Centre de Physique Théorique*- CNRS - Luminy, Case 907
F–13288 Marseille Cedex 9 - France

The staggered charge-order phase of the extended Hubbard model in the atomic limit

C. BORGS[1,†] J. JĘDRZEJEWSKI[2], and R. KOTECKÝ[3‡]

Abstract

We study the phase diagram of the extended Hubbard model in the atomic limit. At zero temperature, the phase diagram decomposes into six regions: three with homogeneous phases (characterized by particle densities $\rho = 0$, 1, and 2 and staggered charge density $\Delta = 0$) and three with staggered phases (characterized by the densities $\rho = \frac{1}{2}$, 1, and $\frac{3}{2}$ and staggered densities $|\Delta| = \frac{1}{2}$, 1, and $\frac{1}{2}$). Here we use Pirogov-Sinai theory to analyze the details of the phase diagram of this model at low temperatures. In particular, we show that for any sufficiently low nonzero temperature the three staggered regions merge into one staggered region S, without any phase transitions (analytic free energy and staggered order parameter Δ) within S.

Key-Words : Hubbard model, Atomic Limit, Staggered Charge-Order, Pirogov-Sinai Theory.

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anonymous ftp or gopher : cpt.univ-mrs.fr

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*Unité Propre de Recherche 7061
[1]School of Mathematics, Institute for Advanced Study, Princeton
[2]Institute of Theoretical Physics, Wrocław University
[3]Centre de Physique Théorique, CNRS, Marseille
[†]DFG Heisenberg Fellow
[‡]On leave from Center for Theoretical Study, Charles University, Prague; partly supported by the grants GAČR 202/93/0449 and GAUK 376

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1. Introduction

The theory of strongly correlated electron systems is nowadays a subject of vigorous research. The interest in these systems is stimulated, to a large extent, by attempts at explaining the mechanism of high-temperature superconductivity [MRR90, Dag94], the phenomenon of electron localization in narrow-band systems [IILM75] and properties of quasi one-dimensional conductors [Hub79], to name a few. Among the models that are most frequently studied is the Hubbard model augmented by a nearest neighbour interaction. This model, known as the extended Hubbard model, is defined by the following Hamiltonian

$$H_t = -t \sum_{\langle \boldsymbol{i},\, \boldsymbol{j} \rangle, \sigma} \left(c^*_{\boldsymbol{i},\, \sigma} c_{\boldsymbol{j},\, \sigma} + h.c. \right) + U \sum_{\boldsymbol{i} \in \Lambda} n_{\boldsymbol{i}, \uparrow} n_{\boldsymbol{i}, \downarrow} + W \sum_{\langle \boldsymbol{i},\, \boldsymbol{j} \rangle} n_{\boldsymbol{i}} n_{\boldsymbol{j}} - \left(\mu + zW + \frac{U}{2} \right) \sum_{\boldsymbol{i} \in \Lambda} n_{\boldsymbol{i}}. \tag{1.1}$$

In (1.1) we used the following notation: at each site $\boldsymbol{i}$ of a d-dimensional bipartite lattice Λ, with z nearest neighbours, there are creation and annihilation operators $c^*_{\boldsymbol{i},\, \sigma}$ and $c_{\boldsymbol{i},\, \sigma}$ of the electron with up and down spin, $\sigma = \uparrow, \downarrow$, that satisfy the canonical anticommutation relations, while $n_{\boldsymbol{i},\, \sigma} := c^*_{\boldsymbol{i},\, \sigma} c_{\boldsymbol{i},\, \sigma}$ and $n_{\boldsymbol{i}} := n_{\boldsymbol{i},\, \uparrow} + n_{\boldsymbol{i},\, \downarrow}$. The first term of the Hamiltonian (1.1) stands for the isotropic nearest neighbour hopping of electrons, the second one is the familiar on-site Hubbard interaction, the third term represents the isotropic nearest neighbour interaction, and the last one the contribution of the particle reservoir characterized by the chemical potential μ. We have introduced the shift $zW + \frac{U}{2}$ in order to move the hole-particle symmetry point (the half-filled band) to the value $\mu = 0$. Originally, the second and the third terms were supposed to simulate the effect of the Coulomb repulsion between the electrons, hence only positive U and W were considered. Later on, in various applications of the model, the parameters t, U and W represented the effective interaction constants that take into account also other interactions (for instance with phonons). Therefore U and W could take negative values as well. In this paper U will be allowed to change its sign while W always stays positive.

The so called narrow band case of the extended Hubbard model, i.e. $|t| \ll |U|$, is of special interest in physical applications of the model. It has been studied by means of various approximate methods in many papers (see for instance [Lor82] and references quoted there). These studies revealed the existence of staggered charge-order at the hole-particle symmetry point. The staggered charge-order is characterized by a nonvanishing order parameter

$$\Delta = \lim_{\Lambda \nearrow \infty} |\Lambda|^{-1} \sum_{\boldsymbol{i} \in \Lambda} \varepsilon_{\boldsymbol{i}} \langle n_{\boldsymbol{i}} \rangle, \tag{1.2}$$

where $\varepsilon_{\boldsymbol{i}}$ assumes two values, 1 or -1, depending on to which sublattice of the bipartite lattice Λ the site $\boldsymbol{i}$ belongs, and $\langle \cdot \rangle$ stands for the Gibbs state.

Rigorously, the existence of staggered charge order has so far only been established in the so called atomic limit $t \to 0$ [Jęd94]. While the above mentioned approximate results suggest that the staggered charge order persists in the corresponding narrow band model, the methods used in [Jęd94] unfortunately do not allow to establish this rigorously, because they rely on the reflection positivity of the atomic limit model which fails to be true for nonzero t.

Here we propose to study the atomic limit of the model (1.1) using a different strategy, based on the by now classical methods of Pirogov and Sinai [PS75], see also [Zah84,BI89]. On the one hand, these methods will allow us to study detailed properties of the low temperature phase diagram in the atomic limit, on the other hand they allow for an extension to nonzero t, treating the narrow band Hubbard model as a quantum perturbation of the $t=0$ model, and leading to the rigorous proof of staggered charge order in the narrow band Hubbard model [BK94].

In the atomic limit, it is convenient to rewrite the Hamiltonian (1.1) in a form that makes the hole-particle symmetry apparent. Namely, introducing $Q_{\boldsymbol{i}} := n_{\boldsymbol{i}} - 1$, we have

$$H = \lim_{t\to 0} H_t = \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} Q_{\boldsymbol{i}} Q_{\boldsymbol{j}} + \frac{U}{2} \sum_{\boldsymbol{i}\in\Lambda} Q_{\boldsymbol{i}}^2 - \mu \sum_{\boldsymbol{i}\in\Lambda} Q_{\boldsymbol{i}}, \tag{1.3}$$

where we passed to dimensionless parameters U and μ, setting $W = 1$. Note that in the atomic limit all operators appearing in the Hamiltonian commute. Therefore, the model (1.3) can be viewed as a two-component classical lattice gas or, equivalently, as the classical gas with four possible states 0, $\uparrow$, $\downarrow$, 2 in each site, that correspond to an empty site, a singly occupied site with spin $\uparrow$ or $\downarrow$, and a doubly occupied site, respectively.

FIG.1. GROUND STATE PHASE DIAGRAM. There are three open regions H_-, H_0 and H_+ with no staggered charge order ($\Delta = 0$), and three open regions $S_{\{+,0\}}$, $S_{\{+,-\}}$, and $S_{\{-,0\}}$, with staggered charge order $|\Delta| = 1/2$, $|\Delta| = 1$, and $|\Delta| = 1/2$, respectively.

