

Global C^* -Dynamics and Its KMS States of Weakly Inhomogeneous Bipolaronic Superconductors

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We establish the limiting dynamics of a class of inhomogeneous bipolaronic models for superconductivity which incorporate deviations from the homogeneous models strong enough to require disjoint representations. The models are of the Hubbard type and the thermodynamics of their homogeneous part has been already elaborated by the authors. Now the dynamics of the systems is evaluated in terms of a generalized perturbation theory and leads to a C^* -dynamical system over a classically extended algebra of observables. The classical part of the dynamical system, expressed by a set of 15 nonlinear differential equations, is observed to be independent from the perturbations. The KMS states of the C^* -dynamical system are determined on the state space of the extended algebra of observables. The subsimplices of KMS states with unbroken symmetries are investigated and used to define the “type” of a phase. The KMS phase diagrams are worked out explicitly and compared with the thermodynamic phase structures obtained in the preceding works.

KEY WORDS: Classically extended observable algebra; inhomogeneous bipolaronic superconductors; global C^* -dynamics; KMS states; types of KMS states; KMS phase diagrams; physical phase diagrams.

1. INTRODUCTION

Already in the early theoretical treatments of superconductivity not only the equilibrium values but also the time dependent behaviour of the collective variables—in first line of the complex gap parameter—have been studied. Its rigorous microscopic derivation is, however, still an open problem for tempered interactions. For a class of long-range interactions recent developments^(3,4) in operator algebraic meanfield theory made

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accessible even a more ambitious dynamical program, namely the so-called *global limiting dynamics*, which is understood as the combination of the classical macro-dynamics with the (effective) quantum dynamics for the microscopic degrees of freedom. Both the macroscopic and microscopic parts of the limiting dynamics, interrelated by so-called cocycle equations, are uniquely determined by the original family of local Hamiltonians. From that input it is then derived by a systematic treatment, involving a C^* -extension of the quasi-local lattice algebra—but without any space for ad hoc assumptions—the limiting dynamics in form of a C^* -dynamical system.

We have previously⁽³⁾ carried through this scheme for a model class, which includes the strong coupling BCS-model. In the latter, by definition, not only the pairing interaction but also the kinetic energy is momentum independent for electrons near the Fermi surface. This renders the model homogeneous, that is invariant under permutations of the one lattice point observables, which are taken from a 16-dimensional quasi-spin algebra. The natural set of collective variables comprises, therefore, 15 parameters, of which only three seem to be of direct physical relevance in equilibrium.

The generalization of the dynamics from homogeneous to weakly inhomogeneous long range models has been worked out in ref. 4 for the case of equilibrium representations. The effective dynamics, which describes only small fluctuations about the equilibrium in this representation, is obtained by the thermodynamic limit of a net of local perturbation series, with the homogeneous dynamics as zeroth order term.

In the present investigation we combine both techniques for the first time and elaborate the limiting collective dynamics of a weakly inhomogeneous bipolaronic superconductor model. In various theoretical groups, cf. especially ref. 5 and references therein, this model is considered relevant for certain high- T_c aspects. It has a more involved operator structure than the BCS-Hamiltonian. First, in order to comprise also antiferromagnetic background features, connected with so-called charge ordering aspects, a bipartite lattice structure is introduced in our formulation, reflecting itself in the doubling of the operators in the quasilocal algebra. Second it involves two kinds of interactions, originating from the original hopping and Coulomb interaction terms, respectively. This leads, beside the phase angle correlations in the superconducting region, to the appearance of a second ordering phenomenon, which creates different charge densities in the two sub-lattices, and thus breaks spontaneously the sub-lattice exchange symmetry of the local input interactions.

As mentioned above, we extend in our approach the quasilocal algebra of the microscopic observables to a larger C^* -algebra, comprising also classical collective variables. (This contrasts the usual strategy for

homogeneous meanfield-models, where the weak closure of the represented quasilocal C^* -algebra is employed, leading to a von Neumann algebra with only the equilibrium values of the collective variables in its center.) Their dynamical evolution may be expressed by a set of nonlinear differential equations, but it is still part of a quantum mechanical, C^* -dynamical system.

This form of an Heisenberg dynamics is essential for the discussion of the thermodynamical aspects, especially of the KMS- and minimal free energy states, since the fundamental investigations in this area start from abstract C^* -dynamical systems. Especially, it is also a prerequisite to apply the theory of metastable states as formulated, e.g., in refs. 6 and 7. Since we deal here with an explicitly given type of Heisenberg dynamics, we do not need the more technical concepts of C^* -dynamical systems.

In Section 2 we translate the model assumptions into asymptotic relations for the interaction parameters, clarifying especially, what it means to be near the homogenization average.

The second step in Section 2 deals with the appropriate extension of the quasilocal algebra to comprise also the possible values of the collective observables, which here appear in the nontrivial center of the C^* -algebra \mathcal{C}_{cl} . This leads to a universal shape of the sectorial decomposition of the states (in terms of a subcentral measure), which is basic for all later arguments.

In Section 3 the homogeneous dynamics is elaborated, the structure of which is known in principle from the algebraic meanfield theory, here constituting the zeroth order of perturbation theory. Its classical part can be expressed on an 15-dimensional parameter space. The one-cell operators, which specify the physical meaning of the coordinates, are given in Appendix A, the equations for the modified phase angle dynamics are written out in Appendix B.

The rather new step is the perturbation theory of Section 4 for the long-range interacting inhomogeneous models. It is demonstrated, that the model assumptions allow for a generalized perturbational treatment in arbitrary, faithful representations of the classically extended C^* -algebra. The convergence estimations, which are based on commutator expressions quite similar to those in ref. 4, are independent from the representation, and in this sense "algebraic." In this way there is no need to require the states of the perturbed system to be normal to the unperturbed ones.

In Section 5 we determine the homogeneous and inhomogeneous KMS-states and analyze their properties.

In the last Section we classify the KMS-states according to their symmetry types and arrive at KMS-phase diagrams, which are definitely richer than the thermodynamic phase diagrams for the minimal free energy states. In contradistinction to short range interactions, the KMS-condition is

shown here not to be equivalent with the minimal free energy condition, but only with the stationarity condition, providing the principal possibility of metastable states in the above mentioned sense. Since we concentrate here on the dynamical foundation of thermodynamic features, deduced from the global C^* -dynamical system of the bipolaronic superconductor by the KMS-condition, we have deferred the elaboration of many mathematical details, especially the extensibility of the relevant inhomogeneous microscopic states to the classical observables, to a later occasion.

2. THE QUASILOCAL MODEL FRAMEWORK AND ITS EXTENSION

2.1. The Local Model Hamiltonians

Let us first briefly review the quasilocal, algebraic framework, which has been also the starting point for our previous, purely thermo-statistical discussions refs. 1 and 2: The C^* -algebra \mathfrak{A} of observables for the electronic system of our model is specified as it is usual in the frame of operator algebraic many body physics (see refs. 8, 9, 7 and references therein) by the algebras for each local subregion of the lattice. As mentioned in the Introduction we are dealing with a bipartite lattice in configuration space \mathfrak{R} , but we denote the local regions simply by $A \in \mathfrak{Q} := \{A' \subset \mathfrak{R} \mid |A'| < \infty\}$ and express the bipartite structure in terms of the composite site-algebra $\mathfrak{B} := \tilde{\mathfrak{B}} \otimes \tilde{\mathfrak{B}}$ with $\tilde{\mathfrak{B}} \cong \mathbb{M}_2(\mathbb{C})$ for each lattice site $i \in \mathfrak{R}$. Then the local algebras of observables for each $A \in \mathfrak{Q}$ are given by $\mathfrak{A}_A = \bigotimes_{i \in A} \mathfrak{B}_i$, where \mathfrak{B}_i is an isomorphic copy of \mathfrak{B} , placed on the lattice site i . The canonical embedding of \mathfrak{A}_A into $\mathfrak{A}_{A'}$, whenever $A \subset A'$, is a prerequisite for the C^* -inductive limit construction (cf. ref. 10). It leads to the smallest C^* -algebra containing all local algebras, hence the naming “quasilocal algebra:”

$$\mathfrak{A} := \bigotimes_{i \in \mathfrak{R}} \mathfrak{B}_i := \overline{\bigcup_{A \in \mathfrak{Q}} \mathfrak{A}_A}^{\|\cdot\|}$$

It is physically the set of all purely microscopic observables, for which it is the characteristic feature to be independent from the (macro) state of the environment. In order to make explicit the bipartite structure of this observable algebra we introduce the notation $c^1 := c \otimes \mathbb{1} \in \mathfrak{B}$ and $c^2 := \mathbb{1} \otimes c \in \mathfrak{B}$ for $c \in \tilde{\mathfrak{B}}$. For $a \in \mathfrak{B}$ we write $a_i \in \mathfrak{A}$ to designate the operator $\dots \otimes \mathbb{1} \otimes a \otimes \mathbb{1} \otimes \dots$, where a is situated at the i th component of the tensor product. The annihilation (creation) operator for a pair of phonon dressed electrons, a bipolaron, at the lattice site i is denoted by $b_i^{r(*)} \in \mathfrak{B}_i$,

$r \in \{1, 2\}$. They fulfill the commutation relations for so-called hard-core bosons:

$$\begin{aligned} [b_i^{r*}, b_j^s] &= b_i^{r*} b_j^s - b_j^s b_i^{r*} = \delta_{rs} \delta_{ij} (2\hat{n}_i^r - \mathbb{1}) \\ \{b_i^{r*}, b_j^s\} &= b_i^{r*} b_j^s + b_j^s b_i^{r*} = \delta_{rs} \delta_{ij} \mathbb{1}, \quad (b_i^r)^2 = 0 \end{aligned}$$

for all $r, s \in \{1, 2\}$ and all $i \in \mathfrak{R}$, where we have introduced the bipolaronic number operator $\hat{n}_i^r := b_i^{r*} b_i^r$ at site i .

