Limiting Gibbs States and Phase Transitions of a Bipartite Mean-Field Hubbard Model

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In the frame of operator-algebraic quantum statistical mechanics we calculate the grand canonical equilibrium states of a bipartite, microscopic mean-field model for bipolaronic superconductors (or anisotropic antiferromagnetic materials in the quasispin formulation). Depending on temperature and chemical potential, the sets of statistical equilibrium states exhibit four qualitatively different regions, describing the normal, superconducting (spin-flopped), charge ordered (antiferromagnetic), and coexistence phases. Besides phase transitions of the second kind, the model also shows phase transitions of the first kind between the superconducting and the charge ordered phases. A unique limiting Gibbs state is found in its central decomposition for all temperatures, even in the coexistence region, if the thermodynamic limit is performed at fixed particle density (magnetization).

1. INTRODUCTION

The aim of this paper is the determination of the phase diagrams and of the limiting Gibbs states of a homogenized Hubbard like model. The original Hamiltonian with short range interaction was introduced in refs. 1 and 2 (see also ref. 3) for systems with bipolaronic interactions leading to superconductivity of condensed bipolarons:

$$H = v \sum_{\langle i; j \rangle} \hat{n}_i \hat{n}_j - 2t \sum_{\langle i; j \rangle} (b_i^* b_j + b_i b_j^*)$$

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Here b_i^* is the creation operator of a bipolaron at the site i, $\hat{n}_i$ the corresponding occupation number operator, and $\sum_{\langle i; j \rangle}$ the sum over nearest neighbours. In ref. 4, the model is discussed in the context of high-T_c superconductors. In the quasispin formulation the Hamiltonian describes an anisotropic antiferromagnet. The same kind of interaction can be found in the literature for lattice gas models of liquid helium.[5, 6] In many investigations, the equilibrium states of this model at finite temperatures are treated in various mean-field approximations. It was observed that, depending on some "parameters", a first order phase transition (e.g., for the anisotropic antiferromagnet) can split up into two transitions of second order (a supersolid phase in a lattice gas model of liquid helium, resp. a superconductive and charge ordered phase in the above noted bipolaronic systems). This effect is related with the problem of "bicritical" and "tetracritical" points, discussed more or less phenomenologically in the literature.[7-10] We focus here on a microscopical derivation of the equilibrium states by means of the limiting grand canonical ensemble. It is in this set up where the first order transition takes place. The splitting of the first order phase transition into two continuous phase transitions will be treated elsewhere, using an ensemble with suppressed particle fluctuations.[11]

The macroscopic-thermodynamic properties of the model will be deduced in the frame of operator-algebraic quantum statistical mechanics.[12, 13] With the intention of using the generalized mean-field frame, we replace the original Hamiltonian with nearest neighbour interaction by a homogeneous one, which is obtained by a certain form of symmetrization. Symmetrizing usual interactions (which are only translation invariant) over the lattice is the systematic way to obtain the mean-field approximation in terms of a new quasi-microscopic model. If the original interaction is an element of the largest Banach space of interactions used in ref. 14, the resulting mean-field model obtained by symmetrization falls into the class, which is in virtue of rigorous developments[15-18] completely under theoretical control. The existence of the limiting equilibrium and non-equilibrium dynamics (with nontrivial classical part) and of the limiting free energy density as well as the validity of so-called variational principles are ensured. Depending, however, on the kind of symmetrization, various mean-field schemes may arise: If it is performed for the above bipolaronic model uniformly over the whole lattice, we find the analogue to the mean-field ansatz in refs 19 and 20. If a bipartite sub-lattice structure is retained during the symmetrization, the ansatz of refs. 1 and 2 is found. Only the clear separation of these procedures avoids the confusion, which has arosen in the literature. This is why details of the second procedure will be described in Section 2 leading to the basic model Hamiltonian of this paper. (For another scheme of a mean-field like approximation of the Hubbard model, cf. ref. 21.)

We evaluate the thermodynamic properties, especially the different phase regions, of our model with a special emphasis on the so-called limiting Gibbs states. These are by definition the accumulation points of the net of the local (here grand canonical) equilibrium states. One knows by a variational principle, that the limiting Gibbs states minimize the limiting free energy density. They are special equilibrium states, which exhibit still the (internal) symmetries of the original local Hamiltonians, even in the case of phase transitions. The set of all eqilibrium states for a given temperature and interaction—defined just by minimizing the free energy density—is a w^*-compact face and a Bauer-simplex of the statistical state space. Its extremal boundary are the pure phase states, which in general have a lower symmetry than the limiting Gibbs states. If the extremal boundary is just one orbit of the broken symmetry group its ergodic mean is the only fully invariant equilibrium state and coincides thus with each of the limiting Gibbs states. In this most frequent case of a unique limiting Gibbs state, its unique extremal decomposition (which coincides with the algebraic central decomposition into pair-wise disjoint factor states) covers all pure phase states and thus determines all of the equilibrium states by various forms of mixing the pure phases. (Note that the free energy density is an affine funtion of the states and retains its minimal value during this mixing of minimal pure phase states.)

The usual strategy in many body physics is to approximate directly the pure phase states by introducing appropriate, symmetry breaking boundary conditions while going into the thermodynamic limit. For lattice systems these are in first line additional interactions with the environment (including the zero interaction for "free boundary conditions"). Other forms of subsidiary conditions may be represented by singular external interactions. For mean-field models it has been demonstrated in ref. 22 that for each pure phase there is a net of perturbations, which vanish in the thermodynamic limit, such that the modified limiting Gibbs state is the prescribed pure phase state. Since there is, however, no systematic way to obtain all pure phases in the latter manner, the determination of the limiting Gibbs states for free boundary conditions has some advantages, if it can be carried through at all.

The limiting Gibbs states are most frequently determined via a net of local reduced Hamiltonians with fixed chemical potential. In the coexistence region the particle density is a multi-valued function of temperature and chemical potential. We are able to demonstrate that a given particle density (instead of the chemical potential) determines *a unique limiting Gibbs state in the coexistence region of the first order phase transition.* The proof of uniqueness for such a case was an open problem for a long time (comp. ref. 23). Especially it is described in ref. 24, how at the

first Van der Waals conference in 1937 it was still a controversial question, whether statistical mechanics is able to produce instead of the meta- and instable parts of the isotherms for a fluid the stable coexistence line with variable particle density at fixed β and μ.

Emphasizing the superconductor interpretation another central point is to describe the nature of the superdonducting condensate, which most concisely is charcterized by the mathematical form of the condensed pair operators. These operators can be formed in the GNS-representation over the limiting Gibbs state by averaging the normal pair operators (in the representation dependent strong operator topology). It belongs to the advantages of such simplified models as the considered one, that these operators can be calculated explicitly, allowing for a comparison with the general idea of Goldstone bosons.

The paper is organized as follows: In Section 2, we give a sketch of the necessary operator-algebraic framework, define the local Hamiltonians and their symmetrization, and introduce the essential internal symmetries. In Section 3, the concepts of general equilibrium and of pure phase states are introduced, and the limiting Gibbs states are formulated with the aid of their central decomposition. In Subsections 3.1 and 3.2 we determine the limiting Gibbs state at fixed chemical potential μ, resp. particle density n. In particular, we demonstrate a unique limiting Gibbs state in each phase region, even in the coexistence region of the first order phase transition (Theorem 3.3). In the Conclusions we discuss beside other things the condensed pair operators in the superconducting phase.

Altogether, the present model discussion is intended to illustrate the general scheme of operator-algebraic mean-field theory. The arising phase diagram, with two different kinds of broken symmetry, provides a non-trivial application for the thermodynamic formalism as worked out in ref. 25. The introduction of (weak) inhomogeneities by site dependent terms in the interactions and a kind of continuum limit for the momenta seem to be possible in a rigorous form. These modifications would make more transparent the connections to further models for strongly correlated electronic systems (cf., e.g., contributions in refs. 26 and 27).

2. INTRODUCTION OF THE MODEL

The first step for introducing the quantum statistical formalism in the thermodynamic limit is to specify the quasi-local C^*-algebra of observables for the infinite lattice. On each lattice site we consider a quantum system with a finite number of relevant levels which we represent at first by a matrix-algebra $\mathfrak{B}$. Later on we introduce a bi-partite lattice structure and combine two $\mathfrak{B}$'s to the cell algebra $\mathfrak{B}$. The explicit taking into account of

the sub-lattice structure helps to avoid a confusion in the literature and leads to the appropriate symmetrization which is performed in accordance with the general microscopic mean-field strategy.

