertheless, it is still an approximately symmetric one.

A main feature of all approximately symmetric nets of Hamiltonian densities is their association with a continuous energy function on the set of all pure phase states, cf. Remark Often the local Hamiltonians are expressed in terms of another net of local selfadjoint operators $(\Phi_X)_{X\in\mathcal{L}}$, the *potential*, such that

$$H_\Lambda = \sum_{X\subseteq\Lambda} \Phi_X\,. \tag{2.4}$$

The largest Banach space of translation invariant potentials used in [6] is characterized by the finiteness of the norm $\sum_{X\ni 0} \|\Phi_X\|/|X|$. In [30] it is demonstrated that the resulting Hamiltonian (2.4) from this potential class lead by symmetrization $j_{\Lambda\Lambda}(H_\Lambda)$ to a mean–field model of our considered class.

The structure of the set of equilibrium states of the infinite lattice system strongly depends on additional symmetries besides the homogeneity. Therefore, we introduce a group H of internal symmetries:

Definition 2.5 (Internal Symmetries)

An internal symmetry is defined by an element u of the compact group $\mathsf{U}(\mathcal{B})$ of unitary and anti–unitary elements of $\mathcal{B}$ acting as $\mathrm{Ad}_u : \mathcal{B} \longrightarrow \mathcal{B}$ *where*

$$\mathrm{Ad}_u x = \begin{cases} uxu^* & u \text{ unitary} \\ ux^*u^* & u \text{ anti–unitary} \end{cases}\,.$$

$\mathsf{U}(\mathcal{B})$ is implemented on $\mathcal{A}$ as a group of (anti–) automorphisms $\Theta_{\mathsf{H}} \subset \mathrm{Aut}(\mathcal{A})$ by linear and continuous extension of $\Theta_u(\bigotimes_{i\in\mathcal{R}} x_i) := \bigotimes_{i\in\mathcal{R}} \mathrm{Ad}_u(x_i)$ for all $u \in \mathsf{U}(\mathcal{B})$ and $\bigotimes_{i\in\mathcal{R}} x_i \in \mathcal{A}_0$. Θ_u is called compatible with a given set of local Hamiltonians $\{H_\Lambda \mid \Lambda \in \mathcal{L}\}$, if

$$\Theta_u(H_\Lambda) = H_\Lambda, \quad \textit{for all } \Lambda \in \mathcal{L}\,.$$

The set of all compatible transformations constitutes the internal symmetry group, which is simply denoted by H, when the reference to the model is evident.

Remark 2.6

The compact group H has a unique Haar measure $\mu_{\mathsf{H}} : \mathcal{C}(\mathsf{H}) \to \mathbb{C}$, which becomes relevant if we decompose H–symmetric thermodynamic equilibrium states.

Each $u \in \mathsf{H}$ has a representing matrix $M(u) = (m_{kn}(u))$ with regard to the chosen basis $\hat{e} = (\hat{e}_1, \ldots, \hat{e}_{n_\mathcal{B}})$ defined by

$$u\hat{e}_n u^* = \sum_{k=1}^{n_\mathcal{B}} m_{kn}(u)\hat{e}_k\,. \tag{2.5}$$

$M(u)$ has real matrix elements because $\hat{e}$ is self–adjoint and one has $M(u_1u_2) = M(u_1)M(u_2)$ for all $u_1, u_2 \in \mathsf{H}$.

If we consider the above case of a two particle interaction Eqs. (2.1)–(2.3), a given closed group $\mathsf{H} \subseteq \mathsf{U}(\mathcal{B})$ is compatible with H_Λ (or $\widetilde{H}_\Lambda$), $\Lambda \in \mathcal{L}$, if for all $u \in \mathsf{H}$ holds: $M(u)\varepsilon = \varepsilon$ and $M(u)wM(u)^T = w$.

The total symmetry group of a model from our considered class is then given by

$$\mathsf{G} := \mathsf{P} \times \mathsf{H} \text{ and}$$

$$(\sigma_1, u_1) \circ (\sigma_2, u_2) := (\sigma_1 \circ \sigma_2, u_1 \circ u_2)\,.$$

The prescription

$$\Theta_g := \Theta_u \circ \Theta_\sigma = \Theta_\sigma \circ \Theta_u \quad \forall g = (\sigma, u) \in \mathsf{G}$$

defines the implementation of G as a group of (anti–) automorphisms of $\mathcal{A}$.

From the general point of view another important symmetry group consists of the lattice translations. For every $j \in \mathbb{Z}^d$ one may define

$$\alpha_j(\bigotimes_{i\in\mathbb{Z}^d} x_i) := \bigotimes_{i\in\mathbb{Z}^d} x_{i+j}, \quad \forall \bigotimes_{i\in\mathbb{Z}^d} x_i \in \mathcal{A}_0$$

and take the linear extension and norm closure to get a $*$–automorphism $\alpha_j \in \mathrm{Aut}(\mathcal{A})$. This means that every observable x_i at the i–th site is translated by a lattice vector with the integer coordinates $j \in \mathbb{Z}^d$. The translation invariant states

$$\mathcal{S}^1(\mathcal{A}) = \{\varphi \in \mathcal{S}(\mathcal{A}) \mid \varphi \circ \alpha_j = \varphi,\ \forall j \in \mathbb{Z}^d\}$$

play a great role in the theory of lattice systems [4, 6, 31]. Here we concentrate on the stronger permutation symmetry.

In the multi–lattice model of [23] there are considered r equal sublattices (comp. Subsect. 2.1 above), which means

$$n(q) =: \widetilde{n} \quad \text{for all } q \in \{1, \ldots, r\}$$

and the group H represents the "restriction" of the usual space group of the considered 3–dimensional lattice "to one cell" (cf. Fig. 2.1). The space group, translating and rotating the lattice points in the usual way, induces permutations of the sublattice indices. Thus H will contain a subgroup of

$$\mathsf{U}_{\mathsf{S}_r} = \{u_\pi : \mathcal{B} \to \mathcal{B},\ \pi \in \mathsf{S}_r\}$$

with u_π defined as

$$\mathcal{B} \to \mathcal{B},\ \bigotimes_{i=1}^{r} b_i \longmapsto \bigotimes_{i=1}^{r} b_{\pi(i)}$$

and the group of permutations of the sublattice indices

$$\mathsf{S}_r = \{\pi : \{1, \ldots, r\} \to \{1, \ldots, r\} \mid \pi \text{ bijective}\}.$$

Other typical examples for an internal symmetry are gauge transformations, spin rotations, and (anti–unitary) spin inversions.

2.3. Decomposition of G–Invariant States

A direct method to get insight into the phase transitions and spontaneous symmetry breaking of our models is to construct the equilibrium or Gibbs states in the thermodynamic limit. Most important in this respect is the variational principle for the limiting Gibbs states [3], see also [17, 18]. Nevertheless, the structure of these states has only been examined in detail for a small number of models, e.g. [13, 23, 24]. In contrast to the trivial phase structure of the finite subsystems we expect a rich nontrivial phase structure in the thermodynamic limit.

For all $\beta > 0$, the local Gibbs state $\omega_\Lambda^\beta \in \mathcal{S}(\mathcal{A})$ is given by

$$\left\langle \omega_\Lambda^\beta ; A \right\rangle := \langle \tau ; \exp(-\beta H_\Lambda)\, A \rangle \,/\, \langle \tau ; \exp(-\beta H_\Lambda) \rangle$$

for all $\Lambda \in \mathcal{L}$ and $A \in \mathcal{A}$,

where τ is the unique tracial state of Prop. 2.1. Note, that $\omega_\Lambda^\beta \in \mathcal{S}(\mathcal{A})$ is the unique β–KMS–state of the dynamics arising from the local Hamiltonian H_Λ. Each w^*–accumulation point $\omega^\beta \in \mathcal{S}(\mathcal{A})$ of the net $\{\omega_\Lambda^\beta, \Lambda \in \mathcal{L}\}$ is called a *limiting Gibbs state.*

Using the symmetries of our local Hamiltonians we find at once the symmetries of the local and the limiting Gibbs states:

Lemma 2.7

(i) $\omega_\Lambda^\beta \circ \Theta_\sigma = \omega_\Lambda^\beta$ *for all* $\sigma \in \mathsf{P}(\Lambda)$ *and all* $\Lambda \in \mathcal{L}$,
(ii) $\omega_\Lambda^\beta \circ \Theta_u = \omega_\Lambda^\beta$ *for all* $u \in \mathsf{H}$ *and all* $\Lambda \in \mathcal{L}$,
(iii) Every limiting Gibbs state ω^β *is an element of*

$$\mathcal{S}^{\mathsf{G}}(\mathcal{A}) := \{\omega \in \mathcal{S}(\mathcal{A}) \mid \omega \circ \Theta_g = \omega \text{ for all } g \in \mathsf{G}\}.$$

Note, that the H–symmetry of the local Hamiltonians H_Λ is not necessary to induce the G–invariance of the corresponding limiting Gibbs state. In [32] there are given criteria for the G–symmetry of the limiting Gibbs state which are approached by non–symmetric local Gibbs states.

For further analysis one has to decompose the states in $\mathcal{S}^{\mathsf{G}}(\mathcal{A})$ into easier accessible ones. Fortunately a theorem of convex decomposition theory tells us that on the subset

$$\mathcal{S}^{\mathsf{P}}(\mathcal{A}) = \{\omega \in \mathcal{S}(\mathcal{A}) \mid \omega \circ \Theta_\sigma = \omega,\ \forall \sigma \in \mathsf{P}\} \supset \mathcal{S}^{\mathsf{G}}(\mathcal{A})$$

of the state space containing the limiting Gibbs states, there is a unique decomposition into classically pure (i.e. factorial) states.

Let us recall here, that a state $\varphi \in \mathcal{S}(\mathcal{A})$ is called a factor state, if in the GNS–representation $(\pi_\varphi, \mathcal{H}_\varphi, \Omega_\varphi)$ (with representation Hilbert space $\mathcal{H}_\varphi$, cyclic vector Ω_φ and representation morphism $\pi_\varphi : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\varphi)$) the von Neumann algebra $\mathcal{M}_\varphi := \overline{\pi_\varphi(\mathcal{A})}^{w}$ has a trivial center. This indicates, that in the statistical ensemble given by φ the classical observables have fixed sharp values and φ is classically pure. Two states φ and ψ are called macroscopically different if their von Neumann algebras $\mathcal{M}_\varphi$ and $\mathcal{M}_\psi$ contain different classical (central) observables. For every state $\varphi \in \mathcal{S}(\mathcal{A})$ there is a canonical decomposition into factor states, which are pairwise macroscopically different (disjoint), the so–called central decomposition by means of the so–called central measure. This decomposition is very important for thermodynamics, since the factor states of the central decomposition are interpreted — at least in the equilibrium case — as the pure phase states of the system [4, 7]. It is a great advantage of the class of systems with permutation symmetry, that we have here in any case only one decomposition into factor states, which is then identical to the central decomposition. A pure phase is thus to be identified with a permutation invariant factor state.

Proposition 2.8

(i) The convex, $\sigma(\mathcal{A}^*,\mathcal{A})$–compact set $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ is a Bauer simplex, i.e., every $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ has a unique barycentric decomposition

$$\omega = \int_{\mathcal{S}^{\mathsf{P}}(\mathcal{A})} \varphi \, \mathrm{d}\mu_\omega(\varphi),$$

where the probability measure μ_ω is supported by the extreme boundary $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ of $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$, and $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ is w^*–closed.

(ii) For $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ the following statements are equivalent:

a) ω is extremal in $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$.

b) ω is a factor state.

c) ω is a product state: There exists a $\phi \in \mathcal{S}(\mathcal{B})$ such that $\omega = \otimes\phi$, i.e.

$$\Big\langle \omega ; \bigotimes_{i \in \mathcal{R}} x_i \Big\rangle = \prod_{i \in \mathcal{R}} \langle \phi ; x_i \rangle \,, \text{ for } \bigotimes_{i \in \mathcal{R}} x_i \in \mathcal{A}_0 .$$

(iii) The decomposition of (i) is the central decomposition of ω.

PROOF: [4, Chapt. 4] and [33, 34], or [17, Chapt. 1.3].

Although the limiting Gibbs states ω^β are elements of $\mathcal{S}^{\mathsf{G}}(\mathcal{A})$ (cf. Lemma 2.7 iii) every φ in the support of μ_{ω^β} is in general only an element of $\mathcal{S}^{\mathsf{G}'}(\mathcal{A})$ where G' is an (invariant) subgroup of G. That is, the pure phase states may have a lower symmetry than the limiting Gibbs states ω^β, a phenomenon called *spontaneous symmetry breaking*. From Theorem 2.8 it follows, that all pure phase states are still in $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$, giving the inclusion relation

$$\mathsf{P} \subset \mathsf{G}' \subset \mathsf{G}$$

for the symmetry group G' of the pure phases. Although the set P does not intersect with the group of lattice translations (with the exception of the unit), every state $\varphi \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ is also translation invariant. The simplex of all translation invariant states $\mathcal{S}^{\mathsf{I}}(\mathcal{A})$ is less well behaved than $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$, since its extreme boundary is even w^*–dense in $\mathcal{S}^{\mathsf{I}}(\mathcal{A})$, which is typical for a Poulsen simplex [35] and contradicts the closedness of the extreme boundary of a Bauer simplex.

In the following sections we are concerned with the determination of the states in the support of the limiting Gibbs states ω^β. We close the present section with a result which under favourable circumstances even determines the central measure. We consider for this the mapping

$$\Theta_u^* : \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A}) \to \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A}),$$
$$\langle \Theta_u^*(\varphi) ; A \rangle := \langle \varphi ; \Theta_{u^*}(A) \rangle$$
$$\text{for all } u \in \mathsf{H} \text{ and } A \in \mathcal{A},$$

which is obviously a bijection on $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and define for some $\varphi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ the orbit

$$\mathcal{O}_{\mathsf{H}}(\varphi) := \{ \Theta_u^*(\varphi) \mid u \in \mathsf{H} \}. \tag{2.6}$$

Proposition 2.9

For $\omega \in \mathcal{S}^{\mathsf{G}}(\mathcal{A})$ the following statements are equivalent:

(i) $\omega \in \partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$.

(ii) There exists a $\varphi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ such that the central measure μ_ω of ω is concentrated on $\mathcal{O}_{\mathsf{H}}(\varphi)$.

If (i) or (ii) is valid, one has (using the Haar measure μ_{H} of H)

(iii) $\mu_\omega(f) = \int_{\mathsf{H}} f(\Theta_u^*(\varphi)) \, \mathrm{d}\mu_{\mathsf{H}}(u)$ for all $f \in \mathcal{C}(\mathcal{S}(\mathcal{A}))$.

(iv) $\omega = \int_{\mathsf{H}} \Theta_u^*(\varphi) \, \mathrm{d}\mu_{\mathsf{H}}(u)$.

PROOF: We give an outline of the main ideas.
(i)⇒(ii): If $\varphi \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ the average over H

$$M(\varphi) := \int_{\mathsf{H}} \Theta_u^*(\varphi) \, \mathrm{d}\mu_{\mathsf{H}}(u)$$

leads to an element in $\mathcal{S}^{\mathsf{G}}(\mathcal{A})$. Since $M(\omega) = \omega$, the convex set

$$K_\omega := \{ \psi \in \mathcal{S}^{\mathsf{P}}(\mathcal{A}) \mid M(\psi) = \omega \}$$

is non–empty and can be shown to be w^*–closed. Its non–void extreme boundary $\partial_e K_\omega$ is contained in $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$. Choose a $\varphi \in \partial_e K_\omega \cap \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$. Then the Haar measure on $\mathcal{O}_{\mathsf{H}}(\varphi)$ defines an orthogonal measure on $\mathcal{S}(\mathcal{A})$, which must be the central measure in virtue of Theorem 2.8 (i). This implies also the relations (iii) and (iv) for the central measure.

(ii)⇒(i): If ω satisfies condition (ii) then the central decomposition is given by (iv) in which we may replace H by G. Then the ensemble average $\langle \omega\,; A\rangle$ may be replaced by an G–average, where G is norm asymptotic abelian. An argument from ergodic theory tells us then, that ω must be extremal G–invariant.

3. Limiting Gibbs States and Symmetry Breaking

3.1. Free Energy Functional

In this section we characterize the set of extremal states in $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ on which the probability measure μ_{ω^β} of each limiting Gibbs state is concentrated. This will be achieved by means of the density of the free energy, which is the appropriate thermodynamic potential when the temperature is a free adjustable parameter for the system in consideration [36]. There exist various approaches to determine the support of the measure μ_{ω^β}, the most important ones are described in [10, 18] (see also [17]), [37], and especially [3] for the large model class we are working with.

Because the local Hilbert spaces are finite dimensional, the restriction of every $\varphi \in \mathcal{S}(\mathcal{A})$ to the local algebra $\mathcal{A}_\Lambda$ may be written as

$$\langle \varphi\,; A\rangle = \mathrm{tr}_\Lambda(\varrho^\varphi_\Lambda A), \quad \text{for all } A \in \mathcal{A}_\Lambda,$$

where $\varrho^\varphi_\Lambda \in \mathcal{B}(\mathcal{H}_\Lambda)$ is the corresponding density operator and tr_Λ is the usual trace on the Hilbert space $\mathcal{H}_\Lambda$.

