Low-Temperature Phase Diagrams of Quantum Lattice Systems. II. Convergent Perturbation Expansions and Stability in Systems with Infinite Degeneracy.

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Abstract

We study groundstates and low-temperature phases of quantum lattice systems in statistical mechanics: quantum spin systems and fermionic or bosonic lattice gases. The Hamiltonians of such systems have the form

$$H = H_0 + tV,$$

where H_0 is a classical Hamiltonian, V is a quantum perturbation, and t is the perturbation parameter. Conventional methods to study such systems cannot be used when H_0 has infinitely many groundstates. We construct a unitary conjugation transforming H to a form that enables us to find its low-energy spectrum (to some finite order > 1 in t) and to understand how the perturbation tV lifts the degeneracy of the groundstate energy of H_0. The purpose of the unitary conjugation is to cast H in a form that enables us to determine the low-temperature phase diagram of the system. Our main tools are a generalization of a form of Rayleigh-Ritz analytic perturbation theory analogous to Nekhoroshev's form of classical perturbation theory and an extension of Pirogov-Sinai theory.

Contents

1 Introduction

In this paper, we study quantum lattice systems which, in a sense made precise below, are small quantum perturbations of classical lattice systems. Our main concern is the analysis of the structure of groundstates of such systems and of their low-temperature phase diagrams. Our results extend those presented in an earlier paper [10]. In this paper, we develop a perturbative method that enables us to analyze how small quantum perturbations of classical lattice systems lift accidental (in particular infinite) degeneracies of the classical groundstates. Once such degeneracies have been recognized to be lifted by the perturbation one can hope to apply the variant of Pirogov-Sinai theory developed in [10] to analyze the low-temperature phase diagram. The necessary modifications of the tools developed in [10], in order to make them applicable to the systems studied in the present paper, will be explained.

We consider quantum systems on a ν-dimensional lattice $\mathbb{Z}^\nu$. Such systems consist of the following data: To each lattice site $x \in \mathbb{Z}^\nu$ is associated a copy $\mathcal{H}_x$ of some Hilbert space, $\mathcal{H}$. To each finite subset X of the lattice is associated an algebra of operators $\mathcal{F}_X$ —the local field algebra. For systems with fermions, this algebra is larger than the algebra of linear operators acting on $\otimes_{x\in X}\mathcal{H}_x$ [see Section 4.2]. The physics of the system is encoded in an interaction, $\Phi = \{\Phi_X\}$, which is a map from finite subsets $X \subset \mathbb{Z}^\nu$ to (self-adjoint) operators of an algebra $\mathcal{A}_X \subseteq \mathcal{F}_X$ —the local observable algebra. For instance, for fermions $\mathcal{A}_X$ is the even part of $\mathcal{F}_X$, i.e., the subalgebra generated by products of two creation or annihilation operators.

In this paper we continue the investigations started in [10] of systems which are small "quantum" perturbations of classical lattice systems. We consider interactions of the form

$$\Phi = \Phi_0 + Q = \{\Phi_{0X}\} + \{Q_X\} \tag{1.1}$$

where, for all X, Φ_{0X} and Q_X belong to the observable algebra $\mathcal{A}_X$, and we define Hamiltonians of a system confined to a finite subset Λ of $\mathbb{Z}^\nu$ by

$$H_\Lambda = H_{0\Lambda} + V_\Lambda, \tag{1.2}$$

where $H_{0\Lambda} := \sum_{X\subset\Lambda} \Phi_{0X}$ and $V_\Lambda := \sum_{X\subset\Lambda} Q_X$.

Our general assumptions on the interactions are as follows.

(i) Φ_0 is a classical, finite range, translation-invariant interaction. "Classical" means here that there exists a tensor product basis of $\otimes_{x\in X}\mathcal{H}_x$ such that, for all X, Φ_{0X} is diagonal in this basis.

(ii) The perturbation interaction $Q = \{Q_X\}$ is translation-invariant and has finite range or decays exponentially with the size of X, i.e.,

$$\|Q\|_r := \sum_{X\ni 0} \|Q_X\| e^{rs(X)} < \infty, \tag{1.3}$$

for some $r > 0$. Here $\|\cdot\|$ denotes the Hilbert-Schmidt norm and $\mathrm{s}(X)$ —the "size" of X— is the cardinality of the smallest connected subset of $\mathbb{Z}^\nu$ which contains X. Moreover we assume that the perturbation is small, i.e., $\|Q\|_r$ is small enough.

In [10] systems in which the only effect of the quantum perturbation is to cause small deformations of the phase diagram of Φ_0 are analyzed. For the case of spin systems, a comparable analysis has also been presented in [3]. The methods of [10] are applicable to interactions of the form (1.2) satisfying (i) and (ii) under the following additional condition:

(**H**) Φ_0 is a classical interaction with a *finite* number of periodic groundstates and it satisfies the Peierls condition, [15]. The latter is a condition for the stability of the groundstates and requires that there is a non-zero minimum energy per unit interface ("contour") separating two groundstates (see Section 5.1).

Quantum perturbations can also have the more drastic effect of breaking the degeneracies of the groundstates of Φ_0. In this paper we study such systems. We consider an interaction whose unperturbed part Φ_0 has infinitely degenerate groundstates but the degeneracy is reduced to a finite number by the perturbation Q. We ask the following question: Does the ordering induced by the perturbation survive at finite temperatures? In this paper we develop tools to answer such questions. These tools together with the contour expansion methods of [10] (or [3] for spin systems), in the slightly generalized form of Section 5, enable us to study the low-temperature phase diagrams of a large class of quantum lattice systems.

The basic idea is to construct equivalent interactions displaying explicitly the part of the interaction relevant for the low-temperature behaviour of the system. Let us consider an interaction of the form $\Phi = \Phi_0 + tQ$ satisfying conditions (i) and (ii) with t the perturbation parameter. We develop a perturbation technique to partially block-diagonalize the Hamiltonian $H_\Lambda(t)$: under certain hypotheses [**(P1)** of Sect.4.4] on the interaction Φ_0, we prove the following result: There exists a family of unitary operators $U_\Lambda^{(n)}(t)$, labelled by the finite regions Λ with the following properties:

(a) The operators $U_\Lambda^{(n)}(t)$ determines a map

$$\Phi(t) \longmapsto \Phi^{(n)}(t) \tag{1.4}$$

between interactions, i.e., the transformed Hamiltonians

$$H_\Lambda^{(n)}(t) := U_\Lambda^{(n)}(t)\,[H_{0\Lambda} + tV_\Lambda]\,U_\Lambda^{(n)}(t)^{-1} \tag{1.5}$$

can be written as sums of local terms which correspond to an interaction $\Phi^{(n)}(t)$. Moreover, if $\Phi(t)$ decays exponentially so does $\Phi^{(n)}(t)$, for t small enough, albeit with a slower rate of decay.
The key point is that the unitary transformation has to preserve the *locality* of the interaction. This is achieved by constructing a unitary transformation which is the exponential of a sum of local terms and by using commutativity of operators with disjoint regions of localization.

(b) The Hamiltonian $H_\Lambda^{(n)}(t)$ can be cast in the form

$$H_\Lambda^{(n)}(t) := \widetilde{H}_{0\Lambda}(t) + \tilde{V}_\Lambda(t), \tag{1.6}$$

where the leading part, $\widetilde{H}_{0\Lambda}(t)$, is of finite range, and the new perturbation, $\tilde{V}_\Lambda(t)$ can be expressed in terms of interactions with exponential decay. If the perturbation lifts the infinite degeneracy of the groundstate of $\widetilde{H}_{0\Lambda}(t)$, then $U_\Lambda^{(n)}(t)$ is chosen in such a way that $\widetilde{H}_{0\Lambda}(t)$ has a (t-dependent) gap between its groundstate energy and the rest of its spectrum. If $\widetilde{H}_{0\Lambda}(t)$ has a finite number of groundstates and satisfies the Peierls condition, then the low-temperature expansion methods of [10] can be applied (with minor adaptations described in Section 5.2). As a result, we can find the zero-temperature phases of the transformed interaction $\Phi^{(n)}(t)$ (hence of the original interaction $\Phi(t)$) and determine which of these phases survive at low-temperatures.

