

Effective Interactions Due to Quantum Fluctuations

Roman Kotecký^{1,2,*}, Daniel Ueltschi^{3,**}

¹ Center for Theoretical Study, Charles University, Jilská 1, 110 00 Praha 1, Czech Republic

² Department of Theoretical Physics, Charles University, V Holešovičkách 2, 180 00 Praha 8, Czech Republic.
E-mail: kotecky@cucc.ruk.cuni.cz

³ Institut de Physique Théorique, EPF Lausanne, CH-1015 Lausanne, Switzerland

Received: 28 April 1998 / Accepted: 19 March 1999

Abstract: A class of quantum lattice models is considered, with Hamiltonians consisting of a classical (diagonal) part and a small off-diagonal part (e.g. hopping terms). In some cases when the classical part has an infinite degeneracy of ground states, the quantum perturbation may stabilize some of them. The mechanism of this stabilization stems from effective potential created by the quantum perturbation.

Conditions are found when this strategy can be rigorously controlled and the low temperature phase diagram of the full quantum model can be proven to be a small deformation of the zero temperature phase diagram of the classical part with the effective potential added. As illustrations we discuss the asymmetric Hubbard model and the Bose–Hubbard model.

Contents

1. Introduction	290
2. Assumptions and Statements	293
2.1 Classical Hamiltonian with quantum perturbation	293
2.2 The effective potential	296
2.3 Stability of the dominant states	297
2.4 Characterization of stable phases	299
2.5 Phase diagram	301
3. Examples	303
3.1 The asymmetric Hubbard model	303
3.2 The Bose–Hubbard model	305
4. Contour Representation of a Quantum Model	308

* Partly supported by the grants GAČR 202/96/0731 and GAUK 96/272.

** Present address: Department of Mathematics, Rutgers University, 110 Frelinghuysen Road, Piscataway, NJ 08854-8019, USA. E-mail: ueltschi@math.rutgers.edu

5. Exponential Decay of the Weight of the Contours	320
6. Expectation Values of Local Observables and Construction of Pure States	328
A. General Expression for the Effective Potential	333

1. Introduction

Physics of a large number of quantum particles at equilibrium is very interesting and difficult at the same time. Interesting, because it is treating such macroscopic phenomena as magnetization, crystallisation, superfluidity or superconductivity. And difficult, because their study has to combine Quantum Mechanics and Statistical Physics.

A natural approach is to decrease difficulties arising from this combination by starting from only one aspect. Thus one can use only Quantum Mechanics and treat the particles first as independent, trying next to add small interactions. In the present paper we are concerned with the other approach. Namely, to start with a model treated by Classical Statistical Physics, adding next a small quantum perturbation. Another simplification is to consider lattice systems (going back to a physical justification for the modeling process, we can invoke applications to condensed matter physics).

Quantum systems studied here have Hamiltonians consisting of two terms. The first term is a classical interaction between particles; formally, this operator is “function” of the position operators of the particles and it is diagonal with respect to the corresponding basis in occupation numbers. The second term is an off-diagonal operator that we suppose to be small with respect to the interaction. A typical example for this is a hopping matrix.

The aim of the paper is to show that a *new effective interaction* appears that is due to the combination of the potential and the kinetic term. An explicit formula is computed, and sufficient conditions are given in order that the low temperature behaviour is controlled by the sum of the original diagonal interaction and the effective potential. To be more precise, it is rigorously shown that the phase diagram of the original quantum model is only a small perturbation of the phase diagram of a classical lattice model with the effective interaction.

Thus, we will start by recalling some standard ideas of Classical Statistical Mechanics of lattice systems. The Peierls argument for proving the occurrence of a first order phase transition in the Ising model [Pei,Dob,Gri] marks the beginning of the perturbative studies of the low temperature regimes of classical lattice models. Partition functions and expectation values of observables may be expanded with respect to the excitations on top of the ground states, interpreting the excitations in geometric terms as *contours*. These ideas and methods are referred to as the Pirogov–Sinai theory; they were first introduced in [PS,Sin] and later further extended [Zah,BI,BS].

The intuitive picture is that a low temperature phase is essentially a ground state configuration with small excitations. A phase is stable whenever it is improbable to install a large domain with another phase inside. For such an insertion one has to pay on its boundary, it is excited (two phases are separated by excitations), but, on the other side, one may gain on its volume if its *metastable free energy* (its ground energy minus the contribution of small thermal fluctuations) is smaller than the one of the external phase. It is important to take into account the fluctuations since they can play a role in determining which phase is dominant. A standard example here is the Blume–Capel model with an external field slightly favouring the “+1” phase; at low temperatures, the “0” phase may be still selected because it has more low energy excitations (theory of such dominant states chosen by thermal fluctuations may be found in [BS]).

The partition function of a quantum system $\text{Tr} e^{-\beta H}$ may be expressed using the Duhamel expansion (or Trotter formula), yielding a classical contour model in a space with one more (continuous) dimension. If the corresponding classical model (the diagonal part only) has stable low temperature phases, and if the off-diagonal terms of the Hamiltonian are small, the contours have low probability of occurrence and it is possible to extend the Peierls argument to quantum models [Gin]. More generally, one can formulate a ‘‘Quantum Pirogov–Sinai theory’’ [BKU1, DFF1], in order to establish that (i) low temperature phases are very close to ground states of the diagonal interaction (more precisely: the density matrix $\frac{1}{Z} e^{-\beta H}$ is close to the projection operator $|g\rangle\langle g|$, where $|g\rangle$ is the ground state of the diagonal interaction only) and (ii) low temperature phase diagrams are small deformations of zero temperature phase diagrams of the interactions.

So far we have only discussed the case when the effect of the quantum perturbation is small, and the features of the phases are due to the classical interaction between the particles. It may happen, however, that the classical interaction alone is not sufficient to choose the low temperature behaviour. This is the case in the two models we introduce now and use later for illustration of our general approach.

- **The asymmetric Hubbard model.** It describes hopping spin $\frac{1}{2}$ particles on a lattice $\Lambda \subset \mathbb{Z}^v$. A basis of its Hilbert space is indexed by classical configurations $n \in \{0, \uparrow, \downarrow, 2\}^\Lambda$, and the Hamiltonian

$$H = - \sum_{\|x-y\|_2=1} \sum_{\sigma=\uparrow,\downarrow} t_\sigma c_{x\sigma}^\dagger c_{y\sigma} + U \sum_x n_{x\uparrow} n_{x\downarrow} - \mu \sum_x (n_{x\uparrow} + n_{x\downarrow}) \quad (1.1)$$

(the hopping parameter t_σ depends on the spin of the particle). In the atomic limit $t_\uparrow = t_\downarrow = 0$ the ground states are all the configurations with exactly one particle at each site. The degeneracy equals $2^{|\Lambda|}$, which means that it has nonvanishing residual entropy at zero temperature. The case $t_\uparrow \neq t_\downarrow = 0$ corresponds to the Falicov–Kimball model (see [GM]); in this case, spin- \downarrow electrons behave as classical particles. Here, we shall consider the strongly asymmetric Hubbard model, with $U \gg t_\uparrow \gg t_\downarrow$.

- **The Bose–Hubbard model.** We consider bosons moving on a lattice $\Lambda \subset \mathbb{Z}^2$. They interact through on-site, nearest neighbour and next nearest neighbour repulsive potentials. A basis of its Hilbert space is the set of all configurations $n \in \mathbb{N}^\Lambda$, and its Hamiltonian:

$$H = -t \sum_{\|x-y\|_2=1} a_x^\dagger a_y + U_0 \sum_x (n_x^2 - n_x) + U_1 \sum_{\|x-y\|_2=1} n_x n_y + U_2 \sum_{\|x-y\|_2=\sqrt{2}} n_x n_y - \mu \sum_x n_x. \quad (1.2)$$

For $U_0 \geq 4U_1 - 4U_2$ and $U_1 \geq 2U_2$, and if $0 < \mu < 8U_2$, the ground states of the potential part are those generated by $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, i.e. any configuration with alternatively a ferromagnetic and an empty line is a ground state (and similarly in the other direction);

see Fig. 2 in Sect. 3. The degeneracy is of the order $2^{\frac{1}{2}|\Lambda|^{\frac{1}{2}}}$ (if Λ is a square), there is no residual entropy. Actually, we shall add to (1.2) a generalized hard-core condition that prevents more than N bosons to be present at the same site; this condition has technical motivations, and does not change the physics of the model.

In these two situations, the smallest quantum fluctuations yield an effective interaction, and this interaction stabilizes phases displaying long-range order (there is neither superfluidity nor superconductivity).

Beside of the low temperature Gibbs states, the effective potential may have an influence in situations with interfaces; it has been shown in [DMN] that rigid 100 and 111 interfaces occur in the Falicov–Kimball model at low temperature.

In the case where classical and quantum particles are mixed in one model, like the Falicov–Kimball model, a method using Peierls argument was proposed by Kennedy and Lieb [KL]; it was extended in [LM] to situations that are not covered by the present paper, namely to cases of such mixed systems with continuous classical variables.

Results very similar to ours have already been obtained by Datta, Fernández, Fröhlich and Rey-Bellet [DFFR]. Their approach is different, however. Starting from a Hamiltonian $H(\lambda) = H^{(0)} + \lambda V$, $H^{(0)}$ being a diagonal operator with infinitely many ground states, and V the quantum perturbation, the idea is to choose an antisymmetric matrix $S = \lambda S^{(1)} + \lambda^2 S^{(2)}$ in such a way that the operator $H^{(2)}(\lambda) = e^S H(\lambda) e^{-S}$, expanded with the help of Lie-Schwinger series, turns out to be diagonal, up to terms of order λ^3 or higher. If the diagonal part of $H^{(2)}$ has a finite number of ground states and the excitations cost strictly positive energy, it can be shown that the ground states are stable. It is possible to include higher orders in this perturbation scheme (see [DFFR]).

In fact, our first intention was to study the stability of the results of [BS] with respect to a quantum perturbation, and we began the present study as a warm-up and the first simple step towards this goal. This simple step turned out however to be rather involved. Even though, at the end, the paper contains results similar to that of [DFFR], we think that the subject is important enough to justify an alternative approach, and that there are some advantages in an explicit formula for the effective potential and sufficient conditions for it to control the low temperature behaviour that may be useful in explicit applications.

The intuitive background of this paper owes much to the work of Bricmont and Slawny [BS] discussing the situation with infinite degeneracy of ground states, where only a finite number of ground states is dominating as a result of thermal fluctuations, and to the paper of Messenger and Miracle-Solé [MM] which was useful to understand the structure of the quantum fluctuations. Having expanded the partition function $\text{Tr} e^{-\beta H}$ using the Duhamel formula and having defined *quantum contours* as excitations with respect to a well chosen classical configuration, we identify the smallest quantum contours (that we call *loops*). Given a set of big quantum contours, we can replace the sum over sets of loops by an *effective interaction* acting on the quantum configurations without loops. This effective interaction is long-range, but decays exponentially quickly with respect to the distance. This allows, for a class of models, to have an explicit control on the approximation given by the effective interaction allowing to prove rigorous statements about the behaviour of original quantum model.

An important model that does not fall into the class of models we can treat is the (symmetric) Hubbard model. Take $U = 1$ and $t_\uparrow = t_\downarrow = t$ in (1.1). Computing the effective potential stemming from one transition of a particle to a neighbouring site and back, we find an antiferromagnetic interaction of strength t^2 . On the other hand, it is possible to make two transitions as a result of which the spins of nearest neighbours are interchanged,

$$|n_x, n_y\rangle = |\downarrow, \uparrow\rangle = -c_{x\downarrow}^\dagger c_{y\downarrow} c_{y\uparrow}^\dagger c_{x\uparrow} |\uparrow, \downarrow\rangle.$$

It turns out that this brings the factor t^2 , which is of the same order as the strength of the effective interaction. In this case we cannot ensure the stability of the phases selected by the effective potential – we would need a stronger effective interaction. Otherwise the system jumps easily from a configuration with one particle per site to another such configuration, i.e. from a classical ground state to another classical ground state. We call

quantum instability this property of the system. In the Hubbard model it is a manifestation of a continuous symmetry of the system, namely the rotation invariance.

In Sect. 2 the ideas discussed above are introduced with precise definitions. The effective potential is written down in Sect. 2.2 – actually, we restrict here to lowest orders; the general formula is not that pleasant, and is therefore hidden in the appendix. The results of the paper are summarized in Theorems 2.2 (a characterization of stable pure phases) and 2.3 (the structure of the phase diagram); experts will recognize standard formulations of Pirogov–Sinai theory. Taking into account that our aim is to describe in a rigorous way the behaviour of a quantum system, some care must be given to the introduction of stable phases. We define them with the help of an external field perturbation of the state constructed with periodic boundary conditions. In Sect. 3 we apply the results to our two illustrative examples. The rest of the paper is devoted to the construction of a contour representation (Sect. 4), the proof of the exponential decay of the weights of the contours (Sect. 5), and, finally, the proofs of our claims with the help of contour expansions of the expectation values of local observables and the standard Pirogov–Sinai theory (Sect. 6).

Let us end this introduction by noting that given a model which enters our setting, it is not a straightforward task to apply our theorems. One still has to separate the correct leading orders that determine the behaviour of effective interaction. This situation has the utmost advantage that it should bring much more pleasure to users, since the most interesting part of the job remains to be done – to get intuition and to understand how the system behaves.

2. Assumptions and Statements

2.1. Classical Hamiltonian with quantum perturbation. Let \mathbb{Z}^v , $v \geq 2$, be the hypercubic lattice. We use $|x - y| := \|x - y\|_\infty$ to denote the distance between two sites $x, y \in \mathbb{Z}^v$. Ω is the finite state space of the system at site $x = 0$, $|\Omega| = S < \infty$. Our standard setting will be to consider the system on a finite torus $\Lambda = (\mathbb{Z}/L\mathbb{Z})^v$ (i.e. a finite hypercube with periodic boundary conditions). With a slight abuse of notation we identify Λ with a subset of \mathbb{Z}^v and always assume that it is sufficiently large (to surpass the range of considered finite range interactions). A *classical configuration* n_Λ (occasionally we suppress the index and denote it n) is an element of Ω^Λ . If $A \subset \Lambda$, the restriction of n_Λ to A is also denoted by n_A . \mathcal{H}_Λ is the (finite-dimensional) Hilbert space spanned by the classical configurations, i.e. the set of vectors

$$|v\rangle = \sum_{n_\Lambda} a_{n_\Lambda} |n_\Lambda\rangle, \quad a_{n_\Lambda} \in \mathbb{C},$$

with the scalar product

$$\langle v|v'\rangle = \sum_{n_\Lambda} a_{n_\Lambda}^* a'_{n_\Lambda}.$$

Given two configurations $n_A \in \Omega^A$ and $n'_{A'} \in \Omega^{A'}$, with $A \cap A' = \emptyset$, it is convenient to define $n_A n'_{A'} \in \Omega^{A \cup A'}$ to be the configuration coinciding with n_A on A and with $n'_{A'}$ on A' .

The Hamiltonian is a sum of two terms, $H_\Lambda = V_\Lambda + T_\Lambda$. The former is the quantum equivalent of a classical interaction, the latter is the quantum perturbation – the notation was chosen such because we have in mind models where V represents the potential

energy of quantum particles, that is diagonal in the basis of occupation number operators, and T represents the kinetic energy. It helps considerably to assume that V_Λ is the quantum equivalent of a classical “block interaction”, that is, an interaction that has support on blocks of a given size in \mathbb{Z}^v . More precisely, let $R_0 \in \frac{1}{2}\mathbb{N}$ be the range of the interaction, and $U_0(x)$ be the R_0 -neighbourhood of $x \in \mathbb{Z}^v$:

$$U_0(x) = \begin{cases} \{y \in \mathbb{Z}^v : |y - x| \leq R_0\} & \text{if } R_0 \in \mathbb{N} \\ \{y \in \mathbb{Z}^v : |y - (x_1 + \frac{1}{2}, \dots, x_v + \frac{1}{2})| \leq R_0\} & \text{otherwise.} \end{cases} \quad (2.1)$$

When R_0 is half-integer, $U_0(x)$ is a block of integer size $2R_0 \times \dots \times 2R_0$ whose center is at distance $\frac{1}{2}$ of x . Then we assume the following structure for V_Λ .

Assumption 1 (Classical Hamiltonian). *There exists a classical periodic block interaction Φ of range R_0 (i.e. a collection of functions $\Phi_x : \Omega^{U_0(x)} \rightarrow \mathbb{R} \cup \{\infty\}$, $x \in \mathbb{Z}^v$) and period ℓ_0 such that*

$$V_\Lambda |n_\Lambda\rangle = \sum_{x \in \Lambda} \Phi_x(n_{U_0(x)}) |n_\Lambda\rangle;$$

for any torus $\Lambda \subset \mathbb{Z}^v$ of side L that is a multiple of ℓ_0 and any $n_\Lambda \in \Omega^\Lambda$.

Let us suppose that a fixed collection of reference local configurations $G_0(x) \subset \Omega^{U_0(x)}$ is given, for all sites of \mathbb{Z}^v .¹ Let $G_A = \{g_A \in \Omega^A : g_{U_0(x)} \in G_0(x) \text{ for all } U_0(x) \subset A\}$, $A \subset \mathbb{Z}^v$, and $G = G_{\mathbb{Z}^v}$. Finally, we set

$$\bar{A} = \cup_{U_0 \cap A \neq \emptyset} U_0 = \{y : \text{dist}(y, A) \leq 2R_0\}. \quad (2.2)$$

We assume that the local energy gap of excitations is uniformly bounded from below, while the spread of local energies of reference states is not too big (Fig. 1):

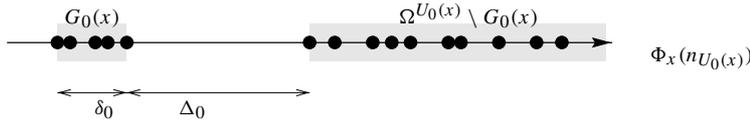


Fig. 1. Illustration for Assumption 2. The image of Φ_x decomposes into two sets separated by a gap Δ_0 ; the spread of the set of small values is bounded by δ_0

Assumption 2 (Energy gap for classical excitations). *There exist constants $\Delta_0 > 0$ and $\delta_0 < \infty$ such that:*

- For any $x \in \mathbb{Z}^v$ and any $n_{U_0(x)} \notin G_0(x)$, one has the lower bound

$$\Phi_x(n_{U_0(x)}) - \max_{g_{U_0(x)} \in G_0(x)} \Phi_x(g_{U_0(x)}) \geq \Delta_0, \quad (2.3)$$

¹ In some situations $G_0(x)$ is simply the set of all ground configurations of Φ_x . When discussing the full phase diagram, however, we will typically extend the interaction Φ_x to a class of interactions by adding certain “external fields”. The set $G_0(x)$ then will actually play the role of ground states of the interaction with a particular value of external fields (the point of maximal coexistence of ground state phase diagram).

• and,

$$\max_{g_{U_0(x)}, g'_{U_0(x)} \in G_0(x)} |\Phi_x(g_{U_0(x)}) - \Phi_x(g'_{U_0(x)})| \leq \delta_0. \quad (2.4)$$

For later purpose, we note the following consequence of Assumption 2.

Property. *Let Φ satisfy Assumption 2, R be such that $R^\nu \leq \Delta_0/\delta_0$, and $A \subset \mathbb{Z}^\nu$ with $\text{diam } A \leq R$. Then any pair of configurations $g_A \in G_A$ and $n_A \notin G_A$ satisfies the lower bound*

$$\sum_{x, U_0(x) \subset A} [\Phi_x(n_{U_0(x)}) - \Phi_x(g_{U_0(x)})] \geq R^{-\nu} \Delta_0. \quad (2.5)$$

Proof. Since $n_A \notin G_A$, there exists at least one site x , $U_0(x) \subset A$ such that $n_{U_0(x)} \notin G_0(x)$. From the assumption, this implies that

$$\sum_{x, U_0(x) \subset A} [\Phi_x(n_{U_0(x)}) - \Phi_x(g_{U_0(x)})] \geq \Delta_0 - \sum_{y \in A, y \neq x} \delta_0.$$

Using $|A| \leq R^\nu$, we obtain the property. \square

The quantum perturbation T_Λ is supposed to be a periodic quantum interaction. Namely, T_Λ is a sum of local operators $T_{\mathbf{A}}$, $T_\Lambda = \sum_{\mathbf{A}} T_{\mathbf{A}}$, where $T_{\mathbf{A}}$ has support $\text{supp } \mathbf{A} = A \subset \Lambda$ and \mathbf{A} is, in general, a pair (A, α) , where the index α specifies $T_{\mathbf{A}}$ from a possible finite set of operators with the same support. We found it useful to label quantum interactions $T_{\mathbf{A}}$ not only by the interaction domain A , but also, say, by quantum numbers of participating creation and annihilation operators. Thus, for example, the term \mathbf{A} might, in the case of the Hubbard model, be a pair $(\langle x, y \rangle, \uparrow)$ corresponding to the operator $T_{\mathbf{A}} = c_{x,\uparrow}^\dagger c_{y,\uparrow}$. We refer to \mathbf{A} as a *quantum transition*.

Assumption 3 (Quantum perturbations). *The collection of operators $T_{\mathbf{A}}$ is supposed to be periodic,² with period ℓ_0 , with respect to the translations of $\text{supp } \mathbf{A}$. The interactions $T_{\mathbf{A}}$ are assumed to satisfy the following condition, for fermions or bosons, respectively:*

- (Fermions) $T_{\mathbf{A}}$ is a finite sum of even monomials in creation and annihilation operators of fermionic particles at a given site, i.e.

$$T_{\mathbf{A}} = \sum_{\substack{(x_1, \sigma_1), \dots, (x_k, \sigma_k) \\ (y_1, \sigma'_1), \dots, (y_\ell, \sigma'_\ell)}} \tilde{T}(\{x_i, \sigma_i, y_j, \sigma'_j\}) c_{x_1, \sigma_1}^\dagger \cdots c_{x_k, \sigma_k}^\dagger c_{y_1, \sigma'_1} \cdots c_{y_\ell, \sigma'_\ell}$$

with $x_i, y_i \in A$ and σ_i, σ'_i are the internal degrees of freedom, such as spins; $\tilde{T}(\cdot)$ is a complex number. $k + \ell$ must be an even number. The creation and annihilation operators satisfy the anticommutation relations

$$\{c_{x,\sigma}^\dagger, c_{y,\sigma'}^\dagger\} = 0, \quad \{c_{x,\sigma}, c_{y,\sigma'}\} = 0, \quad \{c_{x,\sigma}^\dagger, c_{y,\sigma'}\} = \delta_{x,y} \delta_{\sigma,\sigma'}.$$

² By taking the least common multiple, we can always suppose the same periodicity for Φ and T . Moreover, whenever a torus Λ is considered, we suppose that its side is a multiple of ℓ_0 .

- (Spins or bosons) *The matrix element*

$$\langle n_\Lambda | T_\mathbf{A} | n'_\Lambda \rangle$$

is zero whenever $n_{\Lambda \setminus A} \neq n'_{\Lambda \setminus A}$ and otherwise it depends on n_A and n'_A only.

In both cases T is supposed to have an exponential decay with respect to its support: defining $\|T\|$ to be

$$\|T\| = \sup_{\mathbf{A}, A \subset \mathbb{Z}^v} \left[\max_{n_A, n'_A \in \Omega^A} |\langle n'_A | T_\mathbf{A} | n_A \rangle| \right]^{1/|A|}, \quad (2.6)$$

we assume that $\|T\| < \infty$.

When stating our theorems, we shall actually suppose $\|T\|$ to be sufficiently small. Notice also that we do not assume that T is of finite range, the exponential decay suffices.

2.2. The effective potential. In this section we define the effective potential that results from quantum fluctuations. It is due to a succession of “quantum transitions”, that is, it involves terms of the form $\langle g | T_\mathbf{A} | n \rangle$. What are the sequences $(\mathbf{A}_1, \dots, \mathbf{A}_k)$ to take into account? There is no general answer to this question, it depends on the model and on the properties of the phases under observation. In the case where the Hamiltonian is of the form $V + \lambda T$, λ being a perturbation parameter, one could restrict to all sequences that contain less than, say, 4 transitions (or 2, or 17...). But we can also consider models with more than one parameter. Let us say that the choice of the suitable sequence requires some physical intuition.

