Equilibrium States and Phase Transitions of some FCC-Multi-Lattice Systems *

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The general formalism which connects quantum statistical and thermodynamical phase structures, developed previously, is applied here to a class of FCC-multi-lattice systems with four sublattices. A careful treatment of the symmetries gives insights into the origins of the rich phase structure. Arguments for the existence of the limiting Gibbs states are provided. A microscopic foundation of the Landau scenario for phase transitions, which predicts the active directions and the order parameters, is formulated for the considered models.

1. Introduction

In a previous paper the present authors have investigated the conceptual frame for the discussion of thermodynamic equilibrium states of a rather general class of long-range interacting quantum mechanical multi-lattice systems. For these models there exists a canonical set of macroscopic *field variables* (*contact variables* in the notion of [1] and [2]) and of conjugate *density variables*. The reduction of the quantum statistical state space (which equals the mathematical state space of the underlying quasi-local C^*-algebra) to the thermodynamic state space had been performed in terms of a certain mapping. This has given a well defined relation between the quantum statistical and the thermodynamic notions. Various properties of pure phase states and mixed phase states have been formulated and interrelated with each other on both the statistical and the thermodynamic level of description.

Within this conceptual framework we discuss here a special class of FCC-multi-lattice models with four sublattices of equal (relative) size. The considered models originate from several sources in the literature and were also treated as short range interacting models with Monte Carlo methods (cf. also the discussion in Section 3). They have interpretations as meta-magnetic spin systems, as metallic alloys, and as hydrogenium gas placed on interstitial lattice sites in a host metal. We shall discuss the various phase structures mainly in terms of the magnetic spin language.

The symmetry of the considered Hamiltonians is introduced by starting from a global FCC-lattice space group. This O_h^5-group contains elements which leave the sublattices invariant as well as transform them into each other. By homogenization of the interactions within one sublattice (some authors even neglect these one-lattice forces completely [3, 4]) we arrive at a description, where the original space group symmetry essentially shows up as the S_4-symmetry of the interlattice permutations, which may be expressed as transformations of the unit cells into itselves. These transformations have the nature of internal symmetries which may be spontaneously broken in contradistinction to the permutations within the separate sublattices.

Having specified the class of Hamiltonians according the symmetry criteria, the evaluation of the thermodynamic phase structure follows the pattern worked out in [5]. The Haar measure of the internal symmetries, the partition function, free energy density and self-consistency equations are readily written down. The essential work consists in the numerical determination of those solutions of the self-consistency equations which give absolute minima of the free energy density. That is, one has then for all temperature and external field values the sets of the thermodynamic equilibrium states expressed by the specific extensive coordinates (which in general are not simplices as, e.g., the states of the triple point of water). The general theory, however, associates with these data the set of quantum statistical equilibrium states in a

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unique fashion, which always are simplices in an infinite-dimensional space and have the pure phase states as the extreme boundary. From general reasoning one knows that this set of pure phase states is decomposable into orbits of broken internal symmetries. We use here a certain symbolism with arrows to denote the orbit structure for broken S_4-symmetry. The calculation of the specific entropy is helpful, since it has to be constant on each orbit. If only one orbit turns up, the existence of the limiting Gibbs states is ensured. We have here, however, also the interesting case that two orbits with different entropy values show up. This is connected with phase transitions of the first kind, which also inherit typical features of phase transitions of the second kind. There are many arguments for the existence of the limiting Gibbs state also in this case but we don't work them out here.

We check the Landau scenario for phase transitions starting from the microscopic theory and calculating the free energy expansion from the thermodynamic functions determined before. The active directions and order parameters are derived from the interaction matrix and are compared with proposals in the literature.

In this way we hope to demonstrate the fruitfulness of model investigations in which the exact relationships between thermodynamics and quantum statistics can be elaborated.

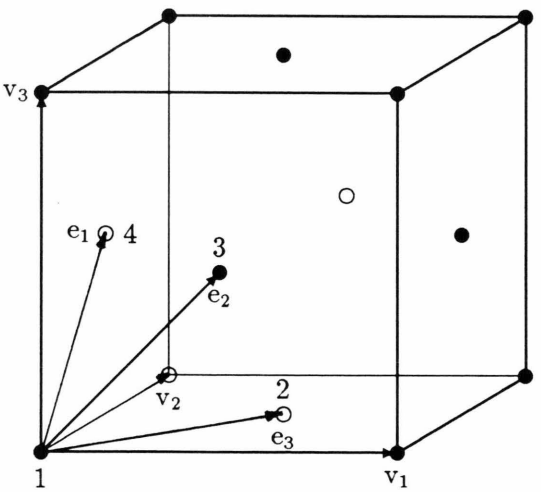

Fig. 1. Conventional unit cell of the face centered cubic (FCC) lattice (cf., e.g., [6]) with the primitive translation vectors e_1, e_2, e_3 and the four simple cubic sublattices (the FCC-lattice is the infinite periodic extension of the above cell in the directions of v_1, v_2, v_3).

2. Lattice Algebra and Symmetries

As starting point we consider a particular three-dimensional Bravais lattice, the face-centered cubic lattice

$$\Gamma_c^f = \left\{ x \in \mathbb{R}^3; x = \sum_{i=1}^{3} n_i e_i, n_i \in \mathbb{Z} \right\},$$

where the basis vectors are visualized in Figure 1. The associated space group is defined by (2.1)

$$O_h^5 = \{(D \mid t) \in O(3) \times \Gamma_c^f; (D \mid t)x = Dx + t \in \Gamma_c^f \ \forall x \in \Gamma_c^f\}$$

(cf., e.g., [6] Fig. 1.3, Table 1.4). It is symmorphic and has the cubic group O_h as point group.

There are many and quite different model discussions (cf. [3, 4, 7]) which suggest to decompose Γ_c^f into four sublattices. We make here the following choice.

Definition 2.1: *The four sublattices of Γ_c^f are given by the following formulas, where $a>0$ and $\{v_i; 1 \geq i \geq 3\}$ is an orthonormal base system in $\mathbb{R}^3$:*

$$\text{sublattice } 1 := \{x = (\textstyle\sum_{k=1}^{3} i_k v_k)\, a;\ i_k \in \mathbb{Z}\}, \tag{2.2}$$

$$\text{sublattice } 2 := \{x = [(i_1 + \tfrac{1}{2}) v_1 + (i_2 + \tfrac{1}{2}) v_2 + i_3 v_3]\, a;\ i_k \in \mathbb{Z}\},$$

$$\text{sublattice } 3 := \{x = [(i_1 + \tfrac{1}{2}) v_1 + i_2 v_2 + (i_3 + \tfrac{1}{2}) v_3]\, a;\ i_k \in \mathbb{Z}\},$$

$$\text{sublattice } 4 := \{x = [i_1 v_1 + (i_2 + \tfrac{1}{2}) v_2 + (i_3 + \tfrac{1}{2}) v_3]\, a;\ i_k \in \mathbb{Z}\}.$$

In Fig. 1 we have indicated the origins of the four sublattices (1, 2, 3, 4). The edge of the cube has length a.

Obviously the total set of variable vector indices is isomorphic to

$$\mathscr{R} := \mathbb{Z}^3 \times \{1, \ldots, 4\}.$$

For every element $(i, q) \in \mathscr{R}$ the first index $i \in \mathbb{Z}^3$ gives the triple of cartesian coordinates and the second index $q \in \{1, \ldots, 4\}$ indicates the sublattice. By inspection of Fig. 1 we get, for example, for the vectors $0, e_1, e_2, e_3$ in Γ_c^f the coordinates (0, 0, 0, 1), (0, 0, 0, 4), (0, 0, 0, 3), (0, 0, 0, 2) in $\mathscr{R}$, respectively. The action of O_h^5 on Γ_c^f induces an action of O_h^5 on $\mathscr{R}$ in a unique manner, by which in general the sublattice indices are changed.

For the formulation of the thermodynamical limit one has to choose a set of local lattice regions $\{\underline{\Lambda}; \underline{\Lambda} \subset \mathscr{R}, |\underline{\Lambda}| < \infty\}$, where $|\underline{\Lambda}|$ denotes the cardinality of $\underline{\Lambda}$. The requirement that in $\underline{\Lambda}$ each sublattice region is of equal size may be expressed by

$$\underline{\Lambda} = \bigcup_{i \in \Lambda} i \times \{1, \ldots, 4\}, \quad \Lambda \subseteq \mathbb{Z}^3, \tag{2.3}$$

that is by joining finitely many unit cells, the latter being given by the index set $\{1, \ldots, 4\}$, with which one

may associate the usual primitive elementary cell of Γ_c^f containing in fact just four edge points. This point of view has an important consequence for the symmetries in our models, for which we assume homogeneity of the interactions within the sublattices. This is expressed as invariance under permutations $p: \mathbb{Z}^3 \to \mathbb{Z}^3$, which act on $\mathscr{R}$ as

$$\mathscr{R} \ni (i, q) \overset{p}{\mapsto} (p(i), q) \in \mathscr{R} . \tag{2.4}$$

The group of all such permutations p, which leave all points i outside a certain finite region $\Lambda \subset \mathbb{Z}^3$ (depending on p) invariant, is denoted by P. Permutations of $\mathscr{R}$, which transform one sublattice into another one in the same fashion for all sublattice points, are induced by permutations in the unit cells and constitute therefore the group S_4. They act on $\mathscr{R}$ as

$$\mathscr{R} \ni (i, q) \overset{\pi}{\mapsto} (i, \pi(q)) \in \mathscr{R} . \tag{2.5}$$

The connection between these groups and the space group O_h^5 is considered in the following.

Lemma 2.2: *Let the groups O_h^5, P and S_4 act in $\mathscr{R}$ as described above. Then it holds:*

(i) *For every $R \in O_h^5$ and every $q \in \{1, \ldots, 4\}$ there is a rotation-reflection A_R of $\mathbb{Z}^3$, a unit cell permutation $\pi_R \in \mathsf{S}_4$ and a translation $t_{R,q} \in \mathbb{Z}^3$ such that*

$$R(i, q) = (A_R i + t_{R,q}, \pi_R(q)), \quad \forall i \in \mathbb{Z}^3 . \tag{2.6}$$

Moreover there is a decomposition (in $\mathbb{Z}^3$)

$$t_{R,q} = t_R + t'_{R,q} \tag{2.7}$$

such that $t'_{R,q}$ is "small" in the sense that the absolute values of its components are not larger than 2. (Observe that a unit step corresponds to one lattice constant a (cf. Figure 1!).

(ii) *For every $\pi \in \mathsf{S}_4$ there is an $R \in O_h^5$ such that $\pi = \pi_R$ in the sense of* (2.6).

(iii) *If $\underline{\Lambda}$ is as in* (2.3) *a union of unit cells and $R \in O_h^5$ then $R\underline{\Lambda}$ is again a union of unit cells up to four "small" translations (which are not larger than two lattice constants).*

Remark: The small translations are due to the fact, that the origins of the different sublattices do not coincide.