Definition 3.1 (Thermodynamic Functionals)

Given the quasi–local algebra $\mathcal{A}$, its state space $\mathcal{S}(\mathcal{A})$, and the local Hamiltonians H_Λ, $\Lambda \in \mathcal{L}$. Denote $\widetilde{h} := (h_\Lambda)_{\Lambda\in\mathcal{L}}$, $h_\Lambda = H_\Lambda/|\Lambda|$. For all $\varphi \in \mathcal{S}(\mathcal{A})$ and $\beta > 0$ we define the density of the

(i) internal energy: $u(\widetilde{h},\varphi) := \lim_\Lambda \frac{1}{|\Lambda|}\langle \varphi\,; H_\Lambda\rangle = \lim_\Lambda \langle\varphi\,; h_\Lambda\rangle$,

(ii) entropy: $s(\varphi) := \lim_\Lambda -\frac{1}{|\Lambda|}\mathrm{tr}_\Lambda(\varrho^\varphi_\Lambda \ln(\varrho^\varphi_\Lambda))$,

(iii) free energy: $f(\beta,\widetilde{h},\varphi) := u(\widetilde{h},\varphi) - \frac{1}{\beta}s(\varphi)$,

if the corresponding limits exist.*

On $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$, a subset of the state space $\mathcal{S}(\mathcal{A})$ containing the equilibrium states and their central support for our model class, the thermodynamic functionals are well–defined:

Proposition 3.2

For all $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and $\widetilde{h} \in \widetilde{\mathcal{Y}}$ it holds: The limits in Def. 3.1 exist and define w^*–continuous and affine functionals on $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$. For all $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$, $\widetilde{h} \to u(\widetilde{h},\omega)$ is linear and $\widetilde{h} \to f(\beta,\widetilde{h},\omega)$ is affine on $\widetilde{\mathcal{Y}}$.

SKETCH OF THE PROOF: We will only sketch the proof of the convergence of the density functionals and refer for details to [3] and [18].

(i) At first we look at a factorial state $\otimes\phi \in \partial_{\mathrm{e}}\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ with $\phi \in \mathcal{S}(\mathcal{B})$ and a family of local Hamiltonians densities $\widetilde{h}$ given by an arbitrary but fixed polynomial Q in the densities $m_\Lambda(\hat{e}^1),\ldots,m_\Lambda(\hat{e}^{n_\mathcal{B}})$ (comp. (2.3)). Then one finds immediately that

$$\begin{aligned} u(\widetilde{h},\otimes\phi) &= \lim_\Lambda \left\langle \otimes\,\phi\,; \frac{H_\Lambda}{|\Lambda|}\right\rangle \\ &= \lim_\Lambda \langle \otimes\phi\,; Q(m_\Lambda(\hat{e}^1),\ldots,m_\Lambda(\hat{e}^{n_\mathcal{B}}))\rangle \\ &= Q(\langle\phi\,;\hat{e}^1\rangle,\ldots,\langle\phi\,;\hat{e}^{n_\mathcal{B}}\rangle). \end{aligned}$$

If we use an arbitrary $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$, it follows with Theorem 2.8 (i) that

$$u(\widetilde{h},\omega) = \lim_\Lambda \left\langle \otimes\,\phi\,; \frac{H_\Lambda}{|\Lambda|}\right\rangle = \int_{\partial_{\mathrm{e}}\mathcal{S}^{\mathsf{P}}(\mathcal{A})} u(\widetilde{h},\varphi)\,\mathrm{d}\mu_\omega(\varphi).$$

Using that such a polynomial Hamiltonian is defined up to a term vanishing in norm for large $\Lambda \in \mathcal{L}$ (compare the remarks before (2.3)) by a symmetric net in $\mathcal{Y}$ and that the symmetric nets approximate the approximately symmetric ones in norm we find that the stated limit exists for the whole model class. The w^*–continuity and the affinity on $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ is obvious. The linearity of $\widetilde{h} \to u(\widetilde{h},\omega)$ follows from Definition 3.1.

(ii) In [37, 38], a similar result is obtained for the relative entropy which corresponds to $s(\varphi)$, $\varphi \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$, up to an constant if the trace state τ is chosen as reference. Here we follow [18, 17], and set $S_\Lambda(\omega) := -\mathrm{tr}_\Lambda(\varrho^\omega_\Lambda \ln(\varrho^\omega_\Lambda))$ for $\omega \in \mathcal{S}(\mathcal{A})$ and $\Lambda \in \mathcal{L}$. Using the subadditivity [4, Prop. 6.2.24]

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

$$\text{for } \Lambda, \Omega \in \mathcal{L}\text{ , with } \Lambda\cap\Omega = \emptyset$$

---

*By $\lim_\Lambda$ we denote the net limit for $\Lambda \in \mathcal{L}$

and $S_\Lambda(\omega) = S_{\sigma(\Lambda)}(\omega)$ for $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and $\sigma \in \mathsf{P}$, one can prove the pointwise existence of

$$\lim_{\Lambda} \frac{S_\Lambda(\omega)}{|\Lambda|} = s(\omega) = \inf\left\{\frac{S_\Lambda(\omega)}{|\Lambda|} \mid \Lambda \in \mathcal{L}\right\}$$

for all $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$.

The affinity of $\mathcal{S}^{\mathsf{P}}(\mathcal{A}) \ni \omega \longrightarrow s(\omega)$ directly follows from the convex and a concave–like behaviour of the local entropy S_Λ [4, Prop. 6.2.25].

For a factor state $\otimes\varrho \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ (we identify a state $\phi \in \mathcal{S}(\mathcal{B})$ with the corresponding density matrix ϱ_ϕ) it holds

$$s(\otimes\varrho) = \lim_{\Lambda} \frac{1}{|\Lambda|} S_\Lambda(\otimes\varrho) = \lim_{\Lambda} \frac{1}{|\Lambda|} \sum_{k\in\Lambda} S_{\{k\}}(\otimes\varrho))$$
$$= -\mathrm{tr}_{\mathcal{B}}(\varrho \ln(\varrho)) =: S_{\mathcal{B}}(\varrho)$$

and we find $s(\omega) = \int_{\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})} S_{\mathcal{B}}(\varrho)\, \mathrm{d}\mu_\omega(\otimes\varrho)$. Then s is w^*–continuous because $S_{\mathcal{B}}(\varrho)$ is so and $\mathcal{S}^{\mathsf{P}}(\mathcal{A}) \rightarrow \mathrm{M}_1^+(\mathcal{S}^{\mathsf{P}}(\mathcal{A})), \omega \longmapsto \mu_\omega$ is weakly continuous, where M_1^+ are the positive normed Radon measures ([39, Theorem II.4.1] using $\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ is a Bauer simplex).

Remark 3.3

In [3] it is elaborated, that $\widetilde{\mathcal{Y}}$ *is a vector space and* $\|x\| := \lim_\Lambda \|x_\Lambda\|$ *defines a seminorm on* $\widetilde{\mathcal{Y}}$*. The function*

$$j : \widetilde{\mathcal{Y}} \longrightarrow C(\mathcal{S}(\mathcal{B}), \mathbb{C}),$$
$$x \longrightarrow [j(x)](\phi) := \lim_{\Lambda} \langle \otimes\phi\,; x_\Lambda \rangle\,,\ \forall \phi \in \mathcal{S}(\mathcal{B})$$

maps $\widetilde{\mathcal{Y}}$ *isometrically onto* $C(\mathcal{S}(\mathcal{B}), \mathbb{C})$*, the continuous functions on* $\mathcal{S}(\mathcal{B})$*. The seminorm defines an equivalence relation on* $\widetilde{\mathcal{Y}}$ *and the corresponding quotient space is isomorphic to* $C(\mathcal{S}(\mathcal{B}), \mathbb{C})$*.*

If we look at a given model $\widetilde{h} \in \widetilde{\mathcal{Y}}$ *with local Hamiltonians* H_Λ *we find that* $[j(\widetilde{h})](\phi) = u(\widetilde{h}, \otimes\phi)$ *for all* $\otimes\phi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$*. Thus, for each continuous function* $\mathcal{S}(\mathcal{B}) \ni \phi \longrightarrow \widetilde{u}(\otimes\phi)$*, there exists a mean–field model* $\widetilde{h}$ *in our model class* $\widetilde{\mathcal{Y}}$*, such that* $\widetilde{u}$ *becomes its functional of the internal energy* $u(\widetilde{h}, \cdot)$ *on the pure phase states.*

The main information on the limiting Gibbs states ω^β is obtained by a variational principle for the free energy density which determines the maximal possible central support of μ_{ω^β}.

Theorem 3.4 (Principle of Minimal Free Energy Density)

For a model in our model class with $\widetilde{h} \in \widetilde{\mathcal{Y}}$*, we set* $f(\beta, \widetilde{h}) := \inf\{f(\beta, \widetilde{h}, \omega) \mid \omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})\} = \inf\{f(\beta, \widetilde{h}, \otimes\phi) \mid \otimes\phi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})\}$*. Each* w^**–accumulation point* ω^β *of* $\{\omega_\Lambda^\beta \mid \Lambda \in \mathcal{L}\}$ *is an element of the* w^**–compact face*

$$\mathcal{S}(\beta, \widetilde{h}) := \{\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A}) \mid f(\beta, \widetilde{h}, \omega) = f(\beta, \widetilde{h})\},$$

which here is also a Bauer simplex. The corresponding central measure μ_{ω^β} *is concentrated on the set*

$$\partial_e \mathcal{S}(\beta, \widetilde{h}) := \{\otimes\phi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A}) \,|\, f(\beta, \widetilde{h}, \varphi) = f(\beta, \widetilde{h})\}$$

and coincides with the unique Choquet decomposition in $\mathcal{S}(\beta, \widetilde{h})$*.*

PROOF: The minimum principle of the free energy density for the limiting Gibbs states is proved for our model class in [3]. Cf. also [18] for a more explicit argumentation which may be adapted to the used model class. The proof essentially uses that the local Gibbs states ω_Λ^β are given by a minimum principle for the local free energies (densities), see e.g. [4, Chapt. 5.3]. The infimum $f(\beta, \widetilde{h})$ is attained in the extreme boundary $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ due to Bauer's maximum principle [4], which is applicable here since $f(\beta, \widetilde{h}, \cdot)$ is w^*–continuous and affine (and thus convex).

3.2. Selfconsistency–Equations and Limiting Gibbs States

The minimum principle of the free energy density allows to determine the pure phase set $\partial_e \mathcal{S}(\beta, \widetilde{h})$ which is also a prerequisite to calculate limiting Gibbs states as shown in Section 2.3. Nevertheless, one should keep in mind that a free energy density functional gives a coarsened description of the underlying microscopically defined model. For example, there exist (not at all pathological) models with the same free energy density functional but totally different (even disjoint) limiting Gibbs states [3, 40, 32, 41]. In the following we will look for additional conditions to determine the states $\otimes\phi$ in the central support $\partial_e \mathcal{S}(\beta, \widetilde{h})$ of the limiting Gibbs states ω^β and conditions for uniqueness of the latter in terms of internal symmetries.

Let us fix in this subsection the model interaction $\widetilde{h}$ and drop the symbol $\widetilde{h}$.

As stated in Theorem 2.8 (ii), the states $\otimes\phi \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ are parametrized by $\mathcal{S}(\mathcal{B})$. Moreover, $\mathcal{S}(\mathcal{B})$ can be *parametrized* by a compact convex subset M of $\mathrm{I\!R}^{n_\mathcal{B}}$ as the expectation values for the basis $\hat{e}$ of $\mathcal{B}$ chosen in Sect. 2.2: Set

$$v : \mathcal{S}(\mathcal{B}) \longrightarrow \mathrm{I\!R}^{n_\mathcal{B}},\ \varrho \longmapsto v(\varrho) := \quad \mathrm{tr}_\mathcal{B}(\varrho\hat{e}) =: m \tag{3.1}$$

$$\text{with} \quad v(\mathcal{S}(\mathcal{B})) = \qquad : M, \tag{3.2}$$

which is an affine, continuous map with the convex closed image M. To prove the injectivity of v we introduce the contragradient basis $\check{e}$ of $\mathcal{B}$ which satisfies $\mathrm{tr}_\mathcal{B}(\check{e}^k\hat{e}^l) = \delta_{kl}$ for $1 \le k, l \le n_\mathcal{B}$. For given $m \in M$ we find that $m \bullet \check{e} := \sum_{i=1}^{n_\mathcal{B}} m_i\check{e}^i$ is the unique inverse $v^{-1}(m)$ of v on M. Obviously $M \subset \mathrm{I\!R}^{n_\mathcal{B}}$ is also a continuous parametrization of $\partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and M contains all vectors $m \in \mathrm{I\!R}^{n_\mathcal{B}}$ for which there is a $\omega \in \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ (not only in $\partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$) with $\lim_\Lambda \langle\omega\,; m_\Lambda(\hat{e})\rangle = m$.

We are now able to give a necessary condition for a state $\varphi \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ to have minimal free energy density. We use the M–parametrization of $\partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and write for $m \in M$

$$\begin{aligned} &u(m) := u(\otimes v^{-1}(m)), \quad s(m) := s(\otimes v^{-1}(m)),\\ &f(\beta, m) := f(\beta, \otimes v^{-1}(m)) \end{aligned} \tag{3.3}$$

instead of $u(\otimes\phi)$, $s(\otimes\phi)$, and $f(\beta, \otimes\phi)$ for $\phi \in \mathcal{S}(\mathcal{B})$.

Proposition 3.5 (Pure Phase Selfconsistency–Equation)

If $M \ni m \to u(m)$ is a continuously differentiable function on M, it holds the following necessary condition for an extremal permutation invariant state in $\partial_e\mathcal{S}(\beta)$: For each $\otimes\varrho$ in $\partial_e\mathcal{S}(\beta)$ (we identify a state $\phi \in \mathcal{S}(\mathcal{B})$ with its corresponding density matrix ϱ_ϕ) it must be satisfied:

$$\begin{aligned} &\varrho = \frac{\exp(-\beta h(\varrho))}{\mathrm{tr}(\exp(-\beta h(\varrho)))},\\ &\textit{with } h(\varrho) := \sum_{i=1}^{n_\mathcal{B}} \frac{\partial u}{\partial m_i}(v(\varrho))\,\hat{e}^i. \end{aligned} \tag{3.4}$$

SKETCH OF THE PROOF: The selfconsistency condition is a consequence of the necessary extremal condition for minimizers ϱ of $f(\beta, \otimes\varrho)$ under the constraints that $m \in M$, i.e. ϱ positive and $\mathrm{tr}(\varrho) = 1$ [18, 3].

A short calculation using Prop. 3.5 shows that every extremal permutation invariant state $\otimes\varrho$ with minimal free energy density is locally given by

$$\langle\otimes\varrho\,; A\rangle = \mathrm{tr}_\Lambda(\varrho_\Lambda A), \quad A \in \mathcal{A}_\Lambda$$

with the density matrix

$$\varrho_\Lambda = \frac{\exp(-\beta h_\Lambda^{\mathrm{eff}})}{\mathrm{tr}_\Lambda(\exp(-\beta h_\Lambda^{\mathrm{eff}}))}, \quad \text{where } h_\Lambda^{\mathrm{eff}} = \sum_{i\in\Lambda}[h(\varrho)]_i$$

is an effective Hamiltonian, in which the original interaction is substituted by the sum of interactions of each particle with an effective field $(\partial u/\partial m_i)(v(\varrho))$.

It should be emphasized that the fixpoint equation (3.4) is a direct *implication* of the principle of minimal free energy involving the local Hamiltonians in their exact form. The same result may be also derived indirectly by the combination of [10] with [9]. In the usual way of handling our model class (3.4) is introduced as an *ansatz* to be solved selfconsistently — which is the reason for calling (3.4) a selfconsistency–equation — involving only mean–field Hamiltonians. Note, that not all solutions ϱ of (3.4) define equilibrium states in $\partial_e\mathcal{S}(\beta)$, because there are also solutions for saddle points and maxima of the free energy density. Nevertheless, all solutions of (3.5) — at least for models with symmetric nets of local Hamiltonian densities — are KMS–states of a corresponding limiting dynamics as is seen by inspection, cf. e.g. [42]. Thus not all KMS–states have a microscopic foundation in terms of the thermodynamic limit of local equilibrium states.

In the sequel we will convert the matrix equation (3.4) into an equivalent system of coupled scalar equations for the expectation values $v(\varrho) \in \mathrm{I\!R}^{n_\mathcal{B}}$ which is more appropriate for a numerical treatment.

Definition 3.6 (Selfconsistency–Equation on the Parameter Space)

Let be $\beta > 0$ and $u : M \to \mathrm{I\!R}^{n_\mathcal{B}}$ continuously differentiable. Then set $y(m) := [\mathrm{grad}\, u](m) \in \mathrm{I\!R}^{n_\mathcal{B}}$ for $m \in M \subset \mathrm{I\!R}^{n_\mathcal{B}}$. We introduce the following quantities:

(i) Molecular–field partition function:

$$\begin{aligned} &Z_\beta : \mathrm{I\!R}^{n_\mathcal{B}} \longrightarrow \mathrm{I\!R},\\ &x \longrightarrow Z_\beta(x) := \mathrm{tr}_\mathcal{B}(\exp(-\beta\, x \bullet \hat{e})), \end{aligned}$$

(ii) Vector–valued fixpoint function:

$$\widetilde{F}_\beta : M \longrightarrow \mathbb{R},$$
$$m \longrightarrow \widetilde{F}_\beta(m) := -\frac{1}{\beta}\,\mathrm{grad}(\ln Z_\beta)(y(m)),$$

(iii) Extremal free energy density (values of $f(\beta,\cdot)$ for solutions of (3.4)):

$$\widetilde{f}(\beta,\cdot) : M \longrightarrow \mathbb{R},\ m \longrightarrow \widetilde{f}(\beta,m),$$
$$\widetilde{f}(\beta,m) := u(m) - y(m)\bullet m - \frac{1}{\beta}\ln Z_\beta(y(m)),$$

(iv) Sets of fixpoints of $\widetilde{F}_\beta$:

$$L(\beta) := \{m \in M \mid m = \widetilde{F}_\beta(m)\},$$
$$M(\beta) := \big\{m \in L(\beta) \mid \widetilde{f}(\beta,m) = \inf\{\widetilde{f}(\beta,m') \mid m' \in L(\beta)\}\big\}.$$

At this point we come back to our example of (2.1), (2.3): Here the internal energy density is given by $u(m) = \varepsilon \bullet m + m \bullet wm$ and thus we have

$$y(m) = \varepsilon + 2\,w\,m,$$
$$\widetilde{f}(\beta,m) = -m \bullet wm - \frac{1}{\beta}\ln\Big(\mathrm{tr}_{\mathcal{B}}(\exp(-\beta(\varepsilon \bullet \hat{e} + 2\,m \bullet w\hat{e})))\Big).$$

These are the expressions for the minimal free energy usually used in mean–field approximations for models with two particle interaction.