In the sequel, we shall present and discuss the phase diagram of the model (1.3) on the lattice $\mathbb{Z}^d$. The ground state phase diagram is shown in Fig. 1. The (U,μ) plane decomposes into six open regions. In each of the regions H_-, H_0, and H_+, there is a unique homogeneous ground state, whose particle density ρ, given by

$$\rho = \lim_{\Lambda\nearrow\mathbb{Z}^d} |\Lambda|^{-1} \sum_{\boldsymbol{i}\in\Lambda} \langle Q_{\boldsymbol{i}} + 1\rangle, \tag{1.4}$$

equals 0, 1, and 2, respectively. The remaining three regions $S_{\{+,-\}}$, $S_{\{+,0\}}$ and $S_{\{-,0\}}$ are characterized by staggered charge-order. Namely, in the region $S_{\{a,b\}}$ there are two staggered ground states, denoted $[a,b]$ and $[b,a]$, with $Q_{\boldsymbol{i}} = a$ on one sublattice and $Q_{\boldsymbol{i}} = b$ on the complementary sublattice. Note that the staggered order parameter Δ is nonvanishing in the whole staggered region S and jumps from $|\Delta| = 1$ to $|\Delta| = \frac{1}{2}$ at the boundary between $S_{\{+,-\}}$ and $S_{\{-,0\}}$ or $S_{\{+,0\}}$.

Using reflection positivity it has been shown [Jęd94] that the staggered long range order in the region S persists at small temperatures $T \equiv \frac{1}{k\beta} > 0$, provided one stays sufficiently far away from the boundary between S and the homogeneous regions H_a, $a = 0, \pm$. However, this does not exclude existence of a phase transition inside the staggered region S. Namely, in view of the discontinuity of Δ at the zero-temperature transition lines, one could expect that Δ reveals a phase transition at nonvanishing temperatures as well. Indeed, mean field arguments [MRC84] predict a first order transition surface emerging from the zero temperature transition line separating $S_{\{+,-\}}$ from $S_{\{+,0\}}$ and similarly for the line separating $S_{\{+,-\}}$ from $S_{\{-,0\}}$,

Using a suitable notion of restricted ensembles we are able to analyze this question rigorously. Our main result here is to show the absence of any such phase transition, in contrast to the above mentioned mean field results.

Theorem A. *Consider the complement S of the union of closed homogeneous regions $\bar{H}_a$, $a = 0, \pm$,*

$$S = \mathbb{R}^d \setminus (\bar{H}_- \cup \bar{H}_0 \cup \bar{H}_+),$$

and let

$$S^{(\epsilon)} = \{x \in S \mid \operatorname{dist}(x, S^c) > \epsilon\}.$$

For $d \geq 2$ and any $\epsilon > 0$ there exists a constant $\beta_0 < \infty$ (depending on ϵ and d) such that, for all $\beta_0 < \beta < \infty$ and $(U, \mu) \in S^{(\epsilon)}$, there are exactly two phases[1], *$\langle - \rangle_{\text{even}}$ and $\langle - \rangle_{\text{odd}}$. Moreover, $\Delta > 0$ for the phase $\langle - \rangle_{\text{even}}$, $\Delta < 0$ for $\langle - \rangle_{\text{odd}}$, and both the free energy density, $f(\beta, U, \mu)$, and the staggered order parameters of the two phases, $\Delta_{\text{even}}(\beta, U, \mu)$ and $\Delta_{\text{odd}}(\beta, U, \mu)$, are real analytic functions of U and μ in $S^{(\epsilon)}$.*

Remark. As mentioned before, the zero temperature staggered order parameter Δ jumps from $\Delta = \pm 1$ to $\Delta = \pm\frac{1}{2}$ at the boundary between $S_{\{+,-\}}$ and $S_{\{+,0\}}$ or $S_{\{-,0\}}$. It is interesting to relate this jump to the smooth behaviour for $T = \frac{1}{k\beta} > 0$. As we will see in Section 3, the crossover between these two behaviours is described by a hyperbolic tangent. Taking, e.g., the order parameter of the even phase in the vicinity of the boundary between, say, $S_{\{+,-\}}$ and $S_{\{+,0\}}$, one obtains that

$$\Delta \sim \frac{3}{4} + \frac{1}{4} \tanh\Big(\frac{2d - \mu - U/2}{kT}\Big)$$

as $T \to 0$.

Turning to the homogeneous regions H_a, $a = 0, \pm$, we use standard Pirogov-Sinai theory to discuss the low temperature behaviour inside the corresponding regions $H_a^{(\epsilon)}$. This enables us to prove analyticity, unicity and translation invariance of the homogeneous phases.

As for the boundaries between the staggered region S and the homogeneous regions H_a, we note that the zero temperature coexistence line between H_0 and $S_{\{+,-\}}$ gives rise to

[1] As usual, a phase is defined as an extremal Gibbs state which is periodic in all d lattice directions.

a coexistence line surface of the two staggered phases with the homogeneous one. With decreasing β, this surface bends towards negative U, i.e., above the ground state coexistence line between H_0 and $S_{\{+,-\}}$ the corresponding homogeneous phase is stable [Jęd94].

The remaining part of the zero temperature boundary between S and the homogeneous regions is of similar type as the boundary between staggered and homogeneous phases in the antiferromagnetic Ising model. For example, at the boundary between $S_{\{+,-\}}$ and H_+, it is possible to join the staggered phase $[+,-]$, without any energy cost, to the second staggered phase $[-,+]$, going through the homogeneous phase stable in H_+ (see [Jęd94] and also Section 2 below for a more detailed explanation). We therefore expect that this phase boundary turns, for nonzero temperatures, into a second order transition line. Actually, in the limit $U \to -\infty$ the extended Hubbard model in the atomic limit becomes equivalent to the Ising antiferromagnet (with homogeneous external field μ) where this fact was rigorously proven [KY93]. In a similar way one expects that all other boundaries between homogeneous and staggered phases, except for the boundary between H_0 and $S_{\{+,-\}}$ already considered above, correspond to second order transition.

We summarize our knowledge of the phase diagram of the extended Hubbard model in the atomic limit in the following theorem (see also Fig. 2).

FIG.2. PHASE DIAGRAM AT LOW TEMPERATURES. Thin lines denote the conjectured second order transitions, while the thick line, separating the two phase staggered region S from the homogeneous region H_0, is first order. Shaded are regions over which we have no rigorous control (they shrink to the zero temperature lines with $\beta \to \infty$).

Theorem B. *Let $d \geq 2$ and β be sufficiently large. Then there exist open regions $H_a(\beta)$, $a = 0, \pm$, and $S(\beta)$, where $H_0(\beta)$, and $S(\beta)$ touch on a curve,*

$$L(\beta) = \partial S(\beta) \cap \partial H_0(\beta) \neq \emptyset,$$

such that the following statements are true:

i) *For $(U, \mu) \in S(\beta)$ there exist exactly two phases, a phase $\langle - \rangle_{\text{even}}$ with $\Delta > 0$ and a phase $\langle - \rangle_{\text{odd}}$ with $\Delta < 0$. These phases are periodic with period 2 and both the free energy density, $f(\beta, U, \mu)$, and the staggered order parameters of the two phases, $\Delta_{\text{even}}(\beta, U, \mu)$ and $\Delta_{\text{odd}}(\beta, U, \mu)$, are real analytic functions of U and μ in $S(\beta)$.*

ii) *For $(U, \mu) \in H_a(\beta)$, $a = 0, \pm$, there is exactly one phase $\langle - \rangle_a$. For this phase, $\Delta = 0$, it is translation invariant, and the free energy density, $f(\beta, U, \mu)$, is a real analytic function of U and μ in in $H_a(\beta)$.*

iii) *On the boundary $L(\beta)$ between $S(\beta)$ and $H_0(\beta)$, the three phases $\langle - \rangle_a$, $\langle - \rangle_{\text{even}}$, and $\langle - \rangle_{\text{odd}}$ coexist. Furthermore, all periodic Gibbs states on this line are a convex combination of those three phases.*

iv) *As $\beta \to \infty$, $H_a(\beta) \to H_a$, $a = 0, \pm$, and $S(\beta) \to S$.*

Proof of Theorems A and B. Theorems A and B are immediate consequences of Propositions 1 – 4 that are stated and proved in Section 3. □

Before passing to the Propositions 1 – 4 we turn to a new representation of the model (1.3) in terms of spin 1 variables and then to a detailed examination of its ground state phase diagram.