Proof: (i) Every $R \in O_h^5$ is a finite product of the three translations $(1, e_k)$, $1 \le k \le 3$, and of four generating elements $(D_l, 0)$, $1 \le l \le 4$, of the point group O_h. (One may choose for D_1 the inversion and for D_l, $2 \le l \le 4$, a rotation around an l-fold axis of the cube.) Direct calculations show, that the $R = (D_l, 0)$, $1 \le l \le 4$, satisfy (2.6) with $t_{R,q}$ small (the components are in fact equal to -1, 0 or $+1$). The other elements of O_h have the form $(D_l, 0)^{-1}(D_k, 0)(D_l, 0)$, $1 \le l, k \le 4$, and fulfill (2.6) again with $t_{R,q}$ small. On the other hand, one finds for $R = (1, e_k)^2$, $1 \le k \le 3$, that

$$R(i, q) = (i + t_R, q) .$$

If $R = (1, \sum_{k=1}^3 z_k e_k)$, we write $z_k = 2u_k + v_k$, $v_k = 0$ or 1 ($z_k, u_k \in \mathbb{Z}$). Then

$$R(i, q) = (i + t_R + t_{R,q}, \pi_R(q))$$

with $t_{R,q}$ small (i.e., that again the components are equal to -1, 0 or $+1$).

Now, since O_h^5 is symmorphic, every $R \in O_h^5$ has the form $R = R_2 \circ R_1$ with $R_2 \in O_h$ and $R_1 = (1, \sum_{k=1}^3 z_k e_k)$, which leads to

$$\begin{aligned} R(i, q) &= R_2(i + t_{R_1} + t_{R_1,q}, \pi_{R_1}(q)) \\ &= (A_{R_2}(i + t_{R_1}) + A_{R_2} t_{R_1,q} + t_{R_2, \pi_{R_1}(q)}, \pi_{R_2 R_1}(q)), \end{aligned}$$

where we have a sum of small translations and a rotated small translation with components in $[-1, +1]$ which gives a small translation with components in $[-2, +2]$, which proves (i).

(ii) For every transposition (=interchange of two elements) $\pi \in \mathsf{S}_4$ one finds by direct calculation space group elements $R := (\sigma, 0)$ or $R := (\sigma, e_k)$ with $\sigma \in O_h$ a rotation-reflection and $e_k \in \mathbb{R}^3$ a base vector, such that

$$R(i, q) = (\sigma i + e_k + t'_{R,q}, \pi(q))$$

for all (i, q). Since an arbitrary element $\pi \in \mathsf{S}_4$ is a product of transpositions we have proved (ii).

(iii) In virtue of (2.3), (2.6), and (2.7) we obtain

$$\begin{aligned} R\underline{\Lambda} &= \bigcup_{q=1}^4 \bigcup_{i \in \Lambda} (A_R i + t_R + t'_{R,q}, \pi_R(q)) \\ &= \bigcup_{q'=1}^4 (\Lambda_R + t'_{R, \pi_R^{-1}(q')}, q') \end{aligned}$$

where $\Lambda_R = A_R \Lambda + t_R$ is independent of q and the $t'_{R, \pi_R^{-1}(q)}$ are small translations with components in $[-2, +2]$. □

The quantum mechanical algebra of observables of the lattice system is obtained by associating with every $(i, q) =: r \in \mathscr{R}$ an algebra $\mathscr{A}_r$, which here is assumed *-isomorphic to the 2×2-matrix algebra $\mathscr{M}^{(2)}$ for all $r \in \mathscr{R}$. (In the notation of [5] we have $d = 3$, $r = 4$, the

number of sublattices, not to be confused with our variable r, and $n(q)=2$, $1\leq q\leq 4$.) For every $i\in\mathbb{Z}^3$ the algebra $\mathscr{A}_i:=\bigotimes_{q=1}^{4}\mathscr{A}_{(i,q)}$ is *-isomorphic to $\mathscr{B}:=\bigotimes_{q=1}^{4}\mathscr{M}^{(2)}$. The *-isomorphisms between the $\mathscr{A}_r$ and $\mathscr{M}^{(2)}$ and between the $\mathscr{A}_i$ and $\mathscr{B}$ will not be made explicit by a symbol.

For every finite multi-lattice region $\underline{\Lambda}\subset\mathscr{R}$, not necessarily of the form (2.3), we associate the algebra

$$\mathscr{A}_{\underline{\Lambda}}:=\bigotimes_{r\in\underline{\Lambda}}\mathscr{A}_r\,. \tag{2.8}$$

If $\underline{\Lambda}$ is associated with $\Lambda\subset\mathbb{Z}^3$ as in (2.3) we write

$$\mathscr{A}_{\underline{\Lambda}}=\mathscr{A}_{\Lambda}=\bigotimes_{i\in\Lambda}\mathscr{A}_i=\bigotimes_{(i,q)\in\underline{\Lambda}}\mathscr{A}_{(i,q)}\,. \tag{2.9}$$

If $\underline{\Lambda}\subset\underline{\Lambda}'$ we define (as in [5])

$$\eta_{\underline{\Lambda}',\underline{\Lambda}}(A):=A\otimes\mathbb{1}_{\underline{\Lambda}'\setminus\underline{\Lambda}}\,,\quad A\in\mathscr{A}_{\underline{\Lambda}}\,, \tag{2.10}$$

where $\mathbb{1}_{\underline{\Lambda}'\setminus\underline{\Lambda}}$ is the unit operator of $\mathscr{A}_{\underline{\Lambda}'\setminus\underline{\Lambda}}$, corresponding to the complementary set of $\underline{\Lambda}$ *in* $\underline{\Lambda}'$. That is, $\eta_{\underline{\Lambda}',\underline{\Lambda}}$ embeds $\mathscr{A}_{\underline{\Lambda}}$ *-isomorphically into $\mathscr{A}_{\underline{\Lambda}'}$. The C^*-inductive limit of this system of local algebras and embedding morphisms [8] gives the so-called quasi-local algebra [9]

$$\mathscr{A}=\bigotimes_{r\in\mathscr{R}}\mathscr{A}_r=\bigotimes_{i\in\mathbb{Z}^3}\mathscr{A}_i\,, \tag{2.11}$$

where we have taken into account the associative law of (infinite) C^*-algebraic tensor products [8] (with minimal cross norm). There exist canonical *-isomorphisms

$$\eta_{\underline{\Lambda}}\colon\mathscr{A}_{\underline{\Lambda}}\to\mathscr{A} \tag{2.12}$$

for every finite multi-lattice set $\underline{\Lambda}$ [8], which embed the local algebras directly into the quasi-local algebra of the infinite lattice system.

The structure of the observable algebra is relevant for a concise discussion of the symmetries. In general an element g of a symmetry group shifts the region $\underline{\Lambda}$ into the region $\underline{\Lambda}_g$ and acts on the observables as an (anti-)isomorphism with

$$\alpha_g^{\underline{\Lambda}}(\mathscr{A}_{\underline{\Lambda}})=\mathscr{A}_{\underline{\Lambda}_g}\,. \tag{2.13}$$

In order to piece the local symmetry transformations together to a global transformation the compatibility conditions with the embedding operators

$$\eta_{\underline{\Lambda}'_g,\underline{\Lambda}_g}\circ\alpha_g^{\underline{\Lambda}}=\alpha_g^{\underline{\Lambda}'}\circ\eta_{\underline{\Lambda}',\underline{\Lambda}} \tag{2.14}$$

for all Λ, Λ' with $\Lambda\subset\Lambda'$ are necessary and sufficient. The resulting transformation α_g is an (anti-)automorphism of $\mathscr{A}$.

The above mentioned spatial symmetries act on local observables as follows ($A_r\in\mathscr{A}_r$):

$$\alpha_R^{\underline{\Lambda}}\Big(\bigotimes_{r\in\underline{\Lambda}}A_r\Big):=\bigotimes_{r\in\underline{\Lambda}}\mathscr{A}_{Rr}\,,\quad R\in O_h^5\,, \tag{2.15}$$

$$\Theta_p^{\underline{\Lambda}}\Big(\bigotimes_{r\in\underline{\Lambda}}A_r\Big):=\bigotimes_{r\in\underline{\Lambda}}\mathscr{A}_{pr}\,,\quad p\in\mathsf{P}\,, \tag{2.16}$$

$$\Theta_\pi^{\underline{\Lambda}}\Big(\bigotimes_{r\in\underline{\Lambda}}A_r\Big):=\bigotimes_{r\in\underline{\Lambda}}\mathscr{A}_{\pi r}\,,\quad \pi\in\mathsf{S}_4\,. \tag{2.17}$$

Since they are (by linear extension) local isomorphisms and satisfy (2.14) they represent the three groups by automorphisms α_R, Θ_p and Θ_π in $\mathscr{A}$.

If I is a spin inversion in $\mathscr{A}_r$ (implemented by an anti-unitary operator) then

$$\Theta_I^{\underline{\Lambda}}\Big(\bigotimes_{r\in\underline{\Lambda}}A_r\Big):=\bigotimes_{r\in\underline{\Lambda}}I(\mathscr{A}_r) \tag{2.18}$$

satisfies again (2.14) and leads to an anti-automorphism Θ_I in $\mathscr{A}$ (cf. also (3.13)).

In our model discussion we restrict the $\underline{\Lambda}$ to the case of unit cell unions (2.3) and designate them – as in (2.9) – by the associated Λ. The set of all finite Λ is denoted by $\mathscr{L}$. Since $\mathscr{A}_\Lambda$ is finite dimensional the Hamiltonian h_Λ for this region is bounded and an element of $\mathscr{A}_\Lambda$. A model is invariant under a symmetry group G, which acts via (anti-)automorphisms α_g, $g\in\mathsf{G}$, in $\mathscr{A}$, if

$$\alpha_g^{\Lambda}(h_\Lambda)=h_{\Lambda_g}\,,\quad\forall\Lambda\in\mathscr{L},\quad g\in\mathsf{G}, \tag{2.19}$$

where Λ_g is again the g-transformed region of Λ. It is well defined, if the original action of G in $\mathscr{R}$ maps unit cells onto unit cells. This is the case for (2.16), (2.17), (2.18), but not in general for (2.15). Since we are mainly interested in very large regions $\underline{\Lambda}$ it seems physically justified for mean field interactions to drop the small translations in (2.7). That is, we neglect the small shifts the sublattices may experience with respect to each other under a space group action R. These modified space group actions $\bar{R}$ map now unit cells onto unit cells, and are introduced only to motivate the special form of our model interactions.