We illustrate the essential features of our theory through an example. Consider a quarter-filled lattice, Λ, of spin-1/2 fermions, described by a Hamiltonian of the form given in (1.2), with

$$H_{0\Lambda} = U \sum_{<xy>\subset\Lambda} n_x n_y - J \sum_{<xy>\subset\Lambda} \sigma_x^{(3)}\sigma_y^{(3)} n_x n_y + U_0 \sum_{x\subset\Lambda} n_{x\uparrow} n_{x\downarrow} \tag{1.7}$$

and

$$V_\Lambda(t) = -t \sum_{\substack{<xy>\subset\Lambda \\ \sigma=\uparrow,\downarrow}} \{c_{x\sigma}^* c_{y\sigma} + c_{y\sigma}^* c_{x\sigma}\} \tag{1.8}$$

where

$$n_x = \sum_{\sigma=\uparrow,\downarrow} n_{x\sigma} = \sum_{\sigma=\uparrow,\downarrow} c_{x\sigma}^* c_{x\sigma}. \tag{1.9}$$

The operators $c_{x\sigma}^*(c_{x\sigma})$ are the usual fermionic creation and annihilation operators and the sum, $\sum_{\langle xy\rangle}(\cdot)$, is over pairs of nearest neighbour sites. We study this system for the range of parameters $U_0 >> U > J >> t > 0$. The hopping term tV_Λ is treated as a perturbation of $H_{0\Lambda}$. It is seen that the groundstate of $H_{0\Lambda}$ at zero temperature corresponds to a "checkerboard configuration" and has a macroscopic degeneracy, since the spins of the particles can be oriented arbitrarily. Using our perturbation method, we can construct a unitary operator $U_\Lambda^{(1)}(t)$ which transforms the Hamiltonian $H_\Lambda(t)$ to the following form:

$$\begin{aligned} H_\Lambda^{(1)}(t) &= U_\Lambda^{(1)}(t)\,[H_{0\Lambda} + tV_\Lambda]\,U_\Lambda^{(1)}(t)^{-1} \\ &:= \widetilde{H}_{0\Lambda}(t) + \widetilde{V}_\Lambda(t), \end{aligned} \tag{1.10}$$

where $\widetilde{V}_\Lambda(t)$ consists of terms which are of order one or higher in the perturbation parameter t. We prove that

- *To order* t^2, $\widetilde{H}_{0\Lambda}(t)$ has four degenerate groundstates each of which corresponds to a "checkerboard configuration" with all spins aligned.
- The remainder $\widetilde{V}_\Lambda(t)$ can be expressed as a sum of interactions whose strength decays exponentially with the size of their supports.

Thus, in this model the quantum perturbation tV_Λ has a degeneracy-breaking effect that allows the application of the contour expansion methods of [10] —in the version summarized in Theorem 5.2 below— to study the Hamiltonian $H_\Lambda^{(1)}(t)$. One then concludes that, at zero temperature, the ferromagnetic ordering of the groundstates of $\widetilde{H}_{0\Lambda}(t)$ persists in the presence of the quantum perturbation $\widetilde{V}_\Lambda(t)$. Moreover, the long range order, characterizing the groundstate of $H_\Lambda^{(1)}(t)$, survives at low-temperatures, with a bound on the critical temperature which depends on t. In Section 5 we also study the less-easy-to-treat phase diagram of the antiferromagnetic regime ($J < 0$). Further examples are presented in [11].

The paper is organized as follows:

In Section 2 we establish some notations and recall some basic facts from operator theory.

In Section 3 we explain the general ideas of our perturbation scheme by first considering a general quantum mechanical Hamiltonian (not necessarily defined on a lattice) acting on a finite-dimensional Hilbert space. We study finite-dimensional perturbation theory, in order to clarify the purely algebraic aspects of this theory in a context where all our formal expansions are actually given by norm-convergent series. We consider a finite interval of the spectrum of the Hamiltonian which is separated from the rest of the spectrum by a spectral gap Δ. The spectral interval may consist of a single eigenvalue or a group of closely spaced eigenvalues. As long as the perturbation parameter $t << \Delta$, we can apply our perturbation scheme to determine the perturbation of the eigenvalues in the given spectral interval. If the underlying Hilbert space is infinite-dimensional, we extend our theory to study the effect of the perturbation on an isolated part of the point spectrum, provided the perturbation is relatively bounded with respect to the unperturbed Hamiltonian.

In Section 4 we introduce interactions and lattice Hamiltonians and we adapt the perturbation scheme to the latter. This forces us to refine the methods developed in Section 3 because the perturbation V_Λ is not relatively bounded w.r.t. to $H_{0\Lambda}$

uniformly in Λ as Λ increases to $\mathbb{Z}^\nu$. In the absence of relative boundedness the standard theorems of analytic perturbation theory cannot be used. Only for a special class of models, methods have been devised (see e.g. [13, 12, 18, 17, 1]) to overcome this difficulty and convergence of the perturbation series for the groundstate energy density has been proved [1]. In this paper we develop a systematic method which is applicable to a broader class of lattice Hamiltonians.

In Section 5 we present a slight generalization of Pirogov-Sinai theory and show how to combine it with the partial block-diagonalization procedure to obtain a description of phase diagrams at low-temperatures.

In Section 6 we illustrate our methods on some examples.

2 Notations and mathematical preliminaries

2.1 Lie-Schwinger series

We consider a finite-dimensional complex Hilbert space $\mathcal{H}$. Let $\mathcal{L}(\mathcal{H})$ denote the $*$-algebra of all linear operators acting on $\mathcal{H}$. It is a finite-dimensional linear space and when equipped with the scalar product

$$(A\,,\,B) \;=\; \mathrm{tr}(A^*B);\;\; A,B \,\in\, \mathcal{L}(H) \tag{2.1}$$

it forms a Hilbert space, which we denote by $\mathcal{L}_2$. The Hilbert-Schmidt norm is given by

$$\|A\| = \sqrt{\mathrm{tr}(A^*A)}\;. \tag{2.2}$$

We define

$$\mathrm{ad}A(B) \;=\; [A,B]\,, \tag{2.3}$$

for A, B in $\mathcal{L}(\mathcal{H})$, and use the conventions

$$\mathrm{ad}^0A(B) \;=\; B \qquad \text{and} \qquad \mathrm{ad}^nA(B) \;=\; \Big[A, \mathrm{ad}^{n-1}A(B)\Big]\;. \tag{2.4}$$

Let $\mathcal{S}$ and $\mathcal{A}$ be the subspaces of $\mathcal{L}(\mathcal{H})$ consisting of selfadjoint and antiselfadjoint operators. Then

$$A\in\mathcal{S} \Longrightarrow \left\{\begin{array}{l}\mathrm{ad}A\colon \mathcal{S}\longrightarrow\mathcal{A}\\ \mathrm{ad}A\colon \mathcal{A}\longrightarrow\mathcal{S}\end{array}\right. \quad ; \quad A\in\mathcal{A} \Longrightarrow \left\{\begin{array}{l}\mathrm{ad}A\colon \mathcal{S}\longrightarrow\mathcal{S}\\ \mathrm{ad}A\colon \mathcal{A}\longrightarrow\mathcal{A}\end{array}\right. . \tag{2.5}$$

In our calculations, the following identity will play an important role:

$$\begin{aligned} e^ABe^{-A} &= B + [A,B] + \frac{1}{2!}[A,[A,B]] + \cdots \\ &:= \sum_{n=0}^{\infty}\frac{1}{n!}\,\mathrm{ad}^nA(B)\;. \end{aligned} \tag{2.6}$$

The formula is known as the Lie-Schwinger series.