As is described in ref. 5, under certain conditions the following Hamiltonian is a useful approximation for the electronic part of the considered class of systems:

$$H_A = \frac{1}{|A|} \left(\sum_{i_1, i_2 \in A} v_{i_1 i_2} \hat{n}_{i_1}^1 \hat{n}_{i_2}^2 - 2 \sum_{i_1, i_2 \in A} (t_{i_1 i_2} b_{i_1}^{1*} b_{i_2}^2 + \bar{t}_{i_1 i_2} b_{i_1}^1 b_{i_2}^{2*}) \right) \in \mathfrak{A}_A \quad (2.1)$$

Here, the first part of the interaction, the distance-dependent, static Coulomb term, has to be symmetric, $v_{i_1 i_2} = v_{i_2 i_1} \in \mathbb{R}$, whereas the spatially inhomogeneous hopping term for pairs, as an intrinsically dynamical, phase-shifting potential, might well be complex with, $t_{i_1 i_2} = \bar{t}_{i_2 i_1}$.

For the present models it is a well established strategy to assume long range behaviour in the sense that the interactions behave at large distances like a non vanishing constant. Thus the following spatially homogeneous model should serve well as reference system:

$$H_A^0 = \frac{1}{|A|} \left(v \sum_{i_1, i_2 \in A} \hat{n}_{i_1}^1 \hat{n}_{i_2}^2 - 2t \sum_{i_1, i_2 \in A} b_{i_1}^{1*} b_{i_2}^2 + b_{i_1}^1 b_{i_2}^{2*} \right) \in \mathfrak{A}_A \quad (2.2)$$

We assume for the occurring constants, the averaged interaction potentials, that $v, t > 0$.

The local Hamiltonians H_A^0 lead, of course, to a treatable model in virtue of their high symmetry. Especially they are invariant under the group of permutations $\mathcal{P}(A)$ of the lattice sites in the local sublattice A ,

$$\Theta_\sigma(H_A^0) = H_A^0 \quad \text{for all } \sigma \in \mathcal{P}(A) \quad \text{and all } A \in \mathfrak{A}$$

where Θ_σ is first defined on the elementary tensors by $\Theta_\sigma(\otimes_{i \in A} a_i) := \otimes_{i \in A} a_{\sigma(i)}$, with $a_i \in \mathfrak{A}$ and with $\sigma(i) = i$ outside from A , and then linearly and continuously extended to all of \mathfrak{A} . The group of all (finite) permutations is introduced as

$$\mathcal{P} = \bigcup_{A \in \mathfrak{A}} \mathcal{P}(A) \quad (2.3)$$

Both the original and homogenized Hamiltonians possess so-called internal symmetries, which act within each one-lattice-site algebra in the same manner. For this we recognize here the symmetry under the permutation of the two sublattices, which forms together with the identity the two-point symmetric group S_2 , and the symmetry under gauge transformations, which constitute the one-dimensional torus group $SU(1)$ (cf., e.g., ref. 1). Thus we have as the total group of internal symmetries for our models $S_2 \times SU(1)$, with the unique Haar measure $d\mu_h$.

The indicated internal symmetries act in \mathfrak{A} via C^* -automorphisms, which are again uniquely determined by the way they transform elementary tensors:

$$\alpha_v \left(\bigotimes_{i \in \mathfrak{R}} a_i \right) := \bigotimes_{i \in \mathfrak{R}} v a_i v^* \quad (2.4)$$

Here v is a unitary in \mathfrak{B} and a_i is an arbitrary element in \mathfrak{B} , both of them embedded into $\mathfrak{B}_i \subset \mathfrak{A}$.

In order to formulate the symmetry operations also in the Schrödinger picture recall that the set of states $\mathfrak{S}(\mathfrak{A})$, which consists of all expectation functionals, is a w^* -compact and convex subset of the dual Banach space \mathfrak{A}^* . If a group G acts via automorphisms α_g , $g \in G$, in \mathfrak{A} the dual transformations v_g , defined by

$$\langle v_g(\varphi); A \rangle := \langle \varphi; \alpha_{g^{-1}}(A) \rangle \quad (2.5)$$

transform the states accordingly. We denote the subset of all permutation invariant states by \mathfrak{S}^P .

We still have to make mathematically precise, in which sense the homogenized model should be near a given inhomogeneous one. For this we introduce for each A the difference operator

$$P_A := H_A - H_A^0 = \frac{1}{|A|} \left(\sum_{i_1, i_2 \in A} \delta v_{i_1 i_2} \hat{n}_{i_1}^1 \hat{n}_{i_2}^2 - 2 \sum_{i_1, i_2 \in A} (\delta t_{i_1 i_2} b_{i_1}^{1*} b_{i_2}^2 + \bar{\delta} t_{i_1 i_2} b_{i_1}^1 b_{i_2}^{2*}) \right) \quad (2.6)$$

between the original and the homogeneous Hamiltonian, where

$$\delta v_{i_1 i_2} := v_{i_1 i_2} - v \quad \text{and} \quad \delta t_{i_1 i_2} := t_{i_1 i_2} - t$$

In usual mathematical treatments of perturbed C^* -dynamical systems the net of perturbations has to be uniformly bounded. In the more recent developments of algebraic meanfield theory $\{P_A \mid A \in \mathfrak{Q}\}$ would be a so-called “quasi-symmetric” net (cf. refs. 11 and 12). We found however (see

refs. 4 and 13), that much weaker conditions on the perturbations allow still for a mathematically well established, dynamical perturbation theory. We, therefore, postulate the following relations for our class of bipolaronic models:

General Assumption for the Model Class 2.1. The averages of the inhomogeneous interactions have to exist in the thermodynamic limit

$$v = \lim_{\mathcal{A} \in \mathfrak{Q}} \frac{1}{|\mathcal{A}|^2} \sum_{i_1, i_2 \in \mathcal{A}} v_{i_1 i_2}, \quad t = \lim_{\mathcal{A} \in \mathfrak{Q}} \frac{1}{|\mathcal{A}|^2} \sum_{i_1, i_2 \in \mathcal{A}} t_{i_1 i_2} \quad (2.7)$$

Further the limits

$$\begin{aligned} \lim_{i_2 \rightarrow \infty} \delta v_{i_1 i_2} = \delta v_{i_1}, \quad \lim_{i_2 \rightarrow \infty} \delta t_{i_1 i_2} = \delta t_{i_1} \\ \text{with} \quad \lim_{i_1 \rightarrow \infty} \delta v_{i_1} = 0 \quad \text{and} \quad \lim_{i_1 \rightarrow \infty} \delta t_{i_1} = 0 \end{aligned} \quad (2.8)$$

as well as

$$\begin{aligned} \lim_{\mathcal{A} \in \mathfrak{Q}} \frac{1}{|\mathcal{A}|} \sum_{i_1, i_2 \in \mathcal{A}} |\delta v_{i_1 i_2} - \delta v_{i_1} - \delta v_{i_2}| = 0 \\ \lim_{\mathcal{A} \in \mathfrak{Q}} \frac{1}{|\mathcal{A}|} \sum_{i_1, i_2 \in \mathcal{A}} |\delta t_{i_1 i_2} - \delta t_{i_1} - \bar{\delta} t_{i_2}| = 0 \end{aligned} \quad (2.9)$$

have to exist with the given limiting values. Here $\lim_{\mathcal{A} \in \mathfrak{Q}}$ always denotes the net limit over the index set \mathfrak{Q} .

Let us emphasize that we do not use any summability condition for δt_i or δv_i , so that $\|P_{\mathcal{A}}\|$ may tend with increasing \mathcal{A} to infinity in a rather strong sense.

2.2. The Classically Extended Algebra of Observables

It is well known that the so-called “mean-field operators,” the spatial averages of one-cell operators,

$$m_{\mathcal{A}}(a) := \frac{1}{|\mathcal{A}|} \sum_{i \in \mathcal{A}} a_i = \frac{1}{|\mathcal{A}|} \sum_{i \in \mathcal{A}} T_i a_0 \quad \text{with} \quad a \in \mathfrak{B} \quad (2.10)$$

(T_i a lattice translation) which occur in $H_{\mathcal{A}}^0$ (cf., Eq. (3.2)) explicitly, but in a hidden form also in $H_{\mathcal{A}}$, do not converge in the norm topology and,

therefore, have no limit in \mathfrak{A} . They may, however, converge in a weaker topology to limits outside of \mathfrak{A} . The set of states, which can be resolved by the meanfield operators, is $\mathfrak{E}^P \subset \mathfrak{S}(\mathfrak{A})$, the set of all permutation invariant states. In the meanfield expectations an arbitrary state may be replaced by its spatial, permutation invariant average. On the other side, each meanfield operator assumes all its possible expectation values already in \mathfrak{E}^P . The convex, compact set \mathfrak{E}^P is a Bauer simplex having a compact extremal boundary $\partial_e \mathfrak{E}^P$.⁽¹⁴⁾ Thus there exists a unique decomposition for each state $\omega \in \mathfrak{E}^P(\mathfrak{A})$ into states of the extremal boundary, the latter being just the factor states of \mathfrak{E}^P and the only states of the product form $\otimes \rho$ with $\rho \in \mathfrak{S}(\mathfrak{B})$.