2.1. The Quasi-Local Algebra

We start with a lattice $\mathscr{H}$ with two dimensional quantum systems at each site $i \in \mathscr{H}$. The corresponding algebra of observables is given by $\mathfrak{B}_i \cong \mathfrak{B} \cong M_2(\mathbb{C})$ for all $i \in \mathscr{H}$. The local algebra $\mathfrak{A}_{\tilde{\Lambda}} := \bigotimes_{i \in \tilde{\Lambda}} \mathfrak{B}_i$ for $\tilde{\Lambda} \in \mathfrak{L} = \{ \tilde{\Lambda}' \subset \mathscr{H} \mid |\tilde{\Lambda}'| < \infty \}$ includes the observables of a finite subregion $\tilde{\Lambda} \subset \mathscr{H}$. With the usual set-inclusion and the corresponding canonical embedding of analgebra $\mathfrak{A}_{\tilde{\Lambda}}$ into $\mathfrak{A}_{\tilde{\Lambda}'}$, provided $\tilde{\Lambda} \subset \tilde{\Lambda}'$, the C^*-inductive limit[28] gives the appropriate abstract quasi-local C^*-algebra $\mathfrak{A}$ of the infinitely extended lattice system:

$$\mathfrak{A} := \bigotimes_{i \in \mathscr{H}} \mathfrak{B}_i \tag{2.1}$$

The local algebras $\mathfrak{A}_{\tilde{\Lambda}}$ may be considered as subalgebras of $\mathfrak{A}$ and then it holds

$$\mathfrak{A} = \overline{\bigcup_{\tilde{\Lambda} \in \mathfrak{L}} \mathfrak{A}_{\tilde{\Lambda}}}^{\|\cdot\|}$$

Especially, a certain model is defined by a family of local Hamiltonians $H_{\tilde{\Lambda}}$ for each finite lattice region $\tilde{\Lambda} \in \mathfrak{L}$, where $H_{\tilde{\Lambda}}$ is in $\mathfrak{A}_{\tilde{\Lambda}} \subset \mathfrak{A}$.

An isomorphic algebra, more suitable for our purpose, is constructed by rearranging the original lattice into two equally sized sub-lattices (see Fig. 1). Then we form a new lattice point by collecting one point of each sub-lattice. Again, the set of the twofold sites is a lattice, now denoted
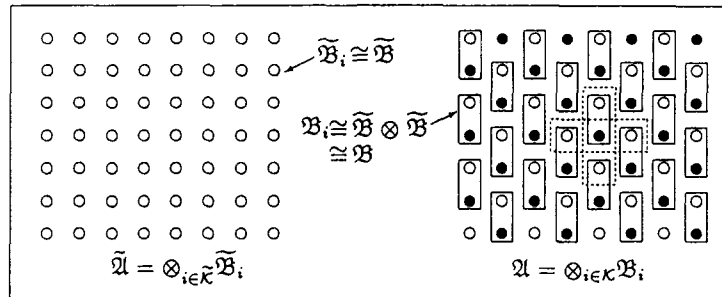

Fig. 1. Sub-lattices and the quasi-local algebra.

by $\mathcal{H}$. The C^*-inductive limit of the local algebras $\mathfrak{A}_\Lambda$, $\Lambda \in \mathfrak{L} := \{\Lambda' \subset \mathcal{H} \mid |\Lambda'| < \infty\}$ leads now to

$$\mathfrak{A} := \bigotimes_{i \in \mathcal{H}} \mathfrak{B}_i \tag{2.2}$$

where the $\mathfrak{B}_i$ are isomorphic to $\mathfrak{B} = \tilde{\mathfrak{B}} \otimes \tilde{\mathfrak{B}} \cong M_4(\mathbb{C})$, for all $i \in \mathcal{H}$. Obviously, $\tilde{\mathfrak{A}}$ and $\mathfrak{A}$ are algebraically isomorphic. Nevertheless, the second form $\mathfrak{A}$ is more suitable to treat our mean-field approximation with a sublattice structure and leads to another type of internal and permutation symmetries than by using $\tilde{\mathfrak{A}}$.

2.2. The Local Pairing Interaction and Its Microscopic Mean-Field Version

As an example for a net of local Hamiltonians $H_{\tilde{\Lambda}}$, $\tilde{\Lambda} \in \tilde{\mathfrak{L}}$, we consider a certain kind of Hubbard–Hamiltonians for a system with local pairing interactions:

$$H_{\tilde{\Lambda}} = \tilde{v} \sum_{\langle i;j \rangle \in \tilde{\Lambda}} \hat{n}_i \hat{n}_j - 2\tilde{t} \sum_{\langle i;j \rangle \in \tilde{\Lambda}} (b_i^* b_j + b_i b_j^*) \in \tilde{\mathfrak{A}}_{\tilde{\Lambda}} \tag{2.3}$$

The summation $\sum_{\langle i;j \rangle \in \tilde{\Lambda}}$ runs over nearest neighbors $i, j \in \tilde{\Lambda}$, $b_i^{(*)}$ is the annihilation (creation) operator of a local pair at the lattice site i, and $\hat{n}_i := b_i^* b_i$ is the occupation number operator. They are characterized in the "pair-algebra" by the following commutation relations (typical for hard-core Bosons; for the relation of this algebra to the CAR-algebra, see ref. 29):

$$[b_i^*; b_j] = b_i^* b_j - b_j b_i^* = \delta_{ij}(2\hat{n}_i - 1), \quad \{b_i^*; b_i\} = b_i^* b_i + b_i b_i^* = 1, \quad b_i^2 = 0$$

The operators $b_i^{(*)}$ and $\hat{n}_i$ are represented by 2×2-matrices embedded in $\tilde{\mathfrak{A}}_{\{i\}} \subset \tilde{\mathfrak{A}}$:

$$b_i = 1 \otimes \cdots \otimes 1 \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes 1 \cdots \qquad \hat{n}_i = 1 \otimes \cdots \otimes 1 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes 1 \cdots$$

$$\uparrow \qquad\qquad\qquad\qquad\qquad\qquad \uparrow$$
$$\text{site } i \qquad\qquad\qquad\qquad\qquad \text{site } i \tag{2.4}$$

The constant $\tilde{v}$ in Eq. (2.3) is an effective (Coulomb-) interaction between neighboring sites, and $\tilde{t}$ describes the hopping frequency of a local pair. We assume both $\tilde{v}$ and $\tilde{t}$ to be positive. Besides these two interactions, we shall

consider a term which is linear in the particle number. It will be treated explicitly in Section 3 as a part of the chemical potential μ. The Hamiltonian (2.3) is motivated in refs. 1–3 (cf. also ref. 19) for bipolaronic interactions. For an overview and more complicated models see ref. 4. Obviously, if we write $H_{\tilde{\Lambda}}$ in the quasispin representation, it is similar to the Hamiltonian of an anisotropic antiferromagnet.

The simplest way to introduce mean-field versions is to replace $H_{\tilde{\Lambda}}$ by $\widetilde{\text{sym}}_{\tilde{\Lambda}} H_{\tilde{\Lambda}}$, where $\widetilde{\text{sym}}_{\tilde{\Lambda}}$: $\mathfrak{A}_{\tilde{\Lambda}} \to \mathfrak{A}_{\tilde{\Lambda}}$ is given by

$$\widetilde{\text{sym}}_{\tilde{\Lambda}} := \frac{1}{|\tilde{\Lambda}|!} \sum_{\sigma} \Theta_{\sigma} \tag{2.5}$$

The summation runs over all bijections $P(\tilde{\Lambda})$ of $\mathscr{K}$ with $P(\tilde{\Lambda}) :=$ $\{\sigma: \mathscr{K} \to \mathscr{K} \mid \sigma(i) = i \text{ for } i \notin \tilde{\Lambda}\}$. Θ is a representation of $P(\tilde{\Lambda})$ in $\text{Aut}(\mathfrak{A})$, defined by

$$\Theta_{\sigma}\left(\bigotimes_{i \in \tilde{\Lambda}'} x_i \right) := \bigotimes_{i \in \tilde{\Lambda}'} x_{\sigma(i)} \quad \text{for} \quad \tilde{\Lambda}' \in \mathfrak{L} \quad \text{and} \quad \bigotimes_{i \in \tilde{\Lambda}'} x_i \in \mathfrak{A}_{\tilde{\Lambda}'}$$

The family of symmetrized Hamiltonians $\widetilde{\text{sym}}_{\tilde{\Lambda}} H_{\tilde{\Lambda}}$, arising from $H_{\tilde{\Lambda}}$ in Eq. (2.3), leads to a simple mean-field model as treated in ref. 19. It shows in the thermodynamic limit a phase with condensed local pairs below some critical temperature (which depends, of course, on the particle density n, or the chemical potential μ). The essential properties of the condensed particle structure in this model are the same as in the BCS-model if the lattice of momenta for the BCS-model is replaced by a lattice in configuration space.[20, 30]

For physical reasons the local Hamiltonians $H_{\tilde{\Lambda}} \in \mathfrak{A}_{\tilde{\Lambda}}$, $\tilde{\Lambda} \in \mathfrak{L}$, in Eq. (2.3) should, however, be considered as elements of $\mathfrak{A}_{\Lambda}$, $\Lambda \in \mathfrak{L}$, where a bipartite sub-lattice structure has been incorporated. If the bi-partite lattice has the property that each nearest neighbour of a site in sub-lattice 1 is an element of sub-lattice 2 and vice versa, there are only products of operators in different sub-lattices in $H_{\tilde{\Lambda}}$. Thus we distinguish the operators b_i^1, b_i^2 and $\hat{n}_i^1$, $\hat{n}_i^2$ for $i \in \mathscr{K}$ (they are represented as in Eq. (2.4), except that the matrices have to be embedded in $M_2(\mathbb{C}) \otimes \mathbb{1}$ resp. $\mathbb{1} \otimes M_2(\mathbb{C})$ according to the sub-lattice index 1 or 2). Now we symmetrize with respect to $\Lambda \in \mathfrak{L}$ and arrive at

$$H_{\Lambda}^{\text{MFH}} = \frac{z(\Lambda)}{|\Lambda|} \left(\tilde{v} \sum_{i_1, i_2 \in \Lambda} \hat{n}_{i_1}^1 \hat{n}_{i_2}^2 - 2\tilde{t} \left(\sum_{i_1, i_2 \in \Lambda} b_{i_1}^{1*} b_{i_2}^2 + b_{i_1}^1 b_{i_2}^{2*} \right) \right) \in \mathfrak{A}_{\Lambda} \tag{2.6}$$

with $x^1 = x \otimes \mathbb{1}$, $x^2 = \mathbb{1} \otimes x \in \mathfrak{B}$ for $x \in \widetilde{\mathfrak{B}}$. Here, $z(\Lambda)$ is the averaged number of nearest neighbors in Λ. The limit $\lim_{\Lambda \to \mathscr{K}} z(\Lambda) = z$ exists if Λ tends towards $\mathscr{K}$ in the sense of van Hove.[13] z is the sum of the number of nearest neighbors in sub-lattice 2 of a site in sub-lattice 1 (or vice versa).

