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LOW TEMPERATURE PHASE DIAGRAMS OF FERMIONIC LATTICE SYSTEMS

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Abstract.

We consider fermionic lattice systems with Hamiltonian $H = H^{(0)} + \lambda H_Q$, where $H^{(0)}$ is diagonal in the occupation number basis, while H_Q is a suitable "quantum perturbation". We assume that $H^{(0)}$ is a finite range Hamiltonian with finitely many ground states and a suitable Peierls condition for excitations, while H_Q is a finite range or exponentially decaying Hamiltonian that can be written as a sum of even monominals in the fermionic creation and annhilation operators. Mapping the d dimensional quantum system onto a *classical* contour system on a $d+1$ dimensional lattice, we use standard Pirogov-Sinai theory to show that the low temperature phase diagram of the quantum system is a small perturbation of the zero temperature phase diagram of the classical system, provided λ is sufficiently small. Particular attention is paid to the sign problems arrising from the fermionic nature of the quantum particles.

As a simple application of our methods, we consider the Hubbard model with an addidional nearest neighbor repulsion. For this model, we rigorously establish the existence of a paramagnetic phase with commensurate staggered charge order for the narrow band case at sufficiently low temperatures.

1. Introduction

In recent years, the Hubbard model has become one of the most important models in the theory of strongly correlated electron systems. Since its invention by Hubbard and others [1–3], it has been used to describe, amoung others, antiferromagnetism [4], ferromagnetism [5], paramagnetism [6], the metal-insulator transition [7–9], and, more recently, high-T_c superconductivity [10, 11].

As already pointed out by Hubbard in his original paper [1], the standard Hubbard model is a very crude approximation to the actual behaviour of electrons in these systems. Many terms, some of which may drastically change the phase diagram, have been neglected. The largest and most important of these terms is the nearest neighbor Coulomb repulsion. The modification of the Hubbard model which contains this term is usually referred to as the *extended Hubbard model*. Most relevant for physical applications is the so called narrow band case of this model,

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characterized by a hopping constant t that is small with respect to the Coulomb interaction.

In this paper we rigorously establish the existence of a low temperature phase with staggered charge order in the narrow band extended Hubbard model in $d \geq 2$ dimensions. This phase is characterized by an electron density which, rather than being constant, varies from one sublattice to the next of a bipartite lattice Λ. While the existence of such a phase has been predicted by many authors (see e.g. [12–16]), the only previous rigorous results consider the atomic limit $t = 0$ [17, 18].

In order to obtain our results for the narrow band extended Hubbard model, we combine the methods of reference [18] with our recent extension of Pirogov-Sinai theory to quantum spin systems [19] to obtain a convergent expansion about the atomic limit. Actually, this expansion will be derived for a more general class of strongly interacting fermionic lattice system, see Section 3 below.

The extended Hubbard model is defined by the Hamiltonian

$$\begin{aligned} H_\Lambda = -t \sum_{\langle x,y\rangle} \big(c^\dagger_{x,\uparrow} c_{y,\uparrow} + c^\dagger_{x,\downarrow} c_{y,\downarrow} + c^\dagger_{y,\uparrow} c_{x,\uparrow} + c^\dagger_{y,\downarrow} c_{x,\downarrow}\big) \\ + U \sum_x \hat n_{x,\uparrow} \hat n_{x,\downarrow} + W \sum_{\langle x,y\rangle} \hat n_x \hat n_y - \big(\mu + zW + \frac{U}{2}\big) \sum_x \hat n_x \end{aligned} \tag{1.1}$$

where the second and fourth sum run over the points x of a bipartite lattice Λ with constant coordination number z, while the first and third sum run over the set $B(\Lambda)$ of all nearest neighbor pairs $\langle x, y\rangle$ in Λ. The symbols $c^\dagger_{x,\sigma}$ and $c_{x,\sigma}$, denote the creation and annihilation operators of the electron with up and down spin, $\sigma = \uparrow, \downarrow$, while $\hat n_{x,\sigma} := c^\dagger_{x,\sigma} c_{x,\sigma}$ and $\hat n_x := \hat n_{x,\uparrow} + \hat n_{x,\downarrow}$ are the corresponding number operators. As usual, the electron creation and annihilation operators satisfy canonical anticommutation relations.

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[1] $\mu = 0$. 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.

Before stating our main result for the narrow band model at low temperatures, we recall the ground state diagram of the atomic limit model ($t = 0$). In order to simplify the notation, we restrict ourselves to the simple hypercubic lattice $\mathbb{Z}^d$, although our results should hold for other bipartite lattices as well. Observing that

[1]For more general biparite lattices where the coordination number z varies from sublattice to sublattice, one would need a shift which is different for the two sublattices. Even though our methods do not require any symmetry between the two sublattices and would allow us to analyse this asymmetric model as well, we don't consider it here in order to simplify our notation.

the potential term in (1.1) can be written as a sum over pair potentials,

$$H_\Lambda = -t \sum_{\langle x,y\rangle\in B(\Lambda)} \left(c^\dagger_{x,\uparrow}c_{y,\uparrow} + c^\dagger_{x,\downarrow}c_{y,\downarrow} + c^\dagger_{y,\uparrow}c_{x,\uparrow} + c^\dagger_{y,\downarrow}c_{x,\downarrow}\right) + \sum_{\langle x,y\rangle\in B(\Lambda)} v(\hat n_x, \hat n_y)\,, \tag{1.2}$$

with

$$v(\hat n_x, \hat n_y) = W\big(\hat n_x - 1\big)\big(\hat n_y - 1\big) + \frac{U}{4d}\Big((\hat n_x - 1)^2 + (\hat n_y - 1)^2\Big) - \frac{\mu}{2d}\big(\hat n_x + \hat n_y - 2\big)\,, \tag{1.3}$$

the ground states of the $t = 0$ model are easily determined. The corresponding ground state diagram is shown in Figure 1. One finds three regions H_a, $a = 0, 1, 2$ with homogeneous particle density $\langle \hat n_x\rangle = a$, and three regions $S_{\{a,b\}}$, $\{a, b\} = \{0, 1\}, \{0, 2\}, \{1, 2\}$ with a commensurate charge density wave: $\langle \hat n_x\rangle = \rho + (-1)^x\Delta$, where $\rho = \frac{a+b}{2}$ and $\Delta = \pm\frac{b-a}{2}$.

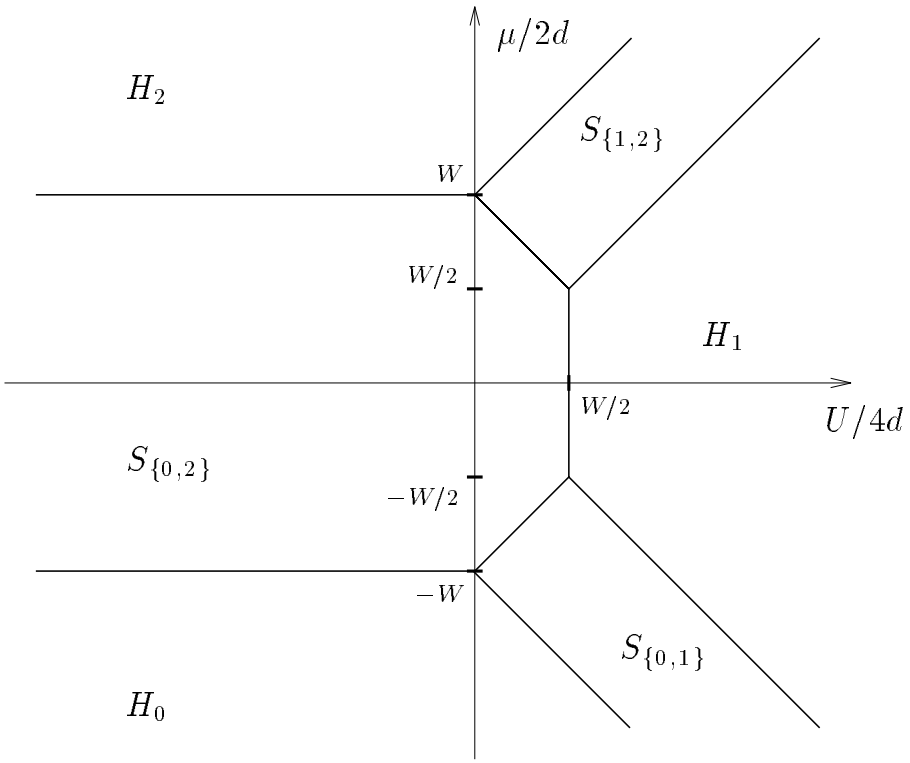

FIG.1. GROUND STATE PHASE DIAGRAM OF THE $t = 0$ MODEL

In this paper we will prove that, for all $\epsilon > 0$, and for all (U, μ) in the subregion

$$S^{(\epsilon)}_{\{0,2\}} = \big\{(U,\mu)\in\mathbb{R}^2 \,\big|\, U < 2d(W-\epsilon)\,,\ |\mu| < 2d\min\{W-\epsilon\,,\ W-\epsilon-U/4d\}\big\} \tag{1.4}$$

of the region $S_{\{0,2\}} = S^{(0)}_{\{0,2\}}$, the staggered charge order persists for sufficiently low temperatures and sufficiently small t. We also establish that the corresponding phase is paramagnetic,[2] see Section 2 for the precise statements of our results.

[2]It would be very interesting to establish the existence of a phase with ferro- or antiferromagnetic order in this model. Unfortunately, this is a very difficult task, due to the Goldstone boson which is expected as a consequence of spontaneous symmetry breaking of the corresponding continuous symmetry. Note that this problem does not arise in the asymetric $t - J$ model studied in [20], where the symmetry to be broken is a discrete symmetry.

The more general class of fermionic systems we consider is described by a Hamiltonian $H = H^{(0)} + \lambda H_Q$, where $H^{(0)}$ is diagonal in the occupation number basis, while H_Q is a suitable "quantum perturbation". We assume that $H^{(0)}$ is a finite range Hamiltonian with finitely many ground states and a suitable Peierls condition for excitations, while H_Q is a finite range or exponentially decaying Hamiltonian that can be written as a sum of even monominals in the fermionic creation and annhilation operators. For these models, we derive a convergent cluster expansion about the "classical theory" with $\lambda = 0$, folowing closely the methods used in [19]: In a first step, we use the Duhamel-Phillips (or Schwinger-Dyson) expansion to derive a path integral representation of the model. In the next step, we block the configurations contributing to the path integral onto lattice configurations on a suitable space-time lattice $\Lambda \times \{1, 2, \ldots, M\}$. Applying Pirogov-Sinai theory [21,22] in the form developed in [23] to the resulting classical contour system, we obtain our main results.

Namely, we determine the stable phases in dependence on the external parameters (construction of the phase diagram), and show that the corresponding infinite volume states are periodic, pure states with exponential clustering for truncated expectation values. We also control the thermodynamic limit for periodic boundary conditions and prove that it is a convex combination of the stable states with equal weight for each of them. Finally, we discuss conservation laws for the quantum system in a general setup. Under the condition that the full Hamiltonian commutes with an operator Q_Λ, we show that the density $\rho_Q = \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \langle Q_\Lambda \rangle$ in the ground state $\langle \cdot \rangle$ of the quantum system exactly coincides with the density of the corresponding classical ground state, see Section 3.6 for the precise statement.

In a parallel work, Datta, Fröhlich and Fernández [20] have also derived convergent expansions for fermionic lattice systems, leading to results that are similar to ours. In contrast to our methods that are based on renormalization group ideas and the reduction to a contour model on a space-time lattice with a subsequent application of standard Pirogov-Sinai theory, they study directly the contour model emerging from the functional integral, extending Pirogov-Sinai theory to contour models with continuous time.

The organization of this paper is as follows. In the next section, we state our main result concerning the extended Hubbard model, Theorem 2.1. In Section 3, we define the general model and state our results in this case. Section 4 is devoted to the derivation of the contour representation of the model, paying particular attention to the factorization properties of the signs coming from the permutation of fermions. In Section 5 we proof exponential decay of contours and use these bound, together with standard cluster expansion methods, to prove the results of Section 3. Theorem 2.1 is proved in Section 6.

2. Statement of Results for the Extended Hubbard Model

For any even L we consider a finite box $\Lambda = \Lambda(L) = \{-L/2, \ldots, L/2 - 1\}^d$ with L^d points, the fermionic creation and annhilation operators $c^\dagger_{x,\sigma}$ and $c_{x,\sigma}$ ($x \in \Lambda$, $\sigma = \uparrow, \downarrow$), the corresponding Fock-space $\mathcal{H}_\Lambda$, the algebra $\mathcal{A}_\Lambda$ that is generated by even monominals in the creation and annhilation operators and the algebra of local observables, $\mathcal{A} = \cup \mathcal{A}_\Lambda$, where the union runs over all finite sets $\Lambda \subset \mathbb{Z}^d$.