The procedure is the following. First we guess a list \mathcal{S} of sequences of quantum transitions, and we apply the formulæ (2.8)–(2.10) below to compute the effective potential. Then we must answer positively two questions:

- Does \mathcal{S} contains all the quantum transitions that actually play a role?
- Are other quantum effects negligible?

The mathematical formulation of these conditions is the subject of Assumptions 5 and 6 below. Notice that there is some freedom in the choice of \mathcal{S} ; indeed, it is harmless to include more transitions than what is necessary. Simply, it decreases the number of computations to guess the minimal set \mathcal{S} . Let us now state the formulæ for the effective potential.

Equations are rather simple in the case where \mathcal{S} contains sequences of no more than 4 transitions; we restrict to that situation in this section, and postpone the general expression, that is quite involved, to the appendix.

Let us decompose $\mathcal{S} = \mathcal{S}^{(2)} \cup \mathcal{S}^{(3)} \cup \mathcal{S}^{(4)}$, with $\mathcal{S}^{(k)}$ denoting the list of sequences with exactly k transitions, and write

$$\Psi = \Psi^{(2)} + \Psi^{(3)} + \Psi^{(4)}. \quad (2.7)$$

Here $\Psi^{(k)}$ is the contribution to the effective potential due to the fluctuations from $\mathcal{S}^{(k)}$.

Let

$$\phi_A(n_A; g_A) = \sum_{x, U_0(x) \subset A} \left[\Phi_x(n_{U_0(x)}) - \Phi_x(g_{U_0(x)}) \right].$$

Then, for any connected $A \subset \mathbb{Z}^v$ and $g_A \in G_A$, we define

$$\Psi_A^{(2)}(g_A) = - \sum_{\substack{(\mathbf{A}_1, \mathbf{A}_2) \in \mathcal{S}^{(2)} \\ \mathbf{A}_1 \cup \mathbf{A}_2 = A}} \sum_{n_A \notin G_A} \frac{\langle g_A | T_{\mathbf{A}_1} | n_A \rangle \langle n_A | T_{\mathbf{A}_2} | g_A \rangle}{\phi_A(n_A; g_A)}, \quad (2.8)$$

$$\Psi_A^{(3)}(g_A) = - \sum_{\substack{(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3) \in \mathcal{S}^{(3)} \\ \mathbf{A}_1 \cup \mathbf{A}_2 \cup \mathbf{A}_3 = A}} \sum_{n_A, n'_A \notin G_A} \frac{\langle g_A | T_{\mathbf{A}_1} | n_A \rangle \langle n_A | T_{\mathbf{A}_2} | n'_A \rangle \langle n'_A | T_{\mathbf{A}_3} | g_A \rangle}{\phi_A(n_A; g_A) \phi_A(n'_A; g_A)}. \quad (2.9)$$

The expression for $\Psi^{(4)}$ becomes more complicated (we shall see in Sect. 4 that clusters of excitations are actually occurring here),

$$\begin{aligned} \Psi_A^{(4)}(g_A) &= \\ &= - \sum_{\substack{(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4) \in \mathcal{S}^{(4)} \\ \mathbf{A}_1 \cup \mathbf{A}_2 \cup \mathbf{A}_3 \cup \mathbf{A}_4 = A}} \left[\sum_{n_A, n'_A, n''_A \notin G_A} \frac{\langle g_A | T_{\mathbf{A}_1} | n_A \rangle \langle n_A | T_{\mathbf{A}_2} | n'_A \rangle \langle n'_A | T_{\mathbf{A}_3} | n''_A \rangle \langle n''_A | T_{\mathbf{A}_4} | g_A \rangle}{\phi_A(n_A; g_A) \phi_A(n'_A; g_A) \phi_A(n''_A; g_A)} \right. \\ &\quad \left. - \frac{1}{2} \sum_{n_A, n'_A \notin G_A} \frac{\langle g_A | T_{\mathbf{A}_1} | n_A \rangle \langle n_A | T_{\mathbf{A}_2} | g_A \rangle \langle g_A | T_{\mathbf{A}_3} | n'_A \rangle \langle n'_A | T_{\mathbf{A}_4} | g_A \rangle}{\phi_A(n_A; g_A) + \phi_A(n'_A; g_A)} \left\{ \frac{1}{\phi_A(n_A; g_A)} + \frac{1}{\phi_A(n'_A; g_A)} \right\}^2 \right]. \end{aligned} \quad (2.10)$$

Property (2.5) implies that all the denominators are strictly positive.

These equations simplify further if $T_{\mathbf{A}}$ is a monomial in creation and annihilation operators; indeed in the sums over intermediate configurations only one element has to be taken into account.

Notice, finally, that the diagonal terms in T are not playing any role in the previous definitions; we consider that they are small, since otherwise we would have included them into the diagonal potential.

2.3. Stability of the dominant states. The aim of rewriting a class of quantum transitions in terms of the effective potential was to get control over stable low temperature phases. To this end, the three conditions, expressed first only vaguely and then in precise terms in the following Assumptions 4, 5, and 6, must be met. Namely, we suppose that

- the Hamiltonian corresponding to the sum $\Phi + \Psi$ of the classical (diagonal) and effective interactions has a finite number of ground configurations, and its excitations have strictly positive energy;³
- the list \mathcal{S} contains all the lowest quantum fluctuations;
- there is no “quantum instability”; the transition probability from a “ground state” g to another “ground state” g' is small compared to the energy cost of the excitations.

³ Again, when exploring a region of phase diagram at once, we have a fixed finite set of reference configurations that, strictly speaking, turn out to be ground configurations of the corresponding Hamiltonian for a particular value of “external fields”. See below for a more detailed formulation.

Each component of the effective interaction Ψ_A is a mapping $G_A \rightarrow \mathbb{R}$; let us first extend it to $\Omega^A \rightarrow \mathbb{R}$ by putting $\Psi_A(n_A) = 0$ if $n_A \notin G_A$. To give a precise meaning to the first condition, we suppose that a finite number of periodic reference configurations $D \subset G$ is given such that the interaction $\Phi + \Psi$ satisfies the Peierls condition with respect to D . We choose a formulation in which it is very easy to verify the condition and, in addition, it takes into account the fact that the configurations from D are not necessarily translation invariant. Namely, we will formulate the condition in terms of a block potential Υ that is equivalent to $\Phi + \Psi$ and is chosen in a suitable way. Of course, in many particular cases this is not necessary and the condition as stated below is valid directly for $\Phi + \Psi$. However, in several important cases treated in Sect. 3, the interaction $\Phi + \Psi$ turns out not to be the so-called m -potential and the use of the equivalent m -potential Υ not only simplifies the formulation of the Peierls condition, but also makes the task of its verification much easier.

We will consider the interactions φ and ϕ to be *equivalent*⁴ if, for any finite torus Λ and any configuration $n \in \Omega^\Lambda$, one has

$$\sum_{A \subset \Lambda^{\text{per}}} \varphi_A(n_A) = \sum_{A \subset \Lambda^{\text{per}}} \phi_A(n_A).$$

Assumption 4 (Peierls condition). *There exist a finite set of periodic configurations $D \subset G$ with the smallest common period L_0 , a constant Δ such that $\Delta > \|T\|^k$ for some finite constant k , and a periodic block interaction $\Upsilon = \{\Upsilon_x\}$ (with period ℓ_0) that is equivalent to $\Phi + \Psi$ such that the following conditions are satisfied. The interaction Υ is of a finite range⁵ $R \in \frac{1}{2}\mathbb{N}$ such that*

$$R^v \leq \Delta_0/\delta_0,$$

with the constants δ_0 and Δ_0 determined by the interaction Φ in Assumption 2. We denote by $U(x)$ the R -neighbourhood of x . The value $\Upsilon_x(d_{U(x)})$ is supposed to be translation invariant with respect to x for any $d \in D$, and the interaction Υ satisfies the following conditions:

- For any $x \in \Lambda$ and any n with $n_{U_0(x)} \notin G_{U_0(x)}$, one has

$$\Upsilon_x(n_{U(x)}) - \max_{g \in G} \Upsilon_x(g_{U(x)}) \geq \frac{1}{2} \Delta_0.$$

- For any $x \in \Lambda$ and any n with $n_{U(x)} \notin D_{U(x)}$, one has

$$\Upsilon_x(n_{U(x)}) - \min_{d \in D} \Upsilon_x(d_{U(x)}) \geq \Delta.$$

The following assumption is a condition demanding that the list \mathcal{S} should contain all transitions that are relevant for the effective potential. For this, we evaluate the diagonal

⁴ The usual notion of (physically) equivalent interactions (see [Geo,EFS]) is slightly weaker, but we will not need it here.

⁵ We will suppose, taking larger R if necessary, that it is larger or equal to the range R_0 of Φ , as well as to half of the range of the effective interaction Ψ and to L_0 .

terms arising from any sequence of transitions that *does not* appear in \mathcal{S} ; it will have to be small compared to the Peierls constant Δ . We define

$$\mathbf{m}(T_{\mathbf{A}_1}, \dots, T_{\mathbf{A}_k}) = \max_{g_A \in G_A} \max_{n_A^1, \dots, n_A^{k-1} \notin G_A} |\langle g_A | T_{\mathbf{A}_1} | n_A^1 \rangle \langle n_A^1 | T_{\mathbf{A}_2} | n_A^2 \rangle \dots \langle n_A^{k-1} | T_{\mathbf{A}_k} | g_A \rangle|, \quad (2.11)$$

where $A = \cup_{j=1}^k \bar{A}_j$.

Assumption 5 (Completeness of the set of quantum transitions). *There exists a finite number ε_1 such that for any sequence $(\mathbf{A}_1, \dots, \mathbf{A}_m) \notin \mathcal{S}$ with connected $\cup_{i=1}^m \bar{A}_i$ one has*

$$\mathbf{m}(T_{\mathbf{A}_1}, \dots, T_{\mathbf{A}_{k_1}}) \mathbf{m}(T_{\mathbf{A}_{k_1+1}}, \dots, T_{\mathbf{A}_{k_2}}) \dots \mathbf{m}(T_{\mathbf{A}_{k_{n-1}+1}}, \dots, T_{\mathbf{A}_m}) \leq \varepsilon_1 \Delta.$$

In general, it is not true that the main effect of quantum fluctuations results in a diagonal effective interaction. A sufficient condition for this to occur is that all possible transitions between *different* configurations g and g' have small contribution compared to Δ .

Assumption 6 (Absence of quantum instability). *There exists a finite number ε_2 such that for any sequence $(\mathbf{A}_1, \dots, \mathbf{A}_m)$, and any $g_A, g'_A \in G_A$ ($A = \cup_{j=1}^m \bar{A}_j$), $g_A \neq g'_A$, one has*

$$\left| \langle g_A | T_{\mathbf{A}_1} \dots T_{\mathbf{A}_m} | g'_A \rangle \right| \leq \varepsilon_2 \Delta.$$

When formulating our theorems, we shall suppose that ε_1 and ε_2 are small, more precisely: smaller than a constant that does not depend on T .

2.4. Characterization of stable phases. Notice first that the specific energy per lattice site of the configuration $d \in D$, defined by

$$e(d) = \lim_{\Lambda \nearrow \mathbb{Z}^v} \frac{1}{|\Lambda|} \sum_{A \subset \Lambda} [\Phi_A(d_A) + \Psi_A(d_A)], \quad (2.12)$$

is equal, according to Assumption 4, to $\Upsilon_x(d_{U(x)})$ (whose value does not depend on x).

Our first result concerns the existence of the thermodynamic limit for the state under periodic boundary conditions. Taking L_0 to be the smallest common period of periodic configurations from D , we always consider in the following the limit over tori $\Lambda \nearrow \mathbb{Z}^v$ whose sides are multiples of L_0 and ℓ_0 .

Theorem 2.1 (Thermodynamic limit). *Suppose that the Assumptions 1–6 are satisfied. There exist constants $\varepsilon_0 > 0$ (independent of T) and $\beta_0 = \beta_0(\Delta)$ such that the limit*

$$\langle K \rangle_\beta^{\text{per}} = \lim_{\Lambda \nearrow \mathbb{Z}^v} \frac{\text{Tr } K e^{-\beta H_\Lambda}}{\text{Tr } e^{-\beta H_\Lambda}} \quad (2.13)$$

*exists whenever $\varepsilon_1, \varepsilon_2, \|T\| \leq \varepsilon_0$ in Assumptions 5 and 6, $\beta \geq \beta_0$, and K is a local observable.*⁶

⁶ A local observable, here, is a finite sum of *even* monomials in creation and annihilation operators, in the case of fermion systems.

Notice the logic of constants in the theorem above (as well as in the remaining two theorems stated below). The constant ε_0 is given by the context (lattice, phase space, range and periodicity of the model, and Φ , but does not depend on T). Then, for any T such that $\|T\|$ and both ε_1 and ε_2 are smaller than ε_0 one can choose β_0 (depending on Δ that is determined in terms of T through the effective potential Ψ) such that the claim is valid for the given T and any $\beta \geq \beta_0(\Delta)$. With $\|T\| \rightarrow 0$ we may have to go to lower temperatures (higher β) to keep the control. Of course, if Δ does not vanish with vanishing $\|T\|$ (i.e. Assumption 4 is valid for Φ alone) as was the case in [BKU1, DFF1], one can choose the constant β_0 uniformly in $\|T\|$.

If there are coexisting phases for a given temperature and Hamiltonian, the state $\langle \cdot \rangle_\beta^{\text{per}}$ will actually turn out to be a linear combination of several pure states. A standard way how to select such a pure state is to consider a thermodynamic limit with a suitably chosen fixed boundary condition. In many situations to which the present theory should apply, this approach is not easy to implement. The classical part of the Hamiltonian might actually consist only of on-site terms and to make the system “feel” the boundary, the truly quantum terms must be used. One possibility is, of course, to couple the system with the boundary with the help of the effective potential. The problem here is, however, that since we are interested in a genuine quantum model, we would have to introduce the effective potential directly in the finite volume quantum state. Expanding this state, in a similar manner as it will be done in the next section, we would actually obtain a new, boundary dependent effective potential. One can imagine that it would be possible to cancel the respective terms by assuming that the boundary potential satisfies certain “renormalizing self-consistency conditions”. However, the details of such an approach remain to be clarified.

Here we have chosen another approach. Namely, we construct the pure states by limits of states $\langle \cdot \rangle_\beta^{\Phi^\alpha \text{ per}}$, defined by (2.13) with $H_\Lambda = V_\Lambda^{\Phi^\alpha} + T_\Lambda$, where Φ^α is a perturbation of the interaction Φ suitably chosen in such a way that one approaches the coexistence point from the one-phase region. Consider thus \mathcal{F}_{R_0} , the space of all periodic interactions of range R_0 . We say that a state $\langle \cdot \rangle_\beta^{\phi \text{ per}}$, $\phi \in \mathcal{F}_{R_0}$, is *thermodynamically stable* if it is insensitive to small perturbations:

$$\langle K \rangle_\beta^{\phi, \text{ per}} = \lim_{\alpha \rightarrow 0} \langle K \rangle_\beta^{(\phi + \alpha \psi) \text{ per}} \quad (2.14)$$

for every $\psi \in \mathcal{F}_{R_0}$ and every local observable K . We define now a state $\langle \cdot \rangle_\beta^*$ to be a *pure state* (with classical potential Φ and quantum interaction T) if there exists a function $(0, \alpha_0) \ni \alpha \rightarrow \Phi^\alpha \in \mathcal{F}_{R_0}$ so that $\lim_{\alpha \rightarrow 0^+} \Phi^\alpha = \Phi$, the states $\langle \cdot \rangle_\beta^{\Phi^\alpha \text{ per}}$ are thermodynamically stable, and

$$\langle K \rangle_\beta^* = \lim_{\alpha \rightarrow 0^+} \langle K \rangle_\beta^{\Phi^\alpha \text{ per}} \quad (2.15)$$

for every local observable K .

Theorem 2.2 (Pure low temperature phases). *Under Assumptions 1–6 and for any $\eta > 0$, there exist $\varepsilon_0 > 0$ (independent of T) and $\beta_0 = \beta_0(\Delta)$ such that if $\varepsilon_1, \varepsilon_2, \|T\| \leq \varepsilon_0$ and $\beta \geq \beta_0$, there exists for every $d \in D$ a function $f^\beta(d)$ such that the set $Q = \{d \in D; \text{Re } f^\beta(d) = \min_{d' \in D} \text{Re } f^\beta(d')\}$ characterizes the set of pure phases. Namely, for any $d \in Q$:*

a) The function $f^\beta(d)$ is equal to the free energy of the system, i.e.

$$f^\beta(d) = -\frac{1}{\beta} \lim_{\Lambda \nearrow \mathbb{Z}^v} \frac{1}{|\Lambda|} \log \text{Tr} e^{-\beta H_\Lambda}.$$

b) There exists a pure state $\langle \cdot \rangle_\beta^d$. Moreover, it is close to the state $|d_\Lambda\rangle$ in the sense that for any bounded local observable K and any sufficiently large Λ , one has

$$\left| \langle K \rangle_\beta^d - \langle d_\Lambda | K | d_\Lambda \rangle \right| \leq \eta \text{supp } K \|K\|$$

where $\text{supp } K$ is the support of the operator K .

c) There is exponential decay of correlations in the state $\langle \cdot \rangle_\beta^d$, i.e. there exists a constant $\xi^d > 0$ such that

$$\left| \langle K K' \rangle_\beta^d - \langle K \rangle_\beta^d \langle K' \rangle_\beta^d \right| \leq \|\text{supp } K\| \|\text{supp } K'\| \|K\| \|K'\| e^{-\text{dist}(\text{supp } K, \text{supp } K')/\xi^d}$$

for any bounded local observables K and K' .

d) The state $\langle \cdot \rangle_\beta^{\text{per}}$ is a linear combination of the states $\langle \cdot \rangle_\beta^d$, $d \in \mathcal{Q}$, with equal weights,

$$\langle K \rangle_\beta^{\text{per}} = \frac{1}{|\mathcal{Q}|} \sum_{d \in \mathcal{Q}} \langle K \rangle_\beta^d$$

for each local observable K .

2.5. Phase diagram. We now turn to the phase diagram at low temperatures. Let r be the number of dominant states, i.e. $r = |D|$. To be able to investigate the phase diagram, we suppose that $r - 1$ suitable “external fields” are added to the Hamiltonian H_Λ . Or, in other words, we suppose that the classical potential Φ and quantum interaction T depend on a vector parameter $\mu = (\mu_1, \dots, \mu_{r-1}) \in \mathcal{U}$, where \mathcal{U} is an open set of \mathbb{R}^{r-1} . The dependence should be such that the parameters μ remove the degeneracy on the set D of dominant states. One way to formulate this condition is to assume a nonsingularity of the matrix of derivatives $\left(\frac{\partial e^\mu(d_j)}{\partial \mu_i} \right)$.

Assumption 7. The potential Φ and the quantum perturbation T are differentiable with respect to μ and there exists a constant $M < \infty$ such that

$$\max_{n \in \Omega^{\mathbb{Z}^v}} \left| \frac{\partial}{\partial \mu_i} \Phi_x(n_{U_0(x)}) \right| \leq M$$

for all $x \in \mathbb{Z}^v$, and

$$\|T\| + \sum_{i=1}^{r-1} \left\| \frac{\partial T}{\partial \mu_i} \right\| \leq M$$

for all $\mu \in \mathcal{U}$.

Further, there exists a point $\mu_0 \in \mathcal{U}$ such that

$$e^{\mu_0}(d) = e^{\mu_0}(d') \text{ for all } d, d' \in D,$$

and the inverse of the matrix of derivatives

$$\left(\frac{\partial}{\partial \mu_i} [e^\mu(d_j) - e^\mu(d_r)] \right)_{1 \leq i, j \leq r-1}$$

has a uniform bound for all $\mu \in \mathcal{U}$.

Notice that if for some $d \in D$ one has $e^\mu(d) = e^\mu := \min_{d' \in D} e^\mu(d')$, then, according to the Peierls condition (Assumption 4), the configuration d is actually a ground state of Υ . Thus, the assumption above implies that the zero temperature phase diagram has a regular structure: there exists a point $\mu_0 \in \mathcal{U}$ where all energies $e^{\mu_0}(d)$ are equal, $e^{\mu_0}(d) = e^{\mu_0}$, r lines ending in μ_0 with $r - 1$ ground states, $\frac{1}{2}r(r - 1)$ two-dimensional surfaces whose boundaries are the lines above with $r - 2$ ground states, \dots , r open $(r - 1)$ -dimensional domains with only one ground state. Denoting the $(r - |Q|)$ -dimensional manifolds corresponding to the coexistence of a given set $Q \subset D$ of ground states by

$$\mathfrak{M}^*(Q) = \left\{ \mu \in \mathcal{U}; \operatorname{Re} e^\mu(d) = \min_{d' \in D} \operatorname{Re} e^\mu(d') \text{ if } d \in Q, \text{ and} \right. \\ \left. \operatorname{Re} e^\mu(d) > \min_{d' \in D} \operatorname{Re} e^\mu(d') \text{ if } d \notin Q \right\}, \quad (2.16)$$

we can summarize the above structure by saying that the collection $\mathcal{P}^* = \{\mathfrak{M}^*(Q)\}_{Q \subset D}$ determines a *regular phase diagram*. Notice, in particular, that $\cup_{Q \subset D} \mathfrak{M}^*(Q) = \mathcal{U}$, $\mathfrak{M}^*(Q) \cap \mathfrak{M}^*(Q') = \emptyset$ whenever $Q \neq Q'$, while for the closures, $\overline{\mathfrak{M}^*(Q)} \cap \overline{\mathfrak{M}^*(Q')} = \overline{\mathfrak{M}^*(Q \cup Q')}$. Here we set $\mathfrak{M}(\emptyset) = \emptyset$.

The statement of the following theorem is that the similar collection $\mathcal{P} = \{\mathfrak{M}(Q)\}_{Q \subset D}$ of manifolds corresponding to existence of corresponding stable pure phases for the full model is also a regular phase diagram and differs only slightly from \mathcal{P}^* . To measure the distance of two manifolds \mathfrak{M} and \mathfrak{M}' , we introduce the Hausdorff distance

$$\operatorname{dist}_H(\mathfrak{M}, \mathfrak{M}') = \max \left(\sup_{\mu \in \mathfrak{M}} \operatorname{dist}(\mu, \mathfrak{M}'), \sup_{\mu \in \mathfrak{M}'} \operatorname{dist}(\mu, \mathfrak{M}) \right).$$

Theorem 2.3 (Low temperature phase diagram). *Under Assumptions 1–7 there exist $\varepsilon_0 > 0$ and $\beta_0 = \beta_0(\Delta)$ such that if $\|T\| + \sum_{i=1}^{r-1} \left\| \frac{\partial}{\partial \mu_i} T \right\| \leq \varepsilon_0$, $\varepsilon_1, \varepsilon_2 \leq \varepsilon_0$, and $\beta \geq \beta_0$, there exists a collection of manifolds $\mathcal{P}^\beta = \{\mathfrak{M}^\beta(Q)\}_{Q \subset D}$ such that*

- (a) *The collection \mathcal{P}^β determines a regular phase diagram;*
- (b) *If $\mu \in \mathfrak{M}^\beta(Q)$, the corresponding stable pure state $\langle \cdot \rangle_\beta^d$ exists for every $d \in Q$ and satisfies the properties b), c), and d), from Theorem 2.2;*
- (c) *The Hausdorff distance dist_H between the manifolds of \mathcal{P}^β and their correspondent in \mathcal{P}^* is bounded,*

$$\operatorname{dist}_H(\mathfrak{M}^\beta(Q), \mathfrak{M}^*(Q)) \leq O(e^{-\beta} + \|T\| + \sum_{i=1}^{r-1} \left\| \frac{\partial T}{\partial \mu_i} \right\|),$$

for all $Q \subset D$.

The proofs of these theorems are given in the rest of the paper. Expansions of the partition function and expectation values of local observables are constructed, and interpreted as contours of a classical model in one additional dimension. Then we show that the assumptions for using the standard Pirogov–Sinai theory are fulfilled, and, with some special care to be taken due to our definition of stability, the validity of the three theorems follows.

3. Examples

3.1. The asymmetric Hubbard model. The usual Hubbard model describes spin- $\frac{1}{2}$ fermions on a lattice, interacting with an on-site repulsion. The kinetic energy of the particles is modelled by a hopping operator. There are many interesting questions with this model, much less rigorous results; see [Lieb] for a review.