Proposition 2.3: *A* P*-invariant four-lattice model is invariant under the modified space group, if and only if it is* S_4*-invariant.*

Proof: If we drop in (2.6) and (2.7) the small translations we obtain for $R\in O_h^5$ the modified transforma-

tion

$$\bar{R}(i, q) = (A_R i + t_R, \pi_R(q)) \tag{2.20}$$

which applied to $\underline{\Lambda}$ maps Λ bijectively onto $\Lambda_R = A_R \Lambda + t_R$. If Λ runs through $\mathscr{L}$ this does Λ_R, too. For every $R \in O_h^5$ and every $\Lambda \in \mathscr{L}$ there is a $p_R \in \mathsf{P}$ localized in $\Lambda \cup \Lambda_R$ such that

$$\bar{R}(i, q) = (p_R i, \pi_R(q)) \tag{2.21}$$

for all $(i, q) \in \underline{\Lambda}$. This decomposition of $\bar{R}$ carries over to the corresponding local automorphisms, since they are – according to (2.15)–(2.17) – totally determined by the lattice transformations. Thus

$$\alpha_{\bar{R}}(h_\Lambda) = p_R \circ \pi_R(h_\Lambda) = \pi_R(h_{\Lambda_R}), \tag{2.22}$$

where P-invariance has been applied. If (2.22) equals h_{Λ_R} due to modified O_h^5-invariance, we obtain S_4-invariance because of Lemma 2.2(ii). On the other hand S_4-invariance in every Λ_R implies modified O_h^5-invariance in every $\Lambda \in \mathscr{L}$. □

If now $\underline{\Lambda}$ is a union of unit cells over Λ then

$$\Theta_\pi\left(\bigotimes_{i \in \Lambda} A_i\right) = \bigotimes_{i \in \Lambda} u_\pi^i A_i u_\pi^{i*}, \tag{2.23}$$

where u_π^i is a unitary representation of S_4 in the unit cell Hilbert space $\bigotimes_{q=1}^{4} \mathbb{C}^2$. Generally we call symmetries which arise in this way from (anti-)unitary operators in the unit cell Hilbert space internal symmetries of the multi-lattice theory. We shall consider only models, whose internal invariance group comprises S_4 (but may well contain additional elements as I of (2.18)). The total internal invariance group of a model is called H. The entire symmetry group of a permutation invariant model is then

$$\mathsf{G} = \mathsf{P} \times \mathsf{H}, \tag{2.24}$$

as was generally postulated in [5].

The point we want to emphasize is, that the original space group invariance of our homogeneous models (cf. also the discussion after formula (3.10)) appears here partly as the sublattice permutation group P and partly as the internal symmetry group S_4. Whereas the P-invariance is never broken, one has for the internal symmetries the principal possibility of a spontaneous symmetry break down in equilibrium states. In fact, it is the broken S_4-invariance combined with spontaneous magnetization effects, which leads to complicated phase diagrams in the considered models.

3. Model Hamiltonians

The model Hamiltonians we want to analyze in this section are of the general type

$$h_\Lambda(\varepsilon) = |\Lambda| \left\{ \sum_{i=1}^{n_{\mathscr{B}}} \varepsilon_i m_\Lambda(\hat{e}_i) + \sum_{i,k=1}^{n_{\mathscr{B}}} m_\Lambda(\hat{e}_i) w_{ik} m_\Lambda(\hat{e}_k) \right\} \tag{3.1}$$

considered in [5], where $n_{\mathscr{B}}$ denotes the dimension of $\mathscr{B}$ as a vector space, $\hat{e}_i$ $(i = 1, \ldots, n_{\mathscr{B}})$ is a self-adjoint matrix basis in $\mathscr{B}$ and $\varepsilon = (\varepsilon_i) \in \mathbb{R}^{n_{\mathscr{B}}}$ and $w = (w_{ik}) \in \mathscr{B}(\mathbb{R}^{n_{\mathscr{B}}})$ respectively, are the energy or field vector and the interaction matrix. The density observables $m_\Lambda(\hat{e}_i)$ $(i = 1, \ldots, n_{\mathscr{B}})$ are given by

$$m_\Lambda(\hat{e}_i) = \frac{1}{|\Lambda|} \sum_{k \in \Lambda} \eta_k(\hat{e}_i)$$

where we again denote with η_k the embedding isomorphism of the algebra $\mathscr{A}_{\{k\}}$ $(\equiv \mathscr{B})$ of one cell $k \in \Lambda$ into the algebra $\mathscr{A}$ of the infinite system.

The Hamiltonians (3.1) are covariant under the group G of Sect. 2, i.e.,

$$\Theta_g h_\Lambda(\varepsilon) = h_{\Lambda_g}(\varepsilon)$$

for every $g = (p, u) \in \mathsf{G} = \mathsf{P} \times \mathsf{H}$, if and only if ε and w fulfill

$$\begin{aligned} M(u)\,\varepsilon &= \varepsilon \\ M(u)\, w\, M(u)^T &= w \end{aligned} \tag{3.2}$$

where for every $u \in \mathsf{H}$ the representing matrix $M(u) = (m_{kn}(u)) \in \mathscr{B}(\mathbb{R}^{n_{\mathscr{B}}})$ is given by

$$u \hat{e}_n u^* = \sum_{k=1}^{n_{\mathscr{B}}} m_{kn}(u)\, \hat{e}_k \tag{3.3}$$

(cf. also [5]).

With the Pauli matrix

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

we define first the "spin"-observables in the unit cell

$$\left.\begin{aligned} s_1 &:= \sigma_z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \\ s_2 &:= \mathbb{1} \otimes \sigma_z \otimes \mathbb{1} \otimes \mathbb{1} \\ s_3 &:= \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z \otimes \mathbb{1} \\ s_4 &:= \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \sigma_z \end{aligned}\right\} \in \mathscr{B} \tag{3.4}$$

and the particle number

$$n_q := \tfrac{1}{2}(\mathbb{1}_{\mathscr{B}} + s_q) \quad (q = 1, \ldots, 4). \tag{3.5}$$

By the *-isomorphy of $\mathscr{B}$ with $\mathscr{A}_i$, $i \in \mathbb{Z}^3$, we have the spin-observables now also at each lattice point i. (The

term "particle number" for the operators n_q is connected with the "lattice gas" interpretation of our special model system.) We next introduce as an "space-average" of the operators $s_q, n_q \in \mathscr{B}$ for finite sets $\Lambda \in \mathscr{L}$ the density observables of the spins

$$s_\Lambda^q := m_\Lambda(s_q) \tag{3.6}$$

and of the particle number

$$n_\Lambda^q := m_\Lambda(n_q) = \tfrac{1}{2}(\mathbb{1}_\Lambda + s_\Lambda^q) \tag{3.7}$$

in the q-th sublattice ($q=1,\ldots,4$). The local Hamiltonians for the four-sublattice system considered here can now be written as

$$\tilde{h}_\Lambda := |\Lambda| \left\{ \sum_{q=1}^{4} (E_q - \mu)\, n_\Lambda^q + \sum_{q,t=1}^{4} \tilde{w}_{qt}\, n_\Lambda^q\, n_\Lambda^t \right\} \tag{3.8}$$

or, equivalently, as

$$\tilde{h}_\Lambda = \sum_{q=1}^{4} \sum_{k \in \Lambda} (E_q - \mu)\, \eta_k(n_q) + \sum_{q,t=1}^{4} \frac{\tilde{w}_{qt}}{|\Lambda|} \sum_{i,k \in \Lambda} \eta_i(n_q)\, \eta_k(n_t). \tag{3.9}$$

The $E_q \in \mathbb{R}$ are one particle energies and μ is the chemical potential of the particles being in the same chemical state; the $\tilde{w}_{qt} \in \mathbb{R}$ denote the 4×4 interaction parameters. With the definitions (3.6), (3.7) we re-express the Hamiltonians (3.8) as Hamiltonians of magnetic systems

$$h_\Lambda := |\Lambda| \left\{ \sum_{q=1}^{4} B_q\, s_\Lambda^q + \sum_{q,t=1}^{4} w_{qt}\, s_\Lambda^q\, s_\Lambda^t \right\}, \tag{3.10}$$

where we omit terms proportional $\mathbb{1}_\Lambda$ and define

$$w_{ik} := \frac{\tilde{w}_{ik}}{4}, \quad B_i := \frac{E_i - \mu}{2} + 4 \sum_{k=1}^{4} w_{ik}\,.$$

Some remarks should be made concerning the peculiar nature of the local Hamiltonians (3.8) (resp. (3.10)). On the one hand they provide a microscopic description of the thermodynamic behaviour of the considered system. On the other hand they are not "first principle" Hamiltonians but can be considered as approximations of Hamiltonians with translationally invariant and short-range interaction usually used to describe order-disorder phenomena on a physically defined lattice (cf., e.g., [7]). The special type of approximation used here and called "homogeneization" consists of two steps. The first step is to choose a sublattice structure which mimics the different kinds of short-range behaviour of the "first principle" interaction [10]. The second step is to calculate the average interaction energy which has the i-th point in the q-th sublattice with some point i' in the q'-th sublattice considering all pairs $(i, i') \in \Lambda \times \Lambda$.

In [7], e.g., the considered sublattice structure is used to simplify a translational invariant interaction ranging only over nearest and next-nearest neighbours with exchange interaction parameters J_{nn} and J_{nnn}. Each FCC lattice point has 12 nearest neighbours, 4 on every of the three *other* sublattices and 6 next-nearest neighbours on the *same* sublattice (cf. Figure 1). In the Hamiltonian (3.10) the interaction of one spin of the q-th sublattice with all spins of the t-th sublattice is given by w_{qq} if $q=t$ and by $2w_{qt}$ if $q \neq t$, respectively. So we arrive at

$$\begin{aligned} &w_{12} = w_{13} = w_{14} = w_{23} = w_{24} = w_{34} = 2J_{nn}\,, \\ &w_{11} = w_{22} = w_{33} = w_{44} = 6J_{nnn}\,. \end{aligned} \tag{3.11}$$

This form of the interaction matrix is not only motivated by the above *ansatz* concerning the range of the interaction, but can be shown to be a consequence of the S_4-invariance as described in Section 2. To that end we relate the Hamiltonians (3.10) to the general ones of (3.1) using the definition in (3.4) and (3.6).

Definition 3.1: (i) *Self-adjoint basis of* $\mathscr{B}$:

$$\hat{e} := (s_1, s_2, s_3, s_4, \ldots)$$

with arbitrary fixed basis elements $\hat{e}_i$ $(i=5,\ldots,n_{\mathscr{B}})$;

(ii) *energy or field vector, respectively,*

$$\varepsilon := (B_1, B_2, B_3, B_4, 0, \ldots, 0) \in \mathbb{R}^{n_{\mathscr{B}}};$$

(iii) *interaction matrix*

$$w = \begin{pmatrix} (w_{ik})_{i,k \in \mathbb{N}_4^*} & 0 \\ 0 & 0 \end{pmatrix} \in \mathscr{B}(\mathbb{R}^{n_{\mathscr{B}}})\,.$$

With the representing matrices

$$M(u_\pi) = \begin{pmatrix} (\delta_{k\pi(i)})_{k,i \in \mathbb{N}_4^*} & \cdots \\ 0 & \ddots \end{pmatrix}, \quad \pi \in \mathsf{S}_4\,,$$

according to (3.3) condition (3.2) puts constraints on ε and w. But because S_4 simply permutes *all* the sublattice indices one has the following result.