With the minimum principle, Theorem 3.4, and the fixpoint condition (3.4), the equivalence of the sets $\partial_e\mathcal{S}(\beta)$ and $M(\beta)$ follows:

Proposition 3.7 (Equivalence of Statistical and Thermodynamical Selfconsistency)

For all $\otimes\varrho \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ the two statements

(i) ϱ is a solution of (3.4),

(ii) $v(\varrho) \in L(\beta)$,

are equivalent, and the two statements

(iii) $\otimes\varrho \in \partial_e\mathcal{S}(\beta)$,

(iv) $v(\varrho) \in M(\beta)$,

are also equivalent. Each state obeying one of these four conditions fulfills

$$f(\beta,\otimes\varrho) = \widetilde{f}(\beta,v(\varrho)) \tag{3.5}$$

and it holds

$$\inf\{f(\beta,\otimes\varphi) \mid \otimes\varphi \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})\} = \inf\{\widetilde{f}(\beta,m) \mid m \in L(\beta)\}. \tag{3.6}$$

PROOF: Applying v to (3.4) shows that ϱ being a solution of (3.4) is equivalent to $v(\varrho)$ being in $L(\beta)$. Thus (3.4) and the parametrization v of $\mathcal{S}(\mathcal{B})$ implies (i)⇔(ii) as well as (3.5) and (3.6). From this (iii)⇔(iv) follows.

The determination of the support of the limiting Gibbs states is now reduced to the problem of finding the minimal solutions $M(\beta)$ of the coupled set

$$m = \widetilde{F}_\beta(m)$$

of nonlinear equations which can be determined at least numerically. If one finds $M(\beta)$ to be an orbit

$$\widetilde{\mathcal{O}}_{\mathsf{H}}(m) := \{M(u^*)^T m \mid u \in \mathsf{H}\} \tag{3.7}$$

for some $m \in M(\beta)$, then there is only one accumulation point of the net $\{\omega_\Lambda^\beta \mid \Lambda \in \mathcal{L}\}$, the *unique limiting Gibbs state*:

Proposition 3.8

(i) With the bijective mapping $v : \mathcal{S}(\mathcal{B}) \longrightarrow M$ it holds

$$v^{-1} \circ M(u^*)^T = \mathrm{Ad}_u^* \circ v^{-1},\ \forall u \in \mathsf{H}. \tag{3.8}$$

Thus we have for $m \in M$: $\otimes v^{-1}(M(u^*)^T m) = \Theta_u^*(\otimes v^{-1}(m))$ and $\otimes v^{-1}\left(\widetilde{\mathcal{O}}_{\mathsf{H}}(v(\varrho))\right) = \mathcal{O}_{\mathsf{H}}(\otimes\varrho)$ for $\otimes\varrho \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$. The following statements are equivalent:

(a) There exists a $m \in M(\beta)$ with $M(\beta) = \widetilde{\mathcal{O}}_{\mathsf{H}}(m)$.

(b) There exists a $\varphi \in \partial_e\mathcal{S}(\beta)$ with $\partial_e\mathcal{S}(\beta) = \mathcal{O}_{\mathsf{H}}(\varphi)$.

(ii) If one statement in (i) is valid, then there exists the net limit

$$\omega^\beta := w^*\text{-}\lim_\Lambda \omega_\Lambda^\beta = \int_{\mathsf{H}} \otimes\varrho_u^\beta\, \mathrm{d}\mu_{\mathsf{H}}(u).$$

Here the product states $\otimes\varrho_u^\beta \in \partial_e\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ are defined by

$$\otimes\varrho_u^\beta := \otimes v^{-1}(M(u^*)^T m) = \Theta_u^*(\otimes v^{-1}(m))$$

for some $m \in M(\beta)$. The density matrix $\varrho_u^\beta = v^{-1}(M(u^*)^T m)$ is given explicitly by

$$\varrho_u^\beta = \frac{\exp\left(-\beta\, y(M(u^*)^T m) \bullet \hat{e}\right)}{\mathrm{tr}_{\mathcal{B}}(\exp\left(-\beta\, y(M(u^*)^T m) \bullet \hat{e}\right))}.$$

For $y(m)$, see Definition 3.6.

PROOF: (i) Equation (3.8) follows by direct inspection (use (2.5), (2.6), and (3.7)) and implies the equivalence of $m \in M(\beta) = \widetilde{\mathcal{O}}_{\mathsf{H}}(m)$ and $\otimes v^{-1}(m) \in \partial_e \mathcal{S}(\beta) = \mathcal{O}_{\mathsf{H}}(\otimes v^{-1}(m))$.

(ii) Because $\mathcal{S}(\mathcal{A})$ is compact the net $\{\omega_\Lambda^\beta, \Lambda \in \mathcal{L}\}$ has at least one accumulation point $\omega^\beta \in \mathcal{S}^{\mathsf{G}}(\mathcal{A})$, Lemma 2.7 (ii). The assumption $M(\beta) = \widetilde{\mathcal{O}}_{\mathsf{H}}(m)$ resp. $\partial_e \mathcal{S}(\beta) = \mathcal{O}_{\mathsf{H}}(\otimes v^{-1}(m))$ implies together with Theorem 3.4 and Prop. 2.9 that each limiting Gibbs state has the same central decomposition and $\{\omega_\Lambda^\beta \mid \Lambda \in \mathcal{L}\}$ has only one accumulation point

$$\omega^\beta := w^*\text{-}\lim_\Lambda \omega_\Lambda^\beta.$$

The central decomposition is given by the Haar measure on $\mathcal{O}_{\mathsf{H}}(\otimes v^{-1}(m))$

$$\omega = \int_{\mathsf{H}} \Theta_u^*(\otimes v^{-1}(m))\, \mathrm{d}\mu_{\mathsf{H}}(u).$$

It remains to determine $\Theta_u^*(\otimes v^{-1}(m))$. With Def. 3.6 and Prop. 3.7 we have:

$$\begin{aligned}
\Theta_u^*(\otimes v^{-1}(m)) &= \Theta_u^*(\otimes \frac{\exp(-\beta\, y(m) \bullet \hat{e})}{\mathrm{tr}_{\mathcal{B}}(\exp(-\beta\, y(m) \bullet \hat{e}))}) \\
&= \otimes \frac{u \exp(-\beta\, y(m) \bullet \hat{e})\, u^*}{\mathrm{tr}_{\mathcal{B}}(\exp(-\beta\, y(m) \bullet \hat{e})\, u^* u)} \\
&= \otimes \frac{\exp(-\beta\, y(m) \bullet u\hat{e}u^*)}{\mathrm{tr}_{\mathcal{B}}(\exp(-\beta\, y(m) \bullet u\hat{e}u^*))} \\
&= \otimes \frac{\exp(-\beta\, (M(u)y(m)) \bullet \hat{e})}{\mathrm{tr}_{\mathcal{B}}(\exp(-\beta\, (M(u)y(m)) \bullet \hat{e}))} \\
&= \otimes \frac{\exp\left(-\beta\, (y(M(u^*)^T m)) \bullet \hat{e}\right)}{\mathrm{tr}_{\mathcal{B}}(\exp\left(-\beta\, (y(M(u^*)^T m)) \bullet \hat{e}\right))},
\end{aligned}$$

where we used that $y(m) = [\mathrm{grad}(u)](m)$ is the gradient of the internal energy y. Due to the H–symmetry of all H_Λ we also have $u(m) = u(M(v^*)^T m)$ for all $m \in M$ and $v \in \mathsf{H}$.

By Prop. 3.8 (i) each orbit in $\partial_e \mathcal{S}(\beta)$ may be mapped onto an orbit in $M(\beta)$ and vice versa. In the general case $\partial_e \mathcal{S}(\beta)$ may contain more than one H–orbit. The general form of the limiting Gibbs states is then more complicated.

Proposition 3.9

(i) Each limiting Gibbs state has the general form

$$\omega^\beta = \int_{\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})} [\int_{\mathsf{H}} \Theta_u^*(\varphi_\psi)\, \mathrm{d}\mu_{\mathsf{H}}(u)] \mathrm{d}\nu(\psi)$$

where ν is a probability measure on $\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$, uniquely determined by ω^β, and every φ_ψ is in $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ and uniquely determined up to a transformation Θ_u^* for some $u \in \mathsf{H}$.

(ii) The energy and entropy densities decompose in a non–trivial way only over $\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$ and have the form

$$u(\omega^\beta) = \int_{\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})} u(\psi)\, \mathrm{d}\nu(\psi)$$

and

$$s(\omega^\beta) = \int_{\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})} s(\psi)\, \mathrm{d}\nu(\psi).$$

They are constant on every H*–orbit.*

PROOF: (i) Since the permutation group P is a subgroup of G, also G acts in a norm asymptotic manner in $\mathcal{A}$. Thus $\mathcal{S}^{\mathsf{G}}(\mathcal{A})$ is a Choquet simplex [4, Chapter 4.3]. Since every limiting Gibbs state is in $\mathcal{S}^{\mathsf{G}}(\mathcal{A})$ there is a unique decomposition of the form

$$\omega^\beta = \int_{\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})} \psi\, \mathrm{d}\nu(\psi)\,,$$

where we have restricted the decomposing measure from $\mathcal{S}(\mathcal{A})$ to $\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$. In virtue of Prop. 2.9 (iv) every $\psi \in \partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$ has a central decomposition of the form

$$\psi = \int_{\mathsf{H}} \Theta_u^*(\varphi_\psi)\, \mathrm{d}\mu_{\mathsf{H}}(u)$$

for some $\varphi_\psi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$. Any other $\varphi'_\psi \in \partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ giving this unique decomposition must be an element of $\mathcal{O}_{\mathsf{H}}(\varphi_\psi)$.

(ii) Restricted to $\partial_e \mathcal{S}^{\mathsf{P}}(\mathcal{A})$ both $u(\varphi)$ and $s(\varphi)$ are invariant under the Θ_u^*–transformations for all $u \in \mathsf{H}$ (cf. Def. 3.1 and Def. 2.5). Since $u(\varphi)$ and $s(\varphi)$ are affine and w^*–continuous, they may be taken into the integral of an orthogonal decomposition.

From Prop. 3.9 we see that a limiting Gibbs state is uniquely specified by the measure ν on $\partial_e \mathcal{S}^{\mathsf{G}}(\mathcal{A})$ and the family $\{\varphi_\psi \mid \psi \in \mathrm{supp}\, \nu\}$ of pure phase states.

In [23, 24], there are given examples, where supp ν consists of two G–invariant states, which in turn have non–trivial decompositions into extremal permutation invariant states. To the best of our knowledge, such a case with several non–trivial orbits has not been discussed before (in rigorous terms).

In general however, there is no method to deduce from the minimal set $\mathcal{S}(\beta)$ of the free energy the complete form of the limiting Gibbs states. Thus one does not know, whether all elements of $\partial_e \mathcal{S}(\beta)$ appear as pure phase states in the central decompositions of the limiting Gibbs states. This would be desirable, since all physical features of infinite systems should be approximable by the properties of finite systems. On the other hand, one may argue that all states in the minimal set $\mathcal{S}(\beta)$ are stable configurations of the macroscopic system under consideration and should be realizable equilibrium states at the temperature β. As a working hypothesis for our subsequent investigations we shall assume this point of view.

4. Thermodynamic Formalism for Functionals and Functions

In the preceding investigations we have considered the thermodynamic potentials, i.e., the densities of energy, entropy and free energy as (affine, w^*–continuous) functionals on $\mathcal{S}^{\mathrm{P}}(\mathcal{A})$. Especially, the free energy density is of interest due to the minimum principle of the free energy density for limiting Gibbs states, Theorem 3.4. Moreover, this minimum value is the thermodynamic limit of the local free energy densities in equilibrium:

Proposition 4.1

Let be $f(\beta, \widetilde{h})$ the minimal free energy of Theorem 3.4 for the family of local Hamiltonians H_Λ, $\Lambda \in \mathcal{L}$. It holds

$$\begin{aligned} f(\beta,\widetilde{h}) &= \lim_{\Lambda} \frac{1}{|\Lambda|}\Big(\Big\langle \omega_\Lambda^\beta ; H_\Lambda \Big\rangle \\ &\qquad + \frac{1}{\beta}\,\mathrm{tr}_\Lambda(e^{-\xi_\Lambda - \beta H_\Lambda} \ln(e^{-\xi_\Lambda - \beta H_\Lambda}))\Big) \\ &= -\lim_{\Lambda} \frac{1}{|\Lambda|}\,\frac{1}{\beta}\,\ln \mathrm{tr}_\Lambda(e^{-\beta H_\Lambda}). \end{aligned}$$

PROOF: Choose an arbitrary increasing sequence of local regions Λ_n with w^*-$\lim_{n\to\infty}\omega_{\Lambda_n} = \omega \in \mathcal{S}^{\mathrm{P}}(\mathcal{A})$. Due to an $\varepsilon/3$ argument $\lim_\Lambda \frac{1}{|\Lambda|}\langle \omega_\Lambda ; H_\Lambda\rangle = u(\widetilde{h}, \omega)$ holds. A similar asymptotic behaviour holds for the entropy. Let be $\varepsilon > 0$. For $k \equiv k(\varepsilon)$ and sufficiently large n we have

$$\begin{aligned} &-\frac{1}{|\Lambda_n|}\mathrm{tr}_\Lambda(e^{-\xi_{\Lambda_n} - \beta H_{\Lambda_n}} \ln(e^{-\xi_{\Lambda_n} - \beta H_{\Lambda_n}})) \\ &\geq -\frac{1}{|\Lambda_k|}\mathrm{tr}_\Lambda(e^{-\xi_{\Lambda_k} - \beta H_{\Lambda_k}} \ln(e^{-\xi_{\Lambda_k} - \beta H_{\Lambda_k}})) - \varepsilon \end{aligned}$$

(see e.g. the proof of Lemma 4.2 in [18]). These convergence relations allow to adopt the arguments in the proof of [18, Theorem 4.3] to our model class. See also [3].

In the following we formulate a variational principle for the free energy as a functional of the net $\mathcal{L} \ni \Lambda \to H_\Lambda/|\Lambda|$, which assumes for the mean–field models under consideration a very concise form.

4.1. Variational Principles for Mean–Field Interactions

In Def. 3.1 and Prop. 3.2 the internal energy, the entropy, and the free energy density have been introduced. Now let H_Λ, $\Lambda \in \mathcal{L}$, be a net of finite volume Hamiltonians with densities $h_\Lambda := H_\Lambda/|\Lambda|$ and denote the net $(h_\Lambda)_{\Lambda\in\mathcal{L}}$ by $\widetilde{h}$. In Remark 3.3 we have introduced the surjective mapping $j : \widetilde{\mathcal{Y}} \to \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{C})$ with

$$[j(\widetilde{h})](\varrho) = u(\widetilde{h}, \otimes\varrho) =: h(\varrho), \tag{4.1}$$

for all $\otimes\varrho \in \partial_e \mathcal{S}^{\mathrm{P}}(\mathcal{A})$. In this sense, the internal energy $u(\widetilde{h}, \cdot)$ is a continuous functional of the pure phase states of the system (parametrized by $\mathcal{S}(\mathcal{B})$). Since j is not injective, u gives a coarsened description of the model which does not consider microscopic details. Since we are interested in this section mainly in the thermodynamic properties of the system, we assume that a certain model at the thermo–statistical stage is characterized by a continuous function $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$ instead of the net $\widetilde{h}$ of local Hamiltonian densities. In correspondence to the properties of the original internal energy, we define for given $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$ and $\omega \in \mathcal{S}^{\mathrm{P}}(\mathcal{A})$:

$$u(h, \omega) := \int_{\mathcal{S}(\mathcal{B})} h(\varrho)\, \mathrm{d}\,\mu_\omega(\varrho), \tag{4.2}$$

where μ_ω is the central measure of ω, parametrized in terms of $\mathcal{S}(\mathcal{B})$. With the equivalence of the positive normed regular Borel measures $\mathrm{M}_1^+(\mathcal{S}(\mathcal{B}))$

and $\mathcal{S}(\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}))$, we define u on the whole of $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$ by

$$\begin{aligned} &u : \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}) \times \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*, \\ &(h,\alpha) \longrightarrow \langle \alpha\,; h\rangle := \int_{\mathcal{S}(\mathcal{B})} h(\varphi)\,\mathrm{d}\,\mu_\alpha(\varphi) \end{aligned} \tag{4.3}$$

with the measure μ_α corresponding to $\alpha \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$. In an analogous way we introduce an entropy density as a w^*–upper semicontinuous functional on $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$:

$$\begin{aligned} &s : \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^* \longrightarrow \mathbb{R} \cup -\infty, \\ &\alpha \longrightarrow \begin{cases} -\displaystyle\int_{\mathcal{S}(\mathcal{B})} \mathrm{tr}_{\mathcal{B}}(\varrho \ln \varrho)\,\mathrm{d}\,\mu_\alpha(\varrho) & \\ \qquad\qquad \text{for } \alpha \in \mathcal{S}\ (\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})), & \\ -\infty \qquad \text{otherwise,} & \end{cases} \end{aligned} \tag{4.4}$$

which is consistent with Definition 3.1 because of Proposition 3.2. That is: $s(\alpha) = s(\omega)$, when α is the central measure of $\omega \in \mathcal{S}^{\mathrm{P}}(\mathcal{A})$. Then the free energy density is introduced such that it corresponds to $f(\beta,\widetilde{h},\omega)$ in Section 3.1:

$$\begin{aligned} &f(\beta,\cdot,\cdot) : \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}) \times \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^* \longrightarrow \mathbb{R} \cup +\infty, \\ &(h,\alpha) \longrightarrow f(\beta,h,\alpha) : \\ &\qquad = u(h,\alpha) - \frac{1}{\beta}s(\alpha) = \langle \alpha\,; h\rangle - \frac{1}{\beta}s(\alpha). \end{aligned} \tag{4.5}$$

With this transcription the equilibrium free energy is:

$$\begin{aligned} f(\beta,j(\widetilde{h})) &:= \inf\{f(\beta,j(\widetilde{h}),\alpha) \mid \alpha \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*\} \\ &= \inf\{f(\beta,j(\widetilde{h}),\omega) \mid \omega \in \mathcal{S}(\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}))\}. \end{aligned} \tag{4.6}$$

As above, (4.5) and (4.6) are consistent with Def. 3.1 and Theorem 3.4, i.e. it holds with Prop. 3.2 and (4.1): $f(\beta,h,\alpha) = f(\beta,j(\widetilde{h}),\alpha) = f(\beta,\widetilde{h},\omega)$ if α is the central measure of $\omega \in \mathcal{S}^{\mathrm{P}}(\mathcal{A})$ and thus $f(\beta,h) = f(\beta,j(\widetilde{h})) = f(\beta,\widetilde{h})$. The set of states $\omega \in \mathcal{S}\ (\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}))$ with $f(\beta,j(\widetilde{h}),\omega) = f(\beta,j(\widetilde{h}))$ obviously corresponds to $\mathcal{S}(\beta,\widetilde{h})$ and the variational problems in Theorem 3.4 and (6.6) characterize the same states. The analysis of the consequences of the minimum principle will be performed by using methods of convex analysis [20, 21, 43].