It is natural to think of the model as describing *one* kind of particles, that can be in two different states because of their spins. But since the Hamiltonian conserves the total magnetization, we can adopt a different point of view, namely to imagine having two different kinds of particles, the \uparrow and \downarrow ones; each kind of particle obeys the Pauli exclusion principle which prevents them from being at the same site. Whenever two particles of different kinds are at the same site, there is an energy cost of U .

The natural phase space is the Fock space of antisymmetric wave functions on Λ . It is isomorphic to \mathcal{H}_Λ if we take for the state space $\Omega = \{0, \uparrow, \downarrow, 2\}$. Particles with different spins being different, it becomes natural to consider that they have different masses, hence different hopping coefficients. The Hamiltonian is written in (1.1). If we set $t_\downarrow = 0$, we obtain the Falicov–Kimball model [GM]; in the following, we consider the situation $t_\downarrow \ll t_\uparrow \ll U$ (strongly asymmetric Hubbard model). This model has for classical interaction

$$\Phi_x(n_x) = \begin{cases} 0 & \text{if } n_x = 0 \\ -\mu & \text{if } n_x = \uparrow \text{ or } n_x = \downarrow \\ U - 2\mu & \text{if } n_x = 2 \end{cases} \quad (3.1)$$

($R_0 = 0$). We choose the chemical potential such that $0 < \mu < U$. The set G is here the set of ground states of Φ , i.e.

$$G = \{n \in \Omega^{\mathbb{Z}^v} : n_x = \uparrow \text{ or } n_x = \downarrow \text{ for any } x \in \mathbb{Z}^v\}.$$

Assumption 2 holds with $\Delta_0 = \min(\mu, U - \mu)$ and $\delta_0 = 0$.

The quantum perturbation is defined to be

$$T_{\mathbf{A}} = \begin{cases} t_\uparrow c_{x\uparrow}^\dagger c_{y\uparrow} & \text{if } \mathbf{A} = (\langle x, y \rangle, \uparrow) \\ t_\downarrow c_{x\downarrow}^\dagger c_{y\downarrow} & \text{if } \mathbf{A} = (\langle x, y \rangle, \downarrow) \end{cases}, \quad (3.2)$$

and we always have $A = \{x, y\}$ for a pair of nearest neighbours $x, y \in \mathbb{Z}^v$. $\|T\| = |t_\uparrow|^{\frac{1}{2}}$ (if $|t_\uparrow| \geq |t_\downarrow|$).

The sequence \mathcal{S} of transitions that we consider is

$$\mathcal{S} = \{(\mathbf{A}, \mathbf{A}') : \mathbf{A} = (\langle x, y \rangle, \uparrow) \text{ and } \mathbf{A}' = (\langle y, x \rangle, \uparrow) \\ \text{for some } x, y \in \mathbb{Z}^v, \|x - y\|_2 = 1\}.$$

The effective potential is given by Eq. (2.8). For any $x, y \in \mathbb{Z}^v$, nearest neighbours, any configuration n such that $|n\rangle = c_{x\uparrow}^\dagger c_{y\uparrow}^\dagger |g\rangle$, $g \in G$, has an increase of energy of

$$\phi_{\{x,y\}}(n_{\{x,y\}}; g_{\{x,y\}}) = U.$$

Furthermore we have

$$\begin{aligned} & \langle g_{\{x,y\}} | c_{x\uparrow}^\dagger c_{y\uparrow}^\dagger c_{y\uparrow}^\dagger c_{x\uparrow} | g_{\{x,y\}} \rangle + \langle g_{\{x,y\}} | c_{y\uparrow}^\dagger c_{x\uparrow}^\dagger c_{x\uparrow}^\dagger c_{y\uparrow} | g_{\{x,y\}} \rangle \\ &= \begin{cases} 1 & \text{if } g_{\{x,y\}} \in \{(\uparrow, \downarrow), (\downarrow, \uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \quad (3.3)$$

Therefore

$$\Psi_{\{x,y\}}(g_{\{x,y\}}) = \begin{cases} -t_\uparrow^2/U & \text{if } g_{\{x,y\}} \in \{(\uparrow, \downarrow), (\downarrow, \uparrow)\} \\ 0 & \text{otherwise.} \end{cases} \quad (3.4)$$

This interaction is nearest-neighbour and can be inscribed in blocks $2 \times \dots \times 2$. We take $R = \frac{1}{2}$ and choose for the physically equivalent interaction Υ ,

$$\Upsilon_x(n_{U(x)}) = \Phi_x(n_x) + \frac{1}{2^{v-1}} \sum_{\{y,z\} \subset U(x)} \Psi_{\{y,z\}}(n_{\{y,z\}}). \quad (3.5)$$

The set D has two elements, namely the two chessboard configurations $d^{(1)}$ and $d^{(2)}$; if $(-1)^x := \prod_{i=1}^v (-1)^{x_i}$,

$$d_x^{(1)} = \begin{cases} \uparrow & \text{if } (-1)^x = 1 \\ \downarrow & \text{if } (-1)^x = -1 \end{cases}, \quad d_x^{(2)} = \begin{cases} \uparrow & \text{if } (-1)^x = -1 \\ \downarrow & \text{if } (-1)^x = 1 \end{cases}.$$

To find the Peierls constant Δ of Assumption 4, let us make the following observation. Consider a cube $2 \times \dots \times 2$ in \mathbb{Z}^v , that we denote C , and a configuration n_C on it. First, only configurations with one particle per site need to be taken into account, the others having an increase of energy of the order U . If $n_C \in G_C$, then all edges of the cubes are either ferromagnetic, or antiferromagnetic. If a spin at a site is flipped, then exactly v edges are changing of state. Since any configuration can be created by starting from the chessboard one, and flipping the spins at some sites, we see that the minimum number of ferromagnetic edges, for configurations that are not chessboard, is v . This leads to $\Delta = \frac{v}{2^{v-1}} \frac{t_\uparrow^2}{U}$.

The maximum of the expression in Assumption 5 is equal to $\max(t_\downarrow^2, t_\uparrow^4)$. The constant ε_1 can be chosen to be $\frac{2^{v-1}U}{v} \max(t_\downarrow^2/t_\uparrow^2, t_\uparrow^2)$. For Assumption 6 the expression has maximum equal to $|t_\downarrow t_\uparrow|$ and we can take $\varepsilon_2 = \frac{2^{v-1}U}{v} |t_\downarrow/t_\uparrow|$ (we cannot suppose this to be very small in the symmetric Hubbard model; the effective potential is not strong enough in order to forbid the model to jump from one g to another g').

Our results for the asymmetric Hubbard model can be stated in the following theorem (see also [KL, DFF2]):

Theorem 3.1 (Chessboard phases in asymmetric Hubbard model). *Consider the lattice \mathbb{Z}^v , $v \geq 2$, and suppose $0 < \mu < U$. Then for any $\delta > 0$, there exist $t, \alpha > 0$ and $\beta_0(t_\uparrow) < \infty$ ($\lim_{t_\uparrow \rightarrow 0} \beta_0(t_\uparrow) = \infty$) such that if $|t_\uparrow| \leq t$, $|t_\downarrow| \leq \alpha |t_\uparrow|$, and $\beta \geq \beta_0$,*

- the free energy exists in the thermodynamic limit with periodic boundary conditions, as well as expectation values of observables.
- There are two pure periodic phases, $\langle \cdot \rangle_\beta^{(1)}$ and $\langle \cdot \rangle_\beta^{(2)}$, with exponential decay of correlations.
- One of these pure phases, $\langle \cdot \rangle_\beta^{(1)}$, is a small deformation of the chessboard state $|d^{(1)}\rangle$:

$$\langle n_{x\uparrow} \rangle_\beta^{(1)} \begin{cases} \geq 1 - \delta & \text{if } (-1)^x = 1 \\ \leq \delta & \text{if } (-1)^x = -1 \end{cases} \quad \langle n_{x\downarrow} \rangle_\beta^{(1)} \begin{cases} \leq \delta & \text{if } (-1)^x = 1 \\ \geq 1 - \delta & \text{if } (-1)^x = -1. \end{cases}$$

The other pure phase, $\langle \cdot \rangle_\beta^{(2)}$, is a small deformation of $|d^{(2)}\rangle$.

To construct the two pure phases, one way is to consider the Hamiltonian

$$H_\Lambda(h) = H_\Lambda - h \sum_{x \in \Lambda} (-1)^x (n_{x\uparrow} - n_{x\downarrow}).$$

Then

$$\langle \cdot \rangle_\beta^{(1)} = \lim_{h \rightarrow 0^+} \langle \cdot \rangle_\beta^{\text{per}}(h)$$

and

$$\langle \cdot \rangle_\beta^{(2)} = \lim_{h \rightarrow 0^-} \langle \cdot \rangle_\beta^{\text{per}}(h),$$

where $\langle \cdot \rangle_\beta^{\text{per}}(h)$ is defined by (2.13) with Hamiltonian $H_\Lambda(h)$.

3.2. The Bose–Hubbard model. This model was introduced by Fisher *et al.* [FWGF] and may describe ^4He absorbed in porous media, or Cooper pairs in superconductors, . . . It is extremely simple, but has very interesting phase diagram with insulating and superfluid domains [FWGF]. Rigorous results mainly concern the insulating phases; when the classical model [(1.2) with $t = 0$] has a finite number of ground states, existence of Gibbs states that are close to projection operators onto the classical ground states can be proven for small t and large β ; moreover, the compressibility vanishes in the ground states of the quantum model [BKU2].

If $U_0 = \infty$, $U_1 = U_2 = 0$ and $\mu = 0$, we obtain a model of hard-core bosons; the reflection positivity technique [DLS] shows that the model has off-diagonal long-range order at low enough temperature, hence has superfluid behaviour.

On-site repulsion U_0 discourages too high occupancy of sites, so it is physically harmless to introduce a generalized hard-core constraint, namely that there cannot be more than N bosons at the same site. As a consequence the local state space is $\Omega = \{0, 1, 2, \dots, N\}$ and is finite.

We restrict our discussion to the two-dimensional case. The range R_0 is equal to $\frac{1}{2}$, and the classical interaction is

$$\begin{aligned} \Phi_x(n_{U_0(x)}) = & \frac{1}{4} \sum_{y \in U_0(x)} (U_0 n_x^2 - U_0 n_x - \mu n_x) + \\ & + \frac{1}{2} U_1 \sum_{\substack{y, z \in U_0(x) \\ \|y-z\|_2=1}} n_y n_z + U_2 \sum_{\substack{y, z \in U_0(x) \\ \|y-z\|_2=\sqrt{2}}} n_y n_z. \end{aligned} \quad (3.6)$$

Remark that we have [BKU2]

$$\begin{aligned} \Phi_x(n_{U_0(x)}) &= \left(\frac{1}{4}U_0 - U_1 + U_2\right) \sum_{y \in U_0(x)} \left(n_y - \frac{1}{2}\right)^2 + \left(\frac{1}{4}U_1 - \frac{1}{2}U_2\right) \\ &\cdot \sum_{\substack{y, z \in U_0(x) \\ \|y-z\|_2=1}} \left(n_y + n_z - \frac{1}{2}\right)^2 + U_2 \left(\sum_{y \in U_0(x)} n_y - \frac{1}{2} - \frac{\mu}{8U_2}\right)^2 + C \end{aligned} \quad (3.7)$$

with a constant C independent of n . When the chemical potential satisfies $0 < \mu < 8U_2$, $\Phi_x(n_{U_0(x)})$ is minimum if $n_{U_0(x)} = \begin{pmatrix} \bullet & \circ \\ \circ & \circ \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, or any configuration obtained from $\begin{pmatrix} \bullet & \circ \\ \circ & \circ \end{pmatrix}$ by rotation. Hence we define

$$G_0(x) = \left\{ \begin{pmatrix} \bullet & \circ \\ \circ & \circ \end{pmatrix}, \begin{pmatrix} \circ & \bullet \\ \circ & \circ \end{pmatrix}, \begin{pmatrix} \circ & \circ \\ \circ & \bullet \end{pmatrix}, \begin{pmatrix} \circ & \circ \\ \bullet & \circ \end{pmatrix} \right\}$$

for any $x \in \mathbb{Z}^{\nu}$. Here, G is the set of ground states of the interaction Φ , so that $\delta_0 = 0$. Since $\Phi_x(n_{U_0(x)}) - \Phi_x(g_{U_0(x)}) \geq \frac{1}{4} \min(\mu, 8U_2 - \mu)$, for any $n_{U_0(x)} \notin G_{U_0(x)}$, $g_{U_0(x)} \in G_{U_0(x)}$, Assumption 2 holds with $\Delta_0 = \frac{1}{36} \min(\mu, 8U_2 - \mu)$ (the factor $\frac{1}{36}$, rather than $\frac{1}{4}$, has been chosen in view of Assumption 4, see below).

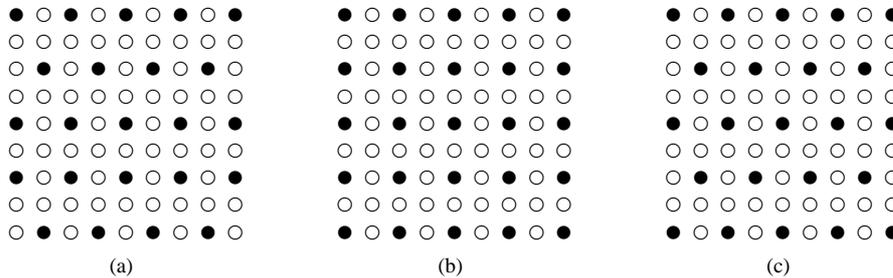
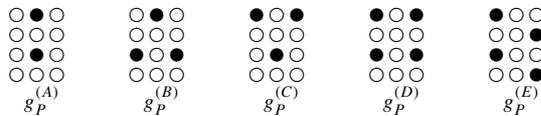


Fig. 2. Configurations that minimize the diagonal interaction; (a) a general configuration; (b) and (c) two natural candidates that may be selected by lowest quantum fluctuations. Actually, candidate (c) dominates, because it allows for more freedom in the moves of bosons.

We take as a sequence of transitions for the smallest quantum fluctuations

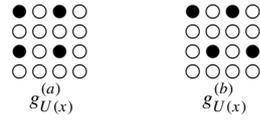
$$S = \{(\mathbf{A}, \mathbf{A}') : \mathbf{A} = \langle x, y \rangle \text{ and } \mathbf{A}' = \langle y, x \rangle \text{ for some } x, y \in \mathbb{Z}^2, \|x - y\|_2 = 1\}.$$

The effective potential follows from (2.8). Let $P_{xy} = \{z : |z - x| \leq 1 \text{ or } |z - y| \leq 1\}$ and more generally we denote by P any 3×4 or 4×3 rectangle. Up to rotations and reflections, we have to take into account five configurations, namely



We find $\Psi_P(g_P^{(A)}) = -t^2/2U_1$, $\Psi_P(g_P^{(C)}) = -t^2/4U_2$, and $\Psi_P(g_P^{(B)}) = \Psi_P(g_P^{(D)}) = \Psi_P(g_P^{(E)}) = 0$.

We can choose $R = \frac{3}{2}$; $U(x)$ is a block 4×4 centered on $(x_1 + \frac{1}{2}, x_2 + \frac{1}{2})$. The configurations $g_{U(x)} \in G_{U(x)}$ are (up to rotations and reflections)



We choose for Υ

$$\Upsilon_x(n_{U(x)}) = \frac{1}{9} \sum_{y, U_0(y) \subset U(x)} \tilde{\Phi}_y(n_{U_0(y)}) + \frac{1}{2} \sum_{P \subset U(x)} \Psi_P(n_P), \quad (3.8)$$

with $\tilde{\Phi}_y(n_{U_0(y)}) = \Phi_y(n_{U_0(y)}) - \min_{g \in G} \Phi_y(n_{U_0(y)})$. Which configurations, among the four generated by $g^{(a)}$ and the eight generated by $g^{(b)}$, allow for more quantum fluctuations? The effective potential yields

$$\begin{aligned} \Upsilon_x(g_{U(x)}^{(a)}) &= -\frac{t^2}{2U_1}, \\ \Upsilon_x(g_{U(x)}^{(b)}) &= -\frac{t^2}{4U_1} - \frac{t^2}{8U_2}. \end{aligned}$$

We see that the set of dominant states D is formed by all the configurations generated by $g^{(b)}$ (recall that $U_1 > 2U_2$). Heuristically, there is more freedom for the bosons to move in $g^{(b)}$, since they can go to a nearest-neighbour site and feel a small repulsion of strength U_2 ; as for bosons of the configuration $g^{(a)}$, any nearest-neighbour move brings them at distance 1 of another boson, and they feel a bigger repulsion U_1 .

As a result we can choose $\Delta = t^2(\frac{1}{8U_2} - \frac{1}{4U_1})$ in Assumption 4. The maximum of the expression in Assumption 5 is $\varepsilon_1 = t^2(\frac{1}{8U_2} - \frac{1}{4U_1})^{-1}$. In Assumption 6 we have $\varepsilon_2 = 0$, because $g \neq g'$ means that g and g' must differ on a whole row, and the matrix element is zero for any finite m .

These eight dominant states bring eight pure periodic phases, $\langle \cdot \rangle^{(1)}, \dots, \langle \cdot \rangle^{(8)}$; each one can be constructed by adding a suitable field in the Hamiltonian (e.g. the projector onto the dominant state).

Theorem 3.2 (Bose–Hubbard model). *Consider the Bose–Hubbard model on the lattice \mathbb{Z}^2 with a generalized hard-core, and suppose $U_0 \geq 4(U_1 - U_2)$, $U_1 > 2U_2$ and $0 < \mu < 8U_2$. There exist $t_0 > 0$ and $\beta_0(t) < \infty$ ($\lim_{t \rightarrow 0} \beta_0(t) = \infty$) such that if $t \leq t_0$ and $\beta \geq \beta_0$,*

- *the free energy exists in the thermodynamic limit with periodic boundary conditions, as well as expectation values of observables,*
- *there are 8 pure periodic phases with exponential decay of correlations.*

Each of these eight phases is a perturbation of a dominant state d , and the expectation value of any local operator is close to its value in the state d , see Theorem 2.2 for more precise statement.

Similar properties hold for other quarter-integer density phases. Equation (3.7) may be generalized so as to exhibit gaps for the spectrum of Φ , cf. [BKU2].

4. Contour Representation of a Quantum Model

Our Hamiltonian has periodicity $\ell_0 < \infty$. Without loss of generality, however, one can consider only translation invariant Hamiltonians, applying the standard trick. Namely, if Ω is the single site phase space, we let $\Omega' = \Omega^{\{1, \dots, \ell_0\}^\nu}$; $S' = |\Omega'| = S^{\ell_0^\nu}$. Then we consider the torus $\Lambda' \subset \mathbb{Z}^\nu$, $\ell_0^\nu |\Lambda'| = |\Lambda|$, each point of which is representing a block of sites in Λ of size ℓ_0^ν , and identify

$$\Omega'^{\Lambda'} \simeq \Omega^\Lambda.$$

Constructing \mathcal{H}' as the Hilbert space spanned by the elements of $\Omega'^{\Lambda'}$, it is clear that \mathcal{H}' is isomorphic to \mathcal{H} . The new translation invariant interactions Φ' and T' are defined by resumming, for each $A \subset \Lambda'$, the corresponding contributions with supports in the union of corresponding blocks. Notice the change in range of interactions. Namely, it decreased to $\lceil R/\ell_0 \rceil$ (the lowest integer bigger or equal to R/ℓ_0).

From now on, keeping the original notation \mathcal{H} , S , \dots , we suppose that the Hamiltonian is translation invariant.

The partition function of a quantum model is a trace over a Hilbert space. But expanding $e^{-\beta H}$ with the help of the Duhamel formula we can reformulate it in terms of the partition function of a classical model in a space with one additional dimension (the extra dimension being continuous). In this section we present such an expansion, leading to a contour representation, of the partition function $Z_\Lambda^{\text{per}} := \text{Tr} e^{-\beta H_\Lambda}$ in a finite torus Λ^{per} .

Expansion with the help of the Duhamel formula yields

$$e^{-\beta H_\Lambda} = \sum_{m \geq 0} \sum_{\substack{\mathbf{A}_1, \dots, \mathbf{A}_m \\ \tilde{A}_i \subset \Lambda^{\text{per}}}} \int_{0 < \tau_1 < \dots < \tau_m < \beta} d\tau_1 \dots d\tau_m \\ e^{-\tau_1 V_\Lambda} T_{\mathbf{A}_1} e^{-(\tau_2 - \tau_1) V_\Lambda} T_{\mathbf{A}_2} \dots T_{\mathbf{A}_m} e^{-(\beta - \tau_m) V_\Lambda}. \quad (4.1)$$

Inserting the expansion of unity $\mathbb{1}_{\mathcal{H}_\Lambda} = \sum_{n_\Lambda} |n_\Lambda\rangle \langle n_\Lambda|$ to the right of operators $T_{\mathbf{A}_j}$, we obtain

$$Z_\Lambda^{\text{per}} = \sum_{n_\Lambda} e^{-\beta V_\Lambda(n_\Lambda)} + \sum_{m \geq 1} \sum_{n_\Lambda^1, \dots, n_\Lambda^m} \sum_{\substack{\mathbf{A}_1, \dots, \mathbf{A}_m \\ \tilde{A}_i \subset \Lambda^{\text{per}}}} \int_{0 < \tau_1 < \dots < \tau_m < \beta} d\tau_1 \dots d\tau_m \\ e^{-\tau_1 V_\Lambda(n_\Lambda^1)} \langle n_\Lambda^1 | T_{\mathbf{A}_1} | n_\Lambda^2 \rangle e^{-(\tau_2 - \tau_1) V_\Lambda(n_\Lambda^2)} \dots \langle n_\Lambda^m | T_{\mathbf{A}_m} | n_\Lambda^1 \rangle e^{-(\beta - \tau_m) V_\Lambda(n_\Lambda^1)}. \quad (4.2)$$

For notational simplicity, we wrote $V_\Lambda(n_\Lambda)$ instead of $\langle n_\Lambda | V_\Lambda | n_\Lambda \rangle$. This expansion can be interpreted as a classical partition function on the $(\nu+1)$ -dimensional space $\Lambda \times [0, \beta]$. Namely, calling the additional dimension “time direction”, the partition function Z_Λ^{per} is a (continuous) sum over all space-time configurations $\mathbf{n}_\Lambda = \mathbf{n}_\Lambda(\tau)$, $\tau \in [0, \beta]$, and all possible transitions at times corresponding to discontinuities of $\mathbf{n}_\Lambda(\tau)$. Notice that $\mathbf{n}_\Lambda(\tau)$ is periodic in the time direction. Thus, actually, we obtain a classical partition function on the $(\nu+1)$ -dimensional torus $\mathbb{T}_\Lambda = \Lambda^{\text{per}} \times [0, \beta]_{\text{per}}$ with a circle $[0, \beta]_{\text{per}}$ in the time direction (for simplicity we omit in \mathbb{T}_Λ a reference to β). Introducing the *quantum configuration* $\omega_{\mathbb{T}_\Lambda}$ consisting of the space-time configuration $\mathbf{n}_\Lambda(\tau)$ and the transitions (\mathbf{A}_i, τ_i) at corresponding times, we can rewrite (4.2) in a compact form

$$Z_{\Lambda}^{\text{per}} = \int d\omega_{\mathbb{T}_{\Lambda}} \rho(\omega_{\mathbb{T}_{\Lambda}}) \quad (4.3)$$

with $\rho(\omega_{\mathbb{T}_{\Lambda}})$ standing for the second line of (4.2).

Now, we are going to specify excitations within a space-time configuration \mathbf{n} and identify classes of small excitations – *the loops*⁷ – and large ones – *the quantum contours*.

A configuration $n \in \Omega^{\mathbb{Z}^v}$ is said to be in the state $g \in G$ at site x whenever $n_{U_0(x)} = g_{U_0(x)}$ (notice that, in general, g is not unique). If there is no such $g \in G$, the configuration n is said to be *classically excited* at x . We use $E(n)$ to denote the set of all classically excited sites of $n \in \Omega^{\mathbb{Z}^v}$. For any $\Lambda \subset \mathbb{Z}^v$, let us consider the set \mathcal{Q}_{Λ} of quantum configurations on the torus \mathbb{T}_{Λ} . Whenever $\omega \in \mathcal{Q}_{\Lambda}$, its *boundary* $\mathbf{B}^{(0)}(\omega) \subset \mathbb{T}_{\Lambda}$ is defined as the union

$$\mathbf{B}^{(0)}(\omega) = (\cup_{\tau \in [0, \beta]} (E(\mathbf{n}(\tau)) \times \tau)) \cup (\cup_{i=1}^m (\bar{A}_i \times \tau_i)).$$

The sets $\bar{A}_i \times \tau_i \subset \mathbb{T}_{\Lambda}$ represent the effect of the operator T and for this reason are called *quantum transitions*. It is worth noticing that the set $\mathbf{B}^{(0)}(\omega)$ is closed.