We take (2.6) as our basic model Hamiltonian, which will lead via the thermodynmic limit to a much richer phase structure than that being obtained by the uniform symmetrization (2.5).

2.3. Symmetries of the Mean-Field Hamiltonian

By construction $H_\Lambda^{\mathrm{MFH}} \in \mathfrak{A}$ is invariant under all permutations $\sigma \in \mathsf{P}(\Lambda)$ of $\Lambda \in \mathfrak{L}$:

$$\Theta_\sigma(H_\Lambda^{\mathrm{MFH}}) = H_\Lambda^{\mathrm{MFH}}, \qquad \text{for all} \quad \sigma \in \mathsf{P}(\Lambda) \quad \text{and} \quad \Lambda \in \mathfrak{L}$$

Besides exhibiting spatial homogeneity in each sublattice, the model is invariant with respect to the internal symmetries *gauge transformations* and *interchange of sub-lattices*. Quite generally internal symmetries are introduced as follows: For all unitary $u \in \mathfrak{B}$, there is a unique C^*-automorphism α_u of $\mathfrak{A}$ such that

$$\alpha_u \left(\bigotimes_{j=1}^{\infty} a_j \right) = \bigotimes_{j=1}^{\infty} u a_j u^*, \qquad \forall \bigotimes_{j=1}^{\infty} a_j \in \mathfrak{A} \tag{2.7}$$

The gauge group arises in this way from the transformations

$$\mathbb{T} := \{ v(\theta) = \exp(i\theta\hat{n}) \mid \theta \in [0, 2\pi[\}$$

with $\hat{n} = \hat{n}^1 + \hat{n}^2$, giving locally the explicit form

$$\alpha_{v(\theta)}^\Lambda(A) = e^{i\theta N_\Lambda} A \, e^{-i\theta N_\Lambda} \qquad \forall A \in \mathfrak{A}_\Lambda, \quad \forall \theta \in \mathbb{R} \tag{2.8}$$

where the local particle number operator is

$$N_\Lambda = \sum_{i \in \Lambda} \hat{n}_i, \qquad \text{for all} \quad \Lambda \in \mathfrak{L} \tag{2.9}$$

In the case of our two sub-lattices, the corresponding exchange group is given by $\mathsf{S}_2 := \{ \mathbb{1}, u_{12} \} \subset \mathfrak{B}$ with $u_{12}(x \otimes y) = y \otimes x$ for $x, y \in \widetilde{\mathfrak{B}}$. The corresponding automorphisms α_u, $u \in \mathsf{S}_2$, of $\mathfrak{A}$ are obtained via Eq. (2.7). A straightforward calculation shows for each $\Lambda \in \mathfrak{L}$

$$\alpha_v \circ \alpha_u(H_\Lambda^{\mathrm{MFH}}) = \alpha_u \circ \alpha_v(H_\Lambda^{\mathrm{MFH}}) = H_\Lambda^{\mathrm{MFH}} \qquad \text{for all} \quad u \in \mathsf{S}_2 \text{ and } v \in \mathbb{T}$$

$$\tag{2.10}$$

The group generated by S_2 and $\mathbb{T}$ is denoted by H. It is a compact subgroup of the group of all unitaries in $\mathfrak{B}$ and thus has a unique Haar measure μ_H.

In the case $\tilde{v} = 4\tilde{t}$ with $\mu = 2z(\Lambda)\,\tilde{t}$ (this corresponds to half filling), there are even more internal symmetries—essentially SO(3)—but this case will be excluded here. (Only for $\tilde{v} > 4\tilde{t}$ we will find the first order phase transition we are interested in.)

3. THE PURE PHASES AND THE LIMITING GIBBS STATES

The unique equilibrium state of a system in the finite region $\Lambda \in \mathfrak{L}$ with local Hamiltonian H_Λ at inverse temperature $\beta = 1/k_B T > 0$ (with absolute temperature T and Boltzmann constant k_B) is given by the local Gibbs state $\omega^{\beta, H_\Lambda}$ as an element in the state space $\mathfrak{S}(\mathfrak{A}_\Lambda)$ of the local algebra $\mathfrak{A}_\Lambda$

$$\omega^{\beta, H_\Lambda}: \mathfrak{A}_\Lambda \longrightarrow \mathbb{C}, \qquad A \longmapsto \langle \omega^{\beta, H_\Lambda}; A \rangle := \frac{\mathrm{tr}(\exp\{-\beta H_\Lambda\}\,A)}{\mathrm{tr}(\exp\{-\beta H_\Lambda\})} \qquad (3.1)$$

Without changing the notation we consider $\omega^{\beta, H_\Lambda}$ as a state on $\mathfrak{A}$ by continuation by means of the trace state. In addition to the inverse temperature β, we introduce the chemical potential μ via $H_\Lambda(\mu) = H_\Lambda - \mu N_\Lambda$, in order to fix a given particle density n in the state $\omega^{\beta, H_\Lambda(\mu)}$, such that $(1/|\Lambda|)\langle \omega^{\beta, H_\Lambda(\mu)}; N_\Lambda \rangle = n$.

Now, a limiting Gibbs state $\omega^{\beta, \mu}$ is by definition a weak*-accumulation point of the net $(\omega^{\beta, H_\Lambda(\mu)})_{\Lambda \in \mathfrak{L}}$. The state space $\mathfrak{S}(\mathfrak{A})$ of $\mathfrak{A}$ is weak*-compact, $\mathfrak{A}$ containing a unit, such that at least one accumulation point exists.[2] Since H_Λ^{MFH} is invariant under permutations $\sigma \in P(\Lambda)$, each limiting Gibbs state has to be homogeneous, i.e., it is an element of $\mathfrak{S}^P(\mathfrak{A}) = \{\omega \in \mathfrak{S}(\mathfrak{A}) \mid \omega \circ \Theta_\sigma = \omega$ for all $\sigma \in P = \bigcup_{\Lambda \in \mathfrak{L}} P(\Lambda)\}$. The set of all permutation invariant states $\mathfrak{S}^P(\mathfrak{A})$ has a well known structure: $\mathfrak{S}^P(\mathfrak{A})$ is a Bauer simplex[31] with (compact) extremal boundary $\partial_e \mathfrak{S}^P(\mathfrak{A}) = \{\bigotimes \varrho \mid \varrho \in \mathfrak{S}(\mathfrak{B})\}$, where $\bigotimes \varrho$ denotes the product state with $\langle \bigotimes \varrho; \bigotimes_{i \in \Lambda} x_i \rangle = \prod_{i \in \Lambda} \mathrm{tr}(\varrho x_i)$ for all $\Lambda \in \mathfrak{L}$ and $\bigotimes_{i \in \Lambda} x_i \in \mathfrak{A}$. The decomposition of a state $\omega \in \mathfrak{S}^P(\mathfrak{A})$ into extremal homogeneous states coincides with the central decomposition[12] of ω into classically pure states (factorial states). We parametrize the central measure μ_ω by the compact set $\mathfrak{S}(\mathfrak{B})$ and write

$$\omega = \int_{\mathfrak{S}(\mathfrak{B})} \bigotimes \varrho \; d\mu_\omega(\varrho) \qquad (3.2)$$

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[2] Convergence in the weak*-topology is simply the convergence of all expectation values.

Moreover, concerning the internal symmetries H (gauge transformations $\mathbb{T}$ and interchange of sub-lattices S_2) we additionally find that a limiting Gibbs state $\omega^{\beta,\mu}$ satisfies $\omega^{\beta,\mu} \circ \alpha_h = \omega^{\beta,\mu}$, for all $h \in H$. The subset of H-invariant states in $\mathfrak{S}^P(\mathfrak{A})$ is denoted by $\mathfrak{S}^H(\mathfrak{A})$. Again, $\mathfrak{S}^H(\mathfrak{A})$ is a simplex, since P times H is a so-called large group of automorphisms,[32] the extremal boundary of $\mathfrak{S}^H(\mathfrak{A})$ being denoted by $\partial_e \mathfrak{S}^H(\mathfrak{A})$. Since $\mathfrak{S}^H \subseteq \mathfrak{S}^P(\mathfrak{A})$, all elements $\omega \in \partial_e \mathfrak{S}^H(\mathfrak{A})$ are decomposed uniquely into elements of $\partial_e \mathfrak{S}^P(\mathfrak{A})$.