2. Structure of ground states and restricted ensembles

In order to rewrite the model (1.3) in terms of a classical spin system, we recall that all operators appearing in (1.3) commute. However, fixing all the eigenvalues $S_{\boldsymbol{i}}$ of the operators $Q_{\boldsymbol{i}}$, $S_{\boldsymbol{i}} \in \{-,0,+\}$, does not completely specify the state of the system, because $S_{\boldsymbol{i}} = 0$ corresponds to two possibilities $n_{\boldsymbol{i},\uparrow} = 1$ and $n_{\boldsymbol{i},\downarrow} = 0$ or $n_{\boldsymbol{i},\uparrow} = 0$ and $n_{\boldsymbol{i},\downarrow} = 1$. In the partition function of the classical spin model, this leads to a factor of 2 for every singly occupied site, and therefore to an overall factor $2^{\sum_{\boldsymbol{i}\in\Lambda}(1-Q_{\boldsymbol{i}}^2)}$. In this way the quantum system (1.3) is mapped onto an antiferromagnetic spin 1 model, with

$$H = \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} S_{\boldsymbol{i}} S_{\boldsymbol{j}} + \frac{\tilde{U}}{2} \sum_{\boldsymbol{i}\in\Lambda} S_{\boldsymbol{i}}^2 - \mu \sum_{\boldsymbol{i}\in\Lambda} S_{\boldsymbol{i}}, \tag{2.1}$$

where

$$\tilde{U} = U - 2\beta^{-1} \ln 2. \tag{2.2}$$

It is useful to rewrite the Hamiltonian (2.1) as a sum over nearest neighbour terms $h(S_{\boldsymbol{i}}, S_{\boldsymbol{j}})$, namely

$$H = \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} h(S_{\boldsymbol{i}}, S_{\boldsymbol{j}}), \tag{2.3}$$

where we introduced the energy per pair of nearest neighbour sites

$$h(S_{\boldsymbol{i}}, S_{\boldsymbol{j}}) = S_{\boldsymbol{i}} S_{\boldsymbol{j}} + \frac{\tilde{U}}{4d}(S_{\boldsymbol{i}}^2 + S_{\boldsymbol{j}}^2) - \frac{\mu}{2d}(S_{\boldsymbol{i}} + S_{\boldsymbol{j}}). \tag{2.4}$$

This form of the Hamiltonian makes the task of constructing the ground state phase diagram, i.e. determining the six regions H_a, $a = 0, \pm$, $S_{\{+,-\}}$, $S_{\{+,0\}}$, and $S_{\{-,0\}}$, mentioned in previous section, an easy exercise. The energies of the nearest neighbour spin configurations are

$$\begin{aligned}
h(+,+) &= 1 + \tfrac{\tilde{U}}{2d} - \tfrac{\mu}{d}, && (2.5a)\\
h(+,0) &= 0 + \tfrac{\tilde{U}}{4d} - \tfrac{\mu}{2d}, && (2.5b)\\
h(+,-) &= -1 + \tfrac{\tilde{U}}{2d}, && (2.5c)\\
h(0,-) &= 0 + \tfrac{\tilde{U}}{4d} + \tfrac{\mu}{2d}, && (2.5d)\\
h(0,0) &= 0. && (2.5e)\\
h(-,-) &= 1 + \tfrac{\tilde{U}}{2d} + \tfrac{\mu}{d}, && (2.5f)
\end{aligned}$$

Using (2.5), we find three homogeneous regions

$$H_+ := \Big\{(U,\mu) \mid \frac{\mu}{2d} > \max\Big\{1, 1 + \frac{\tilde{U}}{4d}\Big\}\Big\}, \tag{2.6a}$$

with minimal energy pairs $(+,+)$,

$$H_- := \Big\{(U,\mu) \mid -\frac{\mu}{2d} > \max\Big\{1, 1 + \frac{\tilde{U}}{4d}\Big\}\Big\}, \tag{2.6b}$$

with minimal energy pairs $(-,-)$, and

$$H_0 := \Big\{(U,\mu) \mid \max\Big\{\Big|\frac{\mu}{2d}\Big|, \frac{1}{2}\Big\} < \frac{\tilde U}{4d}\Big\}, \tag{2.6c}$$

with minimal energy pairs $(0,0)$; and three staggered regions

$$S_{\{+,-\}} := \Big\{(U,\mu) \mid \Big|\frac{\mu}{2d}\Big| < \min\Big\{1, 1-\frac{\tilde U}{4d}\Big\} \quad \text{and} \quad \frac{\tilde U}{4d} < \frac{1}{2}\Big\}, \tag{2.7a}$$

with minimal energy pairs $(+,-)$ and $(-,+)$,

$$S_{\{+,0\}} := \Big\{(U,\mu) \mid \frac{\tilde U}{4d} < \frac{\mu}{2d} < 1+\frac{\tilde U}{4d} \quad \text{and} \quad \frac{\tilde U}{4d} < \frac{\mu}{2d}\Big\}, \tag{2.7b}$$

with minimal energy pairs $(+,0)$ and $(0,+)$, and

$$S_{\{-,0\}} := \Big\{(U,\mu) \mid \frac{\tilde U}{4d} < -\frac{\mu}{2d} < 1+\frac{\tilde U}{4d} \quad \text{and} \quad \frac{\tilde U}{4d} < -\frac{\mu}{2d}\Big\}, \tag{2.7c}$$

with minimal energy pairs $(-,0)$ and $(0,-)$. Thus, in each of the regions H_a, $a = 0, \pm$, there is a unique homogeneous ground configuration $\{S_{\boldsymbol{i}} = a\}_{\boldsymbol{i}\in\Lambda}$. On the other hand, in each of the regions $S_{\{a,b\}}$ there are exactly two ground configurations, such that, when on one sublattice $S_{\boldsymbol{i}} = a$, on the complementary one $S_{\boldsymbol{i}} = b$, and vice versa. In order to relate the formulae (2.6) and (2.7) to Fig. 1, we notice that $U = \tilde U$ for $\beta = \infty$.

At this moment, let us remark that the above analysis of ground configurations shows that the components h of H (cf. (2.4)) constitute a so called m–potential [Sla87]. Moreover, since in each of the regions H_+, H_0, H_-, $S_{\{+,-\}}$, $S_{\{+,0\}}$, and $S_{\{-,0\}}$ there are only finitely many ground configurations, one can readily apply standard Pirogov–Sinai theory to study the low temperature properties of the corresponding phases, away from the boundaries of these regions.

On the boundaries of the regions H_+, H_0, H_-, $S_{\{+,-\}}$, $S_{\{+,0\}}$, and $S_{\{-,0\}}$, the structure of the ground states is more complicated. Combining the minimal energy pair configurations of the corresponding adjacent regions, one can construct infinitely many ground configurations everywhere, except for the boundary between $S_{\{+,-\}}$ and H_0. On the latter boundary there are exactly three ground configurations, namely, those that correspond to the adjacent regions. This, of course, places also this case into the realm of standard Pirogov-Sinai theory.