Chosing periodic boundary conditions, we define the partition function at the

inverse temperature $\beta = 1/kT$ as

$$Z^{\beta}_{\mathrm{per},\Lambda} = \mathrm{Tr}\, \mathcal{H}_\Lambda e^{-\beta H_\Lambda}\,, \tag{2.1}$$

and the expectation value of an observable $\Psi \in \mathcal{A}_\Lambda$,

$$\langle \Psi \rangle^{\beta}_{\mathrm{per},\Lambda} = \frac{1}{Z^{\beta}_{\mathrm{per},\Lambda}} \mathrm{Tr}\, \mathcal{H}_\Lambda \Psi\, e^{-\beta H_\Lambda}\,. \tag{2.2}$$

Assuming for a moment that the corresponding limit exits for all local observables $\Psi \in \mathcal{A}$, we define the infinite volume Gibbs state

$$\langle \Psi \rangle^{\beta}_{\mathrm{per}} = \lim_{\Lambda \to \mathbb{Z}^d} \langle \Psi \rangle^{\beta}_{\mathrm{per},\Lambda}\,, \tag{2.3}$$

where the limit is taken along cubic boxes $\Lambda(L)$ of even side length L.[3]

Next, we define, for an arbitrary periodic state $\langle\cdot\rangle$ on $\mathcal{A}$, the density,

$$\rho = \lim_{\Lambda \to \infty} |\Lambda|^{-1} \sum_{x \in \Lambda} \langle n_x \rangle\,, \tag{2.4}$$

and the staggered density,

$$\Delta = \lim_{\Lambda \nearrow \infty} |\Lambda|^{-1} \sum_{x \in \Lambda} (-1)^x \langle n_x \rangle,\,. \tag{2.5}$$

Introducing, in addition to the number operators

$$\hat{n}_x = \hat{n}_{x,\uparrow} + \hat{n}_{x,\downarrow}\,, \quad \hat{n}_{x,\sigma} = c^\dagger_{x,\sigma} c_{x,\sigma}\,, \tag{2.6}$$

also the spin operators

$$S^3_x = \tfrac{1}{2}\big(\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow}\big)\,, \quad S^+_x = c^\dagger_{x,\uparrow} c_{x,\downarrow} \quad \text{and} \quad S^-_x = c^\dagger_{x,\downarrow} c_{x,\uparrow}\,. \tag{2.7}$$

our main theorem is:

Theorem 2.1. *For $d \geq 2$ there are constants $C_1 = C_1(d) < \infty$ and $C_2 = C_2(d) > 0$ such that, for $0 < \epsilon < W$, $\beta\epsilon > C_1$, $|t| < \epsilon C_2$ and all $(U,\mu) \in S^{(\epsilon)}_{\{0,2\}}$:*

i) The thermodynamic limit (2.3) *exists for all local observables $\Psi \in \mathcal{A}$. It is a convex combination,*

$$\langle\cdot\rangle^{\beta}_{\mathrm{per}} = \tfrac{1}{2}\langle\cdot\rangle^{\beta}_{\mathrm{even}} + \tfrac{1}{2}\langle\cdot\rangle^{\beta}_{\mathrm{odd}}\,, \tag{2.8}$$

of two pure states $\langle\cdot\rangle^{\beta}_{\mathrm{even}}$ and $\langle\cdot\rangle^{\beta}_{\mathrm{odd}}$ with charge density waves

$$\begin{aligned} \langle \hat{n}_x \rangle^{\beta}_{\mathrm{even}} &= \rho + (-1)^x \Delta\,, \qquad x \in \mathbb{Z}^d \\ \langle \hat{n}_x \rangle^{\beta}_{\mathrm{odd}} &= \rho - (-1)^x \Delta\,, \qquad x \in \mathbb{Z}^d\,, \end{aligned} \tag{2.9}$$

where $\Delta > 0$. Here $\Delta = \Delta_{\mathrm{even}} = -\Delta_{\mathrm{odd}}$ and $\rho = \rho_{\mathrm{even}} = \rho_{\mathrm{odd}}$ are given by (2.4) *and* (2.5).

[3] The existence of the limit (2.3) in the relevant region (1.4) is part of our results.

ii) For all $x \in \mathbb{Z}^d$, *and* $m =$ even *or* odd, $\langle \vec{S}_x \rangle_m^\beta = 0$.

iii) Let $t_x(\cdot)$ *be the translation by* $x \in \mathbb{Z}^d$, *and let* $\Psi, \Phi \in \mathcal{A}$ *be arbitrary local observables. Then, for* $m =$ even *or* odd, *and all* $x \in \mathbb{Z}^d$

$$\left| \langle \Psi \, t_x(\Phi) \rangle_m^\beta - \langle \Psi \rangle_m^\beta \langle t_x(\Phi) \rangle_m^\beta \right| \le C(\Psi, \Phi) e^{-|x|/\xi} \,. \tag{2.10}$$

Here $C(\Psi, \Phi) < \infty$ *and* $\xi < \infty$ *are constants.*

iv) At zero temperature, the compressibility $\partial\rho/\partial\mu$ *vanishes for all* $(U, \mu) \in S^{(\epsilon)}_{\{0,2\}}$.

Remarks.

i) By Statement iii), $\langle \cdot \rangle^\beta_{\rm even}$ and $\langle \cdot \rangle^\beta_{\rm odd}$ are pure phases.

ii) Statement ii) implies the absence of magnetic ordering in the phases $\langle \cdot \rangle^\beta_{\rm even}$ and $\langle \cdot \rangle^\beta_{\rm odd}$. Our methods can actually be extended to include non-zero magnetic fields, giving paramagnetism in the usual sense.

3. General Setting and Results

In this section, we state our results for a general class of fermionic models on $\mathbb{Z}^d$. We consider a finite index set $\Sigma = \{1, 2, \ldots, |\Sigma|\}$ labelling internal degrees of freedom, finite subsets $\Lambda \subset \mathbb{Z}^d$, fermionic creation and annhilation operators $c^\dagger_{x,\sigma}$ and $c_{x,\sigma}$ labelled by indices $\underline{x} = (x, \sigma) \in \underline{\Lambda} = \Lambda \times \Sigma$, the corresponding Fock-space $\mathcal{H}_\Lambda$, the algebra $\mathcal{A}_\Lambda$ that is generated by even monominals in the creation and annhilation operators, and the algebra of local observables, $\mathcal{A} = \cup \mathcal{A}_\Lambda$, where the union runs over all finite sets $\Lambda \subset \mathbb{Z}^d$. In order to define an occupation number basis in $\mathcal{H}_\Lambda$, we introduce an arbitrary total order on $\mathbb{Z}^d \times \Sigma$. We then define, for a classical configuration $\boldsymbol{n} : \mathbb{Z}^d \times \Sigma \to \{0, 1\}$: $(x, \sigma) \mapsto n_{x,\sigma}$, the vector $|\boldsymbol{n}\rangle_\Lambda$ as

$$|\boldsymbol{n}\rangle_\Lambda = \mathcal{P} \prod_{\underline{x} \in \underline{\Lambda}} (c^\dagger_{\underline{x}})^{n_{\underline{x}}} |0\rangle_\Lambda \,, \tag{3.1}$$

where $|0\rangle_\Lambda$ is the Fock vacuum in $\mathcal{H}_\Lambda$, and $\mathcal{P}$ denotes ordering with respect to the order on $\mathbb{Z}^d \times \Sigma$. Finally we define the projection operator onto the classical state $\boldsymbol{n}$ in a finite set $U \subset \mathbb{Z}^d$ as

$$P_U(\boldsymbol{n}) = \prod_{\underline{x} \in U \times \Sigma} P_{\underline{x}}(\boldsymbol{n}) \tag{3.2a}$$

where

$$P_{\underline{x}}(\boldsymbol{n}) = n_{\underline{x}}(c^\dagger_{\underline{x}} c_{\underline{x}}) + (1 - n_{\underline{x}})(1 - c^\dagger_{\underline{x}} c_{\underline{x}}) \tag{3.2b}$$

and U is a finite subset of $\mathbb{Z}^d$. Note that $P_U(\boldsymbol{n})$ is a local observable in $\mathcal{A}_\Lambda$ provided $U \subset \Lambda$.

We assume that the Hamiltonian H of the model is a sum of two terms,

$$H = H^{(0)} + \lambda H_Q \,, \tag{3.3}$$

where the "classical part" $H^{(0)}$ is diagonal in the occupation number basis and the "quantum part" H_Q is a sum of even monominals in the creation and annhilation operators. In order to prove the results of this paper, we will need several additional assumption on the classical and the quantum part of the Hamiltonian. We start with the assumptions on the classical part.

3.1. Assumptions on the classical model.

Since $H^{(0)}$ is diagonal in the occupation number basis, it defines a classical lattice gas with $|\Sigma|$ different species, occupation numbers $n_{x,\sigma}$ in $\{0,1\}$, configurations $\boldsymbol{n} : \mathbb{Z}^d \times \Sigma \to \{0,1\}$, $(x,\sigma) \mapsto n_{x,\sigma}$, and a suitable Hamilton function $H^{(0)}(\boldsymbol{n})$. We assume that this Hamilton function is given in terms of finite range, translation invariant interactions, depending on a vector parameter $\mu \in \mathcal{U}$, where $\mathcal{U}$ is an open subset of $\mathbb{R}^\nu$. Due to these assumptions, $H^{(0)}(\boldsymbol{n})$ can be written in the form

$$H^{(0)}(\boldsymbol{n}) = \sum_x \Phi_x(\boldsymbol{n}), \tag{3.4}$$

where $\Phi_x(\boldsymbol{n}) \in \mathbb{R}$ depends on $\boldsymbol{n}$ only via the occupation numbers $n_{y,\sigma}$ for which $\mathrm{dist}(x,y) \leq R_0$, where R_0 is a finite number. In our notation we supress the dependence of $H^{(0)}$ and Φ_x on μ.

As usually, a configuration $\boldsymbol{g}$ which minimizes the Hamiltonian (3.4) is called a ground state configuration. For the purpose of this paper, we will assume that the number of ground states of the Hamiltonian (3.4) is finite, and that all of them are periodic. More precisely, we will assume that there is a finite number of periodic configurations $\boldsymbol{g}^{(1)}, \ldots, \boldsymbol{g}^{(r)}$, with (specific) energies

$$e_m = e_m(\mu) = \lim_{\Lambda \to \mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \Phi_x(\boldsymbol{g}^{(m)}), \tag{3.5}$$

such that for each $\mu \in \mathcal{U}$, the set of ground states $G(\mu)$ is a subset of $\{\boldsymbol{g}^{(1)}, \ldots, \boldsymbol{g}^{(r)}\}$. Obviously, $G(\mu)$ is given by those configurations $\boldsymbol{g}^{(m)}$ for which $e_m(\mu)$ is equal to the "ground state energy"

$$e_0 = e_0(\mu) = \min_m e_m(\mu). \tag{3.6}$$

Note that we may assume, without loss of generality, that $\Phi_x(\boldsymbol{g}^{(m)})$ is independent of the point x for all ground state configurations $\boldsymbol{g}^{(m)}$, because this condition can always be achieved by averaging $\Phi_x(\boldsymbol{n})$ in (3.4) over the minimal common period L_0 of $\boldsymbol{g}^{(1)}, \ldots, \boldsymbol{g}^{(r)}$.

Our goal will be to prove that the low temperature phase diagram of the quantum model is a small perturbation of the classical ground state diagram provided the quantum perturbation is sufficiently small. In order to formulate and prove this statement, we need some assumptions on the structure of the ground state diagram. Here we assume that for some value of $\mu_0 \in \mathcal{U}$ all states in $\{\boldsymbol{g}^{(1)}, \ldots, \boldsymbol{g}^{(r)}\}$ are ground states,

$$e_m(\mu_0) = e_0(\mu_0) \qquad \text{for all} \qquad m = 1, \ldots, r, \tag{3.7}$$

that $e_m(\mu)$ are C^1 functions in $\mathcal{U}$, and that the matrix of derivatives

$$E = \Big(\frac{\partial e_m(\mu)}{\partial \mu_i} \Big) \tag{3.8}$$

has rank $r-1$ for all $\mu \in \mathcal{U}$, with uniform bounds on the inverse of the corresponding submatrices. We remark that this condition implies that the zero temperature phase diagram has the usual structure of a $\nu - (r-1)$ dimensional coexistence surface

S_0 where all states $\boldsymbol{g}^{(m)}$ are ground states, r different $\nu-(r-1)-1$ dimensional surfaces S_n ending in S_0 where all states but the state $\boldsymbol{g}^{(m)}$ are ground states, ...

Next, we formulate a suitable Peierls condition. Recalling that $\Phi_x(\boldsymbol{n})$ does not depend on $n_{y,\sigma}$ if $\mathrm{dist}(x,y) > R_o$, we define $U(x)$ as the minimal set of points y such that $\Phi_x(\boldsymbol{n})$ depends on $n_{y,\sigma}$.[4] We then introduce, for a given configuration $\boldsymbol{n}$, the notion of excited sites $x \in \mathbb{Z}^d$. We say that a site x is in the *state* $\boldsymbol{g}^{(m)}$ if the configuration $\boldsymbol{n}$ coincides with the configuration $\boldsymbol{g}^{(m)}$ on $U(x)$; a site is *excited*, if it is not in any of the states $\boldsymbol{g}^{(1)},\dots,\boldsymbol{g}^{(r)}$. Given this notation, the Peierls assumption used in this paper is that there exists a constant $\gamma_{\mathrm{cl}} > 0$, independent of μ, such that

$$\Phi_x(\boldsymbol{n}) \geq e_0(\mu) + \gamma_{\mathrm{cl}} \qquad \text{for all excited sites } x \text{ of all configurations } \boldsymbol{n}. \tag{3.9}$$

Finally, we assume that the derivatives of Φ_x are uniformly bounded in $\mathcal{U}$. More explicitely, we assume that there is a constant $C_0 < \infty$, such that

$$\Big|\frac{\partial}{\partial\mu_i}\Phi_x(\boldsymbol{n})\Big| \leq C_0 \tag{3.10}$$

for all $i = 1,\dots,\nu$, $\mu \in \mathcal{U}$, $x \in \mathbb{Z}^d$, and all configurations $\boldsymbol{n}$.

Remarks.

i) Given the assumptions stated in this subsection, standard Pirogov-Sinai theory implies that the low temperature phase diagram of the classical model has the same topological structure as the corresponding zero temperature phase diagram (see above).

ii) Let $\hat{n}_{\underline{x}}$ be the number operator $c^\dagger_{\underline{x}} c_{\underline{x}}$. Recalling that all these operators commute with each other, we define

$$H^{(0)}_x = \Phi_x(\hat{\boldsymbol{n}})\,. \tag{3.11}$$

With this definition, $H^{(0)}$ is the formal sum

$$H^{(0)} = \sum_x H^{(0)}_x\,. \tag{3.12}$$

3.2. Assumptions on the quantum perturbation.

We assume that H_Q is given in the form

$$H_Q = \sum_A t_A h_A \tag{3.13}$$

where the sum runs over sequences $A = (\tilde{a}_1,\dots,\tilde{a}_{2k})$ of labels $\tilde{a}_i = (a_i,\alpha_i,\epsilon_i) \in \mathbb{Z}^d \times \Sigma \times \{-1,1\}$, $t_A \in \mathbb{C}$ is a suitable hopping parameter, and

$$h_A = c(\tilde{a}_{2k})c(\tilde{a}_{2k-1})\dots c(\tilde{a}_1)\,, \tag{3.14a}$$

[4] If H is given as a sum of the form $\sum_M \phi_M$, where ϕ_M depends only on $n_{y,\sigma}$ with $y \in M$, then $U(x)$ is the union over all M such that $x \in M$.

with

$$c((a,\alpha,\epsilon)) = \begin{cases} c^\dagger_{a,\alpha} & \text{if} \quad \epsilon = +1 \\ c_{a,\alpha} & \text{if} \quad \epsilon = -1\,. \end{cases} \tag{3.14b}$$

It will be convenient to assume that the creation and annihilation operators in H_Q have been ordered in such a way that for each sequence $A = (\tilde{a}_1, \ldots, \tilde{a}_{2k})$ contributing to (3.13) there exists $\ell \in \{0, 1, \ldots, 2k\}$ such that
i) $\epsilon_i = -1$ for $1 \leq i \leq \ell$ and $\epsilon_i = +1$ for $i > \ell$, and
ii) with respect to the given order on $\mathbb{Z}^d \times \Sigma$ one has $(a_1, \alpha_1) < (a_2, \alpha_2) < \cdots < (a_\ell, \alpha_\ell)$, and $(a_{\ell+1}, \alpha_{\ell+1}) > (a_{\ell+2}, \alpha_{\ell+2}) > \cdots > (a_{2k}, \alpha_{2k})$.
In the sequel, we call such a sequence a *standard sequence* and write $\mathcal{A}_o$ for the set of all standard sequences.