$\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})$ with the norm topology and $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$ with the w^*–topology are a *pairing* in the sense of [21, Chapter 3]. (Note that we use in this subsection the notation $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R}) \times \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^* \ni (h,\alpha) \to \langle\alpha\,;h\rangle$ which arises from the duality relation on $\mathcal{A}$. In contrast to [21], the positions of h and α are exchanged.) Now (4.6) directly implies that $f(\beta,h)$ is the concave conjugate function of $\frac{1}{\beta}\,s$:

$$\begin{aligned} f(\beta,h) &= \left[\frac{1}{\beta}\,s\right]^*(h) \\ &= \inf\left\{\langle\alpha\,;h\rangle - \frac{1}{\beta}s(\alpha) \mid \alpha \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{C})^*\right\}. \end{aligned}$$

The convex or concave conjugate of a function is a generalization of the Legendre transformation and sometimes called Fenchel transform. The biconjugate $\left[\frac{1}{\beta}\,s\right]^{**}$ of $\frac{1}{\beta}\,s$ is obtained by a second conjugation, leading to [21, Theorem 5]

$$\begin{aligned} &[f(\beta,\cdot)]^*(\alpha) \\ &\qquad = \inf\{\langle\alpha\,;h\rangle - f(\beta,h) \mid h \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})\} \\ &\qquad = \left[\frac{1}{\beta}\,s\right]^{**}(\alpha) = \mathrm{cl}(\mathrm{co}\,\frac{1}{\beta}\,s)(\alpha) \end{aligned}$$

for all $\alpha \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$. co is the concave hull of a function and cl coincides in our case with the w^*–upper semicontinuous hull (since we are dealing with proper concave functions, i.e. $\infty > f(\beta,h)$, $\frac{1}{\beta}s(\omega) \not\equiv -\infty$). Moreover, $\frac{1}{\beta}s$ is an affine w^*–upper semicontinuous functional, (4.4), and thus $\mathrm{cl}(\mathrm{co}\,\frac{1}{\beta}\,s)(\alpha) = \frac{1}{\beta}\,s(\alpha)$, which leads to a consistent thermodynamic formalism:

Theorem 4.2

The minimal free energy is a concave upper semicontinuous functional on $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})$ *and the entropy on* $\mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^*$ *is an affine* w^**–upper semicontinuous functional on* $\mathrm{M}_1^+(\mathcal{S}(\mathcal{B}))$ *and it holds*

$$f(\beta,\cdot) = \left[\frac{1}{\beta}\,s\right]^* \ \textit{and}\ s = \beta\left[f(\beta,\cdot)\right]^*.$$

We see that the entropy and the free energy contain the same amount of thermodynamic information. This quality is also expressed by their differentiability properties, leading to a geometrical characterization of the set

$$\mathcal{S}(\beta,h) := \{\alpha \in \mathcal{C}(\mathcal{S}(\mathcal{B}),\mathbb{R})^* \mid f(\beta,h,\alpha) = f(\beta,h)\}.$$

For some fixed $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$, $\mathcal{S}(\beta, h)$ corresponds to the set $\mathcal{S}(\beta, \tilde{h})$ of states with minimal free energy as introduced in Theorem 3.4. For $\omega \in \mathcal{S}(\beta, h)$ it holds

$$f(\beta, h) = \langle \omega ; h \rangle - \frac{1}{\beta}\, s(\omega) = \langle \omega ; h - h' \rangle + f(\beta, h', \omega)$$
$$\geq \langle \omega ; h - h' \rangle + f(\beta, h'). \tag{4.7}$$

This is exactly the defining relation for ω being an element of the *subgradient set* $\partial f(\beta, h)$ of the concave function $f(\beta, h)$ at h (as in [20] we use for simplicity the term *subgradient* instead of the more appropriate one *supergradient*).

Proposition 4.3

For all $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$ *it holds*

$$\mathcal{S}(\beta, h) = \partial f(\beta, h).$$

Thus the subgradient $\partial f(\beta, h)$ *of* $f(\beta, h)$ *uniquely determines the set* $\mathcal{S}(\beta, h)$ *of states with minimal free energy density for the model with internal energy* $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$.

PROOF: In (4.7) we have shown that $\mathcal{S}(\beta, h) \subseteq \partial f(\beta, h)$. Now assume that $\alpha \in \partial f(\beta, h)$. It holds [21, Theorem 12, Corollary 12 A]

$$h \in \partial \left(\frac{1}{\beta}\, s(\omega)\right) \iff \omega \in \partial f(\beta, h), \tag{4.8}$$

thus we have $h \in \partial \frac{1}{\beta}\, s(\alpha)$ and it follows for all $\alpha' \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})^*$

$$f(\beta, h, \alpha) = \langle \alpha ; h \rangle - \frac{1}{\beta}\, s(\alpha)$$
$$\leq \langle \alpha' ; h \rangle - \frac{1}{\beta}\, s(\alpha') = f(\beta, h, \alpha').$$

This is exactly the minimum condition which implies α to be an element of $\mathcal{S}(\beta, h)$.

The above Theorem 4.2 and Proposition 4.3 show that the chosen model class (Definition 2.3) gives indeed a consistent thermodynamic formalism. Proposition 4.2 is the mean–field analog to [6, Theorem II.3.4]. Similar duality principles can be found in [44, 45] in the context of perturbed KMS–states. The connection to large deviation principles is discussed in [30]. Related discussions are also performed in [22].

In Figure 4.1 we have sketched the convex duality between $\frac{1}{\beta} s(\alpha)$ and $f(\beta, h)$ in the case that $\mathcal{S}(\mathcal{B})$ has three points, represented by the corners of the upper triangle in the 0–plane. The affine function $\mathcal{S}(\mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})) \ni \omega \to \frac{1}{\beta} s(\omega)$ is visualized by the oblique triangle. This whole triangle is Fenchel transformed into the corner, which is in the middle of the minimal free energy density surface of the lower diagram. The corresponding normalized interaction is $h(\varrho) = -\frac{1}{\beta} s(\varrho)$, $\varrho \in \mathcal{S}(\mathcal{B})$, giving the free energy the value zero, which has all states $\omega \in \mathcal{S}(\mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R}))$ as subgradient. (In the lower diagram each point in the 0–plane corresponds to a class $[h] := \{h + c \mid c \in \mathbb{R}\}$ of continuous functions for some suitably chosen normalized $h \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathbb{R})$. Since the continuous functions over three points are $\mathbb{R}^3$, their classes are $\mathbb{R}^2$.) The upper one–dimensional edges are transformed into the lower one–dimensional edges. That means, that any interaction of the lower edge has the upper edge as the set of equilibrium states, and all these interactions are physically equivalent in the sense of [6]. In the same sense all interactions in the lower flat surface parts are physically equivalent with just one common equilibrium state given by a corner of the upper entropy triangle. Moreover, we have illustrated

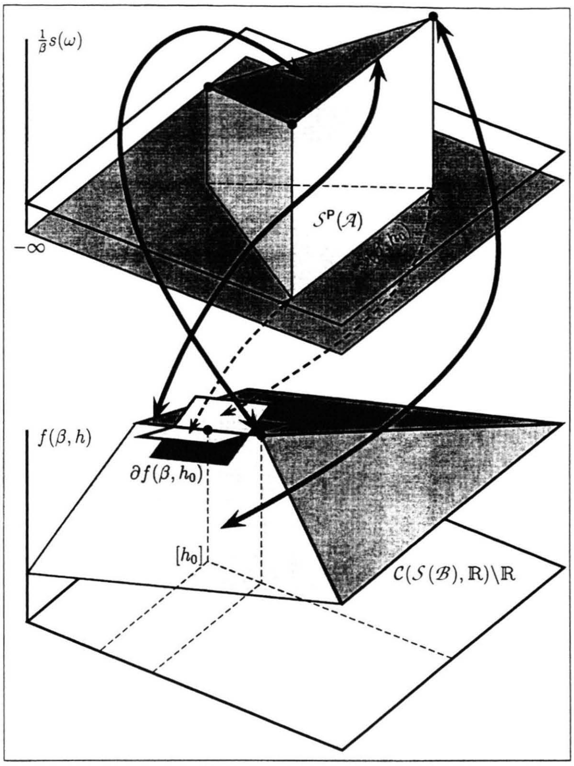

Fig. 4.1. Convex duality between $\frac{1}{\beta}s$ and $f(\beta, \cdot)$.

for a certain $h_0 \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathrm{I\!R})$ the subgradient and the corresponding set $\mathcal{S}(\beta, h_0)$ of states with minimal free energy (comp. Proposition 4.3).

In reality $\mathcal{S}(\mathcal{B})$ is a continuum and constitutes the extremal points of the infinite dimensional simplex $\mathcal{S}(\mathcal{C}(\mathcal{S}(\mathcal{B}), \mathrm{I\!R}))$. Nevertheless, our oversimplified diagram may give an idea, how a whole thermodynamic theory may be described in terms of the boundary structure of an *affine* entropy functional.

4.2. *Variation of Densities and External Field Parameters*

For thermodynamic applications it is more appropriate to convert the thermodynamic functionals into functions of a finite set of relevant macroscopic state variables. Here we choose the temperature β and an $n_{\mathcal{B}}$–tupel of external field variables ε as state variables (comp. ε in the examples (2.1), (2.3)). These so–called contact variables [36] vary in the range

$$E := \mathrm{I\!R}_+ \backslash \{0\} \times \mathrm{I\!R}^{n_{\mathcal{B}}} \ni (\beta, \varepsilon).$$

In many special applications ε will only vary in a hyperplane of $\mathrm{I\!R}^{n_{\mathcal{B}}}$, a case which will be treated in Section 4.3. Our thermodynamical system Σ is specified by a set of interactions W_Λ, $\Lambda \in \mathcal{L}$, with $\Lambda \to \frac{W_\Lambda}{|\Lambda|}$ approximately symmetric, and the corresponding continuous function $w := j((\frac{W_\Lambda}{|\Lambda|})_{\Lambda \in \mathcal{L}}) \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathrm{I\!R})$. In order to make explicit the ε–dependence we write instead of H_Λ the symbol $H_\Lambda(\varepsilon) := \sum_{i \in \Lambda} \varepsilon \bullet \hat{e}^i + W_\Lambda$ for a local Hamiltonian with given interaction. This leads to the symbols $h_\Lambda(\varepsilon) = H_\Lambda(\varepsilon)/|\Lambda|$, $\widetilde{h}(\varepsilon) = (h_\Lambda(\varepsilon))_{\Lambda \in \mathcal{L}}$, and $j(\widetilde{h}(\varepsilon)) = h(\varepsilon) \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathrm{I\!R})$. Starting from the non–equilibrium free energy functional $f(\beta, h, \alpha)$ from (4.5), we insert first $h(\varepsilon)$ for h and restrict the variability of h by varying $\varepsilon \in \mathrm{I\!R}^{n_{\mathcal{B}}}$, only. For states $\omega \in \mathcal{C}(\mathcal{S}(\mathcal{B}), \mathrm{I\!R})^*$ we want to use the m–parametrization introduced by the mapping $v : \mathcal{S}(\mathcal{B}) \to M \subset \mathrm{I\!R}^{n_{\mathcal{B}}}$ of (3.1) and restrict, therefore, ω to the point measures on M which we identify with the points in M. Thus we define the non–equilibrium free energy function

$$\begin{aligned} f(\beta, \cdot, \cdot) &: \mathrm{I\!R}^{n_{\mathcal{B}}} \times M \longrightarrow \mathrm{I\!R}, \\ (\varepsilon, m) &\longrightarrow f(\beta, \varepsilon, m) := f(\beta, h(\varepsilon), \alpha) \end{aligned} \tag{4.9}$$

with the the free energy functional from (4.5) on the right hand side and the point measure α on $\mathcal{S}(\mathcal{B})$ localized at $v^{-1}(m)$ (for the compatibility of the notation, see also (3.3)). Varying m in M gives all (possibly non–equilibrium) pure phase states $\otimes v^{-1}(m)$, resp. their free energy values in (4.9). The equilibrium free energy value may, therefore, be obtained by

$$f(\beta, \varepsilon) := f(\beta, h(\varepsilon)) = \inf \{ f(\beta, \varepsilon, m) \mid m \in M \}$$

$$\text{(from (4.6))}. \tag{4.10}$$

In the above manner we identify the various free energy expressions by their respective arguments.

With M as a subset of $\mathrm{I\!R}^{n_{\mathcal{B}}}$ we introduce a natural duality relation on $\mathrm{I\!R}^{n_{\mathcal{B}}}$ by

$$\begin{aligned} \langle \varepsilon \, ; m \rangle := \langle v^{-1}(m) \, ; \varepsilon \bullet \hat{e} \rangle &= \sum_{i=1}^{n_{\mathcal{B}}} \varepsilon_i \, \langle v^{-1}(m) \, ; \hat{e} \rangle \\ &= \sum_{i=1}^{n_{\mathcal{B}}} \varepsilon_i m_i. \end{aligned} \tag{4.11}$$

We need further the potential function

$$w(m) := [j((\frac{W_\Lambda}{|\Lambda})_{\Lambda \in \mathcal{L}})](v^{-1}(m)), \; m \in M \tag{4.12}$$

and the function

$$\sigma(\beta, m) := -w(m) + \frac{1}{\beta} \, s(m), \; m \in M, \tag{4.13}$$

where the entropy is given by

$$s(m) := s(\alpha), \; m \in M, \tag{4.14}$$

with $s(\alpha)$ from (4.4) and the point measure α on $\mathcal{S}(\mathcal{B})$ localized at $v^{-1}(m) \in \mathcal{S}(\mathcal{B})$ (the compatibility with $s(m)$ from (3.3) is still guaranteed).

We are now going to analyze the properties and the informational contents of the statistically derived free energy function $f(\beta, \varepsilon, m)$.

Proposition 4.4

The minimal free energy $\varepsilon \to f(\beta, \varepsilon)$ is a continuous concave function in ε, which increases monotonously in $\varepsilon_k \in \mathrm{I\!R}$, if the basis element $\hat{e}^k \in \mathcal{B}$, $k \in \{1, \ldots, n_{\mathcal{B}}\}$, is a positive operator.

PROOF: Concavity: Let be $\varepsilon_1 \neq \varepsilon_2 \in \mathrm{I\!R}^{n_{\mathcal{B}}}$ and $0 \leq \lambda \leq 1$. With Theorem 3.4 and the parametrization of $\partial_e \mathcal{S}^{\mathrm{P}}(\mathcal{A})$ by $\mathcal{S}(\mathcal{B})$ resp. M and (3.3) we have

$$\begin{aligned} &f(\beta,\lambda\varepsilon_1+(1-\lambda)\varepsilon_2)\\ &\quad=\inf\left\{\langle\lambda\varepsilon_1+(1-\lambda)\varepsilon_2\,;m\rangle-\sigma(\beta,m)\mid m\in M\right\}\\ &\quad\geq\lambda f(\beta,\varepsilon_1)+(1-\lambda)f(\beta,\varepsilon_2).\end{aligned}$$

Continuity: The following inequality is valid (see e.g. [6]):

$$\begin{aligned} &\left|-\frac{1}{\beta}\ln\operatorname{tr}_\Lambda(e^{-\beta H_\Lambda(\varepsilon)})+\frac{1}{\beta}\ln\operatorname{tr}_\Lambda(e^{-\beta H_\Lambda(\varepsilon')})\right|\\ &\quad\leq\|H_\Lambda(\varepsilon)-H_\Lambda(\varepsilon')\|=\left\|\sum_{i\in\Lambda}(\varepsilon-\varepsilon')\bullet\hat{e}^i\right\|\\ &\quad\leq\mathrm{const}|\Lambda|\,|\varepsilon-\varepsilon'|\,.\end{aligned}$$

Using the convergence of the finite volume free energy density (Proposition 4.1 it follows

$$\left|f(\beta,\varepsilon)-f(\beta,\varepsilon')\right|\leq\mathrm{const}\,|\varepsilon-\varepsilon'|\,.$$

Monotony: For $\varepsilon'_k\geq\varepsilon_k$ and $\varepsilon'_l=\varepsilon_l$ for $l\neq k$ we have

$$-\beta H_\Lambda(\varepsilon')\leq-\beta H_\Lambda(\varepsilon).$$

The monotony of $f(\beta,\varepsilon)$ follows with the monotony of $\mathcal{A}_\Lambda\ni A=A^*\to\ln\operatorname{tr}_\Lambda(e^A)$ and Proposition 4.1.