The next step is to identify the smallest quantum excitations – those consisting of a sequence of transitions from the list \mathcal{S} . First, let us use $\mathcal{B}^{(0)}(\omega)$ to denote the set of connected components of $\mathbf{B}^{(0)}(\omega)$ (so that $\mathbf{B}^{(0)}(\omega) = \cup_{B \in \mathcal{B}^{(0)}(\omega)} B$). To any $B \in \mathcal{B}^{(0)}(\omega)$ that is not wrapped around the cylinder (i.e., for which there exists a time $\tau_B \in [0, \beta]_{\text{per}}$ with $B \cap (\mathbb{Z}^v \times \tau_B) = \emptyset$) we assign its sequence of transitions, $S(B, \omega)$, ordered according to their times (starting from τ_B to β and proceeding from 0 to τ_B) as well as the smallest box \tilde{B} containing B . Here, a box is any subset of $\mathbb{T}_{\mathbb{Z}^v}$ of the form $A \times [\tau_1, \tau_2]$ with connected $A \subset \mathbb{Z}^v$ and $[\tau_1, \tau_2] \subset [0, \beta]_{\text{per}}$ (if $\tau_1 > \tau_2$, we interpret the segment $[\tau_1, \tau_2]$ as that interval in $[0, \beta]_{\text{per}}$ (with endpoints τ_1 and τ_2) that contains the point $0 \equiv \beta$).

We would like to declare the excitations with $S(B, \omega) \in \mathcal{S}$ to be small. However, we need to be sure that there are no other excitations in their close neighbourhood. If this were the case, we would “glue” the neighbouring excitations together. This motivates the following iterative procedure.

Given ω , let us first consider the set $\mathcal{B}_0^{(0)}(\omega)$ of those components $B \in \mathcal{B}^{(0)}(\omega)$ that are not wrapped around the cylinder and for which $S(B, \omega) \in \bar{\mathcal{S}}$, where $\bar{\mathcal{S}}$ is the set of all subsequences of sequences from \mathcal{S} . Next, we define the first extension of the boundary,

$$\mathbf{B}^{(1)}(\omega) = (\cup_{B \in \mathcal{B}^{(0)}(\omega) \setminus \mathcal{B}_0^{(0)}(\omega)} B) \cup (\cup_{B \in \mathcal{B}_0^{(0)}(\omega)} \tilde{B}).$$

Using $\mathcal{B}^{(1)}(\omega)$ to denote the set of connected components of $\mathbf{B}^{(1)}(\omega)$ and $\mathcal{B}_0^{(1)}(\omega) \subset \mathcal{B}^{(1)}(\omega)$ the set of those components B in $\mathcal{B}^{(1)}(\omega)$ that are not wrapped around the cylinder and for which⁸ $S(B, \omega) \in \bar{\mathcal{S}}$, we define

$$\mathbf{B}^{(2)}(\omega) = (\cup_{B \in \mathcal{B}^{(1)}(\omega) \setminus \mathcal{B}_0^{(1)}(\omega)} B) \cup (\cup_{B \in \mathcal{B}_0^{(1)}(\omega)} \tilde{B}).$$

Iterating this procedure, it is clear that after a finite number of steps we obtain the final extension of the boundary,

$$\mathbf{B}(\omega) = (\cup_{B \in \mathcal{B}^{(k)}(\omega) \setminus \mathcal{B}_0^{(k)}(\omega)} B) \cup (\cup_{B \in \mathcal{B}_0^{(k)}(\omega)} B). \quad (4.4)$$

⁷ Even though the present framework is more general, the name comes from thinking about simplest excitations in Hubbard type models. Namely, a jump of an electron to a neighbouring site and returning afterwards to its original position.

⁸ A set $B \in \mathcal{B}_0^{(1)}(\omega)$ may actually contain several original components from $\mathcal{B}_0^{(0)}(\omega)$. We take for $S(B, \omega)$ the sequence of all transitions in all those components.

Here, every $B \in \mathcal{B}_0^{(k)}(\omega)$ is a box of the form $A \times [\tau_1, \tau_2]$ (that is not wrapped around the cylinder) and $S(B, \omega) \in \bar{\mathcal{S}}$. Let us denote $\mathcal{B}(\omega) \equiv \mathcal{B}_0^{(k)}(\omega)$ and consider the set $\mathcal{B}_0(\omega) \subset \mathcal{B}(\omega)$ of all those sets $B \in \mathcal{B}_0^{(k)}(\omega)$ for which actually $S(B, \omega) \in \mathcal{S}$ and, moreover, $n_A(\tau_1 - 0) = n_A(\tau_2 + 0)$. Finally, let $\mathcal{B}_1(\omega) = \mathcal{B}(\omega) \setminus \mathcal{B}_0(\omega)$ – “1” for “large”: it represents the set of all excitations of ω that are not loops. Taking, for any closed $B \subset \mathbb{T}_\Lambda$, the restriction \mathbf{n}_B of a space-time configuration \mathbf{n} to be defined by $(\mathbf{n}_B)_x(\tau) = \mathbf{n}_x(\tau)$ for any $x \times \tau \in B$, we introduce the useful notion of the restriction ω_B of a quantum configuration ω to B as to consist of \mathbf{n}_B and those quantum transitions from ω that are contained in B , $A \times \tau \subset B$ (we suppose here that ω and B are such that no transition intersects both B and its complement; we do not define ω_B in this case).

Now the loops and the quantum contours can be defined. First, the *loops* of a quantum configuration ω are the triplets $\xi \equiv (B, \omega_B, g_A^\xi)$; $B \equiv A \times [\tau_1, \tau_2] \in \mathcal{B}_0(\omega)$ is the *support* of the loop ξ and $g_A^\xi = n_A(\tau_1 - 0) = n_A(\tau_2 + 0)$, a restriction of a configuration $g \in G$. (While the configuration g is not unique, its restriction to A is determined by the loop ξ in a unique way.) We say that ξ is *immersed* in g . Given a quantum configuration ω , we obtain a new configuration $\check{\omega}$ by erasing all loops (B, ω_B, g_A^ξ) , i.e. for each ξ we remove all the transitions in its support B and change the space-time configuration on B into $g \in G$ into which ξ is immersed. Let us remark that $\mathcal{B}(\check{\omega}) = \mathcal{B}_1(\omega)$. Notice that, since we started our construction from (4), we have automatically $\text{diam } A \geq 2R_0$ for a support $A \times [\tau_1, \tau_2]$ of any loop ξ .

Remark. The procedure described here to identify the loops of a quantum configuration is rather intricate. This is so because we consider a quite general class of models; when studying a special model, it is possible to give a more explicit definition of the loops, and to avoid this iteration.

Quantum contours of a configuration ω will be constructed by extending pairs (B, ω_B) with $B \in \mathcal{B}_1(\omega)$ by including also the regions of nondominating states from G . Namely, summing over loops we will see that “loop free energy” favours the regions with dominating configurations from $D \subset G$. However, to recognize the influence of loops, we have to look on regions of size comparable to the size of loops. This motivates the following definitions with $U(x) = \{y \in \mathbb{Z}^v, |x - y| \leq R\}$ being an extension of the original neighbourhood $U_0(x)$. Thus, we enlarge the set $E(n)$ of classically excited sites to $\tilde{E}(n)$, with

$$\tilde{E}(n) = \{x \in \mathbb{Z}^v : n_{U(x)} \neq g_{U(x)} \text{ for any } g \in G\} \quad (4.5)$$

and we introduce the set $F(n)$ of *softly excited sites* by

$$F(n) = \{x \in \mathbb{Z}^v \setminus \tilde{E}(n) : n_{U(x)} \neq d_{U(x)} \text{ for any } d \in D\}. \quad (4.6)$$

Then, for a quantum configuration such that $\omega = \check{\omega}$, we define the new extended boundary

$$\mathbf{B}_e(\check{\omega}) = \bigcup_{\tau \in [0, \beta]_{\text{per}}} \left([\tilde{E}(\mathbf{n}(\tau)) \cup F(\mathbf{n}(\tau))] \times \tau \right) \bigcup_{i=1}^m \left(\left[\bigcup_{x \in A_i} U(x) \right] \times \tau_i \right), \quad (4.7)$$

and if $\omega \neq \check{\omega}$, we set $\mathbf{B}_e(\omega) = \mathbf{B}_e(\check{\omega})$. Notice that $\mathbf{B}(\check{\omega}) \subset \mathbf{B}_e(\omega)$, since the first set is the union of classical excitations, quantum transitions and boxes; obviously the classical excitations and the quantum transitions also belong to $\mathbf{B}_e(\omega)$, and the boxes being such that their diameter is smaller than $2R$ and they contain $U_0(x)$ -excited sites

at each time, they are $U(x)$ -excited. Decomposing $\mathbf{B}_e(\boldsymbol{\omega})$ into connected components, we get our quantum contours, namely $\gamma = (B, \boldsymbol{\omega}_B)$. Notice that the configuration $\boldsymbol{\omega}_B$ contains actually also the information determining which dominant ground state lies outside B . We call the set B the *support* of γ , $B = \text{supp } \gamma$, and introduce also its “truly excited part”, the *core*, core $\gamma \subset \text{supp } \gamma$, by taking

$$\text{core } \gamma = \text{supp } \gamma \cap \left(\bigcup_{\tau \in [0, \beta]_{\text{per}}} (\tilde{E}(\mathbf{n}(\tau)) \times \tau) \cup \bigcup_{i=1}^m \left(\left[\bigcup_{x \in A_i} U(x) \right] \times \tau_i \right) \right). \quad (4.8)$$

Finally, notice that if the contour is not wrapped around the torus in its spatial direction, there exists a space-time configuration $\boldsymbol{\omega}^\gamma$ and we have $B = \mathbf{B}_e(\boldsymbol{\omega}^\gamma)$.

A set of quantum contours $\Gamma = \{\gamma_1, \dots, \gamma_k\}$ is called admissible if there exists a quantum configuration $\boldsymbol{\omega}^\Gamma \in \mathcal{Q}_\Lambda$ which has Γ as set of quantum contours; clearly, if $\boldsymbol{\omega}^\Gamma$ exists, it is unique under the assumption that it contains no loop (i.e. $\boldsymbol{\omega}^\Gamma = \check{\boldsymbol{\omega}}^\Gamma$). We use \mathcal{D}_Λ to denote the set of all collections Γ of admissible quantum contours, and extend the notions of core and support to sets of contours, namely core $\Gamma = \bigcup_{\gamma \in \Gamma} \text{core } \gamma$, $\text{supp } \Gamma = \bigcup_{\gamma \in \Gamma} \text{supp } \gamma$.

Given $\Gamma \in \mathcal{D}_\Lambda$, a set of loops $\Xi = \{\xi_1, \dots, \xi_\ell\}$ is said to be admissible and compatible with Γ if there exists $\boldsymbol{\omega}^{\Gamma \cup \Xi}$ which has Ξ as a set of loops and Γ as a set of quantum contours (it is also unique whenever it exists). More explicitly,

- two loops $\xi = (B, \boldsymbol{\omega}_B, g_A^\xi)$ and $\xi' = (B', \boldsymbol{\omega}'_{B'}, g_A^{\xi'})$ are compatible, $\xi \sim \xi'$, iff $B \cup B'$ is not connected;
- a loop $\xi = (B, \boldsymbol{\omega}_B, g_A^\xi)$, with $B = A \times [\tau_1, \tau_2]$, is compatible with Γ , $\xi \sim \Gamma$, iff

$$\begin{aligned} B \cup \mathbf{B}(\boldsymbol{\omega}^\Gamma) &\text{ is not connected,} \\ g_A^\xi &= \mathbf{n}_A^\Gamma(\tau) \text{ for all } \tau \in [\tau_1, \tau_2]; \end{aligned}$$

- a collection of loops $\Xi = \{\xi_1, \dots, \xi_\ell\}$ is admissible and compatible with Γ iff any two loops from Ξ are compatible and each loop from Ξ is compatible with Γ .

We use $\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)$ to denote the set of all admissible collections Ξ that are compatible with Γ .

The conditions of admissibility and compatibility above can be, for any given set of transitions $\{\mathbf{A}_1, \dots, \mathbf{A}_m\}$, formulated as a finite number of restrictions on corresponding transition times $\{\tau_1, \dots, \tau_m\}$. Given the restrictions on admissibility of $\Gamma \in \mathcal{D}_\Lambda$, the restrictions on Ξ to belong to $\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)$ factorize. As a result, the partition function Z_Λ^{per} in (4.3) can be rewritten in terms of integrations over \mathcal{D}_Λ and $\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)$ [the summation over Γ and Ξ accompanied with the integration, *a priori* over the interval $[0, \beta]$, over times τ_i of corresponding transitions, subjected to the above formulated restrictions, cf. (4.2)]. Furthermore the contribution of $\Gamma \cup \Xi$ factorizes as a contribution of Γ times a product of terms for $\xi \in \Xi$ [BKU1, DFF1],⁹ we get

$$Z_\Lambda^{\text{per}} = \int_{\mathcal{D}_\Lambda} d\Gamma \int_{\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)} d\Xi \rho(\boldsymbol{\omega}^{\Gamma \cup \Xi}) = \int_{\mathcal{D}_\Lambda} d\Gamma \rho(\boldsymbol{\omega}^\Gamma) \int_{\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)} d\Xi \prod_{\xi \in \Xi} z(\xi). \quad (4.9)$$

⁹ For spin or boson systems factorization is true simply because any two operators with disjoint supports commute. In the case of fermion systems there is an additional sign due to anticommutation relations between creation and annihilation operators, and factorization is no more obvious. That it indeed factorizes was nicely proved in Sect. 4.2 of [DFF1].

Here, using $\{(\mathbf{A}_i, \tau_i), i = 1, \dots, m\}$ to denote the quantum transitions of $\Gamma \cup \Xi$, we put

$$\rho(\omega^{\Gamma \cup \Xi}) = \prod_{i=1}^m \langle \mathbf{n}_{A_i}^{\Gamma \cup \Xi}(\tau_i - 0) | T_{A_i} | \mathbf{n}_{A_i}^{\Gamma \cup \Xi}(\tau_i + 0) \rangle \exp \left\{ - \int_{\mathbb{T}_\Lambda} d(x, \tau) \Phi_x(\mathbf{n}_{U_0(x)}^{\Gamma \cup \Xi}(\tau)) \right\}, \quad (4.10)$$

where $\int_B d(x, \tau)$ is the shorthand for $\int_0^\beta d\tau \sum_{x: x \times \tau \in B}$ (used here for $B = \mathbb{T}_\Lambda$). Similarly for $\rho(\omega^\Gamma)$. Further, the weight of a loop $\xi = (B, \omega_B, g_A)$ with the set of quantum transitions $\{(\mathbf{A}_i, \tau_i), i = 1, \dots, \ell\}$ and \mathbf{n} the space-time configuration corresponding to ω_B , is

$$z(\xi) = \exp \left\{ - \int_0^\beta d\tau \sum_{x, U_0(x) \subset A} [\Phi_x(\mathbf{n}_{U_0(x)}(\tau)) - \Phi_x(g_{U_0(x)})] \right\} \langle g_{A_1} | T_{A_1} | \mathbf{n}_{A_1}(\tau_1 + 0) \rangle \times \\ \times \langle \mathbf{n}_{A_2}(\tau_2 - 0) | T_{A_2} | \mathbf{n}_{A_2}(\tau_2 + 0) \rangle \dots \langle \mathbf{n}_{A_\ell}(\tau_\ell - 0) | T_{A_\ell} | g_{A_\ell} \rangle. \quad (4.11)$$

Given $\Gamma \in \mathcal{D}_\Lambda$, the second integral in (4.9) is over the collections of loops that interact only through a condition of non-intersection. This is the usual framework for applying the cluster expansion of polymers. The only technical difficulty is that the set of our loops is uncountable (the loops depend on continuous transition times), and thus we cannot simply quote the existing literature. Nevertheless, the needed extension is rather straightforward and often implicitly used.

Given a collection $\mathcal{C} = (\xi_1, \dots, \xi_n)$ of loops, we define the truncated function

$$\Phi^T(\mathcal{C}) = \frac{1}{n!} \varphi^T(\mathcal{C}) \prod_{\xi \in \mathcal{C}} z(\xi), \quad (4.12)$$

with

$$\varphi^T(\mathcal{C}) = \varphi^T(\xi_1, \dots, \xi_n) = \begin{cases} 1 & \text{if } n = 1, \\ \sum_{\mathcal{G}} \prod_{e(i,j) \in \mathcal{G}} (\mathbb{I}[\xi_i \sim \xi_j] - 1) & \text{if } n \geq 2, \end{cases}$$

where the sum is over all connected graphs \mathcal{G} of n vertices. Notice that $\Phi^T(\mathcal{C}) = 0$ whenever \mathcal{C} is not a cluster, i.e. if the union of the supports of its loops is not connected. We use \mathcal{L}_Λ and \mathcal{C}_Λ to denote the set of all loops and clusters, respectively, and use $\int_{\mathcal{C}_\Lambda} d\mathcal{C}$ as a shorthand for $\sum_{n \geq 1} \int_{\mathcal{L}_\Lambda} d\xi_1 \dots \int_{\mathcal{L}_\Lambda} d\xi_n$, in obvious meaning. Whenever $\Gamma \in \mathcal{D}_\Lambda$ is fixed, we use $\mathcal{L}_\Lambda(\Gamma)$ to denote the set of all loops compatible with Γ and write $\mathcal{C} \in \mathcal{C}_\Lambda(\Gamma)$ whenever the cluster \mathcal{C} contains only loops from $\mathcal{L}_\Lambda(\Gamma)$. Again, $\int_{\mathcal{C}_\Lambda(\Gamma)} d\mathcal{C}$ is a shorthand for $\sum_{n \geq 1} \int_{\mathcal{L}_\Lambda(\Gamma)} d\xi_1 \dots \int_{\mathcal{L}_\Lambda(\Gamma)} d\xi_n$. Finally, we also need similar integrals conditioned by the time of the first transition encountered in the loop ξ or the cluster \mathcal{C} . Namely, using \mathcal{C} to denote the support of \mathcal{C} , i.e. the union of the supports of the loops of \mathcal{C} , and $I_{\mathcal{C}} = \{\tau_1(\mathcal{C}), \tau_2(\mathcal{C})\}$ to denote its vertical projection,¹⁰ $I_{\mathcal{C}} = \{\tau \in [0, \beta]_{\text{per}}; \mathbb{Z}^v \times \tau \cap \mathcal{C} \neq \emptyset\}$, we use $\mathcal{C}_\Lambda^{(x, \tau)}$ for the set of all clusters $\mathcal{C} \in \mathcal{C}_\Lambda$ with the first transition time $\tau_1(\mathcal{C}) = \tau$, for which their first loop ξ_1 with support $B_1 = A_1 \times [\tau_1(\mathcal{C}), \tau_2]$, contains the site x , $A_1 \ni x$. Then $\int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi$ and $\int_{\mathcal{C}_\Lambda^{(x, \tau)}} d\mathcal{C}$ are shorthands for the corresponding integrals with first transition time fixed – formally one replaces $\int d\xi_1$ by $\int \mathbb{I}[A_1 \ni x] \delta(\tau_1(\xi_1) - \tau) d\xi_1$. With this notation we can formulate the cluster expansion lemma.

¹⁰ Again, if $\tau_1 > \tau_2$, the segment $[\tau_1, \tau_2] \subset [0, \beta]_{\text{per}}$ contains the point $0 \equiv \beta$.

Lemma 4.1 (Cluster expansion). *For any $c \in \mathbb{R}$, $\alpha_1 < (4R_0)^{-\nu}$, $\alpha_2 < R^{-2\nu} \Delta_0$ and $\delta > 0$, there exists $\varepsilon_0 > 0$ such that whenever $\|T\| \leq \varepsilon_0$ and $\Gamma \in \mathcal{D}_\Lambda$, we have the loop cluster expansion,*

$$\int_{\mathcal{D}_\Lambda^{\text{loop}}(\Gamma)} d\Xi \prod z(\xi) = \exp \left\{ \int_{\mathcal{C}_\Lambda(\Gamma)} d\mathbf{C} \Phi^{\mathbf{T}}(\mathbf{C}) \right\}. \quad (4.13)$$

Moreover, the weights of the clusters are exponentially decaying (uniformly in Λ and β):

$$\int_{\mathcal{C}_\Lambda} d\mathbf{C} \mathbb{I}[C \ni (x, \tau)] |\Phi^{\mathbf{T}}(\mathbf{C})| \prod_{\xi \in \mathbf{C}} e^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \leq \delta \quad (4.14)$$

and

$$\int_{\mathcal{C}_\Lambda^{(x, \tau)}} d\mathbf{C} |\Phi^{\mathbf{T}}(\mathbf{C})| \prod_{\xi \in \mathbf{C}} e^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \leq \delta \quad (4.15)$$

for every $(x, \tau) \in \mathbb{T}_\Lambda$.

Proof. One can follow any standard reference concerning cluster expansions for continuum systems, for example [Bry]. We are using here [Pfi] whose formulation is closer to our purpose. Assuming that inequality (4.15) holds true, we have a finite bound

$$\sum_{n \geq 1} \frac{1}{n!} \int_{\mathcal{L}_\Lambda(\Gamma)^n} d\xi_1 \dots d\xi_n |\varphi^{\mathbf{T}}(\xi_1, \dots, \xi_n)| \prod_{i=1}^n |z(\xi_i)| \leq \delta \beta |\Lambda|. \quad (4.16)$$

Lemma 4.1 then follows from Lemma 3.1 of [Pfi]. Let us turn to the proof of the two inequalities. Let

$$f(\xi) = |z(\xi)| e^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2 |B|}.$$

Skipping the conditions $\xi_j \sim \Gamma$, we define

$$\begin{aligned} I_n = n & \left[\int_{\mathcal{L}_\Lambda} d\xi_1 \mathbb{I}[B_1 \ni (x, \tau)] + \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi_1 \right] \\ & \cdot \int_{\mathcal{L}_\Lambda^{n-1}} d\xi_2 \dots d\xi_n |\varphi^{\mathbf{T}}(\xi_1, \dots, \xi_n)| \prod_{i=1}^n f(\xi_i) \end{aligned} \quad (4.17)$$

(it does not depend on $(x, \tau) \in \mathbb{T}_\Lambda$). The lemma will be completed once we shall have established that $I_n \leq n! (\frac{1}{2} \delta)^n$ (assuming that $\delta \leq 1$; otherwise, we show that $I_n \leq n!/2^n$). From Lemma 3.4 of [Pfi], we get

$$|\varphi^{\mathbf{T}}(\xi_1, \dots, \xi_n)| \leq \sum_{\mathcal{T} \text{ tree on } n \text{ vertices}} \prod_{e(i, j) \in \mathcal{T}} \mathbb{I}[B_i \cup B_j \text{ connected}]. \quad (4.18)$$

Denoting d_1, \dots, d_n the incidence numbers of vertices $1, \dots, n$, we first proceed with the integration on the loops $j \neq 1$ for which $d_j = 1$; in the tree \mathcal{T} , such j shares an edge only with one vertex i . The incompatibility between ξ_i and ξ_j , with $\xi_i = (B_i, \omega_{B_i}^{(i)}, g_{A_i}^{(i)})$, $B_i = A_i \times [\tau_1^{(i)}, \tau_2^{(i)}]$, and similarly for ξ_j , means that either $B_j \cup [A_i \times \tau_1^{(i)}]$ is connected,

or $[A_j \times \tau_1^{(j)}] \cup B_j$ is connected. Hence, the bound for the integral over the ξ_j that are incompatible with ξ_i is

$$\begin{aligned} & \int_{\mathcal{L}_\Lambda} d\xi_j \mathbb{I}[B_j \cup B_i \text{ connected}] f(\xi_j) \\ & \leq 2\nu|A_i| \int_{\mathcal{L}_\Lambda} d\xi_j \mathbb{I}[B_j \ni (x, \tau)] f(\xi_j) + 2\nu|B_i| \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi_j f(\xi_j) \quad (4.19) \\ & \leq 2\nu(|A_i| + \alpha|B_i|) \left(\int_{\mathcal{L}_\Lambda} d\xi_j \mathbb{I}[B_j \ni (x, \tau)] f(\xi_j) + \frac{1}{\alpha} \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi_j f(\xi_j) \right). \end{aligned}$$

(The constant α has been introduced in order to match with the conditions of the next lemma). Then

$$\begin{aligned} I_n & \leq n(2\nu)^{n-1} \sum_{\mathcal{T} \text{ tree of } n \text{ vertices}} \left[\int_{\mathcal{L}_\Lambda} d\xi_1 \mathbb{I}[B_1 \ni (x, \tau)] + \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi_1 \right] \\ & \quad f(\xi_1) \left(|A_1| + \alpha|B_1| \right)^{d_1} \\ & \quad \prod_{j=2}^n \left[\int_{\mathcal{L}_\Lambda} d\xi_j \mathbb{I}[B_j \ni (x, \tau)] f(\xi_j) \left(|A_j| + \alpha|B_j| \right)^{d_j-1} \right. \\ & \quad \left. + \frac{1}{\alpha} \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi_j f(\xi_j) \left(|A_j| + \alpha|B_j| \right)^{d_j-1} \right]. \quad (4.20) \end{aligned}$$

Now summing over all trees, knowing that the number of trees with n vertices and incidence numbers d_1, \dots, d_n is equal to

$$\frac{(n-2)!}{(d_1-1)! \dots (d_n-1)!} \leq \frac{(n-1)!}{d_1!(d_2-1)! \dots (d_n-1)!},$$

we find a bound

$$\begin{aligned} I_n & \leq n!(2\nu)^{n-1} (1 + \alpha) \left[\int_{\mathcal{L}_\Lambda} d\xi \mathbb{I}[B \ni (x, \tau)] f(\xi) e^{|A| + \alpha|B|} \right. \\ & \quad \left. + \frac{1}{\alpha} \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi f(\xi) e^{|A| + \alpha|B|} \right]^n. \quad (4.21) \end{aligned}$$

We conclude by using the following lemma which implies that the quantity between the brackets is small. \square

Lemma 4.2. *Let $\alpha_1 < (4R_0)^{-\nu}$ and $\alpha_2 < R^{-2\nu} \Delta_0$. For any $c \in \mathbb{R}$ and $\delta > 0$, there exists $\varepsilon_0 > 0$ such that whenever $\|T\| \leq \varepsilon_0$ the following inequality holds true,*

$$\begin{aligned} & \int_{\mathcal{L}_\Lambda} d\xi \mathbb{I}[B \ni (x, \tau)] |z(\xi)| e^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2|B|} \\ & + \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi |z(\xi)| e^{(c - \alpha_1 \log \|T\|)|A| + \alpha_2|B|} \leq \delta, \end{aligned}$$

where (x, τ) is any space-time site of \mathbb{T}_Λ .