More precisely we have:[25, 35] $\omega \in \partial_e \mathfrak{S}^H(\mathfrak{A})$, if and only if there exists a $\otimes \varrho_\omega \in \partial_e \mathfrak{S}^P(\mathfrak{A})$ with

$$\omega = \int_H \otimes \varrho_\omega \circ \alpha_h \, d\mu_H(h) \tag{3.3}$$

That is, ω is obtained in this case from an extremal permutation invariant state by the minimal form of an H-symmetrization procedure. Spontaneous symmetry breaking takes place if $\{\otimes \varrho_\omega\} \neq \mathcal{O}_H(\otimes \varrho_\omega) :=$ $\{\otimes \varrho_\omega \circ \alpha_h \mid h \in H\}$.[33, 34] In this case the central measure μ_ω of ω becomes certainly non-trivial. Obviously, μ_ω is concentrated on the orbit $\mathcal{O}_H(\otimes \varrho_\omega)$ and may be determined with the help of μ_H and the broken symmetry (possibly a subgroup of H). If $\omega \in \mathfrak{S}^H(\mathfrak{A})$ but $\omega \notin \partial_e \mathfrak{S}^H(\mathfrak{A})$, there is no general method to find μ_ω, a case which is treated in Subsection 3.2 below.

Assume for the Hamiltonian $H_A^{MFH}(\mu)$, Eq. (3.1), that $\tilde{z}(\Lambda) > 0$. Then this parameter can be eliminated if we make the following transformation:

$$\frac{\tilde{v}}{\tilde{t}} \longrightarrow v, \qquad \frac{\mu}{\tilde{z}(\Lambda)} \longrightarrow \mu, \qquad \beta \tilde{z}(\Lambda) \to \beta,$$

i.e., we set $\tilde{z}(\Lambda) = 1$ and neglect the Λ-dependence of $z(\Lambda)$. This allows to perform all limits with respect to the whole index set $\mathfrak{L}$. If the Λ-dependence of $z(\Lambda)$ is treated explicitly, the limits have to be performed along a suited subnet in the sense of van Hove but all results remain unchanged. Finally, we suppress in the following the index MFH of $H_A^{MFH}(\mu)$, and write for the net of local reduced Hamiltonians, which define the grand canonical equilibrium states to be discussed,

$$\Lambda \longrightarrow H_\Lambda(\mu) = -\mu \sum_{i \in \Lambda} (\hat{n}_i^1 + \hat{n}_i^2) + \frac{v}{|\Lambda|} \sum_{i_1, i_2 \in \Lambda} \hat{n}_{i_1}^1 \hat{n}_{i_2}^2$$

$$-\frac{2}{|\Lambda|} \sum_{i_1, i_2 \in \Lambda} (b_{i_1}^{1*} b_{i_2}^2 + b_{i_1}^1 b_{i_2}^{2*}) \tag{3.4}$$

3.1. The Pure Phases and the Limiting Gibbs States at Fixed Chemical Potential

In the first step we calculate the equilibrium states of the model, defined by the local Hamiltonians $H_A(\mu)$ of Eq. (3.4) at fixed $\beta > 0$ and fixed $\mu \in \mathbb{R}$. This problem fits into the general scheme of refs. 15–18 (see also ref. 35):

The starting point is that each limiting Gibbs state $\omega^{\beta,\mu}$ of a model (from a well characterized class) minimizes the functional of the free energy density restricted here to the domain $\mathfrak{S}^P(\mathfrak{A})$:

$$\mathfrak{S}^P(\mathfrak{A}) \ni \omega \to f(\beta, \mu, \omega) := \lim_{A \in \mathfrak{L}} f_A(\beta, H_A(\mu), \omega) \tag{3.5}$$

where the functionals of the local free energy density are as usual

$$f_A(\beta, H_A, \cdot): \mathfrak{S}(\mathfrak{A}) \to \mathbb{R},$$

$$\omega \to f_A(\beta, H_A, \omega) := \frac{1}{|A|}\left(\langle \omega; H_A \rangle + \frac{1}{\beta} \operatorname{tr}_A(\varrho_A^\omega \ln \varrho_A^\omega)\right) \tag{3.6}$$

with ϱ_A^ω being the density matrix of $\omega|_{\mathfrak{A}_A}$.

The limit of $f_A(\beta, H_A, \omega)$ in Eq. (3.5) exists according to refs. 15 and 17. Moreover, $\omega \to f(\beta, \mu, \omega)$ is an affine functional on $\mathfrak{S}^P(\mathfrak{A})$. Due to the affinity of $f(\beta, \mu, \cdot)$, all states $\otimes \varrho$ in the support of the central measure $\mu_{\beta,\mu}$ of $\omega^{\beta,\mu}$ minimize the free energy density as well and belong to the set of the statistical pure phase states.

The stationarity of the free energy density leads for the pure phase product states to a necessary condition, which writes for the one-cell components $\varrho \in \mathfrak{S}(\mathfrak{B})$ as the self consistency equation:

$$\varrho = \frac{\exp(-\beta h_{\mathrm{eff}}(\varrho))}{\operatorname{tr}(\exp(-\beta h_{\mathrm{eff}}(\varrho)))} \tag{3.7}$$

The effective one-cell Hamiltonian $h_{\mathrm{eff}}(\varrho)$, depending on the pure phase to be determined, can be written down quite generally, even for non-polynomial mean-field interactions (being the total differential of the internal energy density as a function of the pure phase components). It belongs to the merits of operator-algebraic mean-field theory to have clarified the connection between the original local, model defining Hamiltonians and the effective Hamiltonians via representation theory in the thermodynamic limit. Let us remark that the summed-up, effective one-cell Hamiltonians constitute only part of the dynamical Hamiltonians associated uniquely

with the representation. For our quadratic interaction one arrives at an expression, which coincides up to additive constants—without any physical meaning—with the result of the formal mean-field manipulations

$$h_{\text{eff}}(\varrho) = (v\,\mathrm{tr}(\varrho\hat{n}^2) - \mu)\,\hat{n}^1 - 2(\mathrm{tr}(\varrho b^2)\,b^{1*} + \mathrm{tr}(\varrho b^{2*})\,b^1)$$

$$+ (v\,\mathrm{tr}(\varrho\hat{n}^1) - \mu)\,\hat{n}^2 - 2(\mathrm{tr}(\varrho b^1)\,b^{2*} + \mathrm{tr}(\varrho b^{1*})\,b^2) \qquad (3.8)$$

The solutions ϱ of Eq. (3.7) have to be evaluated for fixed $\mu \in \mathbb{R}$. There are in principle 4 types of solutions of Eq. (3.7), each of them characterizing a type of product state with a certain broken internal symmetry (see Table 1).

A numerical analysis shows, however, that there are only 3 types of the above solutions with *minimal* free energy density: The N-, the S-, and the CO-solutions, which constitute the different pure-phase regions of the model system, namely the *normal*, *superconducting*, and *charge ordered* phases, cf., Fig. 2.

Defining the set $\mathfrak{S}(\beta, \mu)$ of equilibrium states for given temperature and chemical potential (i.e., for a given point in the phase diagram of Fig. 2) as *all* minimal states of the free energy density (with the parameters β and μ), one concludes that this is a face of $\mathfrak{S}^P(\mathfrak{A})$: A minimizing state can only be decomposed into minimizing states. Hence the extremal boundary of $\mathfrak{S}(\beta, \mu)$, that are by definition all of the equilibrium pure phase states, is the intersection of $\partial_e \mathfrak{S}^P(\mathfrak{A})$ with $\mathfrak{S}(\beta, \mu)$ (being a direct consequence of the face property). Since the decomposition over $\partial_e \mathfrak{S}^P(\mathfrak{A})$ is unique, the decomposition of an equilibrium state into pure phases is unique, too, and $\mathfrak{S}(\beta, \mu)$ is a (Bauer) simplex. This means the other way

Table 1.   **Solutions of the Self-Consistency Equation (3.7), Broken Symmetries and the Corresponding Phase States**