From the arguments in Sect. 4.1 it follows that also the function $\mathbb{R}^{n_\mathcal{B}}\ni\varepsilon\to f(\beta,\varepsilon)$ is in general not differentiable. For a thermodynamic formalism at the level of functions we need thus again the Fenchel transform instead of the Legendre transformation. In order to allow a compact formulation of the transformations of $f(\beta,\varepsilon)$ and $\sigma(\beta,m)$ we extend the continuous functions $M\ni m\to\sigma(\beta,m)$, $f(\beta,\varepsilon,m)$ to semi–continuous functions on $\mathbb{R}^{n_\mathcal{B}}$ by setting

$$\begin{aligned} &f(\beta,\varepsilon,m):=\infty\quad\text{and}\\ &\sigma(\beta,m):=-\infty\quad\text{for } m\in\mathbb{R}^{n_\mathcal{B}}\backslash M.\end{aligned}\tag{4.15}$$

With this choice of the extension it is guaranteed that the statistical information is still contained in their values on M although they are considered in the following as functions on $\mathbb{R}^{n_\mathcal{B}}$. Then we rewrite the free energy function (4.9)

$$\begin{aligned} f(\beta,\varepsilon,m)&=\langle\varepsilon\,;m\rangle-\sigma(\beta,m)\\ &=\sum_{i=1}^{n_\mathcal{B}}\varepsilon_i m_i-\sigma(\beta,m),\quad m\in\mathbb{R}^{n_\mathcal{B}}.\end{aligned}\tag{4.16}$$

The minimal relation (4.10) shows then that $f(\beta,\varepsilon)$ is the Fenchel transform of $\sigma(\beta,m)$ and *not* of $\frac{1}{\beta}\,s(m)$:

$$\begin{aligned} f(\beta,\varepsilon)&=\inf\{f(\beta,\varepsilon,m)\mid m\in M\}\\ &=\inf\{f(\beta,\varepsilon,m)\mid m\in\mathbb{R}^{n_\mathcal{B}}\}\\ &=\inf\{\langle\varepsilon\,;m\rangle-\sigma(\beta,m)\mid m\in M\}\\ &=\inf\{\langle\varepsilon\,;m\rangle-\sigma(\beta,m)\mid m\in\mathbb{R}^{n_\mathcal{B}}\}\,,\end{aligned}\tag{4.17}$$

or short $f(\beta,\cdot)=[\sigma(\beta,\cdot)]^*$. The reason is, of course, that the natural duality relation at the level of thermodynamic functions uses only part of the energy expectation value. Now $\sigma(\beta,m)$ is not concave in m and has in general plaits in its graph.

For given $\varepsilon\in\mathbb{R}^{n_\mathcal{B}}$ the corresponding equilibrium values of m are

$$M(\beta,\varepsilon):=\{m\in\mathbb{R}^{n_\mathcal{B}}\mid f(\beta,\varepsilon,m)=f(\beta,\varepsilon)\}\subseteq M.\tag{4.18}$$

Using (4.17) we find

$$\begin{aligned} \sigma(\beta,m)&=-w(m)+\frac{1}{\beta}s(m)\leq\langle\varepsilon\,;m\rangle-f(\beta,\varepsilon),\\ &\forall\varepsilon\in\mathbb{R}^{n_\mathcal{B}},\ \forall m\in\mathbb{R}^{n_\mathcal{B}}.\end{aligned}\tag{4.19}$$

Equality holds in (4.19), iff $m\in M(\beta,\varepsilon)$. In order to get a general variational principle from (4.19), we introduce the concave upper semicontinuous envelope function

$$\hat{\sigma}(\beta,\ \cdot\ ):\mathbb{R}^{n_\mathcal{B}}\to\mathbb{R},\tag{4.20}$$

$$\begin{aligned} \hat{\sigma}(\beta,m)&:=\inf\left\{\,\langle\varepsilon\,;m\rangle+c\mid\varepsilon\in\mathbb{R}^{n_\mathcal{B}},c\in\mathbb{R}\text{ with}\right.\\ &\qquad\left.\langle\varepsilon\,;m'\rangle+c\geq\sigma(\beta,m'),\ \forall m'\in\mathbb{R}^{n_\mathcal{B}}\right\}\\ &=\inf\left\{\,\langle\varepsilon\,;m\rangle+c\mid\varepsilon\in\mathbb{R}^{n_\mathcal{B}},c\in\mathbb{R}\text{ with}\right.\\ &\qquad\left.\langle\varepsilon\,;m'\rangle+c\geq\sigma(\beta,m'),\ \forall m'\in M\right\}.\end{aligned}$$

Using [20, Theorem 12.1], we have $\hat{\sigma}(\beta,\cdot)=\mathrm{cl}(\mathrm{co}\,\sigma(\beta,\cdot))$ (comp. Section 4.1). Moreover, $\hat{\sigma}(\beta,m)$ is continuous in M°, the relative interior of M [20, Theorem 10.1] and $v^{-1}(M^\circ)$ are the faithful states on $\mathcal{B}$.

Proposition 4.5

For all $m\in\mathbb{R}^{n_\mathcal{B}}$ *it holds:*

$$\inf\{\langle\varepsilon\,;m\rangle-f(\beta,\varepsilon)\mid\varepsilon\in\mathbb{R}^{n_\mathcal{B}}\}=\hat{\sigma}(\beta,m),$$

i.e. $\hat{\sigma}(\beta,\cdot)=[f(\beta,\cdot)]^*$ *and especially* $\hat{\sigma}(\beta,m)=-\infty$ *for* $m\in\mathbb{R}^{n_\mathcal{B}}\backslash M$.

PROOF: Although Prop. 4.5 can be reduced to standard results in convex analysis [20, 21, 43], we give here an elementary proof in order to reformulate some typical arguments within our context.

First we consider $m \in M$: With (4.19) and (4.20) we have for all $m \in M$:

$$\hat{\sigma}(\beta, m) \leq \inf\left\{\langle \varepsilon\,; m\rangle - f(\beta, \varepsilon) \mid \varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}\right\}.$$

Define the subgraph

$$\Gamma := \{(m', y') \in M \times \mathbb{R} \mid y' \leq \hat{\sigma}(\beta, m')\}.$$

Due to (4.20), Γ is a convex closed set in $\mathbb{R}^{n_{\mathcal{B}}} \times \mathbb{R}$ [20, Part II]. For the given $m \in M$ choose an arbitrary $y \in \mathbb{R}$ with $\hat{\sigma}(\beta, m) < y$, i.e., $(m, y) \notin \Gamma$. According to the Hahn–Banach Theorem [4, Theorem 2.3.22C] there is a $\Phi \in (\mathbb{R}^{n_{\mathcal{B}}} \times \mathbb{R})^*$ with

$$\Phi(m, y) > \sup\{\Phi(m', y') \mid (m', y') \in \Gamma\}.$$

Since $(\mathbb{R}^{n_{\mathcal{B}}} \times \mathbb{R})^*$ is isomorphic to $(\mathbb{R}^{n_{\mathcal{B}}} \times \mathbb{R})$ there is a tupel $(-\alpha, a)$ which corresponds to Φ, where $\alpha \in \mathbb{R}^{n_{\mathcal{B}}}$ and a may be chosen equal to 1 (use that $m \in M$). Then

$$\begin{aligned}
-\langle \alpha\,; m\rangle + y &> \sup\{-\langle \alpha\,; m'\rangle + y' \mid (m', y') \in \Gamma\} \\
&= \sup\{-\langle \alpha\,; m'\rangle + \hat{\sigma}(\beta, m') \mid m' \in M\} \\
&= -\inf\{\langle \alpha\,; m'\rangle - \hat{\sigma}(\beta, m') \mid m' \in M\} \\
&\geq -\inf\{\langle \alpha\,; m'\rangle - \sigma(\beta, m') \mid m' \in M\} \\
&= -\inf\{\langle \alpha\,; m'\rangle + w(m') - \frac{1}{\beta} s(m') \mid m' \in M\} \\
&= -f(\beta, \alpha).
\end{aligned}$$

Thus $y > \langle \alpha\,; m\rangle - f(\beta, \alpha) \geq \hat{\sigma}(\beta, m)$, which proves the infimum property of $\hat{\sigma}(\beta, m)$ since y is an arbitrary constant greater than $\hat{\sigma}(\beta, m)$.

Now consider the case $m \in \mathbb{R}^{n_{\mathcal{B}}} \backslash M$. Equation (4.20) implies $\hat{\sigma}(\beta, m) = -\infty$ for $m \in \mathbb{R}^{n_{\mathcal{B}}} \backslash M$. Assume that

$$\inf\{\langle \varepsilon\,; m\rangle - f(\beta, \varepsilon) \mid \varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}\} = C_1 > -\infty.$$

Then we have for all $\varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}$

$$\begin{aligned}
C_1 &\leq \langle \varepsilon\,; m\rangle - f(\beta, \varepsilon) \\
&= \langle \varepsilon\,; m\rangle - \inf\{\langle \varepsilon\,; m'\rangle - \sigma(\beta, m') \mid m' \in M\} \\
&\leq \langle \varepsilon\,; m\rangle - \inf\{\langle \varepsilon\,; m'\rangle \mid m' \in M\} + C_2
\end{aligned}$$

because the entropy s and the interaction w are finite on M. Again using the Hahn–Banach Theorem, we find some $\varepsilon_1 \in \mathbb{R}^{n_{\mathcal{B}}}$ such that

$$\langle \varepsilon_1\,; m\rangle - \langle \varepsilon_1\,; m'\rangle \geq C_3 > 0, \ \forall m' \in M.$$

Now choose $\varepsilon = -\lambda\varepsilon_1$ with $\lambda > \frac{|C_1 - C_2|}{C_3}$. It follows

$$\begin{aligned}
&\langle \varepsilon\,; m\rangle - \inf\{\langle \varepsilon\,; m'\rangle \mid m' \in M\} \\
&\quad = \sup\{\langle -\lambda\varepsilon_1\,; m\rangle - \langle -\lambda\varepsilon_1\,; m'\rangle \mid m' \in M\} \\
&\quad \leq -\lambda C_3 < -|C_1 - C_2|.
\end{aligned}$$

Thus C_1 cannot be finite.

The variational relation in Prop. 4.5 shows that $\hat{\sigma}(\beta, m)$ is the Fenchel transform of $f(\beta, \varepsilon)$ which is appropriate to treat not necessarily differentiable concave functions. From the general argument, that the double Fenchel transform is the original function for an upper semicontinuous proper concave function [20, Sect. 12] it follows:

Corollary 4.6

For all $\varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}$ *it holds*

$$\begin{aligned}
f(\beta, \varepsilon) &= \inf\{\langle \varepsilon\,; m\rangle - \sigma(\beta, m) \mid m \in \mathbb{R}^{n_{\mathcal{B}}}\} \\
&= \inf\{\langle \varepsilon\,; m\rangle - \sigma(\beta, m) \mid m \in M\} \\
&= \inf\{\langle \varepsilon\,; m\rangle - \hat{\sigma}(\beta, m) \mid m \in \mathbb{R}^{n_{\mathcal{B}}}\} \\
&= \inf\{\langle \varepsilon\,; m\rangle - \hat{\sigma}(\beta, m) \mid m \in M\},
\end{aligned}$$

i.e. $f(\beta, \cdot) = [\sigma(\beta, \cdot)]^* = [\hat{\sigma}(\beta, \cdot)]^* = [f(\beta, \cdot)]^{**}$.

Comparing this with Theorem 3.4, one may have the impression, that not only $m \to \sigma(\beta, m)$ but also its concave envelope $m \to \hat{\sigma}(\beta, m)$ alone contains the full thermodynamic information of the considered system. The following investigation shows, however, that this is not quite correct.

Before elaborating this, let us remark that the pure phase state entropy density $s(m)$ which is also equal to $-\mathrm{tr}_{\mathcal{B}}(v^{-1}(m)\ln(v^{-1}(m))))$ from (3.3) is a strictly concave continuous bounded function on M, see e.g. [44]. Moreover, $s(m)$ is infinitely differentiable in the interior M° of M (which corresponds to the faithful states on $\mathcal{B}$) as can be seen immediately with the contragradient basis $\check{e}$, giving $s(m) = -\mathrm{tr}_{\mathcal{B}}(m \bullet \check{e}\ln(m \bullet \check{e}))$. With the cyclic permutation property of $\mathrm{tr}_{\mathcal{B}}$ one calculates by power series expansion that

$$\frac{\partial s(m)}{\partial m_l} = -\mathrm{tr}_{\mathcal{B}}\left(\check{e}_l(\ln(m \bullet \check{e}) + 1)\right)$$

and

$$\frac{\partial^n s(m)}{\partial m_{l_1}\dots\partial m_{l_n}} = \frac{(-1)^{n-1}}{(n-2)!}\mathrm{tr}_{\mathcal{B}}\left(\check{e}_{l_1}\cdots\check{e}_{l_n}(m\bullet\check{e})^{-n+1}\right) \tag{4.21}$$

for $n \geq 2$ and $1 \leq l_1, \dots l_n \leq n_{\mathcal{B}}$, whenever the right hand sides are well defined. This is the case, if $m \bullet \check{e}$ is invertible, i.e. is the density matrix of a faithful state on $\mathcal{B}$. By continuity of the affine bijection v this holds for $m \in M^\circ$. Thus if the interaction term w is differentiable, $\sigma(\beta, m)$ is differentiable in $m \in M^\circ$. The differentiability of $\hat{\sigma}(\beta, m)$ is in general not given for all $m \in M^\circ$, but only in a dense subset. The set of points $m \in M^\circ$ where $\hat{\sigma}(\beta, m)$ is not differentiable has zero measure [20, Theorem 25.5].

Definition 4.7

The set

$$M^p(\beta) := \bigcup_{\varepsilon\in\mathrm{IR}^{n_{\mathcal{B}}}} M(\beta,\varepsilon)$$

gives all pure phase minimal m–values for a fixed $\beta > 0$. The absolute concavity region *of $\sigma(\beta,\cdot)$ is* defined *as*

$$M^c(\beta) := \{m \in M \mid \sigma(\beta,m) = \hat{\sigma}(\beta,m)\}.$$

A subgradient $m \in \partial f(\beta,\varepsilon) \subset \mathrm{IR}^{n_{\mathcal{B}}}$ of the function $\varepsilon \to f(\beta,\varepsilon)$ at $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ is defined by

$$f(\beta,\varepsilon') \leq f(\beta,\varepsilon) + \langle \varepsilon' - \varepsilon\,; m\rangle\,,\ \forall\varepsilon' \in \mathrm{IR}^{n_{\mathcal{B}}}. \tag{4.22}$$

The set of subgradients of the free energy for fixed β is given for unspecified ε by

$$M^g(\beta) := \bigcup_{\varepsilon\in\mathrm{IR}^{n_{\mathcal{B}}}} \partial f(\beta,\varepsilon).$$

The set $M^p(\beta)$ is defined by means of $f(\beta,\varepsilon,m)$ via (4.18) in a way that it lifts to the statistical level and parametrizes all statistical pure phase states of the system for a given interaction and varying external fields. $M^g(\beta)$ is according to (4.22) defined by means of the equilibrium function $\varepsilon \to f(\beta,\varepsilon)$ alone and is a union of the convex subsets $\partial f(\beta,\varepsilon) \subset \mathrm{IR}^{n_{\mathcal{B}}}$. It is a natural notion for the thermodynamics with functions, but has no direct connection with the statistical level. Finally $M^c(\beta)$ is defined with the possibly non–concave function $\sigma(\beta,m)$ alone. We study the relations between these sets.

Theorem 4.8

With the notations of Definition 4.7 it holds

(i) $M^c(\beta)\cap M^\circ \subseteq M^c(\beta)\cap M^g(\beta) \subseteq M^p(\beta) \subseteq M^c(\beta)$,

(i)) if the interaction w is continuously differentiable on M we have

$$M^c(\beta)\cap M^\circ = M^c(\beta)\cap M^g(\beta) = M^p(\beta).$$

PROOF: (i) Let be $m \in M^c(\beta)\cap M^\circ$. Since $\hat{\sigma}(\beta,m) = \sigma(\beta,m)$ is subdifferentiable [20, Theorem 23.4] we have $\varepsilon \in \partial\hat{\sigma}(\beta,m)$ for some $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$. Thus $m \in \partial f(\beta,\varepsilon)$ [20, Theorem 23.5] and $m \in M^g(\beta)\cap M^c(\beta)$.

If $m \in M^g(\beta)$, there is some $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ such that $m \in \partial f(\beta,\varepsilon)$. Then it holds

$$\hat{\sigma}(\beta,m) = \langle\varepsilon\,;m\rangle - f(\beta,\varepsilon) \leq \langle\varepsilon'\,;m\rangle - f(\beta,\varepsilon'),$$
$$\forall\varepsilon' \in \mathrm{IR}^{n_{\mathcal{B}}}.$$

If additionally $m \in M^c(\beta)$ it follows

$$\begin{aligned}\inf\{f(\beta,\varepsilon,m') \mid m' \in M\} &= \inf\{\langle\varepsilon\,;m'\rangle - \sigma(\beta,m') \mid m' \in M\}\\ &= f(\beta,\varepsilon) = \langle\varepsilon\,;m\rangle - \sigma(\beta,m)\end{aligned}$$

and we have $m \in M(\beta,\varepsilon) \subset M^p(\beta)$.

If $m \in M^p(\beta)$, there is some ε such that

$$\begin{aligned}f(\beta,\varepsilon) = f(\beta,\varepsilon,m) &= \langle\varepsilon\,;m\rangle - \sigma(\beta,m)\\ &= \inf\{\langle\varepsilon\,;m'\rangle - \sigma(\beta,m') \mid m' \in M\}\\ &= \inf\{\langle\varepsilon\,;m'\rangle - \hat{\sigma}(\beta,m') \mid m' \in M\}\\ &= \langle\varepsilon\,;m\rangle - \hat{\sigma}(\beta,m).\end{aligned}$$

Thus $\hat{\sigma}(\beta,m) = \sigma(\beta,m)$ and $m \in M^c(\beta)$.