There is an important difference between the infinitely degenerated boundaries shared by staggered and homogeneous regions and those shared by two staggered regions. In the first case, i.e. on the boundary between, say, H_+ and $S_{\{+,-\}}$, the minimal energy pairs of both regions, namely the pairs $(+,+)$, $(+,-)$ and $(-,+)$, can be combined into an arbitrary configuration made out of "+" and "−", as long as no nearest neighbour pair of minuses is present. Mutatis mutandis, the same is true for the other infinitely degenerate boundaries between staggered and homogeneous regions. One therefore obtains the same structure of ground states as in the Ising antiferromagnet at the critical field, presumably giving rise to surfaces of second order transitions at nonzero temperature.

In the second case, i.e. on the boundaries shared by two staggered regions, the situation is different. Considering for instance the region S_+ that consists of $S_{\{+,-\}}$, $S_{\{+,0\}}$, and the boundary shared by these regions, we introduce two disjoint classes of configurations, $\mathcal{G}^+_{\text{even}}$ and $\mathcal{G}^+_{\text{odd}}$. Namely, we define $\mathcal{G}^+_{\text{even}}$ as the set of all configurations, for which $S_{\boldsymbol{i}} = +$ on the even sublattice, while $S_{\boldsymbol{i}} = 0$ or $-$ on the odd sublattice, and the set $\mathcal{G}^+_{\text{odd}}$ by interchanging the role of the two sublattices. Then, for all points in S_+, every ground configuration falls into one of these two disjoint classes. This already suggests to use, in S_+, a version of Pirogov-Sinai theory with the sets $\mathcal{G}^+_{\text{even}}$ and $\mathcal{G}^+_{\text{odd}}$ playing the role of restricted ensembles [BKL85] that replace the ground states[2]. The same remark applies to the region S_- made of $S_{\{+,-\}}$, $S_{\{-,0\}}$ and their shared boundary, and the corresponding sets $\mathcal{G}^-_{\text{even}}$ and $\mathcal{G}^-_{\text{odd}}$.

[2]Notice that different configurations from $\mathcal{G}^+_{\text{even}}$ (and similarly $\mathcal{G}^+_{\text{odd}}$) attain, in general, different energies. In particular, only on the boundary between $S_{\{+,-\}}$ and $S_{\{+,0\}}$, all configurations from $\mathcal{G}^+_{\text{even}}$ are ground configurations. As a consequence, the version of the Pirogov-Sinai theory for lattice systems with residual entropy [GS88, SGL89] does not apply here. Namely, it would need in our case an assumption that everywhere in the coexistence region S_+ all configurations from $\mathcal{G}^+_{\text{even}}$ (and $\mathcal{G}^+_{\text{odd}}$) are ground configurations.

3. Proof of Theorems A and B

As mentioned above, Theorems A and B are an immediate consequence of the following four Propositions.

Proposition 1. *Consider the regions*

$$H_a^{(\epsilon)} = \{x \in H_a \mid \operatorname{dist}(x, H_a^c) > \epsilon\}, \qquad a = 0, \pm.$$

For $d \geq 2$ there exists a constant $b = b(d) > 0$, such that for all $\epsilon < \infty$, $\beta > b/\epsilon$, and $(U,\mu) \in H_a^{(\epsilon)}$, there is exactly one phase $\langle - \rangle_a$. For this phase $\Delta = 0$, it is translation invariant, and the free energy density $f(\beta, U, \mu)$ is analytic in

$$\mathcal{H}_a^{(\epsilon)} = \left\{ (\beta, U, \mu) \in \mathbb{C}^3 \mid \operatorname{Re}\beta \geq b/\epsilon, \left(\frac{\operatorname{Re}\beta U}{\operatorname{Re}\beta}, \frac{\operatorname{Re}\beta\mu}{\operatorname{Re}\beta} \right) \in H_a^{(\epsilon)} \right\}. \tag{3.1}$$

Proof. Except for the last statement, the proposition follows immediately from standard Pirogov-Sinai theory [PS75, Mar75, Zah84]: Given the relations (2.5) and (2.6), one gets, for a suitable constant $\alpha = \alpha(d) > 0$ and $(U,\mu) \in H_a^{(\epsilon)}$, the inequality

$$\beta h(b,c) \geq \beta h(a,a) + \beta\alpha\epsilon \tag{3.2}$$

provided $(b,c) \neq (a,a)$. As a consequence, all excitations of the ground state (a,a) are exponentially suppressed, with a "Peierls constant" $\tau = \tilde{\alpha}\beta\epsilon$ where $\tilde{\alpha} > 0$ depends only on the dimension d.

In order to prove the last statement of the proposition, one needs a representation in terms of a convergent contour expansion inside $\mathcal{H}_a^{(\epsilon)}$, where the Hamiltonian H is complex. This situation has been dealt with in [BI89]. In order to prove the corresponding Peierls condition, one needs a relation of the form (3.2) for the *real part* of βH, namely

$$\operatorname{Re}\beta h(b,c) \geq \operatorname{Re}\beta h(a,a) + (\operatorname{Re}\beta)\alpha\epsilon\,. \tag{3.3}$$

This leads to the regions $\mathcal{H}_a^{(\epsilon)}$. $\square$

Proposition 2. *Consider the regions $S_{\{a,b\}}$ and the corresponding sets $S_{\{a,b\}}^{(\epsilon)}$, $\{a,b\} = \{+,-\}$, $\{+,0\}$, $\{-,0\}$. For $d \geq 2$ there exists a constant $b = b(d) > 0$, such that for all $\epsilon < \infty$, $\beta > b/\epsilon$, and $(U,\mu) \in S_{\{a,b\}}^{(\epsilon)}$, there exist exactly two phases, the phase $\langle - \rangle_{\text{even}}$ with $\Delta > 0$ and the phase $\langle - \rangle_{\text{odd}}$ with $\Delta < 0$. These phases are periodic with period 2 and the free energy density, $f(\beta,U,\mu)$, as well as the corresponding staggered order parameters, $\Delta_{\text{even}}(\beta,U,\mu)$ and $\Delta_{\text{odd}}(\beta,U,\mu)$, are analytic in*

$$\mathcal{S}_{\{a,b\}}^{(\epsilon)} = \left\{ (\beta, U, \mu) \in \mathbb{C}^3 \mid \operatorname{Re}\beta \geq b/\epsilon, \left(\frac{\operatorname{Re}\beta U}{\operatorname{Re}\beta}, \frac{\operatorname{Re}\beta\mu}{\operatorname{Re}\beta} \right) \in S_{\{a,b\}}^{(\epsilon)} \right\}. \tag{3.4}$$

Proof. Again, the proof is standard, except for the last statement. Actually, in view of the essential singularities associated with first-order phase transitions [Isa84], the analyticity proof in the coexistence regions $\mathcal{S}_{\{a,b\}}^{(\epsilon)}$ is more subtle than that in the single phase regions $\mathcal{H}_a^{(\epsilon)}$.