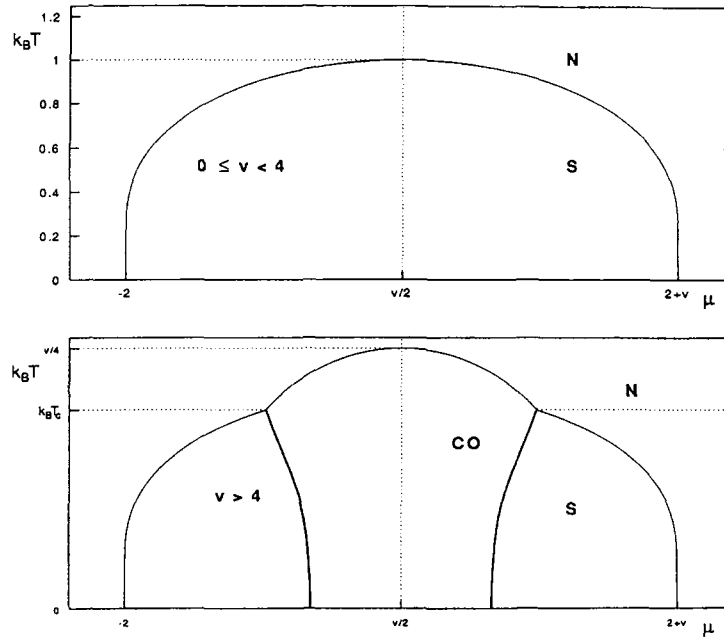| State	Broken symmetry	Macroscopic pure phase
$\mathrm{tr}(\varrho\hat{n}^1) = \mathrm{tr}(\varrho\hat{n}^2),$ $\mathrm{tr}(\varrho b^1) = \mathrm{tr}(\varrho b^2) = 0$		Normal phase (N)
$\mathrm{tr}(\varrho\hat{n}^1) = \mathrm{tr}(\varrho\hat{n}^2),$ $\mathrm{tr}(\varrho b^1) = \mathrm{tr}(\varrho b^2) \neq 0$	gauge invariance	Superconducting phase (S)
$\mathrm{tr}(\varrho\hat{n}^1) \neq \mathrm{tr}(\varrho\hat{n}^2),$ $\mathrm{tr}(\varrho b^1) = \mathrm{tr}(\varrho b^2) = 0$	sub-lattice permutations	Charge ordered phase (CO)
$\mathrm{tr}(\varrho\hat{n}^1) \neq \mathrm{tr}(\varrho\hat{n}^2),$ $\mathrm{tr}(\varrho b^1) \neq \mathrm{tr}(\varrho b^2) \neq 0$	sub-lattice permutations gauge invariance	"Mixed" phase (M)

Fig. 2. (T, μ)-phase diagrams for different values of v. The phase transitions N-S and N-CO are of the second kind, while the transition S-CO is of the first kind.

round, that all states in $\mathfrak{S}(\beta, \mu)$ are obtained by various (may be continuous) ways of mixing the pure phases.

Since a limiting Gibbs state retains all of the (permutation and) internal symmetries, its unique extremal decomposition measure must be H-invariant. If the pure phases constitute just a single H-orbit there is only one invariant probability measure providing just one limiting Gibbs state by integrating over the pure phases. In the interiors of the thermodynamic phase regions of our model, determined by the selfconsistency equations, we find in fact just one H-orbit of the pure phases and are thus able to write down the unique limiting Gibbs states. According to formula (3.3) each of the limiting Gibbs states is extremal H-invariant and cannot be decomposed into other H-invariant states.

In the N-phase region we find a limiting Gibbs state $\omega^{\beta, \mu} \in \partial_e \mathfrak{S}^P(\mathfrak{A})$ of the following form:

$$\omega_N^{\beta, \mu} = \bigotimes \varrho, \quad \text{with } \varrho = \exp(-\xi - \beta h_{\text{eff}}) \quad \text{and} \quad h_{\text{eff}} = \left(v \frac{n}{2} - \mu \right)(\hat{n}^1 + \hat{n}^2)$$

$$(3.9)$$

The limiting Gibbs state in the CO-phase region is given by

$$\omega_{CO}^{\beta,\mu} = \tfrac{1}{2} \otimes \varrho_{12} + \tfrac{1}{2} \otimes \varrho_{21}, \qquad \text{with} \quad \varrho_{ik} = \exp(-\xi - \beta h_{\text{eff}}^{ik})$$

$$\text{and} \quad h_{\text{eff}}^{ik} = (vn^i - \mu)\,\hat{n}^1 + (vn^k - \mu)\,\hat{n}^2 \qquad \text{for} \quad i \neq k = 1, 2 \tag{3.10}$$

with a two-component orbit of gauge invariant pure phase states, which have broken lattice-exchange symmetry. In the S-phase region the limiting Gibbs state is a continuous integral (defined in the w^*-topology):

$$\omega_S^{\beta,\mu} = \int_0^{2\pi} \otimes \varrho_\vartheta \frac{d\vartheta}{2\pi}, \qquad \text{with} \quad \varrho_\vartheta = \exp(-\xi - \beta h_{\text{eff}}^\vartheta) \qquad \text{and}$$

$$h_{\text{eff}}^\vartheta = \left(v\frac{n}{2} - \mu \right) \hat{n}^1 - \Delta(\mathrm{e}^{-i\vartheta} b^{1*} + e^{i\vartheta} b^1)$$

$$+ \left(v\frac{n}{2} - \mu \right) \hat{n}^2 - \Delta(e^{-i\vartheta} b^{2*} + e^{i\vartheta} b^2) \quad \text{for} \quad \vartheta \in [0, 2\pi[\tag{3.11}$$

The broken gauge symmetry in the pure phase states gives rise to the macroscopic phase angle and the non-vanishing expectations for the pair operators. These typical features for super conductivity are here not combined with charge ordering.

The determination of the mean-field values $n^1 = \mathrm{tr}(\varrho\hat{n}^1)$, $n^2 = \mathrm{tr}(\varrho\hat{n}^2)$, $(\Delta/2)\,e^{-i\vartheta} = \mathrm{tr}(\varrho b^1) = \mathrm{tr}(\varrho b^2)$, and $n = n^1 + n^2$ are part of the self-consistency problem for $\varrho = \varrho, \varrho_{ik}, \varrho_\vartheta$ in Eq. (3.7).

We see from the above formulas, that the different phase regions have not only different broken symmetries in the pure phase states but that even the sets of equilibrium states $\mathfrak{S}(\beta,\mu)$ are topologically inequivalent.[25] Both aspects characterize a phase transition while crossing the boundaries of the phase regions, when one uses the (quantum) statistical state concept, and not that of usual phenomenological thermodnamics. In this statistical conceptual frame one would define a phase transition of the second kind by a smooth variation of the pure phases, resp. of the sets $\mathfrak{S}(\beta,\mu)$ in the sense of ref. 25 and a phase transition of the first kind by a discontinous variation of these statistical equilibrium states. The transition "point" (what is statistically the set $\mathfrak{S}(\beta,\mu)$) of a phase transition of the second kind is then by definition a critical point.

Our evaluations of the pure phase states show that the phase transitions N-CO and N-S are of second kind, while the S-CO phase transition is of first kind, which is seen, e.g., by the discontinuous variation of the
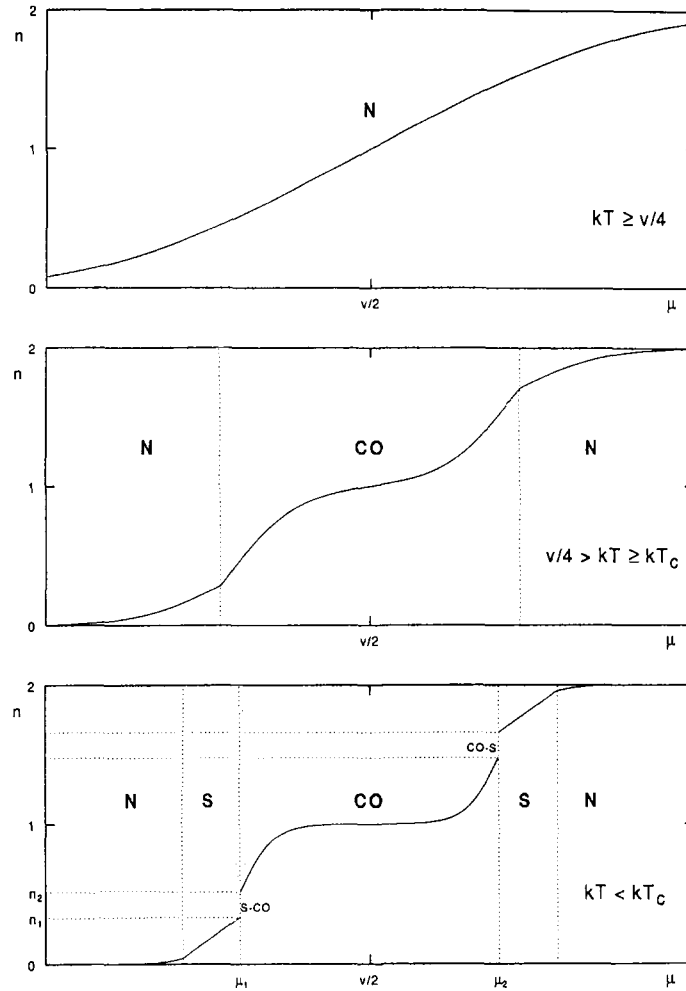
Fig. 3. $n(\mu)$ for various temperatures at $v > 4$. T_c is the largest temperature where the S-phase exists, comp. Figs. 2 and 4. For further details, see Subsection 3.2.

particle density (cf. below). The latter aspect is illustrated in Fig. 3. More precisely there is on the boundaries N-CO and N-S still a unique N-phase solution (as a special case of an H-orbit), which smoothely develops into the different CO-resp. S-phase solutions. In contrast to this, there exist two orbits of solutions on the S-CO boundary, corresponding to the broken gauge symmetry and to the broken sub-lattice exchange symmetry. Thus Eq. (3.3) cannot be used to construct a limiting Gibbs state. In order to get

an H-invariant equilibrium state one has rather to integrate the pure phases over the two seperate orbits and to mix the results:

$$\omega_\lambda^{\beta,\mu} = \lambda\omega_{CO}^{\beta,\mu} + (1-\lambda)\omega_S^{\beta,\mu}, \qquad \lambda \in [0,1] \tag{3.12}$$

Since every H-invariant state obtained by integrating over the previously calculated pure phase states must have the form (3.12), this holds true also for the limiting Gibbs states, where their value $\lambda \in [0, 1]$ is not determined and the question of uniqueness is not solved up to now.