Given the above representation of H_Q (we sometimes call it the standard form for H_Q), our assumptions on H_Q are now formulated in terms of the coefficients t_A. First, in order to assure that the quantum perturbation is selfadjoint, we assume that

$$\bar{t}_A = t_{A^\star}\,, \tag{3.15}$$

where the bar denotes complex conjugation, and $A^\star$ is the sequence

$$A^\star = (\tilde{a}^\star_{2k}, \ldots, \tilde{a}^\star_1)\,, \tag{3.16a}$$

with

$$(a,\alpha,\epsilon)^\star = (a,\alpha,-\epsilon)\,. \tag{3.16b}$$

Note that $A^\star$ is a standard sequence if and only if A is a standard sequence.

Next, we assume that the hopping parameters t_A are translation invariant, and that that t_A and its derivatives decays sufficiently fast in the support of the sequence A, defined as the minimal connected set containing A. To state this more precisely, for $A = (\tilde{a}_1, \ldots, \tilde{a}_{2k})$, we consider connected sets of bonds B that connect all points in $\{a_1, \cdots, a_{2k}\}$. Restricting ourselves to those of minimal size, we define B_0 as the first in some arbitrary (but fixed) lexiographic order, and define the *support*, $\operatorname{supp} A$, of A as the union of all points which are connected by this minimal set B_o. Note that by definition $\operatorname{supp} A$ depends only on the set $\{a_1, \cdots, a_{2k}\}$. As a consequence $\operatorname{supp} A = \operatorname{supp} A^\star$.

Introducing, for each $\gamma \geq 0$, the Sobolev norm

$$||\boldsymbol{t}||_\gamma = \sum_{A: x \in \operatorname{supp} A} \left(|t_A| + \sum_{i=1}^{\nu} \Big| \frac{\partial}{\partial \mu_i} t_A \Big| \right) e^{\gamma |\operatorname{supp} A|}\,, \tag{3.17}$$

our decay assumption for the quantum perturbation is the assumption that

$$||\boldsymbol{t}||_{\gamma_Q} < \infty \tag{3.18}$$

for a sufficiently large constant γ_Q.

Remarks.

i) For a finite range quantum perturbation, this assumption is obviously fulfilled for any $\gamma_Q < \infty$.

ii) If the quantum perturbation is of infinite range, we need that $|t_A|$ and $|\partial t_A / \partial \mu_i|$ decay exponentially fast in the size of the support of A. Assuming exponential decay with a sufficiently large decay constant γ, and observing that the number of connected sets B of size s that contain a given point $x \in \mathbb{Z}^d$ is bounded by $(2d)^{2s}$, while the number of standard sequences A with $\operatorname{supp} A = B$ is bounded by $2^{2|B||\Sigma|}$, the condition (3.18) can be satisfied provided $\gamma > \gamma_Q + 2\log(2d) + 2|\Sigma| \log 2$.

3.3. Finite volume states for the quantum system.

In order to discuss the phase diagram of the quantum spin system, we will consider suitable finite volume states $\langle\cdot\rangle^{\beta}_{q,\Lambda}$ which are analogues of the classical states with boundary condition q, with $q = 1, \dots, r$. Given a finite set $\Lambda \subset \mathbb{Z}^d$, we define $\hat{n}^{(q,\Lambda)}_{\underline{x}}$ as the number $g^{(q)}_{\underline{x}}$ if $x \in \Lambda^c = \mathbb{Z}^d \setminus \Lambda$, and as the operator $c^{\dagger}_{\underline{x}} c_{\underline{x}}$ if $x \in \Lambda$. With this definition, the operators

$$H^{(0)}_{q,x} = \Phi_x(\hat{\boldsymbol{n}}^{(q,\Lambda)}), \tag{3.19}$$

$$H^{(0)}_{q,\Lambda} = \sum_{x\in\Lambda} H^{(0)}_{q,x} \tag{3.20}$$

and

$$H_{q,\Lambda} = H^{(0)}_{q,\Lambda} + \lambda \sum_{A:\mathrm{supp}\, A\subset\Lambda} t_A h_A \tag{3.21}$$

are selfadjoint operators in $\mathcal{H}_\Lambda$ provided $\lambda \in \mathbb{R}$ (recall that the sets $\mathrm{supp}\, A$ have been chosen in such a way that $\mathrm{supp}\, A = \mathrm{supp}\, A^\star$).

Given the Hamiltonian with boundary conditions q, we introduce the quantum state $\langle\cdot\rangle^{\beta}_{q,\Lambda}$ by

$$\langle\Psi\rangle^{\beta}_{q,\Lambda} = \frac{1}{Z^{\beta}_{q,\Lambda}} \mathrm{Tr}\,_{\mathcal{H}_\Lambda}(\Psi\, e^{-\beta H_{q,\Lambda}}), \tag{3.22}$$

where

$$Z^{\beta}_{q,\Lambda} = \mathrm{Tr}\,_{\mathcal{H}_\Lambda} e^{-\beta H_{q,\Lambda}}. \tag{3.23}$$

We close this section with the definition of the support and norm of a local observable Ψ . Recalling that, by definition, any local observable Ψ is a finite sum of the form

$$\Psi = \sum_A \lambda^{\Psi}_A h_A, \tag{3.24}$$

where the h_A are even monominals in creation and annihilation operators (cf. (3.13)), we say that Ψ is given in its *standard form*, if all sequences contributing to (3.24) are standard sequences. Let now Ψ be a local observable, and let (3.24) be its standard form. Then the support of Ψ is defined as

$$\mathrm{supp}\,\Psi = \bigcup_{A:\lambda^{\Psi}_A\neq 0} \mathrm{supp}\, A, \tag{3.25}$$

and its norm as

$$||\Psi|| = \sum_{A\in\mathcal{A}_0} \left|\lambda^{\Psi}_A\right|. \tag{3.26}$$

3.4. Statement of results for non-zero temperatures.

In order to state our results in the form of a theorem we introduce, for each x in $\mathbb{Z}^d$ and any local obserbable $\Psi \in \mathcal{A}$, the corresponding translate $t_x(\Psi)$. Defining finally $\Lambda(L)$ as the box

$$\Lambda(L) = \Big\{ x \in \mathbb{Z}^d \;\Big|\; -\frac{L}{2} \le x_i < \frac{L}{2} \quad \text{for all} \quad i = 1, \dots, d \Big\}, \tag{3.27}$$

our main results are stated in the following two theorems.

Theorem 3.1. *Let $d \geq 2$ and let $H = H^{(0)} + \lambda H_Q$ be a Hamiltonian satisfying the assumptions of Section 3.1 and 3.2. Then there are constants $0 < \gamma_0 = \gamma_0(d, |\Sigma|) < \infty$ and $\alpha = \alpha(d, |\Sigma|) > 0$ such that for all $\gamma \geq \gamma_0$, all finite $\beta \geq \beta_0 = \gamma/\gamma_{\rm cl}$ and all $\lambda \in \mathbb{C}$ with*

$$|\lambda| \leq \lambda_0 := \frac{1}{2e\beta_0(\gamma)||\boldsymbol{t}||_\gamma} \tag{3.28}$$

there are functions $f_q(\mu, \beta)$, $q = 1, \ldots, r$, continuously differentible in μ, such that the following statements hold true whenever

$$a_q(\mu, \beta, \lambda) := \mathrm{Re}\, f_q(\mu, \beta) - \min_m \mathrm{Re}\, f_m(\mu, \beta) = 0\,. \tag{3.29}$$

i) The infinite volume free energy corresponding to $Z^\beta_{q,\Lambda(L)}$ exists and is equal to f_q:

$$f_q = -\frac{1}{\beta} \lim_{L\to\infty} \frac{1}{|\Lambda(L)|} \log Z^\beta_{q,\Lambda(L)}. \tag{3.30}$$

ii) The infinite volume limit

$$\langle \Psi \rangle^\beta_q = \lim_{L\to\infty} \langle \Psi \rangle^\beta_{q,\Lambda(L)} \tag{3.31}$$

exists for all local observables Ψ and has the same period as the corresponding classical ground state $\boldsymbol{g}^{(q)}$.

iii) For all local observables Ψ and Φ, there exists a constant $C_{\Psi,\Phi} < \infty$, such that

$$\big|\langle \Psi t_x(\Phi)\rangle^\beta_q - \langle \Psi\rangle^\beta_q \langle t_x(\Phi)\rangle^\beta_q\big| \leq C_{\Psi,\Phi} e^{-\alpha\gamma|x|}. \tag{3.32}$$

iv) The projection operators $P^{(m)}_x = P_{U(x)}(g^{(m)})$ onto the "classical states" $g^{(m)}_{U(x)}$ obey the bounds

$$\big|\langle P^{(m)}_x\rangle^\beta_q - \delta_{m,q}\big| < Ce^{-\gamma}\,, \tag{3.33}$$

where $C < \infty$ is a constant that depends only on d and $|\Sigma|$.

v) With $C < \infty$ as above, and C_0 as in (3.10), one has

$$|f_q(\mu, \beta) - e_q(\mu)| \leq Ce^{-\gamma} \tag{3.34a}$$

and

$$\Big|\frac{d}{d\mu_i}\big(f_q(\mu, \beta) - e_q(\mu)\big)\Big| \leq CC_0e^{-\gamma}\,. \tag{3.34b}$$

Remarks.

i) Following the usual terminology of Pirogov-Sinai theory, we call a phase with $a_q = 0$ *stable*. By (3.34b) and our assumptions on the derivative matrix (3.8), the matrix

$$F = \Big(\frac{\partial \mathrm{Re}\, f_m(\mu, \beta)}{\partial \mu_i}\Big) \tag{3.34}$$

has rank $r-1$, and the inverse of the corresponding submatrix is uniformly bounded in $\mathcal{U}$, provided γ is sufficiently large. By the inverse function theorem, statement v) of the Theorem therefore implies that the phase diagram of the quantum system has the same structure as the zero temperature phase diagram of the classical sytem,

with a $\nu-(r-1)$ dimensional coexistence surface $\tilde{S}_0$ where all states are stable, r different $\nu-(r-1)-1$ dimensional surfaces $\tilde{S}_n$ ending in $\tilde{S}_0$ where all states but the state m are stable, $\cdots$.

ii) Choosing β sufficiently large and λ sufficiently small, the bounds (3.33) can be made arbitrary sharp. In this sense, the quantum states $\langle\cdot\rangle_q$ are small perturbations of the corresponding classical state whenever q is stable.

iii) While Theorem 3.1 is stated (and proven) for general complex λ, the physical situation corresponds, of course, to real values of λ, as required by the self-adjointness of the Hamiltonian H. The "meta-stable free energies" f_q are real in this case[5], making the real part in (3.29) and (3.34) superfluous.

iv) As stated, Theorem 3.1 is only valid for $\beta<\infty$. Some care is needed when stating the corresponding results for zero temperature, since the thermodynamic limit and the limit of zero temperature, in general, do not commute. Theorem 3.1 *does* hold for zero temperature, if $f_q(\mu,\beta)$ is replaced by

$$f_q(\mu)=\lim_{\beta\to\infty} f_q(\mu,\beta) \tag{3.35}$$

and the equalities (3.30) and (3.31) are replaced by

$$f_q(\mu)=-\lim_{L\to\infty}\lim_{\beta\to\infty}\frac{1}{\beta|\Lambda(L)|}\log Z^\beta_{q,\Lambda(L)} \tag{3.30$'$}$$

and

$$\langle\Psi\rangle_q=\lim_{L\to\infty}\lim_{\beta\to\infty}\langle\Psi\rangle^\beta_{q,\Lambda(L)}\,. \tag{3.31$'$}$$

For a statement concerning the possibility to interchange the order of limits see Section 3.5 below.

In order to state the next theorem, we define states with periodic boundary conditons on $\Lambda(L)$. To this end, we consider the torus $\Lambda_{\rm per}(L)=\big(\mathbb{Z}/L\mathbb{Z}\big)^d$ and the corresponding Hamiltonian

$$H_{{\rm per},\Lambda(L)}=\sum_{x\in\Lambda_{\rm per}(L)}H^{(0)}_x+\lambda\sum_{A:\ \mathrm{supp}\,A\subset\Lambda_{\rm per}(L)}t_A h_A\,, \tag{3.36}$$

where the second sum goes over sequences A whose support $\mathrm{supp}\,A$ does not wind around the torus $\Lambda_{\rm per}(L)$. With these definitions, we then introduce the quantum state with periodic boundary conditions as

$$\langle\cdot\rangle^\beta_{{\rm per},\Lambda(L)}=\frac{1}{Z^\beta_{{\rm per},\Lambda(L)}}\mathrm{Tr}\,\mathcal{H}_{\Lambda(L)}(\cdot\,e^{-\beta H_{{\rm per},\Lambda(L)}}), \tag{3.37}$$

where

$$Z^\beta_{{\rm per},\Lambda(L)}=\mathrm{Tr}\,\mathcal{H}_{\Lambda(L)}e^{-\beta H_{{\rm per},\Lambda(L)}}. \tag{3.38}$$

[5]Given our constructions in Section 4 and 5, the proof of this fact is identical to the corresponding proof in [19].

