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Spectral Phase Diagrams in Different Ensembles for Bipolaronic Superconductors

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Abstract. We start from the set of KMS–states for the global C^*–dynamics of a class of weakly inhomogeneous bipolaronic superconductors, which we have determined in a previous work. We discuss the spectral properties of the generator for the unitary implementation of the global Heisenberg dynamics in the GNS–representation over those KMS–states, which have minimal free energy density and unbroken internal symmetries. It is shown that the stable and hence macroscopically detectable part of such a spectrum is given by the spectrum of the homogenized model. The stable energy values depend on the temperature and doping of the system and lead to so–called spectral phase diagrams. The latter are meant to supplement the thermodynamic phase diagrams elaborated in earlier investigations. The different behaviour of the stable spectra for phase transitions of the first and second kind is especially significant. A classification of the factor types for the pure phase states – occurring in the central decomposition of the stable invariant KMS–states – is carried through. As a remarkable fact we found in certain phase regions a dense subset of pure phase states, which belong to factors of type III_1, having type III_λ states with $\lambda \lneq 1$ in each neighborhood. Thus, in these weakly inhomogeneous quantum lattice systems one has representations with dynamical relaxation features.

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1 Introduction and Preliminary Results

For the characterization of the macro–states of a many body system one uses not only the traditional thermodynamic potentials but frequently also parameters, which arise directly from the microscopic–statistical treatment of the pertinent models, being often related to certain ordering phenomena. For superconductors such a parameter is in first line the so–called gap. In the present investigation we analyze the spectral properties of a class of bipolaronic superconductor models and reveal peculiar stability features for certain energy values. Only these stable eigen–energies, which are invariants of the model class, are well–defined functions of the thermodynamic state variables. This is not so for the first excitation energy over the equilibrium state, which depend on the very details of the interaction potentials. Since each preparation of a macro–system produces a different kind of impurities and defects, the macroscopically relevant gap has to be associated with the stable part of a many body spectrum. These stable eigen–energies, which are not restricted to the superconducting phase region, are the main topic of the present work. In dependence of the temperature and density they illustrate characteristic features of the thermodynamic phases and of the phase transitions.

The model class treated here may be derived from Hubbard–like Hamiltonians [1], [2], [3].

$$H = \sum_{\langle i,j\rangle,\sigma} t_{ij}\, c^*_{i\sigma} c_{j\sigma} - \frac{1}{2}|v| \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} + \frac{1}{2} \sum_{\langle i,j\rangle,\sigma,\sigma'} w_{ij}\, n_{i\sigma} n_{j\sigma'},$$

where $\langle i,j\rangle$ indicates as usual summation over nearest neighbors. By means of perturbation theory, canonical transformations, and the introduction of pair operators $b_i^{(*)}$, one arrives at bipolaronic model Hamiltonians

$$H = \sum_{\langle i,j\rangle} v_{ij} n_i n_j - 2 \sum_{\langle i,j\rangle} t_{ij} b_i^* b_j. \tag{1.1}$$

Many treatments of such kinds of models, aimed to describe high–T_c superconducting features, involve anti–ferromagnetic effects and thus are connected with a bipartite sublattice structure. Here our model is treated from the outset on a bipartite lattice $\mathcal{K}$ in position space. Especially the algebra of observables has to reflect this structure and is, therefore, constructed over a composite one site–algebra $\mathfrak{B} = \widetilde{\mathfrak{B}} \otimes \widetilde{\mathfrak{B}}$, where $\widetilde{\mathfrak{B}} \cong \mathbb{M}_2(\mathbb{C})$. Below we will see that $\widetilde{\mathfrak{B}}$ describes the observables of a fermion pair, while $\mathfrak{B}$ describes the operators of two such pairs in different sublattices. As usual we form for each local sublattice region $\Lambda \in \mathfrak{L} := \{\Lambda' \subset \mathcal{K} \mid |\Lambda'| < \infty\}$ the algebra $\mathfrak{A}_\Lambda := \otimes_{i\in\Lambda} \mathfrak{B}_i$, where $\mathfrak{B}_i$ is an isomorphic copy of $\mathfrak{B}$, placed at site i. The algebra $\mathfrak{A}$ of the infinite lattice is the union of all local observables, mathematically obtained by the C^*–inductive limit of $\mathfrak{A}_\Lambda$, $\Lambda \in \mathfrak{L}$ with the canonical embedding of $\mathfrak{A}_\Lambda$ in $\mathfrak{A}_{\Lambda'}$, for $\Lambda \subset \Lambda'$ [4]:

$$\mathfrak{A} := \bigotimes_{i\in\mathcal{K}} \mathfrak{B}_i.$$

The local algebras $\mathfrak{A}_\Lambda$ can be considered as subalgebras of $\mathfrak{A}$, justifying the notation $\mathfrak{A} = \overline{\bigcup_{\Lambda\in\mathfrak{L}} \mathfrak{A}_\Lambda}^{\|\cdot\|}$. A specific model is characterized by the set of all local Hamiltonians $H_\Lambda \in \mathfrak{A}_\Lambda \subset \mathfrak{A}, \Lambda \in \mathfrak{L}$. Dropping the nearest neighbor subsidiary condition and employing now sublattice indices we get from

(1.1) our inhomogeneous model Hamiltonians [1], [5], [6], [7]:

$$H_\Lambda = \sum_{i_1,i_2\in\Lambda} v_{i_1i_2}\hat{n}^1_{i_1}\hat{n}^2_{i_2} - 2\sum_{i_1,i_2\in\Lambda}(t_{i_1i_2}b^{1*}_{i_1}b^2_{i_2} + \bar{t}_{i_1i_2}b^1_{i_1}b^{2*}_{i_2}) \quad \in \mathfrak{A}_\Lambda. \tag{1.2}$$

We use the notation $x^1 = x\otimes\mathbb{1}$, $x^2 = \mathbb{1}\otimes x \in \mathfrak{B}$ for $x\in\widetilde{\mathfrak{B}}$. Then $b^{r(*)}_i$, $r=1,2$ is the annihilation (creation) operator of a local pair (bipolaron) at site i in sublattice r, and $\hat{n}^r_i := b^{r*}_i b^r_i$ is the number operator. One stipulates the commutation relations, which are characteristic for so–called hard core Bosons:

$$[b^{r*}_i, b^r_j] = b^{r*}_i b^r_j - b^r_j b^{r*}_i = \delta_{ij}\,(2\hat{n}^r_i - \mathbb{1}), \quad \{b^{r*}_i, b^r_i\} = b^{r*}_i b^r_i + b^r_i b^{r*}_i = \mathbb{1}, \quad b^{r2}_i = 0,$$

for $r=1,2$ and $i\in\mathcal{K}$. All commutators between operators in different sublattices vanish.
Without specifying the asymptotic behavior of the interaction constants in (1.2) the models are far from being sufficiently described. In our previous investigations the above models have been treated under the extreme long range assumption namely, that the interaction constants $v_{i_1i_2}$ and $t_{i_1i_2}$ are only weak deviations from their average values v and t. More precisely we have required the following relations for a model to be in the allowed class:

Model Assumptions: For the interaction constants in H_Λ we stipulate:

$$v = \lim_{\Lambda\in\mathfrak{L}}\frac{1}{|\Lambda|^2}\sum_{i_1,i_2\in\Lambda} v_{i_1,i_2}, \qquad t = \lim_{\Lambda\in\mathfrak{L}}\frac{1}{|\Lambda|^2}\sum_{i_1,i_2\in\Lambda} t_{i_1,i_2}, \tag{1.3}$$

and with the abbreviations

$$\delta v_{i_1,i_2} := v_{i_1,i_2} - v \quad \text{and} \quad \delta t_{i_1,i_2} := t_{i_1,i_2} - t \tag{1.4}$$

we demand

$$\lim_{i_1\to\infty}\delta v_{i_1,i_2} = \delta v_{i_1}, \quad \lim_{i_1\to\infty}\delta t_{i_1,i_2} = \delta t_{i_1}, \quad \lim_{i_1\to\infty}\delta v_{i_1} = 0, \quad \lim_{i_1\to\infty}\delta t_{i_1} = 0, \tag{1.5}$$

as well as

$$\lim_{\Lambda\in\mathfrak{L}}\frac{1}{|\Lambda|^2}\sum_{i_1,i_2}|\delta v_{i_1,i_2} - \delta v_{i_1} - \delta v_{i_2}| = 0, \quad \lim_{\Lambda\in\mathfrak{L}}\frac{1}{|\Lambda|^2}\sum_{i_1,i_2}|\delta t_{i_1,i_2} - \delta t_{i_1} - \overline{\delta t}_{i_2}| = 0. \tag{1.6}$$

The foregoing describes analytically, in which sense the actual models are perturbations of the homogenized model

$$H^0_\Lambda = \frac{1}{|\Lambda|}\Big(v\sum_{i_1,i_2\in\Lambda}\hat{n}^1_{i_1}\hat{n}^2_{i_2} - 2t\sum_{i_1,i_2\in\Lambda}\big(b^{1*}_{i_1}b^2_{i_2} + b^1_{i_1}b^{2*}_{i_2}\big)\Big) \quad \in \mathfrak{A}_\Lambda. \tag{1.7}$$

As we have stated in previous papers, the local difference Hamiltonians

$$P_\Lambda := H_\Lambda - H^0_\Lambda \tag{1.8}$$

form in general a strongly unbounded net of operators, and the equilibrium states of two different models involving the same external parameters may be *macroscopically different*, that is mathematically *disjoint*.

General Strategy: The following investigation is based on the results in [5] on the global C^*–dynamical system and its KMS–states for the inhomogeneous model introduced above . The physically stable KMS–states corresponding to the canonical and the grand–canonical ensemble, which are invariant under the internal symmetries of the model, are derived in [5] and [8]. We briefly review the results from [8] and [5] and then derive the spectral properties of the unitary implementation of the global C^*–dynamical model system. One main result of our approach is, that under the above model assumptions the main features of the collective structure of the inhomogeneous models are the same as those of the homogeneous one.

Symmetries: Our inhomogeneous models H_Λ of (1.2) have as spatial symmetry the hidden permutation invariance. In fact, only H^0_Λ is strictly invariant under the action of the permutation group $\mathsf{P}(\Lambda)$ of Λ:

$$\Theta_\sigma(H^0_\Lambda) = H^0_\Lambda, \quad \text{for all } \sigma \in \mathsf{P}(\Lambda) \text{ and } \Lambda \in \mathfrak{L},$$

where $\Theta_\sigma : \mathfrak{A} \to \mathfrak{A}$ is defined on elementary tensors by $\Theta_\sigma(\otimes_i x_i) := \otimes_i x_{\sigma(i)}$ (for $i \notin \Lambda$, we have $\sigma(i) = i$).
Besides the homogeneity of the Hamiltonian, there are additional symmetries, the so–called internal symmetries, which leave each one–lattice point algebra $\mathfrak{B}_i$ invariant, and are exact symmetries also for the inhomogeneous Hamiltonians. These are the gauge transformations and the exchange transformations of sublattice indices [1]. The group of the internal symmetries is therefore given by $\mathsf{S}_2 \times \mathsf{SU}(1)$ where S_2 is the two–point symmetric group.