Lemma 3.2: *Equations* (3.2) *hold if and only if the field and interaction parameters of Def.* 3.1 *are given by*

(i) $$\varepsilon_q = \begin{cases} B & \text{if } q=1,\ldots,4 \\ 0 & \text{otherwise;} \end{cases}$$

(ii) $$w_{qt} = \begin{cases} w_0 & \text{if } 1 \leq q \neq t \leq 4 \\ w_1 & \text{if } 1 \leq q = t \leq 4 \\ 0 & \text{otherwise.} \end{cases}$$

Proof: The S_4-operations induce arbitrary permutations π of the parameter indices $1 \leq q, t \leq 4$. Since $q=t$, iff $\pi(q)=\pi(t)$, the set of double indices decomposes into two S_4-orbits. □

If $B=0$ the Hamiltonians (3.10)

$$h_\Lambda = |\Lambda| \sum_{q,t=1}^{4} w_{qt}\, s_\Lambda^q\, s_\Lambda^t$$

have the additional invariance under (z-)spin inversion $I(s_q)=-s_q$ (which gives $\Theta_I^\Lambda(s_\Lambda^q)=-s_\Lambda^q$). Let us here assume that I is the inversion of all spins in the three space directions. Then the interpretation as inversion of angular momentum observables requires the implementation by means of anti-unitary operators, which may be effectuated, e.g., by

$$u_I := \sigma_I \otimes \sigma_I \otimes \sigma_I \otimes \sigma_I\,,$$

where

$$\sigma_I = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} C, \tag{3.12}$$

C being a complex conjugation in $\mathbb{C}^2$. Then

$$I(A) = u_I\, A^*\, u_I^{-1}, \quad \forall A \in \mathscr{B}\,. \tag{3.13}$$

Observe that $u_I^2=-1$ and $I^2=$identity transformation. As described in (2.18) we obtain the global spin inversion Θ_I as an anti-automorphism of $\mathscr{A}$.

Proposition 3.3: *The internal symmetry groups* H *of the local model Hamiltonians* $\{h_\Lambda(\varepsilon);\ \Lambda \in \mathscr{L}\}$ *in dependence of the external field* $\varepsilon_q = B$, $1 \leq q \leq 4$, *are given by*

$$\mathsf{H} = \begin{Bmatrix} \mathsf{S}_4 \cup I\mathsf{S}_4 & \text{if} \quad B=0 \\ \mathsf{S}_4 & \text{otherwise} \end{Bmatrix}.$$

The finite groups H *have the normalized Haar-measures*

$$\mu_{\mathsf{H}}(f) = \frac{1}{n(\mathsf{H})} \sum_{u \in \mathsf{H}} f(u), \quad f\colon \mathsf{H} \to \mathbb{C}\,,$$

where

$$n(\mathsf{H}) = \begin{Bmatrix} 2 \cdot 4! & \text{if} \quad B=0 \\ 4! & \text{otherwise} \end{Bmatrix}.$$

Proof: According to the preceding discussion, the local Hamiltonians are invariant under H. Every other symmetry transformation, which does not affect the s_q, acts as the identity transformation on the considered observables and is incorporated in the unit element e of H. Since $I^2=e$ and $I\pi I=\pi$, $\pi \in \mathsf{S}_4$, H is a group in the case $B=0$, too.

Every symmetry transformation involving the s_q only, must be of the form $u s_q u^{-1} = c\, s_{\pi(q)}$, where $c \in \mathbb{R}$, with $c^2=1$. Thus we have taken into account all possibilities.

The form of the Haar measure for finite groups is standard. □

4. Equilibrium States and Phase Transitions

The equilibrium states we want to consider in this section are on the one hand the *local Gibbs states* $\omega_\Lambda^{\beta\varepsilon}$ ($\Lambda \in \mathscr{L}$) defined by

$$\langle \omega_\Lambda^{\beta\varepsilon};\, A\rangle := \langle \tau;\, \eta_\Lambda(e^{-\beta h_\Lambda(\varepsilon)})\, A\rangle / \langle \tau;\, \eta_\Lambda(e^{-\beta h_\Lambda(\varepsilon)})\rangle\,,$$

$A \in \mathscr{A}$, where τ is the unique trace state on $\mathscr{A}$ given by

$$\left\langle \tau;\ \bigotimes_{i \in \mathbb{Z}^3} A_i \right\rangle = \prod_{i \in \mathbb{Z}^3} \mathrm{tr}_{\mathscr{B}}\{A_i\}/\mathrm{tr}_{\mathscr{B}}\{\mathbb{1}\}\,.$$

On the other hand there are the accumulation points of the net $\{\omega_\Lambda^{\beta\varepsilon};\ \Lambda \in \mathscr{L}\}$, which describe the considered system in the thermodynamic limit and are called *limiting Gibbs states.*

Since the model Hamiltonians $h_\Lambda(\varepsilon)$ of Sect. 3 are invariant under P and H the local as well as the limiting Gibbs states are invariant under P and H, too. We have argued in [5, 11] that each state in the w^*-closed, convex subset $\mathscr{S}^P(\mathscr{A})$ of permutation invariant states in $\mathscr{S}(\mathscr{A})$ has a unique (central) decomposition

$$\omega = \int_{\mathscr{S}^P} \varphi\, \mathrm{d}\mu_\omega(\varphi)\,, \tag{4.1}$$

where the (central) probability measure μ_ω is concentrated on the extremal boundary $\partial_e \mathscr{S}^P$. The states $\varphi \in \partial_e \mathscr{S}^P$ have product form $\varphi = \bigotimes_{i \in \mathbb{Z}^d} \Phi$, $\Phi \in \mathscr{S}(\mathscr{B})$ and are factor states; thus they have sharp macroscopic observables which is the reason for their interpretation as pure phase states. This means that each limiting Gibbs state can be uniquely written as convex combination (4.1) of pure phase states, which are permutation invariant but are in general not invariant under all elements of H, which is a concise form of spontaneous symmetry breaking. Since the symmetry under the permutation group P is never broken in our general class of models we restrict the following considerations to the subset $\mathscr{S}^P$ and refer to it as *state space.*

The limiting Gibbs states of the considered systems resp. their central decomposition will not be com-

puted directly via (sub)net convergence of $\{\omega_\Lambda^{\beta\varepsilon}; \Lambda \in \mathscr{L}\}$, but indirectly using the minimum principle for the specific free energy and symmetry arguments. The latter method does not require to diagonalize the local Hamiltonians explicitly, which is in most cases impossible. We recall some results derived in [11].

On the state space $\mathscr{S}^P$ the specific energy

$$u(\varepsilon, \varphi) = \lim_{\Lambda} \langle \varphi; h_\Lambda(\varepsilon)\rangle / |\Lambda| \tag{4.2}$$

and the specific entropy [1]

$$s(\varphi) = \lim_{\Lambda} - \mathrm{tr}_\Lambda \{\varrho_\Lambda^\varphi \ln \varrho_\Lambda^\varphi\}/|\Lambda| \tag{4.3}$$

can be shown to exist, i.e., the net limits exist, and so does the specific free energy

$$f(\beta, \varepsilon, \varphi) = u(\varepsilon, \varphi) - \beta^{-1} s(\varphi). \tag{4.4}$$

Each limiting Gibbs state is a member of the set of *equilibrium states*

$$\mathscr{S}(\beta, \varepsilon) = \{\varphi \in \mathscr{S}^P;\ f(\beta, \varepsilon, \varphi) = \inf f(\beta, \varepsilon, \mathscr{S}^P)\} \tag{4.5}$$

which is a convex, w^*-closed subset of $\mathscr{S}^P$, since $f(\beta, \varepsilon, .)$ is affine and w^*-continuous. It has therefore by the Krein-Millman theorem a large extreme boundary $\partial_e \mathscr{S}(\beta, \varepsilon)$ which can be written as

$$\partial_e \mathscr{S}(\beta, \varepsilon) = \{\varphi \in \partial_e \mathscr{S}^P;\ f(\beta, \varepsilon, \varphi) = \inf f(\beta, \varepsilon, \partial_e \mathscr{S}^P)\} \tag{4.6}$$

since $f(\beta, \varepsilon, .)$ takes its minimal value on the extremal permutation invariant states. The central measure of each limiting Gibbs state according to (4.1) is concentrated on $\partial_e \mathscr{S}(\beta, \varepsilon)$, so this set contains all pure phase equilibrium states of the infinite system. In order to calculate $\partial_e \mathscr{S}(\beta, \varepsilon)$ two mappings were introduced in [5]. Denoting the density matrices in $\mathscr{B}$ with W the bijective, w^*-continuous mapping

$$j:\ W \to \partial_e \mathscr{S}^P, \quad \varrho \mapsto \bigotimes_{i \in \mathbb{Z}^d} \mathrm{tr}_{\mathscr{B}}\{\varrho\, .\} \tag{4.7}$$

is a *finite dimensional* parametrization of the extremal permutation invariant states in the infinite dimensional state space $\mathscr{S}^P(\mathscr{A})$. The affine, continuous and bijective mapping

$$v:\ W \xrightarrow{\text{onto}} M, \quad \varrho \mapsto \mathrm{tr}_{\mathscr{B}}\{\varrho\, \hat{e}\} \tag{4.8}$$

gives a characterization of each density matrix by an $n_{\mathscr{B}}$-tupel of expectation values for the fixed basis elements $\hat{e}$. The elements of the convex, closed set $M \subseteq \mathbb{R}^{n_{\mathscr{B}}}$ are therefore called specific extensive coordinates. The combined mapping $v \circ j^{-1}$: $\partial_e \mathscr{S}^P \to M$ plays a role in the transition from the quantum statistical to the thermodynamical picture considered in the next section.

Evaluating the variational condition in (4.6) ensues that each $\varphi \in \partial_e \mathscr{S}(\beta, \varepsilon)$ is described by a density matrix

$$j^{-1}(\varphi) =: \varrho = e^{-\beta h(\varrho)}/\mathrm{tr}_{\mathscr{B}}\{e^{-\beta h(\varrho)}\} \in W \tag{4.9}$$

with an effective Hamiltonian

$$h(\varrho) = (\varepsilon + 2 w v(\varrho)) \bullet \hat{e} \in \mathscr{B}\,. \tag{4.10}$$

The self-referring relation (4.9) – the expectation values $v(\varrho)$ of the density matrix ϱ enter the right-hand side – is transformed in [5] into a coupled set of nonlinear equations for the component of $v(\varrho)$: (4.9) combined with (4.8) yields the so-called self-consistency equations

$$v(\varrho) = \mathrm{tr}_{\mathscr{B}}\{e^{-\beta h(\varrho)}\, \hat{e}\}/\mathrm{tr}_{\mathscr{B}}\{e^{-\beta h(\varrho)}\} \tag{4.11}$$

which can be written as

$$v(\varrho)_i = -\beta^{-1} \frac{\partial}{\partial m_i} \ln Z_\beta(\varepsilon + 2 w v(\varrho)) =: \{\tilde{F}_{\beta\varepsilon}(v(\varrho))\}_i \tag{4.12}$$

$(i = 1, \ldots, n_{\mathscr{B}})$, where $Z_\beta(m) = \mathrm{tr}_{\mathscr{B}}\{e^{-\beta m \bullet \hat{e}}\}$ and $\tilde{F}_{\beta\varepsilon}(m)$ are the partition function and the vector-valued fixpoint function respectively $(m \in \mathbb{R}^{n_{\mathscr{B}}})$.