We start with the observation that a Peierls condition of the form (3.3), namely

$$\mathrm{Re}\ \beta h(c,d) \geq \mathrm{Re}\ \beta h(a,b) + (\mathrm{Re}\ \beta)\alpha\epsilon \qquad \text{for all} \qquad \{c,d\} \neq \{a,b\}\,, \tag{3.5}$$

is valid in all of $\mathcal{S}^{(\epsilon)}_{\{a,b\}}$. Introducing truncated contour models as in [Zah84, BI89] to expand about the two staggered ground states $[a,b]$ and $[b,a]$, one therefore obtains a convergent cluster expansion for the corresponding "truncated free energies" f_{even} and f_{odd}. Next we note that

$$f_{\mathrm{even}}(\beta,U,\mu) = f_{\mathrm{odd}}(\beta,U,\mu) \qquad \text{for all} \qquad (\beta,U,\mu) \in \mathcal{S}^{(\epsilon)}_{\{a,b\}}$$

due to the translation symmetry of the model. As a consequence,

$$\mathrm{Re}\,(\beta f_{\mathrm{even}}(\beta,U,\mu)) = \mathrm{Re}\,(\beta f_{\mathrm{odd}}(\beta,U,\mu)) \qquad \text{for all} \qquad (\beta,U,\mu) \in \mathcal{S}^{(\epsilon)}_{\{a,b\}}\,.$$

The results of [BI89] then imply that both the even and the odd phase are stable in all of $\mathcal{S}^{(\epsilon)}_{\{a,b\}}$, implying in particular that the truncated free energies are equal to the corresponding "physical free energy" $f(\beta,U,\mu)$ obtained as the limit of (logarithms of) finite volume partition functions. As a consequence, $f(\beta,U,\mu)$ can be expressed as an absolutely convergent sum of analytic terms, implying that $f(\beta,U,\mu)$ is analytic itself. The stability of both the even and the odd phase also implies the convergence of the contour expansion for the staggered order parameters $\Delta_{\mathrm{even}}(\beta,U,\mu)$ and $\Delta_{\mathrm{odd}}(\beta,U,\mu)$, yielding their analyticity in $\mathcal{S}^{(\epsilon)}_{\{a,b\}}$. $\square$

Remark. Let us note the differences between the situation of Proposition 2 and the phase coexistence of, say, an Ising ferromagnet at zero field h. In the situtation of Proposition 2, where the two phases $\langle - \rangle_{\mathrm{even}}$ and $\langle - \rangle_{\mathrm{odd}}$ can be obtained from each other by a translation, $f_{\mathrm{even}} = f_{\mathrm{odd}}$ troughout the complex region $\mathcal{S}^{(\epsilon)}_{\{a,b\}}$, a statement which is stronger than the stability condition $\mathrm{Re}\,(\beta f_{\mathrm{even}}) = \mathrm{Re}\,(\beta f_{\mathrm{odd}})$. For the Ising model, on the other hand, the symmetry relating the two phases $\langle - \rangle_{+}$ and $\langle - \rangle_{-}$ requires a change of the sigh of h. As a consequence, no open neighbourhood $\mathcal{U} \subset \mathbb{C}$ of $h = 0$ can be found such that both the plus and the minus phase are stable in $\mathcal{U}$. Furthermore, on the coexistence line $\mathrm{Re}\, h = 0$ where both phases are stable, $f_+ \not\equiv f_-$, even though the weaker condition $\mathrm{Re}\,(\beta f_+) = \mathrm{Re}\,(\beta f_-)$ is true for $\mathrm{Re}\, h = 0$.

Proposition 3. *Let R be the union of H_0, $S_{\{+,-\}}$ and their common boundary, and let $R^{(\epsilon)} = \{x \in R \mid \mathrm{dist}(x, R^c) > \epsilon\}$. For $d \geq 2$ there exists a constant $b = b(d) > 0$, such that for all $\epsilon < \infty$ and $\beta > b/\epsilon$ there exist a curve $L(\beta)$, separating $R^{(\epsilon)}$ into two open regions $R^{(\epsilon)}_0$ and $R^{(\epsilon)}_{\{+,-\}}$, such that the following statements are true.*

i) In $R^{(\epsilon)}_0$, there exits exactly one phase $\langle - \rangle_0$. This phase is translation invariant with $\Delta = 0$.

ii) In $R^{(\epsilon)}_{\{+,-\}}$ there are exactly two phases $\langle - \rangle_{\mathrm{even}}$ and $\langle - \rangle_{\mathrm{odd}}$, characterized by $\Delta > 0$ and $\Delta < 0$. Both phases are periodic with period 2.

iii) On the boundary $L(\beta)$ between $R^{(\epsilon)}_0$ and $R^{(\epsilon)}_{\{+,-\}}$, all three phases $\langle - \rangle_0$, $\langle - \rangle_{\mathrm{even}}$ and $\langle - \rangle_{\mathrm{odd}}$ coexist. Furthermore, all periodic Gibbs states on this curve are a convex combination of these three phases.

iv) As a function of U and μ, the free energy f is real analytic in $R^{(\epsilon)} \setminus L(\beta)$, and the staggered order parameters of the two phases $\langle - \rangle_{\mathrm{even}}$ and $\langle - \rangle_{\mathrm{odd}}$, $\Delta_{\mathrm{even}}(\beta,U,\mu)$ and $\Delta_{\mathrm{odd}}(\beta,U,\mu)$, are real analytic in $R^{(\epsilon)}_{\{+,-\}}$.

Proof. Again the proof is standard. One now introduces three different truncated contour models: one for the excitations about the homogeneous configuration $(0,0)$ and two for the excitations about the two staggered configurations $(+,-)$ and $(-,+)$. In the region $R^{(\epsilon)}$, and more generally in the complex region

$$\mathcal{R}^{(\epsilon)} = \{(U,\mu) \mid (\operatorname{Re} U, \operatorname{Re} \mu) \in R^{(\epsilon)}\}\,, \tag{3.6}$$

the model again satisfies a suitable Peierls condition provided $\beta\epsilon$ is big enough. This leads to the convergence of the cluster expansion for the corresponding truncated free energies f_0, f_{even} and f_{odd} in $\mathcal{R}^{(\epsilon)} \supset R^{(\epsilon)}$.

Given the "degeneracy removing condition"

$$\frac{d}{dU}\Big(h(+,-) - h(0,0)\Big) = \frac{1}{2d} > 0 \tag{3.7}$$

and the symmetry relation

$$f_{\text{even}}(U,\mu) = f_{\text{odd}}(U,\mu)\,, \tag{3.8}$$

the proof of statement i) – iii) is now an easy application of the methods of [Zah84]. Actually, the complex analogue of (3.7), namely the degeneracy removing condition

$$\frac{d}{d\operatorname{Re} U}\Big(\operatorname{Re} h(+,-) - \operatorname{Re} h(0,0)\Big) = \frac{1}{2d} > 0\,, \tag{3.9}$$

together with the validity of (3.8) in the complex region $\mathcal{R}^{(\epsilon)}$ leads to the existence of a phase transition surface $\mathcal{S}(\beta)$ that separates $\mathcal{R}^{(\epsilon)}$ into two open regions: a region $\mathcal{R}_0^{(\epsilon)}$ in which $\operatorname{Re}(\beta f_0(U,\mu)) < \operatorname{Re}(\beta f_{\text{even}}(U,\mu))$ and $f(U,\mu) = f_0(U,\mu)$, and a region $\mathcal{R}_{\{+,-\}}^{(\epsilon)}$ in which $\operatorname{Re}(\beta f_0(U,\mu)) > \operatorname{Re}(\beta f_{\text{even}}(U,\mu))$ and $f(U,\mu) = f_{\text{even}}(U,\mu)$, see [BI89][3]. As a consequence, the free energy f of the model can be rewritten as a convergent sum of analytic terms in both $\mathcal{R}_0^{(\epsilon)}$ and $\mathcal{R}_{\{+,-\}}^{(\epsilon)}$, leading to the analyticity of f in $\mathcal{R}^{(\epsilon)} \setminus \mathcal{L}(\beta)$ and hence the real analyticity of f in $R^{(\epsilon)} \setminus L(\beta)$. In a similar way, one obtains the real analyticity of the charged order parameters $\Delta_{\text{even}}(\beta,U,\mu)$ and $\Delta_{\text{odd}}(\beta,U,\mu)$. $\square$

Proposition 4. *Consider the regions $S_\pm$ introduced in the last section, and the corresponding sets $S_\pm^{(\epsilon)}$. For $d \geq 2$ and $m = \pm$ there exists a constant $b = b(d) > 0$, such that for all $\epsilon < \infty$, $\beta > b/\epsilon$, and $(U,\mu) \in S_m^{(\epsilon)}$, there exist exactly two phases, a phase $\langle - \rangle_{\text{even}}$ with $\Delta > 0$ and a phase $\langle - \rangle_{\text{odd}}$ with $\Delta < 0$. These phases are periodic with period 2 and both the free energy density, $f(\beta,U,\mu)$, and the corresponding staggered order parameters, $\Delta_{\text{even}}(\beta,U,\mu)$ and $\Delta_{\text{odd}}(\beta,U,\mu)$, are real analytic functions of U and μ in $S_m^{(\epsilon)}$.*