(ii) We only have to show $M^p(\beta) \subseteq M^\circ$. The rest follows with (i). Now let be $m \in M^p$, i.e. there is some ε such that $m \in M(\beta,\varepsilon)$. Then we have $m \in L(\beta,\varepsilon)$ (Def. 3.6 and Prop. 3.7). Thus $v^{-1}(m)$ is a solution of (3.4) which obviously is faithful on $\mathcal{B}$, and $m \in M^\circ$ follows.

For fixed $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ we find quite similar results as in Theorem 4.8:

Proposition 4.9

With the notations of Def. 4.7 it holds for a continuously differentiable interaction w:

(i) $\mathrm{conv} M(\beta,\varepsilon) = \partial f(\beta,\varepsilon) = m(\mathcal{S}(\beta,\varepsilon))$, *with* $m(\omega) := \langle \omega\,;\hat{e}_l\rangle = \lim_\Lambda \frac{1}{|\Lambda|}\langle\omega\,;\sum_{k\in\Lambda}\hat{e}_k\rangle$ *for* $\omega\in\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ *and some arbitrary* $l\in\mathcal{R}$.

(ii) $\partial_e[\partial f(\beta,\varepsilon)] \subseteq M(\beta,\varepsilon)$.

PROOF: (i) $\mathrm{conv} M(\beta,\varepsilon) = m(\mathcal{S}(\beta,\varepsilon))$ follows from the Bauer–simplex property of $\mathcal{S}(\beta,\varepsilon)$ (Theorem 3.4), the affinity of $\mathcal{S}^{\mathsf{P}}(\mathcal{A})\ni\omega\to f(\beta,\varepsilon,\omega)$, and the affinity of v.

Now we show $\mathrm{conv} M(\beta,\varepsilon) = \partial f(\beta,\varepsilon)\cap M^\circ$: If $m\in M(\beta,\varepsilon)$, it follows

$$\begin{aligned}\langle\varepsilon'\,;m\rangle - f(\beta,\varepsilon') &\geq \langle\varepsilon'\,;m\rangle - f(\beta,\varepsilon',m) = \sigma(\beta,m)\\ &= \langle\varepsilon\,;m\rangle - f(\beta,\varepsilon,m) = \langle\varepsilon\,;m\rangle - f(\beta,\varepsilon),\end{aligned}$$

i.e. $m\in\partial f(\beta,\varepsilon)$. With the solutions $L(\beta,\varepsilon)$ of (3.4) in M it follows that $m\in M^\circ$. Since $\partial f(\beta,\varepsilon)$ is convex [20, Theorem 23.2], we have $\mathrm{conv} M(\beta,\varepsilon)\subseteq\partial f(\beta,\varepsilon)\cap M^\circ$.

The other way round let be $m\in\partial f(\beta,\varepsilon)\cap M^\circ$. In this case we have $\mathrm{cl}_M(\mathrm{co}_M\, f(\beta,\varepsilon,m)) = \mathrm{co}_M\, f(\beta,\varepsilon,m)$, since $m\in M^\circ$ [20, Theorem 7.4]. Here co_M (cl_M) denotes the convex hull (closure) of $f(\beta,\varepsilon,\cdot) : M\to\mathbb{R}$ on M. For $m\in\partial f(\beta,\varepsilon)$ it is $\varepsilon\in\partial\hat{\sigma}(\beta,m)$ [20, Theorem 23.5] and

$$\begin{aligned}\mathrm{cl}_M(\mathrm{co}_M f(\beta,\varepsilon,m')) &= \langle\varepsilon\,;m'\rangle - \hat{\sigma}(\beta,m')\\ &\geq \langle\varepsilon\,;m\rangle - \hat{\sigma}(\beta,m) = \mathrm{cl}_M(\mathrm{co}_M f(\beta,\varepsilon,m)),\\ &\text{for all } m'\in M.\end{aligned}$$

Thus we have $\mathrm{cl}_M(\mathrm{co}_M f(\beta,\varepsilon,m)) = \inf\{\mathrm{cl}_M(\mathrm{co}_M\, f(\beta,\varepsilon,m'))\mid m'\in M\}$. Moreover, it is $m\in M^\circ$, i.e. $\mathrm{co}_M f(\beta,\varepsilon,m) = \inf\{\mathrm{cl}_M(\mathrm{co}_M f(\beta,\varepsilon,m'))\mid m'\in M\} = f(\beta,\varepsilon)$, and $m\in M_{\min} := \{m'\in M\mid \mathrm{cl}_M(\mathrm{co}_M\, f(\beta,\varepsilon,m')) = f(\beta,\varepsilon)\}$. It remains to show that $m\in M_{\min}$ implies $m\in\mathrm{conv} M$. But

$$\begin{aligned}\mathrm{co}_M f(\beta,m,\varepsilon) = \inf\Big\{\sum_{i=1}^n \lambda_i f(\beta,\varepsilon,m_i)\Big|\\ 0<\lambda_i\leq 1, i=1,\dots,n, \text{ for some}\\ n\in\mathbb{N} \text{ and } \sum_{i=1}^n\lambda_i = 1, \sum_{i=1}^n\lambda_i m_i = m\Big\}\end{aligned}$$

and $m\in\mathrm{conv}\, M(\beta,\varepsilon)$.

Finally, use [20, Corollary 6.5.2]: Since $\partial f(\beta,\varepsilon)\subset M$ and $\partial f(\beta,\varepsilon)\cap M^\circ\neq\emptyset$, the relative interior of $\partial f(\beta,\varepsilon)$ is a non–empty subset of M° [20, Theorem 6.2]. With [20, Theorem 6.5] we find

$$\begin{aligned}\mathrm{conv}\, M(\beta,\varepsilon) &= \partial f(\beta,\varepsilon)\cap M^\circ = \mathrm{cl}(\partial f(\beta,\varepsilon)\cap M^\circ)\\ &= \mathrm{cl}(\partial f(\beta,\varepsilon))\cap\mathrm{cl}(M^\circ) = \partial f(\beta,\varepsilon)\cap M = \partial f(\beta,\varepsilon).\end{aligned}$$

(ii) Directly follows from $\mathrm{conv} M(\beta,\varepsilon) = \partial f(\beta,\varepsilon)$ in (i).

By means of Theorem 4.8 and Proposition 4.9 we have a characterization of pure phase states of the system at a given finite temperature $\beta>0$: Take an interior point $m\in M^\circ$ which also belongs to the absolute concavity region $M^c(\beta)$ of $\sigma(\beta,m)$. Then you can find a field–tupel $\varepsilon=\varepsilon(m)$, such that $m\in M(\beta,\varepsilon)$. Thus $\varrho = \otimes v^{-1}(m)\in\partial_e\mathcal{S}(\beta,\varepsilon)$, and all pure phase states arise in this way. In contrast, if $m\notin M^c(\beta)$ it is according to Theorem 4.8 (ii) not in $M^p(\beta)$ and cannot parametrize a pure phase state with minimal free energy. Especially, if $\hat{\sigma}$ is affine on a convex subset $M'\subset M$ with $\hat{\sigma}(\beta,m)>\sigma(\beta,m)$ for all $m\in M'$, such m are candidates for expectation values of $\hat{e}$ in states ω from the interior of $\mathcal{S}(\beta,\varepsilon)$, that are mixed phase states.

Concerning the differentiability of $f(\beta,\varepsilon)$ and the connection to limiting Gibbs states with non–trivial central decompositions we introduce the notion of a tangent state, comp. [6]:

Definition 4.10

A state $\omega\in\mathcal{S}^{\mathsf{P}}(\mathcal{A})$ *is called a tangent state of* $f(\beta,\varepsilon)$ *at* ε *with gradient* $m(\omega) := \langle\omega\,;\hat{e}_l\rangle = \lim_\Lambda\frac{1}{|\Lambda|}\langle\omega\,;\sum_{k\in\Lambda}\hat{e}_k\rangle$ *for an arbitrary* $l\in\mathcal{R}$ *if* $m(\omega)$ *is a subgradient of* $f(\beta,\varepsilon)$ *at* ε.

Observe that the gradient of a tangent state fulfills

$$\langle\varepsilon'\,;m(\omega)\rangle \geq [f(\beta,\varepsilon+\lambda\varepsilon') - f(\beta,\varepsilon)]/\lambda$$

and

$$\langle\varepsilon'\,;m(\omega)\rangle \leq [f(\beta,\varepsilon-\lambda\varepsilon') - f(\beta,\varepsilon)]/(-\lambda)$$

for all $\lambda>0$. Consequently, $\langle\varepsilon'\,;m(\omega)\rangle$ has the unique value $\langle\varepsilon'\,;\nabla_\varepsilon f(\beta,\varepsilon)\rangle$, if the latter exists.

Proposition 4.11

If $\omega\in\mathcal{S}(\beta,\varepsilon)$*, then* ω *is a tangent state on* $f(\beta,\varepsilon)$ *at* ε.

PROOF: From the minimal principle at $\varepsilon+\varepsilon'$ we obtain for $\omega\in\mathcal{S}\,(\beta,\varepsilon)$ and all $\varepsilon'\in\mathbb{R}^{n_{\mathcal{B}}}$

$$f(\beta,\varepsilon+\varepsilon') \leq f(\beta,\varepsilon+\varepsilon',\omega) = \langle\varepsilon'\,;m(\omega)\rangle + f(\beta,\varepsilon).$$

Here $f(\beta,\varepsilon+\varepsilon',\omega)$ is the free energy density from Def. 3.1 (iii) of the model with local Hamiltonians $H_\Lambda(\varepsilon+\varepsilon')$ in the state ω.

Thus if $\mathcal{S}(\beta, \varepsilon)$ contains more than one state, the free energy is not differentiable at ε. A special situation may be described in terms of limiting Gibbs states.

Corollary 4.12

If there are more than one limiting Gibbs states or there is a non–factorial limiting Gibbs state of the model with local Hamiltonians $H_\Lambda(\varepsilon)$, $\Lambda \in \mathcal{L}$, then $f(\beta, \varepsilon)$ is not differentiable at ε.

PROOF: Since all limiting Gibbs states together with their components of the central decomposition are in $\mathcal{S}(\beta, \varepsilon)$, both assumptions of the corollary lead to more than one element in $\mathcal{S}(\beta, \varepsilon)$.

We see, that the free energy function $f(\beta, \cdot) : \mathrm{IR}^{n_{\mathcal{B}}} \longrightarrow \mathrm{IR}$ contains the complete information on all possible m–values, which may arise in thermodynamic equilibrium at the temperature β, since they appear as (generalized) gradients. For the discrimination between pure phase and mixed phase m–values one needs however the function $\sigma(\beta, \cdot) : M \longrightarrow \mathrm{IR}$. One is reminded on the *primitive surface* (here given by $\sigma(\beta, m)$) and the *derived or ruled surface* (here given by $\hat{\sigma}(\beta, m)$) of the geometric thermodynamics of Gibbs [46, 47]. Observe, however, that the correct thermodynamic potentials $f(\beta, \cdot) : \mathrm{IR}^{n_{\mathcal{B}}} \longrightarrow \mathrm{IR}$ and $s : M \longrightarrow \mathrm{IR}$ have no unstable parts! Instead of $\sigma(\beta, \cdot)$ we could have used, of course, the combination

$$f(\beta, \varepsilon, m) = \langle \varepsilon \, ; m \rangle - \sigma(\beta, m), \qquad m \in M.$$

This non–equilibrium free energy contains also the complete thermodynamic information.

Finally let us mention, that the operator–algebraic pure phase concept as extremal states in $\mathcal{S}(\beta, \varepsilon)$ is completely confirmed by the foregoing discussion of the thermodynamic functions in the sense, that it leads to a commonly accepted point of view in phenomenological thermodynamics.

4.3. Variation of H*–Symmetric Field Parameters*

Corollary 4.12 tells us that the function $f(\beta, \cdot) : \mathrm{IR}^{n_{\mathcal{B}}} \longrightarrow \mathrm{IR}$ is not differentiable if and only if there is more than one pure phase state with minimal free energy density. This is the situation for low temperatures in the case where a phase transition has taken place. For later applications we choose here ε such that $H_\Lambda(\varepsilon)$ is always H–symmetric and we expect that the minimal free energy remains differentiable in this subspace also if a second order phase transition takes place. Moreover, we determine the concave conjugate of $f(\beta, \varepsilon)$, restricted to the subspace of H–symmetric fields.

In Definition 2.5 and Remark 2.6 we have introduced the internal symmetries H on $\mathcal{B}$ and $\mathcal{A}$. Now we consider the action of H on the parametrization M of $\mathcal{S}(\mathcal{B})$: Let be $v_i(\varphi)$ the i–th component of $v(\varphi)$ for some $\varphi \in \mathcal{S}(\mathcal{B})$. Then we find for arbitrary $u \in \mathrm{H}$

$$\begin{aligned} v_i(\mathrm{Ad}^*_u \varphi) &= \big\langle \mathrm{Ad}^*_u \varphi \, ; \hat{e}^i \big\rangle = \big\langle \varphi \, ; \mathrm{Ad}_{u^*} \hat{e}^i \big\rangle \\ &= \sum_{k=1}^{n_{\mathcal{B}}} m_{ki}(u^*) v_k(\varphi) = \big(M(u^{-1})^T v(\varphi) \big)_i , \end{aligned} \tag{4.23}$$

and $M(u^{(-1)})^T m \in M$ for all $m \in M$ and $u \in \mathrm{H}$.

Now consider the free energy density $f(\beta, \varepsilon, m)$ for a H–invariant interaction w and H–invariant fields ε, i.e. we have $w \circ M(u)^T = w$ and $M(u)\varepsilon = \varepsilon$ for all $u \in \mathrm{H}$. Obviously, the set $E(\mathrm{H})$ of H–invariant fields $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ is a linear subspace of $\mathrm{IR}^{n_{\mathcal{B}}}$. We find

$$\begin{aligned} & f(\beta, \varepsilon, M(u)^T m) \\ &= \big\langle M(u)^T m \, ; \varepsilon \big\rangle + w(M(u)^T m) - \frac{1}{\beta} s(M(u)^T m) \\ &= f(\beta, \varepsilon, m). \end{aligned} \tag{4.24}$$

Thus $m \longrightarrow f(\beta, \varepsilon, m)$ is invariant under the transformations $M(u)^T$ for all $u \in \mathrm{H}$ and $m \in M$.

Proposition 4.13

Let H *be the group of internal symmetries with action on $\mathcal{B}$ according to (2.5). Then we define the symmetrization operator $\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u)$ on $\mathrm{IR}^{n_{\mathcal{B}}}$ by*

$$\Big\langle m \, ; \int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u) \, \varepsilon \Big\rangle := \int_{\mathrm{H}} \langle m \, ; M(u)\varepsilon \rangle \; \mathrm{d}\mu_{\mathrm{H}}(u), \qquad \forall m, \varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}.$$

It satisfies

$$\Big(\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u) \Big)^2 = \int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u)$$

and $E(\mathrm{H}) = \big[\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u) \big] \, \mathrm{IR}^{n_{\mathcal{B}}}$.

PROOF: Obviously, $\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u)$ is well defined. The properties of $\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u)$ follow by standard argumentation.

Remark 4.14

In general the H*–symmetrization $\int_{\mathrm{H}} M(u) \, \mathrm{d}\mu_{\mathrm{H}}(u)$ is not selfadjoint. Nevertheless, one can choose a* *basis $\hat{e}'$ of $\mathcal{B}$ such that the symmetrization becomes an orthogonal projection in this representation. Thus we assume that the basis $\hat{e}$ is chosen such that $\int_{\mathsf{H}} M(u)\,\mathrm{d}\mu_{\mathsf{H}}(u)$ becomes selfadjoint and constitutes the orthogonal projection*

$$P_{\mathsf{H}} := \int_{\mathsf{H}} M(u)\,\mathrm{d}\mu_{\mathsf{H}}(u). \tag{4.25}$$

We denote the restriction of $f(\beta,\cdot) : \mathrm{I\!R}^{n_{\mathcal{B}}} \longrightarrow \mathrm{I\!R}$ to $E(\mathsf{H})$ by $f_{\mathsf{H}}(\beta,\cdot)$. In Proposition 4.5 we have determined the concave conjugate of the minimal free energy density on $\mathrm{I\!R}^{n_{\mathcal{B}}}$. Here we repeat this calculation on $E(\mathsf{H})$ and define for all m in $\mathrm{I\!R}^{n_{\mathcal{B}}}$

$$\hat{\sigma}^0_{\mathsf{H}}(\beta,\cdot) : \mathrm{I\!R}^{n_{\mathcal{B}}} \longrightarrow \mathrm{I\!R} \cup -\infty, \tag{4.26}$$

$$m \rightarrow \hat{\sigma}^0_{\mathsf{H}}(\beta,m) := \inf\{\langle m\,;\varepsilon\rangle - f_{\mathsf{H}}(\beta,\varepsilon) \,|\, \varepsilon \in E(\mathsf{H})\},$$

$$\hat{\sigma}_{\mathsf{H}}(\beta,\cdot) : E(\mathsf{H}) \longrightarrow \mathrm{I\!R} \cup -\infty, \tag{4.27}$$

$$m \rightarrow \hat{\sigma}_{\mathsf{H}}(\beta,m) := \inf\{\langle m\,;\varepsilon\rangle - f_{\mathsf{H}}(\beta,\varepsilon) \,|\, \varepsilon \in E(\mathsf{H})\}.$$

It holds

$$\begin{aligned}
&\hat{\sigma}^0_{\mathsf{H}}(\beta, M(u)^T m) \\
&\quad = \inf\{\langle M(u)^T m\,;\varepsilon\rangle - f_{\mathsf{H}}(\beta,\varepsilon) \mid \varepsilon \in E(\mathsf{H})\} \\
&\quad = \hat{\sigma}^0_{\mathsf{H}}(\beta,m),
\end{aligned}$$

i.e. $\hat{\sigma}^0_{\mathsf{H}}(\beta,m)$ is invariant under the transformations which arise from H. In the next steps we clarify the relation between $\hat{\sigma}^0_{\mathsf{H}}(\beta,m)$ and $\hat{\sigma}(\beta,m)$.