According to Def. 3.1 the effective hamiltonians of (4.10) for the model systems considered here have the following two properties:

(i) Only the expectation values

$$v(\varrho)_i = \mathrm{tr}_{\mathscr{B}}(\varrho\, s_i) =: m_i \in [-1, +1] \quad (i = 1, \ldots, 4)$$

enter $h(\varrho)$;

(ii) $h(\varrho) \in \mathrm{span}\{s_1, s_2, s_3, s_4\}$.

The equations (4.11) are therefore *self-consistent* only in the first four components. The remaining $v(\varrho)_i$ $(i = 5, \ldots, n_{\mathscr{B}})$ give the expectation values of $\hat{e}_i$ $(i = 5, \ldots, n_{\mathscr{B}})$ as functions of the $v(\varrho)_i$ $(i = 1, \ldots, 4)$. This is the reason for reducing the thermodynamic density variables onto the interval $\times_{i=1}^4 [-1, +1]$.

Proposition 4.1: *With* $\beta \in \mathbb{R}_+^* = \mathbb{R}_+ \setminus \{0\}$, ε, w *according to Lemma* 3.2 *and* $m \in \times_{i=1}^4 [-1, +1]$ *one has the*

(1) *partition function:* $Z_\beta(m) = \prod_{i=1}^4 2\cosh(\beta m_i)$;

(2) *vector-valued fixpoint function:*

$$\{\tilde{F}_{\beta\varepsilon}(m)\}_i = -\tanh\left\{\beta\left(\varepsilon_i + 2\sum_{k=1}^{4} w_{ik}\, m_k\right)\right\} \quad (i = 1, \ldots, 4);$$

[1] Restricted to $\mathscr{A}_\Lambda$ there is a one-to-one relation between states $\varphi \in \mathscr{S}(\mathscr{A})$ and density matrices $\varrho_\Lambda^\varphi \in \mathscr{A}_\Lambda$.

(3) *values of the specific free energy for every solution of* $m = \tilde{F}_{\beta\varepsilon}(m)$:

$$\tilde{f}(\beta, \varepsilon, j \circ v^{-1}(m)) = \sum_{i,k=1}^{4} w_{ik}\, m_i\, m_k - \beta^{-1} \ln \left\{ \prod_{i=1}^{4} 2 \cosh \beta \left(\varepsilon_i + 2 \sum_{k=1}^{4} w_{ik}\, m_k \right) \right\}.$$

Proof: (1) From [5], Sect. 2.5, we have

$$Z_\beta(m) = \mathrm{tr}_{\mathscr{B}} \left\{ \exp\left(-\beta \sum_{i=1}^{4} m_i\, s_i \right) \right\} = \mathrm{tr}_{\mathscr{B}} \left\{ \prod_{i=1}^{4} e^{-\beta m_i s_i} \right\} = \mathrm{tr}_{\mathscr{B}} \{ \otimes_{i=1}^{4} e^{-\beta m_i \sigma_z} \}$$
$$= \prod_{i=1}^{4} \mathrm{tr}_{\mathscr{M}^2} \{ e^{-\beta m_i \sigma_z} \} = \prod_{i=1}^{4} \{ 2 \cosh(\beta m_i) \};$$

(2) with $\ln Z_\beta(m) = \sum_{i=1}^{4} \ln\{2 \cosh(\beta m_i)\}$:

$$\{\tilde{F}_{\beta\varepsilon}(m)\}_i = -\beta^{-1} \frac{\partial(\ln Z_\beta)}{\partial m_i} (\varepsilon + 2 w v(\varrho)) = -\tanh\left(\beta \varepsilon_i + 2 \sum_{k=1}^{4} w_{ik} m_k \right);$$

(3) immediately. □

We denote by $M(\beta, \varepsilon) \subseteq M$ the set of solutions of the coupled equations (4.11) resp. (4.12) with minimal free energy. $\partial_e \mathscr{S}(\beta, \varepsilon)$ and $M(\beta, \varepsilon)$ are equivalent descriptions of the system's equilibrium pure phase states, the former in quantum statistical, the latter in thermodynamical state space. Both are generally the union of several H-orbits mapped onto each other by $v \circ j^{-1}$: $\partial_e \mathscr{S}^P \to M$. We recall that

$$O_{\mathsf{H}}(\varphi) = \{ \Theta_u^* \varphi = \varphi \circ \Theta_{u^*};\ u \in \mathsf{H} \}$$

resp. $\tilde{O}_{\mathsf{H}}(m) = \{ M(u^*)^T m;\ u \in \mathsf{H} \}$

with $\varphi \in \partial_e \mathscr{S}^P$ and $m = v \circ j^{-1}(\varphi)$ are equivalent orbits in $\partial_e \mathscr{S}^P$ resp. M.

Proposition 4.2: *With* $\beta \in \mathbb{R}_+^*$, ε, w *of Lemma* 3.2, $m \in \mathbb{R}^{n_{\mathscr{A}}}$ *it holds:*

(i) *If* $\varepsilon \neq 0$ *and* $M(\beta, \varepsilon) = \tilde{O}_{\mathsf{H}}(m)$ *then the net* $\{\omega_\Lambda^{\beta\varepsilon};\ \Lambda \in \mathscr{L}\}$ *has the unique limiting Gibbs state*

$$\omega_m^{\beta\varepsilon} = \frac{1}{4!} \sum_{\pi \in \mathsf{S}_4} \varphi_\pi^{\beta\varepsilon},$$

where the product states $\varphi_\pi^{\beta\varepsilon} \in \partial_e \mathscr{S}^P$ *are defined by*

$$\varphi_\pi^{\beta\varepsilon} \left(\bigotimes_{i \in \mathbb{Z}^3} A_i \right) = \prod_{i \in \mathbb{Z}^3} \mathrm{tr}_{\mathscr{B}}(\exp(-\beta t_\pi \bullet \hat{e})\, A_i) / \mathrm{tr}_{\mathscr{B}}(\exp(-\beta t_\pi \bullet \hat{e}))$$

and

$$\hat{e} = (s_1, s_2, s_3, s_4, \ldots)$$
$$(t_\pi)_i = \varepsilon_i + 2 \sum_{k=1}^{4} w_{ik}\, m_{\pi^{-1}(k)} \qquad i = 1, \ldots, 4$$
$$(t_\pi)_i = 0 \qquad i > 4$$

and $\bigotimes_{i \in \mathbb{Z}^3} A_i \in \mathscr{A}$.

(ii) *If* $\varepsilon = 0$ *and* $M(\beta, \varepsilon) = \tilde{O}_{\mathsf{H}}(m)$ *the net* $\{\omega_\Lambda^{\beta\varepsilon};\ \Lambda \in \mathscr{L}\}$ *has the unique limiting Gibbs state*

$$\omega^{\beta\varepsilon} = \tfrac{1}{2}(\omega_m^{\beta\varepsilon} + \omega_{-m}^{\beta\varepsilon})$$

where $\omega_m^{\beta\varepsilon}$ *and* $\omega_{-m}^{\beta\varepsilon}$ *are defined in* (i).

Proof: (i) and (ii) are implied by the orbit analysis in [5, Sect. 2.5], by Prop. 3.3 and Eq. (4.12) of the present paper, and by the action of Θ_I^* onto the $\omega_m^{\beta\varepsilon}$. □

If $M(\beta, \varepsilon)$ decomposes into finitely or countably many H-orbits the limiting Gibbs states have the form

$$\omega^{\beta\varepsilon} = \sum_{k=1}^{n} \lambda_k\, \omega_k^{\beta\varepsilon} \tag{4.13}$$

($\lambda_k \geq 0$, $\sum_{k=1}^{n} \lambda_k = 1$, $n \in \mathbb{N} \cup \{\infty\}$), where the $\omega_k^{\beta\varepsilon}$ are the pure phase S_4-orbit states given in Prop. 4.2(i). The relative weights are uniquely determined by $\omega^{\beta\varepsilon}$ [5]. An example for the case with two S_4-orbits is already provided in Prop. 4.2(ii), where the representation (4.13) is obtained by extending the group of inner symmetries S_4 to $\mathsf{S}_4 \cup I\mathsf{S}_4$ which determines the relative weights of the two S_4-orbit states. Unfortunately this method cannot be taken as a general rule to determine the λ_k's of (4.13) uniquely if the pure phases of different orbits differ in their entropy values.

By the following procedure we have calculated numerically the sets $M(\beta, \varepsilon)$ for two representative combinations (w_0, w_1) of the interaction parameters which are motivated by considerations in Section 5. For every element of a uniformly distributed net of *starting points* in $\times_{i=1}^{4}[-1, +1]$ one nearby solution of the coupled set of nonlinear equations (4.12) has been calculated by means of methods of numerical mathematics (cf., e.g., [12]). This step has been repeated with denser and denser nets until there were no

Table 1. The sets $M(\beta, \varepsilon)$ for $w_0 < 0$, $w_1 = -w_0$, and $m = m(\beta, \varepsilon) < 0$.

	$B=0$	$B>0$
$0 < \beta \leq \beta_c$	$\{(0, 0, 0, 0, \ldots)\}$	$\{(m, m, m, m, \ldots)\}$
$\beta_c < \beta \leq \infty$	$\{(m, m, m, m, \ldots)\} \cup \{(-m, -m, -m, -m, \ldots)\}$	$\{(m, m, m, m, \ldots)\}$

Table 2. The limiting Gibbs states $\omega^{\beta\varepsilon}$ for $w_0 < 0$, $w_1 = -w_0$.

	$B=0$	$B>0$
$0 < \beta \leq \beta_c$	$(\downarrow\downarrow\downarrow\downarrow)$	
$\beta_c < \beta \leq \infty$	$\frac{1}{2}(\downarrow\downarrow\downarrow\downarrow) + \frac{1}{2}(\uparrow\uparrow\uparrow\uparrow)$	$(\downarrow\downarrow\downarrow\downarrow)$

new solutions to be found. The free energy of each solution has been calculated and the solutions with minimal free energy have ben selected. The structure of the resulting sets $M(\beta, \varepsilon)$ is summarized in the Tables 1 and 3. The equilibrium states in the latter one are given by

$$m^{(1)} = (m_a, m_b, m_b, m_b, \ldots),$$
$$m^{(2)} = (m_c, m_c, m_d, m_d, \ldots),$$
$$\bar{m} \quad = (m_e, m_e, m_e, m_e, \ldots)$$

and the components (which are of course functions of the temperature and the fields) obey the restrictions $m_a > 0 > m_b$, $m_c > 0 > m_d$ and $0 \geq m_e$. The Tables 2 and 4 show the ensuing limiting Gibbs states according to (4.13) where we have used special symbols to denote the *type* of the S_4-orbit states, which show up in their central decompositions.