We now want to give a more explicit characterization of the elements in $\partial_e \mathfrak{E}^P$. Since the single site algebras \mathfrak{B}_i of our model are of the form $\mathfrak{B} = \mathbb{M}_2(\mathbb{C}) \otimes \mathbb{M}_2(\mathbb{C}) \cong \mathbb{M}_4(\mathbb{C})$, we may use the Lie-algebra \mathcal{G} for the Lie-group $\mathbf{SU}(4)$ to introduce a distinguished antihermitian basis $\{\beta^1, \dots, \beta^{15}\}$, resp. the hermitian counterpart $\{i\beta^1, \dots, i\beta^{15}\}$. This basis is given in Appendix A. A parameterization of $\partial_e \mathfrak{E}^P$ can then be introduced by the evaluation of the 15 nontrivial, independent coordinates and leads to the affine homeomorphism

$$\mathfrak{S}(\mathfrak{B}) \ni \rho \mapsto (\langle \rho; i\beta^1 \rangle, \dots, \langle \rho; i\beta^{15} \rangle) =: x_\rho \in \mathbb{R}^{15}$$

The preceding formula discloses, that $\mathfrak{S}(\mathfrak{B})$ may also be considered as a subset $E_{\mathcal{G}}$ of \mathcal{G}^* , the dual space of the Lie algebra \mathcal{G} . In order to conform with previous notational conventions (ranging back to geometric quantization), we consider $\partial_e \mathfrak{E}^P(\mathfrak{A})$ as parameterized in terms of the differentiable manifold $E_{\mathcal{G}}$, keeping nevertheless often the symbol ρ for its elements instead of x_ρ . We write in this sense for the extremal decomposition in \mathfrak{E}^P :

$$\varphi = \int_{E_{\mathcal{G}}} \otimes \varrho \, d\mu_\varphi(\varrho), \quad \varphi \in \mathfrak{E}^P \quad (2.11)$$

In view of these considerations we base the dynamics of our models on the following observable algebra.

Definition 2.2. The *classically-extended observable-algebra* is defined as the C^* -algebra

$$\mathcal{C}_{\mathcal{G}} \cong \mathfrak{A} \otimes \mathcal{C}(E_{\mathcal{G}}) \cong \mathcal{C}(E_{\mathcal{G}}, \mathfrak{A}) \quad (2.12)$$

where $\mathcal{C}(E_{\mathcal{G}}, \mathfrak{A})$ are the continuous functions from $E_{\mathcal{G}}$ into \mathfrak{A} .

Not all states on $\mathcal{C}_{\mathcal{G}}$ are physically relevant, since their values for the collective variables should be deduceable from their values on the quasilocal

observables, that is, they should be “microscopically extended.” The implications of this subsidiary condition will be elaborated elsewhere. For the decomposition of the equilibrium states, the following results are basic.

Proposition 2.3. (i) For each state $\omega \in \mathfrak{S}(\mathcal{C}_{\mathcal{G}})$ there is a Borel measure μ_ω and a μ_ω -a.e. unique measurable function $E_{\mathcal{G}} \ni \varrho \rightarrow \omega_\varrho \in \mathfrak{S}(\mathcal{C}_{\mathcal{G}})$, providing the following integral decomposition of ω (called the *sector decomposition*):

$$\langle \omega; A \rangle = \int_{E_{\mathcal{G}}} \langle \omega_\varrho; A(\varrho) \rangle d\mu_\omega(\varrho) \quad A \in \mathcal{C}_{\mathcal{G}} \quad (2.13)$$

(ii) For each state $\omega \in \mathfrak{S}(\mathcal{C}_{\mathcal{G}})$ the measure μ_ω is (after transposition to a measure on $\mathfrak{S}(\mathcal{C}_{\mathcal{G}})$) subcentral.

(iii) The foregoing decomposition is the central decomposition, iff the component states ω_ϱ are factor states μ_ω -a.e.

3. THE GLOBAL DYNAMICS OF THE HOMOGENEOUS SYSTEM

We assume throughout the following that we have an arbitrary but fixed representation of \mathfrak{A} , in which all meanfield limits exist in the weak topology and which is extended to a faithful representation of $\mathcal{C}_{\mathcal{G}}$ in the same Hilbert space. The σ -weak and strong operator topologies, employed for the subsequent limits, refer always to this representation. Since $\mathcal{C}_{\mathcal{G}}$ is isomorphic to its representation, we omit the representation symbol.

The reduced local Hamiltonian of the homogeneous system is obtained by subtracting the chemical and electrostatic potential energy

$$H_A^{r0}(\mu) := H_A^{r0} := H_A^0 - \mu N_A := H_A^0 - \mu \sum_{i \in A} (\hat{n}_i^1 + \hat{n}_i^2) \quad (3.1)$$

H_A^{r0} can be expressed as a polynomial in the local space averaged operators $m_A(i\beta^l)$:

$$\begin{aligned} H_A^{r0} &= |A| Q(m_A(i\beta^1), \dots, m_A(i\beta^{15})) \\ &= |A| v(2m_A(i\beta^{15})^2 + 2m_A(i\beta^{14})^2 + m_A(i\beta^3) - m_A(i\beta^7)) \\ &\quad \times (2m_A(i\beta^8)^2 + 2m_A(i\beta^9)^2 + m_A(i\beta^3) + m_A(i\beta^7)) \\ &\quad - |A| 2t(4m_A(i\beta^8) m_A(i\beta^{15}) + 4m_A(i\beta^9) m_A(i\beta^{14})) \\ &\quad - |A| \mu(2m_A(i\beta^{15})^2 + 2m_A(i\beta^{14})^2 + 2m_A(i\beta^8)^2 \\ &\quad + 2m_A(i\beta^9)^2 + 2m_A(i\beta^3)) \end{aligned} \quad (3.2)$$

We introduce the reduced local homogeneous Heisenberg dynamics

$$\tau_t^{0,A}(\cdot) = \exp\{itH_A^{r0}\} \cdot \exp\{-itH_A^{r0}\}$$

and obtain analogously as in ref. 3—which for itself is a modification of the general strategy developed in ref. 15—the following results for its thermodynamic limit:

Theorem 3.1. (i) For the net of local Hamiltonians $\{H_A^{r0} \mid A \in \mathcal{Q}\}$ there exists a unique C^* -dynamical system $(\tau_t^0)_{t \in \mathbb{R}}$ (that is a point wise norm continuous group of $*$ -automorphisms) on $\mathcal{C}_{\mathcal{G}}$, such that for each $A \in \mathcal{C}_{\mathcal{G}}$, which necessarily possesses a local approximation $A = s\text{-lim}_{A \in \mathcal{Q}} A_A$, it holds:

$$\tau_t^0(A) = s\text{-lim}_{A \in \mathcal{Q}} \exp\{itH_A^{r0}\} A_A \exp\{-itH_A^{r0}\} \quad \text{for all } t \in \mathbb{R} \quad (3.3)$$

(ii) For each $\varrho \in E_{\mathcal{G}}$ and each t we introduce a C^* -automorphism $\tau_t^{0\varrho}$, which acts on local elements $A \in \mathfrak{A}$ as

$$\tau_t^{0\varrho}(A) = \left(\bigotimes_{i \in \mathfrak{R}} \exp\{ith_i^0(\varrho)\} \right) A \left(\bigotimes_{i \in \mathfrak{R}} \exp\{-ith_i^0(\varrho)\} \right) \quad (3.4)$$

With this sector dependent dynamics the action of the global τ_t^0 on $A = (\varrho \mapsto A(\varrho)) \in \mathcal{C}_{\mathcal{G}}$ has the explicit form

$$\tau_t^0(A)(\varrho) = \tau_t^{0\varrho}(A(\gamma_t(\varrho))) \quad (3.5)$$

Here, at each lattice site i we have the same one-cell Hamiltonian $h^0(\varrho) \in \mathfrak{B}$, of the form

$$\begin{aligned} h^0(\varrho) &= \sum_{l=1}^{15} \frac{\partial Q}{\partial x_j}(\varrho)(i\beta^j) \\ &= v(\langle \varrho; \hat{n}^2 \rangle \hat{n}^1 + \langle \varrho; \hat{n}^1 \rangle \hat{n}^2) - 2t(\langle \varrho; b^2 \rangle b^{1*} + \langle \varrho; b^{2*} \rangle b^1) \\ &\quad - 2t(\langle \varrho; b^1 \rangle b^{2*} + \langle \varrho; b^{1*} \rangle b^2) - \mu(\hat{n}^1 + \hat{n}^2) \end{aligned} \quad (3.6)$$

Making use of the structure constants C_l^{kj} of the Lie-algebra \mathcal{G} , the classical flow $(\gamma_t)_{t \in \mathbb{R}}$ on $E_{\mathcal{G}}$ is given by the vector field

$$\lambda^{\varrho}: \mathbb{R}^{15} \rightarrow \mathbb{R}^{15}, \quad (\lambda^{\varrho}(\varrho))_k = \sum_{j=1}^{15} \frac{\partial Q}{\partial x_j}(\varrho) \left(\sum_{l=1}^{15} C_l^{kj} x_l(\varrho) \right) \quad (3.7)$$

in terms of the differential equation

$$\frac{d\gamma_t(\varrho)}{dt} = \lambda \mathcal{Q}(\gamma_t(\varrho)) \quad \text{for } \varrho \in E_{\mathcal{G}}, \quad t \in \mathbb{R} \tag{3.8}$$

Its explicit form in special coordinates is given in Appendix B.

Proof. (i) follows from ref. 11 with [12, Prop. 4.2] (cf. also refs. 16 and 17).

(ii) is an immediate consequence from (i), where the flow and the effective single site Hamiltonian are calculated from Eq. (3.2). ■

4. THE GLOBAL DYNAMICS OF THE INHOMOGENEOUS SYSTEM

As the starting point we first calculate the limit of the local Heisenberg generators in increasing regions for the perturbed system, which act on a fixed local observable $A_A \in \mathfrak{A}_A$. For such kinds of limits we use weaker-than-norm topologies (the strong operator topology and the σ -weak topology) in our fixed representation. The subsequent elaboration, based on the evaluation of commutators shows, that our results do not depend on the representation.

Introducing $H_{A'}^r(\mu) := H_{A'}^r := H_A - \mu N_A$ we investigate the existence and form of the limit:

$$\text{s-lim}_{A' \in \mathfrak{Q}} [H_{A'}^r, A_A] = \text{s-lim}_{A' \in \mathfrak{Q}} [H_{A'}^0, A_A] + \text{s-lim}_{A' \in \mathfrak{Q}} [P_{A'}, A_A]$$

where $H_{A'}^0$, H_A and $P_{A'}$ are from Eqs. (3.1), (2.1) and (2.6).