If H_0 is a selfadjoint operator acting on $\mathcal{H}$ then $\mathrm{ad}H_0$ is a selfadjoint operator acting on $\mathcal{L}_2$ since

$$\begin{aligned}(\mathrm{ad}H_0(A), B) &= \mathrm{tr}((A^* H_0 - H_0 A^*)B) \\ &= \mathrm{tr}(A^* \, \mathrm{ad}H_0(B)) \\ &= (A, \mathrm{ad}H_0(B)) \; . \end{aligned} \tag{2.7}$$

2.2 Spectrum of H_0

Let $\sigma(H_0)$ denote the spectrum of a selfadjoint operator H_0. [In the present situation it is simply the set of eigenvalues of H_0.] We write $\sigma(H_0)$ as a union of disjoint subsets,

$$\sigma(H_0) = \bigcup_{j=1}^{N} I_j \tag{2.8}$$

such that

$$\mathrm{dist}(I_i, I_j) \; := \; \min_{E \in I_i, E' \in I_j} |E - E'| \; \geq \; \Delta \tag{2.9}$$

where Δ is some positive number. The size of Δ will be inversely related to the size of the perturbations amenable to our treatment.

Let P_i be the spectral projection of H_0 associated with I_i, i.e,

$$P_i = \sum_{a:\, E_a \in I_i} P_a \; , \tag{2.10}$$

P_a being the orthogonal projection onto the eigenspace of H_0 corresponding to the eigenvalue E_a. Also,

$$\sum_{i=1}^{N} P_i = \mathbf{1}, \quad (\text{partition of unity}), \tag{2.11}$$

where $\mathbf{1}$ is the identity operator.
An operator $V \in \mathcal{L}(H)$ can be decomposed into a diagonal and an off-diagonal part with respect to the partition of unity chosen in eqn.(2.11), as follows:

$$V = V^d + V^{\mathrm{od}} \tag{2.12}$$

$$V^d := \sum_j P_j V P_j \tag{2.13}$$

$$V^{\mathrm{od}} := \sum_{i \neq j} P_i V P_j \; . \tag{2.14}$$

The space of all off-diagonal operators,

$$\mathcal{O} = \{A^{\mathrm{od}} := \sum_{i \neq j} P_i A P_j \, : \, A \in \mathcal{L}(H), 1 \leq i, j \leq N\}, \tag{2.15}$$

can be written as a direct sum

$$\mathcal{O} = \bigoplus_{i \neq j} \mathcal{O}^{ij} \ , \tag{2.16}$$

where

$$\mathcal{O}^{ij} = \{A^{(ij)} := P_i A P_j : A \in \mathcal{L}(H), 1 \leq i, j \leq N, i \neq j\} \tag{2.17}$$

is the space of all off-diagonal operators with non-vanishing matrix elements between the j^{th} and the i^{th} subspace. It is an invariant subspace for $\mathrm{ad}H_0$.
Note: (ij) is an ordered pair. $\mathcal{O}^{ij}$ is orthogonal to $\mathcal{O}^{kl}$ if $(ij) \neq (kl)$ with respect to the scalar product, eqn.(2.1).
We define

$$\mathrm{ad}^{-1} H_0(V^{\mathrm{od}}) \ := \int \mathrm{d}P_E \frac{V^{\mathrm{od}}}{E - E'} \mathrm{d}P_{E'} \tag{2.18}$$

Using the partition of unity,

$$\mathbf{1} = \int \mathrm{d}P_E \tag{2.19}$$

one sees that

$$[H_0, \mathrm{ad}^{-1} H_0(V^{\mathrm{od}})] = V^{\mathrm{od}} \tag{2.20}$$

2.3 Properties of $\mathrm{ad}H_0$ and $\mathrm{ad}^{-1}H_0$

(i) Some useful immediate algebraic properties are the linearity of $\mathrm{ad}^n A(\bullet)$:

$$\mathrm{ad}^n A(t_1 B + t_2 C) \ = \ t_1 \mathrm{ad}^n A(B) + t_2 \mathrm{ad}^n A(C) \ , \tag{2.21}$$

and the multilinearity of $\mathrm{ad}^n \bullet (B)$:

$$\mathrm{ad}^n t A(B) \ = \ t^n \mathrm{ad}^n A(B) \ , \tag{2.22}$$

$$\mathrm{ad}^n \sum_{i=1}^{k} A_i(B) \ = \ \sum_{i_1=1}^{k} \cdots \sum_{i_n=1}^{k} \mathrm{ad}A_{i_1}\Big(\mathrm{ad}A_{i_2} \cdots (\mathrm{ad}A_{i_n}(B)) \cdots\Big) \ . \tag{2.23}$$

(ii) If H_0 is a selfadjoint operator, then

$$\begin{array}{c} \mathrm{ad}^{-1} H_0 : \mathcal{S} \longrightarrow \mathcal{A} \\ \mathrm{ad}^{-1} H_0 : \mathcal{A} \longrightarrow \mathcal{S} \ . \end{array} \tag{2.24}$$

This can be read off from (2.18).
(iii) For all $V \in \mathcal{O}^{ij}$

$$|(V, \mathrm{ad}\, H_0(V))| \geq \Delta(V, V) \ , \tag{2.25}$$

where the scalar product is defined by eqn.(2.1) and

$$\Delta := \min_{i \neq j} \mathrm{dist}(I_i, I_j) \tag{2.26}$$

is interpreted as the minimum spectral gap of H_0.

Proof:

$$\begin{aligned}(V, \mathrm{ad}\, H_0(V)) &= \mathrm{tr}(V^* H_0 V - V^* V H_0) \\ &= \mathrm{tr}(P_j V^* H_0 V P_j - P_j V^* V H_0 P_j),\end{aligned} \tag{2.27}$$

since $V = P_i V P_j$ because $V \in \mathcal{O}^{ij}$. Moreover

$$V = \sum_{\substack{a,b: \\ E_a \in I_i, E_b \in I_j}} V_{ab} \, , \tag{2.28}$$

with

$$V_{ab} := P_a V P_b \, . \tag{2.29}$$

Thus,

$$(V, \mathrm{ad}\, H_0(V)) = \sum_{\substack{a,b: \\ E_a \in I_i, E_b \in I_j}} (E_a - E_b)\, \mathrm{tr}(V_{ba}^* V_{ab}) \, . \tag{2.30}$$

The operator $V_{ba}^* V_{ab}$ is positive and hence $\mathrm{tr}(V_{ba}^* V_{ab}) \geq 0$. Moreover, since the factors $(E_a - E_b)$ in each term of the sum have the same sign, we have that

$$\begin{aligned}|(V, \mathrm{ad}\, H_0(V))| &= \sum_{\substack{a,b: \\ E_a \in I_i, E_b \in I_j}} |E_a - E_b|\, \mathrm{tr}(V_{ba}^* V_{ab}) \\ &\geq \mathrm{dist}(I_i, I_j) \sum_{\substack{a,b: \\ E_a \in I_i, E_b \in I_j}} \mathrm{tr}(V_{ba}^* V_{ab}) \, ,\end{aligned} \tag{2.31}$$

where $\mathrm{dist}(I_i, I_j)$ is defined by eqn.(2.9). Finally,

$$\begin{aligned}(V, V) &= \mathrm{tr}(V^* V) \\ &= \sum_{\substack{a,b: \\ E_a \in I_i, E_b \in I_j}} \mathrm{tr}(V_{ba}^* V_{ab}) \, .\end{aligned} \tag{2.32}$$