We write

$(\downarrow\downarrow\downarrow\downarrow)$ if $m_1 = m_2 = m_3 = m_4 \leq 0$,
$(\uparrow\uparrow\uparrow\uparrow)$ if $m_1 = m_2 = m_3 = m_4 \geq 0$,
$(\uparrow\downarrow\downarrow\downarrow)$ if $m_1 > 0$, $m_2 = m_3 = m_4 \leq 0$,
$(\uparrow\uparrow\downarrow\downarrow)$ if $m_1 = m_2 > 0$, $m_3 = m_4 \leq 0$

each symbol designating the states of a whole S_4-orbit. $(\uparrow\downarrow\downarrow\downarrow)$, e.g., stands for all pure phase states which arise from the special one with $m_1 > 0$, $m_2 = \ldots = m_4 \leq 0$ by application of the S_4-transformations. The detailed *form* of the pure phase states depends, of course, on the values of the m_q-coordinates.

The restriction to positive B-values ($\varepsilon = (B, B, B, B, 0, \ldots, 0)$) is possible due to the fact that the self-consistency equations $m = \tilde{F}_{\beta\varepsilon}(m)$ as well as the specific free energy $f(\beta, \varepsilon, j \circ v^{-1}(m))$ are invariant under the mapping $(m, B) \mapsto (-m, -B)$.

To discuss the phase transition behaviour of our model system we recall the definitions given in [5].

Definition 4.3: (i) *A* phase transition *is a continuous curve of the form*

$$\gamma = \{(\beta(t), \varepsilon(t)) \in \mathbb{R}_+^* \times \mathbb{R}^{n_\infty} =: E;\ t \in I \subset \mathbb{R}\} \quad (4.14)$$

on which a qualitative change of the sets $M(\beta, \varepsilon) \subseteq M$ occurs, i.e., the number of the connected components and/or the dimensions of the connected components undergo a change. A point $(\beta^0, \varepsilon^0) \in \gamma$, which has different types of equilibrium sets $M(\beta, \varepsilon)$ in every neighbourhood, is called a transition point.

(ii) *A phase transition is called to be of* first or second kind *resp. if the set function*

$$t \mapsto M(\gamma(t))$$

is discontinuous or continuous resp. at the transition point (β^0, ε^0). Transition points of phase transitions of the second kind are called critical points.

A neighbourhood of a set $M(\beta, \varepsilon)$ can be simply constructed by the union of usual neighbourhoods (e.g., open balls) of its elements. The notion of *continuity of set functions* is more difficult to define (cf. [5]). Here the intuitive idea is sufficient, that the equilibrium states $M(\gamma(t))$ change continuously with changing t if *corresponding* elements of $M(\gamma(t))$ and $M(\gamma(t'))$ are close together whenever t and t' are so.

Examining the numerically computed results in Table 1 and 3 we arrive at the following statements concerning the transition points $(\beta, \varepsilon) \in E$ according to Def. 4.3(i) for phase transitions of our model system. We recall that $\varepsilon = (B, B, B, B, 0, \ldots, 0)$. In the case $w_0 < 0$, $w_1 = -w_0$ (Table 1) the sets $M(\beta, \varepsilon)$ have two elements for $\beta \geq \beta_c$ and $B = 0$ and one element otherwise, so there is a qualitative change on each continuous curve γ passing the points $(\beta, 0) \in E$, $\beta \geq \beta_c$. According to the numerical analysis the two solutions in $M(\beta, \varepsilon)$, $\beta > \beta_c$ and $B = 0$, are a finite distance apart

Table 3. The sets $M(\beta, \varepsilon)$ for $w_0 > 0$, $w_1 = -3w_0$ (cf. the text for an explanation of the symbols).

	$0 \le B < B_{c_1}$	$B = B_{c_1}$	$B_{c_1} < B < B_{c_2}$	$B = B_{c_2}$	$B_{c_2} < B$
$0 < \beta \le \beta_c$	$\tilde{O}_H(\bar{m})$				
$\beta_c < \beta \le \infty$	$\tilde{O}_H(m^{(2)})$	$\tilde{O}_H(m^{(1)}) \cup \tilde{O}_H(m^{(2)})$	$\tilde{O}_H(m^{(1)})$	$\tilde{O}_H(\bar{m}) \cup \tilde{O}_H(m^{(1)})$	$\tilde{O}_H(\bar{m})$

Table 4. The limiting Gibbs states $\omega^{\beta\varepsilon}$ for $w_0 > 0$, $w_1 = -3w_0$, $0 \le \lambda, \lambda' \le 1$.

	$0 \le B < B_{c_1}$	$B = B_{c_1}$	$B_{c_1} < B < B_{c_2}$	$B = B_{c_2}$	$B_{c_2} < B$
$0 < \beta \le \beta_c$	$(\downarrow\downarrow\downarrow\downarrow)$				
$\beta_c < \beta \le \infty$	$(\uparrow\uparrow\downarrow\downarrow)$	$\lambda(\uparrow\downarrow\downarrow\downarrow) + (1-\lambda)(\uparrow\uparrow\downarrow\downarrow)$	$(\uparrow\downarrow\downarrow\downarrow)$	$\lambda'(\downarrow\downarrow\downarrow\downarrow) + (1-\lambda')(\uparrow\downarrow\downarrow\downarrow)$	$(\downarrow\downarrow\downarrow\downarrow)$

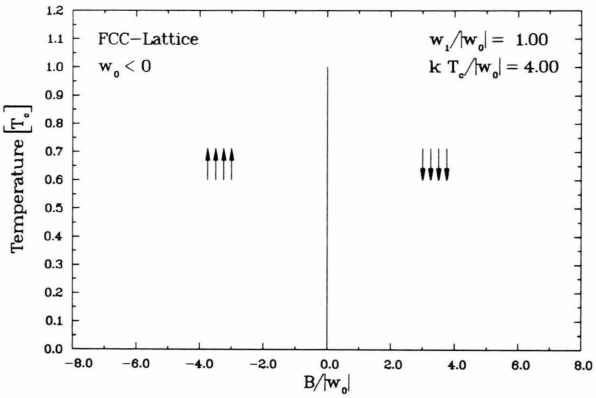

Fig. 2. Phase regions and transition points for $w_0 < 0$.

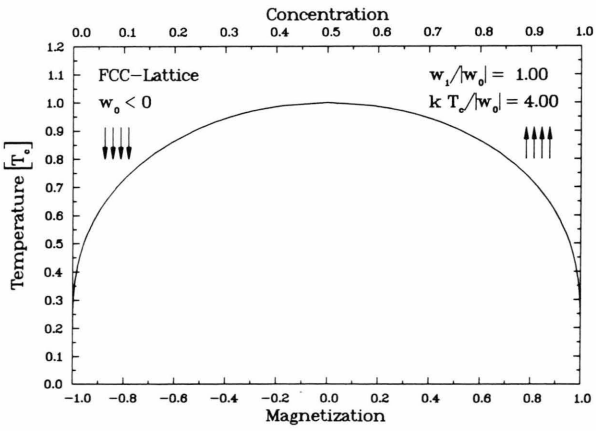

Fig. 3. Phase regions for $w_0 < 0$ depending on temperature and magnetization ($m = \sum_{q=1}^{4} m_q/4$) resp. concentration ($= (m+1)/2$).

because $m < 0$, but approach each other and finally are equal as β tends to β_c. So we conclude that there is a discontinuous change of the equilibrium sets for every process passing through the points $(\beta, 0)$, $\beta > \beta_c$, and a continuous one for every process through $(\beta_c, 0)$. The former phase transitions are therefore of first kind, while the latter are of second kind. Figure 2 shows the transition points in the B-T-diagram ($T = 1/k\beta$), while Fig. 3 displays the different phase regions in terms of the temperature and the magnetization (per cell). Some more comments on the figures follow the discussion of the second model class which we have evaluated numerically.

In the case $w_0 > 0$, $w_1 = -3w_0$ (Table 3) the situation is more complicated. Above a critical inverse temperature β_c there exist two critical fields $0 < B_{c_1}(\beta) < B_{c_2}(\beta)$. If $\beta > \beta_c$ and $0 \le B < B_{c_1}(\beta)$ the sets $M(\beta, \varepsilon)$ contain one orbit with six elements according to S_4-symmetry; if $\beta > \beta_c$ and $B = B_{c_1}(\beta)$ there are two orbits with ten elements altogether; if $\beta > \beta_c$ and $B_{c_1}(\beta) < B < B_{c_2}(\beta)$ there is one orbit with four elements; finally if $\beta > \beta_c$ and $B = B_{c_2}(\beta)$ there are two orbits with five elements. In all other combinations of β and B the set $M(\beta, \varepsilon)$ has only one element. According to numerical analysis the critical fields $B_{c_1}(\beta)$ and $B_{c_2}(\beta)$ tend to zero and the several elements in each of the above given sets $M(\beta, \varepsilon)$, $\beta > \beta_c$, approach each other as $\beta \downarrow \beta_c$. So we conclude that every phase transition passing through the points $(\beta, \varepsilon) \in E$, $\beta > \beta_c$ and $B = B_{c_1}(\beta)$ or $B = B_{c_2}(\beta)$, is of first kind because independently of the direction of approach the sets $M(\beta, \varepsilon)$ are enlarged discontinuously by a new orbit of pure phase states.

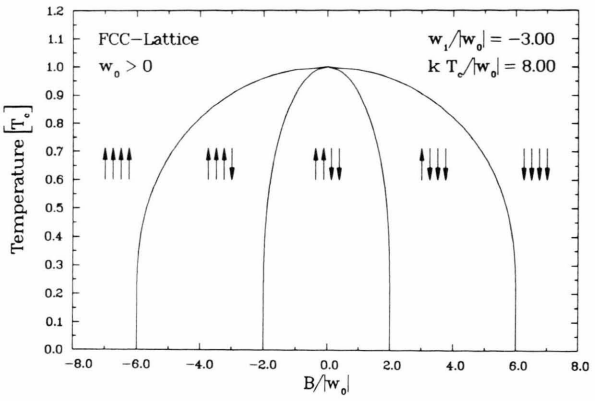

Fig. 4. Phase regions and transition points for $w_0 > 0$.

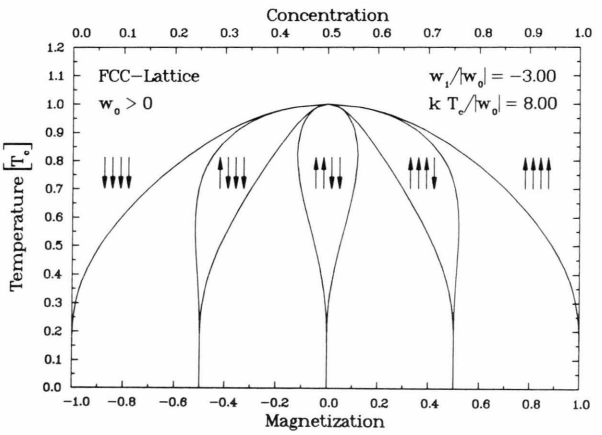

Fig. 5. Phase regions for $w_0 > 0$ depending on temperature and magnetization resp. concentration.