The dependency of the various phases from the particle density is quite generally of interest for applications. Thus we calculate the relationship between $\mu \in \mathbb{R}$ and $n = n^1 + n^2 \in]0, 2[$. We find for each of the pure phases a certain function $\mu(n)$ which is determined by the solutions of Eq. (3.7):

$$\text{N-phase: } \mu_N = \frac{v}{2}n - \frac{2}{\beta}\text{artanh}(1-n), \qquad \text{S-phase: } \mu_S = \left(\frac{v}{2}+2\right)n - 2,$$

$$\text{CO-phase: } \mu_{CO} = \frac{v}{2}n - \frac{1}{\beta}\text{artanh}\left(\frac{2-2n}{1+(1-n)^2-\Delta n^2}\right)$$

with $\Delta n = n^2 - n^1$. We can invert these equations in the regions of their validity and find a strictly monotonous function $\mathbb{R} \ni \mu \to n(\mu)$. This function is continuous (i.e., $n_N(\mu) = n_S(\mu)$, $n_N(\mu) = n_{CO}(\mu)$) on the N-S and the N-CO boundaries, while it changes discontinuously on the S-CO boundary. This makes explicit the analytical background for the already mentioned Fig. 3.

Using the function $n(\mu)$, we have plotted a (T, n)-phase diagram in Fig. 4. Here, the critical chemical potential μ of the S-CO transition is constant over a coexistence region of the two phases, where in its interior a pure phase state with the corresponding particle density does not exist. The N-S and the N-CO boundary can be calculated explicitly by a Landau expansion of the free energy density. One finds along these boundaries the critical temperatures as functions of the densities:

$$T_{N-S} = \frac{n-1}{\text{artanh}(n-1)}, \qquad T_{N-CO} = \frac{v}{4}n(2-n)$$

Our derived coexistence region contrasts the findings in refs. 1 and 2, where there is obtained a pure M-phase (listed in our Table 1 also as a pure phase, being however instable in our set up), and where *all* phase transitions are continuous. (We come back to this point in ref. 11.)
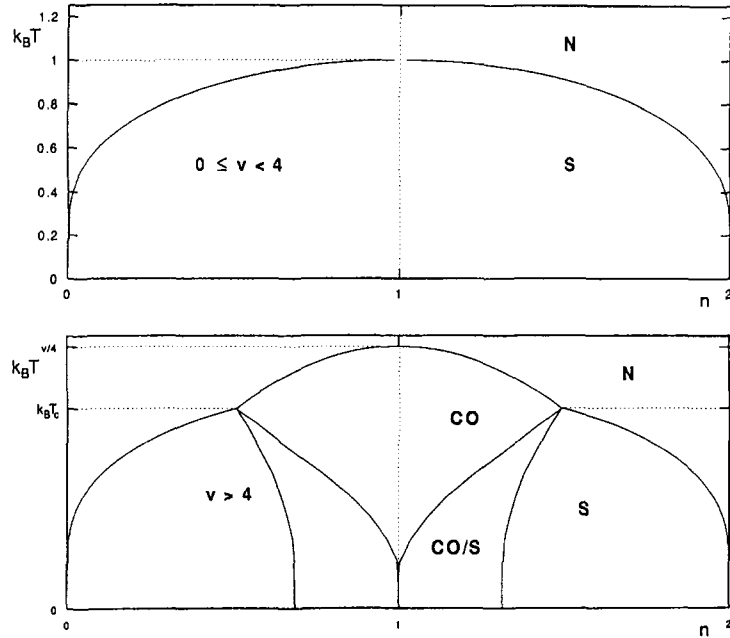
Fig. 4. (T, n)-phase diagram for different values of v.

3.2. The Limiting Gibbs States at Fixed Particle Density

In order to investigate the uniqueness of the limiting Gibbs states on the S-CO phase boundary we perform the thermodynamic limit at a fixed particle density $n \in {]}0, 2[$, i.e., we determine for each local region $A \in \mathfrak{L}$ a $\mu_A \in \mathbb{R}$ such that $(1/|A|)\langle \omega^{\beta H_A(\mu_A)}; N_A \rangle = n$. Then we have to analyze the convergence properties of the corresponding chemical potentials μ_A in the thermodynamic limit. They are a consequence of the concavity and the convergence of the free energy densities, (3.5), (3.6). The arguments for the convergence of the local chemical potentials outside the coexistence region can be taken over from ref. 20 (where BCS- and mean-field Hubbard models on the uniform lattice are treated at fixed particle density while going into the thermodynamic limit). Here, we have to consider this convergence also in the additional S-CO transition with its discontinuous variation of the particle density. We assume that $v > 4$, which implies that this transition exists indeed for low temperatures $T < T_c$ (cf. Fig. 2, lower diagram).

The differentiation of the respective free energy densities allows us to determine the particle densities on the local, as well as on the global level (Lemma A.1).

Lemma 3.1. Let be $\beta > \beta_c > 0$, $\mu \in \mathbb{R}$, and $\mu \neq \mu_1, \mu_2$, where $\mu_{1,2} = \mu_{1,2}(\beta)$ are the chemical potentials at which the S-CO transition takes place.

(i) For $A \in \mathfrak{L}$, $n_A(\mu) := \langle \omega^{\beta, H_A(\mu)}; N_A/|A| \rangle$ and $n \in]0, 2[$, there exists a unique $\mu_A = \mu_A(n) \in \mathbb{R}$, such that $n_A(\mu_A) = n$.

(ii) Define

$$n(\mu) := \lim_{A \in \mathfrak{L}} n_A(\mu)$$

which limit exists. Then there exists for all $n \in]0, 2[$, a unique $\mu_0 \in \mathbb{R}$, such that $n(\mu_0) = n$. Here, we choose for all n in the two coexistence regions of the S-CO transition the values $\mu_0 = \mu_1$ or $\mu_0 = \mu_2$, respectively (comp. Fig. 3, lower diagram). (We usually suppress the β-dependency of μ_A and μ_0 and write only occasionally, for the sake of clarity, $\mu_A(n)$ and $\mu_0(n)$.)

Proof. See Appendix A.

In the next step we prove the convergence of the chemical potentials μ_A at fixed particle density:

Proposition 3.2. For $\beta > \beta_c$ let $n \in]0, 2[$ be arbitrarily given and $\mu_A(n)$, $\mu_0(n)$ as in Lemma 3.1. Then it holds:

$$\lim_{A \in \mathfrak{L}} \mu_A(n) := \mu_0(n)$$

Proof. We prove the convergence along a sequence of local regions $(A_n)_{n \in \mathbb{N}}$, such that $A_n \subset A_{n+1}$, and show that for all $A \in \mathfrak{L}$ there is a $n \in \mathbb{N}$ with $A \subset A_n$.

First we choose $n \in]0, 2[$ such that $\mu_0 \in \mathbb{R}\backslash\{\mu_1, \mu_2\}$. The convergence $n_{A_k}(\mu) \xrightarrow{k \to \infty} n(\mu)$ along such a sequence of local regions A_k is uniform on compact convex sets [36, Theorem 25.7]. The convergence $\lim_{A \in \mathfrak{L}} \mu_A = \mu_0$ for all $n \in]0, 2[$ with $\mu_0 \neq \mu_1, \mu_2$ then follows as in the proof of Prop. 3.5 in ref. 20.

Now let us assume that n is in one of the two coexistence regions of the S-CO transition, i.e., $\mu_0(n) = \mu_1$ or μ_2. We set $\mu_0 = \mu_1$ and denote by $n_{1,2}$, $n_1 < n_2$, the boundary points of the possible particle densities in the coexistence region, i.e., we have $n \in [n_1, n_2]$. Then choose an arbitrary $\varepsilon > 0$ and $\tilde{n}_1$, $\tilde{n}_2$ with

$$n_1 - \varepsilon < \tilde{n}_1 < n_1, \qquad n_2 < \tilde{n}_2 < n_1 + \varepsilon \qquad (3.14)$$

There exist $\mu_1^{\pm\varepsilon}$ with

$$n(\mu_1^{-\varepsilon}) = n_1 - \varepsilon, \qquad n(\mu_1^{+\varepsilon}) = n_2 + \varepsilon$$

and due to the monotonicity we have

$$\mu_1^{-\varepsilon} < \mu_0(n) = \mu_1 < \mu_1^{+\varepsilon}$$

With the continuity of $\mu(n)$ it follows

$$\lim_{\varepsilon \to 0} \mu_1^{\pm\varepsilon} = \mu_1 \tag{3.15}$$

For each finite subsystem with $\Lambda_k \in \mathfrak{L}$, there are $\mu_{\Lambda_k}(\tilde{n}_1)$, $\mu_{\Lambda_k}(\tilde{n}_2)$ such that $n(\mu_{\Lambda_k}(\tilde{n}_{1,2})) = \tilde{n}_{1,2}$. Now use the uniform convergence of $\lim_{k \to \infty} (-d/d\mu) f_{\Lambda_k}(\beta, H_{\Lambda_k}(\mu), \omega^{\beta, H_{\Lambda_k}(\mu)}) = -(d/d\mu) f(\beta, \mu, \omega^{\beta, \mu})$ in a suitably chosen closed interval to find a $k_0 \in \mathbb{N}$ such that for all $k > k_0$ [36, Theorem 25.7]

$$\mu_{\Lambda_k}(\tilde{n}_1) \in [\mu_1^{-\varepsilon}, \mu_1], \qquad \mu_{\Lambda_k}(\tilde{n}_2) \in [\mu_1, \mu_1^{+\varepsilon}]$$