Proof. Let us first consider the integral over ξ such that its box contains a given space-time site. We denote by ℓ_1 the number of quantum transitions of ξ at times bigger than τ , and ℓ_2 the number of the other quantum transitions. The integral over ξ can be done by summing over $(\ell_1 + \ell_2)$ quantum transitions $\mathbf{A}_1^1, \dots, \mathbf{A}_{\ell_1}^1, \mathbf{A}_1^2, \dots, \mathbf{A}_{\ell_2}^2$, by summing over $(\ell_1 + \ell_2)$ configurations $n_{A_j}^{i,j}$, and by integrating over times $\tau_1^1 < \dots < \tau_{\ell_1}^1$, $\tau_1^2 < \dots < \tau_{\ell_2}^2$. Let us do the change of variables $\tilde{\tau}_1^1 = \tau_1^1 - \tau$, $\tilde{\tau}_2^1 = \tau_2^1 - \tau_1^1, \dots, \tilde{\tau}_{\ell_1}^1 = \tau_{\ell_1}^1 - \tau_{\ell_1-1}^1$, and $\tilde{\tau}_1^2 = \tau - \tau_1^2, \dots, \tilde{\tau}_{\ell_2}^2 = \tau_{\ell_2-1}^2 - \tau_{\ell_2}^2$. Then we can write the following upper bound:

$$\begin{aligned} & \int_{\mathcal{L}_\Lambda} d\xi \mathbb{I}[B \ni (x, \tau)] |z(\xi)| e^{(c-\alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \\ & \leq \sum_{\ell_1, \ell_2 \geq 1} \sum_{\substack{\mathbf{A}_1^1, \dots, \mathbf{A}_{\ell_2}^2 \\ \cup_{i,j} \tilde{A}_j^i = A \ni x \\ A \text{ connected}}} \sum_{n_{A_1^1}^{1,1}, \dots, n_{A_{\ell_2}^2}^{2,\ell_2} \notin G_A} \int_0^\infty d\tilde{\tau}_1^1 \dots d\tilde{\tau}_{\ell_2}^2 \prod_{i=1,2} \prod_{j=1}^{\ell_i} |\langle n_A^{i,j} | T_{\mathbf{A}_j^i} | n_A^{i,j+1} \rangle| \\ & \quad e^{(c-\alpha_1 \log \|T\|)|\tilde{A}_j^i|} e^{-\tilde{\tau}_j^i \sum_{y, U_0(y) \subset A} [\Phi_y(n_{U_0(y)}^{i,j}) - \Phi_y(g_{U_0(y)})]} e^{\tilde{\tau}_j^i R^v \alpha_2}, \end{aligned} \quad (4.22)$$

where $g_A \in G_A$ is the configuration in which the loop ξ is immersed (if the construction does not lead to a possible loop, we find a bound by picking any $g_A \in G_A$). Remark that we neglected a constraint on the sum over configurations, namely $n_{A_1^1}^{1,1} = n_{A_1^1}^{2,1}$. It is useful to note that the sums over ℓ_1, ℓ_2 and over the quantum transitions are finite, otherwise they cannot constitute a loop.

Using the definition (2.6) of $\|T\|$, we have

$$|\langle n'_A | T_{\mathbf{A}} | n_A \rangle| \leq \|T\|^{|A|}.$$

Furthermore

$$\sum_{x, U_0(x) \subset A} [\Phi_x(n_{U_0(x)}^{i,j}) - \Phi_x(g_{U_0(x)})] \geq R^{-v} \Delta_0,$$

as claimed in Property (2.5). Hence we have, since the number of configurations on A is bounded with $S^{|A|}$,

$$\begin{aligned} & \int_{\mathcal{L}_\Lambda} d\xi \mathbb{I}[B \ni (x, \tau)] |z(\xi)| e^{(c-\alpha_1 \log \|T\|)|A| + \alpha_2 |B|} \\ & \leq \sum_{\ell_1, \ell_2 \geq 1} \sum_{\substack{\mathbf{A}_1^1, \dots, \mathbf{A}_{\ell_2}^2 \\ \cup_{i,j} \tilde{A}_j^i = A \ni x \\ A \text{ connected}}} \prod_{i=1,2} \prod_{j=1}^{\ell_i} \frac{[\|T\|^{1-\alpha_1(4R_0)^v} S e^{c(4R_0)^v}]^{|\tilde{A}_j^i|}}{R^{-v} \Delta_0 - R^v \alpha_2}. \end{aligned} \quad (4.23)$$

This is a small quantity since the sums are finite, by taking $\|T\|$ small enough. Now we turn to the second term, namely

$$\int_{\mathcal{L}_\Lambda^{(x,\tau)}} d\xi |z(\xi)| e^{(c-\alpha_1 \log \|T\|)|A| + \alpha_2 |B|}.$$

The proof is similar; we first sum over the number of transitions ℓ , then over ℓ transitions $\mathbf{A}_1, \dots, \mathbf{A}_\ell$ with $A = \cup_i \bar{A}_i \ni x$, A connected. Then we choose $\ell - 1$ intermediate configurations. Finally, we integrate over $\ell - 1$ time intervals. The resulting equation looks very close to (4.23) and is small for the same reasons. \square

Now, we single out the class of *small clusters*. Namely, a cluster is small if the sequence of its quantum transitions belongs to the list \mathcal{S} . To be more precise, we have to specify the order of transitions: considering a cluster $\mathbf{C} \equiv (\xi_1, \dots, \xi_k)$ and using $S(\xi^{(\ell)})$, $\ell = 1, \dots, k$, to denote the sequence of quantum transitions of the loop $\xi^{(\ell)} = (B^{(\ell)}, \omega_{B^{(\ell)}}, g_A^{\xi^{(\ell)}})$, $S(\xi^{(\ell)}) \equiv S(B^{(\ell)}, \omega_{B^{(\ell)}})$, we take the sequence $S(\mathbf{C})$ obtained by combining the sequences $S(\xi^{(1)}), \dots, S(\xi^{(k)})$ in this order. A cluster \mathbf{C} is said to be *small* if $S(\mathbf{C}) \in \mathcal{S}$, it is *large* otherwise. We use $\mathcal{C}_\Lambda^{\text{small}}$ to denote the set of all small clusters on the torus \mathbb{T}_Λ .

The local contribution to the energy at time τ , when the system is in a state $\mathbf{n}_{U_0(x)}(\tau)$, is $\Phi_x(\mathbf{n}_{U_0(x)}(\tau))$. Similarly, we will introduce the local contribution of loops (and small clusters of loops) in the expansion of the partition function – the effective potential $\Psi_A^\beta(\mathbf{n}_A(\tau))$. The latter is a local quantity in the sense that it depends on \mathbf{n} only on the set A at time τ . An explicit expression of $\Psi_A^\beta(g_A)$ with $g \in G$ is, in terms of small clusters,

$$\Psi_A^\beta(g_A) := - \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \frac{\Phi^\Gamma(\mathbf{C})}{|I_C|} \mathbb{I}[\mathbf{C} \sim g_A, A_C = A, I_C \ni 0]. \quad (4.24)$$

Here, again, \mathbf{C} is the support of \mathbf{C} , A_C its horizontal projection onto \mathbb{Z}^v , $A_C = \{x \in \mathbb{Z}^v; x \times [0, \beta]_{\text{per}} \cap \mathbf{C} \neq \emptyset\}$, and I_C its vertical projection, $|A_C|$ and $|I_C|$ their corresponding areas, and the condition $\mathbf{C} \sim g_A$ means that each loop of \mathbf{C} is immersed in the ground state g . Notice that the “horizontal extension” of any small cluster is at most $2R$: if \mathbf{C} is a small cluster, $\text{diam}(A_C) \leq 2R$. The definitions introduced to write the effective potential (see the appendix) are now clear, once we identify the effective potential Ψ defined in (A.1) as the limit $\beta \rightarrow \infty$ of (4.24). Namely,

$$\Psi = \lim_{\beta \rightarrow \infty} \Psi^\beta.$$

Our assumptions in Sect. 2.3 concern the limit $\beta \rightarrow \infty$ of the effective potential, but at non zero temperature we have to work with Ψ^β . To trace down the difference, we introduce $\psi^\beta = \Psi^\beta - \Psi$. Notice that (4.24) implies $\Psi_A^\beta(n_A) = 0$ whenever $n_A \notin G_A$ or $\text{diam} A < 4R_0$.

Recalling that if $C \subset \mathbb{T}_\Lambda$, \tilde{C} is the smallest box containing C , we introduce, for any cluster $\mathbf{C} \in \mathcal{C}_\Lambda^{\text{small}}$, the function

$$\Phi^\Gamma(\mathbf{C}; \Gamma) = \frac{\Phi^\Gamma(\mathbf{C})}{|I_C|} \int_{I_C} d\tau \left(\mathbb{I}[\mathbf{C} \sim \Gamma] - \mathbb{I}[\mathbf{n}_{A_C}^\Gamma(\tau) \in G_{A_C}, \mathbf{C} \sim \mathbf{n}_{A_C}^\Gamma(\tau)] \right). \quad (4.25)$$

Here, the first indicator function in the parenthesis singles out the clusters each loop of which is compatible with Γ , while the second indicator concerns the clusters for which $\mathbf{n}_{A_C}^\Gamma(\tau) \in G_{A_C}$ and each of their loops is immersed in the configuration $\mathbf{n}_{A_C}^\Gamma(\tau)$ (extended as a constant to all the time interval I_C). Observing that $\Phi^\Gamma(\mathbf{C}; \Gamma) = 0$ whenever $\tilde{C} \cap \text{core } \Gamma = \emptyset$, we split the integral over small clusters into its bulk part expressed in terms of the effective potential and boundary terms “decorating” the quantum contours from Γ .

Lemma 4.3. *For any fixed $\Gamma \in \mathcal{D}_\Lambda$, one has*

$$\begin{aligned} \int_{\mathcal{C}_\Lambda^{\text{small}}(\Gamma)} d\mathbf{C} \Phi^{\text{T}}(\mathbf{C}) &= - \int_{\mathbb{T}_\Lambda} d(A, \tau) \Psi_A(\mathbf{n}_A^\Gamma(\tau)) \\ &\quad - \int_{\mathbb{T}_\Lambda} d(A, \tau) \psi_A^\beta(\mathbf{n}_A^\Gamma(\tau)) + \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \Phi^{\text{T}}(\mathbf{C}; \Gamma). \end{aligned}$$

The term $\Phi^{\text{T}}(\mathbf{C}; \Gamma)$ vanishes whenever $\tilde{\mathcal{C}} \cap \text{core } \Gamma = \emptyset$.

Similarly as $\int d(x, \tau)$, the shorthand $\int d(A, \tau)$ means $\sum_A \int d\tau$.

Proof. To get the equality of integrals, it is enough to rewrite

$$\int_{\mathcal{C}_\Lambda^{\text{small}}(\Gamma)} d\mathbf{C} \Phi^{\text{T}}(\mathbf{C}) = \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \Phi^{\text{T}}(\mathbf{C}) \mathbb{I}[\mathbf{C} \sim \Gamma] \quad (4.26)$$

and

$$- \int_{\mathbb{T}_\Lambda} d(A, \tau) \Psi_A^\beta(\mathbf{n}_A^\Gamma(\tau)) = \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \frac{\Phi^{\text{T}}(\mathbf{C})}{|\mathbf{C}|} \int_{I_C} d\tau \mathbb{I}[\mathbf{n}_{A_C}^\Gamma(\tau) \in G_{A_C}, \mathbf{C} \sim \mathbf{n}_{A_C}^\Gamma(\tau)]. \quad (4.27)$$

Moreover, whenever $\tilde{\mathcal{C}} \cap \text{core } \Gamma = \emptyset$, the configuration $\mathbf{n}_{A_C}^\Gamma(\tau)$ belongs to G_{A_C} , and it is constant, for all $\tau \in I_C$. Under these circumstances, the condition $\mathbf{C} \sim \Gamma$ is equivalent to $\mathbf{C} \sim \mathbf{n}_{A_C}^\Gamma(\tau)$ and the right hand side of (4.25) vanishes. \square

Whenever $\Gamma \in \mathcal{D}_\Lambda$ is fixed, let $W_d(\Gamma) \subset \mathbb{T}_\Lambda$ be the set of space-time sites in the state d , i.e.

$$W_d(\Gamma) = \{(x, \tau) \in \mathbb{T}_\Lambda : \mathbf{n}_{U(x)}^\Gamma(\tau) = d_{U(x)}\}.$$

Notice that

$$\mathbb{T}_\Lambda = \text{supp } \Gamma \cup \bigcup_{d \in D} W_d(\Gamma); \quad W_d(\Gamma) \cap W_{d'}(\Gamma) = \emptyset \text{ if } d \neq d',$$

and the set $\text{supp } \Gamma \cap W_d(\Gamma)$ is of measure zero (with respect to the measure $d(x, \tau)$ on \mathbb{T}_Λ). Let us recall that the equivalent potential Υ satisfies the equality $\sum_{x \in \Lambda} \Upsilon_x(n_{U(x)}) = \sum_{A \subset \Lambda} (\Phi_A(n_A) + \Psi_A(n_A)) + \text{const}|\Lambda|$ for any configuration n on the torus Λ ; actually, we can take $\text{const} = 0$, since Υ and $\Upsilon' = \Upsilon + \text{const}$ are also physically equivalent, and Υ' satisfies the same assumptions as Υ .

Lemma 4.4. *The partition function (4.9) can be rewritten as*

$$Z_\Lambda^{\text{per}} = \int_{\mathcal{D}_\Lambda} d\Gamma \prod_{d \in D} e^{-|W_d(\Gamma)|e(d)} \prod_{\gamma \in \Gamma} z(\gamma) e^{\mathcal{R}(\Gamma)}.$$

Here the weight $z(\gamma)$ of a quantum contour $\gamma = (B, \omega_B)$ with the sequence of transitions $(\mathbf{A}_1, \dots, \mathbf{A}_m)$ at times (τ_1, \dots, τ_m) is

$$z(\gamma) = \prod_{i=1}^m \langle \mathbf{n}_{A_i}^\gamma(\tau_i - 0) | T_{\mathbf{A}_i} | \mathbf{n}_{A_i}^\gamma(\tau_i + 0) \rangle \exp \left\{ - \int_B d(x, \tau) \Upsilon_x(\mathbf{n}_{U(x)}^\gamma(\tau)) \right\}. \quad (4.28)$$

The rest $\mathcal{R}(\Gamma)$ is given by

$$\mathcal{R}(\Gamma) = \int_{\mathcal{C}_\Lambda(\Gamma) \setminus \mathcal{C}_\Lambda^{\text{small}}(\Gamma)} d\mathbf{C} \Phi^T(\mathbf{C}) - \int_{\mathbb{T}_\Lambda} d(A, \tau) \psi_A^\beta(\mathbf{n}_A^\Gamma(\tau)) + \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \Phi^T(\mathbf{C}; \Gamma). \quad (4.29)$$

Proof. Using Lemmas 4.1 and 4.3 to substitute in (4.9) the contribution of loops by the action of the effective potential, we get

$$\begin{aligned} Z_\Lambda^{\text{per}} &= \int_{\mathcal{D}_\Lambda} d\Gamma \left\{ \prod_{i=1}^m \langle \mathbf{n}_{A_i}^\Gamma(\tau_i - 0) | T_{A_i} | \mathbf{n}_{A_i}^\Gamma(\tau_i + 0) \rangle \right\} \\ &\quad \cdot \exp \left\{ - \int_{\mathbb{T}_\Lambda} d(A, \tau) (\Phi_A(\mathbf{n}_A^\Gamma(\tau)) + \Psi_A(\mathbf{n}_A^\Gamma(\tau))) \right\} e^{\mathcal{R}(\Gamma)}. \end{aligned} \quad (4.30)$$

Replacing $\Phi + \Psi$ by the physically equivalent potential Υ , we get

$$\begin{aligned} Z_\Lambda^{\text{per}} &= \int_{\mathcal{D}_\Lambda} d\Gamma \left\{ \prod_{i=1}^m \langle \mathbf{n}_{A_i}^\Gamma(\tau_i - 0) | T_{A_i} | \mathbf{n}_{A_i}^\Gamma(\tau_i + 0) \rangle \right\} \\ &\quad \exp \left\{ - \int_{\text{supp } \Gamma} d(x, \tau) \Upsilon_x(\mathbf{n}_{U(x)}^\Gamma(\tau)) \right\} \prod_{d \in D} e^{-e(d)|W_d(\Gamma)|} e^{\mathcal{R}(\Gamma)}. \end{aligned} \quad (4.31)$$

We get our lemma by observing that the product over quantum transitions and the first exponential factorize with respect to the quantum contours, as was the case for the loops (for fermions the sign arising because of anticommutation relations also factorizes; we again refer to [DFF1] for the proof). \square

Our goal is to obtain a classical lattice system in $\nu + 1$ dimensions. Thus we introduce a discretization of the continuous time direction, by choosing suitable parameters $\tilde{\beta} > 0$ and $N \in \mathbb{N}$ with $\beta = N \frac{\tilde{\beta}}{\Delta}$.¹¹ Setting \mathbb{L}_Λ to be the $(\nu + 1)$ -dimensional discrete torus $\mathbb{L}_\Lambda = \Lambda \times \{0, 1, \dots, N - 1\}^{\text{per}}$ – let us recall that Λ has periodic boundary conditions in all spatial directions – and using $C(x, t) \subset \mathbb{R}^{\nu+1}$ to denote, for any $(x, t) \in \mathbb{L}_\Lambda$, the cell centered in $(x, \frac{\tilde{\beta}}{\Delta}t)$ with vertical length $\tilde{\beta}/\Delta$, we have $\mathbb{T}_\Lambda = \cup_{(x,t) \in \mathbb{L}_\Lambda} C(x, t)$.

For any $M \subset \mathbb{L}_\Lambda$, we set $C(M)$ to be the union of all cells centered at sites of M , $C(M) = \cup_{(x,t) \in M} C(x, t) \subset \mathbb{T}_\Lambda$. Conversely, if $B \subset \mathbb{T}_\Lambda$, we take $M(B) \subset \mathbb{L}_\Lambda$ to be the smallest set such that $C(M(B)) \supset B$. Given a connected¹² set $M \subset \mathbb{L}_\Lambda$ and a collection of quantum contours $\Gamma \in \mathcal{D}_\Lambda$, we define

$$\begin{aligned} \varphi(M; \Gamma) &= \int_{\mathcal{C}_\Lambda(\Gamma) \setminus \mathcal{C}_\Lambda^{\text{small}}(\Gamma)} d\mathbf{C} \mathbb{I}[M(C) = M] \Phi^T(\mathbf{C}) + \\ &\quad + \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \mathbb{I}[M(C) = M, C \not\subset C(\text{supp } \Gamma)] \Phi^T(\mathbf{C}; \Gamma) - \\ &\quad - \int_{M(A \times \tau) = M} d(A, \tau) \psi_A^\beta(\mathbf{n}_A^\Gamma(\tau)) \end{aligned} \quad (4.32)$$

¹¹ Note the difference from [BKU1]; here the vertical length of a unit cell $\tilde{\beta}/\Delta$ depends on $\|T\|$, since so does the quantum Peierls constant Δ .

¹² Connectedness in \mathbb{L}_Λ is meant in the standard way via nearest neighbours.

and

$$\tilde{\mathcal{R}}(\Gamma) = \int_{C_{\Lambda}^{\text{small}}} d\mathbf{C} \mathbb{I}[C \subset C(\text{supp } \Gamma)] \Phi^{\mathbf{T}}(\mathbf{C}; \Gamma). \quad (4.33)$$

We have separated the contributions of the small clusters inside

$$C(\text{supp } \Gamma) \equiv C(M(\text{supp } \Gamma)),$$

because they are not necessarily a small quantity, and it is impossible to expand them. On the contrary, $\varphi(M; \Gamma)$ is small, and hence it is natural to write

$$e^{\mathcal{R}(\Gamma)} = e^{\tilde{\mathcal{R}}(\Gamma)} \sum_{\mathcal{M}} \prod_{M \in \mathcal{M}} \left(e^{\varphi(M; \Gamma)} - 1 \right), \quad (4.34)$$

with the sum running over all collections \mathcal{M} of connected subsets of \mathbb{L}_{Λ} .

Let $\text{supp } \mathcal{M} = \cup_{M \in \mathcal{M}} M$. Given a set of quantum contours $\Gamma \in \mathcal{D}_{\Lambda}$ and a collection \mathcal{M} , we introduce contours on \mathbb{L}_{Λ} by decomposing the set $M(\text{supp } \Gamma) \cup \text{supp } \mathcal{M}$ into connected components [notice that if $(x, t) \notin M(\text{supp } \Gamma) \cup \text{supp } \mathcal{M}$, then $C(x, t) \subset \cup_{d \in D} W_d(\Gamma)$]. Namely, a *contour* Y is a pair $(\text{supp } Y, \alpha_Y)$, where $\text{supp } Y \subset \mathbb{L}_{\Lambda}$ is a (non-empty) connected subset of \mathbb{L}_{Λ} , and α_Y is a labeling of connected components F of $\partial C(\text{supp } Y)$, $\alpha_Y(F) = 1, \dots, r$. We write $|Y|$ for the length (area) of the contour Y , i.e. the number of sites in $\text{supp } Y$. A set of contours $\mathcal{Y} = \{Y_1, \dots, Y_k\}$ is *admissible* if the contours are mutually disjoint and if the labeling is constant on the boundary of each connected component of $\mathbb{T}_{\Lambda} \setminus \cup_{Y \in \mathcal{Y}} C(\text{supp } Y)$. Finally, given an admissible set of contours \mathcal{Y} , we define $\mathcal{W}_d(\mathcal{Y})$ to be the union of all connected components M of $\mathbb{L}_{\Lambda} \setminus \cup_{Y \in \mathcal{Y}} \text{supp } Y$ such that $C(M)$ has label d on its boundary.