Proof of Proposition 4. Without loss of generality, we may assume that $(U,\mu) \in S_+$. In order to prove the proposition, we introduce an auxiliary Ising variable $\sigma_{\boldsymbol{i}} = \sigma(S_{\boldsymbol{i}})$ as

$$\sigma(S_{\boldsymbol{i}}) = \begin{cases} + & \text{if} \quad S_{\boldsymbol{i}} = + \\ - & \text{if} \quad S_{\boldsymbol{i}} \in \{0,-\} \end{cases}\,, \tag{3.10}$$

[3] In the language of [Zah84, BI89], $\mathcal{R}_0^{(\epsilon)}$ is the region where the homogeneous phase is stable, and $\mathcal{R}_{\{+,-\}}^{(\epsilon)}$ is the region where the two staggered phases are stable.

and rewrite the model (2.1) in terms of an effective Hamiltonian $H^{\mathrm{eff}}(\sigma)$. We then prove that the Hamiltonian H^{eff} has two ground states g^{even} and g^{odd}, corresponding to the restricted ensembles $\mathcal{G}^{+}_{\mathrm{even}}$ and $\mathcal{G}^{+}_{\mathrm{odd}}$ introduced at the end of the last section,

$$g^{\mathrm{even}}_{\boldsymbol{i}} = \epsilon_{\boldsymbol{i}} \quad \text{and} \quad g^{\mathrm{odd}}_{\boldsymbol{i}} = -\epsilon_{\boldsymbol{i}}\,, \tag{3.11}$$

and that the excitation above these ground states obey a suitable Peierls condition. Here, as in Section 1, $\epsilon_{\boldsymbol{i}} = +1$ on the even and $\epsilon_{\boldsymbol{i}} = -1$ on the odd sublattice.

We start with some notation. We consider a box $\Lambda = [1, L]^d \cap \mathbb{Z}^d$, its boundary $\partial\Lambda = \{\boldsymbol{i} \in \Lambda^c \mid \mathrm{dist}(\boldsymbol{i}, \Lambda) = 1\}$, the set $B(\Lambda)$ of nearest neighbour bonds $\langle \boldsymbol{i}, \boldsymbol{j}\rangle$ with at least one endpoint in Λ, and the union of Λ and its boundary, $\bar{\Lambda} = \Lambda \cup \partial\Lambda$. Here, as in the sequel, $\mathrm{dist}(\cdot,\cdot)$ denotes the ℓ_1 distance in $\mathbb{Z}^d$. As usual, we call two sets V, $V' \in \mathbb{Z}^d$ adjacent or touching if $\mathrm{dist}(V, V') = 1$, and a set $V \subset \mathbb{Z}^d$ connected if for any two points $\boldsymbol{i}, \boldsymbol{j} \in V$ there is a sequence of adjacent points in V that joins $\boldsymbol{i}$ to $\boldsymbol{j}$.

Keeping in mind that we want to construct finite temperature states $\langle - \rangle_m$ which are small perturbations of the restricted ensembles $\mathcal{G}^{+}_{m}$, $m =$ "even" or "odd", we introduce an effective Hamiltonian $H^{\mathrm{eff}}_{\Lambda}(\sigma_\Lambda \mid m)$ in Λ with the boundary conditions $m =$ even, odd, by

$$e^{-\beta H^{\mathrm{eff}}_{\Lambda}(\sigma_\Lambda|m)} = \sum_{\substack{S_{\bar{\Lambda}}:\ \sigma(S_{\boldsymbol{i}})=\sigma_{\boldsymbol{i}},\, \boldsymbol{i}\in\Lambda \\ \sigma(S_{\boldsymbol{i}})=g^m_{\boldsymbol{i}},\, \boldsymbol{i}\in\partial\Lambda}} \prod_{\langle \boldsymbol{i},\boldsymbol{j}\rangle \in B(\Lambda)} e^{-\beta h(S_{\boldsymbol{i}}, S_{\boldsymbol{j}})}\,. \tag{3.12}$$

The corresponding finite volume Gibbs states are

$$\langle\,\cdot\,\rangle_{m,\Lambda} = \frac{1}{Z_m(\Lambda)} \sum_{\sigma_\Lambda} \cdot\; e^{-\beta H^{\mathrm{eff}}_{\Lambda}(\sigma_\Lambda|m)} \tag{3.13}$$

with

$$Z_m(\Lambda) = \sum_{\sigma_\Lambda} e^{-\beta H^{\mathrm{eff}}_{\Lambda}(\sigma_\Lambda|m)}. \tag{3.14}$$

Extending the configuration σ_Λ to $\bar{\Lambda}$ by setting $\sigma_{\boldsymbol{i}} = g^m_{\boldsymbol{i}}$ for $\boldsymbol{i} \in \partial\Lambda$, we define a nearest neighbour pair $\langle \boldsymbol{i}, \boldsymbol{j}\rangle \in B(\Lambda)$ as *excited* in the configuration σ_Λ if $\sigma_{\boldsymbol{i}} = \sigma_{\boldsymbol{j}}$ and a point $\boldsymbol{i} \in \bar{\Lambda}$ as *excited* if it is contained in an excited bond. Note that the notion of whether a bond $\langle \boldsymbol{i}, \boldsymbol{j}\rangle$ that joins the volume Λ to its boundary $\partial\Lambda$ is excited or not depends on the boundary condition.

At this point, contours and ground state regions are defined in the standard way: Given a configurations σ_Λ (and one of the two boundary conditions introduced above), the *contours* $Y_1, \cdots, Y_n$ corresponding to the configuration σ_Λ are defined as pairs of the form $Y = (\mathrm{supp}\, Y, \sigma_Y)$, where $\mathrm{supp}\, Y$ is a connected component of the set of excited points and σ_Y is the restriction of $\sigma_{\bar{\Lambda}}$ to $\mathrm{supp}\, Y$. The *ground state regions* are defined as the connected components of the set of points which are not exited. Note that the restriction of $\sigma_{\bar{\Lambda}}$ to a ground state region C is staggered, and hence equal to the restriction of one of the two ground states to C, $\sigma_C = g^m_C$, where $m = m(C)$ may vary from component to component.

An important property of a set of contours $Y_1, \cdots, Y_n$ corresponding to a configuration σ_Λ is that they "match". In order to define this notion, we note that each contour Y determines the value of $\sigma_{\boldsymbol{i}}$ on all points $\boldsymbol{i} \in \bar{\Lambda}$ which touch its support because all bonds joining the support of Y to such a point are not exited. The contour Y therefore determines the value of $m(C)$ for all ground state regions C touching its support. We say that Y attaches a *label* $m(C) = m_Y(C)$ to these ground state regions. *Matching* of the contours $Y_1, \cdots, Y_n$ is the statement that the labels attached to a given ground state region C by different contours are identical and compatible with the boundary condition. A minute of reflection now shows that to each set $\{Y_1, \cdots, Y_n\}$ of matching contours with $\operatorname{dist}(\operatorname{supp} Y_k, \operatorname{supp} Y_l) > 1$, $k \neq l$, there corresponds exactly one configuration σ_Λ. The partition function $Z_m(\Lambda)$ can therefore be expressed as a sum over sets of matching contours, once the Hamiltonian $H_\Lambda^{\text{eff}}(\sigma_\Lambda \mid m)$ has been expressed in terms of $Y_1, \cdots, Y_n$.