With the monotonicity of $n \to \mu_{\Lambda_k}(n)$ it follows

$$\mu_1^{-\varepsilon} \leqslant \mu_{\Lambda_k}(\tilde{n}_1) < \mu_{\Lambda_k}(n) < \mu_{\Lambda_k}(\tilde{n}_2) \leqslant \mu_1^{+\varepsilon} \tag{3.16}$$

Since $\varepsilon > 0$ is arbitrary, we find with Eq. (3.15) for all $n \in [n_1, n_2]$:

$$\lim_{k \to \infty} \mu_{\Lambda_k}(n) = \mu_1, \qquad \forall n \in [n_1, n_2]$$

This is independent of the chosen sequence $(\Lambda_n)_{n \in \mathbb{N}}$. Thus we have $\lim_{\Lambda \in \mathfrak{L}} \mu_\Lambda(n) = \mu_1$, $\forall n \in [n_1, n_2]$, cf. [20, Appendix].

The convergence of the chemical potentials μ_Λ enables us directly to determine the limiting Gibbs states. In order to specify a limiting state with a certain particle density $n \in]0, 2[$, we have to find the w^*-accumulation points of the net $(\omega^{\beta, H_\Lambda(\mu_\Lambda)})_{\Lambda \in \mathfrak{L}}$ prescribing for all $\Lambda \in \mathfrak{L}$ that $\mu_\Lambda = \mu_\Lambda(n)$ according to Lemma 3.1. In order to show that these modified accumulation points satisfy also the variational principle of the free energy density we first observe that $(H_\Lambda(\mu_\Lambda)/|\Lambda|)_{\Lambda \in \mathfrak{L}}$, as a so-called approximately symmetric net, is applicable to the results of ref. 15, and then deduce from the convergence of the chemical potentials that

$$\lim_{\Lambda \in \mathfrak{L}} \frac{1}{|\Lambda|} \|H_\Lambda(\mu_\Lambda) - H_\Lambda(\mu_0)\| = 0$$

Thus both models, with fixed particle density $n \in {]}0, 2{[}$ and with fixed chemical potential μ_0, have the same limiting free energy density as a functional on $\mathfrak{S}^P(\mathfrak{A})$, which is, therefore, also minimal in the limiting equilibrium states with fixed n.

Theorem 3.3. For $\beta > 0$ and $n \in {]}0, 2{[}$, let $\mu_A = \mu_A(n)$ and $\mu_0 = \mu_0(n)$ as in Lemma 3.1.

(i) If n is chosen such that $\mu_0 \neq \mu_1, \mu_2$, we find the unique limiting Gibbs state

$$w^*\text{-}\lim_{A \in \mathfrak{L}} \omega^{\beta, H_A(\mu_A)} = \omega^{\beta, \mu_0}$$

where ω^{β, μ_0} is one of the three cases (3.9), (3.10), (3.11).

(ii) If $\mu_0 = \mu_1$, or $\mu_0 = \mu_2$ (for $\beta > \beta_c$) the limiting Gibbs state is uniquely given by

$$w^*\text{-}\lim_{A \in \mathfrak{L}} \omega^{\beta, H_A(\mu_A)} = \omega_\lambda^{\beta, \mu_0} \qquad \lambda \in [0, 1]$$

where the particle density n uniquely determines the weight λ in the decomposition of $\omega_\lambda^{\beta, \mu_0}$ into S- and CO-phase states (comp. Eq. (3.12)).

(iii) The unique central decomposition (into pure phases) of each limiting Gibbs state is a specialization of

$$\omega_\lambda^{\beta, \mu_0} = \lambda \left(\frac{1}{2} (\otimes \varrho_{12}) + \frac{1}{2} (\otimes \varrho_{21}) \right) + (1 - \lambda) \left(\int_0^{2\pi} \otimes \varrho_\vartheta \, \frac{d\vartheta}{2\pi} \right)$$

where $\lambda \in [0, 1]$. The mean-field values in the one-cell density operators ϱ_x and the $\lambda, (1 - \lambda)$ depend uniquely on (β, n), having trivial values in certain regions.

Proof. (i) The uniqueness of the limiting Gibbs state for a fixed n with $\mu_0(n) \neq \mu_1, \mu_2$ follows from the minimality of the free energy, discussed before 3.3, and from the one-orbit argument.

(ii) For $\mu_0 = \mu_1, \mu_2$ we know, as explained previously, that each limiting Gibbs state $\omega^{\beta, n}$ has the form

$$\omega^{\beta, n} = \lambda \omega_{CO}^{\beta, \mu} + (1 - \lambda) \omega_S^{\beta, \mu}, \qquad \lambda \in [0, 1]$$

with $\omega_{CO}^{\beta,\mu}$ and $\omega_S^{\beta,\mu}$ as in (3.10)–(3.12). Since $\lim_{A\in\mathfrak{L}}(1/|A|)\langle\omega_{CO}^{\beta,\mu}; N_A\rangle =:$
$n_{CO} \neq n_S := \lim_{A\in\mathfrak{L}}(1/|A|)\langle\omega_S^{\beta,\mu}; N_A\rangle$ and $\lim_{A\in\mathfrak{L}}(1/|A|)\langle\omega^{\beta,H_A(\mu_A)}; N_A\rangle$
$=n$, $\lambda\in[0, 1]$ is uniquely determined by $n = \lambda n_{CO} + (1-\lambda)n_S$.

(iii) The decomposition of a permutation invariant state into product states is—as mentioned before—quite generally the unique central decomposition.

The now proven convergence of the local Gibbs states at a fixed particle density n is somewhat subtle in the coexistence region: It depends on the way the net of local chemical potentials $\mu_A(n)$ converges, and not merely on its limit. Consider, e.g., the coexistence region with $n < 1$, where we have the convergence $\lim_{A\in\mathfrak{L}}\mu_A(n) = \mu_1$, but where we have different limiting Gibbs states depending on the n-index of the net. The latter limiting Gibbs states may even be mutually disjoint: Choose for n the particle densities n_{CO} and n_S on the boundary of the coexistence region with corresponding local chemical potentials μ_A^{CO} and μ_A^S. Then it holds $\lim_{A\in\mathfrak{L}}\mu_A^{CO} = \lim_{A\in\mathfrak{L}}\mu_A^S$, but $w^*\text{-}\lim_{A\in\mathfrak{L}}\omega^{\beta,H_A(\mu_A^{CO})} = \omega_{CO}^{\beta,\mu} \neq \omega_S^{\beta,\mu} = w^*\text{-}\lim_{A\in\mathfrak{L}}\omega^{\beta,H_A(\mu_A^S)}$. As we see from (3.10) and (3.11) the pure phase components in the central decompositions of $\omega_{CO}^{\beta,\mu}$ and $\omega_S^{\beta,\mu}$ are all pairwise disjoint factor states being pairwise different homogeneous product states. Thus the central measures (as measures on the set $\partial_e\mathfrak{S}^P(\mathfrak{A})$) are disjoint, and from this we conclude (as, e.g., in ref. 37) that the states $\omega_{CO}^{\beta,\mu}$ and $\omega_s^{\beta,\mu}$ are disjoint for themselves.

4. CONCLUSIONS

Our investigation has been devoted to the determination of the phase diagrams of a model, which occurs for the description of bipolaronic superconductors (and antiferromagnetic materials). The model is originally defined by a family of short range Hamiltonians depending on the finite lattice regions, which are connected with the Hubbard model. After having divided each local lattice into two sublattices a symmetrization of the Hamiltonians over the cells of the bipartite lattices leads to a quasi-microscopic mean-field model canonically associated with the short range model. For its elaboration in the thermodynamic limit a rather recent operator-algebraic scheme is applied, which ensures beside other things the existence of the limiting free energy density and gives a general formula for the effective Hamiltonians occurring in the stationarity conditions of the free energy density (self-consistency equations) for the statistical pure phase states. Besides the thermodynamic limit no further approximations are employed to obtain the typical mean-field expressions in the symmetrized theory, which allow for a numerical evaluation.

In this way all pure phase states which minimize the limiting free energy density are determined and are grouped into the three classes of normal (N), charge ordered (CO), and superconducting (S) states according to the kind of broken symmetry (cf., Table 1). Pure phase states with simultaneous breaking of the gauge invariance and of the sub-lattice exchange symmetry make the free energy stationary, but not minimal in the present model. This two-fold symmetry breaking arises here rather in terms of a coexistence region.