Theorem 3.2. *Let $H^{(0)}$, H_Q, β and λ as in Theorem* 3.1*, and let L_0 be the smallest common period of the ground states $g^{(1)}$, ..., $g^{(r)}$. Assume in addition that λ is real. Then the infinite volume state with periodic boundary conditions,*

$$\langle\Psi\rangle^{\beta}_{\rm per} = \lim_{n\to\infty}\langle\Psi\rangle^{\beta}_{{\rm per},\Lambda(nL_0)} \tag{3.39}$$

exists for all local observables Ψ, and is a convex combination (with equal weights) of the stable states,

$$\langle\Psi\rangle^{\beta}_{\rm per} = \sum_{q\in Q}\frac{1}{|Q|}\langle\Psi\rangle^{\beta}_{q}\,, \tag{3.40}$$

with

$$Q = Q(\mu,\beta,\lambda) = \{q\in\{1,\dots,r\}\mid a_q(\mu,\beta,\lambda)=0\}\,. \tag{3.41}$$

Remark:. The statement of the theorem remains true if the sequence of volumes in (3.39) goes over volumes $\Lambda(L)$ with $L = nL_0(Q)$, where $L_0(Q)$ is the smallest common period of all *stable* ground states $g^{(q)}$, $q\in Q = Q(\mu,\beta,\lambda)$.

3.5. Quantum states at zero temperature.

As discussed in Remark iv) above, some care is needed when considering zero temperature states since the zero temperature limit $\beta\to\infty$ and the thermodynamic limit $\Lambda\to\mathbb{Z}^d$, in general, do not commute. In order to discuss this further, let us consider the modified partition function

$$Z^{\beta,{\rm np}}_{q,\Lambda} = \langle \boldsymbol{g}^{(q)}_{\Lambda}|\, e^{-\beta H_{q,\Lambda}}\,|\boldsymbol{g}^{(q)}_{\Lambda}\rangle\,, \tag{3.42}$$

where np indicates non-periodic boundary conditions. Namely, represented as a contour partition function on a suitable space-time lattice, see Section 4, the partition function $Z^{\beta,{\rm np}}_{q,\Lambda}$ is characterized by the boundary conditions $\boldsymbol{g}^{(q)}_{\Lambda}$ at times 0 and β, instead of the periodic b.c. in time corresponding to $Z^{\beta}_{q,\Lambda}$. As a consequence, $Z^{\beta}_{q,\Lambda}$ might contain contours wrapped around the lattice in time direction, while $Z^{\beta,{\rm np}}_{q,\Lambda}$ does not. Since these contours may force a state that is stable at zero temperature to be unstable at finite β, the cluster expansion for $\log Z^{\beta}_{q,\Lambda}$ might be divergent for arbitrary large β, even though the phase q becomes stable as $\beta\to\infty$.

This phenomen does not occur for $Z^{\beta,{\rm np}}_{q,\Lambda}$ that does not allow for the dangerous contours wrapped around the lattice in time direction. Therefore, the partition function $Z^{\beta,{\rm np}}_{q,\Lambda}$ can be analysed by the convergent expansion provided $\beta\geq\beta_0$ and q is stable for $\beta=\infty$. The same will be true for the modified expectation values

$$\langle\Psi\rangle^{\beta,{\rm np}}_{q,\Lambda} = \langle\Omega^{\beta}_{q,\Lambda}|\,\Psi\,|\Omega^{\beta}_{q,\Lambda}\rangle, \tag{3.43}$$

where

$$|\Omega^{\beta}_{q,\Lambda}\rangle = \frac{1}{\sqrt{Z^{\beta,{\rm np}}_{q,\Lambda}}}e^{-\frac{\beta}{2}H_{q,\Lambda}}\,|\boldsymbol{g}^{(q)}_{\Lambda}\rangle. \tag{3.44}$$

As a consequence, we obtain the following lemma.

Lemma 3.3. *Let $d \geq 2$ and let $H^{(0)}$, H_Q, α, γ, β_0, β and λ be as in Theorem* 3.1. *Let q be a phase with*

$$\lim_{\beta\to\infty} a_q(\mu,\beta,\lambda) = 0, \tag{3.45}$$

and let $\langle\cdot\rangle_q$ and $f_q(\mu)$ be as defined in (3.31′) *and* (3.30′). *Then*

$$\Big|\frac{1}{\beta|\Lambda|}\log Z^{\beta,\mathrm{np}}_{q,\Lambda} + f_q(\mu)\Big| \leq O\big(\frac{1}{\beta} + \frac{1}{\beta_0}\frac{|\partial\Lambda|}{|\Lambda|}\big), \tag{3.46}$$

and

$$\big|\langle\Psi\rangle^{\beta,\mathrm{np}}_{q,\Lambda} - \langle\Psi\rangle_q\big| \leq C_\Psi e^{-\alpha\gamma\min\{\beta/\beta_0,\mathrm{dist}(\mathrm{supp}\,\Psi,\partial\Lambda)\}}, \tag{3.47}$$

where $C_\Psi < \infty$ depends on d, $|\Sigma|$, the norm $||\Psi||$ of Ψ, and the size $|\,\mathrm{supp}\,\Psi|$ of the support of Ψ.

Remarks.
i) Lemma 3.3 implies, in particular, that the limits $\beta\to\infty$ and $\Lambda\to\mathbb{Z}^d$ commute for the modified partition function and expectation values (3.42) and (3.43).
ii) The statement (and the above consequence) of Lemma 3.3 remains true for the unmodified partition function and expectation values, $Z^\beta_{q,\Lambda}$ and $\langle\Psi\rangle^\beta_{q,\Lambda}$, if the phase q is stable for all $\tilde\beta$ in $[\beta,\infty]$, i.e. if $a_q(\mu,\tilde\beta,\lambda) = 0$ for all $\tilde\beta\in[\beta,\infty]$. In fact, the error term $O(\frac{1}{\beta})$ in (3.46) gets replaced by an error term $O(e^{-\beta/\beta_0})$ in this case.

3.6. Low temperature states and global symmetries.

In this section we consider the case in which the Hamiltonian $H_{q,\Lambda}$ commutes with some operator Q_Λ, which is extensive in the sense that

$$Q_\Lambda = \sum_{x\in\Lambda} Q_{x,\Lambda}, \tag{3.48}$$

where $Q_{x,\Lambda}$ are local observables in $\mathcal{A}_\Lambda$ for which $|\,\mathrm{supp}\,Q_{x,\Lambda}|$ and $\|Q_{x,\Lambda}\|$ is uniformly bounded in both x and Λ. A typical example would be the operator of total particle number

$$N_\Lambda = \sum_{\underline{x}\in\underline{\Lambda}} n_{\underline{x}}, \tag{3.49}$$

or the operator of the total number of particles of a given spin σ,

$$N_{\Lambda,\sigma} = \sum_{x\in\Lambda} n_{x,\sigma}. \tag{3.50}$$

In addition to the assumption that Q_Λ is a symmetry of the quantum system,

$$[H_{q,\Lambda}, Q_\Lambda] = 0, \tag{3.51}$$

we will assume that $|\boldsymbol{g}^{(q)}_\Lambda\rangle$ is an eigenstate of Q_Λ,

$$Q_\Lambda\,|\boldsymbol{g}^{(q)}_\Lambda\rangle = \rho^{(q)}_\Lambda|\Lambda|\,|\boldsymbol{g}^{(q)}_\Lambda\rangle, \tag{3.52}$$

and that the classical density $\rho^{(q)}_\Lambda$ has a limit as $\Lambda\to\infty$,

$$\rho^{(q)}_{\mathrm{class}} = \lim_{\Lambda\to\mathbb{Z}^\nu}\rho^{(q)}_\Lambda. \tag{3.53}$$

In the above examples, $\rho^{(q)}_{\text{class}}$ is the average density or the average density of particles with spin σ, respectively, in the classical state $|\boldsymbol{g}^{(q)}_\Lambda\rangle$. The following Theorem states that the "quantum density"

$$\rho^{(q)}_{\text{quant}}(\beta) = \lim_{\Lambda\to\mathbb{Z}^d} \frac{1}{|\Lambda|}\langle Q_\Lambda\rangle^\beta_q \tag{3.54}$$

approaches the classical density $\rho^{(q)}_{\text{class}}$ as $\beta\to\infty$.

Theorem 3.4. *Let $d\geq 2$, let $H^{(0)}$, H_Q, β_0, and λ_0 be as in Theorem* 3.1*., and let $|\lambda|\leq\lambda_0$. Assume that Q_Λ is an operator that is extensive in the sense described above, and that satisfies (3.51) through (3.53) for some q. Then there exist constants $C=C<\infty$ and $c>0$ such that*
i) If q is stable at $\beta=\infty$, i.e. if $\lim_{\beta\to\infty} a_q(\mu,\beta,\lambda)=0$, then

$$\rho^{(q)}_{\text{quant}} \equiv \lim_{\Lambda\to\mathbb{Z}^d}\frac{1}{|\Lambda|}\langle Q_\Lambda\rangle_q = \rho^{(q)}_{\text{class}}\,, \tag{3.55}$$

where $\langle\cdot\rangle_q$ is the zero temperature state defined in (3.31′).
ii) If $\tilde\beta_0\geq\beta_0$ and if q is stable for all $\beta\geq\tilde\beta_0$, then

$$\left|\rho^{(q)}_{\text{quant}}(\beta)-\rho^{(q)}_{\text{class}}\right|\leq Ce^{-\beta c}\,, \tag{3.56}$$

provided $\beta\geq\tilde\beta_0$.

Remark. For many models, the classical density $\rho^{(q)}_{\text{class}}$ is constant in some range of parameters μ. For these models, Theorem 3.4 implies that the compressibilities

$$\chi^{(i)} = \frac{\partial}{\partial\mu_i}\rho^{(q)}_{\text{quant}}(\beta) \tag{3.57}$$

vanish at zero temperature. An example of such a model is the extended Hubbard model in the staggered phase considered in Section 2.

4. Contour Representation

We consider a fixed finite volume $\Lambda=\Lambda(L)=\{x\in\mathbb{Z}^d \mid |x_i|\leq L \text{ for all } i=1,\dots,d\}$, and a fixed value $q\in\{1,\dots,r\}$ for the boundary condition; further, we are not explicitely specifying this in our notation.

Fixing an interger M to be determined later, and setting $\tilde\beta=\beta/M$, we introduce the transfer matrices

$$T^{(0)} = e^{-\tilde\beta H^{(0)}_{q,\Lambda}} \tag{4.1}$$

and

$$T = e^{-\tilde\beta H_{q,\Lambda}}\,, \tag{4.2}$$

and rewrite the partition function $Z_{q,\Lambda}$ as

$$Z_{q,\Lambda} = \operatorname{Tr}_{\mathcal{H}_\Lambda} T^M\,. \tag{4.3}$$

4.1. Duhamel Series and Path Integral Representation.

In a first step, we expand the transfer matrix T around the matrix $T^{(0)}$ using the Duhamel (or Dyson) series for the operator T (for a reference on the Duhamel series, see e.g. [25]). Introducing the family $\mathcal{A}_0$ of all sequences A contributing to (3.21), and, for each multiindex $\boldsymbol{m}\colon \mathcal{A}_0 \to \{0,1,\dots,\}$, the notation

$$|\boldsymbol{m}| = \sum_{A\in\mathcal{A}_0} m_A\,,$$

$$(-\lambda \boldsymbol{t})^{\boldsymbol{m}} = \prod_{A\in\mathcal{A}_0} (-\lambda t_A)^{m_A}\,,$$

$$\boldsymbol{m}! = \prod_{A\in\mathcal{A}_0} m_A!$$

and

$$\int d\boldsymbol{\tau}^{\boldsymbol{m}} = \prod_{A\in\mathcal{A}_0:m_A\neq 0} \int_0^{\tilde\beta} d\tau_A^1 \cdots \int_0^{\tilde\beta} d\tau_A^{m_A}\,,$$

the Duhamel series for the operator T can be written in the form

$$T = \sum_{\boldsymbol{m}} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}}}{\boldsymbol{m}!} \int d\boldsymbol{\tau}^{\boldsymbol{m}}\; T(\boldsymbol{\tau},\boldsymbol{m})\,. \tag{4.4}$$

Here the sum goes over multiindices $\boldsymbol{m}\colon \mathcal{A}_0 \to \{0,1,\dots,\}$, $\boldsymbol{\tau} = \{\tau_A^1,\dots,\tau_A^{m_A}, A\in\mathcal{A}_0\}$, and the operator $T(\boldsymbol{\tau},\boldsymbol{m})$ is obtained from $T^{(0)}$ by "inserting" the operator h_A at the times $\tau_A^1,\dots,\tau_A^{m_A}$, $A\in\mathcal{A}_0$. Formally, it can be defined as follows. For a given $\boldsymbol{m}$ and $\boldsymbol{\tau}$, let $\mathcal{A} = \{A_1,\dots,A_k\}$ be the set of all $A\in\mathcal{A}_0$ with $m_A\neq 0$, $m_i = m_{A_i}$, and $h_i = h_{A_i}$. Let

$$(s_1,\dots,s_{|\boldsymbol{m}|}) = \pi(\tau_{A_1}^1,\dots,\tau_{A_1}^{m_1},\dots,\tau_{A_k}^1,\dots,\tau_{A_k}^{m_k}) \tag{4.5}$$

be a permutation of the times $\boldsymbol{\tau}$ such that $s_1\le s_2\le\cdots\le s_{|\boldsymbol{m}|}$, and set

$$(\tilde h_1,\dots,\tilde h_{|\boldsymbol{m}|}) = \pi(h_1,\dots,h_1,\dots,h_k,\dots,h_k), \tag{4.6}$$

where on the right-hand side each h_i appears exactly m_i times. Then $T(\boldsymbol{\tau},\boldsymbol{m})$ is defined by

$$T(\boldsymbol{\tau},\boldsymbol{m}) = e^{-(\tilde\beta - s_{|\boldsymbol{m}|})H^{(0)}_{q,\Lambda}}\tilde h_{|\boldsymbol{m}|} e^{-(s_{|\boldsymbol{m}|}-s_{|\boldsymbol{m}|-1})H^{(0)}_{q,\Lambda}}\tilde h_{|\boldsymbol{m}|-1}\cdots \\ \cdots e^{-(s_2-s_1)H^{(0)}_{q,\Lambda}}\tilde h_1 e^{-s_1 H^{(0)}_{q,\Lambda}}\,. \tag{4.7}$$

For later reference, we also define the time ordered monminals

$$R(\boldsymbol{\tau},\boldsymbol{m}) = \tilde h_{|\boldsymbol{m}|}\tilde h_{|\boldsymbol{m}|-1}\dots\tilde h_1. \tag{4.8}$$

(Notice that, formally, $R(\boldsymbol{\tau},\boldsymbol{m}) \equiv T_{H^{(0)}\equiv 0}(\boldsymbol{\tau},\boldsymbol{m})$.)