The Global C*–Dynamical System: The limit of the reduced local dynamics

$$\tau^\Lambda_t(\cdot) = \exp\{it\,H^r_\Lambda\} \cdot \exp\{-it\,H^r_\Lambda\} \tag{1.9}$$

with

$$H^r_\Lambda := H_\Lambda - \mu N_\Lambda := H_\Lambda - \mu \sum_{i\in\Lambda} \left(\hat{n}^1_i + \hat{n}^2_i\right) \quad , \tag{1.10}$$

exists as a C^*–dynamical system $(\,\mathcal{C}_\mathcal{G}, \mathbb{R}, \tau_t\,)$ on the classically extend algebra of observables

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

It can be calculated locally by perturbation theory as is shown in [5]. Here $E_\mathcal{G}$ denotes the 15–dimensional differentiable manifold corresponding to the parameterization of $\mathfrak{S}(\mathfrak{B})$ on which the classical part of the limiting dynamics is acting. $\mathcal{C}(E_\mathcal{G})$ are the continuous functions on $E_\mathcal{G}$ and $\mathcal{C}(E_\mathcal{G}, \mathfrak{A})$ are the $\mathfrak{A}$–valued continuous functions on $E_\mathcal{G}$. For obtaining the above results one first calculates the limiting C^*–dynamical system for the homogeneous part of the models

$$\tau^0_t(A) = \underset{\Lambda\in\mathfrak{L}}{\text{s-lim}} \exp\left\{it\left(H^0_\Lambda - \mu N_\Lambda\right)\right\} A_\Lambda \exp\left\{-it\left(H^0_\Lambda - \mu N_\Lambda\right)\right\}, \qquad \forall\ t \in \mathbb{R} \qquad \text{with} \qquad A_\Lambda \in \mathfrak{A}_\Lambda$$

and then determines the sigma–weak limit of this dynamics perturbed by P_Λ

$$\tau_t(A) = \sigma\text{-w-}\lim_{\Lambda' \in \mathfrak{L}} (\tau_t^0)^{P_{\Lambda'}}(A) \qquad \text{for } |t| < t_0 \ .$$

For the explicit form of τ_t see [5].

Invariant KMS–states: The set of KMS–states for the C^*–dynamical system $(\mathcal{C}_\mathcal{G}, \mathbb{R}, \tau_t)$ which are invariant under the group of internal symmetries $\mathsf{S}_2 \times \mathsf{SU}(1)$ forms a subsimplex of the simplex of all KMS–states and is given by the convex combinations of the following, extremal invariant KMS–states

$$\omega = \int_0^{2\pi} \Big(\frac{1}{2} \bigotimes_{i \in \mathcal{K}} \varrho_{12}^{i\vartheta} + \frac{1}{2} \bigotimes_{i \in \mathcal{K}} \varrho_{21}^{i\vartheta} \Big) \frac{\mathrm{d}\vartheta}{2\pi}. \tag{1.11}$$

Here $\varrho_{12}^{i\vartheta}$ and $\varrho_{21}^{i\vartheta}$ are determined by

$$\varrho_{12}^{i\vartheta} := \frac{e^{-\beta h_{12}^{i\vartheta}(\varrho)}}{\mathrm{tr}\{ e^{-\beta h_{12}^{i\vartheta}(\varrho)} \}}, \qquad \text{and} \qquad \varrho_{21}^{i\vartheta} := \frac{e^{-\beta h_{21}^{i\vartheta}(\varrho)}}{\mathrm{tr}\{ e^{-\beta h_{21}^{i\vartheta}(\varrho)} \}}, \tag{1.12}$$

with the following single site Hamiltonians

$$\begin{aligned} h_{12}^{i\vartheta} &:= (vn_2^i - \mu)\,\hat{n}^1 + (vn_1^i - \mu)\,\hat{n}^2 - 2\Delta_2^i \left(e^{-i(\vartheta - \delta\vartheta_i)} b^{1*} + e^{+i(\vartheta - \delta\vartheta_i)} b^1 \right) \\ &\quad - 2\Delta_1^i \left(e^{-i(\vartheta - \delta\vartheta_i)} b^{2*} + e^{+i(\vartheta - \delta\vartheta_i)} b^2 \right) \\ h_{21}^{i\vartheta} &:= (vn_2^i - \mu)\,\hat{n}^2 + (vn_1^i - \mu)\,\hat{n}^1 - 2\Delta_2^i \left(e^{-i(\vartheta - \delta\vartheta_i)} b^{2*} + e^{+i(\vartheta - \delta\vartheta_i)} b^2 \right) \\ &\quad - 2\Delta_1^i \left(e^{-(\vartheta - \delta\vartheta_i)} b^{1*} + e^{+i(\vartheta - \delta\vartheta_i)} b^1 \right) \ . \end{aligned} \tag{1.13}$$

We use here the notation $n_r^i := (1 + \frac{\delta v_i}{v})\, n_r$, $\Delta_r^i := | (1 + \frac{\delta t_i}{t})\, t \langle \varrho ; b^r \rangle | = | 1 + \frac{\delta t_i}{t} |\, \Delta_r$ and $\delta\vartheta_i := -\mathrm{Arg}(1 + \frac{\delta t_i}{t})$, where the values of these expectations can be determined from (1.12), which implies an inhomogeneous selfconsistency equation (similar to the gap equation). The phase difference between the expectation values $\langle \varrho ; b^r \rangle$ in the two sublattices is equal to a multiple of π and is hence set equal to zero. Therefore we set $-\mathrm{Arg}(\langle \varrho ; b^r \rangle) =: \vartheta$. See [5] for a detailed discussion.

The set of invariant KMS–states does not determine the physically stable phases of the system (see [8]). For this we need the additional principle, that the physically stable states be *minimizers of the free energy density.*

Grand Canonical Ensemble: The grand-canonical ensemble is characterized by a fixed chemical potential and a fixed temperature but allows for non vanishing fluctuations of the particle density. The free energy density of KMS–states for the inhomogeneous model is entirely determined by the KMS–states of the homogenized model. As is shown in [8] the function $\mu(n)$ for the homogeneous part of the model may be inverted and we can therefore use the parameterization (β, n) for the set of KMS–states of $(\mathcal{C}_\mathcal{G}, \mathbb{R}, \tau_t)$ instead of the parameters (β, μ). We show in

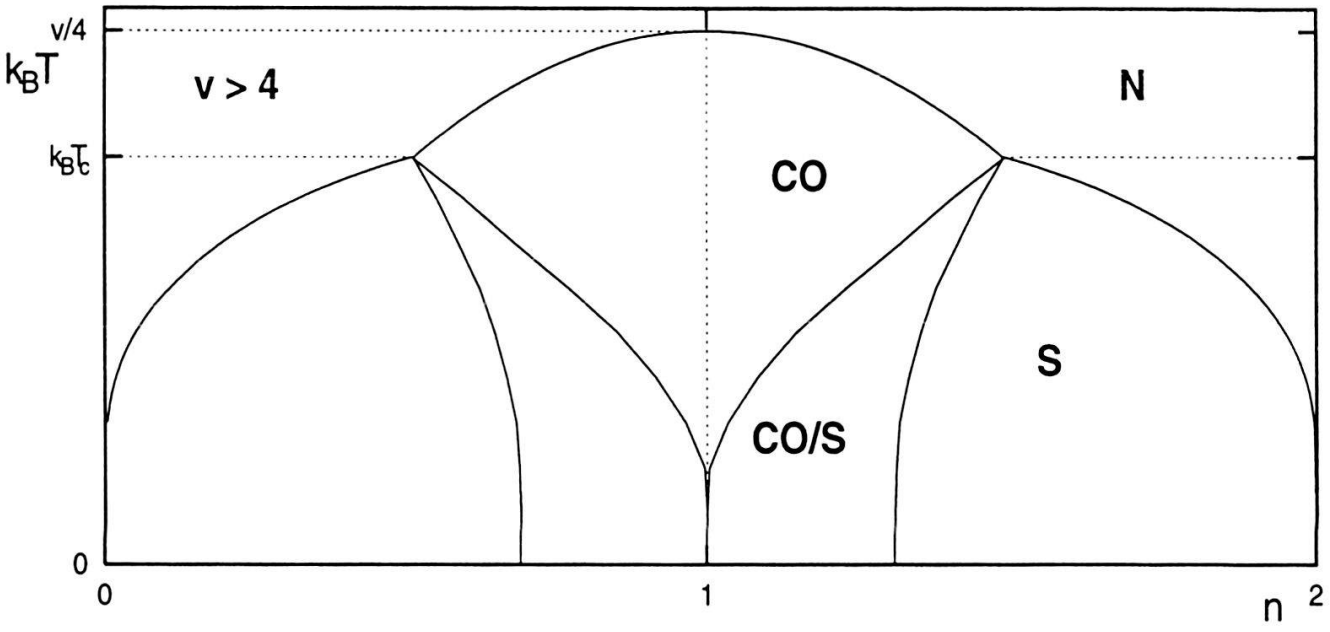

Figure 1.1: (n,T)–phase diagram for the grand canonical ensemble.

Fig. 1.1 the phase diagram of the grand-canonical ensemble given by the invariant KMS–states, which minimize the free energy density. (The phase diagram of all KMS–states is depicted in [5])

The phase structure may also be seen by studying the homogeneous limiting Gibbs states: To fix a certain mean particle density $n \in]0,2[$ in the homogeneous local Gibbs state, we introduce the chemical potential μ via $H^0_\Lambda(\mu) := H^{0r}_\Lambda := H^0_\Lambda - \mu N_\Lambda$, $N_\Lambda := \sum_{i\in\Lambda}(\hat{n}^1_i + \hat{n}^2_i)$. Since $[H^0_\Lambda, N_\Lambda] = 0$, for each $n \in]0,2[$ there is a unique $\mu \in \mathbb{R}$, such that

$$\frac{1}{|\Lambda|}\langle \omega^{\beta,H^0_\Lambda(\mu)} \,;\, N_\Lambda\rangle = n.$$

For each local region Λ, the unique $\mu \in \mathbb{R}$ is denoted by μ_Λ. The remarkable fact is, that the limiting Gibbs state

$$\omega_0^{\beta,n} := \mathrm{w}^*\text{-}\lim_{\Lambda\in\mathfrak{L}} \omega^{\beta,H^0_\Lambda(\mu_\Lambda)} \tag{1.14}$$

is unique for each $n \in]0,2[$ in all phase regions [1].