At this stage a detailed analysis of the indicated phase transitions and critical points in terms of the purely statistical concepts of ref. 25 would have been possible, but has been only briefly touched in the present work. Let us supplement in this connection, that only the upper curves in the diagrams of Figs. 2 and 4 signify simple critical points. In the lower diagrams two bicritical points at T_c are visible. Using an equilibrium ensemble without particle fluctuations, as systematically devised and investigated in ref. 11, the boundaries of the present coexistence regions are transformed into two further critical lines, which meet in tetracritical points.

As one of our main results we have demonstrated how symmetry arguments combined with convex analysis lead to the existence of unique limiting Gibbs states in all of the various phase regions. For obtaining this result the thermodynamic limit was performed first at fixed chemical potential μ and then at fixed particle density n. It is the latter limit, which allows for a unique limiting Gibbs states in the coexistence regions of the S-CO phase transitions. The different mixed phase states with equal β and μ and varying density are locally approximated by means of different nets of local chemical potentials with the same limit. In the coexistence region the (symmetric) limiting Gibbs state has a central decomposition into two orbits of pure phase states with broken symmetry. This strategy for treating the coexistence region may in principle be generalized to a large number of models with discontinuous phase transitions, cf., e.g., ref. 23.

In all the mentioned cases the limiting Gibbs states in their central decompostion contain the full information on all possible phases for given β and μ. They would provide also the natural reference state for reconstructing the quantum theory via the GNS-representation, to treat local dynamical disturbances from equilibrium. (The study of the gap and of other stable spectral features will be performed in a future investigation leading to so-called spectral phase diagrams.) In this representation the phase structure for given β and μ is also reflected by the operator form of the represented fields. Since we have two types of long range order (diagonal long range order for breaking the lattice exchange symmetry and off-diagonal long range order for the broken gauge invariance) we have

two types of field operators at infinity, which characterize the respective condensed particles. Let us mention in our Conclusions only the condensed bipolaron operators, which may be obtained by averaging the normal fields over the lattice.

For the simple mean-field model with homogeneous lattice,[19] we have already shown[20, 30] that the condensed pairs in the superconducting phase show a similar operator structure as in the BCS-model.[38, 39] The only difference is that the limits are performed in configuration or momentum space, respectively. In the S-phase of the pure and mixed phase region we find also in the present model

$$\text{s-lim}_{\substack{\Lambda \in \mathfrak{L}}} \Pi_S \left(\frac{1}{|\Lambda|} \sum_{i \in \Lambda} b_i^{1*} \right) = \text{s-lim}_{\substack{\Lambda \in \mathfrak{L}}} \Pi_S \left(\frac{1}{|\Lambda|} \sum_{i \in \Lambda} b_i^{2*} \right)$$

$$= \text{const} \int_{[0, 2\pi[}^{\oplus} e^{i\vartheta} \mathbb{1}_\vartheta \frac{d\vartheta}{2\pi} \in \mathfrak{M}_S = \Pi_S(\mathfrak{A})''$$

By Π_S we denote the GNS-representation of the limiting Gibbs state $\omega_S^{\beta, \mu}$ in the S-phase region (comp. Eq. (3.11)). Using the central decomposition of $\omega_S^{\beta, \mu}$, we find the direct integral decomposition of the corresponding von Neumann algebra which gives the above explicit form of the condensed local pair operators in terms of their components.

The creation operators for condensed local pairs are purely classical because they are central, i.e., they commute with all observables in the represented quasi-local electron algebra. They have nothing in common with bosonic creation operators. It is an interesting problem, whether this peculiar structure of condensed pair operators is in its basic form a universal feature of superconductivity. Our experiences with BCS- and Hubbard-like mean-field models would confirm this hypothesis, but it seems to be in conflict with the operators for Goldstone bosons, which also should arise from the broken gauge invariance.

In contradistiction to two weakly coupled superconductors, as they occur, e.g., for the spatially separated subsytems of a Josephson junction, the present condensed bipolarons have lost their association with the sub-lattices. First the constant in front of the integral does not depend on the sub-lattice index. More decisively, the central decomposition of the super-conducting limiting Gibbs states exhibits only *one* macroscopic phase. The condensed bipolarons from the sublattices are uniformly phase locked, such that the macroscopic phase variable cannot be used to discriminate between the sublattices. This is typical for a strong coupling, where here this coupling between the different lattices produces even the superconduc-tive phase within each of the sublattices.

Concerning the physical relevance of our model treated in the grand canonical ensemble, one has for the antiferromagnetic interpretation experiments, which confirm the coexistence region.[40–41] In the superconductor language, which we have preferred in our elaboration, the connection with real (high-T_c) substances is rather involved,[43] but a mixed pure phase seems to be envisaged as physically possible. In any case, an experimental discrimination between a mixture of spatially non-separated components to form a pure phase or to form a composite phase presupposes a concisely formulated conceptual background.

APPENDIX. PROOFS OF SUBSECTION 3.2

Lemma A.1. Let be $\beta > 0$, $\mu \in \mathbb{R}$. Denote by μ_1, μ_2 with $\mu_1 < \mu_2$ the chemical potentials where the S-CO phase transition takes place (if there is some). Then it holds:

(i) $\mu \to f_A(\beta, H_A(\mu), \omega^{\beta, H_A(\mu)})$ is a twice differentiable concave function on $\mathbb{R}$.

(ii) $\mu \to f(\beta, \mu, \omega^{\beta, \mu})$:= $\lim_{A \in \mathcal{Q}} f_A(\beta, H_A(\mu), \omega^{\beta, \mu}) = \lim_{A \in \mathcal{Q}} f_A(\beta, H_A(\mu), \omega^{\beta, H_A(\mu)})$ is a differentiable concave function on $]-\infty, \mu_1[$, $]\mu_1, \mu_2[$, and $]\mu_2, \infty[$. If there is no S-CO transition $\mu \to f(\beta, \mu, \omega^{\beta, \mu})$ is differentiable and concave on $\mathbb{R}$.

Proof. (i) Follows by direct inspection, see, e.g., ref. 20.

(i) For the convergence of $A \to f_A(\beta, H_A(\mu), \omega^{\beta, \mu})$, see [17, Theorem 4.3]. The concavity of $\mu \to f(\beta, \mu, \omega^{\beta, \mu})$ is a consequence of the minimum principle for the free energy density of limiting Gibbs states. The differentiability of $\mu \to f(\beta, \mu, \omega^{\beta, \mu})$ has to be verified by explicit calculation of $(d/d\mu) f(\beta, \mu, \omega^{\beta, \mu})$ with the help of (3.7), (3.9)–(3.11) and the limit in (3.5). If there is a S-CO transition at μ_1, μ_2, the corresponding particle density which is the differential of the free energy density changes discontinuously (see also proof of Lemma 3.1 below). These differentiability properties are a general consequence for a mean-field system with the above stated phase transitions.[25]

Proof of Lemma 3.1. (i) follows from $[H_A(\mu), N_A] = 0$ for all $A \in \mathcal{Q}$ and $\sigma(N_A/|A|) \subset [0, 2]$. Moreover, it is

$$\frac{d}{d\mu} f_A(\beta, H_A(\mu), \omega^{\beta, H_A(\mu)}) = -\frac{1}{|A|} \langle \omega^{\beta, H_A(\mu)}; N_A \rangle \qquad (A.1)$$

Due to the concavity of $\mu \to f_A(\beta, H_A(\mu), \omega^{\beta, H_A(\mu)})$ we find that $\mu \to n_A(\mu) = \langle \omega^{\beta, H_A(\mu)}; N_A/|A| \rangle$ is a bijective function $n_A: \mathbb{R} \to]0, 2[$.

(ii)   For a sequence of finite differentiable concave functions $f_i(\mu)$ on an open convex set, pointwise converging to a concave differentiable function $f(\mu)$, we have $\lim_{i \to \infty} (d/d\mu) f_i(\mu) = (d/d\mu) f(\mu)$ [36, Theorem 25.7]. Now choose an arbitrary sequence $(\Lambda_n)_{n \in \mathbb{N}}$ with $\Lambda_n \subset \Lambda_{n+1}$, and for all $A \in \mathfrak{L}$ there is a $n \in \mathbb{N}$, such that $A \subset \Lambda_n$.

According to Lemma A.1, $f_{\Lambda_n}(\beta, H_{\Lambda_n}(\mu), \omega^{\beta, H_{\Lambda_n}(\mu)})$ and $f(\beta, \mu, \omega^{\beta, \mu})$ are differentiable concave functions (for $\mu \neq \mu_1, \mu_2$). The pointwise convergence follows from Lemma A.1(ii). With Eq. (A.1) we find

$$\lim_{n \to \infty} \frac{1}{|\Lambda_n|} \langle \omega^{\beta, H_{\Lambda_n}(\mu)}; N_{\Lambda_n} \rangle = -\frac{d}{d\mu} f(\beta, \mu, \omega^{\beta, \mu})$$

This limit is independent of the chosen sequence $(\Lambda_n)_{n \in \mathbb{N}}$. Thus we have $\lim_{A \in \mathfrak{L}} \langle \omega^{\beta, H_A(\mu)}; N_A/|A| \rangle = -(d/d\mu) f(\beta, \mu, \omega^{\beta, \mu})$ [20, Appendix]. The uniqueness of μ_0 follows with (3.7) and (3.13).

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