Lemma 4.1. With the model assumptions 2.1 for $P_{A'}$ it holds for fixed $A_A \in \mathfrak{A}_A$

$$\text{s-lim}_{A' \in \mathfrak{Q}} [P_{A'}, A_A] = [P_{A'}^{\mathcal{G}}, A_A] \tag{4.1}$$

with

$$P_{A'}^{\mathcal{G}} = \sum_{i \in A} \delta h_i \in \mathcal{C}(E_{\mathcal{G}}, \mathfrak{A}_A) \subset \mathcal{C}(E_{\mathcal{G}}, \mathfrak{A}) \cong \mathcal{C}_{\mathcal{G}} \tag{4.2}$$

where δh_i is given by

$$\begin{aligned} \delta h_i(\varrho) = & \delta v_i(\langle \varrho; \hat{n}^1 \rangle \hat{n}_i^2 + \langle \varrho; \hat{n}^2 \rangle \hat{n}_i^1) - 2\delta t_i(\langle \varrho; b^2 \rangle b_i^{1*} + \langle \varrho; b^1 \rangle b_i^{2*}) \\ & - 2\overline{\delta t}_i(\langle \varrho; b^{1*} \rangle b_i^2 + \langle \varrho; b^{2*} \rangle b_i^1) \end{aligned} \quad (4.3)$$

Proof. The reasoning runs parallel to that in ref. 4. ■

For general quasilocal observables the limiting perturbation series cannot be written down, because of the lack of the limiting perturbation operator. Nevertheless we may announce, as one of our main results, the following structure of a well-defined, algebraic limiting dynamics for the inhomogeneous system:

Theorem 4.2. (i) For each model satisfying the model assumptions 2.1 there exists a unique C^* -dynamical system $(\mathcal{C}_{\mathcal{G}}, \mathbb{R}, \tau_t)$ such that for each $A \in \mathcal{C}(E_{\mathcal{G}}, A_A)$, with $A \in \mathfrak{Q}$, there exists a $t_0 = t_0(A) > 0$ allowing for the limit relation

$$\tau_t(A) = \sigma - w - \lim_{A' \in \mathfrak{Q}} (\tau_t^0)^{P_{A'}}(A) = (\tau_t^0)^{P_A}(A) \quad \text{for } |t| < t_0 \quad (4.4)$$

(ii) Let us introduce the sector dependent automorphism group in \mathfrak{A} :

$$\tau_t^{\mathfrak{q}}(A) = \left(\bigotimes_{i \in \mathfrak{R}} \exp\{ith_i(\varrho)\} \right) A \left(\bigotimes_{i \in \mathfrak{R}} \exp\{-ith_i(\varrho)\} \right), \quad A \in \mathfrak{A} \quad (4.5)$$

where $h_i(\varrho) := h_i^0(\varrho) + \delta h_i(\varrho)$ with h_i^0 from Eq. (3.6) and δh_i from Eq. (4.3), this is

$$\begin{aligned} h_i(\varrho) = & (v + \delta v_i)(\langle \varrho; \hat{n}^1 \rangle \hat{n}_i^2 + \langle \varrho; \hat{n}^2 \rangle \hat{n}_i^1) \\ & - 2(t + \delta t_i)(\langle \varrho; b^2 \rangle b_i^{1*} + \langle \varrho; b^1 \rangle b_i^{2*}) \\ & - 2(t + \overline{\delta t}_i)(\langle \varrho; b^{1*} \rangle b_i^2 + \langle \varrho; b^{2*} \rangle b_i^1) \end{aligned} \quad (4.6)$$

Then it holds for $A = (\varrho \mapsto A(\varrho)) \in \mathcal{C}_{\mathcal{G}}$

$$\tau_t(A)(\varrho) = \tau_t^{\mathfrak{q}}(A(\gamma_t(\varrho))) \quad (4.7)$$

The classical flow γ_t on $E_{\mathcal{G}}$ is the same as in the homogeneous case.

Proof. The proof again parallels the reasoning given in the appendix of ref. 4. ■

5. THE KMS-STATES

The KMS-condition was introduced by refs. 18 and 19 in the context of Greens functions and in ref. 20 in its algebraic version. In the C^* -algebraic formalism a state ω is called a β -KMS-state of the C^* -dynamical system $(\tau_t)_{t \in \mathbb{R}}$ if for all τ_t -analytic elements A, B in the C^* -algebra it holds

$$\langle \omega; A\tau_{i\beta}(B) \rangle = \langle \omega; BA \rangle \tag{5.1}$$

where $i\beta$ is the special imaginary value of time given by the natural temperature β .

The grandcanonical KMS-states, we are interested in, are indexed usually by the two real numbers (β, μ) , where the natural temperature β occurs in Eq. (5.1) and the chemical potential μ is introduced in Eq. (3.1) as a parameter of the reduced dynamics. The set of all β -KMS-states for the (homogeneous) C^* -dynamical system $(\mathcal{C}_{\mathcal{G}}, \mathbb{R}, \tau_t^{(0)}(\mu))$ be denoted by $\mathfrak{S}_{\text{KMS}}^{(0)}(\beta, \mu)$.

5.1. The KMS-States of the Homogeneous Model

First we calculate the extremal KMS-states, the candidates for the pure equilibrium phases, for the homogeneous model.

Proposition 5.1. The extremal β -KMS-states in $\partial_e \mathfrak{S}_{\text{KMS}}^{(0)}(\beta, \mu)$ are exactly the states with the sector decomposition:

$$\omega^0 = \int_{E_{\mathcal{G}}} \omega_{\varrho}^0 \delta(\varrho' - \varrho) d\varrho' = \omega_{\varrho}^0 \tag{5.2}$$

where ω_{ϱ}^0 has as restriction to \mathfrak{A} the homogeneous product state

$$\otimes \varrho \quad \text{with } \varrho \text{ of the form } \varrho = \frac{e^{-\beta h^0(\varrho)}}{\text{tr}\{e^{-\beta h^0(\varrho)}\}} \tag{5.3}$$

$h^0(\varrho)$ being taken from Eq. (3.6).

Thus the point support $\varrho \in E_{\mathcal{G}}$ of the Dirac measure $\delta(\varrho' - \varrho) d\varrho'$ has coordinates, which satisfy the self-consistency equations

$$\langle \varrho; i\beta^l \rangle = \text{tr} \left\{ \frac{e^{-\beta h^0(\varrho)} i\beta^l}{\text{tr}\{e^{-\beta h^0(\varrho)}\}} \right\} \tag{5.4}$$

for all members of the basis $\{i\beta^1, \dots, i\beta^{15}\}$, and, reversely, each solution of Eq. (5.4) determines a homogeneous KMS-state ω_{ϱ}^0 .

The explicit form of $h_i^0(\rho)$ in Eqs. (3.6) and (5.4), and the relations from Eq. (A.2) imply that the KMS-states for the homogeneous limiting dynamics are characterized by the following self-consistency equations for the two real parameters $n_1 := \langle \varrho; \hat{n}^1 \rangle$ and $n_2 := \langle \varrho; \hat{n}^2 \rangle$ and for the two complex parameters $\Delta_1 e^{-i\vartheta_1} := t \langle \varrho; b^1 \rangle$ and $\Delta_2 e^{-i\vartheta_2} := t \langle \varrho; b^2 \rangle$:

$$\begin{aligned} n_1 &= \frac{1}{2} - \frac{vn_2 - \mu}{2\sqrt{(vn_2 - \mu)^2 + 16(\Delta_2)^2}} \tanh\left(\frac{\beta}{2}\sqrt{(vn_2 - \mu)^2 + 16(\Delta_2)^2}\right) \\ n_2 &= \frac{1}{2} - \frac{vn_1 - \mu}{2\sqrt{(vn_1 - \mu)^2 + 16(\Delta_1)^2}} \tanh\left(\frac{\beta}{2}\sqrt{(vn_1 - \mu)^2 + 16(\Delta_1)^2}\right) \\ \Delta_1 e^{i\vartheta_1} &= \frac{t\Delta_2 e^{i\vartheta_2}}{\sqrt{(vn_2 - \mu)^2 + 16(\Delta_2)^2}} \tanh\left(\frac{\beta}{2}\sqrt{(vn_2 - \mu)^2 + 16(\Delta_2)^2}\right) \\ \Delta_2 e^{i\vartheta_2} &= \frac{t\Delta_1 e^{i\vartheta_1}}{\sqrt{(vn_1 - \mu)^2 + 16(\Delta_1)^2}} \tanh\left(\frac{\beta}{2}\sqrt{(vn_1 - \mu)^2 + 16(\Delta_1)^2}\right) \end{aligned} \quad (5.5)$$

From the last two equations one sees, that only the macroscopic phase difference between the two sublattice systems may be fixed by the above equations. Thus we introduce the new phase variables:

$$\vartheta := (\vartheta_1 + \vartheta_2)/2 \quad \Delta\vartheta := (\vartheta_2 - \vartheta_1)/2 \quad (5.6)$$

In terms of the mentioned six real parameters we give the explicit form of the effective one-cell Hamiltonians for each value of the macroscopic phases and for each distribution of the two electron densities on the sublattices:

$$\begin{aligned} h_{12}^{0\vartheta}(\varrho) &:= (vn_2 - \mu) \hat{n}^1 + (vn_1 - \mu) \hat{n}^2 - 2(\Delta_2 e^{-(i/2)(\vartheta + \Delta\vartheta)} b^{1*} \\ &\quad + \Delta_2 e^{+(i/2)(\vartheta + \Delta\vartheta)} b^1) \\ &\quad - 2(\Delta_1 e^{-(i/2)(\vartheta - \Delta\vartheta)} b^{2*} + \Delta_1 e^{+(i/2)(\vartheta - \Delta\vartheta)} b^2) \\ h_{21}^{0\vartheta}(\varrho) &:= (vn_2 - \mu) \hat{n}^2 + (vn_1 - \mu) \hat{n}^1 - 2(\Delta_2 e^{-(i/2)(\vartheta + \Delta\vartheta)} b^{2*} \\ &\quad + \Delta_2 e^{+(i/2)(\vartheta + \Delta\vartheta)} b^2) \\ &\quad - 2(\Delta_1 e^{-(i/2)(\vartheta - \Delta\vartheta)} b^{1*} + \Delta_1 e^{+(i/2)(\vartheta - \Delta\vartheta)} b^1) \end{aligned} \quad (5.7)$$