Inserting the expansion (4.4) into (4.3), and using the occupation number basis (3.1) to express the trace as a sum of expectation values, we get

$$Z_{q,\Lambda} = \sum_{\boldsymbol{n}} \sum_{\boldsymbol{m}_1} \cdots \sum_{\boldsymbol{m}_M} \Big(\prod_{k=1}^{M} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \langle \boldsymbol{n}| \, T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle \,, \tag{4.9}$$

where $\boldsymbol{m}_k$, $k = 1, \ldots, M$ are multiindices $\boldsymbol{m}_k \colon \mathcal{A}_0 \to \{0, 1, \ldots, \} \colon A \mapsto m_{k,A}$ and $\boldsymbol{\tau}_k = \{\tau_{k,A}^1, \ldots, \tau_{k,A}^{m_{k,A}}, A \in \mathcal{A}_0\}$ are the corresponding integration variables.

Each term on the right hand side of (4.9) can be interpreted, in a standard manner, in terms of a classical path $\boldsymbol{n}(\cdot) \colon [0, \beta] \to \{0, 1\}^{\underline{\Lambda}}$ determined uniquely by the vector $|\boldsymbol{n}\rangle$ and sequences $(\boldsymbol{\tau}_1, \boldsymbol{m}_1), \ldots, (\boldsymbol{\tau}_M, \boldsymbol{m}_M)$. To get the assignement $\tau \mapsto \boldsymbol{n}(\tau)$ we start with the observation that an operator h_A applied to a vector of the form (3.1) yields either zero or again a vector of the form (3.1). Combined with the fact that $H_{q,\Lambda}^{(0)}$ is diagonal in the basis (3.1),

$$H_{q,\Lambda}^{(0)} |\boldsymbol{n}\rangle = \sum_{x \in \Lambda} \Phi_x(\boldsymbol{n}) \, |\boldsymbol{n}\rangle \,, \tag{4.10}$$

we infer that $T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ and $R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ are parallel vectors of $\mathcal{H}_\Lambda$ and that $\langle \boldsymbol{n}| \, T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ is non zero if and only if $\langle \boldsymbol{n}| \, R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ does not vanish. The classical path $\boldsymbol{n}(\cdot)$ is now obtained in the standard way. Starting from $\boldsymbol{n}(0) = \boldsymbol{n}$, $\boldsymbol{n}(\tau)$ is piecewise constant, with a jump whenever

$$\tau = (k-1)\tilde{\beta} + \tau_{k,A}^i \tag{4.11}$$

for some $k \in \{1, \ldots, M\}$, $A \in \mathcal{A}_0$, and $i \in \{1, \ldots, m_{k,A}\}$. At these times, $n(\cdot)$ jumps from $\boldsymbol{n}(\tau)$ to $\boldsymbol{n}(\tau + 0)$ defined by

$$|\boldsymbol{n}(\tau + 0)\rangle := h_{A(\tau)} |\boldsymbol{n}(\tau)\rangle \,, \tag{4.12}$$

with $A(\tau)$ implicitely defined by (4.11). Note that $\boldsymbol{n}(\tau + 0)$ is not defined if the right hand side of (4.12) is zero. It is easy to see, however, that the corresponding terms do not contribute to the right hand side of (4.9), since the matrix elements $\langle \boldsymbol{n}| \, R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ and $\langle \boldsymbol{n}| \, T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ vanish in this case. In a similar way, paths with $\boldsymbol{n}(\beta) \neq \boldsymbol{n}(0) \equiv \boldsymbol{n}$ do not contribute to (4.9). Note also that there may be several values for A, k and i which fulfill (4.11). Since such "events" have measure zero in the integration on the right hand side of (4.9), we may assume, without loss of generality, that this does not happen. Given the above construction and the definition (4.8) of the matrix $T(\boldsymbol{\tau}, \boldsymbol{m})$, one immediately gets the following explicit formula for the vector $T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$ in terms of $R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle$. Namely,

$$\begin{aligned} &T(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots T(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle = \\ &\qquad = \exp\Big\{ - \sum_{x \in \Lambda} \int_0^\beta \Phi_x(\boldsymbol{n}(\tau)) d\tau \Big\} R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle \,. \end{aligned} \tag{4.13}$$

Inserting the equality (4.13) into (4.9), and introducing the symbol $S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\})$ for the "sign"

$$S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}) = \langle \boldsymbol{n}| R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \, |\boldsymbol{n}\rangle \,, \tag{4.14}$$

we obtain the representation

$$Z_{q,\Lambda} = \sum_{\boldsymbol{n}} \sum_{\{\boldsymbol{m}_k\}} \Big(\prod_{k=1}^{M} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \exp\Big\{ - \sum_{x \in \Lambda} \int_0^\beta \Phi_x(\boldsymbol{n}(\tau)) d\tau \Big\} \times \\ \times S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}) \,, \quad (4.15)$$

where the second sum stands for the M sums over $\boldsymbol{m}_1, \dots, \boldsymbol{m}_M$.

Remarks.

i) Note that for x near to the boundary, the value of $\Phi_x(\boldsymbol{n}(\tau))$ depends on the configuration outside Λ, which we assumed to be the ground state configuration $\boldsymbol{g}^{(q)}$ by assuming boundary conditions q. We suppress this dependence in our notation.

ii) As discussed above, configurations $\{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ only contribute to the partition function $Z_{q,\Lambda}$ if they correspond to a classical configuration $\boldsymbol{n}(\cdot)$ with $\boldsymbol{n}(0) = \boldsymbol{n}(\beta)$. To make this condition more explicit, it is convenient to consider time ordered monominals $M_{\underline{x}}(\boldsymbol{\tau}, \boldsymbol{n})$ which are obtained from $R(\boldsymbol{\tau}, \boldsymbol{n})$ by leaving out all creation and annhilation operators $c_{\underline{y}}^\dagger$ and $c_{\underline{y}}$ with $\underline{y} \neq \underline{x}$. A configuration $\{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ then contributes to the partition function $Z_{q,\Lambda}$ if and only if, for each $\underline{x}$, the monominals $M_{\underline{x}}(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots M_{\underline{x}}(\boldsymbol{\tau}_1, \boldsymbol{m}_1)$ are of the form $c_{\underline{x}}^\dagger c_{\underline{x}} c_{\underline{x}}^\dagger \cdots c_{\underline{x}}$ if $n_{\underline{x}} = 1$, and of the form $c_{\underline{x}} c_{\underline{x}}^\dagger c_{\underline{x}} \cdots c_{\underline{x}}^\dagger$ if $n_{\underline{x}} = 0$.

4.2. Ground State Cells, Excited Cells and Contours.

In order to define contours, we introduce a suitable space time lattice, the notion of an elementary cell, and the definition of ground state cells and excited cells. We define the lattices

$$\mathbb{L} = \mathbb{Z}^d \times \tilde{\beta}\{0, \dots, M\}_{\rm per} \quad (4.16a)$$

and

$$\mathbb{L}_\Lambda = \Lambda \times \tilde{\beta}\{0, \dots, M\}_{\rm per} \,, \quad (4.16b)$$

where the index "per" stands for the identification of $(x, 0)$ and $(x, M\tilde{\beta}) = (x, \beta)$, and the continuum tori

$$\mathbb{T} = \mathbb{R}^d \times [0, \beta]_{\rm per} \quad (4.17a)$$

and

$$\mathbb{T}_\Lambda = \{y \in \mathbb{R}^d \mid {\rm dist}(y, \Lambda) \leq \tfrac{1}{2}\} \times [0, \beta]_{\rm per} \,, \quad (4.17b)$$

again with periodic boundary conditions in the "time direction".

An *elementary cell* $C(x, k)$, labbeled by an index $(x, k) \in \mathbb{Z}^d \times \{1, \dots, M\}$ (we identify 0 and M), is now defined as the set

$$C(x, k) = \{y \in \mathbb{R}^d \mid {\rm dist}(y, x) \leq \tfrac{1}{2}\} \times \tilde{\beta}[k-1, k] \,. \quad (4.18)$$

Given a "configuration" $\omega = \{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ contributing to the right hand side of (4.15), we distinguish between elementary cells $C(x, k)$ with constant occupation numbers $n_{x,\sigma}(\tau)$, and those which are "visited" by a hopping term h_A. We define an elementary cell $C(x, k) \subset \mathbb{T}_\Lambda$ to be a *quantum cell*, if $x \in {\rm supp}\, \boldsymbol{m}_k$, where ${\rm supp}\, \boldsymbol{m}_k := \bigcup_{A: m_{k,A} \neq 0} {\rm supp}\, A$, and to be a *classical cell* if $x \notin {\rm supp}\, \boldsymbol{m}_k$. Note that with this definition, the occupation number $n_{x,\sigma}(\tau)$ is constant inside classical cells, so that $n_{x,\sigma}(\tau) = n_{x,\sigma}(k\tilde{\beta}) =: n_\sigma(C(x, k))$ if $C(x, k)$ is a classical cell and

$(k-1)\tilde{\beta} \leq \tau \leq k\tilde{\beta}$. We say that a cell $C(x,k)$ is in the *ground state* m, if all cells $C(y,k)$ with $y \in U(x)$ are classical cells, and $n_\sigma(C(y,k)) = g^{(m)}_{y,\sigma}$. A cell which is not in a ground state is called an *excited cell*, and the set of excited cells corresponding to the configuration ω is denoted by $D = D(\omega)$.

At this point, the definion of contours is standard. One defines a (labeled) contour Y as a pair $(\operatorname{supp} Y, \alpha)$, where $\operatorname{supp} Y \subset \mathbb{T}$ is a finite, connected union of elementary cells, while α is an asignment of labels $\alpha(F)$ to faces of $\partial \operatorname{supp} Y$ which is constant on the boundary of all connected components of $\mathbb{T} \setminus \operatorname{supp} Y$.

The contours $Y_1, \ldots, Y_n$ corresponding to a configuration $\omega = \{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ are then defined by taking the connected components of the set D of excited cells in $\mathbb{T}_\Lambda$ for their supports $\operatorname{supp} Y_1, \ldots, \operatorname{supp} Y_n$ and by taking the labels m of the ground states for the elementary cells C that touch the face F, see above, for the corresponding labels $\alpha_i(F)$. The ground state regions V_m, $m = 1, \ldots, r$, corresponding to ω, on the other hand, are defined as the union of all elementary cells that are in the ground state m.

Note that for each configuration $\omega = \{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ contributing to (4.15), the set of contours corresponding to ω is a set of mutually compatible contours with matching labels and external boundary condition q. Here, as usually, two contours Y and Y' are called *compatible* whenever $\operatorname{supp} Y \cap \operatorname{supp} Y' = \emptyset$, a set $\{Y_1, \ldots, Y_n\}$ of pairwise compatible contours is called a *set with matching labels*, if the labels $\alpha(F)$ of the contours $Y_1, \ldots, Y_n$ are constant on the boundary of each component of $\mathbb{T} \setminus (\operatorname{supp} Y_1 \cap \cdots \cap \operatorname{supp} Y_n)$, and a set of mutually compatible contours with matching labels is said to have *external boundary condition* q if these labels take the value q on the boundary of the infinite component of $\mathbb{T} \setminus (\operatorname{supp} Y_1 \cap \cdots \cap \operatorname{supp} Y_n)$.

Note also that, by our definition of ground state cells, the function $\Phi_x(\boldsymbol{n}(\tau))$ in the exponent in (4.15) is constant and equal to e_m for all (x,τ) in the ground state region V_m. As a consequence, the contribution of the ground state region V_m to the exponent in (4.15) is $-\tilde{\beta}|V_m|e_m$, where $|V_m|$ is the number of elementary cells in V_m.

In a final step, we now sum (and integrate) over all configurations leading to the same set of contours $\{Y_1, \ldots, Y_n\}$. Extracting further the factor $e^{-\sum_m \tilde{\beta} e_m |V_m|}$ for the classical energy of the ground state regions, $\cup_m V_m = \mathbb{T}_\Lambda \setminus (\operatorname{supp} Y_1 \cap \cdots \cap \operatorname{supp} Y_n)$, and denoting the numerical value of the sum over the remaining factors by $\rho(Y_1, \ldots, Y_n)$, we obtain the contour representation

$$Z_{q,\Lambda} = \sum_{\{Y_1,\ldots,Y_n\}} e^{-\sum_m \tilde{\beta}|V_m|e_m} \rho(Y_1, \ldots, Y_n)\,, \tag{4.19}$$

where the sum goes over all sets of mutually compatible contours with matching labels, external boundary condition q, and support $\operatorname{supp} Y_i \subset \mathbb{T}_\Lambda$. Note that the external boundary condition q refers to the set $\{Y_1, \ldots, Y_n\}$, not to the individual contours $Y \in \{Y_1, \ldots, Y_n\}$.

Our goal, now, is to show that it is possible to define contour activities $\rho(Y)$ so that

$$\rho(Y_1, \ldots, Y_n) = \prod_{i=1}^{n} \rho(Y_i)\,, \tag{4.20}$$

and hence

$$Z_{q,\Lambda} = \sum_{\{Y_1,\ldots,Y_n\}} e^{-\sum_m \tilde{\beta}|V_m|e_m} \prod_{i=1}^{n} \rho(Y_i)\,. \tag{4.21}$$

Given this representation, the partition function can then be analysed using a slightly modified version [19] of standard Pirogov-Sinai theory, provided $\rho(Y)$ is decaying sufficiently fast in the size of Y (which will be easy to show, see Section 5).