Hence

$$|(V, \mathrm{ad}\, H_0(V))| \geq \Delta (V, V) \tag{2.33}$$

for all $V \in \mathcal{O}^{ij}$. ∎

It follows from (2.25) that $\sigma\left(\mathrm{ad} H_0|_{\mathcal{O}^{ij}}\right)$ is contained in $(-\infty, -\Delta] \cup [\Delta, \infty)$. Hence the operator norm of its inverse on $\mathcal{O}^{ij}$ obeys the bound

$$\left\| \mathrm{ad}^{-1} H_0 \big|_{\mathcal{O}^{ij}} \right\|_{\mathrm{op}} \leq \frac{1}{\Delta} \, , \tag{2.34}$$

for all i, j. Therefore

$$\left\| \mathrm{ad}^{-1} H_0 \Big|_{\bigoplus_{i \neq j} \mathcal{O}^{ij}} \right\|_{\mathrm{op}} \leq \frac{1}{\Delta} \, . \tag{2.35}$$

3 The Perturbation Scheme

3.1 First order perturbation

Using the above notations the Hamiltonian can be written as

$$H(t) \;=\; H_0 \,+\, tV_1^{\mathrm{d}} \,+\, tV_1^{\mathrm{od}}, \tag{3.1}$$

where the perturbation operator tV_1 $(= tV)$ is decomposed w.r.t the partition of unity chosen in eqn.(2.11). The operator V_1 is assumed to be selfadjoint. [*Note*: The subscript 1 is introduced for notational convenience since later we shall generalize to higher orders.]

To explain the perturbation scheme we first look for a unitary transformation, $U^{(1)}(t)$, which removes the off-diagonal perturbation to order t:

$$U^{(1)}(t) \;:=\; e^{S^{(1)}(t)} \;:=\; e^{tS_1} \tag{3.2}$$

where S_1 is anti-selfadjoint and t is real. The transformed Hamiltonian is

$$\begin{aligned} H^{(1)}(t) &= e^{S^{(1)}(t)}\, H\, e^{-S^{(1)}(t)} \\ &= \sum_{n=0}^{\infty} \frac{t^n}{n!}\, \mathrm{ad}^n S_1(H(t)) \;. \end{aligned} \tag{3.3}$$

The first few terms of the Lie-Schwinger series, eqn.(3.3), give

$$\begin{aligned} H^{(1)}(t) &= H_0 + tV_1^{\mathrm{d}} + tV_1^{\mathrm{od}} + t\,\mathrm{ad}S_1(H_0) + t^2\mathrm{ad}S_1(V_1^{\mathrm{d}}) \\ &\quad + t^2\mathrm{ad}S_1(V_1^{\mathrm{od}}) + \frac{t^2}{2}\mathrm{ad}^2 S_1(H_0) + \mathrm{O}(t^3) \;. \end{aligned} \tag{3.4}$$

We require $H^{(1)}(t)$ to be block-diagonal to order t^2. This criterion leads us to choose S_1 as follows:

$$\mathrm{ad}H_0(S_1) = V_1^{\mathrm{od}}. \tag{3.5}$$

Thus

$$S_1 \;=\; \mathrm{ad}^{-1}H_0(V_1^{\mathrm{od}}) + S_1^0, \tag{3.6}$$

with

$$\mathrm{ad}H_0(S_1^0) = 0, \tag{3.7}$$

i.e., S_1 is defined modulo an operator which commutes with H_0. On choosing S_1^0 to be zero, we can write

$$S_1 \;=\; \mathrm{ad}^{-1}H_0(V_1^{\mathrm{od}}) \tag{3.8}$$

$$\;=\; \int \mathrm{d}P_E \frac{V_1^{\mathrm{od}}}{E-E'}\, \mathrm{d}P_{E'} \;. \tag{3.9}$$

Since V_1 is selfadjoint,

$$S_1{}^* = -S_1 \tag{3.10}$$

as required. Moreover, S_1 is purely off-diagonal with respect to the partition of unity (2.11). ¿From (2.35) we get

$$\|S_1\| \;\le\; \frac{\|V_1^{\rm od}\|}{\Delta} \;. \tag{3.11}$$

On substituting (3.5) into the RHS of (3.4) we obtain

$$\begin{aligned} H^{(1)}(t) \;&=\; H_0 + tV_1^{\rm d} + \frac{t^2}{2}\left[{\rm ad}S_1(V_1^{\rm od})\right]^{\rm d} + \frac{t^2}{2}\left[{\rm ad}S_1(V_1^{\rm od})\right]^{\rm od} \\ &\quad + t^2{\rm ad}S_1(V_1^{\rm d}) + \sum_{n\ge 2} t^{n+1}\frac{n}{n+1!}{\rm ad}^n S_1(V_1^{\rm od}) + \sum_{n\ge 2}\frac{t^{n+1}}{n!}{\rm ad}^n S_1(V_1^{\rm d}) \\ &:=\; H_0^{(1)}(t) + R(t), \end{aligned} \tag{3.12}$$

where

$$H_0^{(1)}(t) := H_0 + tV_1^{\rm d} + \frac{t^2}{2}[{\rm ad}S_1(V_1^{\rm od})]^{\rm d} \tag{3.13}$$

and

$$R(t) \;=\; \frac{t^2}{2}\left[{\rm ad}S_1(V_1^{\rm od})\right]^{\rm od} \;+\; t^2{\rm ad}S_1(V_1^{\rm d}) \;+\; (\text{terms of order} \,\ge 3 \text{ in } t)\;. \tag{3.14}$$

The operator ${\rm ad}S_1(V_1^{\rm d})$ is off-diagonal. Hence the diagonal terms in the remainder $R(t)$ are of order t^3. $H_0^{(1)}(t)$ is block-diagonal, with respect to the partition of unity, eqn.(2.11). The spectrum of each block must be found by direct diagonalization.

3.2 Generalization to higher orders

In this section we shall generalize the ideas of the previous section and find a unitary operator which block-diagonalizes the Hamiltonian to an arbitrary finite order n$\ge$ 2.

Lemma 3.1 *Consider a selfadjoint Hamiltonian of the form $H(t) = H_0 + tV$. Then for any $n \ge 0$ one can find a unitary operator*

$$U^{(n)}(t) := \exp[S^{(n)}(t)], \tag{3.15}$$

where $S^{(n)}(t) = \sum_{j=1}^n t^j\, S_j$, such that the transformed Hamiltonian,

$$H^{(n)}(t) \;=\; U^{(n)}(t)\,H(t)\,{U^{(n)}(t)}^{-1}, \tag{3.16}$$

is block-diagonal up to order t^{n+1}, w.r.t the partition of unity, eqn.(2.11).