Canonical Ensemble: The canonical ensemble which is realized by a fixed temperature and a fixed particle density with vanishing fluctuations can be obtained by adding a perturbation

$$R_\Lambda := g_\Lambda\,|\Lambda|\left(\frac{N_\Lambda}{|\Lambda|} - n\right)^2 \qquad \text{with} \qquad g_\Lambda \longrightarrow \infty\,,\ \frac{g_\Lambda}{|\Lambda|} \longrightarrow 0$$

to the local Hamiltonian H_Λ, that suppresses the fluctuations of the particle density in the thermodynamic limit. Applying this perturbation to the inhomogeneous dynamical system means that the set of KMS–states is reduced to only those KMS–states with vanishing fluctuations of the particle

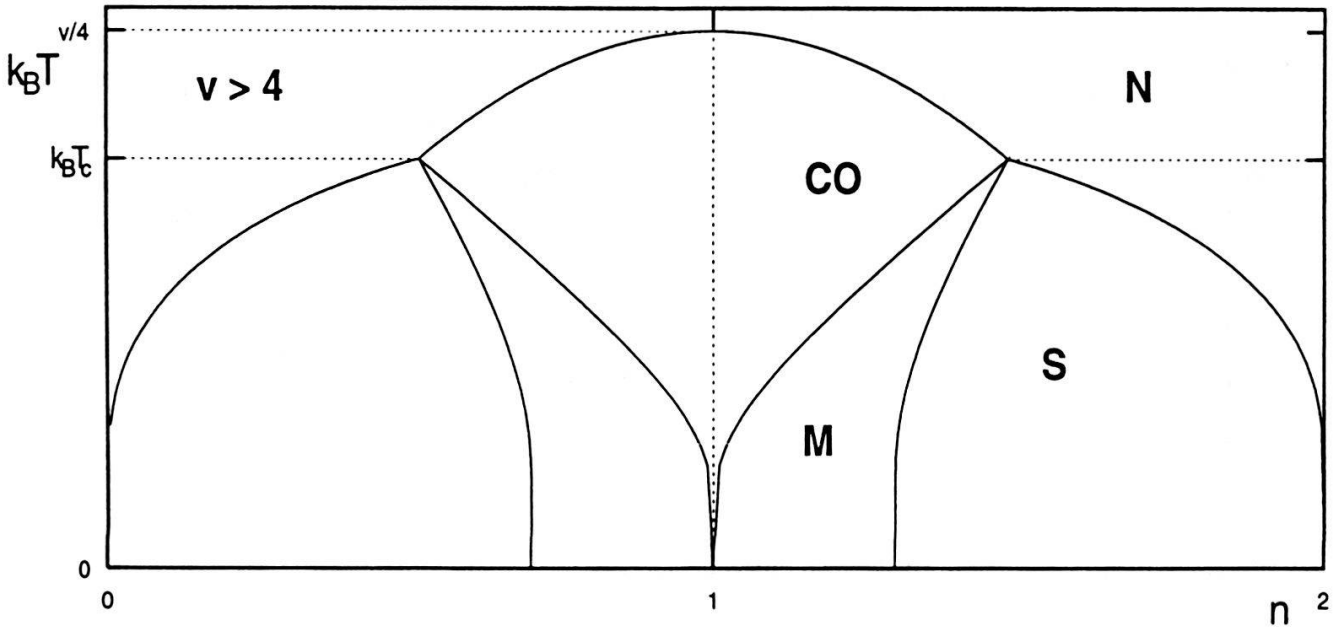

Figure 1.2: (n,T)–phase diagram for the canonical ensemble (thermodynamic limit at particle density $n \in]0,2[$ with suppressed fluctuations [8]).

density.
The free energy density is now given by the Legendre transform of the one for the grand–canonical case. This leads to a different phase diagram for the minimizers of the canonical free energy density as is shown in Fig. 1.2.

In comparison with the grand canonical ensemble the CO–S coexistence region is replaced by the so–called M–phase with broken gauge symmetry *and* broken sublattice exchange symmetry. Note, that the phase boundaries S–M and CO–M are shifted with respect to the previous ones of the CO–S coexistence region. Apart from the choice of v, t, and the parameterization of $\mathfrak{S}(\mathfrak{B})$, these are the boundaries as given in [7].

Again there exist the unique limiting Gibbs states for the homogeneous part of the system [8] which are given by

$$\omega_0^{\beta,n} := \mathrm{w}^*\text{-}\lim_{\Lambda\in\mathfrak{L}} \frac{\langle \omega^{\beta H_\Lambda^0}\,;\, R_\Lambda \cdot R_\Lambda\rangle}{\langle \omega^{\beta H_\Lambda^0}\,;\, R_\Lambda\rangle}. \tag{1.15}$$

The pure phases – resp. the stable extremal KMS–states – of the system are characterized by the broken internal symmetries of the model class (see Table 1.1). Equivalently, each broken symmetry leads to a nontrivial sum or integral in the decomposition formula (1.11) for the extremal invariant KMS–states. See [5] for a detailed discussion.

We close this Section with a list of all extremal invariant KMS–states $\omega^{\beta,n} = \omega_{\mathrm{N}}$, ω_{S}, ω_{CO}, $\omega_{\mathrm{CO/S}}$, ω_{M} occurring in Figs. 1.1 and 1.2 and indicate their central measures.

State	Broken Symmetry	Macroscopic Pure Phase
$\mathrm{tr}(\varrho^i\hat{n}^1) = \mathrm{tr}(\varrho^i\hat{n}^2)$, $\mathrm{tr}(\varrho^i b^1) = \mathrm{tr}(\varrho^i b^2) = 0$		Normal phase (**N**)
$\mathrm{tr}(\varrho^i\hat{n}^1) = \mathrm{tr}(\varrho^i\hat{n}^2)$, $\mathrm{tr}(\varrho^i b^1) = \mathrm{tr}(\varrho^i b^2) \neq 0$	gauge invariance	Superconducting phase (**S**)
$\mathrm{tr}(\varrho^i\hat{n}^1) \neq \mathrm{tr}(\varrho^i\hat{n}^2)$, $\mathrm{tr}(\varrho^i b^1) = \mathrm{tr}(\varrho^i b^2) = 0$	sub–lattice permutations	Charge Ordered phase (**CO**)
$\mathrm{tr}(\varrho^i\hat{n}^1) \neq \mathrm{tr}(\varrho^i\hat{n}^2)$, $\mathrm{tr}(\varrho^i b^1) \neq \mathrm{tr}(\varrho^i b^2) \neq 0$	sub–lattice permutations gauge invariance	'Mixed' phase (**M**)

Table 1.1: Characterization of pure phase states $\otimes\varrho^i$ in terms of broken symmetries and expectation values.

Proposition 1.1
With the notation from eqns. (1.11), (1.12) *and* (1.13) *we find for the extremal* $\mathsf{S}_2 \times \mathsf{SU}(1)$ *invariant KMS–states of the introduced class of inhomogeneous bipolaronic models:*

(i) *In the* ***N–phase region*** *of Figure 1.1 or 1.2 each invariant β–KMS–state* ω_{N} *is obtained from eq.* (1.11) *by setting* $n_1^i = n_2^i =: n^i$ *and* $\Delta_1^i = \Delta_2^i = 0$ *in eq.* (1.13).

(ii) *In the so–called charge–ordered phase, the* ***CO–phase****, the invariant β–KMS–states* ω_{CO} *are obtained from eq.* (1.11) *by setting* $\Delta_1^i = \Delta_2^i = 0$ *in eq.* (1.13).

(iii) *In the superconducting region, the* ***S–phase****, the invariant the β–KMS–states* ω_{S} *are obtained from eq.* (1.11) *by setting* $n_1^i = n_2^i = n^i$, $\Delta_1^i = \Delta_2^i = \Delta^i$ *and* $\delta\vartheta_i = 0$ *in eq.* (1.13).

(iv) *In the* ***CO–S coexistence region*** *each invariant β–KMS–state is decomposed into a state corresponding to the CO– and S–phases, i.e. we have*

$$\omega_{\mathrm{CO/S}} = \omega_\lambda = \lambda\,\omega_{\mathrm{CO}} + (1-\lambda)\,\omega_{\mathrm{S}}, \quad \lambda \in]0,1[. \tag{1.16}$$

The value $\lambda \in]0,1[$ *is determined by the given particle density* $n = \lim_{\Lambda\in\mathfrak{L}} \frac{1}{|\Lambda|}\langle\omega_\lambda\,;\,N_\Lambda\rangle = \lambda\,n_{\mathrm{CO}} + (1-\lambda)\,n_{\mathrm{S}}$ *because we have* $\lim_{\Lambda\in\mathfrak{L}} \frac{1}{|\Lambda|}\langle\omega_{\mathrm{CO}}\,;\,N_\Lambda\rangle = n_{\mathrm{CO}} \neq n_{\mathrm{S}} = \lim_{\Lambda\in\mathfrak{L}} \frac{1}{|\Lambda|}\langle\omega_{\mathrm{S}}\,;\,N_\Lambda\rangle$.

(v) *The invariant β–KMS–state* ω_{M} *in the* ***M–phase*** *region are given directly by eqns.* (1.11) *and* (1.13).

PROOF: [8], [5]. □

2 Equilibrium Representations and Spectra of Effective Hamiltonians

We discuss the KMS–dynamics τ_t and their unitary implementation in the GNS–representations over the above equilibrium states $\omega = \omega_{\mathrm{N}}, \omega_{\mathrm{S}}, \omega_{\mathrm{CO}}, \omega_{\mathrm{CO/S}}, \omega_{\mathrm{M}}$.
The states ω are invariant under τ_t, i.e. $\langle \omega\,;\, \tau_t(A)\rangle = \langle \omega\,;\, A\rangle\ \forall t$, and it is a well known result [9, Theo. 2.3.16 and Cor. 2.3.17] that there exists a unitary implementation of τ_t in the GNS–representation of $\mathcal{C}_\mathcal{G}$ to the state ω, which is decomposed by means of the central measure $\mathrm{d}\,\mu_\omega(\varrho)$ of ω :

$$(\Pi_\omega, \mathcal{H}_\omega, \Omega_\omega) = \int_{E_\mathcal{G}}^{\oplus} (\Pi_\varrho, \mathcal{H}_\varrho, \Omega_\varrho)\, \mathrm{d}\,\mu_\omega(\varrho)$$

with the corresponding von Neumann Algebra

$$\mathfrak{M}_\omega := \Pi_\omega\,(\mathcal{C}_\mathcal{G})'' = \int_{E_\mathcal{G}}^{\oplus} \mathfrak{M}_\varrho\, \mathrm{d}\,\mu_\omega(\varrho) := \int_{E_\mathcal{G}}^{\oplus} \Pi_\varrho\,(\mathcal{C}_\mathcal{G})''\, \mathrm{d}\,\mu_\omega(\varrho)\ .$$

We remark that, because of the states ω being microscopically extended (see [5]), in the case of the stable invariant KMS–states the GNS–representation of $\mathcal{C}_\mathcal{G}$ corresponds to the GNS–representation of $\mathfrak{A}$.
The unitary implementation is introduced by

$$U_t^\omega\, \Pi_\omega(A)\, \Omega_\omega := \tau_t(\Pi_\omega(A))\, \Omega_\omega,$$

and then extended to all of $\mathcal{H}_\omega$. It satisfies indeed

$$\tau_t(M) := U_t^\omega M U_t^{\omega *} \quad \in \mathfrak{M}_\omega, \quad \forall M \in \mathfrak{M}_\omega.$$

The U_t^ω are the only implementing unitaries which leave Ω_ω invariant. Note that τ_t corresponds to the modular automorphism group [9], [10] corresponding to Ω_ω, and U_t^ω is given by

$$U_t^\omega = \Delta_\omega^{-i\frac{t}{\beta}}$$

with the modular operator Δ_ω. The family $t \longrightarrow U_t^\omega$ is a strongly continuous group of unitaries with the selfadjoint generator

$$K^\omega = -\frac{1}{\beta} \ln \Delta_\omega.$$

We will illustrate this result by the two most general forms of KMS–states from Section 1.1, that are the equilibrium states in the coexistence region for the grand-canonical ensemble and the equilibrium states in the mixed phase for the canonical ensemble:

Since a state of the coexistence region $\omega_{\mathrm{CO/S}}$ is the mixture of the disjoint ω_{CO} and ω_{S} states

its GNS–representation of the algebra $\mathcal{C}_\mathcal{G}$ is a direct sum of the GNS–representations over ω_{CO} and ω_{S}:

$$(\mathcal{H}_{\mathrm{CO/S}}, \Pi_{\mathrm{CO/S}}, \Omega_{\mathrm{CO/S}}) = (\mathcal{H}_{\mathrm{CO}} \oplus \mathcal{H}_{\mathrm{S}}, \Pi_{\mathrm{CO}} \oplus \Pi_{\mathrm{S}}, \Omega_{\mathrm{CO}} \oplus \Omega_{\mathrm{S}}) \quad . \tag{2.1}$$