The corresponding one-cell KMS-states have the form:

$$\varrho_{12}^{0\vartheta} := \frac{e^{-\beta h_{12}^{0\vartheta}(\varrho)}}{\text{tr}\{e^{-\beta h_{12}^{0\vartheta}(\varrho)}\}}, \quad \varrho_{21}^{0\vartheta} := \frac{e^{-\beta h_{21}^{0\vartheta}(\varrho)}}{\text{tr}\{e^{-\beta h_{21}^{0\vartheta}(\varrho)}\}} \quad (5.8)$$

This makes explicit, that for our model interaction, only the mentioned six collective variables possibly appear in the extremal KMS-states and constitute the thermodynamic order parameters. The remaining nine collective coordinates do not appear in the effective energy expressions and are not incorporated into our discussion. For the equilibrium indicated by (β, μ) one has to calculate all solutions of the self-consistency equations in order to determine $\partial_e \mathfrak{S}_{\text{KMS}}^0(\beta, \mu)$ in terms of the chosen parameterization. From the above selfconsistency equations it follows, that $\Delta\mathfrak{G}$ can have only the trivial equilibrium values $\mathbb{Z}\pi$, and we fix it at zero

$$\Delta\mathfrak{G} := 0$$

Thus the obtained parameter set

$$E(\beta, \mu) := \{ \varrho \in E_{\mathfrak{G}} \mid \varrho \text{ solves the selfconsistency Eq. (5.4)} \} \quad (5.9)$$

is a subset of \mathbb{R}^5 , which is *compact*, since the order parameters vary in bounded intervals, and the continuous selfconsistency equations have no singular points. Since the elements of $E(\beta, \mu)$ are invariant under γ_t and permutation invariance is ensured for our considered product states, the only symmetries to be discussed are the internal symmetries from $\mathbf{S}_2 \times \mathbf{SU}(1)$.

Proposition 5.2. (i) The sector decomposition

$$\omega^0 = \int_{E(\beta, \mu)} \omega_{\varrho}^0 d\mu_{\omega^0}(\varrho) \quad (5.10)$$

provides an affine homeomorphism

$$\mathfrak{S}_{\text{KMS}}^0(\beta, \mu) \ni \omega^0 \leftrightarrow \mu_{\omega^0} \in M_+^1((\beta, \mu)) \quad (5.11)$$

revealing the set of homogeneous KMS-states as a Bauer simplex (that is a simplex with compact extremal boundary, the latter being here the point measures on $E(\beta, \mu)$).

(ii) If ϱ (resp. x_{ϱ}) is a solution of Eq. (5.4), then also $\gamma_g \varrho$ is so for all $g \in \mathbf{S}_2 \times \mathbf{SU}(1)$. Thus $E(\beta, \mu)$ is a $\mathbf{S}_2 \times \mathbf{SU}(1)$ -invariant set and, therefore, is the union of orbits. We write:

$$E(\beta, \mu) = \bigcup_{v \in V} \mathfrak{D}_{\varrho(v)} \quad (5.12)$$

where the representatives of an orbit are indexed in terms of the index set V , a measurable subset of \mathbb{R}^n , for some $n \leq 5$, which may be chosen compact.

(iii) Associated with each orbit $\mathfrak{O}_{\varrho^{(v)}}$ is a unique invariant KMS-state $\bar{\omega}_v^0$, obtained by mixing with the Haar measure over the orbit. It has the explicit form:

$$\bar{\omega}_v^0 = \int_0^{2\pi} \left(\frac{1}{2} \otimes_{i \in \mathfrak{R}} \varrho_{12}^{0g} + \frac{1}{2} \otimes_{i \in \mathfrak{R}} \varrho_{21}^{0g} \right) \frac{d\vartheta}{2\pi} \quad (5.13)$$

where ϱ_{12}^{0g} and ϱ_{21}^{0g} are determined by Eqs. (5.5) and (5.7) and their parameters are related with the orbit index v . There are four types of invariant KMS-states of the form of Eq. (5.13): (1) The $\mathfrak{S}_2 \times \mathfrak{SU}(1)$ -integral is trivial (normal states); (2) only the \mathfrak{S}_2 -integral is trivial (superconducting states); (3) only the $\mathfrak{SU}(1)$ -integral is trivial (charge ordered states); (4) no orbit integral is trivial (mixed phase states).

(iv) For the set of all invariant KMS-states one has the affine homeomorphism

$$\bar{\mathfrak{E}}_{\text{KMS}}^0(\beta, \mu) \ni \bar{\omega}^0 \leftrightarrow \bar{\mu}_\omega \in M_+^1(V) \quad (5.14)$$

revealing $\bar{\mathfrak{E}}_{\text{KMS}}^0(\beta, \mu)$ to constitute a Bauer simplex. The $\bar{\omega}_v^0$ are exactly the extremal $\mathfrak{S}_2 \times \mathfrak{SU}(1)$ -invariant states in $\bar{\mathfrak{E}}_{\text{KMS}}^0(\beta, \mu)$. Since there are at most four extremal invariant KMS-states, $\bar{\mathfrak{E}}_{\text{KMS}}^0(\beta, \mu)$ is affine isomorphic to a face of a tetrahedron.

5.2. The KMS-States of the Inhomogeneous Model

The treatment of the KMS-states $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ of the inhomogeneous limiting dynamics essentially parallels the homogeneous case, in spite of these states being macroscopically different from each other—for given β and μ —in certain instances.

Proposition 5.3. The extremal β -KMS-states in $\partial_e \mathfrak{E}_{\text{KMS}}(\beta, \mu)$ are exactly the states of the form

$$\omega = \int_{E_g} \omega_{\varrho'} \delta(\varrho' - \varrho) d\varrho' = \omega_\varrho \quad (5.15)$$

where ω_ϱ has as its restriction to \mathfrak{A} the inhomogeneous product state

$$\otimes_{i \in \mathfrak{R}} \varrho_i(\varrho) \quad \text{with} \quad \varrho_i(\varrho) = \frac{e^{-\beta h_i(\varrho)}}{\text{tr}_{\mathfrak{B}} \{ e^{-\beta h_i(\varrho)} \}} \quad (5.16)$$

h_i being taken from Eq. (4.6). The point support of the Dirac measure $\delta(\varrho' - \varrho) d\varrho'$ is uniquely determined for each β -KMS-state by the same self-consistency equations (5.4) as for the homogeneous case, implying:

$$\partial_e \mathfrak{S}_{\text{KMS}}(\beta, \mu) = \{\omega_\varrho \mid \varrho \in E(\beta, \mu)\} \tag{5.17}$$

With the definitions $n_r^i := (1 + (\delta v_i/v)) n_r$, $A_r^i := |(1 + (\delta t_i/t)) t \langle \varrho; b^r \rangle| = |1 + (\delta t_i/t)| A_r$ and $\delta \vartheta_i := -\text{Arg}(1 + (\delta t_i/t))$ we can adopt the notation from Eq. (5.7) for the inhomogeneous case (note, that we set $\Delta \vartheta = 0$):

$$\begin{aligned} h_{12}^{i\vartheta} &:= (vn_2^i - \mu) \hat{n}^1 + (vn_1^i - \mu) \hat{n}^2 - 2A_2^i(e^{-i(\vartheta - \delta \vartheta_i)} b^{1*} + e^{+i(\vartheta - \delta \vartheta_i)} b^1) \\ &\quad - 2A_1^i(e^{-i(\vartheta - \delta \vartheta_i)} b^{2*} + e^{+i(\vartheta - \delta \vartheta_i)} b^2) \\ h_{21}^{i\vartheta} &:= (vn_2^i - \mu) \hat{n}^2 + (vn_1^i - \mu) \hat{n}^1 - 2A_2^i(e^{-i(\vartheta - \delta \vartheta_i)} b^{2*} + e^{+i(\vartheta - \delta \vartheta_i)} b^2) \\ &\quad - 2A_1^i(e^{-i(\vartheta - \delta \vartheta_i)} b^{1*} + e^{+i(\vartheta - \delta \vartheta_i)} b^1) \\ \varrho_{12}^{i\vartheta}(\varrho) &:= \frac{e^{-\beta h_{12}^{i\vartheta}(\varrho)}}{\text{tr}\{e^{-\beta h_{12}^{i\vartheta}(\varrho)}\}} \\ \varrho_{21}^{i\vartheta}(\varrho) &:= \frac{e^{-\beta h_{21}^{i\vartheta}(\varrho)}}{\text{tr}\{e^{-\beta h_{21}^{i\vartheta}(\varrho)}\}} \end{aligned} \tag{5.18}$$

With this definitions let us describe the sets of KMS-states for the inhomogeneous dynamics, observing that the latter has also $S_2 \times \text{SU}(1)$ as an exact internal symmetry group.

Proposition 5.4. (i) The inhomogeneous KMS-states $\omega \in \mathfrak{S}_{\text{KMS}}(\beta, \mu)$ are exactly the states of $\mathfrak{S}(\mathcal{C}_\vartheta)$ which have the sector decomposition

$$\omega = \int_{E(\beta, \mu)} \omega_\varrho d\mu_\omega(\varrho) \tag{5.19}$$

with the ω_ϱ from Prop. 5.3. This provides an affine homeomorphism

$$\mathfrak{S}_{\text{KMS}}(\beta, \mu) \ni \omega \leftrightarrow \mu \in M^1_+(E(\beta, \mu)) \tag{5.20}$$

disclosing the set of inhomogeneous KMS-states to form a Bauer simplex. Associating with each $\omega \in \mathfrak{S}_{\text{KMS}}(\beta, \mu)$ the homogeneous KMS-state $\omega^0 \in \mathfrak{S}_{\text{KMS}}^0(\beta, \mu)$ with the same sectorial decomposition measure establishes an affine homeomorphism between the two sets of KMS-states, which only locally—but not globally—may be expressed in terms of a KMS perturbation expansion.