Consider now any quantum configuration $\omega \in \mathcal{Q}_{\Lambda}$ yielding, together with a collection \mathcal{M} , a fixed set of contours \mathcal{Y} . Summing over all such configurations ω and collections \mathcal{M} , we get the weight to be attributed to the set \mathcal{Y} . Let Γ^{ω} be the collection of quantum contours corresponding to ω , $\cup_{Y \in \mathcal{Y}} \text{supp } Y = M(\text{supp } \Gamma^{\omega}) \cup \text{supp } \mathcal{M}$. Given that the configurations ω are necessarily constant with no transition on $\mathbb{T}_{\Lambda} \setminus C(\cup_{Y \in \mathcal{Y}} \text{supp } Y)$, we easily see that the weight factor splits into a product of weight factors of single contours $Y \in \mathcal{Y}$. Namely, for the weight \mathfrak{z} of a contour Y we get the expression

$$\begin{aligned} \mathfrak{z}(Y) &= \int_{\mathcal{D}_{\Lambda}(Y)} d\Gamma \prod_{\gamma \in \Gamma} z(\gamma) \prod_{d \in D} e^{-e(d)|W_d(\Gamma) \cap C(\text{supp } Y)|} e^{\tilde{\mathcal{R}}(\Gamma)} \\ &\quad \sum_{\mathcal{M}} \mathbb{I}[M(\text{supp } \Gamma) \cup \text{supp } \mathcal{M} = \text{supp } Y] \prod_{M \in \mathcal{M}} \left(e^{\varphi(M; \Gamma)} - 1 \right), \end{aligned} \quad (4.35)$$

where $\mathcal{D}_{\Lambda}(Y)$ is the set of quantum configurations compatible with Y , $\Gamma \in \mathcal{D}_{\Lambda}(Y)$ if $\text{supp } \Gamma \subset \text{supp } Y$ and the labels on the boundary of $\text{supp } \Gamma$ match with labels of Y . Thus, we can finally rewrite the partition function in a form that agrees with the standard Pirogov–Sinai setting, namely

$$Z_{\Lambda}^{\text{per}} = \sum_{\mathcal{Y}} \prod_{d \in D} e^{-\frac{\beta}{\Delta} e(d)|\mathcal{W}_d(\mathcal{Y})|} \prod_{Y \in \mathcal{Y}} \mathfrak{z}(Y), \quad (4.36)$$

with the sum being over all admissible sets of contours on \mathbb{L}_{Λ} .

In the next section we will evaluate the decay rate of contour weights in preparation to apply, in Sect. 6, the Pirogov–Sinai theory to prove Theorems 2.1, 2.2, and 2.3.

5. Exponential Decay of the Weight of the Contours

In this section we show that the weight \mathfrak{z} has exponential decay with respect to the length of the contours. We begin by a lemma proving that the contribution of \mathcal{M} is small, that we shall use in Lemma 5.2 below for the bound of \mathfrak{z} .

Lemma 5.1. *Under Assumptions 1–6, for any $c < \infty$ there exist constants $\beta_0, \tilde{\beta}_0 < \infty$, and $\varepsilon_0 > 0$ such that for any $\beta \geq \beta_0, \tilde{\beta}_0 \leq \tilde{\beta} < 2\tilde{\beta}_0$, and $\|T\|, \varepsilon_1, \varepsilon_2 \leq \varepsilon_0$, one has*

$$\sum_{M \ni (x,t)} |e^{\varphi(M;\Gamma)} - 1| e^{c|M|} \leq 1$$

for any contour Y and any set of quantum contours $\Gamma \in \mathcal{D}_\Lambda(Y)$.

Proof. We show that

$$\sum_{M \ni (x,t)} |\varphi(M; \Gamma)| e^{c|M|} \leq 1.$$

This implies that $|\varphi(M; \Gamma)| \leq 1$ and consequently Lemma 5.1 holds – with a slightly smaller constant c .

Let us consider separately, in (4.32), the three terms on the right hand side: (a) the integral over big clusters, (b) the integral over small clusters, and (c) the expression involving ψ^β .

(a) *Big clusters.* Our aim is to estimate

$$J = \sum_{M \ni (x,t)} e^{c|M|} \int_{\mathcal{C}_\Lambda(\Gamma) \setminus \mathcal{C}_\Lambda^{\text{small}}(\Gamma)} d\mathbf{C} \mathbb{I}[M(\mathbf{C}) = M] |\Phi^T(\mathbf{C})|.$$

Since $M(\mathbf{C}) = M$ and $M \ni (x, t)$, the cell $C(x, t)$ intersects a quantum transition of \mathbf{C} , or it is contained in a box B belonging to a loop of \mathbf{C} (both possibilities may occur at the same time). In the first case we start the integral over clusters by choosing the time for the first quantum transition, which yields a factor $\tilde{\beta}/\Delta$. In the second case we simply integrate over all loops containing the given site. In the same time, given a cluster $\mathbf{C} = (\xi_1, \dots, \xi_n)$, $\xi_i = (B_i, \omega_{B_i}^{(i)}, g_{A_i}^{\xi_i})$ and $B_i = A_i \times [\tau_1^{(i)}, \tau_2^{(i)}]$, the condition $M(\mathbf{C}) = M$ implies that

$$\sum_{i=1}^n \left\{ |A_i| + \frac{\Delta}{\tilde{\beta}} |B_i| \right\} \geq |M|. \quad (5.1)$$

Using it to bound $|M|$, we get the estimate

$$\begin{aligned} J &\leq \frac{\tilde{\beta}}{\Delta} \int_{\mathcal{C}_\Lambda^{(x,\tau)} \setminus \mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} |\Phi^T(\mathbf{C})| \prod_{\xi \in \mathbf{C}} e^{c|A| + c\frac{\Delta}{\tilde{\beta}}|B|} + \\ &+ \int_{\mathcal{C}_\Lambda \setminus \mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \mathbb{I}[C \ni (x, \tau)] |\Phi^T(\mathbf{C})| \prod_{\xi \in \mathbf{C}} e^{c|A| + c\frac{\Delta}{\tilde{\beta}}|B|}. \end{aligned} \quad (5.2)$$

Taking, in Lemma 4.1, the constant c as above as well as $\alpha_1 = \frac{1}{2}(4R_0)^{-\nu}$, $\alpha_2 = c\Delta/\tilde{\beta}$, $\delta = 1$, and choosing the corresponding $\varepsilon_0(c, \alpha_1, \alpha_2, \delta)$, we can bound the second term

of (5.2), for any $\|T\| \leq \varepsilon_0$, with the help of (4.14) once $\tilde{\beta}$ is chosen large enough to satisfy

$$\frac{\tilde{\beta}}{\Delta} > \frac{c}{\Delta_0} R^{2\nu}. \quad (5.3)$$

To estimate the first term of (5.2), we first consider the contribution of those clusters for which

$$\frac{\tilde{\beta}}{\Delta} \leq \prod_{\xi \in \mathbf{C}} \|T\|^{-\frac{1}{2}(4R_0)^{-\nu}|A|}.$$

Applying it together with (5.3) we can directly use the bound (4.15).

Thus it remains to estimate the contribution of those terms for which

$$\frac{1}{2(4R_0)^\nu} \sum_{\xi \in \mathbf{C}} |A| < \frac{\log(\tilde{\beta}/\Delta)}{\log(1/\|T\|)}. \quad (5.4)$$

Let us first fix $\tilde{\beta}$ and $\varepsilon_0 \leq \varepsilon_0(c, \alpha_1, \alpha_2, \delta)$ with the constants c, α_1, α_2 , and δ as above, so that

$$\frac{\tilde{\beta}}{\varepsilon_0} > \frac{c}{\Delta_0} R^{2\nu} \quad (5.5)$$

and, in the same time,

$$\tilde{\beta} \leq \varepsilon_0^{k - \frac{1}{2}k'(4R_0)^{-\nu}} \quad (5.6)$$

for a suitable large k' (we also assume that $\varepsilon_0 \leq 1$). Here k is the constant that appears in Assumption 4, $\Delta(\|T\|) \geq \|T\|^k$. Observing further that $\Delta(\|T\|)$ can be taken to increase with $\|T\|$ (one can always consider a weaker lower bound Δ when taking smaller $\|T\|$), we conclude that (5.3), as well as the condition

$$2(4R_0)^\nu \frac{\log(\tilde{\beta}/\Delta)}{\log(1/\|T\|)} \leq k',$$

are satisfied for every $\|T\| \leq \varepsilon_0$. Thus, it suffices to find an upper bound to

$$J' = \frac{\tilde{\beta}}{\Delta} \int_{\mathcal{C}_\Lambda^{(x,\tau)} \setminus \mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} |\Phi^T(\mathbf{C})| \mathbb{I} \left[\sum_{\xi \in \mathbf{C}} |A| < k' \right]. \quad (5.7)$$

The main problem in estimating this term stems from the factor $1/\Delta$ that may be large if $\|T\|$ is small. Thus, to have a bound valid for all small $\|T\|$, some terms, coming from the integral, that would suppress this factor must be displayed.

The condition $\sum_{\xi \in \mathbf{C}} |A| < k'$ will be used several times by applying its obvious consequences: (i) the number of loops in \mathbf{C} is smaller than k' , (ii) the number of transitions for each loop is smaller than k' , (iii) each transition \mathbf{A} is such that $|A| < k'$, and (iv) the distance between each transition and x is smaller than k' .

Furthermore, we use Assumption 5 to bound the contribution of the transitions of C ; recalling the definition (4.11) of the weight of ξ , we have, for any large C ,

$$\begin{aligned} \prod_{\xi \in C} |z(\xi)| &\leq \varepsilon_1 \Delta \prod_{\xi \in C} \exp \left\{ - \int_B d(x, \tau) [\Phi_x(n_{U_0(x)}^\xi(\tau)) - \Phi_x(g_{U_0(x)}^\xi)] \right\} \\ &\leq \varepsilon_1 \Delta \prod_{\xi \in C} e^{-R^{-2\nu} \Delta_0 |B|}. \end{aligned} \tag{5.8}$$

In the last inequality we used Assumption 2 in the form of the bound (2.5) as well as the lower bound $|\tau_2 - \tau_1| = \frac{|B|}{|A|} \geq \frac{|B|}{R^\nu}$ for the support $B = A \times [\tau_1, \tau_2]$ of the loop ξ .

For any $\xi \in C = (\xi_1, \dots, \xi_n)$, let τ be the time at which the first transition in C occurs (we assume that it happens for the “first” loop ξ_1) and τ^ξ be such that $\tau + \tau^\xi$ is the time at which the first transition in ξ occurs ($\tau^{\xi_1} = 0$). Referring to the condition (i) on the number of loops in C , we get the inequality

$$\sum_{\xi \neq \xi_1} |\tau^\xi| \leq k' \sum_{\xi} |B|,$$

and thus also

$$1 \leq \prod_{\xi} e^{-\frac{\Delta_0}{2k'R^{2\nu}} |\tau^\xi|} \prod_{\xi} e^{\frac{1}{2} R^{-2\nu} \Delta_0 |B|}.$$

Integrating now over the time of the first transition for each $\xi \in C$, $\xi \neq \xi_1$, and taking into account that $|\varphi^T(\xi_1, \dots, \xi_n)| \leq n^{n-2}$, we get

$$J' \leq \tilde{\beta} \varepsilon_1 \sum_{n=1}^{k'} \frac{n^{n-2}}{(n-1)!} \left(\frac{2k'R^{2\nu}}{\Delta_0} \right)^{n-1} \left\{ \int_{\mathcal{L}_\Lambda^{(x, \tau)}} d\xi e^{-\frac{1}{2} R^{-2\nu} \Delta_0 |B|} \mathbb{I}[\xi : k'] \right\}^n. \tag{5.9}$$

Here the constraint $\mathbb{I}[\xi_i : k']$ means that the loop ξ_i satisfies the conditions (ii)–(iv) above. We have then a finite number of finite terms, the contribution of which is bounded by a fixed number $K < \infty$ (depending on ε_0 , $\tilde{\beta}$, and k'). Thus $J' \leq \tilde{\beta} \varepsilon_1 K$ which we can suppose sufficiently small if ε_1 is small.

(b) *Small clusters.* Let us first notice that $|\Phi^T(C; \Gamma)| \leq |\Phi^T(C)|$, and since $M(C) = M$, inequality (5.1) is valid. Moreover C must contain at least one of the two boundary points $(y, t \frac{\tilde{\beta}}{\Delta} \pm \frac{\tilde{\beta}}{2\Delta})$ of some cell $C(y, t)$ for which $\text{dist}(x, y) \leq R$. Indeed, given that C is small and in the same time $\tilde{C} \cap \text{core } \Gamma \neq \emptyset$ (cf. Lemma 4.3), this is the only way to satisfy also $C \not\subset C(\text{supp } \Gamma)$ [cf. (4.32)]. Thus it suffices to use again (4.14) and (5.3) to estimate

$$(2R)^\nu \int_{C_\Lambda^{\text{small}}} dC \mathbb{I}[C \ni (x, \tau)] |\Phi^T(C)| \prod_{\xi \in C} e^{c|A| + c \frac{\Delta}{\tilde{\beta}} |B|}.$$

(c) *Bound for ψ^β .* Finally, we estimate the expression involving ψ^β . We first observe that

$$e^{\alpha\beta} |\psi_A^\beta(g_A)| \leq 1 \tag{5.10}$$

for any $A \subset \mathbb{Z}^v$ and with $\alpha = \frac{1}{2}R^{-2v}\Delta_0$, Indeed,

$$\begin{aligned} e^{\alpha\beta} |\psi_A^\beta(g_A)| &= e^{\alpha\beta} |\Psi_A^\beta(g_A) - \Psi_A(g_A)| = \\ &= e^{\alpha\beta} \left| - \int_{\mathcal{C}_{\Lambda}^{\text{small}}} d\mathbf{C} \mathbb{I}[C \sim g_A, A_C = A, I_C \ni 0, C \subset \Lambda \times [0, \beta]_{\text{per}}, |I_C| = \beta] \frac{\Phi^T(\mathbf{C})}{|I_C|} + \right. \\ &\left. + \int_{\mathcal{C}_{\Lambda}^{\text{small}}} d\mathbf{C} \mathbb{I}[C \sim g_A, A_C = A, I_C \ni 0, C \subset \Lambda \times [-\infty, \infty], |I_C| \geq \beta] \frac{\Phi^T(\mathbf{C})}{|I_C|} \right|. \end{aligned} \quad (5.11)$$

The first integral above corresponds to clusters wrapped around the torus in vertical direction, while the second one assumes integration over all clusters in $\Lambda \times [-\infty, \infty]$. For any \mathbf{C} above $|I_C| \geq \beta$ and thus

$$e^{\alpha\beta} \leq \prod_{\xi \in \mathbf{C}} e^{\alpha|B|}.$$

Observing now that every cluster in both integrals necessarily contains in its support at least one of the points $(x, 0)$, $x \in A$, and using the fact that $\text{diam } A \leq R$, we can bound the first integral by

$$\frac{R^v}{\beta} \int_{\mathcal{C}_{\Lambda}^{\text{small}}} d\mathbf{C} \mathbb{I}[C \ni (x, 0)] |\Phi^T(\mathbf{C})| \prod_{\xi \in \mathbf{C}} e^{\alpha|B|},$$

which can be directly evaluated by (4.14). The same bound can be actually used also for the second integral, once we realize that the estimate (4.14) is uniform in β .

Using now the fact that $\psi_A^\beta = 0$ if $\text{diam } A \geq R$, the condition $M(A \times \{\tau\}) = M$ implies that M has less than R^v sites, hence $e^{c|M|} \leq e^{cR^v}$. Furthermore, referring to (5.10), we have

$$\int_{\mathbb{T}_{\Lambda}} d(A, \tau) |\psi_A^\beta(\cdot)| \mathbb{I}[M(A \times \{\tau\}) = M] e^{c|M|} \leq \frac{\tilde{\beta}}{\Delta} e^{-\frac{1}{2}R^{-2v}\Delta_0\beta + cR^v}, \quad (5.12)$$

which can be made small for β sufficiently large and concludes thus the proof of the lemma. \square

Using Lemma 5.1 and introducing $e_0 = \min_{d \in D} e(d)$, we can estimate the weight \mathfrak{z} of the contours in the discrete space of cells.

Lemma 5.2. *Under Assumptions 1–6, for any $c < \infty$, there exist $\beta_0, \tilde{\beta}_0 < \infty$ and $\varepsilon_0 > 0$ such that for any $\beta \geq \beta_0$, $\tilde{\beta}_0 \leq \tilde{\beta} < 2\tilde{\beta}_0$, and $\|T\|, \varepsilon_1, \varepsilon_2 \leq \varepsilon_0$, one has*

$$|\mathfrak{z}(Y)| \leq e^{-\frac{\tilde{\beta}}{\Delta}e_0|Y|} e^{-c|Y|}$$

for any contour Y .

Proof. For a given Γ (such that $M(\text{supp } \Gamma) \subset \text{supp } Y$) with transitions $\{\mathbf{A}_1, \dots, \mathbf{A}_m\}$ at times $\{\tau_1, \dots, \tau_m\}$, we define $A(\Gamma) = \cup_{i=1}^m \cup_{x \in A_i} [U(x) \times \tau_i]$, $\mathcal{A} = M(A(\Gamma))$, and $\mathcal{E} \subset \text{supp } Y \setminus \mathcal{A}$ to be the set of sites (x, t) such that $\mathbf{n}_{U(x)}^\Gamma(\tau) \notin D_{U(x)}$ for some $(x, \tau) \in C(x, t)$. The latter can be split into two disjoint subsets, $\mathcal{E} = \mathcal{E}^{\text{core}} \cup \mathcal{E}^{\text{soft}}$, with $(x, t) \in \mathcal{E}^{\text{core}}$ whenever $\mathbf{n}_{U(x)}^\Gamma(\tau) \notin G_{U(x)}$ for some $(x, \tau) \in C(x, t)$. The condition $M(\text{supp } \Gamma) \cup \text{supp } \mathcal{M} = \text{supp } Y$ in (4.35) implies the inequality

$$e^{c|Y|} \leq e^{c(2R)^\nu |A(\Gamma)|} e^{c|\mathcal{E}|} \prod_{M \in \mathcal{M}} e^{c|M|}.$$

From definitions (4.35) of $\mathfrak{z}(Y)$ and (4.28) of $z(\gamma)$, and using Assumption 4, we have

$$\begin{aligned} e^{c|Y|} |\mathfrak{z}(Y)| &\leq \sum_{\mathcal{A} \subset \text{supp } Y} e^{-\frac{\tilde{\beta}}{\Delta} \varepsilon_0 |\text{supp } Y \setminus \mathcal{A}|} \\ &\sum_{\mathcal{E} \subset \text{supp } Y \setminus \mathcal{A}} \sum_{\mathcal{E}^{\text{core}} \subset \mathcal{E}} e^{-(\tilde{\beta}-c)|\mathcal{E} \setminus \mathcal{E}^{\text{core}}|} e^{-\left(\frac{\tilde{\beta}}{\Delta} \frac{\Delta_0}{2} (2R)^{-\nu} - c\right) |\mathcal{E}^{\text{core}}|} \times \\ &\times \int_{\mathcal{D}_\Lambda} d\Gamma \mathbb{I} [M(A(\Gamma)) = \mathcal{A}, M(\text{core } \Gamma) = \mathcal{E}^{\text{core}}] \\ &\prod_{i=1}^m |\langle \mathbf{n}_{A_i}^\Gamma(\tau_i - 0) | T_{A_i} | \mathbf{n}_{A_i}^\Gamma(\tau_i + 0) \rangle| e^{c(2R)^\nu |A_i|} \times \\ &\times \exp \left\{ - \int_{C(\mathcal{A})} d(x, \tau) \Upsilon_x(\mathbf{n}_{U(x)}^\Gamma(\tau)) \right\} e^{|\tilde{\mathcal{R}}(\Gamma)|} \sum_{\mathcal{M}, \text{supp } \mathcal{M} \subset \text{supp } Y} \prod_{M \in \mathcal{M}} |e^{\varphi(M; \Gamma)} - 1| e^{c|M|}. \end{aligned} \quad (5.13)$$

All elements in \mathcal{M} are different, because it is so in the expansion (4.34). Therefore we have

$$\begin{aligned} &\sum_{\mathcal{M}, \text{supp } \mathcal{M} \subset \text{supp } Y} \prod_{M \in \mathcal{M}} |e^{\varphi(M; \Gamma)} - 1| e^{c|M|} \\ &\leq \sum_{n \geq 0} \frac{1}{n!} \left[\sum_{M \subset \text{supp } Y} |e^{\varphi(M; \Gamma)} - 1| e^{c|M|} \right]^n \\ &\leq \sum_{n \geq 0} \frac{1}{n!} \left[|Y| \sum_{M \ni (x, t)} |e^{\varphi(M; \Gamma)} - 1| e^{c|M|} \right]^n, \end{aligned} \quad (5.14)$$

and using Lemma 5.1 this may be bounded by $e^{|Y|}$.

In (4.33) clusters are small, and they must contain a space-time site (x, τ) such that there exists x' with $(x', \tau) \in \text{core } \Gamma$ and $\text{dist}(x, x') < R$. So we have the bound

$$|\tilde{\mathcal{R}}(\Gamma)| \leq (2R)^\nu |\text{core } \Gamma| \int_{\mathcal{C}_\Lambda^{\text{small}}} d\mathbf{C} \mathbb{I} [C \ni (x, \tau)] |\Phi^T(\mathbf{C})|,$$

since $|\Phi^T(\mathbf{C}; \Gamma)| \leq |\Phi^T(\mathbf{C})|$. Taking now, in Lemma 4.1, the constants $c = \alpha_1 = \alpha_2 = 0$ and $\delta = \frac{\Delta_0}{4(2R)^{2\nu}}$, and choosing the corresponding ε_0 , we apply (4.14) to get, for any $\|T\| \leq \varepsilon_0$, the bound

$$|\tilde{\mathcal{R}}(\Gamma)| \leq \frac{\Delta_0}{4} (2R)^{-\nu} |\text{core } \Gamma| \leq \frac{\tilde{\beta}}{\Delta} \frac{\Delta_0}{4} (2R)^{-\nu} |\mathcal{E}^{\text{core}}| + \frac{\Delta_0}{4} (2R)^{-\nu} |\text{core } \Gamma \cap C(\mathcal{A})|.$$

Assuming $\tilde{\beta} \geq c$ and $\frac{\tilde{\beta}}{\Delta} \frac{\Delta_0}{4} \geq (2R)^\nu c$ [cf. (5.3)], we bound

$$e^{-(\tilde{\beta}-c)|\mathcal{E} \setminus \mathcal{E}^{\text{core}}|} e^{-\left(\frac{\tilde{\beta}}{\Delta} \frac{\Delta_0}{4} (2R)^{-\nu} - c\right)|\mathcal{E}^{\text{core}}|} \leq 1.$$

Inserting these estimates into (5.13), we get

$$\begin{aligned} e^{c|Y|} |\mathfrak{Z}(Y)| &\leq e^{-\frac{\tilde{\beta}}{\Delta} e_0 |Y|} e^{|Y|} \sum_{\mathcal{A} \subset \text{supp } Y} 3^{|\text{supp } Y \setminus \mathcal{A}|} \int_{\mathcal{D}_{\mathcal{A}}} d\Gamma \mathbb{I}[M(A(\Gamma)) = \mathcal{A}] \\ &\quad \prod_{i=1}^m |\langle \mathbf{n}_{A_i}^\Gamma(\tau_i - 0) | T_{\mathbf{A}_i} | \mathbf{n}_{A_i}^\Gamma(\tau_i + 0) \rangle| e^{c(2R)^\nu |A_i|} \\ &\exp\left\{-\int_{C(\mathcal{A})} d(x, \tau) [\Upsilon_x(\mathbf{n}_{U(x)}^\Gamma(\tau)) - e_0 - \frac{\Delta_0}{4} (2R)^{-\nu} \mathbb{I}[(x, \tau) \in \text{core } \Gamma]]\right\}. \end{aligned} \quad (5.15)$$

To estimate the above expression, we will split the ‘‘transition part’’ of the considered quantum contours into connected components, to be called *fragments*, and deal with them separately. Even though the weight of a quantum contour cannot be partitioned into the corresponding fragments, we will get an upper bound combined from fragment bounds. Consider thus the set

$$\hat{A}(\Gamma) = \text{core } \Gamma \cap C(A(\Gamma))$$

and the fragments $\zeta_i = (B_i, \omega_{B_i})$ on the connected components B_i of $\hat{A}(\Gamma)$, $\hat{A}(\Gamma) = \cup_{i=1}^n B_i$, ω_{B_i} is the restriction of ω^Γ onto B_i .