We give the explicit form of the representing Hilbert space:

$$\mathcal{H}_{\mathrm{CO/S}} = \Big(\mathcal{H}_{12} \oplus \mathcal{H}_{21} \Big) \bigoplus \Big(\int_0^{2\pi \oplus} \mathcal{H}_\vartheta \, \frac{\mathrm{d}\vartheta}{2\pi} \Big) \quad .$$

The generator of the unitary implementation $U_{\mathrm{CO/S}}$ of τ_t in $(\mathcal{H}_{\mathrm{CO/S}}, \Pi_{\mathrm{CO/S}}, \Omega_{\mathrm{CO/S}})$ has the form

$$K^{\mathrm{CO/S}} = K^{\mathrm{CO}} \oplus K^{\mathrm{S}} \quad .$$

A core for $K^{\mathrm{CO/S}}$ is given by $\mathfrak{D}_0^{\mathrm{CO/S}} := \mathfrak{M}_0^{\mathrm{CO/S}} \Omega_{\mathrm{CO/S}}$ where

$$\mathfrak{M}_0^{\mathrm{CO/S}} := \Big\{ \int_{E_\mathcal{G}}^{\oplus} \Pi_\varrho \left(A\left(\varrho\right) \right) \mathrm{d}\mu_{\omega_{\mathrm{CO/S}}}(\varrho) \; =: M_\Lambda \;\Big|\; \text{there is a } \Lambda \in \mathfrak{L} \text{ with } A\left(\varrho\right) \in \mathfrak{A}_\Lambda, \, \forall \varrho \in E_\mathcal{G}, \\ \text{and } \varrho \to A\left(\varrho\right) \text{ is norm continuous} \Big\} \quad .$$

On $\mathfrak{D}_0^{\mathrm{CO/S}}$ the typical element is $M_\Lambda \Omega_{\mathrm{CO/S}}$ and the generator $K^{\mathrm{CO/S}}$ is explicitly given by

$$K^{\mathrm{CO/S}} M_\Lambda \Omega_{\mathrm{CO/S}} = \Big[\, \widetilde{H}_\Lambda^{\mathrm{CO/S}} \, , \, M_\Lambda \, \Big] \, \Omega_{\mathrm{CO/S}},$$

with

$$\begin{aligned} \widetilde{H}_\Lambda^{\mathrm{CO/S}} &= \widetilde{H}_\Lambda^{\mathrm{CO}} \oplus \widetilde{H}_\Lambda^{\mathrm{S}} \\ &= \Big(\sum_{i \in \Lambda} \left(\, v n_2^i - \mu \, \right) \Pi_{12} \left(\, \hat{n}_i^1 \, \right) + \left(\, v n_1^i - \mu \, \right) \Pi_{12} \left(\, \hat{n}_i^2 \, \right) \\ &\qquad \oplus \sum_{i \in \Lambda} \left(\, v n_2^i - \mu \, \right) \Pi_{21} \left(\, \hat{n}_i^2 \, \right) + \left(\, v n_1^i - \mu \, \right) \Pi_{21} \left(\, \hat{n}_i^1 \, \right) \Big) \\ &\qquad \bigoplus \Big(\int_0^{2\pi \oplus} \sum_{i \in \Lambda} \Big(\, [\, v n^i - \mu \,] \, [\, \Pi_\vartheta \left(\, \hat{n}_i^1 \, \right) + \Pi_\vartheta \left(\, \hat{n}_i^2 \, \right) \,] \\ &\qquad - 2\Delta^i \left(\, e^{-i(\vartheta - \delta\vartheta_i)} \Pi_\vartheta \left(\, b_i^{1*} \, \right) + e^{+i(\vartheta - \delta\vartheta_i)} \Pi_\vartheta \left(\, b_i^1 \, \right) \right) \\ &\qquad - 2\Delta^i \left(\, e^{-i(\vartheta - \delta\vartheta_i)} \Pi_\vartheta \left(\, b_i^{2*} \, \right) + e^{+i(\vartheta - \delta\vartheta_i)} \Pi_\vartheta \left(\, b_i^2 \, \right) \right) \Big) \, \frac{\mathrm{d}\vartheta}{2\pi} \Big) . \end{aligned} \tag{2.2}$$

As the second representative example we give the GNS–representation of $\mathcal{C}_\mathcal{G}$ over the state ω_M of the mixed phase

$$(\mathcal{H}_{\mathrm{M}}, \Pi_{\mathrm{M}}, \Omega_{\mathrm{M}}) \quad .$$

A core for the generator K^{M} of the unitary implementation of the inhomogeneous limiting dynamics is given by $\mathfrak{D}_0^{\mathrm{M}} := \mathfrak{M}_0^{\mathrm{M}} \Omega_{\mathrm{M}}$ where

$$\mathfrak{M}_0^{\mathrm{M}} := \Big\{ \int_{E_\mathcal{G}}^{\oplus} \Pi_\varrho \left(A\left(\varrho\right) \right) \mathrm{d}\mu_{\omega_M}(\varrho) \; =: M_\Lambda \;\Big|\; \text{there is a } \Lambda \in \mathfrak{L} \text{ with } A\left(\varrho\right) \in \mathfrak{A}_\Lambda, \, \forall \varrho \in E_\mathcal{G}, \\ \text{and } \varrho \to A\left(\varrho\right) \text{ is norm continuous} \Big\} \quad .$$

K^M is given for each typical element $M_\Lambda \Omega_M$ by

$$K^{\mathrm{M}} M_\Lambda \Omega_{\mathrm{M}} = \left[\widetilde{H}^{\mathrm{M}_\Lambda} , M_\Lambda \right] \Omega_{\mathrm{M}}$$

with

$$\widetilde{H}^{\mathrm{M}_\Lambda} = \int_0^{2\pi} \Big(\Big(\sum_{i\in\Lambda} \Pi_{\mathrm{M}} \left(h_{12}^{i\vartheta} \right) \Big) \oplus \Big(\sum_{i\in\Lambda} \Pi_{\mathrm{M}} \left(h_{21}^{i\vartheta} \right) \Big) \Big) \, \frac{\mathrm{d}\vartheta}{2\pi} \tag{2.3}$$

and $h_{rs}^{i\vartheta}$ from eq. (1.13).

As may be seen from Prop. 1.1 the GNS–representations for all the other invariant KMS–states are special cases of those two given above.
We remark from the explicit formulas above that the generator for the implemented dynamical system has the general from

$$K^\omega = \int_{E_\mathcal{G}}^{\oplus} K^\varrho \, \mathrm{d}\, \mu_\omega \, (\varrho) \quad , \tag{2.4}$$

that is a direct integral over unbounded self–adjoint operators.

For the spectral analysis we first diagonalize the generators of the unitaries implementing the limiting dynamics in the GNS–representations $(\Pi_\varrho, \mathcal{H}_\varrho, \Omega_\varrho)$ for the pure phases.
The eigenvalues and eigenvectors of the selfadjoint generators at finite temperature are derived by means of a generalized Bogoliubov–Valatin transformation. The transformation is motivated by the diagonalization of $h^i(\varrho)$ in terms of quasi–pair operators. With Proposition 1.1 each $h^i(\varrho)$ has the form

$$h^i(\varrho) = h_1^i(\varrho) \otimes \mathbb{1} + \mathbb{1} \otimes h_2^i(\varrho), \tag{2.5}$$

with $h_r^i(\varrho) \in \widetilde{\mathfrak{B}}$ for $r = 1, 2$ and

$$h_r^i(\varrho) = A_r^i \, (\varrho) \, \hat{n} - B_r^i \, (\varrho) \, (e^{-i(\vartheta - \delta\vartheta_i)} b^* + e^{i(\vartheta - \delta\vartheta_i)} b), \tag{2.6}$$

where $A_r^i \, (\varrho) \in \mathbb{R}$, $B_r^i \, (\varrho) \geq 0$ and $\vartheta \in [0, 2\pi[$ are constants which are made explicit below. We introduce the transformation $\chi_{i\varrho}^r$ by its action on a pair operator b^r, $r = 1, 2$, leading to the quasi–pairs

$$q_i^r(\varrho) := \chi_{i\varrho}^r(b_i^r) := \left(u_r^{i\varrho}\right)^2 b_i^{r*} - \left(v_r^{i\varrho}\right)^2 e^{2i(\vartheta - \delta\vartheta_i)} \, b_i^r - u_r^{i\varrho} v_r^{i\varrho} \, e^{i(\vartheta - \delta\vartheta_i)} \, [b_i^r, b_i^{r*}], \tag{2.7}$$

with

$$u_r^{i\varrho} = \frac{1}{\sqrt{2}} \left(1 + \frac{A_r^i \, (\varrho)}{E_r^i \, (\varrho)} \right)^{\frac{1}{2}}, \quad v_r^{i\varrho} = \frac{1}{\sqrt{2}} \left(1 - \frac{A_r^i \, (\varrho)}{E_r^i \, (\varrho)} \right)^{\frac{1}{2}} \text{ and } \quad E_r^i \, (\varrho) = \sqrt{(A_r^i \, (\varrho))^2 + (B_r^i \, (\varrho))^2}.$$

This transformation extends to an automorphism of $\widetilde{\mathfrak{B}}$ and by $\chi_\varrho(\bigotimes_{i\in\Lambda} x_i) := \bigotimes_{i\in\Lambda}[\chi^1_{i\varrho}\otimes\chi^2_{i\varrho}](x_i)$ to $\mathfrak{A}$. In terms of the quasi-pair operators one obtains in fact the diagonal form:

$$H_\Lambda(\varrho) = \sum_{i\in\Lambda}(2E^i_1(\varrho)\, q^{1*}_i(\varrho)q^1_i(\varrho) + 2E^i_2(\varrho)\, q^{2*}_i(\varrho)q^2_i(\varrho)) + \text{const}\,\mathbb{1}_\Lambda.$$

Since $\chi_\varrho(\mathfrak{A}) = \mathfrak{A}$, the following set of vectors is total in $\mathcal{H}_\varrho$:

$$\psi_\varrho(\overline{\Lambda}) := \prod_{i_1\in\Lambda_1} q^{1*}_{i_1}(\varrho) \prod_{i_2\in\Lambda_2} q^1_{i_2}(\varrho) \prod_{i_3\in\Lambda_3} q^{2*}_{i_3}(\varrho) \prod_{i_4\in\Lambda_4} q^2_{i_4}(\varrho)\,\Omega_\varrho, \tag{2.8}$$

for all $\overline{\Lambda} = (\Lambda_1,\Lambda_2,\Lambda_3,\Lambda_4) \in \mathfrak{L}^4$. Moreover, it holds:

$$K^\varrho\psi_\varrho(\overline{\Lambda}) = \Big[\, 2\sum_{i_1\in\Lambda_1} E^{i_1}_1 - 2\sum_{i_2\in\Lambda_2} E^{i_2}_1 + 2\sum_{i_3\in\Lambda_3} E^{i_3}_2 - 2\sum_{i_4\in\Lambda_4} E^{i_4}_2 \,\Big]\psi_\varrho(\overline{\Lambda}), \tag{2.9}$$

implying

$$\sigma(K^\varrho) = \overline{\Big\{\, 2\sum_{i_1\in\Lambda_1} E^{i_1}_1 - 2\sum_{i_2\in\Lambda_2} E^{i_2}_1 + 2\sum_{i_3\in\Lambda_3} E^{i_3}_2 - 2\sum_{i_4\in\Lambda_4} E^{i_4}_2 \mid \overline{\Lambda}\in\mathfrak{L}^4 \,\Big\}}. \tag{2.10}$$

where we have simply set $E^i_r := E^i_r(\varrho)$ because we are dealing here with an extremal equilibrium state corresponding to one point $\varrho \in E_\mathcal{G}$.