(ii) Associated with each orbit $\mathfrak{D}_{\varrho(v)}$ is a unique invariant KMS-state $\bar{\omega}_v$, obtained by mixing via the Haar measure over the orbit. It has the explicit form:

$$\bar{\omega}_v = \int_0^{2\pi} \left(\frac{1}{2} \otimes_{i \in \mathfrak{R}} \varrho_{12}^{i\vartheta} + \frac{1}{2} \otimes_{i \in \mathfrak{R}} \varrho_{21}^{i\vartheta} \right) \frac{d\vartheta}{2\pi} \quad (5.21)$$

where $\varrho_{12}^{i\vartheta}$ and $\varrho_{21}^{i\vartheta}$ are determined by Eqs. (5.18) and their parameters are related with the orbit index v . There are the previous four types of invariant KMS-states:

- (1) The $\mathbf{S}_2 \times \mathbf{SU}(1)$ -integral is trivial (normal states N);
- (2) only the \mathbf{S}_2 -integral is trivial (superconducting states S);
- (3) only the $\mathbf{SU}(1)$ -integral is trivial (charge ordered states CO);
- (4) no orbit integral is trivial (mixed phase states M).

(iii) For the set of all invariant KMS-states one has the affine homeomorphism

$$\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu) \leftrightarrow M_+^1(V) \quad (5.22)$$

showing $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ to be a Bauer simplex, which is affine isomorphic to a *face of the tetrahedron*. The $\bar{\omega}_v$ are exactly the extremal $\mathbf{S}_2 \times \mathbf{SU}(1)$ -invariant states in $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$.

6. THE KMS-PHASE DIAGRAMS

In order to discuss the obtained KMS-states from a thermodynamic point of view, we recall, that here, as in most (quantum) lattice systems, the equilibrium states have a natural partition into “types” according to occurrence and coexistence of the broken internal symmetries. In this respect there is no difference to the (stable) thermodynamic phases, and we may subdivide the space $\mathbb{R}_+ \times \mathbb{R}$ of the external parameters β, μ into regions of equal types in order to draw something like a KMS-phase diagram. The complete KMS-phase structure is given by the bundle

$$P_{\text{KMS}} := \{ \mathfrak{E}_{\text{KMS}}(\beta, \mu) \mid (\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R} \} \quad (6.1)$$

For a concise characterization of the type we coarsen the simplices $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ to the sub-simplices $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ of invariant KMS-states (under internal symmetries). By means of Prop. 5.4 (iii) we map each $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ onto a face of the tetrahedron in an affinely isomorphic manner. Let us combine the symbols for the four extremal points of the tetrahedron to the set $\{N, S, \text{CO}, M\}$. Then each of the 16 subsets of

$\{N, S, CO, M\}$ (including the empty and the total set) gives a symbol, which describes biunivocally a face of the tetrahedron. By the above mentioned affine mapping also each face of $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ is mapped onto a face of the tetrahedron and thus also acquires a subset of $\{N, S, CO, M\}$ as an identifying symbol.

The idea is now, that the simplices of the tetrahedron may serve to characterize the basic structure, that is the type, of $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ as well as of a single KMS-state. This generalizes the notion of a type already introduced for the 4 extremal invariant KMS-states of Section 5, where each for itself constitutes a face of $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$, which is mapped onto an extremal point of the tetrahedron. These are designated by a one-element symbol and are called *elementary types*.

Definition 6.1. (i) The type of $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ is the tetrahedron face (resp. its symbol) onto which $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ is mapped via Prop. 5.4 (iii). This defines in the (β, μ) - or in the (β, n) -parameter space regions of equal type, the boundaries of which giving the “KMS-phase boundaries.”

(ii) The type of a single KMS-state is defined as follows: Form its invariant mean over the internal symmetry group and determine the smallest face of $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$ which contains this invariant KMS-state. The corresponding tetrahedron face (resp. its symbol) is then taken as the type of the given KMS-state.

In general $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ includes invariant states associated with different orbits and their convex combinations, leading to the various faces of $\bar{\mathfrak{E}}_{\text{KMS}}(\beta, \mu)$. Thus the types for the $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ are chosen in principle from 16 possibilities. (The empty set may occur in systems, where there is, e.g., a maximal temperature and β^{-1} is larger.) If there are invariant states in $\mathfrak{E}_{\text{KMS}}(\beta, \mu)$ associated with different orbits then, and only then, one would speak in the case of physical equilibrium states (with minimal free energy) of *phase coexistence*. Note that the convex combination of KMS-states belonging to one orbit is a purely statistical one.

The 5 types of sets of KMS-states, occurring in the present model class, may easily be deduced from the observations, that the normal phase N satisfies the KMS-condition for each (β, μ) and has thus always to be included in the phase type, and that the mixed phase M needs the presence of the S- and CO-solutions of the KMS-condition, obtaining thus all of the three other elementary types necessarily as partners.

The types of the single KMS-states are then given by all possible sub-simplices of the five mentioned ones, including the four elementary types. An arbitrary extremal KMS-states (with broken symmetry) is always mapped—via averaging over one orbit—onto an extremal invariant KMS-

state, and thus obtains an elementary type. Reversely, an extremal invariant KMS-state is decomposed (uniquely) into extremal KMS-states (of the same type), where only the latter are usually called *pure phase states* in statistical mechanics. The invariant (“mixed phase”) M-states are extremal invariant KMS-states and thus are of elementary type rather than being coexistence states.

As is shown in the preceding Section there is an affine homeomorphism between $\mathfrak{S}_{\text{KMS}}(\beta, \mu)$ of a given model and $\mathfrak{S}_{\text{KMS}}^0(\beta, \mu)$ of the associated homogenized model. Now let us take into account, that the type is an affine invariant in order to arrive at




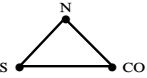
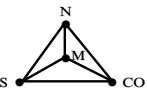
Proposition 6.2. For a model in the considered class the type of the set $\mathfrak{S}_{\text{KMS}}(\beta, \mu)$, for given $(\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R}$, equals the type of $\mathfrak{S}_{\text{KMS}}^0(\beta, \mu)$, where the latter are the KMS-states of the associated homogeneous model. Thus, for fixed (β, μ) the types of the KMS-states, but not the states (with their fluctuations) for themselves, depend only on the averaged model constants v and t .

The 5 types of KMS-sets for our model class are listed in Table 1, together with the back translation into invariant KMS-states. The kind of broken symmetry for the pure phase states is seen from the non-trivial orbit structure of the invariant KMS-states. As mentioned before, a KMS-set which includes the M-type must be affinely isomorphic to the whole tetraeder. States with all 4 elementary phase types occur in this set and would, as physical phases, coexist. The states besides the mixing coefficients λ_i , $i = 1, 2, 3, 4$, are extremal invariant KMS-states. The last one is the invariant M-state in its decomposition into pure phase states. These pure phase states, given by an infinite tensor product over position-dependent one-cell density operators, have the same sharp macroscopic phase angle (with microscopic fluctuations) but different condensate densities (with microscopic fluctuations) on the two sublattices. Since they combine both kinds of symmetry break down, the application of the internal symmetry transformations generates the maximal orbit and makes in this way explicit the M-type character also for these pure phase states. Altogether, each group of nonvanishing λ_i 's specifies the type of the KMS-state, shown in the table, which is obtained by mixing KMS-states of elementary types, imitating phase coexistence.

We may now use the calculational material of ref. 2 for the homogeneous models to draw the KMS-phase diagram. In order to use the more detailing (β, n) -coordinates we observe that the limiting equation

$$n(\beta, \mu) := \lim_{A \in \mathfrak{Q}} \left\langle \omega(\beta, \mu); \frac{N_A}{|A|} \right\rangle \quad (6.2)$$

Table 1. KMS-States Which Are Invariant Under the Internal Symmetry Group $SU(1) \times S_2$

Phase region	Invariant KMS states
	$\omega = \bigotimes_{i \in \mathfrak{R}} \varrho^{iN}$
	$\omega = \lambda \bigotimes_{i \in \mathfrak{R}} \varrho^{iN} + (1 - \lambda) \left(\frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{12}^{iCO} + \frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{21}^{iCO} \right)$ with $\lambda \in [0, 1]$
	$\omega = \lambda \bigotimes_{i \in \mathfrak{R}} \varrho^{iN} + (1 - \lambda) \int_0^{2\pi} \bigotimes_{i \in \mathfrak{R}} \varrho^{i\theta S} \frac{d\theta}{2\pi}$ with $\lambda \in [0, 1]$
	$\omega = \lambda_1 \bigotimes_{i \in \mathfrak{R}} \varrho^{iN} + \lambda_2 \left(\frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{12}^{iCO} + \frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{21}^{iCO} \right) + \lambda_3 \int_0^{2\pi} \bigotimes_{i \in \mathfrak{R}} \varrho^{i\theta S} \frac{d\theta}{2\pi}$ with $\lambda_{1,2,3} \in [0, 1]$ and $\lambda_1 + \lambda_2 + \lambda_3 = 1$
	$\omega = \lambda_1 \bigotimes_{i \in \mathfrak{R}} \varrho^{iN} + \lambda_2 \left(\frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{12}^{iCO} + \frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{21}^{iCO} \right) + \lambda_3 \int_0^{2\pi} \bigotimes_{i \in \mathfrak{R}} \varrho^{i\theta S} \frac{d\theta}{2\pi}$ $+ \lambda_4 \int_0^{2\pi} \left(\frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{12}^{i\theta S} + \frac{1}{2} \bigotimes_{i \in \mathfrak{R}} \varrho_{21}^{i\theta S} \right) \frac{d\theta}{2\pi}$ with $\lambda_{1,2,3,4} \in [0, 1]$ and $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 1$

with $\omega(\beta, \mu) \in \mathfrak{S}_{\text{KMS}}(\beta, \mu)$, may be solved for the function

$$\mathbb{R}_+ \times [0, 2] \ni (\beta, n) \rightarrow \mu(\beta, n) \in \mathbb{R} \tag{6.3}$$

by the same reasoning as in ref. 2. The resulting KMS-phase diagram is pictured in Fig. 1. Before being able to perform a comparison between KMS-phase diagrams and physical phase diagrams we have to introduce the thermodynamic functions over appropriate (nonequilibrium) states of our inhomogeneous models. We do this—without giving existence proofs—for certain microscopically extended states $\omega \in \mathfrak{S}(\mathcal{C}_g)$, and start with their restrictions $\omega_A := \omega|_{\mathcal{A}_A}$, for which there is a unique density operator D_A . In view of the grand canonical ensemble we define the local internal energy density

$$u_A(\beta, \mu; \omega_A) := \left\langle \omega_A; \frac{H_A^r(\mu)}{|A|} \right\rangle \tag{6.4}$$