4.3. Factorization of the contour activities.

In this subsection we prove the factorization (4.20). Let us first introduce the notation $\omega(V)$ for a configuration living on a set $V \subset \mathbb{T}_\Lambda$; namely, such a configuration is given by $\omega(V) = \{\boldsymbol{n}(V), \{\boldsymbol{\tau}_k(V), \boldsymbol{m}_k(V)\}\}$ with $\boldsymbol{n}(V) = \{n_{\underline{x}}, C(x,1) \subset V\}$, $\boldsymbol{m}_k(V) = \{m_{k,A}; \cup_{x \in \mathrm{supp}\, A} C(x,k) \subset V\}$, $\boldsymbol{\tau}_k(V) = \{\boldsymbol{\tau}^i_{k,A}; \cup_{x \in \mathrm{supp}\, A} C(x,k) \subset V\}$. Inspecting now the mapping $\omega \mapsto \{Y_1, \dots, Y_n\}$ assigning a set of mutually compatible contours to a configuration $\omega = \{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ contributing to $Z_{q,\Lambda}$ (see Remark ii) after (4.15) for an explicit condition), we define the indicator function $\chi_{Y_1,\dots,Y_n}(\omega)$ to be 1 if $Y_1, \dots, Y_n$ are the contours corresponding to ω and to be 0 otherwise. Note that this definition implicitely gives $\chi_{Y_1,\dots,Y_n}(\omega) = 0$ if ω does not contribute to $Z_{q,\Lambda}$, since such a configuration does not correspond to a classcial path $\boldsymbol{n}(\tau)$ and hence not to *any* assignment of contours.

The indicator function $\chi_{Y_1,\dots,Y_n}(\omega)$ can now be decomposed into a product

$$\chi_{Y_1,\dots,Y_n}(\omega) = \prod_m \chi_m(\omega(V_m)) \prod_{i=1}^n \chi_{Y_i}(\omega(\mathrm{supp}\, Y_i)). \tag{4.22}$$

Here $\omega(V_m)$ and $\omega(\mathrm{supp}\, Y_i)$ are the corresponding restrictions of the configuration ω. The function $\chi_m(\omega(V_m))$ indicates that $\boldsymbol{m}_k(V_m) = 0$ for all k and $n_{\underline{x}} = g^{(m)}_{\underline{x}}$ for all x such that $C(x,1) \subset V_m$. Given a contour Y and extending the configuration $\omega(\mathrm{supp}\, Y)$ by putting $\boldsymbol{m}_k(\mathbb{T}_\Lambda \setminus \mathrm{supp}\, Y) = 0$ and fixing $n_{\underline{x}} = g^{(m)}_{\underline{x}}$ for every cell $C(x,1) \cap \mathrm{supp}\, Y = \emptyset$ contained in the component of $\mathbb{T}_\Lambda \setminus \mathrm{supp}\, Y$ whose boundary is labeled by $\alpha = m$, the function $\chi_Y(\omega(\mathrm{supp}\, Y))$ indicates that Y is the only contour of this extension of $\omega(\mathrm{supp}\, Y)$. Note that the conditions according to Remark ii) after (4.15) are fullfilled for ω if and only if they are fullfilled for the extension of $\omega(\mathrm{supp}\, Y)$, for all contours Y corresponding to ω, a condition that is, in turn, again implicit in $\chi_Y(\omega(\mathrm{supp}\, Y))$.

Next, we introduce the classical energy $\tilde\beta E(\omega(\mathrm{supp}\, Y))$ of a contour Y:

$$\tilde\beta E(\omega(\mathrm{supp}\, Y)) = \sum_{k=1}^M \sum_{x: C(x,k) \subset \mathrm{supp}\, Y} \int_{(k-1)\tilde\beta}^{k\tilde\beta} \Phi_x(\boldsymbol{n}_Y(\tau))\, d\tau\,, \tag{4.23}$$

where $\boldsymbol{n}_Y(\cdot)$ is the classical path obtained from the above extension of $\omega(\mathrm{supp}\, Y)$ to $\mathbb{T}_\Lambda$. With these notations,

$$\rho(Y_1, \dots, Y_n) = \sum_{\boldsymbol{n}} \sum_{\{\boldsymbol{m}_k\}} \Big(\prod_{k=1}^M \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \chi_{Y_1,\dots,Y_n}(\omega) \times \\ \times S(\omega) \prod_{i=1}^n e^{-\tilde\beta E(\omega(\mathrm{supp}\, Y_i))}\,, \tag{4.24}$$

where $\omega = \{\boldsymbol{n}, \{\tau_k, \boldsymbol{m}_k\}\}$, and $S(\omega) = S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\})$ is given by (4.14).

Thus to prove the factorization (4.20), it remains to show the factorization for the sign $S(\omega)$. Our task is to introduce signs $S(\omega(\operatorname{supp} Y)) \in \{-1, 1\}$ so that, for a configuration ω with contours $\{Y_1, \dots, Y_n\}$, one has

$$S(\omega) = \prod_{i=1}^{n} S(\omega(\operatorname{supp} Y_i)) \,. \tag{4.25}$$

We need some notation. As ususal, the interior $\operatorname{Int} Y$ of a contour $Y = (\operatorname{supp} Y, \alpha)$ is defined as the union of all finite[6] components C of $\mathbb{T} \setminus \operatorname{supp} Y$, while the exterior $\operatorname{Ext} Y$ is defined as the infinite component of $\mathbb{T} \setminus \operatorname{supp} Y$. One says that Y is a contour with external boundary condition q, or shorter: a q-contour, if $\alpha(F) = q$ for all faces F in the boundary of $\operatorname{Ext} Y$, and one defines $\operatorname{Int}_m Y$ as the union of all components C of $\operatorname{Int} Y$ such that $\alpha\big|_{\partial C} = m$. Finally, $V(Y)$ is defined as $\operatorname{supp} Y \cup \operatorname{Int} Y$.

We now proceed by determining the signs of contours one by one, starting from the most inner ones, "erasing" them simultaneously from the configuration ω. Let thus Y_i be a contour with external boundary condition q_i, such that there is no contour Y_j, $j \neq i$, with $\operatorname{supp} Y_j \subset \operatorname{Int} Y_i$. Consider the configuration $\tilde{\omega}$ obtained by extending the configuration $\omega(\mathbb{T}_\Lambda \setminus V(Y_i))$ by taking $\tilde{\boldsymbol{m}}_k(V(Y_i)) = 0$ and $\tilde{n}_{\underline{x}} = g_{\underline{x}}^{(q_i)}$ for all x such that $C(x, 1) \subset V(Y_i)$. We will now introduce the sign $S(\omega(\operatorname{supp} Y_i))$ (independently of the configuration $\omega(\mathbb{T}_\Lambda \setminus V(Y_i))$) in such a way that

$$S(\omega) = S(\omega(\operatorname{supp} Y_i)) S(\tilde{\omega}) \tag{4.26}$$

with $S(\tilde{\omega})$ defined from the configuration $\tilde{\omega}$ by (4.14). Iterating the erasure procedure and formula (4.26), we get a final configuration with no contours and sign $+1$, establishing thus the equality (4.25).

To determine the sign $S(\omega(\operatorname{supp} Y_i))$, we begin by considering for each $x \in \Lambda$ the intersection $I(x)$ of the line $\{x\} \times [0, \beta]_{\mathrm{per}}$ with $V(Y_i)$, $I(x) = (\{x\} \times [0, \beta]_{\mathrm{per}}) \cap V(Y_i)$. If nonempty, the set $I(x)$ is either a union of disjoint intervals $I(x) = \cup_l [k_l^-, k_l^+]$ or $I(x) = [0, \beta]_{\mathrm{per}}$. In the former case ($I(x) \neq [0, \beta]_{\mathrm{per}}$), we use the fact that all boundary cells of $V(Y_i)$ are classic cells with the same ground state $\boldsymbol{g}^{(m)}$ and thus the path $\boldsymbol{n}(\tau)$ (corresponding to ω for which $\chi_Y(\omega(\operatorname{supp} Y_i)) \neq 0$) necessarily attains the values $n_{\underline{x}}(\tau = k_l^-) = n_{\underline{x}}(\tau = k_l^+) = g_{\underline{x}}^{(m)}$. Assuming for a moment that the interval (k_l^-, k_l^+) does not contain the time $\tau = 0$, let us consider the product

$$\tilde{h}_a \cdots \tilde{h}_b \tag{4.27}$$

consisting of those terms h_A in the product $\prod R(\boldsymbol{\tau}_k, \boldsymbol{m}_k)$ for which the times $\tau_{k,A}^i$ fall into the interval (k_l^-, k_l^+). If the corresponding term is to be nonvanishing (i. e. if $\chi_Y(\omega(\operatorname{supp} Y_i)) \neq 0$), there must be in (4.27) the same number of creation and annihilation operators $c_{\underline{x}}^+$ and $c_{\underline{x}}$. Commuting them through all remaining terms until they mutually annihilate, we produce a sign $s_{\underline{x},l}(\omega(\operatorname{supp} Y_i))$. Notice that this sign does not depend on the configuration $\omega(\mathbb{T}_\Lambda \setminus \operatorname{supp} Y_i)$, since if (4.27) contains a term h_A corresponding to any other contour, then necessarily $x \notin \operatorname{supp} A$ and, since A is a product of an even number of creation and annihilation operators, the

[6] In the sense that C is a finite union of unit cells.

operator $c^+_{\underline{x}}$ (resp. $c_{\underline{x}}$) commutes with such h_A producing no additional sign. If the interval (k_l^-, k_l^+) contains the time $\tau = 0$, we consider separately the product of the form (4.27) for the interval $(k_l^-, 0)$, and that for the interval $(0, k_l^+)$. We then commute all creation and annihilation operators $c^+_{\underline{x}}$ and $c_{\underline{x}}$ that correspond to times in $(k_l^-, 0)$ with the remaining operators in the product (4.27) until they hit time zero, and similarly for those in $(0, k_l^+)$. After annihilating all pairs, we will be left with monomials R_+ and R_- in the operators $c^+_{\underline{x}}$ and $c_{\underline{x}}$, such that

$$R_+ \, |\boldsymbol{n}\rangle\langle\boldsymbol{n}| \, R_- = \, |\tilde{\boldsymbol{n}}^{(x)}\rangle\langle\tilde{\boldsymbol{n}}^{(x)}| \,, \tag{4.28}$$

where $\tilde{\boldsymbol{n}}^{(x)}$ is obtained from $\boldsymbol{n}$ by substituting $\tilde{n}_{\underline{x}} = g^{(m)}_{\underline{x}}$ for $n_{\underline{x}}$. Combining the steps described so far, we get a sign $s_{\underline{x}}(\omega(\operatorname{supp} Y_i)) = \prod_l s_{\underline{x},l}(\omega(\operatorname{supp} Y_i))$ and the new state $\tilde{\boldsymbol{n}}^{(x)}$ at $\tau = 0$, with $\tilde{n}_{\underline{x}} = g^{(m)}_{\underline{x}}$, as required by our definition of $\tilde{\omega}$.

If $I(x) = [0, \beta]_{\rm per}$, then the values $n_{\underline{x}}(\tau = 0) = n_{\underline{x}}(\tau = \beta) = n_{\underline{x}}$ and we can reason in a similar fashion as in the first case above. Then *all* operators $c^+_{\underline{x}}$ and $c_{\underline{x}}$ are annihilated after the commutations are performed yielding the sign $s_{\underline{x}}(\omega(\operatorname{supp} Y_i))$, without any change in the state $\boldsymbol{n}$ at time $\tau = 0$. Since all operators $c^+_{\underline{x}}$ and $c_{\underline{x}}$ corresponding to the concerned x have been cancelled, the value of $S(\tilde{\omega})$ does not depend on the state $n_{\underline{x}}$ and we may replace it, without any additional change in sign, by $\tilde{n}_{\underline{x}} = g^{(m)}_{\underline{x}}$.

Iterating the above procedure for all $\underline{x}$ (chosen in a fixed (say, lexicographic) order) such that $I(x)$ is nonempty, we pass to the configuration $\tilde{\omega}$ and produce the sign $S(\omega(\operatorname{supp} Y_i)) = \prod_{\underline{x}} s_{\underline{x}}(\omega(\operatorname{supp} Y_i))$.

5. Exponential Decay of Contour Activities, Proof of Theorems 3.1–3.4

5.1. Bound on the contour activities $\rho(Y)$.

Given the contour representation (4.21), the proof of Theorems 3.1 and 3.2 is an easy exercise in Pirogov-Sinai theory, once a suitable bound on the weights $\rho(Y)$ is established. This is done in this subsection.