To treat the multi-phase representations corresponding to the stable invariant KMS-states from Prop. 1.1 we piece the pure-phase informations together and set

$$q^r_i(\omega) := \int^\oplus_{E_\mathcal{G}} q^r_i(\varrho)\,\mathrm{d}\,\mu_\omega(\varrho) \tag{2.11}$$

leading to

$$\psi_\omega(\overline{\Lambda}) := \prod_{i_1\in\Lambda_1} q^{1*}_{i_1}(\omega) \prod_{i_2\in\Lambda_2} q^1_{i_2}(\omega) \prod_{i_3\in\Lambda_3} q^{2*}_{i_3}(\omega) \prod_{i_4\in\Lambda_4} q^2_{i_4}(\omega)\,\Omega_\omega, \tag{2.12}$$

for $\overline{\Lambda} = (\Lambda_1,\Lambda_2,\Lambda_3,\Lambda_4) \in \mathfrak{L}^4$. In this way one obtains particle operators and states with good quantum numbers, also for the broken symmetry generators. We find for the energy eigenvalues

$$K^\omega\psi_\omega(\overline{\Lambda}) = \int^\oplus_{E_\mathcal{G}} K^\varrho\psi_\varrho(\overline{\Lambda})\,\mathrm{d}\,\mu_\omega(\varrho) \tag{2.13}$$

$$= \int^\oplus_{E_\mathcal{G}} 2\sum_{i_1\in\Lambda_1} E^{i_1}_1(\varrho)\,\psi_\varrho(\overline{\Lambda})\,\mathrm{d}\,\mu_\omega(\varrho) - \int^\oplus_{E_\mathcal{G}} 2\sum_{i_2\in\Lambda_2} E^{i_2}_1(\varrho)\,\psi_\varrho(\overline{\Lambda})\,\mathrm{d}\,\mu_\omega(\varrho) \tag{2.14}$$

$$+ \int^\oplus_{E_\mathcal{G}} 2\sum_{i_3\in\Lambda_3} E^{i_3}_2(\varrho)\,\psi_\varrho(\overline{\Lambda})\,\mathrm{d}\,\mu_\omega(\varrho) - \int^\oplus_{E_\mathcal{G}} 2\sum_{i_4\in\Lambda_4} E^{i_4}_2(\varrho)\,\psi_\varrho(\overline{\Lambda})\,\mathrm{d}\,\mu_\omega(\varrho).$$

The single particle excitations $E^i_r(\varrho)$ are given by

$$E^i_r = \sqrt{(\,v n^i_s - \mu\,)^2 + 16\,(\,\Delta^i_s\,)^2} \qquad \text{with} \qquad r \neq s\ . \tag{2.15}$$

From eqns (2.2) and (2.3) together with eq. (1.13) we find the ϱ–independence $E_1^i = E_1^i(\varrho)$ and $E_2^i = E_2^i(\varrho)$ on the orbits in eq. (2.13). Thus we get as in (2.9)

$$K^\omega \psi_\omega(\overline{\Lambda}) = \Big[2 \sum_{i_1 \in \Lambda_1} E_1^{i_1} - 2 \sum_{i_2 \in \Lambda_2} E_1^{i_2} + 2 \sum_{i_3 \in \Lambda_3} E_2^{i_3} - 2 \sum_{i_4 \in \Lambda_4} E_2^{i_4} \Big] \psi_\omega(\overline{\Lambda}) \tag{2.16}$$

and

$$\Big\{ 2 \sum_{i_1 \in \Lambda_1} E_1^{i_1} - 2 \sum_{i_2 \in \Lambda_2} E_1^{i_2} + 2 \sum_{i_3 \in \Lambda_3} E_2^{i_3} - 2 \sum_{i_4 \in \Lambda_4} E_2^{i_4} \mid \overline{\Lambda} \in \mathfrak{L}^4 \Big\} \subseteq \sigma(K^\omega). \tag{2.17}$$

Note, that the set of $\psi_\omega(\overline{\Lambda})$, $\overline{\Lambda} \in \mathfrak{L}^4$, is, in general, not total in $\mathcal{H}_\omega$, cf. e.g. [11]. While the Hilbert space vectors $\psi_\omega(\overline{\Lambda})$ express quasi–pair excitations they do not include classical particle structures. For the KMS–dynamics these classical parts have only the energy value zero. This is expressed by the equation

$$K^\omega Z \psi_\omega(\overline{\Lambda}) = Z K^\omega \psi_\omega(\overline{\Lambda}), \quad \text{for all } Z \in \mathcal{Z}_\omega := \mathfrak{M}_\omega \cap \mathfrak{M}'_\omega. \tag{2.18}$$

The set $\{ Z\psi_\omega(\overline{\Lambda}) \mid Z \in \mathcal{Z}_\omega, \overline{\Lambda} \in \mathfrak{L}^4 \}$ is total in $\mathcal{H}_\omega$ and thus suited to give the spectral information on K^ω. Especially in the case of ϱ–independent energy values as in (2.17) we may conclude

$$\sigma(K^\omega) = \overline{\left\{ 2 \sum_{i_1 \in \Lambda_1} E_1^{i_1} - 2 \sum_{i_2 \in \Lambda_2} E_1^{i_2} + 2 \sum_{i_3 \in \Lambda_3} E_2^{i_3} - 2 \sum_{i_4 \in \Lambda_4} E_2^{i_4} \mid \overline{\Lambda} \in \mathfrak{L}^4 \right\}} \, .$$

We use the preceding insights in

Theorem 2.1

Let us choose an arbitrary, but fixed tupel $(\beta, n) \in \mathbb{R} \times [0,2]$, observing that then μ is fixed, too. We further select a model of the considered class and study the effective Heisenberg dynamics for a KMS-state belonging to this model.

(i) *In the GNS–representation over every KMS–state ω, independently of its location in the phase diagram, the Heisenberg dynamics can be unitarily implemented, so that the corresponding selfadjoint generator K^ω annihilates the cyclic vector Ω_ω. The spectra of all K^ω are the same.*

(ii) *All $E \in \sigma(K^\omega)$ are limit points of eigenvalues.*

(iii) *$E \in \sigma(K^\omega)$ implies $-E \in \sigma(K^\omega)$, but E, E' does not imply $E + E' \in \sigma(K^\omega)$, in general.*

(iv) *Every $E \in \sigma(K^\omega)$ has infinite multiplicity.*

(v) *The spectrum $\sigma(K^{\omega^0})$ for a homogeneous model is a subgroup of the additive group $\mathbb{R}$, which is made explicit in Table 3.1. It is contained in every $\sigma(K^\omega)$, where ω belongs to a model, which has the given homogenization. It holds the module property:*

$$E \in \sigma(K^\omega) \text{ and } E_o \in \sigma(K^{\omega^0}) \text{ implies } E + E_o \in \sigma(K^\omega).$$

PROOF: (i) We have observed above, that the pure phase spectra for fixed $(\beta, n) \in \mathbb{R} \times [0,2]$ are the same, which then takes over for a mixture of those pure phases in terms of an arbitrary probability measure. (ii) follows directly from the arguments given above. (iii) K^ω involves a commutator and its spectrum is symmetric around zero. For the second assertion observe, that two operators, which excite in application to the cyclic vector two energy eigenstates, may have the product zero, so that the sum of eigenvalues may not be realizable. In each GNS–representation one has the quasi–pair excitations and the central excitations – with zero energy – as the total set of eigenvectors. (iv) This is clear from the explicit formulas above. (v) In the homogeneous case the sums over positive and negative one–particle energies reduce to integer multiples of – at most three different – generator values, which are listed in Table 3.1. From the model assumptions we find for the one–particle spectra

$$\lim_{i\to\infty} E_r^i = E_r \qquad \text{and} \qquad E_r = \lim_{\Lambda\in\mathfrak{L}} \frac{1}{|\Lambda|} \sum_{i\in\Lambda} E_r^i \ .$$

Here the single particle excitations for the homogeneous models are explicitly given by

$$E_r = \sqrt{(\, vn_s - \mu \,)^2 + 16\,(\, \Delta_s \,)^2} \qquad \text{for} \qquad r \neq s \ .$$

with $n_r = \lim_{i\to\infty} n_r^i$ and $\Delta_r = \lim_{i\to\infty} \Delta_r^i$. Thus the homogeneous energy spectra are always accumulation points of the inhomogeneous spectra.

To an arbitrary energy eigenvalue we may add an homogeneous one, because we can approximate the latter in terms of sequences which are localized on Λ regions, which do not intersect with the region belonging to the given eigenvalue (in contrast to the problem of adding arbitrary inhomogeneous eigenvalues). Now replace the given eigenvalue by a sequence of eigenvalues, which approximate a given spectral value. This gives a sequence of sums, eigenvalues plus homogeneous eigenvalue, which converges within the spectrum. ❑

The set of stable energy spectral values for the quasi pairs has much similarity to the set of energy eigenvalues for condensed particles, e.g. condensed Cooper pairs, in spite of the fact, that the latter have central field operators commuting with all other operators, whereas the quasi pair operators have non-trivial commutation relations: Both sets constitute a subgroup of $\mathbb{R}$ which has the module property for the total energy spectrum. In a certain sense we may also in our discrete lattice system formalism state, that the stable spectral values have a high density of states: By being spectral accumulation points there are many quasi pair excitation vectors with close or identical energies.

3 Spectral Phase Diagrams

In the following we will only deal with the stable spectral group generators, which are indentified by the spectrum of the homogenized model. For the convenience of notation we introduce $\frac{n}{2} := \langle \varrho\,;\, \hat{n}^r \rangle$ and $\frac{\Delta}{2} e^{-i\vartheta} := \langle \varrho\,;\, b^r \rangle$ for $r = 1,2$, where we assume, that v and t are both greater than zero and we set $t \equiv 1$.

We use the quasi–pair transformations (2.7) and (2.11) to determine the robust one–particle spectrum for all regions of the phase diagrams in Figures 1.1 and 1.2.

N–Phase: The N–phase states are factor states with $h_{\text{eff}} = (v\frac{n}{2}-\mu)(\hat{n}^1+\hat{n}^2)$, i.e. in the notation of (2.6) it is $A_1 = A_2 = v\frac{n}{2} - \mu$ and $B_1 = B_2 = 0$. This leads to a unique $E^{\text{N}} = E_1^{\text{N}} = E_2^{\text{N}} = |v\frac{n}{2} - \mu|$.