We will now show that this can be done in the form

$$e^{-\beta H_\Lambda^{\text{eff}}(\sigma_\Lambda|m)} = e^{-\beta H_\Lambda^{\text{eff}}(g_\Lambda^m|m)} \prod_{k=1}^{n} z(Y_k) \tag{3.15}$$

where $z(Y_k)$ are contour weights obeying a Peierls condition

$$|z(Y_k)| \leq e^{-\tau|\operatorname{supp} Y|} \tag{3.16}$$

with sufficiently large Peierls constant τ.

We start with an explicit calculation of the Hamiltonian $H_\Lambda^{\text{eff}}(\sigma_\Lambda \mid m)$ for the configuration $\sigma_\Lambda = g_\Lambda^m$ with no contour. In this configuration, each point $\boldsymbol{i} \in \bar{\Lambda}$ with $\sigma_{\boldsymbol{i}} = -$ has $2d$ nearest neighbours $\boldsymbol{j} \in \bar{\Lambda}$ with $\sigma_{\boldsymbol{j}} = +$ if $\boldsymbol{i} \in \Lambda$, and 1 nearest neighbour $\boldsymbol{j} \in \bar{\Lambda}$ with $\sigma_{\boldsymbol{j}} = +$ if $\boldsymbol{i} \in \partial\Lambda$. Since $\sigma_{\boldsymbol{j}} = \sigma(S_{\boldsymbol{j}}) = +$ implies $S_{\boldsymbol{j}} = +$, the summation over the spin variable $S_{\boldsymbol{i}}$ in (3.12) therefore leads to a factor

$$\lambda = \sum_{S_{\boldsymbol{i}}:\sigma(S_{\boldsymbol{i}})=-} e^{-2d\beta h(S_{\boldsymbol{i}},+)} = e^{-2d\beta h(0,+)} + e^{-2d\beta h(-,+)} \tag{3.17}$$

if $\boldsymbol{i} \in \Lambda$, and to a factor

$$\lambda' = \sum_{S_{\boldsymbol{i}}:\sigma(S_{\boldsymbol{i}})=-} e^{-\beta h(S_{\boldsymbol{i}},+)} = e^{-\beta h(0,+)} + e^{-\beta h(-,+)} \tag{3.18}$$

if $\boldsymbol{i} \in \partial\Lambda$. Per bond, this yields the energy

$$h_0^m(\langle \boldsymbol{i}, \boldsymbol{j} \rangle) = \begin{cases} h_0' = -\frac{1}{\beta} \log \lambda' & \text{if } \boldsymbol{i} \in \partial\Lambda \text{ and } \sigma_{\boldsymbol{i}} = g_{\boldsymbol{i}}^m = - \\ h_0 = -\frac{1}{2d\beta} \log \lambda & \text{if } \boldsymbol{i} \in \Lambda \text{ and } \sigma_{\boldsymbol{i}} = g_{\boldsymbol{i}}^m = - \end{cases} . \tag{3.19}$$

For the energy of the configuration g_Λ^m, this gives

$$H_\Lambda^{\text{eff}}(g_\Lambda^m \mid m) = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle \in B(\Lambda)} h_0^m(\langle \boldsymbol{i}, \boldsymbol{j} \rangle) . \tag{3.20}$$

Remark. Obviously, the boundary correction (3.19) does not affect the specific ground state energy

$$e_m = \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} H_\Lambda^{\text{eff}}(g_\Lambda^m \mid m) \tag{3.21}$$

so that $e_{\text{even}} = e_{\text{odd}}$. It does affect, however, the finite volume ground state energies $H_\Lambda^{\text{eff}}(g_\Lambda^m \mid m)$.

In order to calculate the weight $e^{-\beta H_\Lambda^{\mathrm{eff}}(\sigma_\Lambda|m)}$ for a configuration σ_Λ corresponding to a nonempty set of contours $\{Y_1\cdots,Y_n\}$, we extract from (3.12), for each contour $Y\in\{Y_1\cdots,Y_n\}$, the factor

$$\tilde z(Y)=\sum_{S_Y:\sigma(S_i)=\sigma_i}\ \prod_{\langle \boldsymbol{i},\boldsymbol{j}\rangle\in B(Y)} e^{-\beta h(S_{\boldsymbol{i}},S_{\boldsymbol{j}})}\,. \tag{3.22}$$

Here $B(Y)$ is the set of all bonds $\langle \boldsymbol{i},\boldsymbol{j}\rangle\in B(\Lambda)$ such that either

i) both endpoints of $\langle \boldsymbol{i},\boldsymbol{j}\rangle$ are in the support of Y,

or

ii) only one endpoint of $\langle \boldsymbol{i},\boldsymbol{j}\rangle$ lies in the support of Y, and this endpoint corresponds to a value $\sigma_{\boldsymbol{i}}=-1$.

Note that the second class of bonds are those bonds which couple the spin variables in the support of Y to the spin variables in $\bar\Lambda\setminus\operatorname{supp}Y$. The remaining sum in (3.12) can be easily calculated because all points $\boldsymbol{i}\in\Lambda\setminus(\operatorname{supp}Y_1\cup\cdots\cup\operatorname{supp}Y_n)$ with $\sigma_{\boldsymbol{i}}=-$ are not excited. The summation over the corresponding spin variable $S_{\boldsymbol{i}}$ therefore again leads to factors λ and λ', giving a factor $e^{-\beta h_0^m(\langle \boldsymbol{i},\boldsymbol{j}\rangle)}$ for all the bonds in $B(\Lambda)\setminus(B(Y_1)\cup\cdots\cup B(Y_n))$. Extracting the factor

$$\prod_{\langle \boldsymbol{i},\boldsymbol{j}\rangle\in B(Y)} e^{-\beta h_0^m((\langle \boldsymbol{i},\boldsymbol{j}\rangle))}$$

from the activities (3.22), we therefore obtain a representation of the form (3.15), with

$$z(Y)=\sum_{S_Y:\sigma(S_i)=\sigma_i}\ \prod_{\langle \boldsymbol{i},\boldsymbol{j}\rangle\in B(Y)} e^{-\beta(h(S_i,S_j)-h_0^m(\langle \boldsymbol{i},\boldsymbol{j}\rangle))}\,. \tag{3.23}$$

We are left with the proof of the Peierls condition (3.16). We start with the observation that for $(U,\mu)\in S_+^{(\epsilon)}\subset S_+$ and arbitrary values for the spins $S_{\boldsymbol{i}}$ and $S_{\boldsymbol{j}}$,

$$h(S_{\boldsymbol{i}},S_{\boldsymbol{j}})\ge\min\{h(0,+),h(-,+)\}\,, \tag{3.24}$$

while

$$h(S_{\boldsymbol{i}},S_{\boldsymbol{j}})\ge\min\{h(0,+),h(-,+)\}+\alpha\epsilon\,, \tag{3.25}$$

for some dimension dependent constant $\alpha>0$ whenever the bond $\langle \boldsymbol{i},\boldsymbol{j}\rangle$ is excited. Combining (3.24) and (3.25) with the fact that

$$h_0^m(\langle \boldsymbol{i},\boldsymbol{j}\rangle)\le\min\{h(0,+),h(-,+)\}\,, \tag{3.26}$$

we obtain the bound

$$|z(Y)|\le\sum_{S_Y:\sigma(S_i)=\sigma_i}\ \prod_{\langle \boldsymbol{i},\boldsymbol{j}\rangle\in B^*(Y)} e^{-\beta\alpha\epsilon}\,, \tag{3.27}$$

where $B^*(Y)$ is the set of excited bonds in $B(Y)$. Bounding $|B^*(Y)|$ from below by $\frac12|\operatorname{supp}Y|$, and the number of terms in the sum over S_Y from above by $2^{|\operatorname{supp}Y|}$, we obtain the bound (3.16) with