Lemma 4.15

Let be $\beta > 0$ and $\varepsilon \in E(\mathsf{H})$. Then we have for all $\varepsilon^{\perp} \in E(\mathsf{H})^{\perp}$

$$f(\beta,\varepsilon+\varepsilon^{\perp}) \leq f(\beta,\varepsilon) = f_{\mathsf{H}}(\beta,\varepsilon). \tag{4.28}$$

PROOF: For all $u \in \mathsf{H}$ we have $f(\beta,\varepsilon) = f(\beta, M(u)\varepsilon)$ and

$$\begin{aligned}
f(\beta,\varepsilon+\varepsilon^{\perp}) &= \inf\{\langle M(u)^T m\,;\varepsilon+\varepsilon^{\perp}\rangle \\
&\qquad + w(M(u)^T m) - \frac{1}{\beta}s(M(u)^T m) \mid m \in M\} \\
&= f(\beta,\varepsilon + M(u)\varepsilon^{\perp}).
\end{aligned}$$

Assume, that there is a $\varepsilon^{\perp} \in E(\mathsf{H})^{\perp}$ with $f(\beta,\varepsilon+\varepsilon^{\perp}) > f(\beta,\varepsilon)$. Due to $P_{\mathsf{H}}\varepsilon^{\perp} = 0$ it holds

$$\begin{aligned}
f(\beta,\varepsilon) &= f(\beta, P_{\mathsf{H}}(\varepsilon+\varepsilon^{\perp})) \\
&\geq \int_{\mathsf{H}} f(\beta, M(u)(\varepsilon+\varepsilon^{\perp}))d\mu_{\mathsf{H}}(u) \\
&= f(\beta,\varepsilon+\varepsilon^{\perp}) > f(\beta,\varepsilon),
\end{aligned}$$

which is not possible.

In Proposition 4.17 we prove a corresponding result for $\hat{\sigma}(\beta,m)$.

Lemma 4.16

Let be $\beta > 0$. It holds

(i) $\hat{\sigma}^0_{\mathsf{H}}(\beta,m) = \mathrm{cl}\left(\sup\{\hat{\sigma}(\beta,m-m^{\perp}) \mid m^{\perp} \in E(\mathsf{H})^{\perp}\}\right)$ for all $m \in \mathrm{I\!R}^{n_{\mathcal{B}}}$,

(ii) $\hat{\sigma}_{\mathsf{H}}(\beta,m) = \hat{\sigma}^0_{\mathsf{H}}(\beta,m) = \hat{\sigma}(\beta,m)$ for all $m \in E(\mathsf{H})$.

PROOF: (i) $\hat{\sigma}^0_{\mathsf{H}}(\beta,m) = \inf\{\langle m\,;\varepsilon\rangle - f_{\mathsf{H}}(\beta,\varepsilon) \mid \varepsilon \in E(\mathsf{H})\}$ writes with the indicator function $\delta_W(x) := \begin{cases} 0 & x \in W \\ \infty & x \notin W \end{cases}$ for an arbitrary subset W of $\mathrm{I\!R}^{n_{\mathcal{B}}}$ as

$$\begin{aligned}
\hat{\sigma}^0_{\mathsf{H}}(\beta,m) &= \inf\{\langle m\,;\varepsilon\rangle - f(\beta,\varepsilon) + \delta_{E(\mathsf{H})}(\varepsilon) \,|\, \varepsilon \in \mathrm{I\!R}^{n_{\mathcal{B}}}\} \\
&= \left[f(\beta,\cdot) - \delta_{E(\mathsf{H})}\right]^{*}(m).
\end{aligned}$$

$f(\beta,\cdot) = [\hat{\sigma}(\beta,\cdot)]^{*}$ is a closed proper concave function. Since $E(\mathsf{H})$ is a linear subspace of $\mathrm{I\!R}^{n_{\mathcal{B}}}$, $-\delta_{E(\mathsf{H})}$ is also closed and proper concave. Then we find with [20, Theorem 16.4]:

$$\begin{aligned}
\hat{\sigma}^0_{\mathsf{H}}(\beta,m) &= \mathrm{cl}\left([f(\beta,\cdot)]^{*} \Box [-\delta_{E(\mathsf{H})}]^{*}\right)(m) \\
&= \mathrm{cl}\left(\hat{\sigma}(\beta,\cdot) \Box [-\delta_{E(\mathsf{H})}]^{*}\right)(m),
\end{aligned} \tag{4.29}$$

where $\Box$ denotes the infimal convolution. The conjugation of $-\delta_{E(\mathsf{H})}$ is given by $[-\delta_{E(\mathsf{H})}]^{*}(m) = -\delta_{E(\mathsf{H})^{\perp}}(m)$ and we find with (4.29)

$$\hat{\sigma}^0_{\mathsf{H}}(\beta,m) = \mathrm{cl}\left(\sup\{\hat{\sigma}(\beta,m-m^{\perp}) \,|\, m^{\perp} \in E(\mathsf{H})^{\perp}\}\right).$$

(ii) Let be $m \in E(\mathsf{H})$. With Lemma 4.15 we calculate $\hat{\sigma}(\beta,m)$:

$$\begin{aligned}
\hat{\sigma}(\beta,m) &\geq \inf\{\langle P_{\mathsf{H}} m\,;\varepsilon+\varepsilon^{\perp}\rangle - f(\beta,\varepsilon) \mid \\
&\qquad\qquad \varepsilon \in E(\mathsf{H}),\ \varepsilon^{\perp} \in E(\mathsf{H})^{\perp}\} \\
&= \inf\{\langle m\,;\varepsilon\rangle - f_{\mathsf{H}}(\beta,\varepsilon) \mid \varepsilon \in E(\mathsf{H})\} = \hat{\sigma}_{\mathsf{H}}(\beta,m).
\end{aligned}$$

Due to its definition we have $\hat{\sigma}(\beta,m) \leq \hat{\sigma}_{\mathsf{H}}(\beta,m)$ and thus equality holds for all $m \in E(\mathsf{H})$.

Lemma 4.17

For all $\beta > 0$ *it holds*
(i) $\hat{\sigma}_{\mathsf{H}}(\beta, m) = [f_{\mathsf{H}}(\beta, \cdot)]^*(m)$ *for all* $m \in E(\mathsf{H})$,
(ii) $f_{\mathsf{H}}(\beta, \varepsilon) = [\hat{\sigma}_{\mathsf{H}}(\beta, \cdot)]^*(\varepsilon)$ *for all* $\varepsilon \in E(\mathsf{H})$.

Moreover, for all $m \in E(\mathsf{H})$ *and* $m^{\perp} \in E(\mathsf{H})^{\perp}$ *it is* $\hat{\sigma}(\beta, m + m^{\perp}) \leq \hat{\sigma}(\beta, m)$.

PROOF: (i) is valid according to the Definition of $\hat{\sigma}_{\mathsf{H}}(\beta, m)$ in (4.26), and (ii) follows from $f_{\mathsf{H}}(\beta, \cdot) = [f_{\mathsf{H}}(\beta, \cdot)]^{**}$ which holds since $f_{\mathsf{H}}(\beta, \varepsilon)$ is finite on $E(\mathsf{H})$ [20, Corollary 7.4.2]. The inequality follows from Lemma 4.16, because for all $m \in E(\mathsf{H})$ it is

$$
\begin{aligned}
\hat{\sigma}(\beta, m) &= \hat{\sigma}_{\mathsf{H}}(\beta, m) \\
&= \mathrm{cl}\left(\sup\{\hat{\sigma}(\beta, m + m^{\perp}) \mid m^{\perp} \in E(\mathsf{H})^{\perp}\}\right) \\
&\geq \sup\{\hat{\sigma}(\beta, m + m^{\perp}) \mid m^{\perp} \in E(\mathsf{H})^{\perp}\} \\
&\geq \hat{\sigma}(\beta, m + m^{\perp}), \quad \forall m^{\perp} \in E(\mathsf{H})^{\perp}.
\end{aligned}
$$

Let us emphasize that the concave conjugate functions $\hat{\sigma}_{\mathsf{H}}(\beta, m)$ and $f_{\mathsf{H}}(\beta, \varepsilon)$ on $E(\mathsf{H})$ are restrictions of the concave conjugate functions $\hat{\sigma}(\beta, m)$ and $f(\beta, \varepsilon)$ on $\mathbb{R}^{n_{\mathcal{B}}}$. Especially, the full information on $\hat{\sigma}(\beta, \cdot)|_{E(\mathsf{H})}$ may be obtained by experimental data from $f(\beta, \cdot)|_{E(\mathsf{H})}$. Consequently, the subgradient set of $f_{\mathsf{H}}(\beta, \varepsilon)$ still contains information on the pure phase equilibrium states of the system:

Lemma 4.18

Let be $\beta > 0$ *and* $f_{\mathsf{H}}(\beta, \varepsilon)$, P_{H} *as above. For all* $\varepsilon \in E(\mathsf{H})$ *it holds*

$$P_{\mathsf{H}} \partial f(\beta, \varepsilon) = \partial f_{\mathsf{H}}(\beta, \varepsilon).$$

Especially, it holds $P_{\mathsf{H}} \mathrm{conv} M(\beta, \varepsilon) = \partial f_{\mathsf{H}}(\beta, \varepsilon)$.

PROOF: Let be $\varepsilon \in E(\mathsf{H})$ and $m \in \partial f(\beta, \varepsilon)$. Then we have for all $\varepsilon' \in E(\mathsf{H})$

$$
\begin{aligned}
f_{\mathsf{H}}(\beta, \varepsilon + \varepsilon') = f(\beta, \varepsilon + \varepsilon') &\leq \langle m \,; \varepsilon' \rangle + f(\beta, \varepsilon) \\
&= \langle P_{\mathsf{H}} m \,; \varepsilon' \rangle + f_{\mathsf{H}}(\beta, \varepsilon),
\end{aligned}
$$

i.e. $P_{\mathsf{H}} m \in \partial f_{\mathsf{H}}(\beta, \varepsilon)$. The other way round, let be $m \in \partial f_{\mathsf{H}}(\beta, \varepsilon)$. With Lemma 4.15 it holds for arbitrary $\varepsilon' \in E(\mathsf{H})$ and $\varepsilon^{\perp} \in E(\mathsf{H})^{\perp}$

$$
\begin{aligned}
f(\beta, \varepsilon + \varepsilon' + \varepsilon^{\perp}) \leq f(\beta, \varepsilon + \varepsilon') &\leq \langle m \,; \varepsilon' \rangle + f(\beta, \varepsilon) \\
&= \langle m \,; P_{\mathsf{H}}(\varepsilon' + \varepsilon^{\perp}) \rangle + f(\beta, \varepsilon) \\
&= \langle P_{\mathsf{H}} m \,; \varepsilon' + \varepsilon^{\perp} \rangle + f(\beta, \varepsilon) \\
&= \langle m \,; \varepsilon' + \varepsilon^{\perp} \rangle + f(\beta, \varepsilon).
\end{aligned}
$$

Thus $m \in \partial f(\beta, \varepsilon)$ and with $P_{\mathsf{H}} m = m$ we have $m \in P_{\mathsf{H}} \partial f(\beta, \varepsilon)$.

As a consequence of the variation of external field parameters with given symmetry we find differentiability properties of the minimal free energy density — even if there is more than one pure phase equilibrium state (comp. Corollary 4.12):

Corollary 4.19

Let be $\varepsilon \in E(\mathsf{H})$ *and* $\partial_e \mathcal{S}(\beta, \varepsilon) = \mathcal{O}_{\mathsf{H}}(\otimes\varphi)$ *for some* $\varphi \in \mathcal{S}_{\mathcal{B}}$. *Then the subgradient of the free energy* $f_{\mathsf{H}}(\beta, \varepsilon)$ *is a one point set*

$$\partial f_{\mathsf{H}}(\beta, \varepsilon) = \{P_{\mathsf{H}} v(\varphi)\}$$

and $f_{\mathsf{H}}(\beta, \varepsilon)$ *is differentiable in* ε.

PROOF: According to Prop. 3.8 there exists a $m \in M(\beta, \varepsilon)$ such that $M(\beta, \varepsilon) = \widetilde{\mathcal{O}}_{\mathsf{H}}(m)$. Now use Prop. 4.18, $P_{\mathsf{H}} \partial f(\beta, \varepsilon) = \partial f_{\mathsf{H}}(\beta, \varepsilon)$, and $\mathrm{conv} M(\beta, \varepsilon) = \mathrm{conv}\{M(u)^T m \mid u \in \mathsf{H}\}$. With Prop. 4.9 (i) and Prop. 4.18 it follows $\partial f_{\mathsf{H}}(\beta, \varepsilon) = P_{\mathsf{H}} \mathrm{conv}\{M(u)^T m \mid u \in \mathsf{H}\}$. We find $P_{\mathsf{H}} M(u)^T m = P_{\mathsf{H}} m$ for all $u \in \mathsf{H}$, and consequently it is

$$
\begin{aligned}
\partial f_{\mathsf{H}}(\beta, \varepsilon) &= P_{\mathsf{H}} \mathrm{conv}\{M(u)^T m \mid u \in \mathsf{H}\} \\
&= \mathrm{conv}\{P_{\mathsf{H}} m\} = \{P_{\mathsf{H}} m\} = \{P_{\mathsf{H}} v(\varphi)\}.
\end{aligned}
$$

A consequence of Corollary 4.19 is the specification of the directions where $f(\beta, \varepsilon)$ may be not differentiable. In the above case where we have one orbit of pure phase states with minimal free energy density, the restriction $E(\mathsf{H}) \ni \varepsilon \to f_{\mathsf{H}}(\beta, \varepsilon) = f(\beta, \varepsilon)$ is still differentiable. Thus the non–differentiability according to Corollary 4.12 is related to the variation of fields such that the internal symmetry H of the local Hamiltonians $H_{\Lambda}(\varepsilon)$ is lost and the orbital–structure of $M(\beta, \varepsilon)$ destroyed. Further conclusions from this property will be discussed in the next section, where the relation to phase transitions is elaborated.

5. Phase Transitions

We propose here a definition of phase transitions, which seems to be appropriate at least for the discussion of our considered class of models. The general idea is that a phase transition occurs, if the equilibrium properties of a thermodynamic system undergo a "qualitative change". The equilibrium properties are here given by the sets $\mathcal{S}(\beta, \varepsilon)$ in dependence on the parameters (β, ε). The structure of these sets may even be better characterized by their extreme boundaries $\partial_e \mathcal{S}(\beta, \varepsilon)$, the sets of all statistical pure phase states. Two such sets are certainly qualitatively different, if the number of connected components and/or the dimensions of the connected components are different. For quantum lattice models a qualitative change is usually made manifest by a change of the (internal) symmetry group of the pure phase states, that is the set of all symmetry transformations, under which the pure phase state is invariant. This may be accompanied by the change of the topological invariants, but must not necessarily be so. In our frame all features can be seen as well in terms of the parameter sets $M(\beta, \varepsilon)$ for the pure phase states. Usually the symmetry group decreases with decreasing absolute temperature and the degree of order increases correspondingly.

Definition 5.1

For a given quantum lattice model we say that two pure phase states are of the same type, *if they have the same symmetry group. A* phase transition *is then a continuous curve of the form*

$$\gamma = \{(\beta(t), \varepsilon(t)) \mid t \in I_\gamma \subset \mathrm{IR}\} \subset E,$$

on which a qualitative change of the sets $M(\beta, \varepsilon)$ (pure phase equilibrium values of the density observables) occurs, that is, the topological invariants and/or the type of the pure phases undergo a change. A point $\gamma(t_0) = (\beta_0, \varepsilon_0)$, which has both kinds of equilibrium sets in every neighbourhood, is called transition point.

In contradistinction to Ehrenfest's notion of the *order* of a phase transition, which may assume in principle arbitrary natural numbers as values (and to which we return at the end of our discussion) many authors have introduced a division of all phase transitions into two *kinds* (cf., e.g., [36, 48 - 50], and also Wightman in the Introduction of [6]). The basic idea is that some relevant quantity may behave discontinuously or continuously at the transition point. We shall try to reformulate this in terms of our pure phase sets $M(\beta, \varepsilon)$. For this we introduce

Definition 5.2

$\gamma(t_0) = (\beta_0, \varepsilon_0)$ is called a continuity point of the curve γ in Def. 5.1, if for all $\varepsilon > 0$ there exists a $\delta > 0$ such that for all $t \in I_\gamma$ with $|t_0 - t| < \delta$ the sets $M(\gamma(t))$ are contained in the ε–neighbourhood of $M(\gamma(t_0))$ and $M(\gamma(t_0))$ is in the ε–neighbourhoods of $M(\gamma(t))$. Otherwise (β_0, ε_0) is called a discontinuity point of γ. (An ε–neighbourhood of $M(\gamma(t))$ is here the union of all ε–neighbourhoods of the points in $M(\gamma(t))$.)

Definition 5.3

A phase transition γ is called to be of first or second kind *if the transition point is not or is a continuity point. The transition points of phase transitions of the second kind are called* critical points. *An equilibrium state is called a* coexistence state *if it is a mixture of phases with varying types (in contradistinction to a mixture of pure phase states of the same type, which only signifies statistically the non–accurateness of the preparation method).*

An other alternative of the definition of a transition of the first kind which emphasizes the role of the latent heat would be the following one: A phase transition γ is called to be of the first kind if the set function

$$t \longrightarrow \{s \in \mathrm{IR} \mid \exists m \in M(\gamma(t)) \text{ with } s = s(m)\} =: s(M(\gamma(t)))$$

is discontinuous at the transition point $\gamma(t_0)$. Since $s(m)$ is a continuous function on M (see before Def. 4.7) the set function $t \longrightarrow M(\gamma(t))$ must be discontinuous in this case and implies a transition of the first kind according to Definition 5.3. The other way round this alternative definition would not be the logical complement of a second kind transition according to Definition 5.3. Nevertheless, in applications the discontinuous change of $M(\gamma(t))$ at t_0 in general implies a discontinuous behaviour of $s(M(\gamma(t)))$. Thus we work in the following with Definition 5.3 for the kind of a transition.