Proof: We look for an operator of the form

$$S^{(n)} \equiv S^{(n)}(t) = \sum_{j=1}^{n} t^j S_j \ , \tag{3.17}$$

such that

$$S_j^* = -S_j \quad \text{for all } 1 \le j \le n \ , \tag{3.18}$$

and that the transformed Hamiltonian

$$H^{(n)}(t) = e^{S^{(n)}} H(t)\, e^{-S^{(n)}} \tag{3.19}$$

has no off-diagonal terms up to order n. On expanding (3.19) in a Lie-Schwinger series, we obtain

$$H^{(n)}(t) = H_0 + tV_1 + \sum_{j\ge 1} \frac{1}{j!} \mathrm{ad}^j S^{(n)}(H_0) + \sum_{j\ge 1} \frac{t}{j!} \mathrm{ad}^j S^{(n)}(V_1) \ . \tag{3.20}$$

This series converges absolutely for all (real or complex) t. Further, expanding via (2.23), we can write this in the form

$$H^{(n)}(t) = H_0 + \sum_{j=1}^{n} t^j \left[\mathrm{ad}S_j(H_0) + V_j\right] + \sum_{j=n+1}^{\infty} t^j V_j \tag{3.21}$$

where $V_1 := V$ and

$$\begin{aligned} V_j \ := & \sum_{\substack{p\ge 2\,,\, k_1\ge 1 \ldots,\, k_p\ge 1 \\ k_1+\cdots+k_p=j}} \frac{1}{p!}\, \mathrm{ad}S_{k_1}\Big(\mathrm{ad}S_{k_2}\cdots(\mathrm{ad}S_{k_p}(H_0))\cdots\Big) \\ & + \sum_{\substack{p\ge 1\,,\, k_1\ge 1 \ldots,\, k_p\ge 1 \\ k_1+\cdots+k_p=j-1}} \frac{1}{p!}\, \mathrm{ad}S_{k_1}\Big(\mathrm{ad}S_{k_2}\cdots(\mathrm{ad}S_{k_p}(V_1))\cdots\Big) \end{aligned} \tag{3.22}$$

for $j \ge 2$.

In order that the operator $U^{(n)}$ removes all off-diagonal terms up to order t^n from the above series we demand that

$$\left[\mathrm{ad}H_0(S_j)\right]^{\mathrm{od}} = V_j^{\mathrm{od}} \quad \text{for} \quad 1 \le j \le n, \tag{3.23}$$

which uniquely determines the off-diagonal part of S_j. The diagonal part is arbitrary and is chosen to be zero, so that we obtain

$$S_j = \mathrm{ad}^{-1} H_0(V_j^{\mathrm{od}}) \ . \tag{3.24}$$

The system (3.22)/(3.24) has a unique solution that is found recursively starting from V_1. We see that the operators have the right symmetry properties: (2.24) and

(2.5) imply that if $V_1 \in \mathcal{S}$ then $V_j \in \mathcal{S}$ and $S_j \in \mathcal{A}$ for each j. This last fact implies (3.18) and hence the intended unitarity of $U^{(n)}$. The bound (2.35) implies that

$$\|S_j\| \;\leq\; \frac{\|V_j^{\rm od}\|}{\Delta}\,. \tag{3.25}$$

Let us point out, as well, that the definition of the operators S_j is *independent* of n.

Thus, we conclude that the unitary operator $U^{(n)} = e^{S^{(n)}}$, where $S^{(n)}$ is defined through eqs.(3.17), (3.22) and (3.24), transforms the Hamiltonian to

$$H^{(n)}(t) \;=\; H_0 + \sum_{j=1}^{n+1} t^j V_j^{\rm d} + R^{(n)}(t), \tag{3.26}$$

where each $V_j^{\rm d}$ is block-diagonal, and $R^{(n)}(t)$ is a remainder of order $\geq (n+1)$ in t. The diagonal terms in $R^{(n)}(t)$ are of order $(n+2)$. ∎

For example, for $n = 2$, we have from eqn.(3.22)

$$\begin{aligned} V_2 \;&:=\; \frac{1}{2}{\rm ad}S_1\left({\rm ad}S_1(H_0)\right)) + {\rm ad}S_1(V_1^d) + {\rm ad}S_1(V_1^{\rm od}) \\ &=\; {\rm ad}S_1(V_1^d) + \frac{1}{2}{\rm ad}S_1(V_1^{\rm od}), \end{aligned} \tag{3.27}$$

where we have used the relation ${\rm ad}H_0(S_1) = V_1^{\rm od}$.
The operator ${\rm ad}S_1(V_1^d)$ is off-diagonal, since S_1 is off-diagonal. Hence,

$$V_2^{\rm d} \;=\; \frac{1}{2}\Big[{\rm ad}S_1(V_1^{\rm od})\Big]^{\rm d} \tag{3.28}$$

and

$$S_2 \;=\; {\rm ad}^{-1}H_0(V_2^{\rm od}), \tag{3.29}$$

where

$$V_2^{\rm od} \;=\; {\rm ad}S_1(V_1^d) + \frac{1}{2}\Big[{\rm ad}S_1(V_1^{\rm od})\Big]^{\rm od}. \tag{3.30}$$

3.3 Analyticity of $U^{(\infty)}(t)$

As the operators $S^{(n)}$ are polynomials in t, each $U^{(n)}$ is an entire (operator-valued) function of t, which has the bounded entire inverse $e^{-S^{(n)}}$. The successive operators $S^{(n)}$ are obtained by adding terms S_j of higher order, without changing the terms already defined in the preceding steps. In the following theorem we show that the norms of the (n-independent) operators S_j have an at most power-law growth in j, and hence we can take the limit $n \to \infty$ of the expansion (3.17). This yields a transformed Hamiltonian $H^{(\infty)}$ which is completely block-diagonal.

Theorem 3.2 *There is a constant $t_0 > 0$ such that*

$$S^{(\infty)}(t) \;:=\; \lim_{n\to\infty} S^{(n)}(t) \tag{3.31}$$

exists and is an analytic function of t in the disc $\{|t| < t_0\}$. Here $S^{(n)}$ is the operator defined by eqs.(3.17), (3.22) and (3.24). As a consequence:

(i) The operator $U^{(\infty)}(t) := lim_{n\to\infty} U^{(n)}(t)$ exists, is analytic and has a bounded analytic inverse in the disc $\{|t| < t_0\}$. For real t, $U^{(\infty)}(t)$ is unitary.

(ii) This operator $U^{(\infty)}(t)$ defines a block-diagonal transformed Hamiltonian $H^{(\infty)}(t)$ which is an analytic function of t in the disc $\{|t| < t_0\}$. Its series expansion is given by the perturbation series (3.21), with V_j defined by (3.22) and S_j by (3.24).

Proof: Equation (3.22) implies that

$$\begin{aligned} s_j \;\leq\; & \frac{\|H_0\|}{\Delta} \sum_{p=2}^{j} \frac{2^p}{p!} \sum_{\substack{k_1\geq 1 \ldots, k_p \geq 1 \\ k_1+\cdots+k_p=j}} s_{k_1}\, s_{k_2} \ldots s_{k_p} \\ & + \frac{\|V_1\|}{\Delta} \sum_{p=1}^{j-1} \frac{2^p}{p!} \sum_{\substack{k_1\geq 1 \ldots, k_p \geq 1 \\ k_1+\cdots+k_p=j-1}} s_{k_1}\, s_{k_2} \ldots s_{k_p} \;, \end{aligned} \tag{3.32}$$

for $j \geq 2$. We have defined

$$s_j \;:=\; \|S_j\| \;, \tag{3.33}$$

and used the bound (3.25) and the inequality

$$\|\mathrm{ad}A(B)\| \leq 2\|A\|\|B\| \;. \tag{3.34}$$

The sum over all ways of writing an integer as a sum of smaller integers leads us to a recursion relation closely related to the Catalan numbers (these appear, for instance, when counting the number of binary trees, see e.g. [9, problem 13-4]). Indeed, consider the numbers $(B_j)_{j\geq 1}$ recursively defined by the equations:

$$B_1 \;=\; s_1 \tag{3.35}$$

$$B_j \;=\; \frac{1}{a} \sum_{k=1}^{j-1} B_{j-k} B_k \;, \qquad j \geq 2 \;. \tag{3.36}$$

where a satisfies

$$\frac{\|H_0\|}{\Delta} \left(\frac{e^{2a} - 2a - 1}{a} \right) + \frac{\|V_1\|}{2\Delta s_1} \left(e^{2a} - 1\right) \;=\; 1 \;. \tag{3.37}$$

Our proof relies on the following inequality.