From Assumption 4, we have

$$\begin{aligned} &\int_{C(\mathcal{A})} d(x, \tau) \left[\Upsilon_x(\mathbf{n}_{U(x)}^\Gamma(\tau)) - e_0 - \frac{\Delta_0}{4} (2R)^{-\nu} \mathbb{I}[(x, \tau) \in \text{core } \Gamma] \right] \\ &\geq \frac{1}{4} (2R)^{-\nu} \Delta_0 \sum_{i=1}^n |B_i|. \end{aligned}$$

Let us introduce a bound for the contribution of a fragment ζ with transitions \mathbf{A}_j , $j = 1, \dots, k$,

$$\hat{z}(\zeta) = e^{-\frac{1}{4} (2R)^{-\nu} \Delta_0 |B|} \prod_{j=1}^k |\langle \mathbf{n}_{A_j}^\zeta(\tau_1 - 0) | T_{\mathbf{A}_j} | \mathbf{n}_{A_j}^\zeta(\tau_1 + 0) \rangle| e^{c(2R)^\nu |A_j|}.$$

Then, integrating over the set $\mathcal{F}_{C(\mathcal{A})}$ of all fragments in $C(\mathcal{A})$, we get

$$e^{c|Y|} |\mathfrak{Z}(Y)| \leq e^{-\frac{\tilde{\beta}}{\Delta} e_0 |Y|} e^{|Y|} \sum_{\mathcal{A} \subset \text{supp } Y} 3^{|\text{supp } Y \setminus \mathcal{A}|} \sum_{n \geq 0} \frac{1}{n!} \left(\int_{\mathcal{F}_{C(\mathcal{A})}} d\zeta \hat{z}(\zeta) \right)^n. \quad (5.16)$$

Anticipating the bound $\int_{\mathcal{F}_{C(\mathcal{A})}} d\zeta \hat{z}(\zeta) \leq |\mathcal{A}|$, we immediately get the claim,

$$e^{c|Y|} |\mathfrak{Z}(Y)| \leq e^{-\frac{\tilde{\beta}}{\Delta} e_0 |Y|} e^{3|Y|},$$

with a slight change of constant $c \rightarrow c - 3$.

A bound on the integral of fragments. Let us first consider *short* fragments $\zeta = (B, \omega_B)$ satisfying the condition

$$\frac{1}{2} \sum_{j=1}^k |A_j| \leq \frac{\log(\tilde{\beta}/\Delta)}{\log(1/\|T\|)} \leq \log \tilde{\beta} + k \quad (5.17)$$

(if $\|T\| \leq 1$). The integral over the time of occurrence of the first transition yields the factor $\tilde{\beta}/\Delta$. Notice that ζ is not a loop. This follows from the construction of quantum contours and the fact that B is a connected component of $\hat{A}(\Gamma)$, where every transition is taken together with its R -neighbourhood. Thus, either its sequence of transitions does not belong to \mathcal{S} , or the starting configuration does not coincide with the ending configuration. In the first case we use Assumption 5, in the second case Assumption 6, and since (5.17) means that the sum over transitions is bounded, we can write

$$\int_{\mathcal{F}_{C(A)}^{\text{short}}} d\zeta \hat{z}(\zeta) \leq \frac{1}{2} |\mathcal{A}|, \quad (5.18)$$

if ε_1 and ε_2 are small enough, independently of $\|T\|$.

Finally, we estimate the integral over ζ 's that are not short. We have

$$\int_{\mathcal{F}_{C(A)} \setminus \mathcal{F}_{C(A)}^{\text{short}}} d\zeta \hat{z}(\zeta) \leq |\mathcal{A}| \frac{\tilde{\beta}}{\Delta} \int_{\mathcal{F}_{C(A)}^{(x,\tau)} \setminus \mathcal{F}_{C(A)}^{\text{short}}} d\zeta \hat{z}(\zeta). \quad (5.19)$$

Here $\mathcal{F}_{C(A)}^{(x,\tau)}$ is the set of all fragments ζ whose first quantum transition (A_1, τ_1) is such that $x \in A_1$ and $\tau = \tau_1$. Whenever ζ is not short, we have

$$1 \leq \frac{\Delta}{\tilde{\beta}} \prod_{j=1}^k \|T\|^{-\frac{1}{2}|A_j|}.$$

Thus, defining

$$\hat{z}'(\zeta) = e^{-\frac{1}{4}(2R)^{-\nu} \Delta_0 |B|} \prod_{j=1}^k \left[\|T\|^{\frac{1}{2}} e^{c(2R)^\nu + 1} \right]^{|A_j|}, \quad (5.20)$$

we find the bound

$$|\mathcal{A}| \int_{\mathcal{F}(x,\tau)} d\zeta \hat{z}'(\zeta).$$

Here, slightly overestimating, we take for $\mathcal{F}(x, \tau)$ the set of all fragments containing a quantum transition (A, τ) with $x \in A$.

The support B of a fragment $\zeta = (B, \omega_B) \in \mathcal{F}(x, \tau)$, is a finite union of vertical segments (i.e. sets of the form $\{y\} \times [\tau_1, \tau_2] \subset \mathbb{T}_\Delta$) and k horizontal quantum transitions A_1, \dots, A_k .

We will finish the proof by proving by induction the bound

$$\int_{\mathcal{F}(x,\tau;k)} d\zeta \hat{z}'(\zeta) \leq 1 \quad (5.21)$$

with $\mathcal{F}(x, \tau; k)$ denoting the set of fragments from $\mathcal{F}(x, \tau)$ with at most k quantum transitions.

Consider thus a fragment ζ with k horizontal quantum transitions connected by vertical segments. Let (A, τ) be the transition containing the point (x, τ) and let $(A_1, \tau + \tau_1), \dots, (A_\ell, \tau + \tau_\ell)$ be the transitions that are connected by (one or several) vertical segments of the respective lengths $|\tau_1|, \dots, |\tau_\ell|$ with the transition (A, τ) . If we remove all those segments, the fragment ζ will split into the “naked” transition (A, τ) and additional $\bar{\ell} \leq \ell$ fragments $\zeta_1, \dots, \zeta_{\bar{\ell}}$, such that each fragment $\zeta_j, j = 1, \dots, \bar{\ell}$, belongs to $\mathcal{F}(y_j, \tau + \tau_j; k-1)$ with $y_j \in A$. Taking into account that the number of configurations (determining the possible vertical segments attached to A) above and below A is bounded by $S^{2|A|}$ and that the number of possibilities to choose the points y_j is bounded by $|A|^{\bar{\ell}}$, we get

$$\begin{aligned} \int_{\mathcal{F}(x, \tau; k)} d\zeta \hat{z}'(\zeta) &\leq \sum_{A, \text{dist}(A, x) < R} [\|T\|^{\frac{1}{2}} e^{c(2R)^{\nu+1}} S^2]^{|A|} \\ &\quad \sum_{\bar{\ell}=1}^{\infty} \frac{|A|^{\bar{\ell}}}{\bar{\ell}!} \int d\tau_1 \cdots \int d\tau_{\bar{\ell}} e^{-\frac{1}{2}(2R)^{-\nu} \Delta_0(\tau_1 + \cdots + \tau_{\bar{\ell}})} \\ &\quad \prod_{j=1}^{\bar{\ell}} \int_{\mathcal{F}(y_j, \tau + \tau_j; k-1)} d\zeta \hat{z}'(\zeta_j) \\ &\leq \sum_{A, \text{dist}(A, x) < R} [\|T\|^{\frac{1}{2}} S^2 e^{c(2R)^{\nu+2}}]^{|A|} e^{2(2R)^{\nu}/\Delta_0} \leq 1 \end{aligned} \quad (5.22)$$

once $\|T\|$ is sufficiently small. \square

In the application of Pirogov–Sinai theory we shall also need a bound on derivatives of the weight of contours.

Lemma 5.3. *Under Assumptions 1–7, for any $c < \infty$, there exist constants $\alpha, \beta_0, \tilde{\beta}_0 < \infty$ and $\varepsilon_0 > 0$ such that if $\beta \geq \beta_0, \tilde{\beta}_0 \leq \tilde{\beta} < 2\tilde{\beta}_0, \|T\| + \sum_{i=1}^{r-1} \|\frac{\partial}{\partial \mu_i} T\| \leq \varepsilon_0$, and $\varepsilon_1, \varepsilon_2 \leq \varepsilon_0$, one has*

$$\left| \frac{\partial}{\partial \mu_i} \mathfrak{z}(Y) \right| \leq \alpha \tilde{\beta} |Y| e^{-\frac{\tilde{\beta}}{\Delta} c_0^\mu |Y|} e^{-c|Y|}$$

for any contour Y .

Proof. From the definition (4.35) of \mathfrak{z} , one has

$$\begin{aligned} \left| \frac{\partial}{\partial \mu_i} \mathfrak{z}(Y) \right| &\leq \\ &\leq |\mathfrak{z}(Y)| \left\{ \sum_{\gamma \in \Gamma} \left| \frac{\partial}{\partial \mu_i} z(\gamma) \right| + \sum_{d \in D} |W_d \cap C(\text{supp } Y)| \left| \frac{\partial}{\partial \mu_i} e^{\mu}(d) \right| + \left| \frac{\partial}{\partial \mu_i} \tilde{\mathcal{R}}(\Gamma) \right| \right\} \\ &\quad + \int_{\mathcal{D}_\Lambda(Y)} d\Gamma \prod_{\gamma \in \Gamma} |z(\gamma)| \prod_{d \in D} e^{-e^\mu(d) |W_d \cap C(\text{supp } Y)|} e^{|\tilde{\mathcal{R}}(\Gamma)|} \\ &\quad \sum_{\mathcal{M}} \mathbb{I}[\mathcal{M}(\text{supp } \Gamma) \cup \text{supp } \mathcal{M} = \text{supp } Y] \\ &\quad \sum_{M \in \mathcal{M}} \left| e^{\varphi(M; \Gamma)} \frac{\partial}{\partial \mu_i} \varphi(M; \Gamma) \right| \prod_{M' \in \mathcal{M}, M' \neq M} |e^{\varphi(M'; \Gamma)} - 1|. \end{aligned} \quad (5.23)$$

The bound for $|\frac{\partial}{\partial \mu_i} z(\Gamma)|$ is standard, see [BKU1], and $|\frac{\partial}{\partial \mu_i} e^\mu(d)|$ is assumed to be bounded in Assumption 7. For the other terms we have to control clusters of loops. Since we have exponential decay for $z(\xi)$ with any strength (by taking β large and $\|T\|$ small), we have the same for $\frac{\partial}{\partial \mu_i} z(\xi)$ (by taking β larger and $\|T\|$ smaller). The integrals over C can be estimated as before, the only effect of the derivative being an extra factor n (when the clusters have n loops). \square

6. Expectation Values of Local Observables and Construction of Pure States

So far we have obtained an expression (4.36) for the partition function Z_Λ^{per} of the quantum model on torus Λ in terms of that of a classical lattice contour model with the weights of the contours showing an exponential decay with respect to their length. Using the same weights $\mathfrak{z}(Y)$, we can also introduce the partition functions $Z_{\Lambda(L)}^d$ with the torus Λ replaced by a hypercube $\Lambda(L)$ and with fixed boundary conditions d . Namely, we take simply the sum only over those collections \mathcal{Y} of contours whose external contours are labeled by d and are not close to the boundary.¹³ Notice, however, that here we are defining $Z_{\Lambda(L)}^d$ directly in terms of the classical contour model, without ensuring existence of corresponding partition function for the original model. We will use these partition functions only as a tool for proving our theorems that are stated directly in terms of quantum models.

To be more precise, we can extend the definition even more and consider, instead of the torus Λ , any finite set $V \subset \mathbb{L} = \mathbb{Z}^v \times \{0, 1, \dots, N - 1\}^{\text{per}}$. There is a class of contours that can be viewed as having their support contained in $V \subset \mathbb{L}$. For any such contour Y we introduce its interior $\text{Int } Y$ as the union of all finite components of $\mathbb{L} \setminus \text{supp } Y$ and $\text{Int}_d Y$ as the union of all components of $\text{Int } Y$ whose boundary is labelled by d . Recalling that we assumed $v \geq 2$, we note that the set $\mathbb{L} \setminus (\text{supp } Y \cup \text{Int } Y)$ is a connected set, implying that the label $\alpha_Y(\cdot)$ is constant on the boundary of the set $V(Y) = \text{supp } Y \cup \text{Int } Y$. We say that Y is a d -contour, if $\alpha_Y = d$ on this boundary. Two contours Y and Y' are called *mutually external* if $V(Y) \cap V(Y') = \emptyset$. Given an admissible set \mathcal{Y} of contours, we say that $Y \in \mathcal{Y}$ is an *external contour* in \mathcal{Y} , if $\text{supp } Y \cap V(Y') = \emptyset$ for all $Y' \in \mathcal{Y}$, $Y' \neq Y$. The sets \mathcal{Y} contributing to Z_V^d are such that all their external contours are d -contours and $\text{dist}(Y, \partial V) > 1$ for every $Y \in \mathcal{Y}$.

In this way we find ourselves exactly in the setting of standard Pirogov–Sinai theory, or rather, the reformulation for “thin slab” (cylinder \mathbb{L} of fixed temporal size N) as presented in Sects. 5–7 and Appendix of [BKU1]. In particular, for sufficiently large β and sufficiently small $\|T\| + \sum_{i=1}^{r-1} \|\frac{\partial}{\partial \mu_i} T\|$, there exist functions $f^{\beta, \mu}(d)$, metastable free energies, such that the condition $\text{Re } f^{\beta, \mu}(d) = f_0$, with $f_0 \equiv f_0^{\beta, \mu}$ defined by $f_0 = \min_{d' \in D} \text{Re } f^{\beta, \mu}(d')$, characterizes the existence of pure stable phase d . Namely, as will be shown next, a pure stable phase $\langle \cdot \rangle_\beta^d$ exists and is close to the pure ground state $|d\rangle$.

There is one subtlety in the definition of $f^{\beta, \mu}(d)$. Namely, after choosing a suitable $\tilde{\beta}_0$, given β , there exist several pairs $(\tilde{\beta}, N)$ such that $\tilde{\beta} \in (\tilde{\beta}_0, 2\tilde{\beta}_0)$ and $N\tilde{\beta} = \beta$. To be specific, we may agree to choose among them that one with maximal N . The function $f^{\beta, \mu}(d)$ is then uniquely defined for each $\beta > \beta_0$. Notice, however, that while increasing β , we pass, at the particular value $\beta_N = N\tilde{\beta}_0$, from discretization of temporal size N

¹³ In the terminology of Pirogov–Sinai theory we rather mean *diluted partition functions* – see the more precise definition below.

to $N + 1$. As a result, the function $f^{\beta, \mu}(d)$ might be discontinuous at β_N with $\beta = \infty$ being an accumulation point of such discontinuities. Nevertheless, these discontinuities are harmless. They can appear only when $\text{Re } f^{\beta, \mu}(d) > f_0$ and do not change anything in the following argument.

Before we come to the construction of pure stable phases, notice that the first claim of Theorem 2.2 (equality of f_0 with the limiting free energy) is now a direct consequence of the bound

$$\left| Z_{\Lambda}^{\text{per}} - |Q| e^{-\tilde{\beta} f_0 N L^v} \right| \leq e^{-\tilde{\beta} f_0 N L^v} O(e^{-\text{const } L}) \quad (6.1)$$

[cf. [BKU1], (7.14)]. Here $Q = \{d; \text{Re } f^{\beta, \mu}(d) = f_0\}$.

The expectation value of a local observable K is defined as

$$\langle K \rangle_{\Lambda}^{\text{per}} = \frac{\text{Tr } K e^{-\beta H_{\Lambda}}}{\text{Tr } e^{-\beta H_{\Lambda}}}. \quad (6.2)$$

In Sect. 4 we have obtained a contour expression for $Z_{\Lambda}^{\text{per}} = \text{Tr } e^{-\beta H_{\Lambda}}$. We retrace here the same steps for $Z_{\Lambda}^{\text{per}}(K) := \text{Tr } K e^{-\beta H_{\Lambda}}$. The Duhamel expansion (4.1) for $Z_{\Lambda}^{\text{per}}(K)$ leads to an equation analogous to (4.2),

$$\begin{aligned} Z_{\Lambda}^{\text{per}}(K) &= \sum_{m \geq 0} \sum_{n_{\Lambda}^0, \dots, n_{\Lambda}^m} \sum_{\substack{\mathbf{A}_1, \dots, \mathbf{A}_m \\ \mathbf{A}_i \subset \Lambda}} \int_{0 < \tau_1 < \dots < \tau_m < \beta} d\tau_1 \dots d\tau_m \langle n_{\Lambda}^0 | K | n_{\Lambda}^1 \rangle \\ &e^{-\tau_1 V_{\Lambda}(n_{\Lambda}^1)} \langle n_{\Lambda}^1 | T_{\mathbf{A}_1} | n_{\Lambda}^2 \rangle e^{-(\tau_2 - \tau_1) V_{\Lambda}(n_{\Lambda}^2)} \dots \langle n_{\Lambda}^m | T_{\mathbf{A}_m} | n_{\Lambda}^0 \rangle e^{-(\beta - \tau_m) V_{\Lambda}(n_{\Lambda}^0)}. \end{aligned} \quad (6.3)$$

Configurations n_{Λ}^0 and n_{Λ}^1 match on $\Lambda \setminus \text{supp } K$ ($\text{supp } K \subset \Lambda$ is a finite set due to the locality of K), but may differ on $\text{supp } K$ if K is an operator with non-zero off-diagonal terms. Let $\mathcal{Q}_{\Lambda}(K)$ be the set of quantum configurations with $\mathbf{n}_{\Lambda}(\tau)$ that is constant except possibly at $\cup_{i=1}^m (A_i \times \tau_i) \cup (\text{supp } K \times 0)$. Then

$$Z_{\Lambda}^{\text{per}}(K) = \int_{\mathcal{Q}_{\Lambda}(K)} d\omega_{\mathbb{T}_{\Lambda}} \langle n_{\Lambda}^0 | K | n_{\Lambda}^1 \rangle \rho(\omega_{\mathbb{T}_{\Lambda}}). \quad (6.4)$$

We identify loops with the same iteration scheme as in Sect. 4, starting with the set $\mathbf{B}^{(0)}(\omega) \cup (\text{supp } K \times 0)$ instead of $\mathbf{B}^{(0)}(\omega)$ only. This leads to the set $\mathbf{B}^K(\omega)$. Removing the loops, we define $\mathbf{B}_e^K(\omega)$, whose connected components form quantum contours. There is one special quantum contour, namely that which contains $\text{supp } K \times 0$. Let us denote it by γ^K and define its weight [see (4.28)]

$$\begin{aligned} z^K(\gamma^K) &= \langle \mathbf{n}_{\text{supp } K}^{\gamma^K}(-0) | K | \mathbf{n}_{\text{supp } K}^{\gamma^K}(+0) \rangle \prod_{i=1}^m \langle \mathbf{n}_{A_i}^{\gamma^K}(\tau_i - 0) | T_{A_i} | \mathbf{n}_{A_i}^{\gamma^K}(\tau_i + 0) \rangle \\ &\exp \left\{ - \int_B d(x, \tau) \Upsilon_x(\mathbf{n}_{U(x)}^{\gamma^K}(\tau)) \right\}. \end{aligned} \quad (6.5)$$

Let $\Gamma^K = \{\gamma^K, \gamma_1, \dots, \gamma_k\}$ be an admissible set of quantum contours, defining a quantum configuration $\omega^{\Gamma^K} \in \mathcal{Q}_{\Lambda}(K)$. Then we have an expression similar to that of Lemma 4.4,

$$Z_{\Lambda}^{\text{per}}(K) = \int_{\mathcal{D}_{\Lambda}(K)} d\Gamma^K \prod_{d \in D} e^{-|W_d(\Gamma^K)|e(d)} z^K(\gamma^K) \prod_{\gamma \in \Gamma^K \setminus \{\gamma^K\}} z(\gamma) e^{\mathcal{R}(\Gamma^K)}, \quad (6.6)$$

with $\mathcal{R}(\Gamma^K)$ as in (4.29) with Γ replaced by Γ^K .

Next step is to discretize the lattice, to expand $e^{\mathcal{R}(\Gamma^K)}$, and if Y^K is the contour that contains $\text{supp } K \times 0 \subset \mathbb{L}_{\Lambda}$, to define $\mathfrak{z}^K(Y^K)$ [see (4.35)]:

$$\begin{aligned} \mathfrak{z}^K(Y^K) &= \int_{\mathcal{D}_{\Lambda}(Y^K)} d\Gamma^K z^K(\gamma^K) \prod_{\gamma \in \Gamma^K \setminus \{\gamma^K\}} z(\gamma) \prod_{d \in D} e^{-e(d)|W_d(\Gamma^K) \cap C(\text{supp } Y^K)|} e^{\tilde{\mathcal{R}}(\Gamma^K)} \\ &\sum_{\mathcal{M}} \mathbb{I}[M(\text{supp } \Gamma^K \cup \text{supp } \mathcal{M} = \text{supp } Y^K)] \prod_{M \in \mathcal{M}} (e^{\varphi(M; \Gamma^K)} - 1). \end{aligned} \quad (6.7)$$

We also need a bound for $\mathfrak{z}^K(Y^K)$. It is clear that the situation is the same as for Lemmas 5.1 and 5.2, except for a factor $\langle \mathbf{n}_{\text{supp } K}^{\gamma^K}(-0) | K | \mathbf{n}_{\text{supp } K}^{\gamma^K}(+0) \rangle$ that is bounded by $\|K\|$. We can thus summarize:

Lemma 6.1. *Under Assumptions 1–6, for any $c < \infty$, there exist $\beta_0, \tilde{\beta}_0 < \infty$, and $\varepsilon_0 > 0$ such that if $\beta \geq \beta_0$, $\tilde{\beta} \leq \tilde{\beta} < 2\tilde{\beta}_0$ and $\|T\|, \varepsilon_1, \varepsilon_2 \leq \varepsilon_0$, we have*

$$Z_{\Lambda}^{\text{per}}(K) = \sum_{\mathcal{Y}^K = \{Y^K, Y_1, \dots, Y_k\}} \prod_{d \in D} e^{-\frac{\tilde{\beta}}{\Delta} e(d) |\mathcal{W}_d(\mathcal{Y}^K)|} \mathfrak{z}^K(Y^K) \prod_{Y \in \mathcal{Y}^K \setminus \{Y^K\}} \mathfrak{z}(Y), \quad (6.8)$$

for every local observable K , with

$$|\mathfrak{z}^K(Y^K)| \leq \|K\| e^{c|\text{supp } K|} e^{-\frac{\tilde{\beta}}{\Delta} e_0 |Y^K|} e^{-c|Y^K|}$$

for any contour Y^K .

In a similar manner as at the beginning of this section, we can introduce $Z_V^d(K)$ for any $V \subset \mathbb{L}$ by restricting ourselves in the sum (6.8) to the collections \mathcal{Y}^K whose all external contours are d -contours and $\text{dist}(Y, \partial V) > 1$ for every $Y \in \mathcal{Y}^K$. Thus we can define the expectation value

$$\langle K \rangle_V^d = \frac{Z_V^d(K)}{Z_V^d} \quad (6.9)$$

for any $V \subset \mathbb{L}$ and, in particular, the expectation $\langle K \rangle_{\Lambda(L)}^d$ for a hypercube $\Lambda(L)$.