S–Phase: The limiting Gibbs state in the S–phase region has a non–trivial central decomposition according to Prop. 1.1. Nevertheless, each state in the support of the central measure has the effective Hamiltonian $h_{\text{eff}} = (v\frac{n}{2} - \mu)\hat{n}^1 - \Delta(e^{-i\vartheta}b^{1*} + e^{i\vartheta}b^1) + (v\frac{n}{2} - \mu)\hat{n}^2 - \Delta(e^{-i\vartheta}b^{2*} + e^{i\vartheta}b^2)$ and thus it is $A_1 = A_2 = v\frac{n}{2} - \mu$ and $B_1 = B_2 = \Delta$. Consequently we have $E^{\text{S}} = E_1^{\text{S}} = E_2^{\text{S}} = \sqrt{(v\frac{n}{2} - \mu)^2 + \Delta^2}$.
We see that for the N– and the S–phase regions all one–particle excitation energies have the same value, independent of the chosen sublattice and the chosen pure phase state in $\operatorname{supp}\mu_\omega$. Thus the corresponding spectrum of K^ω is given by $\sigma(K^\omega) = E^{\text{N}}\mathbb{Z}$ and $E^{\text{S}}\mathbb{Z}$, respectively.

CO–Phase: The pure phase state $\otimes\varrho$ in $\operatorname{supp}\mu_\omega$ of a charge ordered limiting Gibbs state have different one–particle Hamiltonians in the two sublattices and in general there are different one particle energies $E_1 \neq E_2$. With $h_{\text{eff}}^r = (vn_r - \mu)\hat{n}$, $r = 1, 2$, and $n_1 \neq n_2$ we have either $h_{\text{eff}} = h_{\text{eff}}^1 \otimes \mathbb{1} + \mathbb{1} \otimes h_{\text{eff}}^2$ or $h_{\text{eff}} = h_{\text{eff}}^2 \otimes \mathbb{1} + \mathbb{1} \otimes h_{\text{eff}}^1$. Thus the two energy values are $E_r^{\text{CO}} = |vn_r - \mu|$, $r = 1, 2$, and they are equal for the two pure phase states in $\operatorname{supp}\mu_\omega$ according to Prop. 1.1.

M–Phase: The pure phase states in the M–region lead to one–particle energies as in the charge ordered case, except that here $\Delta_{1,2} \neq 0$ as well. For all states in $\operatorname{supp}\mu_\omega$ we find the single particle excitations $E_r^{\text{M}} = \sqrt{(vn_r - \mu)^2 + \Delta_r^2}$, where in general $n_1 \neq n_2$ and $\Delta_1 \neq \Delta_2$. Due to the independence of these energies from the chosen pure phase state we have found again the one–particle excitations of K^ω.
For the CO– and the M–phase regions it is $E_1 \neq E_2$. Obviously it is

$$\sigma(K^\omega) = \overline{\{2E_1\, n_1 + 2E_2\, n_2 \mid n_1, n_2 \in \mathbb{Z}\}}.$$

There are two possibilities for $\sigma(K^\omega)$ either if E_1 and E_2 are commensurate, or not. If

$$\frac{E_1}{E_2} = \frac{p}{q}, \qquad p, q \in \mathbb{N}$$

then we find

$$\sigma(K^\omega) = E\mathbb{Z}, \quad \text{with } E := \frac{E_1}{p} = \frac{E_2}{q}.$$

In the other case it is $\sigma(K^\omega) = \mathbb{R}$.

CO–S–Phase Coexistence: As given in Prop. 1.1 each state in this region has the form $\omega = \lambda\omega_{\text{S}} + (1 - \lambda)\omega_{\text{CO}}$ with the values $\lambda \in]0, 1[$, depending on the given particle density n. Thus the GNS–representation decomposes as

$$\Pi_{\text{CO/S}} = \Pi_{\text{CO}} \oplus \Pi_{\text{S}}$$

Macroscopic Phase	Spectrum of K^ω
N–region	$2\,E^{\mathrm{N}}\,\mathbb{Z}$
S–region	$2\,E^{\mathrm{S}}\,\mathbb{Z}$
CO–region	$\overline{2\,E_1^{\mathrm{CO}}\,\mathbb{Z}+2\,E_2^{\mathrm{CO}}\,\mathbb{Z}} = \begin{cases} 2\,E^{\mathrm{CO}}\,\mathbb{Z} & \text{if } E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \in \mathbb{Q} \\ \mathbb{R} & \text{if } E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \notin \mathbb{Q} \end{cases}$
M–region	$\overline{2\,E_1^{\mathrm{M}}\,\mathbb{Z}+2\,E_2^{\mathrm{M}}\,\mathbb{Z}} = \begin{cases} 2\,E^{\mathrm{M}}\,\mathbb{Z} & \text{if } E_1^{\mathrm{M}}/E_2^{\mathrm{M}} \in \mathbb{Q} \\ \mathbb{R} & \text{if } E_1^{\mathrm{M}}/E_2^{\mathrm{M}} \notin \mathbb{Q} \end{cases}$
CO/S–coexistence region	$2\,E^{\mathrm{S}}\,\mathbb{Z} \cup (\overline{2\,E_1^{\mathrm{CO}}\,\mathbb{Z}+2\,E_2^{\mathrm{CO}}\,\mathbb{Z}}) = \begin{cases} 2\,E^{\mathrm{S}}\,\mathbb{Z} \cup 2\,E^{\mathrm{CO}} & \text{if } E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \in \mathbb{Q} \\ \mathbb{R} & \text{if } E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \notin \mathbb{Q} \end{cases}$

Table 3.1: Spectra of the macroscopic Hamiltonians K^ω in the various region of the phase diagrams (Figures 1.1 and 1.2).

In the different sectors, corresponding to the CO– and the S–phases respectively, the one–particle energies $E_{1,2}^{\mathrm{CO}}$ and E_{S} differ. They are distinguished in terms of the classical properties (central projections)

$$c_{\mathrm{CO}} := \mathbb{1}_{\mathrm{CO}} \oplus 0 \quad \text{and} \quad c_{\mathrm{S}} := 0 \oplus \mathbb{1}_{\mathrm{S}}.$$

With (2.18), we find for all $Z \in \mathcal{Z}_\omega$ and $\overline{\Lambda} \in \mathfrak{L}^4$

$$K^\omega c_{\mathrm{CO}} Z\,\psi_\omega(\overline{\Lambda}) = \left[2E_1^{\mathrm{CO}}\,(|\Lambda_1| - |\Lambda_2|) + 2E_2^{\mathrm{CO}}\,(|\Lambda_3| - |\Lambda_4|)\right] c_{\mathrm{CO}} Z\,\psi_\omega(\overline{\Lambda}) \tag{3.1}$$

and

$$K^\omega c_{\mathrm{S}} Z\,\psi_\omega(\overline{\Lambda}) = 2E^{\mathrm{S}}\,(|\Lambda_1| - |\Lambda_2| + |\Lambda_3| - |\Lambda_4|)\, c_{\mathrm{S}} Z\,\psi_\omega(\overline{\Lambda}). \tag{3.2}$$

Since these eigenvalues of K^ω are determined by a total set of vectors in $\mathcal{H}_\omega$, the spectrum of K^ω is given by:

$$\sigma(K^\omega) = 2\,E^{\mathrm{S}}\,\mathbb{Z} \cup (\overline{2\,E_1^{\mathrm{CO}}\,\mathbb{Z}+2\,E_2^{\mathrm{CO}}\,\mathbb{Z}}).$$

If E_1^{CO} and E_2^{CO} are incommensurate, we have — as above — $\sigma(K^\omega) = \mathbb{R}$ and $\sigma(K^\omega) = 2\,E^{\mathrm{S}}\,\mathbb{Z} \cup 2\,E^{\mathrm{CO}}\,\mathbb{Z}$ otherwise.

All stable spectra of the effective Hamiltonians in the (possibly multi–phase) equilibrium representations are compiled in Table 3.1. In Figures 3.1 and 3.2 we picture the one–particle energies E^{X} with $\mathrm{X} = \mathrm{N}, \mathrm{S}, \mathrm{CO}, \mathrm{M}, \mathrm{S/CO}$ and their negative mirror values for various fixed temperatures

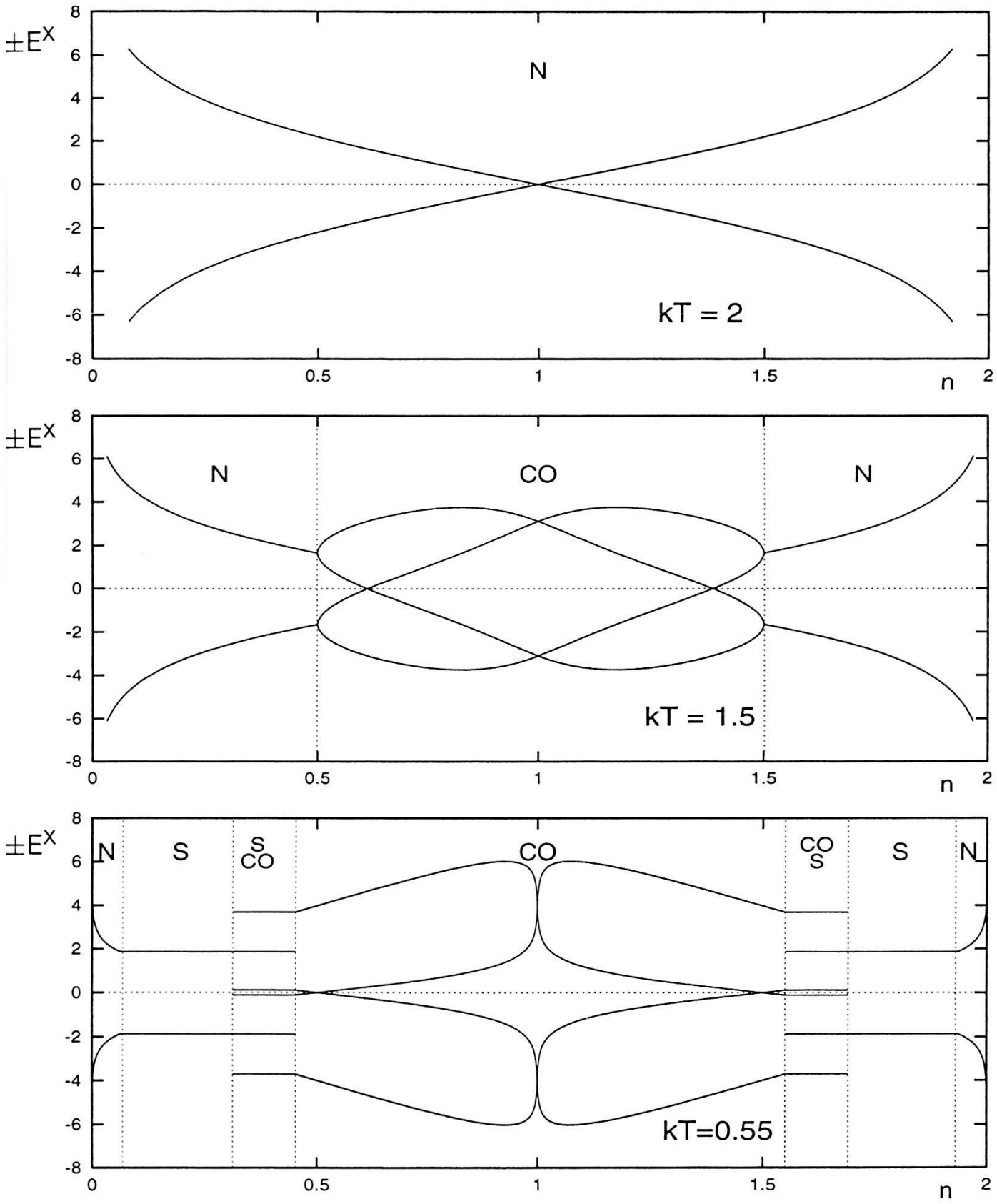

Figure 3.1: One–particle energies E^{X} with $\mathrm{X} = \mathrm{N}, \mathrm{S}, \mathrm{CO}, \mathrm{S/CO}$ of the macroscopic Hamiltonian for the grand canonical ensemble at different temperatures (v=8).