Proposition 5.1. *Let $\lambda \in \mathbb{R}$, $\tilde{\beta} > 0$, and $\gamma_Q \geq 1$ be such that*

$$(e-1)\tilde{\beta}|\lambda|\|t\|_{\gamma_Q} \leq 1. \tag{5.1}$$

Then

$$|\rho(Y)| \leq e^{-(\tilde{\beta}e_0 + \tilde{\gamma})|\operatorname{supp} Y|} \tag{5.2}$$

where

$$\tilde{\gamma} = \min\{\tilde{\beta}\gamma_{\rm cl}, \gamma_Q - 1\} - (1 + |\Sigma|)\log 2. \tag{5.3}$$

Proof. Since $|S(\omega)| = 1$, we get from (4.24) (for $n = 1$) the bound

$$|\rho(Y)| \leq e^{-\tilde{\beta}e_0|\operatorname{supp} Y|} 2^{|\Sigma||\operatorname{supp} Y|} \times$$
$$\times \sum_{X \subset \operatorname{supp} Y} \sum_{\substack{\{\boldsymbol{m}_k\} \\ \cup_k \operatorname{supp} \boldsymbol{m}_k = X}} \Big(\prod_{k=1}^{M} \frac{(|\lambda||\boldsymbol{t}|)^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \tilde{\beta}^{|\boldsymbol{m}_k|} \Big) e^{-\tilde{\beta}\gamma_{\rm cl}|\operatorname{supp} Y \setminus X|}. \tag{5.4}$$

The second sum is over all unions X of unit cells in $\operatorname{supp} Y$ (corresponding to the quantum cells on the right hand side of (4.24)) . The factor $2^{|\Sigma||\operatorname{supp} Y|}$ comes from the sum over occupation numbers $\boldsymbol{n}$, observing that, for a q-contour Y, the occupation numbers are fixed, $n_{x,\sigma} = g^{(q)}_{x,\sigma}$, whenever $C(x,1)\cap\operatorname{supp} Y \neq \emptyset$, and the last factor in (5.4) comes from the fact that all cells in $\operatorname{supp} Y$ that are not quantum cells must be classically excited. In a similar manner as in [19], we use the bound

$$\sum_{m_{k,A}=1}^{\infty} \frac{(|\lambda|\tilde{\beta}|t_A|)^{m_{k,A}}}{m_{k,A}!} \leq (e-1)|\lambda|\tilde{\beta}|t_A|, \tag{5.5}$$

valid whenever $|\lambda|\tilde{\beta}|t_A| \leq 1$, to get

$$|\rho(Y)| \leq e^{-\tilde{\beta}e_0|\operatorname{supp} Y|} 2^{|\Sigma||\operatorname{supp} Y|} \times \\ \times \sum_{X\subset\operatorname{supp} Y} e^{-\tilde{\beta}\gamma_{\mathrm{cl}}|\operatorname{supp} Y\setminus X|} \prod_k \Big(\sum_{\mathcal{B}_k} \prod_{A\in\mathcal{B}_k} (e-1)|\lambda|\tilde{\beta}|t_A|\Big). \tag{5.6}$$

The $\sum_{\mathcal{B}_k}$ is over all finite collections $\mathcal{B}_k \subset \mathcal{A}_0$ such that $\cup_{A\in\mathcal{B}_k} A = X_k$, where, for a fixed $k \in \{1,\dots,M\}$, the set X_k is the union of all unit cells $C(x,k)$ contained in X. Using now (5.1) we get the bound

$$\sum_{\substack{\mathcal{B}_k=\{A_1,\dots,A_\ell\} \\ \cup A_i = X_k}} \prod_{A_i\in\mathcal{B}_k} (e-1)|\lambda|\tilde{\beta}|t_{A_i}| \leq \\ \leq e^{-\tilde{\gamma}_Q|X_k|} \sum_{\ell=1}^{\infty} \frac{1}{\ell!} \prod_{i=1}^{\ell} \Big(\sum_{\substack{A_i\in\mathcal{A}_0 \\ A_i\cap X_k\neq\emptyset}} (e-1)|\lambda|\tilde{\beta}|t_{A_i}| e^{\gamma_Q|\operatorname{supp} A_i|} \Big) \leq \\ \leq e^{-\gamma_Q|X_k|} \sum_{\ell=1}^{\infty} \frac{1}{\ell!} \prod_{i=1}^{\ell} \Big(\sum_{x\in X_k} \sum_{\substack{A_i\in\mathcal{A}_0 \\ A_i\ni x}} (e-1)|\lambda|\tilde{\beta}|t_{A_i}| e^{\gamma_Q|\operatorname{supp} A_i|} \Big) \leq \\ \leq e^{-\gamma_Q|X_k|} \sum_{\ell=1}^{\infty} \frac{1}{\ell!} |X_k|^{\ell} \leq e^{-(\gamma_Q-1)|X_k|}. \tag{5.7}$$

Since

$$\sum_{X\subset\operatorname{supp} Y} e^{-(\gamma_Q-1)|X|} e^{-\tilde{\beta}\gamma_{\mathrm{cl}}|\operatorname{supp} Y\setminus X|} \leq e^{-\min(\tilde{\beta}\gamma_{\mathrm{cl}},\gamma_Q-1)|\operatorname{supp} Y|} 2^{|\operatorname{supp} Y|}, \tag{5.8}$$

we finally get (5.2) with $\tilde{\gamma}$ given by (5.3). □

5.2. Bound on the derivaties $\partial\rho(Y)\,/\,\partial\mu_i$.

Proposition 5.2. *Let $\lambda \in \mathbb{R}$, $\tilde{\beta} > 0$, and $\gamma_Q \geq 1$ be such that (5.1) is satisfied. Then*

$$\Big|\frac{\partial}{\partial\mu_i}\rho(Y)\Big| \leq \big(\tilde{\beta}C_0 + \frac{e}{e-1}\big)|\operatorname{supp} Y| e^{-(\tilde{\beta}e_0+\tilde{\gamma})|Y|}. \tag{5.9}$$

Here C_0 is the constant from (3.10) and $\tilde{\gamma}$ is the constant defined in (5.3).

Proof. We start again from the expression (4.24) for $n = 1$ and bound

$$\Big|\frac{\partial}{\partial\mu_i} e^{-\tilde{\beta}E(\omega(\operatorname{supp} Y))}\Big| \leq \tilde{\beta}\Big|\frac{\partial}{\partial\mu_i} E(\omega(\operatorname{supp} Y))\Big| e^{-\tilde{\beta}E(\omega(\operatorname{supp} Y))} \leq \\ \leq \tilde{\beta}C_0|\operatorname{supp} Y| e^{-\tilde{\beta}E(\omega(\operatorname{supp} Y))} \tag{5.10}$$

with the help of (4.23) and (3.10), as well as

$$\Big|\frac{\partial}{\partial\mu_i}\prod_{k=1}^{M}\frac{(\lambda\boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!}\Big| \le (\prod_{k=1}^{M}\frac{(|\lambda||\boldsymbol{t}|)^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!})\sum_{\bar k,\bar A} m_{\bar k,\bar A}\Big|\frac{\partial}{\partial\mu_i}\log t_{\bar A}\Big|. \tag{5.11}$$

Using then (5.5) and

$$\sum_{m_{\bar k,\bar A}=1}^{\infty} m_{\bar k,\bar A}\frac{(|\lambda|\tilde\beta|t_{\bar A}|)^{m_{\bar k,\bar A}}}{m_{\bar k,\bar A}!}\Big|\frac{\partial t_{\bar A}}{\partial\mu_i}\Big|\frac{1}{|t_{\bar A}|} = \\ = |\lambda|\tilde\beta\Big|\frac{\partial t_{\bar A}}{\partial\mu_i}\Big|\sum_{m_{\bar k,\bar A}=0}^{\infty}\frac{(|\lambda|\tilde\beta|t_{\bar A}|)^{m_{\bar k,\bar A}}}{m_{\bar k,\bar A}!} \le |\lambda|\tilde\beta e\Big|\frac{\partial t_{\bar A}}{\partial\mu_i}\Big|, \tag{5.12}$$

we get

$$\Big|\frac{\partial}{\partial\mu_i}\rho(Y)\Big| \le e^{-\tilde\beta e_0|\operatorname{supp}Y|}2^{|\Sigma||\operatorname{supp}Y|}\sum_{X\subset\operatorname{supp}Y} e^{-\tilde\beta\gamma_{\rm cl}|\operatorname{supp}Y\setminus X|}\times \\ \times\Big\{\tilde\beta C_0|\operatorname{supp}Y|\prod_k\Big(\sum_{\mathcal{B}_k}\prod_{A\in\mathcal{B}_k}(e-1)|\lambda|\tilde\beta|t_A|\Big) + \\ + \sum_{\substack{\bar k,\bar A\\ \bar A\cap X_{\bar k}\neq\emptyset}}|\lambda|\tilde\beta e\Big|\frac{\partial t_{\bar A}}{\partial\mu_i}\Big|\sum_{\substack{\mathcal{B}_{\bar k}\\ \bar A\notin\mathcal{B}_{\bar k}}}\prod_{A\in\mathcal{B}_{\bar k}}(e-1)|\lambda|\tilde\beta|t_{\bar A}|\prod_{k\neq\bar k}\Big(\sum_{\mathcal{B}_k}\prod_{A\in\mathcal{B}_k}(e-1)|\lambda|\tilde\beta|t_A|\Big)\Big\} \tag{5.13}$$

with the sum on the last line running through all $\bar A$ and $\mathcal{B}_{\bar k}$ such that the union of $\bar A$ with all A in $\mathcal{B}_{\bar k}$ is $X_{\bar k}$. Hence

$$\Big|\frac{\partial}{\partial\mu_i}\rho(Y)\Big| \le e^{-\tilde\beta e_0|\operatorname{supp}Y|}2^{|\Sigma||\operatorname{supp}Y|}\times \\ \times\sum_{X\subset\operatorname{supp}Y} e^{-\tilde\beta\gamma_{\rm cl}|\operatorname{supp}Y\setminus X|}\Big\{\tilde\beta C_0|\operatorname{supp}Y| + |X|\frac{e}{e-1}\Big\}e^{-(\gamma_Q-1)|X|}. \tag{5.14}$$

The rest of the proof then follows the same argument as above in the proof of Proposition 5.1. □

5.3. Proof of Theorem 3.1 and 3.2.

Given the representation (4.21) and the bounds of Propositions 5.1 and 5.2, the proof of Theorem 3.1 i) and v) is essentially identical to the proof of Theorem 2.1 i) and v) in [19]. Actually, it is an almost standard application of Pirogov-Sinai theory, with two modifications: the fact that the contour weights $\rho(Y)$ are in general not positive, and the fact that (4.21) describes a contour model in a finite slab, see [19] for the details. The constants can be chosen as follows. Taking any sufficiently large γ, we put $\beta_0 = \gamma/\gamma_{\rm cl}$ and assume that λ fulfils (3.28). Taking now $\gamma_Q = \gamma$ and $\tilde\beta \in [\beta_0, 2\beta_0)$, the condition (5.1) is satisfied and we can infer that the bounds (5.2) and (5.9) are fulfiled with $\tilde\gamma = \gamma - 1 - (1+|\Sigma|)\log 2$. Finally, whenever $\beta \ge \beta_0$, we choose $M \in \mathbb{N}$ so that $\tilde\beta = \beta/M \in [\beta_0, 2\beta_0)$.

In order to prove the remaining parts of Theorem 3.1, we need a representation of the form (4.21) for expectation values of local observables. By linearity and the fact that a local observable is a finite sum of even monominals in the creation annihilation operators, we may restrict ourselves to local observables that are of the form

$$\Psi = h_{A(\Psi)} \qquad \Phi = h_{A(\Phi)}. \tag{5.15}$$

Rewriting the expectation value of a local observable Ψ as

$$\langle \Psi \rangle_{q,\Lambda} = \frac{\operatorname{Tr}_{\mathcal{H}_\Lambda}(\Psi e^{-\beta H_{q,\Lambda}})}{\operatorname{Tr}_{\mathcal{H}_\Lambda}(e^{-\beta H_{q,\Lambda}})} = \frac{\operatorname{Tr}_{\mathcal{H}_\Lambda}(\Psi T^M)}{\operatorname{Tr}_{\mathcal{H}_\Lambda}(T^M)} = \frac{Z^\Psi_{q,\Lambda}}{Z_{q,\Lambda}}, \tag{5.16}$$

we now derive a contour representation for the modified partition function $Z^\Psi_{q,\Lambda}$. Retracing the steps leading to representation (4.15), we get the expression

$$Z^\Psi_{q,\Lambda} = \sum_{\boldsymbol{n}} \sum_{\{\boldsymbol{m}_k\}} \Big(\prod_{k=1}^{M} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \exp\Big\{ - \sum_{x \in \Lambda} \int_0^\beta \Phi_x(\boldsymbol{n}(\tau)) d\tau \Big\} \times \\ \times S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}; \Psi)\,, \tag{5.17}$$

where

$$S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}; \Psi) = \langle \boldsymbol{n} | R(\boldsymbol{\tau}_M, \boldsymbol{m}_M) \cdots R(\boldsymbol{\tau}_1, \boldsymbol{m}_1) \Psi \, | \boldsymbol{n} \rangle\,. \tag{5.18}$$

In order to define the contours corresponding to a configuration $\omega = \{\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\}\}$ we then introduce, in addition to the set of excited cells $D(\omega)$, the $d+1$ dimensional support of Ψ as

$$\mathcal{D}(\Psi) := \bigcup_{x \in \operatorname{supp} \Psi} C(x, 1)\,, \tag{5.19}$$

where we localized the observable Ψ, *by definition*, in the first time slice. Considering all cells in $D(\omega) \cup D(\Psi)$ as excited, we then define the set $\operatorname{supp} Y_\Psi$ as the union of all connected components of $D(\omega)$ that are connected to $D(\Psi)$, and the set $\overline{\operatorname{supp}}\, Y_\Psi$ as $\operatorname{supp} Y_\Psi \cup D(\Psi)$. The contours corresponding to the configuration ω are defined by taking the set $\operatorname{supp} Y_\Psi$, and the remaining components of $D(\omega)$, denoted by $\operatorname{supp} Y_1$, …, $\operatorname{supp} Y_n$ as their support. Since the cell in $D(\Psi)$ have to be considered as excited as well, a slight variance will apear in the definition of the ground state regions V_m, which now, by definition, does not contain the cells in $D(\Psi)$.

With these definitions, we get the contour representation

$$Z^\Psi_{q,\Lambda} = \sum_{Y_\Psi} \sum_{n=0}^{\infty} \sum_{\{Y_1, \ldots, Y_n\}} e^{-\sum_m \tilde{\beta} |V_m| e_m} \rho(Y_\Psi, Y_1, \ldots, Y_n)\,, \tag{5.20}$$

with

$$\rho(Y_\Psi, Y_1, \ldots, Y_n) = \sum_{\boldsymbol{n}} \sum_{\{\boldsymbol{m}_k\}} \Big(\prod_{k=1}^{M} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \chi_{Y_\Psi, Y_1, \ldots, Y_n}(\omega) \times \\ \times S(\omega; \Psi) e^{-\tilde{\beta} E(\omega(\overline{\operatorname{supp}}\, Y_\Psi))} \prod_{i=1}^{n} e^{-\tilde{\beta} E(\omega(\operatorname{supp} Y_i))}\,, \tag{5.21}$$

where $\omega = \{\boldsymbol{n}, \{\tau_k, \boldsymbol{m}_k\}\}$, and $S(\omega;\Psi) = S(\boldsymbol{n}, \{\boldsymbol{\tau}_k, \boldsymbol{m}_k\};\Psi)$ is given by (5.18). Since the observable Ψ is of the form (5.15), the factorization proof now goes through without modifications, leading to the representation

$$Z^{\Psi}_{q,\Lambda} = \sum_{Y_\Psi} \sum_{n=0}^{\infty} \sum_{\{Y_1,\dots,Y_n\}} e^{-\sum_m \tilde\beta |V_m| e_m} \rho(Y_\Psi) \prod_{i=1}^{n} \rho(Y_i)\,, \tag{5.22}$$

with $\rho(Y_i)$ defined as before, and $\rho(Y_\Psi)$ defined by

$$\rho(Y_\Psi) = \sum_{\boldsymbol{n}} \sum_{\{\boldsymbol{m}_k\}} \Big(\prod_{k=1}^{M} \frac{(-\lambda \boldsymbol{t})^{\boldsymbol{m}_k}}{\boldsymbol{m}_k!} \int d\boldsymbol{\tau}_k^{\boldsymbol{m}_k} \Big) \chi_{Y_\Psi(\omega)} S(\omega;\Psi) e^{-\tilde\beta E(\omega(\overline{\mathrm{supp}}\, Y_\Psi))}\,. \tag{5.23}$$

Given the contour representation (5.22), we can now proceed as in [19] to complete the proof of Theorem 3.1. In the same way, Theorem 3.2 follows from the corresponding representation for the modified partition function $Z^{\Psi}_{\mathrm{per},\Lambda} = \langle\Psi\rangle_{\mathrm{per},\Lambda} Z_{\mathrm{per},\Lambda}$.