Claim:

$$s_j \;\le\; B_j \;. \tag{3.38}$$

This is proven by induction in j. Equation (3.38) is obviously true for $j = 1$. Assume that it is true for $j-1$. We leave to the reader the easy inductive proof that (3.35)–(3.36) imply:

$$\sum_{\substack{k_1\ge 1\,\ldots,\,k_p\ge 1\\ k_1+\cdots+k_p=j}} B_{k_1}\,B_{k_2}\ldots.B_{k_p} \;\le\; a^{p-1}B_j \tag{3.39}$$

for any $j \ge 1$. Using this inequality and (3.32) we readily obtain

$$s_j \;\le\; B_j\frac{\|H_0\|}{\Delta}\left(\frac{e^{2a}-2a-1}{a}\right) + B_{j-1}\frac{\|V_1\|}{\Delta}\left(\frac{e^{2a}-1}{a}\right) \;. \tag{3.40}$$

Equations (3.35)–(3.36) imply that

$$\begin{aligned} B_j \;&=\; \frac{1}{a}\Big[2B_{j-1}s_1 + \sum_{k=2}^{j-2} B_{j-k}B_k\Big] \\ &\ge\; \frac{2B_{j-1}s_1}{a} \;. \end{aligned} \tag{3.41}$$

Combining (3.40) with (3.41) we obtain (3.38):

$$\begin{aligned} s_j \;&\le\; B_j\left[\frac{\|H_0\|}{\Delta}\left(\frac{e^{2a}-2a-1}{a}\right) + \frac{\|V_1\|}{2\Delta s_1}\,(e^{2a}-1)\right] \\ &=\; B_j \;, \end{aligned} \tag{3.42}$$

where the last line is a consequence of the choice (3.37) for a.

Inequality (3.38) implies the theorem, because the numbers B_j are the Taylor coefficients of

$$f(x) \;=\; \frac{1-\sqrt{1-(4s_1x/a)}}{2/a} \;. \tag{3.43}$$

This fact can be seen, for instance, by observing that the relations (3.35)–(3.36) imply that the generating series $B(x) := \sum_{j\ge 1} B_j x^j$ satisfies the identity $B(x) = (B^2(x)/a) + s_1x$. Again we refer to problem 13-4 in [9]. Therefore, we conclude that the series defining $S^{(n)}(t)$, $n \ge 1$, are uniformly majorized by the series of $f(t)$ and, hence, so is their limit $n \to \infty$. The radius of analyticity of the latter is bounded below by that of (3.43):

$$t_0 \;\ge\; \frac{a}{4s_1} \;\ge\; \frac{a\Delta}{4\|V_1^{\rm od}\|} \;. \tag{3.44}$$

[The last inequality is due to (3.11).] ∎

Remark: One can obtain an explicit bound on a by combining (3.37) with the inequality $(e^{2a}-2a-1)/a \le e^{2a}-1$. One obtains

$$\Big(e^{2a}-1\Big)\left(\frac{\|H_0\|}{\Delta}+\frac{\|V_1\|}{2\Delta s_1}\right)\;\ge\;1 \tag{3.45}$$

which implies

$$a\;\ge\;\frac{1}{2}\ln\left(1+\frac{\Delta}{\|H_0\|+\frac{\|V_1\|}{2s_1}}\right). \tag{3.46}$$

Since the numbers B_j increase with s_1, we obtain a (larger) majorizing series if we replace s_1 by an upper bound throughout the preceding proof. In particular, if we use the bound $s_1 \le \|V_1^{\rm od}\|/\Delta$ [eqn. (3.11)] we get a (smaller) lower bound on the radius of convergence of $S^{(\infty)}$ given by the rightmost bound in (3.44) with

$$a\;\ge\;\frac{1}{2}\ln\left(1+\frac{\Delta}{\|H_0\|+\frac{\Delta}{2}\left(1+\frac{\|V_1^{\rm d}\|}{\|V_1^{\rm od}\|}\right)}\right). \tag{3.47}$$

3.4 Alternative approach

Instead of using the unitary operators $U^{(n)}(t)=\exp[S^{(n)}(t)]$ defined in Section 3.2, the partial diagonalization can be accomplished by the successive application of simpler operators:

$$\widehat{H}^{(n)}(t)\;=\;\exp[t^n\widehat{S}_n(t)]\cdots\exp[t\widehat{S}_1(t)]\,H(t)\exp[-t\widehat{S}_1(t)]\cdots\exp[-t^n\widehat{S}_n(t)]\,. \tag{3.48}$$

The Lie-Schwinger expansion of this expression yields:

$$\widehat{H}^{(n)}(t)=\sum_{j_n\ge 0}\frac{t^{nj_n}}{j_n!}\cdots\sum_{j_1\ge 0}\frac{t^{j_1}}{j_1!}\,{\rm ad}^{j_n}\widehat{S}_n\Big(\cdots\Big({\rm ad}^{j_1}\widehat{S}_1\Big(H_0+tV\Big)\Big)\cdots\Big) \tag{3.49}$$

Regrouping terms with like powers of t, we obtain, in complete analogy with (3.21)–(3.22),

$$\widehat{H}^{(n)}(t)\;=\;H_0\;+\;\sum_{m=1}^{n}t^m\left[{\rm ad}\widehat{S}_m(H_0)+\widehat{V}_m\right]\;+\;\sum_{m=n+1}^{\infty}t^m\widehat{V}_m \tag{3.50}$$

where $\widehat{V}_1 := V$ and

$$\widehat{V}_j\;:=\;\sum_{\substack{p\ge 2\,,(k_1,\ldots,k_p):\\ 1\le k_1\le\cdots k_p\le n\\ k_1+\cdots+k_p=j}}\left[\prod_{i=1}^{n}\frac{1}{({\rm card}\{j\colon k_j=i\})!}\right]{\rm ad}\widehat{S}_{k_p}\Big(\cdots\Big({\rm ad}\widehat{S}_{k_1}\Big(H_0\Big)\Big)\cdots\Big)$$

$$+ \sum_{\substack{p\geq 1\,,\,(k_1,\ldots,k_p):\\ 1\leq k_1\leq \cdots k_p\leq n\\ k_1+\cdots+k_p=j-1}} \left[\prod_{i=1}^{n} \frac{1}{(\mathrm{card}\{j\colon k_j=i\})!}\right] \mathrm{ad}\widehat{S}_{k_p}\Big(\cdots\Big(\mathrm{ad}\widehat{S}_{k_1}\Big(V\Big)\Big)\cdots\Big) \tag{3.51}$$

for $j \geq 2$. These operators $\widehat{V}_j$ define the operators $\widehat{S}_j$ by the analogue of (3.24)

$$\widehat{S}_j = \mathrm{ad}^{-1}H_0(\widehat{V}_j^{\mathrm{od}}) \; . \tag{3.52}$$

This approach is more convenient for numerical calculations, because expression (3.51) involves less terms than its counterpart (3.22). In the limit $n \to \infty$ the resulting series can also be bounded above by the power series with coefficients s_j satisfying (3.32). Hence, (3.44)–(3.47) are lower bounds for its radius of convergence.