Again, this is exactly the setting discussed in detail in [BKU1]. We can use directly the corresponding results (cf. [BKU1], Lemma 6.1) to prove first that the limiting state $\langle \cdot \rangle_{\beta}^d$ exists. Further, retracing the proof of Theorem 2.2 in [BKU1] we prove that the limit

$$\langle K \rangle_{\beta}^{\text{per}} = \lim_{\Lambda \nearrow \mathbb{Z}^v} \frac{\text{Tr } K e^{-\beta H_{\Lambda}}}{\text{Tr } e^{-\beta H_{\Lambda}}} \quad (6.10)$$

exists for every local K (proving thus Theorem 2.1). Moreover,

$$\langle K \rangle_{\beta}^{\text{per}} = \frac{1}{|Q|} \sum_{d \in Q} \langle K \rangle_{\beta}^d, \quad (6.11)$$

where, again, Q denotes the set of stable phases, $Q = \{d; \operatorname{Re} f^{\beta, \mu}(d) = f_0\}$. Thus we proved the claim d) of Theorem 2.2.

Also the assertion c) follows in standard manner from the contour representation employing directly the exponential decay of contour activities and the corresponding cluster expansion [cf. [BKU1], (2.27)].

Before passing to the proof of b), we shall verify that $\langle \cdot \rangle_{\beta}^d$ is actually a pure stable state according to our definition, i.e. a limit of thermodynamically stable states.¹⁴ To this end, let us first discuss how metastable free energies $f^{\beta, \mu}(d)$ change with μ . The standard construction yields $f^{\beta, \mu}(d)$ in the form of a sum $e^{\mu}(d) + s^{\beta, \mu}(d)$, where $s^{\beta, \mu}(d)$ is the free energy of “truncated” contour model $K'_d(Y)$ [see [BKU1], (5.13) and (5.6)] constructed from the labelled contour model (4.36), which is under control by cluster expansions. As a result, we have bounds of the form $O(e^{-\beta} + \|T\| + \sum_{i=1}^{r-1} \|\frac{\partial T}{\partial \mu_i}\|)$ on $|s^{\beta, \mu}(d)|$ as well as on the derivatives with respect to μ . Hence, in view of Assumption 7, the leading behaviour is yielded by $e^{\mu}(d)$.

Starting thus from a given potential Φ^{μ} with $Q^{\mu} = \{d \in D; \operatorname{Re} f^{\beta, \mu}(d) = f_0^{\mu}\}$, one can easily add to Φ^{μ} a suitable “external field” that favours a chosen $d \in Q^{\mu}$. For example, one can take

$$\Phi_A^{\mu, \alpha}(n) = \Phi_A^{\mu}(n) + \alpha \delta_A^d(n)$$

with δ_A^d defined by taking $\delta_A^d(n) = 0$ for $n_A = d_A$ and $\delta_A^d(n) = 1$ otherwise.¹⁵ Now, since $\frac{\partial e^{\mu, \alpha}(d)}{\partial \alpha}$ is bounded from below by a positive constant (while $\frac{\partial e^{\mu, \alpha}(d')}{\partial \alpha} = 0$ for $d' \neq d$), for any $\alpha > 0$ the only stable phase is d , $\operatorname{Re} f^{\beta, \mu, \alpha}(d) = f_0^{\beta, \mu, \alpha} \equiv \min_{d' \in D} \operatorname{Re} f^{\beta, \mu, \alpha}(d')$, and, in the same time, $\operatorname{Re} f^{\beta, \mu, \alpha}(d') > f_0^{\beta, \mu, \alpha}$ for $d' \neq d$. Thus, $Q^{\mu, \alpha} = \{d\}$ and $\langle \cdot \rangle_{\beta, \mu, \alpha}^d = \langle \cdot \rangle_{\beta, \mu, \alpha}^{\text{per}}$. This state is thermodynamically stable – when adding any small perturbation, metastable free energies will change only a little and that one corresponding to the state d will still be the only one attaining the minimum. The fact that in the limit of vanishing perturbation we recover $\langle \cdot \rangle_{\beta, \mu, \alpha}^d$, as well as the fact that

$$\lim_{\alpha \rightarrow 0+} \langle \cdot \rangle_{\beta, \mu, \alpha}^{\text{per}} \equiv \lim_{\alpha \rightarrow 0+} \langle \cdot \rangle_{\beta, \mu, \alpha}^d = \langle \cdot \rangle_{\beta, \mu}^d,$$

follows by inspecting the contour representations of the corresponding expectations and observing that it can be expressed in terms of converging cluster expansions whose terms depend smoothly on α as well as on the additional perturbation.

To prove, finally, the claim b) of Theorem 2.2, it suffices to show that it is valid for $\langle \cdot \rangle_{\beta, \mu, \alpha}^{\text{per}} = \langle \cdot \rangle_{\beta, \mu, \alpha}^d$ for every $\alpha > 0$. Abbreviating $\langle \cdot \rangle_{\beta, \mu, \alpha}^{\text{per}} = \langle \cdot \rangle^{\text{per}}$ and $H_{\Lambda}^{\mu, \alpha} = H_{\Lambda}$, we first notice that the expectation value of the projector onto the configuration d on $\operatorname{supp} K$, $P_{\operatorname{supp} K}^d := |d_{\operatorname{supp} K}\rangle \langle d_{\operatorname{supp} K}|$, is close to 1, since its complement $\langle (\mathbb{1} - P_{\operatorname{supp} K}^d) \rangle^{\text{per}} = \langle (\mathbb{1} - P_{\operatorname{supp} K}^d) \rangle^d$ is related to the presence of a contour intersecting or surrounding $\operatorname{supp} K$ (loops intersecting $\operatorname{supp} K \times \{0\}$ are considered here as part of quantum contours), whose weight is small. More precisely, for any $\delta > 0$ we have

$$\langle (\mathbb{1} - P_{\operatorname{supp} K}^d) \rangle^{\text{per}} \leq \delta |\operatorname{supp} K|,$$

¹⁴ Recall that, up to now, the state $\langle \cdot \rangle_{\beta}^d$ is defined only in terms of the contour representation [see (6.9), (6.8), and (4.36)], and the only proven connection with a state of original quantum model is the equality (6.11).

¹⁵ Actually, we can restrict δ_A^d only to a particular type of sets A – for example all hypercubes of side R .

whenever $\|T\|$, ε_1 , ε_2 are small enough and β large enough. Furthermore,

$$\begin{aligned} \langle K \rangle_{\Lambda}^{\text{per}} &= \frac{1}{Z_{\Lambda}^{\text{per}}} \left[\text{Tr} (P_{\text{supp } K}^d K P_{\text{supp } K}^d e^{-\beta H_{\Lambda}}) + \right. \\ &\quad \left. + \text{Tr} ((\mathbb{1} - P_{\text{supp } K}^d) K P_{\text{supp } K}^d e^{-\beta H_{\Lambda}}) + \text{Tr} (K (\mathbb{1} - P_{\text{supp } K}^d) e^{-\beta H_{\Lambda}}) \right] \end{aligned} \quad (6.12)$$

and

$$\begin{aligned} \text{Tr} (P_{\text{supp } K}^d K P_{\text{supp } K}^d e^{-\beta H_{\Lambda}}) &= \langle d_{\Lambda} | K | d_{\Lambda} \rangle \text{Tr} (P_{\text{supp } K}^d e^{-\beta H_{\Lambda}}) \\ &= \langle d_{\Lambda} | K | d_{\Lambda} \rangle [\text{Tr} (e^{-\beta H_{\Lambda}}) - \text{Tr} ((\mathbb{1} - P_{\text{supp } K}^d) e^{-\beta H_{\Lambda}})], \end{aligned} \quad (6.13)$$

so that we have

$$\begin{aligned} |\langle K \rangle_{\Lambda}^{\text{per}} - \langle d_{\Lambda} | K | d_{\Lambda} \rangle| &\leq |\langle d_{\Lambda} | K | d_{\Lambda} \rangle| \langle (\mathbb{1} - P_{\text{supp } K}^d) \rangle_{\Lambda}^{\text{per}} \\ &\quad + |\langle (\mathbb{1} - P_{\text{supp } K}^d) K P_{\text{supp } K}^d \rangle_{\Lambda}^{\text{per}}| + |\langle K (\mathbb{1} - P_{\text{supp } K}^d) \rangle_{\Lambda}^{\text{per}}|. \end{aligned} \quad (6.14)$$

The mapping $(K, K') \mapsto \langle K^{\dagger} K' \rangle_{\Lambda}^{\text{per}}$, with any two local operators K, K' , is a scalar product; therefore the Schwarz inequality yields

$$\begin{aligned} |\langle K \rangle_{\Lambda}^{\text{per}} - \langle d_{\Lambda} | K | d_{\Lambda} \rangle| &\leq |\langle d_{\Lambda} | K | d_{\Lambda} \rangle| \langle (\mathbb{1} - P_{\text{supp } K}^d) \rangle_{\Lambda}^{\text{per}} \\ &\quad + \left(\langle (\mathbb{1} - P_{\text{supp } K}^d) \rangle_{\Lambda}^{\text{per}} \right)^{\frac{1}{2}} \left([\langle P_{\text{supp } K}^d K^{\dagger} K P_{\text{supp } K}^d \rangle_{\Lambda}^{\text{per}}]^{\frac{1}{2}} + [\langle K^{\dagger} K \rangle_{\Lambda}^{\text{per}}]^{\frac{1}{2}} \right) \\ &\leq \|K\| \left[\langle (\mathbb{1} - P_{\text{supp } K}^d) \rangle_{\Lambda}^{\text{per}} + 2 \langle (\mathbb{1} - P_{\text{supp } T}^d) \rangle_{\Lambda}^{\text{per}} \right]^{1/2} \\ &\leq \|K\| |\text{supp } K| (\delta + 2\delta^{\frac{1}{2}}). \end{aligned} \quad (6.15)$$

The proof of the remaining Theorem 2.3 is a standard application of the implicit function theorem. Thus, for example, the point $\bar{\mu}_0$ of maximal coexistence, $\text{Re } f^{\beta, \bar{\mu}_0}(d) = \text{Re } f^{\beta, \bar{\mu}_0}(d')$ for every pair $d, d' \in D$, can be viewed as the solution of the vector equation $f(\bar{\mu}_0) = 0$, with $f(\mu) = (\text{Re } f^{\beta, \mu}(d_i) - \text{Re } f^{\beta, \mu}(d_r))_{i=1}^{r-1}$. Now, $f = e + s$, $e(\mu) = (e^{\mu}(d_i) - e^{\mu}(d_r))_{i=1}^{r-1}$, $s(\mu) = (\text{Re } s^{\beta, \mu}(d_i) - \text{Re } s^{\beta, \mu}(d_r))_{i=1}^{r-1}$, with $\|s\|$ as well as $\|\frac{\partial s}{\partial \mu}\|$ bounded by a small constant once $\|T\| + \sum_{i=1}^{r-1} \|\frac{\partial T}{\partial \mu_i}\|$ is sufficiently small and β is sufficiently large. The existence of a unique solution $\bar{\mu}_0 \in \mathcal{U}$ then follows once we notice the existence of the solution $\mu_0 \in \mathcal{U}$ of the equation $e(\mu_0) = 0$ (equivalent with $e^{\mu_0}(d) = e^{\mu_0}(d')$, $d, d' \in D$) and the fact that the mapping

$$\mathcal{T} : \mu \rightarrow A^{-1} \left(\frac{\partial e}{\partial \mu} \Big|_{\mu=\mu_0} (\mu - \mu_0) - f(\mu) \right)$$

with A^{-1} the matrix inverse to $(\frac{\partial e}{\partial \mu})$, is a contraction. To this end it is enough just to recall Assumption 7 and the bounds on $s^{\beta, \mu}(d)$, $d \in D$, and its derivatives.

A. General Expression for the Effective Potential

It is actually a cumbersome task to write down a compact formula for the effective potential in the general case. A lot of notation has to be introduced, and one pays for the generality by the fact that the resulting formulæ look rather obscure; nevertheless, the logic behind the following definitions and equations appeared rather naturally along the steps in Sect. 4. We would like to stress that for typical concrete models, it is entirely sufficient to restrict to the effective potential due to at most 4 transitions, and we can content ourselves with Eqs. (2.8)–(2.10).

We assume that a list \mathcal{S} of sequences of quantum transitions \mathbf{A} is given to represent the leading quantum fluctuations. The particular choice of \mathcal{S} depends on properties of the considered model. Often the obvious choice like “any sequence of transitions not surpassing a given order” is sufficient. In the general case, certain conditions (specified in Assumption 5) involving \mathcal{S} are to be met. For any $g_A \in G_A$, the effective potential Ψ is defined to equal

$$\begin{aligned} \Psi_A(g_A) = & - \sum_{n \geq 1} \frac{1}{n!} \sum_{k_1, \dots, k_n \geq 2} \sum_{\substack{(\mathbf{A}_1^1, \dots, \mathbf{A}_{k_1}^1, \mathbf{A}_1^2, \dots, \mathbf{A}_{k_n}^n) \in \mathcal{S} \\ \cup_{i,j} \bar{A}_j^i = A}} \\ & \prod_{i=1}^n \left\{ \sum_{\substack{n_A^{i,1}, \dots, n_A^{i,k_i-1} \notin G_A}} \mathcal{I}(A_1^i, \dots, A_{k_i}^i; n_A^{i,1} g_{\Lambda \setminus A}, \dots, n_A^{i,k_i-1} g_{\Lambda \setminus A}) \left[\prod_{j=1}^{k_i} \langle n_A^{i,j-1} | T_{A_j^i} | n_A^{i,j} \rangle \right] \right. \\ & \left. \int_{-\infty < \tau_1^i < \dots < \tau_{k_i}^i < \infty} d\tau_1^i \dots d\tau_{k_i}^i \left[\prod_{j=1}^{k_i-1} e^{-(\tau_{j+1}^i - \tau_j^i) \sum_{x, U_0(x) \subset A} [\Phi_x(n_{U_0(x)}^{i,j}) - \Phi_x(g_{U_0(x)})]} \right] \right\} \\ & \frac{\mathbb{I}[\min_{i,j} \tau_j^i < 0 \text{ and } \max_{i,j} \tau_j^i > 0]}{\max_{i,j} \tau_j^i - \min_{i,j} \tau_j^i} \varphi^T(B_1, \dots, B_n). \quad (\text{A.1}) \end{aligned}$$

To begin to decode this formula, notice first that the second sum is over all sequences $(\mathbf{A}_1^1, \dots, \mathbf{A}_{k_1}^1, \mathbf{A}_1^2, \dots, \mathbf{A}_{k_n}^n)$ of transitions that are in the list \mathcal{S} and are just covering the set A , $\cup_{i,j} \bar{A}_j^i = A$. The sum in the braces (for a given $i = 1, \dots, n$) is taken over collections of configurations $n_A^{i,1}, \dots, n_A^{i,k_i-1} \notin G_A$ with $n_A^{i,0} \equiv n_A^{i,k_i} \equiv g_A$, while the integral is taken over “times” attributed to transitions, with the energy term in the exponent taken over the set $A^i = \cup_{j=1}^{k_i} \bar{A}_j^i$.

Finally, there are some restrictions on the sums and integrals encoded in functions $\frac{\mathbb{I}[\min_{i,j} \tau_j^i < 0 \text{ and } \max_{i,j} \tau_j^i > 0]}{\max_{i,j} \tau_j^i - \min_{i,j} \tau_j^i}$, $\varphi^T(B_1, \dots, B_n)$, and $\mathcal{I}(A_1^i, \dots, A_{k_i}^i; n_A^{i,1} g_{\Lambda \setminus A}, \dots, n_A^{i,k_i-1} g_{\Lambda \setminus A})$. The easiest is the first one. One just assumes that the interval between the first and the last of concerned “times” contains the origin and the integrand is divided by the length of this interval. The function $\varphi^T(B_1, \dots, B_n)$ in terms of the sets $B_i = A^i \times [\tau_1^i, \tau_{k_i}^i] \subset \mathbb{Z}^v \times [-\infty, \infty]$, $i = 1, \dots, n$, is the standard factor from the theory of cluster expansions defined as

$$\varphi^T(B_1, \dots, B_n) = \begin{cases} 1 & \text{if } n = 1 \\ \sum_{\mathcal{G}} \prod_{e(i,j) \in \mathcal{G}} (-\mathbb{I}[B_i \cup B_j \text{ is connected}]) & \text{if } n \geq 2 \end{cases}$$

with the sum over all connected graphs \mathcal{G} of n vertices. Connectedness of a set $B \subset \mathbb{Z}^v \times [-\infty, \infty]$ is defined by combining connection in continuous direction with connection in slices $\{x | (x, \tau) \in B\} \subset \mathbb{Z}^v$ through pairs of sites of distance one. The most difficult to define is the restriction given by the function \mathcal{I} that characterizes whether the collection of transitions is connected, in some generalized sense, through the intertwining configurations. A consolation might be that in lowest orders it is always true. Namely, whenever $k \leq 5$,

$$\begin{aligned} & \mathcal{I}(A_1, \dots, A_k; n_A^1 g_{\Lambda \setminus A}, \dots, n_A^{k-1} g_{\Lambda \setminus A}) \\ &= \begin{cases} 1 & \text{if } \cup_j \bar{A}_j \text{ is connected and } \prod_{j=1}^k \langle n_A^{j-1} | T_{A_j} | n_A^j \rangle \neq 0 \\ 0 & \text{if } \cup_j \bar{A}_j \text{ is not connected.} \end{cases} \quad (\text{A.2}) \end{aligned}$$

To define it in a general case, consider $A_1, \dots, A_k \subset \mathbb{Z}^v$ and $n^1, \dots, n^{k-1} \in \Omega^{\mathbb{Z}^v}$. Taking $\bar{A} = \cup_{x \in A} U(x)$ and $E(n) = \{x \in \Lambda : n_{U(x)} \neq g_{U(x)} \text{ for any } g \in G\}$, we consider the set $\hat{B}^{(0)} \subset \mathbb{Z}^{v+1}$,

$$\hat{B}^{(0)} = \bigcup_{j=1}^k [\bar{A}_j \times \{2j-2\}] \cup \bigcup_{j=1}^{k-1} [E(n^j) \times \{2j-1\}].$$

Think of layers, one on top of another – configurations on odd levels interspersed with transitions on even levels. The set $\hat{B}^{(0)}$ decomposes into connected components, $\hat{B}^{(0)} = \cup_{\ell \geq 1} \hat{B}_\ell^{(0)}$. To any $\hat{B}_\ell^{(0)}$, define the box $\tilde{B}_\ell^{(0)} \subset \mathbb{Z}^{v+1}$ as the smallest rectangle containing $\hat{B}_\ell^{(0)}$. Then let $\hat{B}^{(1)} = \cup_{\ell \geq 1} \tilde{B}_\ell^{(0)}$, decompose into connected components $\hat{B}^{(1)} = \cup_{\ell \geq 1} \hat{B}_\ell^{(1)}$, and repeat the procedure until no change occurs any more, i.e. until $\hat{B}^{(m)} = \cup_{\ell \geq 1} \tilde{B}_\ell^{(m)}$. The function \mathcal{I} characterizes whether this final set, the result of the above construction, is connected or not,

$$\mathcal{I}(A_1, \dots, A_k; n^1, \dots, n^{k-1}) = \begin{cases} 1 & \text{if } \hat{B}^{(m)} \text{ is connected} \\ 0 & \text{otherwise.} \end{cases} \quad (\text{A.3})$$

Equations (2.8)–(2.10) are obtained from the general expression (A.1) by considering the cases with one or two loops (i.e. $n = 1, 2$), each loop having no more than 4 transitions ($k_i \leq 4$).

Acknowledgements. We are thankful to Christian Gruber for discussions. R. K. acknowledges the Institut de Physique Théorique at EPFL, and D. U. the Center for Theoretical Study at Charles University for hospitality.

References

- [BI] Borgs, C. and Imbrie, J.: A unified approach to phase diagrams in field theory and statistical mechanics. *Commun. Math. Phys.* **123**, 305–328 (1989)
- [BKU1] Borgs, C., Kotecký, R. and Ueltschi, D.: Low temperature phase diagrams for quantum perturbations of classical spin systems. *Commun. Math. Phys.* **181**, 409–446 (1996)
- [BKU2] Borgs, C., Kotecký, R. and Ueltschi, D.: Incompressible phase in lattice systems of interacting bosons. Unpublished, available at <http://dpwww.epfl.ch/instituts/ipt/publications.html> (1997)
- [BS] Bricmont, J. and Slawny, J.: Phase transitions in systems with a finite number of dominant ground states. *J. Stat. Phys.* **54**, 89–161 (1989)
- [Bry] Brydges, D.C.: A short course on cluster expansions. *Proceeding of Les Houches, Session XLIII*, 129–183 (1986)

- [DFF1] Datta, N., Fernández, R. and Fröhlich, J.: Low-temperature phase diagrams of quantum lattice systems. I. Stability for quantum perturbations of classical systems with finitely-many ground states. *J. Stat. Phys.* **84**, 455–534 (1996)
- [DFF2] Datta, N., Fernández, R. and Fröhlich, J.: Effective Hamiltonians and phase diagrams for tight-binding models. Preprint, math-ph/9809007 (1998)
- [DFFR] Datta, N., Fernández, R., Fröhlich, J. and Rey-Bellet, L.: Low-temperature phase diagrams of quantum lattice systems. II. Convergent perturbation expansions and stability in systems with infinite degeneracy. *Helv. Phys. Acta* **69**, 752–820 (1996)
- [DMN] Datta, N., Messenger, A. and Nachtergaele, B.: Rigidity of interfaces in the Falicov–Kimball model. Preprint, mp-arc 98-267 (1998)
- [Dob] Dobrushin, R.L.: Existence of a phase transition in the two-dimensional and three-dimensional Ising models. *Sov. Phys. Doklady* **10**, 111–113 (1965)
- [DLS] Dyson, F.J., Lieb, E.H. and Simon, B.: Phase transitions in quantum spin systems with isotropic and nonisotropic interactions. *J. Stat. Phys.* **18**, 335–383 (1978)
- [EFS] van Enter, A.C.D., Fernández, R. and Sokal, A.D.: Regularity properties and pathologies of position-space renormalization-group transformations: scope and limitations of Gibbsian theory. *J. Stat. Phys.* **72**, 879–1167 (1993)
- [FWGF] Fisher, M.P.A., Weichman, P.B., Grinstein, G. and Fisher, D.S.: Boson localization and the superfluid-insulator transition. *Phys. Rev. B* **40**, 546–570 (1989)
- [Geo] Georgii, H.-O.: *Gibbs Measures and Phase Transitions*. De Gruyter studies in Mathematics, Berlin–New York: De Gruyter, 1988
- [Gin] Ginibre, J.: Existence of phase transitions for quantum lattice systems. *Commun. Math. Phys.* **14**, 205–234 (1969)
- [Gri] Griffiths, R.B.: Peierls’ proof of spontaneous magnetization of a two-dimensional Ising ferromagnet. *Phys. Rev. A* **136**, 437–439 (1964)
- [GM] Gruber, Ch. and Macris, N.: The Falicov–Kimball model: a review of exact results and extensions. *Helv. Phys. Acta* **69**, 850–907 (1996)
- [KL] Kennedy, T. and Lieb, E.H.: An itinerant electron model with crystalline or magnetic long range order. *Physica A* **138**, 320–358 (1986)
- [LM] Lebowitz, J.L. and Macris, N.: Low-temperature phases of itinerant fermions interacting with classical phonons: the static Holstein model. *J. Stat. Phys.* **76**, 91–123 (1994)
- [Lieb] Lieb, E.H.: The Hubbard model: some rigorous results and open problems. In: *XIth International Congress of Mathematical Physics (Paris, 1994)*, Cambridge, MA: Internat. Press, 1995 pp. 392–412
- [MM] Messenger, A. and Miracle-Solé, S.: Low temperature states in the Falicov–Kimball model. *Rev. Math. Phys.* **8**, 271–299 (1996)
- [Pei] Peierls, R.: On the Ising model of ferromagnetism. *Proceedings of the Cambridge Philosophical Society* **32**, 477–481 (1936)
- [Pfi] Pfister, C.-E.: Large deviations and phase separation in the two-dimensional Ising model. *Helv. Phys. Acta* **64**, 953–1054 (1991)
- [PS] Pirogov, S.A. and Sinai, Ya.G.: Phase diagrams of classical lattice systems. *Theoretical and Mathematical Physics* **25**, 1185–1192 (1975); **26**, 39–49 (1976)
- [Sin] Sinai, Ya.G.: *Theory of Phase Transitions: Rigorous Results*, Oxford–New York–etc.: Pergamon Press, 1982
- [Zah] Zahradník, M.: An alternate version of Pirogov–Sinai theory. *Commun. Math. Phys.* **93**, 559–581 (1984)

Communicated by Ya. G. Sinai