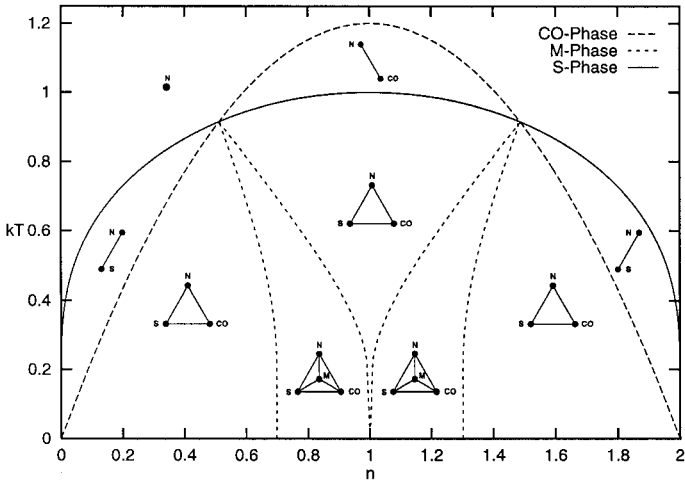


Fig. 1. KMS-phase diagram for the homogeneous as well as for the inhomogeneous limiting KMS dynamics for the parameter settings $t=1$ and $v>4$.

with $H_A^r(\mu)$ the reduced model Hamiltonians, and the local entropy density

$$s_A(\omega_A) := -\frac{\text{tr}_A\{D_A \ln D_A\}}{|A|} \quad (6.5)$$

In case that the limits exist, we write for the limiting free energy density

$$f(\beta, \mu; \omega) = \lim_{A \in \mathfrak{A}} f(\beta, \mu; \omega_A) = \lim_{A \in \mathfrak{A}} [u_A(\beta, \mu; \omega_A) - \beta s_A(\omega_A)] \quad (6.6)$$

For our considered models the limiting internal energy density exists in all microscopically extended states. Omitting in this work technical details we only communicate that there is a sufficiently large class $\mathfrak{S}_{\text{Th}}(\mathcal{C}_g)$ of microscopically extended states—comprising our inhomogeneous KMS-states—in which the limiting entropy density exists with the same value as for the corresponding homogenized states.²

Proposition 6.3. Let $(\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R}$ be arbitrary but fixed.

(i) For $\omega \in \mathfrak{S}_{\text{Th}}(\mathcal{C}_g)$, with the sector components ω_q and the measure $\mu_\omega \in M_+^1(E_g)$ it holds

² A sufficient condition for a state to be in $\mathfrak{S}_{\text{Th}}(\mathcal{C}_g)$ is the convergence of the translation average in the state norm topology.

$$\begin{aligned}
 f(\beta, \mu; \omega) &= \int_{E_{\mathcal{G}}} f(\beta, \mu; \omega_{\varrho}) \, d\mu_{\omega}(\varrho) \\
 &= \int_{E_{\mathcal{G}}} f(\beta, \mu; \omega_{\varrho}^0) \, d\mu_{\omega}(\varrho) \\
 &= f(\beta, \mu; \omega^0) \quad \forall (\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R}
 \end{aligned} \tag{6.7}$$

- (ii) $f(\beta, \mu; \omega)$ is an affine lower semicontinuous function in ω .
- (iii) $f(\beta, \mu; \omega) = f(\beta, \mu; v_g \omega)$, $\forall g \in \mathbf{S}_2 \times \mathbf{SU}(1)$.
- (iv) The function

$$E_{\mathcal{G}} \ni \varrho \rightarrow f(\beta, \mu; \omega_{\varrho}^0)$$

is differentiable in the open subset of invertible one-cell density operators ϱ . It holds

$$E(\beta, \mu) = \{ \varrho \in E_{\mathcal{G}} \mid df(\beta, \mu; \omega_{\varrho}^0) = 0 \} \tag{6.8}$$

$E(\beta, \mu)$ having been defined in (5.9).

- (v) The set

$$M(\beta, \mu) := \{ \varrho \in E_{\mathcal{G}} \mid \varrho \rightarrow f(\beta, \mu; \omega_{\varrho}^0) \text{ is minimal} \}$$

is a non-empty, closed subset of $E(\beta, \mu)$.

- (vi) The set $\mathfrak{S}_{\text{Th}}(\beta, \mu)$ of all absolute minima of the function $\mathfrak{S}_{\text{Th}}(\mathcal{C}_{\mathcal{G}}) \ni \omega \rightarrow f(\beta, \mu; \omega)$ is a w^* -closed sub-simplex of $\mathfrak{S}_{\text{KMS}}(\beta, \mu)$. For $\omega \in \mathfrak{S}_{\text{Th}}(\mathcal{C}_{\mathcal{G}})$ with sector measure μ_{ω} it holds

$$\omega \in \mathfrak{S}_{\text{Th}}(\beta, \mu) \Leftrightarrow \text{supp } \mu_{\omega} \subset M(\beta, \mu) \tag{6.9}$$

- (vii) The type of $\mathfrak{S}_{\text{Th}}(\beta, \mu)$ (as a subset of $\{N, S, \text{CO}, M\}$) is a subset of the type of $\mathfrak{S}_{\text{KMS}}(\beta, \mu)$.
- (viii) It holds the reduction shown in Table 2.

Proof. Besides the technical details, which will be given elsewhere, the results are rather straightforward, if one notes that

$$df(\beta, \mu; \omega_{\varrho}^0) = h(\varrho) - \frac{1}{\beta} (c + \ln \varrho)$$

where c is an unspecified c -number. (The basic manifold is here the convex set $E_{\mathcal{G}}$, on which the differentiation takes place. Since there is the subsidiary condition $\text{tr}_{\mathfrak{B}}(\varrho) = 1$, c remains unspecified in the total differential,

Table 2. Type Reduction of the KMS-States

$\mathfrak{S}_{\text{KMS}}(\beta, \mu)$ type	Minimal free energy principle	$\mathfrak{S}_{\text{Th}}(\beta, \mu)$ type
{N}	—————→	{N}
{N, CO}	—————→	{CO}
{N, S}	—————→	{S}
{N, S, CO}	$f_{\text{CO}} < f_{\text{S}}$ ↘	{CO}
	$f_{\text{CO}} > f_{\text{S}}$ ↘	{S}
{N, S, CO, M}	grand canonical ↘	{S, CO}
	canonical ↘	{M}

but is determined by the normalization afterwards. The tangent space to E_g is isomorphic to \mathfrak{B}^* and the cotangent vectors of the total differential may be realized by—non-unique—elements in $\mathfrak{B}^{**} = \mathfrak{B}$.) Thus $df = 0$ is equivalent to the self-consistency equation (5.4), which in turn is equivalent to the KMS condition. The assertions on $M(\beta, \mu)$ follow from the Bauer minimum principle (cf. e.g., ref. 8) and from the fact that a face of a simplex is a simplex for itself. ■

The thermodynamic phase structure is expressed by the bundle

$$P_{\text{Th}} := \{ \mathfrak{S}_{\text{Th}}(\beta, \mu) \mid (\beta, \mu) \in \mathbb{R}_+ \times \mathbb{R} \} \quad (6.10)$$

In contrast to the equivalence of the KMS-condition with local thermodynamic stability (cf. refs. 21, 22, and 9) we may draw from the proceeding discussion the

Conclusion 6.4. In the present model class the KMS-condition is equivalent to the stationarity of the limiting free energy density, that is to thermodynamic equilibrium (with uniform intensive contact variables) without thermodynamic stability (minimality of the free energy density³). The thermodynamic phase structure P_{Th} differs, in general, significantly from the KMS-Phase structure P_{KMS} (to which it is a “sub substructure”).

³ In the thermodynamic treatment of equilibrium and stability one varies, of course, not ω but macroscopic state variables, beside the fixed β and μ . This is done virtually (Gibbs) or in terms of the composite system approach (refs. 23 and 24, and Wightman’s Introduction in ref. 25).

The specification, which of the present, non absolutely stable KMS-states are in fact metastable, would require a more detailed, numerical investigation of the extremal free energy states.