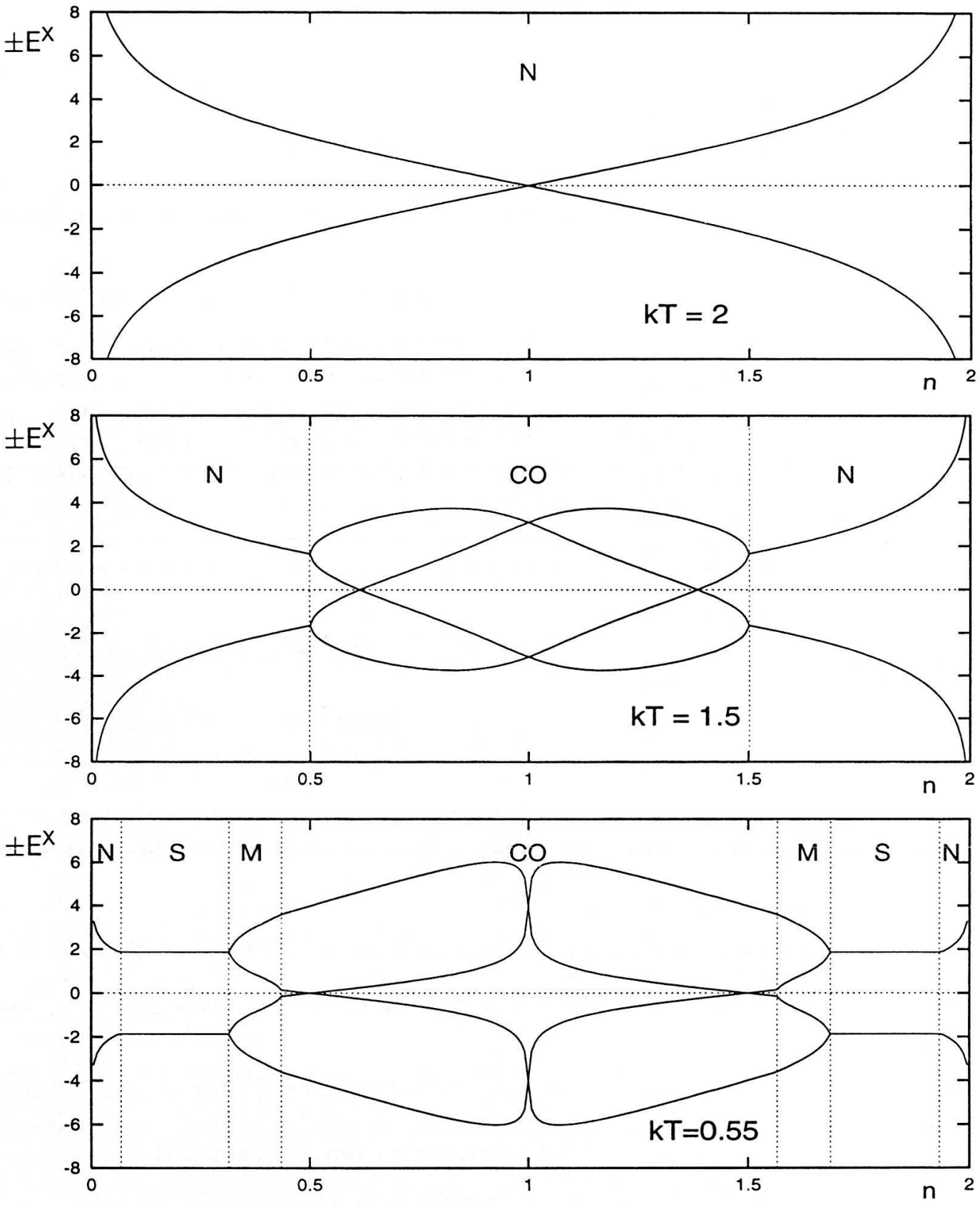

Figure 3.2: One–particle energies E^{X} with $\mathrm{X} = \mathrm{N}, \mathrm{S}, \mathrm{CO}, \mathrm{M}$ for the canonical ensemble (thermodynamic limit at particle density $n \in]0, 2[$ with suppressed fluctuations) for different temperatures (v=8).

in dependence on the total densities n, where first the grand canonical and then the canonical ensembles are used.

The preceding discussion motivates the following definition.

Definition 3.1
For the considered class of weakly inhomogeneous models we introduce the notion of a spectral phase diagram as the bundle

$$P_{Sp} = \{(E^1(\beta,n),...,(E^k(\beta,n)) \Big| (\beta,n) \in \mathbb{R}_+ \times [0,1], \textit{ with } E^l(\beta,n) \textit{ the generators of the stable spectral group } \}. \tag{3.3}$$

4 Classificatory Conclusions

In the foregoing Section we have identified in each effective energy spectrum an additive group, which consists of the integer multiples of certain one particle energies, and which is stable under the allowed perturbations. This group coincides with the spectrum of the homogenized models and depends on the equilibium state, giving rise to the notion of a spectral phase diagram. It is interesting that this structure is related in many cases with the Connes spectrum for the von Neumann algebras of the pure phase equilibrium representations.

4.1 Classification of the factor types of the pure phase representations

Recall, that the Connes spectrum has been introduced to classify the factors of type III. Starting from the W*–dynamical system $(\mathfrak{M}_\varrho, \mathbb{R}, \tau_t^\varrho)$ for the pure phase state ω_ϱ one defines according to Connes first the spectrum

$$\Gamma(\tau^\varrho) := \bigcap \{\mathrm{Sp}(\tau^{\varrho P} \mid P \text{ runs over the time invariant projections in } \mathfrak{M}_\varrho\}, \tag{4.1}$$

where $\tau^{\varrho P}$ is the restriction of τ^ϱ to $P\mathfrak{M}_\varrho P$. The Arveson spectrum $\mathrm{Sp}(\tau^{\varrho P})$ of the restricted automorphism group may be shown to equal the operator spectrum $\sigma(PK_\varrho P)$, K_ϱ the selfadjoint generator of the implementing unitary group, since the cyclic and separating vector Ω_ϱ is also time invariant for the restricted dynamics. Second one introduces the Connes invariant for $\mathfrak{M}_\varrho$

$$\mathrm{S}(\mathfrak{M}_\varrho) := \bigcap_\omega \sigma(\Delta_\omega) \tag{4.2}$$

where ω ranges over all normal faithful states of $\mathfrak{M}_\varrho$, and Δ_ω is the corresponding modular operator. It then holds

$$E \in \Gamma(\tau^\varrho) \Leftrightarrow \exp(-E) \in \mathrm{S}(\mathfrak{M}_\varrho), \tag{4.3}$$

which is one way to express the fact that $\Gamma(\tau^\varrho)$ is a characteristicum of $\mathfrak{M}_\varrho$, independent from the choosen dynamical system. The following cases are discriminated in [12]: If $\mathrm{S}(\mathfrak{M}_\varrho) = [0,\infty[$ then

Macroscopic Phase	λ
N–region	$\exp(-\beta E^{\mathrm{N}})$
S–region	$\exp(-\beta E^{\mathrm{S}})$
CO–region	$\exp(-\beta E^{\mathrm{CO}})$ if $E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \in \mathbb{Q}$, 1 if $E_1^{\mathrm{CO}}/E_2^{\mathrm{CO}} \notin \mathbb{Q}$.
M–region	$\exp(-\beta E^{\mathrm{M}})$ if $E_1^{\mathrm{M}}/E_2^{\mathrm{M}} \in \mathbb{Q}$, 1 if $E_1^{\mathrm{M}}/E_2^{\mathrm{M}} \notin \mathbb{Q}$.

Table 4.1: Factor type of the pure phase state representations in the various regions of the phase diagrams (Figures 1.1 and 1.2).

$\mathfrak{M}_\varrho$ is a factor of type III_1 and if $\mathsf{S}(\mathfrak{M}_\varrho) = \{0\} \cup \{\lambda^n \mid n \in \mathbb{Z}\}$ for some $\lambda \in]0,1[$, it is of type III_λ. If $\mathsf{S}(\mathfrak{M}_\varrho) = \{0,1\}$, $\mathfrak{M}_\varrho$ is of type III_0. If $\mathsf{S}(\mathfrak{M}_\varrho) = \{1\}$ then $\mathfrak{M}_\varrho$ is not of type III.
It has been proved by Connes [12] and, for type III_1, by Haagerup [13], that there is – up to W*–isomorphisms – only one injective factor of type III_λ (c.f. also the overview in [14]). As may be shown in complete analogy to [15] it holds for the homogeneous Hamiltonians K_0^ϱ, belonging to the state ω_ϱ^0 with the $\mathfrak{A}$–restriction $\otimes\varrho$:

$$\mathsf{S}(\mathfrak{M}_\varrho) = \sigma(\exp(-\beta K_0^\varrho)) \tag{4.4}$$

and only one spectrum, the homogeneous one, has to be evaluated for determining the type λ. We can now read out the type λ for $\mathfrak{M}_\varrho$ directly from the spectra in Table 3.1 and are led to Table 4.1.

The short look on the Connes theory on the factors of type III_λ displays a very peculiar stability of the homogeneous spectrum. First it occurs already in each restriction of the dynamics to an arbitrary one–lattice point algebra. Second it is stable not only against the perturbations of our model class but against all perturbations P affiliated with $\mathfrak{M}_\varrho$. Since the $\mathfrak{M}_\varrho$ are hyperfinite they are injective and thus represent the unique factor types III_λ.
In the diagrams 4.1 and 4.2 we illustrate the classification at hand of the numerical results for the one particle spectra for the grand canonical and the canonical ensemble. Note, that for $n = 1$ in the N–phase region the factor of type II_1 can be located . In the M– and the CO–region with $E_1 \neq E_2$ the value of λ is in the hatched region (especially it is $\lambda = 1$, if E_1 and E_2 are incommensurate). There is one exception in this region: if one of the energies $E_{1,2}$ becomes zero, say $E_1 = 0$, then we have $\lambda = \exp(-\beta E_2)$, i.e. $\lambda \neq 1$.