5.4. Proof of Lemma 3.3.

Given the results of Section 4 and 5, the proof of Lemma 3.3 is almost a textbook exercise. We therefore only indicate the main steps, and leave the details to the reader.

Starting with the partition function $Z^{\beta,\mathrm{np}}_{q,\Lambda}$, we note that it has a representation of the form (4.15), with the only difference that the sum over $\boldsymbol{n}$ is replaced by the single term $\boldsymbol{n} = \boldsymbol{g}^{(q)}_\Lambda$. Represented as the partition function of a contour model, $Z^{\beta,\mathrm{np}}_{q,\Lambda}$ is then given as a sum over sets of contours in a volume $V(\Lambda) \subset \mathbb{R}^{d+1}$,

$$V(\Lambda) = \{y \in \mathbb{R}^d \mid \mathrm{dist}(y,\Lambda) \le \tfrac{1}{2}\} \times [0,\beta]\,, \tag{5.24}$$

with boundary condition q on $\partial V(\Lambda)$

The partition function $Z^{\beta,\mathrm{np}}_{q,\Lambda}$ can be analysed by standard Pirogov-Sinai theory as developped in [21–24]. We follow [23,24], with a slight variant in the definition of truncated contour models. Namely, for a contour Y with support $\mathrm{supp}\, Y \subset \mathbb{R}^{d+1}$, we define $\delta(Y)$ as the diameter of the projection of $\mathrm{supp}\, Y$ on $\mathbb{R}^d$, and then proceed by induction on $\delta(Y)$, see [19], equations (5.8) – (5.10). Denoting the corresponding truncated partition functions by $\bar Z^{\mathrm{np}}_q(V(\Lambda))$, we define the truncated free energies

$$\bar f_q(\mu) = -\lim_{V\to\mathbb{R}^{d+1}} \frac{\log \bar Z^{\mathrm{np}}_q(V)}{|V|}\,, \tag{5.25}$$

where V denotes the euclidean volume of V (note that $|V|$ is nothing but the number of elementary cells $C(x,k)$ in V multiplied by $\tilde\beta$).

As usual, the untruncated partition functions $Z^{\beta,\mathrm{np}}_{q,\Lambda}$ and the corresponding truncated partition functions $\bar Z^{\mathrm{np}}_q(V(\Lambda))$ are identical whenever $a_q(\mu) = 0$, where $a_q(\mu) = 0$ is defined as

$$a_q(\mu) = \bar f_q(\mu) - \min_m \bar f_m(\mu)\,. \tag{5.26}$$

For $a_q(\mu) = 0$, the partition function $Z^{\beta,\mathrm{np}}_{q,\Lambda}$ can therefore be analyzed by a convergent cluster expansion, giving a representation for

$$\log Z^{\beta,\mathrm{np}}_{q,\Lambda} + \bar f_q(\mu)\,|V(\Lambda)| = \log Z^{\beta,\mathrm{np}}_{q,\Lambda} + \bar f_q(\mu)\,\beta|\Lambda|$$

in terms of clusters connected to the boundary $\partial V(\Lambda)$. Defining $\partial_i V(\Lambda)$ as the union over all faces in $\partial V(\Lambda)$ that are orthogonal to the direction i, and recalling that an elementary cell $C(x,k)$ has extension $\tilde\beta$ in the "time direction", we therefore get the bound

$$\begin{aligned}\log Z^{\beta,\mathrm{np}}_{q,\Lambda} &= -\bar f_q(\mu)\beta|\Lambda| + O\Big(|\partial_0 V(\Lambda)| + \frac{1}{\tilde\beta}\sum_{i=1}^{d}|\partial_i V(\Lambda)|\Big)\\ &= -\bar f_q(\mu)\beta|\Lambda| + O\Big(|\Lambda| + \frac{\beta}{\tilde\beta}|\partial\Lambda|\Big)\,. \end{aligned} \tag{5.27}$$

In order to complete the proof of (3.46), we need a relation between the truncated free energies $\bar f_q(\mu)$ introduced above and the truncated free energies $f_q(\mu,\beta)$ of the model on the torus $\mathbb{T}$. To this end, we note that the truncated activity of a contour Y with $\operatorname{supp} Y \subset \mathbb{T}$ is the same for both truncated models, as long as the support of Y does not wind arround the torus $\mathbb{T}$. The cluster expansions for $\tilde\beta\bar f_q(\mu)$ and $\tilde\beta f_q(\mu,\beta)$ therefore only differ by terms involving clusters winding arround $\mathbb{T}$ in the time direction. As a consequence,

$$\tilde\beta f_q(\mu,\beta) = \tilde\beta\bar f_q(\mu) + O(e^{-\alpha\gamma(\beta/\tilde\beta)})\,, \tag{5.28}$$

where γ and $\alpha > 0$ are the constants from Theorem 3.1. From (5.28) we get $f_q(\mu) \equiv \lim_{\beta\to\infty} f_q(\mu,\beta) = \bar f_q(\mu)$ and as a consequence

$$a_q(\mu) = \lim_{\beta\to\infty} a_q(\mu,\beta,\lambda)\,. \tag{5.29}$$

Observing finally that $\tilde\beta \in [\beta_0, 2\beta_0)$, see the proof of Theorem 3.1 above, the bound (3.46) follows from (5.27).

As for the proof of (3.47), we note that the above methods also give a convergent cluster expansion for $\langle\Psi\rangle^{\beta,\mathrm{np}}_{q,\Lambda}$ if $a_q(\mu) = 0$. Comparing this cluster expansion to the corresponding cluster expansion in the thermodynamic limit $V(\Lambda) \to \mathbb{R}^{d+1}$, we get

$$\langle\Psi\rangle^{\beta,\mathrm{np}}_{q,\Lambda} = \lim_{\substack{\Lambda\to\mathbb{Z}^d\\ \beta\to\infty}} \langle\Psi\rangle^{\beta,\mathrm{np}}_{q,\Lambda} + O(e^{-\alpha\gamma\min\{\mathrm{dist}(\operatorname{supp}\Psi,\partial\Lambda),\beta/2\tilde\beta\}})\,, \tag{5.30}$$

provided $a_q(\mu) = 0$. In order to complete the proof, we need to controll the limit in (3.31′), showing that it is identical to the limit in the right hand side of (5.30). To this end, we note that the condition $a_q(\mu) = 0$ implies that

$$\tilde\beta a_q(\mu,\beta,\lambda) \le O(e^{-\alpha\gamma(\beta/\tilde\beta)})\,. \tag{5.31}$$

Standard Pirogov-Sinai theory, here in the form derived in [19], on the other hand, gives that $Z_{q,\Lambda}$ and $\langle\Psi\rangle^{\beta}_{q,\Lambda}$ can be analysed by a convergent cluster expansion if

$$\tilde\beta a_q(\mu,\beta,\lambda)\,\mathrm{diam}(\Lambda) \le O(1)\,. \tag{5.32}$$

The limits in (3.30′) and (3.31′) can therefore be analysed by a convergent expansion. Comparing the resulting expansion for $\langle\Psi\rangle_q$ to that for $\langle\Psi\rangle^{\beta,\mathrm{np}}_{q,\Lambda}$, we obtain the desired bound (3.47). □

Proof of Theorem 3.4.

Let $\beta \geq \beta_0$, where β_0 is the constant from Theorem 3.1. Using (3.51), (3.52), Lemma 3.3, and the fact that the norm and support of $Q_{x,\Lambda}$ are uniformly bounded in Λ, we get

$$\Big|\frac{1}{|\Lambda|}\langle Q_\Lambda\rangle_q - \rho_\Lambda^{(q)}\Big| = \frac{1}{|\Lambda|}\Big|\langle Q_\Lambda\rangle_q - \langle Q_\Lambda\rangle_{q,\Lambda}^{\beta,\mathrm{np}}\Big| = \frac{1}{|\Lambda|}\Big|\sum_{x\in\Lambda}\big(\langle Q_{x,\Lambda}\rangle_q - \langle Q_{x,\Lambda}\rangle_{q,\Lambda}^{\beta,\mathrm{np}}\big)\Big| \leq$$
$$\leq \frac{C}{|\Lambda|}\sum_{x\in\Lambda}\exp\{-\alpha\gamma\min\{\mathrm{dist}(\mathrm{supp}\,Q_{x,\Lambda},\partial\Lambda),\beta/\beta_0\}\}. \quad (5.33)$$

Taking the limit $\beta\to\infty$, this gives

$$\Big|\frac{1}{|\Lambda|}\langle Q_\Lambda\rangle_q - \rho_\Lambda^{(q)}\Big| \leq \frac{C}{|\Lambda|}\sum_{x\in\Lambda}\exp\{-\alpha\gamma\,\mathrm{dist}(\mathrm{supp}\,Q_{x,\Lambda},\partial\Lambda)\} \leq O\big(\frac{|\partial\Lambda|}{|\Lambda|}\big) \quad (5.34)$$

which in turn implies the bound (3.55).

In order to prove (3.56), we have to bound the difference of $\langle Q_{x,\Lambda}\rangle_q^\beta$ and $\langle Q_{x,\Lambda}\rangle_q$. Since q is stable for all $\beta\geq\tilde\beta_0$, both $\langle Q_{x,\Lambda}\rangle_q^\beta$ and $\langle Q_{x,\Lambda}\rangle_q$ can be analysed by a convergent cluster expansion. Comparing then the expansions, one obtains a representation for $\langle Q_{x,\Lambda}\rangle_q^\beta - \langle Q_{x,\Lambda}\rangle_q$ that only involves clusters which either wind around the torus $\mathbb{T}$ in the time direction or are contained in infinite volume $\mathbb{R}^{d+1}$ and "do not fit" into the torus $\mathbb{T}$. In either case, one gets only contribution of the order $O\big(e^{-(\beta/\beta_0)\alpha\gamma}\big)$ yielding the bound

$$\Big|\langle Q_{x,\Lambda}\rangle_q - \langle Q_{x,\Lambda}\rangle_q^\beta\Big| \leq Ce^{-(\beta/\beta_0)\alpha\gamma}, \quad (5.35)$$

which in turn implies the bound (3.56).

6. Application to the Extended Hubbard Model: Proof of Theorem 2.1

The claims i) and iii) are a straightforward corollary of Theorem 3.1. For the choice of constants we notice that $\gamma_{\mathrm{cl}}\geq c(d)\epsilon$ everywhere in $S^{(\epsilon)}_{\{0,2\}}$, where $c(d)$ is a strictly positive constant. As a consequence, $\beta_0\sim\frac{1}{\epsilon}$ and $\lambda_0\sim\epsilon$. The bound $|t|<\epsilon C_2$ corresponds to (3.28) (with t replacing λ and $2de^{8\gamma}$ replacing $||\boldsymbol{t}||_\gamma$). The long range order expressed in (2.9) follows from the bound (3.33) and the staggered order of the ground states of $H^{(0)}$ (see [18] for a detailed discussion of the classical states of $H^{(0)}$).

Using Theorem 3.4 for the (quantum) density $\rho(\beta)$ defined in (2.4) and noticing that the density of classical ground state ρ_{class} is actually constant throughout the region $S^{(0)}_{\{0,2\}}$, $\rho_{\mathrm{class}}=1$, we get the claim iv).

To prove ii), we first show that $\langle S_x^3\rangle_m^\beta = 0$. Taking into account Theorem 3.1 ii), it is enough to show that

$$\mathrm{Tr}_{\,\mathcal{H}_\Lambda(L)}(S_x^3\,e^{-\beta H_{m,\Lambda(L)}}) = 0 \quad (6.1)$$

for every $\Lambda(L)$ with even L and $H_{m,\Lambda}$ defined as in (3.21) with $\boldsymbol{g}^{(m)}$ being the corresponding $\{0,2\}$ staggered ground configuration. Using (2.7) and expressing

the trace in terms of the base $|\boldsymbol{n}\rangle$ of occupation numbers $\boldsymbol{n} : \Lambda \times \Sigma \to \{0,1\}$, we want to show that

$$\sum_{\boldsymbol{n}} \langle \boldsymbol{n}| \left(\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow}\right) e^{-\beta H_{m,\Lambda(L)}} |\boldsymbol{n}\rangle = 0. \tag{6.2}$$

Indeed, taking into account that

$$\sum_{\boldsymbol{n}} \langle \boldsymbol{n}| \left(\hat{n}_{x,\uparrow} - \hat{n}_{x,\downarrow}\right) e^{-\beta H_{m,\Lambda(L)}} |\boldsymbol{n}\rangle = \sum_{\boldsymbol{n}} \langle \boldsymbol{n}| e^{-\beta H_{m,\Lambda(L)}} |\boldsymbol{n}\rangle (n_{x,\uparrow} - n_{x,\downarrow}) \tag{6.3}$$

and that the matrix element $\langle \boldsymbol{n}| e^{-\beta H_{m,\Lambda(L)}} |\boldsymbol{n}\rangle$ is symmetric under the overall spin flip $\boldsymbol{n} \to \tilde{\boldsymbol{n}}$, $\tilde{n}_{x,\uparrow} = n_{x,\downarrow}$ and $\tilde{n}_{x,\downarrow} = n_{x,\uparrow}$, we get (6.1).

The Hamiltonian above is invariant under rotations and has actually an identical expression in terms of the creation and annihilation operators of the electron with up and down spin with respect to, say, the 1-axis. To get $\langle S^1_x \rangle^\beta_m = 0$ and $\langle S^2_x \rangle^\beta_m = 0$ it is therefore enough to repeat the above argument in the corresponding occupation number bases. □

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