APPENDIX A. BASIS OF THE LIE ALGEBRA \mathcal{G} OF $SU(4)$

With the Pauli spin matrices $\sigma_x, \sigma_y, \sigma_z$ we define

$$e_1 := \frac{1}{4}(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y), \quad e_2 := \frac{1}{4}(\sigma_x \otimes \sigma_y - \sigma_y \otimes \sigma_x)$$

$$e_3 := \frac{1}{4}(\sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_z)$$

$$e_4 := \frac{1}{2\sqrt{2}}(\sigma_z \otimes \sigma_z), \quad e_5 := \frac{1}{4}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)$$

$$e_6 := \frac{1}{4}(\sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x)$$

$$e_7 := \frac{1}{4}(\mathbb{1} \otimes \sigma_z - \sigma_z \otimes \mathbb{1}), \quad e_8 := \frac{1}{2\sqrt{2}}(\mathbb{1} \otimes \sigma_x)$$

$$e_9 := \frac{1}{2\sqrt{2}}(\mathbb{1} \otimes \sigma_y)$$

$$e_{10} := \frac{1}{2\sqrt{2}}(\sigma_x \otimes \sigma_z), \quad e_{11} := \frac{-1}{2\sqrt{2}}(\sigma_y \otimes \sigma_z), \quad e_{12} := \frac{-1}{2\sqrt{2}}(\sigma_z \otimes \sigma_y)$$

$$e_{13} := \frac{1}{2\sqrt{2}}(\sigma_z \otimes \sigma_x), \quad e_{14} := \frac{1}{2\sqrt{2}}(\sigma_y \otimes \mathbb{1}), \quad e_{15} := \frac{1}{2\sqrt{2}}(\sigma_x \otimes \mathbb{1})$$

With the unitary transformation $V: \mathbb{C}^2 \times \mathbb{C}^2 \rightarrow \mathbb{C}^4 = \mathbb{C} \oplus \mathbb{C}^2$ defined by

$$(1, 0) \otimes (1, 0) \rightarrow (1, 0, 0, 0) = (1, 0) \oplus (0, 0)$$

$$(0, 1) \otimes (0, 1) \rightarrow (0, 1, 0, 0) = (0, 1) \oplus (0, 0)$$

$$(0, 1) \otimes (1, 0) \rightarrow (0, 0, 1, 0) = (0, 0) \oplus (1, 0)$$

$$(1, 0) \otimes (0, 1) \rightarrow (0, 0, 0, 1) = (0, 0) \oplus (0, 1)$$

we define the elements $\beta^k := -iVe_kV^{-1}$ of the basis $\{\beta^1, \dots, \beta^{15}\}$ for the Lie algebra of $SU(4)$. We then have:

$$\begin{aligned}
 i\beta^1 &= \frac{1}{2} \begin{pmatrix} \sigma_x & 0_2 \\ 0_2 & 0_2 \end{pmatrix}, & i\beta^2 &= \frac{1}{2} \begin{pmatrix} \sigma_y & 0_2 \\ 0_2 & 0_2 \end{pmatrix}, & i\beta^3 &= \frac{1}{2} \begin{pmatrix} \sigma_z & 0_2 \\ 0_2 & 0_2 \end{pmatrix} \\
 i\beta^4 &= \frac{1}{2\sqrt{2}} \begin{pmatrix} \mathbb{1} & 0_2 \\ 0_2 & -\mathbb{1} \end{pmatrix}, & i\beta^5 &= \frac{1}{2} \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & \sigma_x \end{pmatrix}, & i\beta^6 &= \frac{1}{2} \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & \sigma_y \end{pmatrix} \\
 i\beta^7 &= \frac{1}{2} \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & \sigma_z \end{pmatrix}, & i\beta^8 &= \frac{1}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_x \\ \sigma_x & 0_2 \end{pmatrix}, & i\beta^9 &= \frac{1}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_y \\ \sigma_y & 0_2 \end{pmatrix} \\
 i\beta^{10} &= \frac{1}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_z \\ \sigma_z & 0_2 \end{pmatrix}, & i\beta^{11} &= \frac{i}{2\sqrt{2}} \begin{pmatrix} 0_2 & \mathbb{1} \\ -\mathbb{1} & 0_2 \end{pmatrix} \\
 i\beta^{12} &= \frac{i}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_x \\ -\sigma_x & 0_2 \end{pmatrix} \\
 i\beta^{13} &= \frac{i}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_y \\ -\sigma_y & 0_2 \end{pmatrix}, & i\beta^{14} &= \frac{i}{2\sqrt{2}} \begin{pmatrix} 0_2 & \sigma_z \\ -\sigma_z & 0_2 \end{pmatrix} \\
 i\beta^{15} &= \frac{1}{2\sqrt{2}} \begin{pmatrix} 0_2 & \mathbb{1} \\ \mathbb{1} & 0_2 \end{pmatrix}
 \end{aligned}$$

which satisfy the orthonormality condition $\text{tr}\{(i\beta^k)^*(i\beta^l)\} = \frac{1}{2}\delta_{kl}$.

The structure constants C_i^{jk} are defined as

$$[\beta^j, \beta^k] = \sum_{l=1}^{15} C_l^{jk} \beta^l \quad (\text{A.1})$$

Finally we want to remark that certain elements of the basis may be interpreted as bipolaronic operators:

$$\begin{aligned}
 b^{1*} &= \frac{1}{2}(b_x^1 + ib_y^1) = \sqrt{2}(e_{15} + ie_{14}) \\
 b^1 &= \frac{1}{2}(b_x^1 - ib_y^1) = \sqrt{2}(e_{15} - ie_{14}) \\
 b^{2*} &= \frac{1}{2}(b_x^2 + ib_y^2) = \sqrt{2}(e_8 + ie_9) \\
 b^{2*} &= \frac{1}{2}(b_x^2 - ib_y^2) = \sqrt{2}(e_8 - ie_9) \\
 b_z^1 &= 2(e_3 - e_7) \\
 b_z^2 &= 2(e_3 + e_7)
 \end{aligned} \quad (\text{A.2})$$

APPENDIX B. THE CLASSICAL PART OF THE LIMITING DYNAMICAL SYSTEM

The classical dynamics $(\gamma_t)_{t \in \mathbb{R}}$ is given by the fifteen dimensional vector field from Eq. (3.7) that constitutes the Hamiltonian flow λ^Q and generates a differential equation for γ_t on the differentiable manifold $E_{\mathcal{G}}$. The part for the coordinates $x_3 = \langle i\beta^3; \varphi_{\varrho} \rangle$, $x_7 = \langle i\beta^7; \varphi_{\varrho} \rangle$, $x_8 = \langle i\beta^8; \varphi_{\varrho} \rangle$, $x_9 = \langle i\beta^9; \varphi_{\varrho} \rangle$, $x_{14} = \langle i\beta^{14}; \varphi_{\varrho} \rangle$ and $x_{15} = \langle i\beta^{15}; \varphi_{\varrho} \rangle$ which correspond to the bipolaronic expectation values $n_1, n_2, \Delta_1, \Delta_2, \mathcal{G}_1$ and \mathcal{G}_2 by Eq. (A.1) decouple from the differential equations for the coordinates $\{x_1, x_2, x_4, x_5, x_6, x_{10}, x_{11}, x_{12}, x_{13}\}$ which do depend on the values of the former mentioned but not vice versa. Therefore we will only give the part of the Hamiltonian flow corresponding to the ‘‘physically relevant’’ mean-field expectation values, which is sufficient to calculate the stationarity condition for the KMS-states:

$$\frac{d\gamma_t(\varrho)_3}{dt} = 0$$

$$\frac{d\gamma_t(\varrho)_7}{dt} = 8t(\gamma_t(\varrho)_8 \gamma_t(\varrho)_{14} - \gamma_t(\varrho)_9 \gamma_t(\varrho)_{15})$$

$$\begin{aligned} \frac{d\gamma_t(\varrho)_8}{dt} = & -4t\gamma_t(\varrho)_{14} (\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) \\ & + 2v\gamma_t(\varrho)_9 (2(\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) - 1)((\gamma_t(\varrho)_{15})^2 + (\gamma_t(\varrho)_{14})^2) \\ & + v\gamma_t(\varrho)_9 (2(-(\gamma_t(\varrho)_7)^2 + (\gamma_t(\varrho)_3)^2) + \gamma_t(\varrho)_7 - \gamma_t(\varrho)_3) \\ & - \mu\gamma_t(\varrho)_9 (2(\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) - 1) \end{aligned}$$

$$\begin{aligned} \frac{d\gamma_t(\varrho)_9}{dt} = & 4t\gamma_t(\varrho)_{15} (\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) \\ & - 2v\gamma_t(\varrho)_8 (2(\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) - 1)((\gamma_t(\varrho)_{15})^2 + (\gamma_t(\varrho)_{14})^2) \\ & + v\gamma_t(\varrho)_8 (2((\gamma_t(\varrho)_7)^2 - (\gamma_t(\varrho)_3)^2) - \gamma_t(\varrho)_7 + \gamma_t(\varrho)_3) \\ & + \mu\gamma_t(\varrho)_8 (2(\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) - 1) \end{aligned}$$

$$\begin{aligned} \frac{d\gamma_t(\varrho)_{14}}{dt} = & 4t\gamma_t(\varrho)_8 (\gamma_t(\varrho)_3 - \gamma_t(\varrho)_7) \\ & + 2v\gamma_t(\varrho)_{15} (2(-\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) + 1)((\gamma_t(\varrho)_8)^2 + (\gamma_t(\varrho)_9)^2) \\ & + v\gamma_t(\varrho)_{15} (2((\gamma_t(\varrho)_7)^2 - (\gamma_t(\varrho)_3)^2) + \gamma_t(\varrho)_7 + \gamma_t(\varrho)_3) \\ & + \mu\gamma_t(\varrho)_{15} (2(\gamma_t(\varrho)_3 - \gamma_t(\varrho)_7) - 1) \end{aligned}$$

$$\begin{aligned} \frac{d\gamma_t(\varrho)_{15}}{dt} = & 4t\gamma_t(\varrho)_9 (-\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) \\ & - 2v\gamma_t(\varrho)_{14} (2(-\gamma_t(\varrho)_3 + \gamma_t(\varrho)_7) + 1)((\gamma_t(\varrho)_8)^2 + (\gamma_t(\varrho)_9)^2) \\ & - v\gamma_t(\varrho)_{14} (2((\gamma_t(\varrho)_7)^2 - (\gamma_t(\varrho)_3)^2) + \gamma_t(\varrho)_7 + \gamma_t(\varrho)_3) \\ & - \mu\gamma_t(\varrho)_{14} (2(\gamma_t(\varrho)_3 - \gamma_t(\varrho)_7) - 1) \end{aligned}$$

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