We start with a necessary condition for the possibility of a phase transition. Intuitively one expects that the interaction w has to be attractive in order to create a non–trivial equilibrium phase structure. This is expressed in terms of convexity properties of w:

Proposition 5.4

If for a given system Σ the interaction w is a convex continuously differentiable function on M, then $M(\beta, \varepsilon)$ contains only one point for all $(\beta, \varepsilon) \in E$, $f(\beta, \varepsilon)$ is differentiable in ε at all $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ and the system does not exhibit a phase transition. For every $(\beta, \varepsilon) \in E$ the system has a unique limiting Gibbs state.

PROOF: Since $m \longrightarrow s(m)$ is strictly concave, $m \longrightarrow w(m)$ is convex, and $m \longrightarrow \langle \varepsilon\,; m\rangle$ is affine, it follows that

$$f(\beta, \varepsilon, m) = \langle \varepsilon\,; m\rangle + w(m) - \frac{1}{\beta}\, s(m)$$

is strictly convex. A strictly convex function on the compact convex set M has a unique minimal point $m(\beta, \varepsilon)$ [20], i.e. $M(\beta, \varepsilon) = \{m(\beta, \varepsilon)\}$. Due to Prop. 4.9 (i) the subgradient $\partial f(\beta, \varepsilon)$ consists of exactly one point for all $\varepsilon \in \mathrm{IR}^{n_{\mathcal{B}}}$ and $\varepsilon \to f(\beta, \varepsilon)$ is differentiable. If $M(\beta, \varepsilon) = \{m(\beta, \varepsilon)\}$, we have $\mathcal{S}(\beta, \varepsilon) = \{\otimes v^{-1} m(\beta, \varepsilon)\} = \partial_e \mathcal{S}(\beta, \varepsilon)$ and all limiting Gibbs states are unique. Of course, the singleton sets $M(\beta, \varepsilon)$ do not change qualitatively for each $(\beta, \varepsilon) \in E$, and no phase transition according to Definition 5.1 is possible.

At any transition point, the "size" of the sets $M(\gamma(t))$ changes. Usually, the amount of pure phase equilibrium states increases with decreasing temperature, i.e. for $\beta > \beta_0$; but there are interesting examples for the reverse case [51]. In general one finds:

Proposition 5.5

Let w be a continuous interaction and γ a continuous curve. For all $t \in I_\gamma$ and $t' \to t$ it holds

$$\lim_{t' \nearrow t} M(\gamma(t')) \subseteq M(\gamma(t)) \supseteq \lim_{t' \searrow t} M(\gamma(t')).$$

PROOF: $M(\beta, \varepsilon)$ is defined as $M(\beta, \varepsilon) = \{m \in M \mid f(\beta, \varepsilon, m) = f(\beta, \varepsilon)\}$ and $(\beta, \varepsilon) \to f(\beta, \varepsilon, m)$ is continuous on E. Since γ is continuous, it follows that $t' \to \inf\{f(\beta(t'), \varepsilon(t'), m) \mid m \in M\}$ is continuous. Thus the inclusion relations follow.

Corollary 5.6

Let w be a continuous interaction. At the transition point $\gamma(t_0) = (\beta_0, \varepsilon_0)$ of a phase transition of the first kind γ, the number of orbits in $M(\gamma(t))$ is increased at least by one orbit of H *for $t \nearrow t_0$ or $t \searrow t_0$.*

PROOF: Since $\gamma(t_0) = (\beta_0, \varepsilon_0)$ is the transition point of a phase transition of the first kind, we have with Definition 5.3:

$$\lim_{t \nearrow t_0} M(\gamma(t)) \neq M(\gamma(t_0)) \text{ or}$$

$$\lim_{t \searrow t_0} M(\gamma(t)) \neq M(\gamma(t_0)).$$

Thus at least one of the inclusions in Prop. 5.5 is proper, and at least one orbit is added.

Next we have a look on the differentiability of the free energy density $f_{\mathsf{H}}(\beta, \varepsilon)$ as introduced in Section 4.3.

Proposition 5.7

(i) Let be $f_{\mathsf{H}}(\beta_0, \cdot)$ not differentiable in $\varepsilon_0 \in E(\mathsf{H})$ and differentiable in a neighbourhood $I \backslash \{\varepsilon_0\}$. If $\gamma(t) = (\beta_0, \varepsilon(t))$ is a continuous curve (with constant inverse temperature $\beta(t) \equiv \beta_0$) through (β_0, ε_0), then there is a phase transition of the first kind at (β_0, ε_0) in the sense of Definition 5.1 and 5.3.

(ii) Let be $\gamma(t) = (\beta_0, \varepsilon(t))$ a phase transition of the second kind (at constant inverse temperature $\beta(t) \equiv \beta_0$) with critical point $\gamma(t_0) = (\beta_0, \varepsilon_0)$. If $M(\gamma(t))$ consists for all $t < t_0$ of one H*–orbit, then $\varepsilon \to f_{\mathsf{H}}(\beta_0, \varepsilon)$ is differentiable at ε_0.*

PROOF: (i) We have with Corollary 4.19: $\partial f_{\mathsf{H}}(\beta, \varepsilon) = \{P_{\mathsf{H}} \mathrm{conv} M(\beta, \varepsilon)\}$. Since $E(\mathsf{H}) \ni \varepsilon \to f_{\mathsf{H}}(\beta_0, \varepsilon)$ is differentiable in $I \backslash \{\varepsilon_0\}$, $\partial f_{\mathsf{H}}(\beta, \varepsilon)$ changes discontinuously at ε_0 and the number of H–Orbits in $M(\beta, \varepsilon)$ increases discontinuously at (β_0, ε_0).

(ii) Since $M(\gamma(t))$ consists of one H–orbit for all $t < t_0$, $P_{\mathsf{H}} \mathrm{conv} M(\gamma(t))$ is a singleton and $f_{\mathsf{H}}(\beta_0, \varepsilon)$ is differentiable for all $\varepsilon(t)$, $t < t_0$. Now $\gamma(t_0)$ is the critical point of a phase transition of the second kind and thus $P_{\mathsf{H}} \mathrm{conv} M(\gamma(t_0)) = \partial f_{\mathsf{H}}(\beta_0, \varepsilon_0)$ is also a singleton, i.e. $\varepsilon \to f_{\mathsf{H}}(\beta_0, \varepsilon)$ is even differentiable at ε_0.

Let us end our investigation with an incorporation of certain ideas of the Landau theory into our scheme. As is well known, Landau [52] based his analysis of structural phase transitions on an expansion of a certain thermodynamic potential $\Phi(\beta, \eta)$ into powers of the so–called *order parameter* η. (We restrict our discussion to the simple case of a scalar order parameter as it is presented in [48]. For a review of more complicated applications cf., e.g., [53].) First we have to clarify, which potential in our treatment would correspond to that of Landau. It must be a potential in which the temperature β and the external field variables ε are fixed, but which nevertheless depends on some non–equilibrium features, which Landau compressed into the notion of an order parameter.

In Def. 3.6 we introduced a mean–field free energy $\widetilde{f}(\beta, m)$, which also depends (via $y(m)$) on ε and varies in our applications over $m \in L(\beta) \subset \mathrm{IR}^{n_{\mathcal{B}}}$, the set of self–consistency values. It is very important to note, that firstly, we have already added a correction term with respect to the *strict* mean–field free energy $-\frac{1}{\beta} Z_\beta(y(m))$ (where the partition function is evaluated with the mean–field Hamiltonian), and that secondly any extension of the domain of definition beyond $L(\beta)$ is no longer in coincidence with the microscopic theory. In our opinion the free energy $f(\beta, \varepsilon, m)$, which we introduced in Def. 3.1 (see also (3.3)) and used in Sect. 4.2 gives the correct free energy value for any pure phase non–equilibrium state with density observables $m \in M \subset \mathbb{R}^{n_{\mathcal{B}}}$, and may be restricted to Landau's potential Φ. In the case of a one–dimensional order parameter one then varies m along a one–parametric curve $\kappa := \{m(\eta) \in M \mid \eta \in \mathbb{R}\}$, here chosen without loss in generality as a straight line in M–space. Since this analysis of phase transitions depends on the series expansion of $f(\beta, \varepsilon, m)$ in m we assume the interaction function w to be analytic.

Proposition 5.8

Let w be an analytic interaction, and $\kappa(\eta) = m^0 + \eta m'$ with $m^0 \in M^\circ$, $m' \in \mathbb{R}^{n_{\mathcal{B}}}$, and $\eta \in I_\kappa \subset \mathbb{R}$ such that $\kappa(\eta) \in M^\circ$. Then the non–equilibrium free energy along κ has an asymptotic expansion in positive integer powers of the curve parameter η at $\eta = 0$ (we use the coefficient symbols of [48]):

$$\begin{aligned}\Phi(\beta, \varepsilon, \eta) &:= f(\beta, \varepsilon, \kappa(\eta)) \\ &\simeq f(\beta, \varepsilon, \kappa(0)) + \alpha\eta + A\eta^2 + B\eta^3 + C\eta^4 + \cdots\end{aligned}$$

where

$$\alpha = \alpha(\beta, \varepsilon) = \sum_{i=1}^{n_{\mathcal{B}}} (\varepsilon - \nabla\sigma(\beta, m^0))_i m'_i,$$

$$A = A(\beta) = \frac{1}{2} \sum_{i,j=1}^{n_{\mathcal{B}}} \frac{\partial^2 \sigma(\beta, m^0)}{\partial m_i \partial m_j} m'_i m'_j,$$

$$B = B(\beta) = \frac{1}{6} \sum_{i,j,k=1}^{n_{\mathcal{B}}} \frac{\partial^3 \sigma(\beta, m^0)}{\partial m_i \partial m_j \partial m_k} m'_i m'_j m'_k,$$

$$C = C(\beta) = \frac{1}{24} \sum_{i,j,k,l=1}^{n_{\mathcal{B}}} \frac{\partial^4 \sigma(\beta, m^0)}{\partial m_i \partial m_j \partial m_k \partial m_l} m'_i m'_j m'_k m'_l.$$

PROOF: The assertion follows from the fact, that the internal energy and the entropy are infinitely differentiable functions on M° and by differentiation of $f(\beta, \varepsilon, m)$ along κ.

In the frequently used case of a quadratic interaction as in (2.3) the derivatives in the coefficients B and C reduce to the differentials of the pure phase state entropy density $s(m)$ from (4.21).

The main point of the Landau theory is to combine the asymptotic expansion of $\eta \to \Phi(\beta, \varepsilon, \eta)$ with symmetry arguments [54, Chapt. VII, Second Order Phase Transitions, 64] in order to get an analytic treatment of phase transitions of the second kind. For this one specifies a curve $\mathbb{R} \supset I_\gamma \ni t \to \gamma(t) = (\beta(t), \varepsilon(t)) \in E$ on which the critical point $\gamma(t_c)$ should be situated. For each $t \in I_\gamma$ one selects a curve $\mathbb{R} \supset I_\kappa \ni \eta \to \kappa^t(\eta) = m^0(t) + \eta m' \in M^\circ$ in the space of non–equilibrium density variables, such that for $\eta = 0$ one has an equilibrium value $m^0(t)$ with minimal free energy for $t \le t_c$. For $t > t_c$ $m^0(t)$ is changed into a local maximal (or saddle) point of the free energy. Usually rather restricted assumptions are formulated to obtain this scenario:

(i) $\alpha(\gamma(t)) = 0$ for all $t \in I_\gamma$,

(ii) $A(\beta(t)) > 0$ for $t < t_c$, and $A(\beta(t)) < 0$ for $t > t_c$ (implying $A(\beta(t_c)) = 0$),

(iii) $B(\beta(t_c)) = 0$ and $C(\beta(t_c)) > 0$.

For the treatments of special models these assumptions have proven to be very useful. From the classificatory point of view they are at the one hand too restricted and on the other hand not strong enough. We propose the following modification, making use of our above developed conceptual frame and appealing to the internal symmetry group H:

Observation 5.9 (Generalized Landau Scenario)

Using the notions of Proposition 5.8 and the subsequent discussion we postulate

(i) $I_\gamma \ni t \to m^0(t)$ is a continuous curve in M°,

(ii) for all $t \in I_\gamma$ $\eta = 0$ is a stationary point of $\eta \to \Phi(\gamma(t), \eta)$,

(iii) $\{\kappa^t(0)\} = M(\gamma(t))$ ($\equiv$ set of equilibrium values) for $t \le t_c$,

(iv) $m^0(t) = M(u)^T m^0(t)$ for all $u \in \mathsf{H}$, $t \in I_\gamma$, and $m' \neq M(u')^T m'$ for a $u' \in \mathsf{H}$,

(v) for $t > t_c$ the absolute minimum of $\eta \to \Phi(\gamma(t), \eta)$ is obtained for $\eta(t) \neq 0$, and

$$M(\gamma(t)) = \left\{ M(u)^T \kappa^t(\eta(t)) \mid u \in \mathsf{H} \right\}. \qquad (5.1)$$

Then $\gamma(t_c)$ is a critical point (i.e. the transition point of a phase transition of the second kind along γ).

PROOF: For $t > t_c$ $M(u')^T \kappa(\eta(t)) \neq \kappa(\eta(t))$ and $M(\gamma(t))$ has more than one element in contrast to $M(\gamma(t'))$, for $t' \le t_c$, and $\gamma(t_c)$ is a transition point of a phase transition along γ.

Using Prop. 5.5 it follows from (iii) for small $t - t_c$ that $M(\gamma(t))$ consists of one H–orbit only. Since $\eta \longrightarrow \Phi(\gamma(t), \eta)$ and all its derivatives are continuous and depend continuously on $t \in I_\gamma$, the minimizing order parameter $t \longrightarrow \eta(t)$ is continuous with $\lim_{t \to t_c} \eta(t) = 0$. Then we have $\lim_{t \to t_c} \kappa^t(\eta(t)) = \lim_{t \to t_c} (m^0(t) + \eta(t) m') = m^0(t_c)$. Since $M(u)^T$ is bounded on $\mathbb{R}^{n_{\mathcal{B}}}$ and leaves $m^0(t)$ invariant, it follows as well $\lim_{t\to t_c} M(u)^T\kappa^t(\eta(t)) = \lim_{t\to t_c}(m^0(t) + \eta(t)M(u)^T m') = m^0(t_c)$. Thus $M(\gamma(t))$ is continuously deformed from a one point set into a non–trivial H–orbit while passing t_c.

The preceding Observation 5.9 may be extended straightforwardly to the case when there are n H–orbits in $M(\gamma(t))$ for $t > t_c$. Then we have to consider n curves $\eta \to \kappa_i^t(\eta) = m^0(t) + \eta m_i'$ with active directions m_i' for $i = 1,\ldots,n$, where we assume for $i \neq j$, that $m_i' \neq c\, M^T(u)m_j'$ for all $c \in \mathrm{IR}$ and $u \in \mathrm{H}$. Condition (iv) must be satisfied for all m_i', $i = 1,\ldots,n$, i.e. there is some $u' \in \mathrm{H}$ such that $m_i' \neq M(u')^T m_i'$. The absolute minima of the Landau potential along the curves κ_i^t are attained for $\eta_i(t) \neq 0$ for $t > t_c$ and

$$M(\gamma(t)) = \left\{M(u)^T\kappa_i^t(\eta_i(t)) \mid u \in \mathrm{H}, i = 1,\ldots,n\right\}. \tag{5.2}$$

Then $\gamma(t_c)$ is a critical point. This extension allows to include the possibility of higher order critical points (intersections of critical lines) into our formulation.

6. Remarks on Model Discussions

One can find the general structures presented in this paper in a number of rigorously treated models. Most of them have a quadratic interaction as in (2.1)–(2.3) or an asymptotic behaviour which leads to this form in the thermodynamic limit. One of the most popular examples is the BCS–model [55 - 57]. Very similar in their pure phase state structure are homogenizations of the Hubbard model [58, 59]. In the notation of Sect. 2 these are models with only one sublattice, i.e. $r = 1$. More general sublattice structures — leading to complex phase diagrams — can be found in spin lattice models (e.g. of an FCC–lattice with $r = 4$, Fig. 2.1 [23]) or lattice dependent symmetrizations of Hubbard models ($r = 2$) [24, 60], which are discussed in connection with models of bipolaronic interactions [61, 62], for high–T_c superconductors [63].

The latter models reveal in a rigorous reformulation a relationship to short range interactions and their systematic treatment in terms of a microscopic mean–field scaling. Besides phase transitions of the first kind they provide also examples for phase transitions of the second type and of multi–critical points (cf. the above cited BCS– or FCC–spin lattice models). They show that the type of the phase transition varies according to the chosen ensemble (multi–lattice mean–field Hubbard models, [24]). Moreover, one can prove that many thermodynamic properties remain robust under certain perturbations, even if they lead to disjoint equilibrium states of the perturbed and unperturbed system [57]. This explains peculiar features of weakly coupled macroscopic quantum systems.

In many applications one is interested in the full quantum statistical information of the macroscopic systems, especially in its local quantum fluctuations. Such aspects may be expressed in terms of the limiting Gibbs states and their associated equilibrium representations.

The results in Sect. 2.3 and give in many situations a scheme to determine the limiting Gibbs states. A problem arises at the transition point of a phase transition of the first kind, where the symmetry properties combined with the free energy minimalization are not sufficient, and all convex combinations of two H–symmetric states are candidates for the limiting Gibbs state [23]. This difficulty is circumvented by the help of additional conditions on the expectation value of the mean–field, which may fluctuate in the coexistence region of the phase transition. For example, if there is a coexistence region with varying particle densities $n \in [n_1, n_2]$, we fix the mean particle density on a certain value by means of the chemical potentials μ_Λ of the finite subsystems in Λ and then perform the thermodynamic limit (grand canonical ensemble). Due to the fixed particle density, the limiting Gibbs state may become unique [24] even in the coexistence region, where for one and the same chemical potential many converging subnets of local equilibrium states exist.

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