3.5 Perturbation theory in infinitely many dimensions

Consider a Hamiltonian

$$H(t) = H_0 + tV \tag{3.53}$$

acting on an infinite-dimensional Hilbert space $\mathcal{H}$, where H_0 is selfadjoint, t is the perturbation parameter, and V is a symmetric operator which is relatively bounded with respect to H_0, i.e.,

(i) $D(V) \supset D(H_0)$,

(ii) for all $\psi \in D(H_0)$ and for some $a, b > 0$

$$\|V\psi\|_2 \;\leq\; a\|H_0\psi\|_2 + b\|\psi\|_2, \tag{3.54}$$

where the symbol $\|\cdot\|_2$ denotes the norm of vectors in the Hilbert space $\mathcal{H}$.

Let I be an isolated part of the spectrum of H_0, i.e., if

$$J \;:=\; \sigma(H_0) \setminus I, \tag{3.55}$$

then

$$\mathrm{dist}(I, J) \;:=\; \min_{\substack{E\in I,\\ E'\in J}} |E - E'| \;\geq\; \Delta \tag{3.56}$$

where Δ is some positive number. We assume that I consists of a finite number of eigenvalues of finite multiplicity.

Let P be the spectral projection of H_0 associated with I. Then

$$P = \frac{1}{2\pi i}\oint_\gamma dz \frac{1}{z - H_0} \tag{3.57}$$

where γ is a closed positively oriented curve in the complex plane enclosing only the segment I of $\sigma(H_0)$. The operator

$$P(t) = \frac{1}{2\pi i} \oint_\gamma dz \frac{1}{z - H(t)} \tag{3.58}$$

exists and is analytic in t for t near zero. $P(t)$ is a finite rank projection operator with $P(0) = P$. For $|\, t \,|$ small, $\operatorname{rank} P(t) = \operatorname{rank} P$, and

$$\lim_{t\to 0} \|P(t) - P\|_{\mathrm{op}} = 0 \, . \tag{3.59}$$

We want to study the effect of the quantum perturbation tV on the segment I of $\sigma(H_0)$. For this purpose we define bounded operators

$$\widetilde{H}_0 = (H_0 + k)P, \tag{3.60}$$

where $k > 0$ is chosen such that $I + k \subset [\delta, \infty)\,, \;\; \delta > 0$, and

$$\begin{aligned} \widetilde{H}(t) &= (H(t) + k)P(t) \\ &= (H_0 + k)P + (H_0 + k)(P(t) - P) + tVP(t) \\ &:= \widetilde{H}_0 + \widetilde{V}(t) \, . \end{aligned} \tag{3.61}$$

The spectrum of $\widetilde{H}_0$ is given by

$$\sigma(\widetilde{H}_0) = \{0\} \cup (I + k). \tag{3.62}$$

The eigenvalue 0 of $\widetilde{H}_0$ is separated from the rest of the spectrum by a finite gap:

$$\begin{aligned} \widetilde{\Delta} &:= \operatorname{dist}\Big[\{0\}, \sigma(\widetilde{H}_0) \setminus \{0\}\Big] \\ &\geq \delta > 0 \, . \end{aligned} \tag{3.63}$$

The operator $\widetilde{V}(t)$ can be treated as a perturbation of the selfadjoint Hamiltonian $\widetilde{H}_0$. The Hamiltonian $\widetilde{H}(t)$, defined in eqn.(3.61), can be analyzed by our perturbation scheme. This is because the operators $\widetilde{H}_0$ and $\widetilde{V}(t)$ have the following properties:

$$\|\widetilde{H}_0\|_{\mathrm{op}} = \text{const.} < \infty \tag{3.64}$$

and

$$\|\widetilde{V}(t)\|_{\mathrm{op}} \to 0, \;\; \text{as } \mathrm{t} \to 0 \tag{3.65}$$

[as one shows by using the Neumann series expansion of $\Big(z - H(t)\Big)^{-1}$]. Hence all the results of Section 3.3 apply, and we conclude, among other things, that there exists a unitary operator $U^{(\infty)}(t)$ such that the Hamiltonian

$$U^{(\infty)}(t)\, \widetilde{H}(t)\, U^{(\infty)}(t)^{-1} \tag{3.66}$$

leaves the subspace $P\mathcal{H}$ invariant and vanishes on the subspace $(1-P)\mathcal{H}$. In particular,

$$U^{(\infty)}(t)\,P(t)\,U^{(\infty)}(t)^{-1}=P\,. \tag{3.67}$$

The problem whose solution we have just sketched has been solved, a long time ago, under considerably more general circumstances. We quote the pertinent results from [16, 21].

Theorem 3.3 *Let R be a connected, simply connected region of the complex plane containing 0. Let $P(t)$ be be a projection-valued analytic function on R. Then there is an analytic family of invertible operators $U(t)$ with*

$$U(t)^{-1}\,P(0)\,U(t)=P(t), \tag{3.68}$$

for all $t\in R$. Moreover, if $P(t)$ is selfadjoint, for real $t\in R$, then we can choose $U(t)$ unitary, for t real.

Remark: The operator $U(t)$ is not unique. Explicit forms for $U(t)$ can be found in [16].

This theorem allows us to define a Hamiltonian

$$U(t)\,\widetilde{H}(t)\,U(t)^{-1} \tag{3.69}$$

where $\widetilde{H}(t)$ is given in eqn.(3.61), with $P(t)$ as in eqn.(3.58). This operator leaves the subspace $\operatorname{Ran}P$ invariant.

Our method yields an explicit construction of operators $U^{(n)}(t)$, for any $n<\infty$, such that

$$U(t)=U^{(\infty)}(t)=\lim_{n\to\infty}U^{(n)}(t), \tag{3.70}$$

(Lemma 3.1 and Theorem 3.2).

4 Quantum lattice systems: Framework and perturbative approach

4.1 Introductory remarks

We now turn to the study of phase diagrams of quantum lattice systems. In [10, 3] a theory was developed for models with a dominant classical part which satisfies the following hypotheses:

(H1) The (periodic) groundstates have an at most finite degeneracy.

(H2) The Peierls condition holds, which roughly means that excited configurations have an energy proportional to the area of the defects.

For low-temperatures and small quantum perturbations, the phase diagrams of such models are shown to be smooth deformations of the zero-temperature phase diagram of the classical part [10, 3]. The treatment is based on an extension of the Pirogov-Sinai theory of classical lattice models [19, 20, 25, 28, 2] to quantum systems.

There have been a number of extensions of the theory to classical systems which violate **(H1)** (eg. [6, 7, 14, 8]), or **(H2)** [8]. The purpose of the present paper is *not* to exploit these extensions, but rather to investigate an intrinsically quantum phenomenon: In many instances, the quantum perturbation effectively removes the infinite degeneracy, or restores the Peierls condition, placing the system within the setting of the standard Pirogov-Sinai approach. The formalization of this fact is through techniques of partial block-diagonalization discussed below: The partially block-diagonalized Hamiltonian acquires a classical leading part that satisfies the hypotheses of Pirogov-Sinai theory.

The theory we develop in the sequel has, therefore, two components: A block-diagonalization scheme within the framework of lattice systems, and a small generalization of the quantum Pirogov-Sinai theory of [10, 3]. In this section we discuss the block-diagonalization process; the Pirogov-Sinai theory is presented in Section 5.

4.2 Basic set-up

We consider a quantum mechanical system on a ν-dimensional lattice $\mathbb{Z}^\nu$. We consider translation-invariant systems, but systems which are invariant under a subgroup of finite index of $\mathbb{Z}^\nu$ can be accommodated with trivial changes. Standard references for this section are [23, 4, 5, 24]. Here we require a slight modification of the usual formalism in order to treat fermionic lattice gases. While minor, these modifications are essential for both, the diagonalization procedure and the Pirogov-Sinai theory (see [10]). For fermionic lattice systems creation or annihilation operators at different sites of the lattice do not commute, but anticommute. But in both parts of our theory we must impose commutativity (or locality) conditions. This is achieved by requiring that interactions belong to a suitable (physically reasonable) class of interactions.