We see that the Connes spectrum is only partially suited to characterize the stable energy spectra. While λ of a factor of type III_λ corresponds in the N– and the S–phase states to well defined one particle energies, this structure is lost completely in the CO– and M–phases. Here, λ jumps discontinuously for continuously varying density n and takes the value $\lambda = 1$ for all pairs E_1 and E_2 with $E_1/E_2 \notin \mathbb{Q}$. Thus the true structure of the spectral phase diagrams cannot be resolved

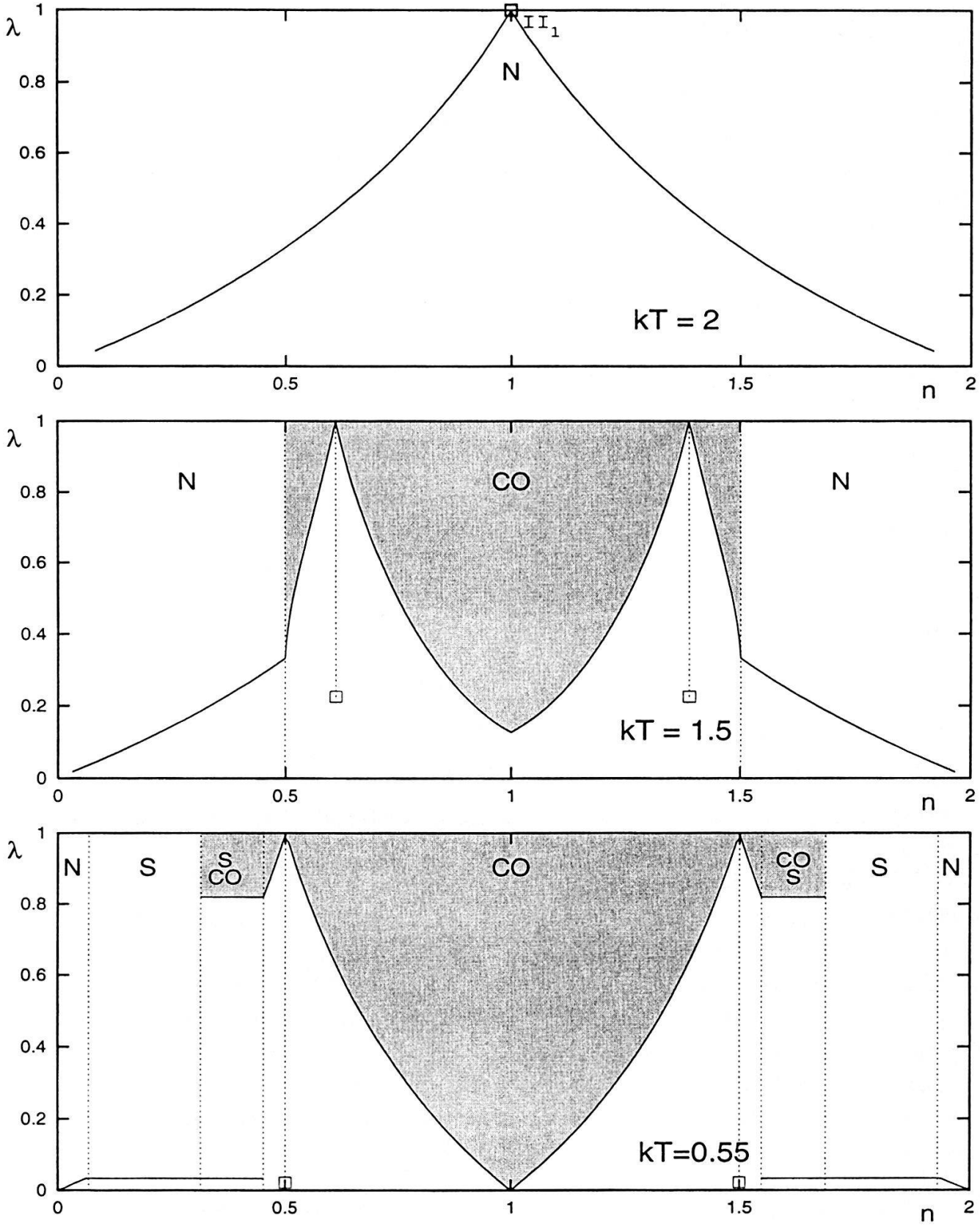

Figure 4.1: Factor type of the pure phase state representations in the grand canonical ensemble at different temperatures (v=8).

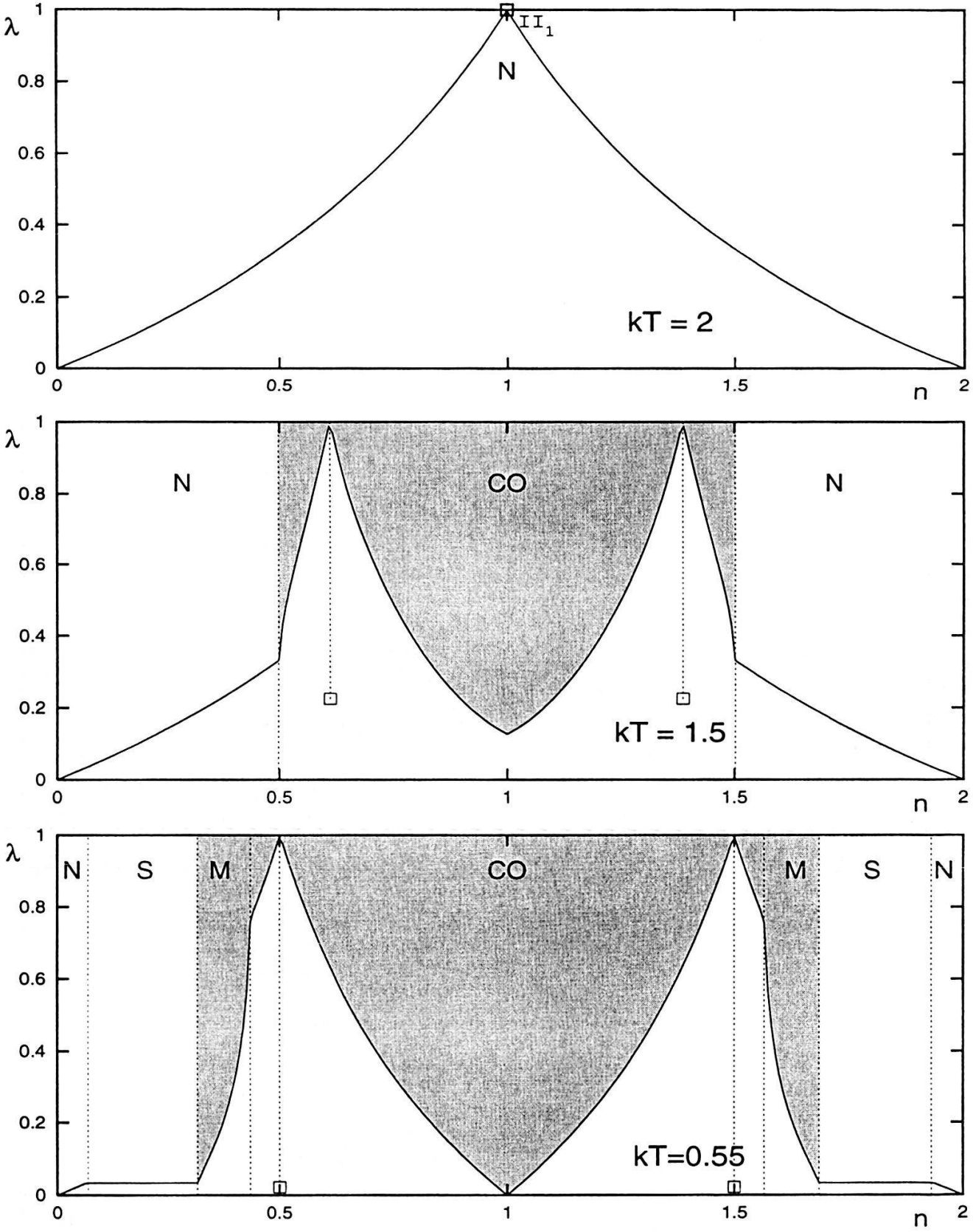

Figure 4.2: Factor type of the pure phase state representations for the canonical ensemble (thermodynamic limit with suppressed fluctuations) at different temperatures (v=8).

from the factor type of the representation. In this sense the correspondence between the spectra of homogeneous lattice systems and the factor type of the representation, as worked out previously for the Weiß–Ising model [16] and the BCS–model [15], seems to be of accidental nature. In the case of two or more different stable one particle energies, which characterize a global inhomogeneity of the collective structure (here charge ordering), one cannot compress this information into one single number.
Also for the ground states, which are obtained in the limit $\beta \to \infty$, we have a similar situation . Beside the loss of reflection anti–symmetry about zero, the spectral phase diagrams at $T = 0$ have qualitatively the same form as in Figures 3.1 and 3.2 for $T > 0$. Nevertheless, all these ground state representations (for the pure ground states) are factors of type I_∞.

In summary, the see that the mathematical classification of the factor representations is not sufficient for our purposes, and we have need for the more detailed spectral phase diagrams.

4.2 Phase Transitions

It is clear from the outset, that the spectral phase diagrams cannot replace the thermodynamic phase diagrams. They rather supplement the purely thermodynamic information and give additional features of the collective phenomena. Nevertheless it is surprising, how well the phase boundaries are reproduced in terms of the spectral behaviour. Thus we want also to inquire, how well the type of a phase transition is exhibited by the spectral phase diagrams. We use the definition and classification of phase transitions as proposed in [17]: A phase transition occurs, if the equilibrium properties of the thermodynamic system undergo a *qualitative change.* The equilibrium properties are given here by the set $\mathfrak{S}_{\mathrm{Th}}(\beta, n)$ of all states ω with minimal free energy density $f(\beta, \mu_0, \omega)$ or $\tilde{f}(\beta, n, \omega)$, respectively. These sets are determined by the pure phase states $\otimes\varrho$ of the extreme boundary with the free energies $f(\beta, \mu_0, \otimes\varrho)$ or $\tilde{f}(\beta, n, \otimes\varrho)$, used for the discussions of the phase diagrams.

Definition 4.1

(i) *The thermodynamic phase structure is given by the bundle*

$$P_{Th} = \{\mathfrak{S}_{Th}(\beta, n) \,|\, (\beta, n) \in \mathbb{R} \times [0, 2]\} \tag{4.5}$$

(ii) *A phase transition is a continuous curve of the form*

$$\gamma = \{(\beta(t), n(t)) \mid t \in \mathbb{R}\},$$

on which a qualitative change of the sets $\mathfrak{S}_{\mathrm{Th}}(\beta, n)$ occurs, that is, the number of connected components and/or the dimensions of the connected components and/or the type of broken symmmetry undergoes a change.

(iii) *A point (β^0, n^0) on a phase transition γ, which has both types of equilibrium sets in every neighbourhood, is called transition point.*

Let us use the partition of phase transitions into two *kinds* (cf., e.g., [18], [19], [20], [21]), where the well known basic idea is that some relevant quantity may behave discontinuously or continuously at the transition point. This leads to

Definition 4.2
A phase transition γ is called to be of the first or the second kind if the set function

$$t \to \mathfrak{S}_{Th}(\gamma(t))$$

is discontinuous or continuous, respectively, at t_0. The transition points $\gamma(t_0) = (\beta_0, n_0)$ of phase transitions of the second kind are called critical points.

These definitions at once imply features of the spectral phase diagrams:

Proposition 4.3

(i) *Let be $(\beta^0, n^0) \in \gamma$ a point where the stable one particle energies change discontinuously. Then (β^0, n^0) is a transition point of a phase transition of the first kind.*

(ii) *Let be $(\beta^0, n^0) \in \gamma$ the critical point of a phase transition of the second kind. Then the stable one particle energies behave continuously at (β^0, n^0). (Nevertheless, there may appear bifurcations!)*

PROOF: Follows directly from the definition of the phase transitions, and their partition into types, if one takes into account that a continuous behaviour of the sets $\mathfrak{S}_{\mathrm{Th}}(\gamma(t))$, as we have introduced it in [17], implies the continuous behaviour of their elements. ❑

Especially, the S/CO–transition in Figure 1.1 is of the first kind and the S/CO-region is the coexistence region of the transition, with two values of $E^{C/O}$ and one value of E^S. The difference to the mixed phase situation M is brought out very clearly, if one compares the two spectral phase diagrams for the different ensembles, i. e., Figure 3.1 with Figure 3.2.
In many cases the dependence, or independence, of the stable energy values on the state parameters is a valuable indication for itself to identify the nature of the collective ordering phenomenon under discussion.

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