$$e^{-\tau}=2e^{-\frac12\beta\alpha\epsilon}\,. \tag{3.28}$$

Given (3.14), (3.15) and (3.16), the partition function (3.14) can be expressed as the partition function of a contour system with exponentially decaying weights,

$$Z_m(\Lambda) = e^{-\beta H_\Lambda^{\mathrm{eff}}(g_\Lambda^m|m)} \sum_{\{Y_1,\cdots,Y_n\}} \prod_{k=1}^{n} z(Y_k) \tag{3.29}$$

where the sum runs over sets $\{Y_1, \cdots, Y_n\}$ of matching contours obeying the compatibility condition that $\mathrm{dist}(\mathrm{supp}\, Y_k, \mathrm{supp}\, Y_l) > 1$ for $k \neq l$. As a consequence, the model can be again analyzed by standard methods, see e.g. [Zah84]. One obtains the existence of the limits

$$\langle - \rangle_m = \lim_{L\to\infty} \langle - \rangle_{m,\Lambda} \tag{3.30}$$

as periodic Gibbs states with $\Delta > 0$ and $\Delta < 0$, respectively, the fact that these states are extremal, and the fact that all other periodic Gibbs states are convex combinations of $\langle - \rangle_{\mathrm{even}}$ and $\langle - \rangle_{\mathrm{odd}}$.

Considering finally a suitable complex neighbourhood of the region $S_+^{(\epsilon)}$, e.g.

$$\mathcal{S}_+^{(\epsilon,\delta)} = \{(U,\mu) \mid (\mathrm{Re}\, U, \mathrm{Re}\, \mu) \in S_+^{(\epsilon)} \quad \text{and} \quad |\mathrm{Im}\, U| < \delta, |\mathrm{Im}\, \mu| < \delta\} \tag{3.31}$$

with δ sufficiently small, one easily establishes a Peierls condition with a slightly smaller Peierls constant $\tau = \tau(\beta, \epsilon, \delta, d)$. The methods of [BI89] then give[4] the free energy density f and the staggered charge-order parameters $\Delta_{\mathrm{even}}(\beta, U, \mu)$ and $\Delta_{\mathrm{odd}}(\beta, U, \mu)$ as convergent sums of analytic terms in $\mathcal{S}_+^{(\epsilon,\delta)}$, implying their analyticity in $\mathcal{S}_+^{(\epsilon,\delta)}$ and hence their real analyticity in $S_+^{(\epsilon)}$. This completes the proof of Proposition 4. $\square$

Remark. It is intriguing to relate the first order jump of the staggered order parameter at $T = 0$ to the analytic behaviour at positive temperatures. To this end, we note that the distribution of the spin variable $S_{\boldsymbol{i}}$ in the restricted ensembles $\mathcal{G}_m^+$ is given by

$$\mu(S_{\boldsymbol{i}}) = \begin{cases} \delta(S_{\boldsymbol{i}}, +) & \text{if} \quad g_{\boldsymbol{i}}^m = + \\ \lambda^{-1} e^{-2d\beta h(S_{\boldsymbol{i}},+)} & \text{if} \quad g_{\boldsymbol{i}}^m = - \end{cases}.$$

The finite temperature excitation above the corresponding ground states $\sigma = g^m$ slightly modify these distributions, leading to corrections of the order $O(e^{-\beta\alpha\epsilon})$. As a consequence, the staggered order parameter Δ in the region $S_+^{(\epsilon)}$ is given by

$$\begin{aligned} \Delta &= \pm\Big(\frac{3}{4} + \frac{1}{4}\tanh\Big(2d\beta(h(0,+) - h(-,+))\Big)\Big) + O(e^{-\beta\alpha\epsilon}) \\ &= \pm\Big(\frac{3}{4} + \frac{1}{4}\tanh\big(\beta(2d - \mu - \tilde{U}/2)\big)\Big) + O(e^{-\beta\alpha\epsilon}), \end{aligned} \tag{3.32}$$

where the plus sign corresponds to the even phase and the minus sign corresponds to the odd phase.

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[4] As in the proof of Proposition 2, we use the fact that, by translation invariance, the corresponding truncated free energies f_{even} and f_{odd} are equal in the whole complex region $\mathcal{S}_+^{(\epsilon,\delta)}$.

References

[BI89] Borgs, C., Imbrie, J., *A Unified Approach to Phase Diagrams in Field Theory and Statistical Mechanics*, Commun. Math. Phys. **123** (1989), 305–328.

[BK94] Borgs, C., Kotecký. R., *Staggered charge order in the narrow band extended Hubbard model* (1994), in preparation.

[BKL85] Bricmont, J., Kuroda, K. and Lebowitz, J.L., *First-order phase transitions in lattice and continuous systems: extension of Pirogov-Sinai theory*, Commun. Math. Phys. **101** (1985), 501–538.

[Dag94] Dagotto, E., *Correlated electrons in high temperature superconductors*, Rev. Mod. Phys. **66** (1994), 763–840.

[GS88] Gruber, C., Sütő, A., *Phase diagrams of lattice systems with residual entropy*, J. Stat. Phys. **52** (1988), 113–142.

[Hub79] Hubbard, J., *Generalized Wigner Lattices and Band Motion Effects*, Quasi One-Dimensional Conductors (Barišić, S., Bjeliš, A., Cooper, J. R. and Leontič, B., eds.), Lecture Notes in Physics **96**, Springer, Berlin, pp. 11–19.

[IILM75] Ionov, S.P., Ionova, G.V., Lubimov, V.S., Makarov, E.F., *Instasbility of crystal lattices with respect to electron density redistributions*, Phys. Stat. Sol. b **71** (1975), 11.

[Isa84] Isakov, S.,N., *Nonanalytic features of first order phase transition in the Ising model.*, Commun. Math. Phys. **95** (1984), 427–433.

[Jęd94] Jędrzejewski, J., *Phase diagrams of extended Hubbard models in the atomic limit*, Physica A **205** (1994), 702–717.

[KY93] Klein, D. and Yang, W.-S., *Absence of first-order phase transitions for antiferromagnetic Systems*, J. Stat. Phys. **70** (1993), 1391–1400.

[Lor82] Lorentz, B., *On the stability of the Wigner crystallized ground state*, Phys. Stat. Sol. b **112** (1982), K47–K49.

[Mar75] Martirosjan D. G., *The problem of an upper estimate of the number of Periodic Gibbs states for the model of a lattice gas*, Usp. Mat. Nauk **30** (1975), 181.

[Mon92] Montorsi, A. (ed.), *The Hubbard Model: A Collection of Reprints*, World Scientific, 1992.

[MRC84] Micnas, R., Robaszkiewicz, S. and Chiao, K.A., *Multicritical behaviour of the extended Hubbard model in the zero-bandwidth limit*, Phys. Rev. **B 29** (1984), 2784–2789.

[MRR90] Micnas, R., Ranninger, R. and Robaszkiewicz, S., *Superconductivity in narrow–band systems with local nonretarded attractive interactions*, Rev. Mod. Phys. **62** (1990), 113–171.

[PS75] Pirogov, S. and Sinai, Ya. G., *Phase diagrams of classical lattice systems*, Theoretical and Mathematical Physics **25** (1975), 1185–1192; **26** (1976), 39–49.

[SGL89] Sütő, A., Gruber, C., Lemberger, P., *Phase diagrams of lattice systems with residual entropy. II. Low temperature expansion*, J. Stat. Phys. **56** (1989), 261–290.

[Sla87] Slawny, J., *Low temperature properties of classical lattice systems: Phase transitions and phase diagrams*, Phase Transitions and Critical Phenomena (C. Domb and J. L. Lebowitz, eds.), vol. 11, Academic Press, New York, 1987, pp. 127–205.

[Zah84] Zahradník, M., *An Alternate Version of Pirogov-Sinai Theory*, Commun. Math. Phys. **93** (1984), 559–581.