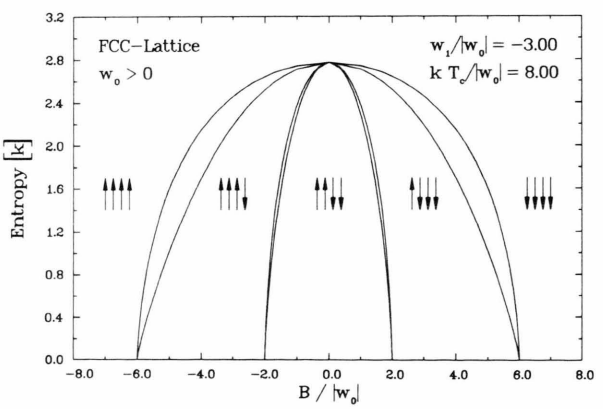

Fig. 6. Values of the entropy $s(m)$ in the transition points of Figure 4.

Every phase transition through $(\beta_c, 0) \in E$ is of second kind on the other hand because it is accompanied by a continuous change of the pure phase states. Figure 4 shows the transition points in the B-T-diagram and Fig. 5 is like Fig. 3 a temperature-magnetization diagram.

The arrow symbols in all figures denote regions where the pure phase states belong to one orbit of the group of inner symmetries and a unique limiting Gibbs state exists. The connected regions without arrows are regions where the pure phase states consist of two orbits and the limiting Gibbs state is a convex combination of the corresponding two S_4-orbit states (cf. Tables 2 and 4), which have different entropy values. These regions are usually called coexistence regions.

Figure 6 shows the entropy (cf. Sect. 5) of the coexisting S_4-orbit states in the transition points of Figure 4. The vertical difference between two curves in Fig. 6 separating two different phase regions multiplied with the corresponding temperature of Fig. 4 gives the latent heat of the first-kind phase transitions.

In Sect. 5 we provide some analytical arguments that the points $(\beta_c, 0) \in E$ in the two considered cases are critical points in the sence of Definition 4.3.

5. Miscroscopic Treatment of the Landau Scenario

We summarize the general ideas worked out in [5] as far as we need them here for the discussion of our model systems.

As is well known Landau based his analysis of phase transitions of second kind [13, 14] (in the english translation of his textbook they are called of *second order* which may be confused with Ehrenfest's notion) on a Taylor expansion of a certain thermodynamic free energy with regard to a so-called order parameter, the equilibrium values of which are determined by a variational principle. Conditions for second-kind phase transitions to occur were given in terms of the properties of the coefficients of this expansion.

The class of models given by the Hamiltonians (3.1) has a specific (thermodynamic) free energy $f(\beta, \varepsilon; m) = f(\beta, \varepsilon, j \circ v^{-1}(m))$ (cf. Eq. (4.4) and [5]) which explicitly reads

$$f(\beta, \varepsilon; m) = \varepsilon \bullet m + m \bullet wm - \beta^{-1} s(m) \quad (m \in M), \quad (5.1)$$

where

$$s(m) = -\mathrm{tr}_{\mathscr{B}}\{v^{-1}(m) \ln v^{-1}(m)\} \quad (5.2)$$

is the specific entropy. $f(\beta, \varepsilon; m)$ seems to us to be the appropriate function for an analysis in the sense of Landau: It depends on the one hand on (intensive) macroscopic parameters (β and ε) and on the other hand on some *non-equilibrium variables* m the equilibrium values of which are determined by the variational principle

$$f(\beta, \varepsilon; \bar{m}) = \inf f(\beta, \varepsilon; M) \tag{5.3}$$

which is the thermodynamic version of (4.6) using the bijective mapping $j \circ v^{-1}$.

Restricting the variation in m to a sufficiently smooth curve $\{\varkappa(\eta) \in M; \eta \in \mathbb{R}\}$, e.g., a straight line, one can expand the function $f(\beta, \varepsilon; \varkappa(\eta))$ into an asymptotic power series[2] with regard to the curve parameter η

$$\begin{aligned} &f(\beta, \varepsilon; \varkappa(\eta)) \\ &\quad = f(\beta, \varepsilon; \varkappa(0)) + \alpha\eta + A\eta^2 + B\eta^3 + C\eta^4 + \dots . \end{aligned} \tag{5.4}$$

Doing this for every temperature-field tupel of a continuous curve $\gamma = \{(\beta, \varepsilon(\beta)); \beta \in \mathbb{R}_+^*\}$ in E (which is a special case of Def. 4.3(i)) the so-called *Landau scenario* can be formulated as follows. There is a phase transition of second kind in $\beta^0 \in \mathbb{R}_+^*$ if the coefficients in Eq. (5.4) fulfill:

$$\begin{aligned} &\alpha(\gamma(\beta)) = 0 \quad \text{for all } \beta, \\ &A(\gamma(\beta)) \quad \begin{cases} > 0 & \text{if } \beta < \beta^0, \\ = 0 & \text{if } \beta = \beta^0, \\ < 0 & \text{if } \beta > \beta^0, \end{cases} \\ &B(\gamma(\beta^0)) = 0, \\ &C(\gamma(\beta^0)) > 0. \end{aligned} \tag{5.5}$$

In [5] arguments are provided that the conditions (5.5) characterize a special case of a second-kind phase transition in the sense of Definition 4.3(ii).

The conditions (5.5) imply that below the (inverse) transition temperature β^0 the equilibrium value of the curve parameter is $\bar{\eta} = 0$ ($A > 0$ implies a convex shape of $f(\beta, \varepsilon; \varkappa(\eta))$ in the vicinity of $\eta = 0$) while above β^0 the equilibrium value will be $\bar{\eta} \neq 0$ ($A < 0$ implies a concave shape). The parameter η of a curve $\varkappa$ leading to (5.5) thus behaves like an order parameter. The curves we consider hereafter enter the coefficients $\alpha, \dots, C$ in terms of their first derivatives $\varkappa'(0)$ only. Directions $\varkappa'(0)$ leading to (5.5) with especially the necessary condition for A are called *active directions.*

[2] $f(\beta, \varepsilon; .)$ is a C^∞-function [5].

The determination of the active directions of our model systems gives an explanation for the occurrence of only two types of phase diagrams in Sect. 4; furtheron we get an analytical formula for the critical temperature and arrive at proposals for order parameters including the ones given in the literature, e.g. in [7].

We first need the specific entropy (5.2) which we have to compute not for all thermodynamic states $m \in M$ but only for the ones in the subset

$$\begin{aligned} v(W_r) := \{&(m_r, \Phi(m_r)) \in M; \\ &m_r := (m_1, \dots, m_4) \in \times_{i=1}^4 [-1, +1]\}, \end{aligned} \tag{5.6}$$

where

$$W_r := \left\{ \varrho \in W;\ \varrho = \varrho(m_r) = \bigotimes_{i=1}^4 \tfrac{1}{2}(\mathbb{1} + m_i \sigma_z),\ m_i \in [-1, +1] \right\} \tag{5.7}$$

is a subset of the one-cell density matrices containing the pure phase density matrices for the model systems considered here according to the general theory (cf. Sect. 3 and 4, esp. Eq. (4.9) and (4.10)). This means with other words that the set $v(W_r)$ contains all solutions of the variational problem (5.3). The map Φ: $\times_{i=1}^4 [-1, +1] \to \mathbb{R}^{n_{\mathscr{B}}-4}$ with values

$$\Phi(m_r) = (\mathrm{tr}_{\mathscr{B}}\{\varrho(m_r)\, \hat{e}_5\}, \dots, \mathrm{tr}_{\mathscr{B}}\{\varrho(m_r)\, \hat{e}_{n_{\mathscr{B}}}\})$$

is C^∞, because all components are fourth-order polynomials in m_i ($i = 1, \dots, 4$), thus making $v(W_r)$ a C^∞-manifold.

Lemma 5.1: *For arguments in $v(W_r)$ the specific entropy $s(m) = -\mathrm{tr}_{\mathscr{B}}\{v^{-1}(m) \ln v^{-1}(m)\}$ has the values*

$$\begin{aligned} &s(m_r, \Phi(m_r)) \\ &\quad = -\sum_{i=1}^4 \left\{ \frac{1+m_i}{2} \ln \frac{1+m_i}{2} + \frac{1-m_i}{2} \ln \frac{1-m_i}{2} \right\} \end{aligned}$$

where $-1 \leq m_i \leq +1$ ($i = 1, \dots, 4$).

Proof: With the definition

$$v^{-1}(m_r, \Phi(m_r)) = \varrho(m_r) = \bigotimes_{i=1}^4 \tfrac{1}{2}(\mathbb{1} + m_i \sigma_z)$$

and the property

$$\begin{aligned} \ln \varrho(m_r) = &\{\ln \tfrac{1}{2}(\mathbb{1} + m_1 \sigma_z)\} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} + \dots \\ &\dots + \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \{\ln \tfrac{1}{2}(\mathbb{1} + m_4 \sigma_z)\} \end{aligned}$$

the above formula can be easily derived. □

The connection between the variational problem (5.3) and its solutions $M(\beta, \varepsilon)$ on the one hand and the

Landau scenario (5.5) on the other hand is established by a suitable choice of the testing curves $\varkappa$. After the previous remarks the sets $M(\beta, \varepsilon)$ are contained in $v(W_r)$. Thus we choose the curves $\varkappa$ to lie in $v(W_r)$, too.

Lemma 5.2: *With ε, w given in Lemma* 3.2, $m^0, m' \in \times_{i=1}^4 [-1, +1]$ *and* $\varkappa(\eta) = (m^0 + \eta m', \Phi(m^0 + \eta m'))$ $(\eta \in \mathbb{R}$, *such that* $m^0 + \eta m' \in \times_{i=1}^4 [-1, +1])$ *the coefficients of the expansion* (5.4) *read:*

$$\alpha = \alpha(\beta, \varepsilon) = \sum_{k=1}^{4} \left\{ \varepsilon_k + 2 \sum_{i=1}^{4} w_{ki} m_i^0 + \beta^{-1} \tfrac{1}{2} \ln \frac{1+m_i^0}{1-m_i^0} \right\} m_k',$$

$$A = A(\beta) = \tfrac{1}{2} \sum_{k,i=1}^{4} \left\{ 2 w_{ki} + \frac{\delta_{ki} \beta^{-1}}{1-(m_i^0)^2} \right\} m_k' m_i',$$

$$B = B(\beta) = -\frac{\beta^{-1}}{6} \sum_{i=1}^{4} \left\{ \frac{-2 m_i^0}{(1-(m_i^0)^2)^2} \right\} m_i'^3,$$

$$C = C(\beta) = \frac{\beta^{-1}}{24} \sum_{i=1}^{4} \left\{ \frac{2(1-(m_i^0)^2)^2 + 8 (m_i^0)^2 (1-(m_i^0)^2)}{(1-(m_i^0)^2)^4} \right\} m_i'^4.$$

Proof: (5.4) shows the first five summands of the power series expansion

$$f(\beta, \varepsilon; \varkappa(\eta)) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\mathrm{d}^n}{\mathrm{d}\eta^n} f(\beta, \varepsilon; \varkappa(\eta))|_{\eta=0} \eta^n$$

the coefficients of which are given above using the chain rule and the restricted model free energy

$$f(\beta, \varepsilon; \varkappa(\eta)) = \varepsilon \bullet \varkappa(\eta) + \varkappa(\eta) \bullet w \varkappa(\eta) + \beta^{-1} \sum_{i=1}^{4} \left\{ \frac{1+\varkappa(\eta)_i}{2} \ln \frac{1+\varkappa(\eta)_i}{2} + \frac{1-\varkappa(\eta)_i}{2} \ln \frac{1-\varkappa(\eta)_i}{2} \right\}.$$

By a suitable choice of the origin m^0 on the curve $\varkappa$ the first and third condition in (5.5) can be fulfilled as we will show later, while the fourth condition holds already for all $m^0 \in \times_{i=1}^4 [-1, +1]$ and all directions $m' \neq 0$. To examine the validity of the second condition it is obviously helpful to know the eigenvalues of the interaction matrix $w = (w_{ik})$. Since the second derivatives of the specific entropy are strictly negative $(-\delta_{ki}/(1-(m_i^0)^2)) - s(m)$ is a strictly concave function (cf. [5]) – there must be necessarily negative eigenvalues of w to provide a sign change of A, which is positive for very small β (high temperature range). The corresponding eigenvectors are the active directions.

Proposition 5.3: *The matrix w given in Lemma* 3.2 *has the following eigenvalues (EV) and eigenspaces (ES):*

(i) $\lambda_1 = w_1 + 3 w_0$ *is a simple EV with ES* $\mathbb{R}_1^{n_{\mathcal{B}}} = \mathbb{R}(1, 1, 1, 1, 0, \ldots, 0)$;

(ii) $\lambda_2 = w_1 - w_0$ *is a threefold EV with ES* $\mathbb{R}_2^{n_{\mathcal{B}}} = \mathrm{span}_{\mathbb{R}} \{b_1, b_2, b_3\}$ *where*

$$b_1 = (1, -1, 0, 0, 0, \ldots, 0)$$
$$b_2 = (1, 0, -1, 0, 0, \ldots, 0)$$
$$b_3 = (1, 0, 0, -1, 0, \ldots, 0).$$

(iii) $\lambda_3 = 0$ *is a* $(n_{\mathcal{B}} - 4)$*-fold EV with ES* $\{\mathbb{R}_1^{n_{\mathcal{B}}} + \mathbb{R}_2^{n_{\mathcal{B}}}\}^{\perp}$.

If $w_0 > 0$, i.e. $\lambda_2 < \lambda_1$, there must be $\lambda_2 < 0$; if $w_0 < 0$, i.e. $\lambda_1 < \lambda_2$, there must be $\lambda_1 < 0$ or else there occurs no phase transition resp. there is a factorial limiting Gibbs state $\omega^{\beta\varepsilon}$ for all temperatures $\beta \in \mathbb{R}_+^*$ and fields $\varepsilon \in \mathbb{R}^{n_{\mathcal{B}}}$.

Proof: (i)–(iii) follows by direct calculation. The second part is implied by [5], Section 4. □

Figure 7 shows the ranges of the interaction parameters where phase transitions can occur and the corresponding active directions. As one sees there are two different connected regions leading to two types of phase diagrams an example of each was given in Sect. 4, where the numerical analysis indicated that in both cases $(\beta, 0) \in E$ is a critical point in the sense of Definition 4.3(ii). We now give an analytical proof.

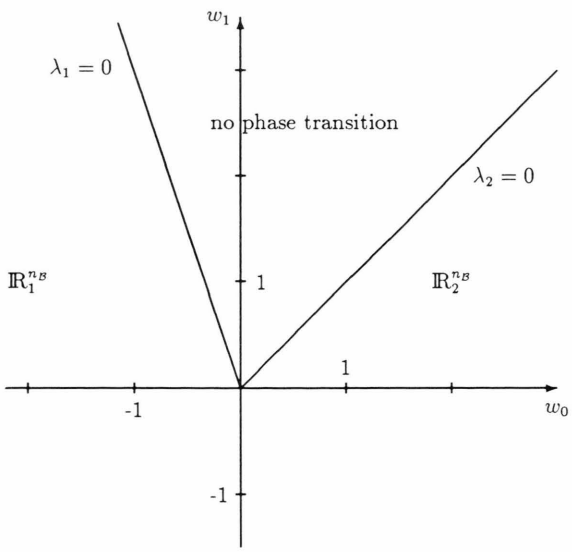

Fig. 7. Active directions for phase transitions in dependence on the interaction parameters w_0 and w_1.

Proposition 5.4: *Let be* m^0 *a solution of* (4.11) *and* $m'=(m'_1,\ldots,m'_4,0,\ldots,0)$ *an arbitrary normalized active direction, i.e.,*

(1) $m'\in\mathbb{R}_1^{n_\mathcal{A}}$ *if* $w_0<0$ *and* $\lambda_1=w_1+3w_0<0$,
(2) $m'\in\mathbb{R}_2^{n_\mathcal{A}}$ *if* $w_0>0$ *and* $\lambda_2=w_1-w_0<0$.

Then the coefficients in Lemma 5.2 *fulfill:*

(i) $\alpha(\beta,\varepsilon)=0$;
(ii) $C(\beta)>0$.

Along the continuous curve

$$\gamma\colon\ \mathbb{R}_+^*\to E,\ \beta\mapsto(\beta,0)$$

there holds additionally

(iii) $B(\beta)=0$,
(iv) $A(\beta)>0$ *if* $\beta<\beta_c$, $A(\beta)<0$ *if* $\beta>\beta_c$,

where the critical temperature

$$\beta_c=\begin{cases}-(2\lambda_1)^{-1} & \text{if}\quad w_0<0\\ -(2\lambda_2)^{-1} & \text{if}\quad w_0>0\end{cases}$$

is determined by $A(\beta)=0$. *In the sense of Def.* 4.3 γ *is then a second-kind phase transition and* $(\beta_c,0)$ *a critical point.*

Proof: (i) m^0 is a solution of

$$m_k^0=-\tanh\beta\left\{\varepsilon_k+2\sum_{i=1}^{4}w_{ki}\,m_i^0\right\}\quad(k=1,\ldots,4)$$

(Prop. 4.1(2)) resp.

$$\operatorname{Artanh} m_k^0=\tfrac{1}{2}\ln\frac{1+m_k^0}{1-m_k^0}=-\beta\left\{\varepsilon_k+2\sum_{i=1}^{4}w_{ki}\,m_i^0\right\},$$

which gives $\alpha(\beta,\varepsilon)=0$.

(ii) $m_i^0\in(-1,+1)$, $i=1,\ldots,4$, which implies $C(\beta)>0$.

(iii), (iv) The solution $m^0=(0,0,0,0,\ldots)$ for $\varepsilon=0$ gives $B(\beta)=0$ for arbitrary $\beta\in\mathbb{R}_+^*$. If $w_0<0$

$$A(\beta)=\lambda_1+(2\beta)^{-1}=0$$

implies $\beta_c=-(2\lambda_1)^{-1}$, while if $w_0>0$

$$A(\beta)=\lambda_2+(2\beta)^{-1}=0$$

implies $\beta_c=-(2\lambda_2)^{-1}$. γ thus fulfills the conditions of the Landau scenario (5.5) being a continuous phase transition in the sense of Def. 4.3(ii) ([15] Prop. 4.51). □

As already mentioned the curve parameters of curves $\varkappa(\eta)=(m^0+\eta m',\Phi(m^0+\eta m'))$ with m' an active direction can serve as order parameters, where the origin m^0 can always be chosen such that above the transition temperature the equilibrium value is $\bar\eta=0$ and below there is $\bar\eta\neq0$. If there are several distinct pure phases below the transition temperature there are sometimes vectorial order parameters in use in the literature. E.g., for the model system considered here, the vectorial order parameters

$$\tilde m_1^{\uparrow\uparrow\downarrow\downarrow}=(m_1+m_2-m_3-m_4)/4,$$
$$\tilde m_2^{\uparrow\uparrow\downarrow\downarrow}=(m_1-m_2-m_3+m_4)/4,$$
$$\tilde m_3^{\uparrow\uparrow\downarrow\downarrow}=(m_1-m_2+m_3-m_4)/4,$$

resp.

$$\tilde m_1^{\uparrow\downarrow\downarrow\downarrow}=[3m_1-(m_2+m_3+m_4)]/6,$$
$$\tilde m_2^{\uparrow\downarrow\downarrow\downarrow}=[3m_2-(m_3+m_4+m_1)]/6,$$
$$\tilde m_3^{\uparrow\downarrow\downarrow\downarrow}=[3m_3-(m_4+m_1+m_2)]/6,$$
$$\tilde m_4^{\uparrow\downarrow\downarrow\downarrow}=[3m_4-(m_1+m_2+m_3)]/6,$$

were introduced in [7] to describe the several superstructures if $w_0>0$. Each component belongs to another pure phase the values ranging from -1 to $+1$ and can be viewed as the projection of a selfconsistent solution $m\in\mathbb{R}^{n_\mathcal{A}}$ onto a special active direction, e.g., $\tilde m^{\uparrow\uparrow\downarrow\downarrow}=\frac{1}{4}(1,1,-1,-1,0,\ldots,0)\bullet m$. Let be m lie on the curve $\varkappa(\eta)=(m^0+\eta m',\ldots)$ with $m^0=(\bar m^0,\bar m^0,\bar m^0,\bar m^0)$ and $m'=\frac{1}{2}(1,1,-1,-1)$ be a normalized active direction in $\mathbb{R}_2^{n_\mathcal{A}}$. Then $\tilde m^{\uparrow\uparrow\downarrow\downarrow}$ can be identified as a multiple of the curve parameter η and thus fits to our scheme.

6. Conclusions

The model systems worked out in the preceding investigation are, to the best of our knowledge, the first rigorously treated models with several symmetry breaking orbits, in spite of the fact that this seems to be not an untypical property of systems with continuous and discontinuous phase transitions.

The rigorous treatment is enabled by the use of a long-range interaction instead of the usual short-range interactions, which can be viewed as a kind of approximation, an idea which should be the subject of future research. The fact that the approximation already covers essential features illustrate the computed phase diagrams which agree with short-range diagrams with respect to their topological structure. Besides that a lot of qualitative results is up to now not available for short-range models as, e.g., the H-orbit structure of the limiting Gibbs states and the general connections between quantum statistical and thermo-

dynamical notions (which leads here to the microscopic foundation of the Landau scenario). In the opinion of the present authors the advanced numerical methods for short range models should be supplemented by structural investigations, even if they may be rigorously carried through for simplified interactions only.

Acknowledgements

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