A quantum lattice system is defined by the following data:

(i) To each lattice site $x \in \mathbb{Z}^\nu$ is associated a Hilbert space $\mathcal{H}_x$ and, for any finite subset $X \subset \mathbb{Z}^\nu$, the corresponding Hilbert space is given by

$$\mathcal{H}_X = \bigotimes_{x \in X} \mathcal{H}_x \,. \tag{4.1}$$

We require that there be a Hilbert space isomorphism $\phi_x : \mathcal{H}_x \longrightarrow \mathcal{H}$, for all $x \in \mathbb{Z}^\nu$. To avoid ambiguities in the definition of the tensor product (4.1), we choose a total ordering (denoted by the symbol $\preceq$) of the sites in $\mathbb{Z}^\nu$. For convenience, we choose the *spiral order*, depicted in Figure 1 for $\nu = 2$, and an analogous ordering for $\nu \geq 3$. This ordering is chosen to have the property that, for any finite set X, the

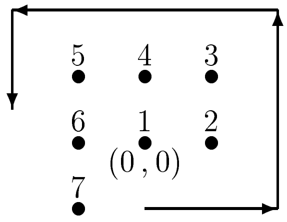

Figure 1: Spiral order in $\mathbb{Z}^2$

set $\overline{X} := \{z \in \mathbb{Z}^\nu, z \preceq X\}$ of lattice sites which are smaller than X, or belong to X, is finite.

(ii) For any finite subset $X \subset \mathbb{Z}^\nu$ two operator algebras acting on $\mathcal{H}_X$ are given

(a) The (local) *field algebra* $\mathcal{F}_X \subset \mathcal{L}(\mathcal{H}_{\overline{X}})$,

(b) the (local) *observable algebra* $\mathcal{A}_X \subseteq \mathcal{F}_X$,

which have the following properties:

1) If $X \subset Y$ and $x \prec y$, for all $x \in X$ and all $y \in Y \setminus X$, then there is a natural embedding of $\mathcal{F}_X$ into $\mathcal{F}_Y$: An operator $B \in \mathcal{F}_X$ corresponds to the operator $B \otimes \mathbf{1}_{\mathcal{H}_{Y\setminus X}}$ in $\mathcal{F}_Y$. In the following, we write B for both operators $B \in \mathcal{F}_X$ and $B \otimes \mathbf{1}_{\mathcal{H}_{Y\setminus X}} \in \mathcal{F}_Y$.

2) For the infinite system, the (quasilocal) field algebra is the norm closure of the union of all local field algebras, i.e.,

$$\mathcal{F} := \overline{\bigcup_{X \nearrow \mathbb{Z}^\nu} \mathcal{F}_X}^{\text{norm}} , \tag{4.2}$$

(the limit being taken through a sequence of increasing subsets of $\mathbb{Z}^\nu$, where increasing refers to the (spiral) ordering defined above). Similarly, the (quasilocal) observable algebra for the infinite system is defined as

$$\mathcal{A} := \overline{\bigcup_{X \nearrow \mathbb{Z}^\nu} \mathcal{A}_X}^{\text{norm}} . \tag{4.3}$$

The group of space translations $\mathbb{Z}^\nu$ acts as a $*$-automorphism group, $\{\tau_a : a \in \mathbb{Z}^\nu\}$ on the algebras $\mathcal{F}$ and $\mathcal{A}$, with

$$\mathcal{F}_{X+a} = \tau_a(\mathcal{F}_X), \quad \mathcal{A}_{X+a} = \tau_a(\mathcal{A}_X), \tag{4.4}$$

for any $X \subset \mathbb{Z}^\nu$ and $a \in \mathbb{Z}^\nu$.

3) Commutativity condition: If $X \cap Y = \emptyset$, then for any $A \in \mathcal{F}_X$, $B \in \mathcal{A}_Y$

$$[A, B] \, = \, 0 \, . \tag{4.5}$$

(iii) An *interaction* $\Phi = \{\Phi_X\}$ is given: This is a map from the finite sets $X \subset \mathbb{Z}^\nu$ to self-adjoint operators Φ_X in the *observable algebra* $\mathcal{A}_X$. The *bonds* of the interaction are the sets X for which the operators Φ_X are not identically zero. We consider translation-invariant interactions, i.e., $\Phi_{X+a} = \tau_a \Phi_X$, for all $X \subset \mathbb{Z}^\nu$ and $a \in \mathbb{Z}^\nu$. The *range* of the interaction is the maximum of the diameters of the sets of the family $R_\Phi = \{X \subset \mathbb{Z}^\nu : X \ni 0 \text{ and } \Phi_X \neq 0\}$. We shall use the ℓ^∞-diameter

$$\mathrm{diam} M \ := \ \max_{x,y \in M} \max_{1 \leq i \leq \nu} |x_i - y_i| \ . \tag{4.6}$$

Some of our interactions will be of finite range, that is, with R_Φ finite. More generally, we shall consider interactions decaying exponentially with the size of their supports, that is, with

$$\|\Phi\|_r \ := \ \sum_{X \ni 0} \|\Phi_X\| e^{r\mathrm{s}(X)} \tag{4.7}$$

finite, for some $r > 0$. Here $\|\cdot\|$ denotes the Hilbert-Schmidt norm and $\mathrm{s}(X)$ denotes the cardinality of the smallest connected subset of $\mathbb{Z}^\nu$ which contains X. We shall denote by

$$\mathcal{B}_r \ := \ \Big\{\Phi \colon \|\Phi\|_r < \infty\Big\} \tag{4.8}$$

the corresponding Banach space of interactions.

Similarly, we can define a Banach space $\mathcal{B}_r^{\mathrm{op}}$ as

$$\mathcal{B}_r^{\mathrm{op}} \ := \ \Big\{\Phi = \{\Phi_X\} : \sum_{X \ni 0} \|\Phi_X\|_{\mathrm{op}}\, e^{rs(X)} < \infty\Big\}, \tag{4.9}$$

where $\|\cdot\|_{\mathrm{op}}$ denotes the operator norm.

Remark: If the Hilbert space $\mathcal{H}_X$ (4.1) is finite-dimensional, as for spin or fermionic systems (see Examples (i) and (ii) below), the Hilbert-Schmidt norm of Φ_X is equivalent to its operator norm $\|\Phi_X\|_{\mathrm{op}}$, i.e.,

$$\|\Phi_X\|_{\mathrm{op}} \leq \|\Phi_X\| \leq \dim(\mathcal{H}_X)\|\Phi_X\|_{\mathrm{op}}, \tag{4.10}$$

where $\dim(\mathcal{H}_X)$ is the dimensionality of $\mathcal{H}_X$ and is given by

$$\dim(\mathcal{H}_X) = \Big(\dim(\mathcal{H})\Big)^{s(X)}, \tag{4.11}$$

with $\mathcal{H}$ being the Hilbert space which is isomorphic to $\mathcal{H}_x$ for all $x \in X$. Hence,

$$\begin{aligned} \sum_{X \ni 0} \|\Phi_X\|_{\mathrm{op}}\, e^{rs(X)} &\leq \sum_{X \ni 0} \|\Phi_X\| e^{rs(X)} \\ &\leq \sum_{X \ni 0} \|\Phi_X\|_{\mathrm{op}}\, e^{r's(X)}, \end{aligned} \tag{4.12}$$

where

$$r' = r + \ln(\dim \mathcal{H}). \tag{4.13}$$

Therefore, if an interaction Φ belongs to a Banach space $\mathcal{B}_r$ for some $r > 0$, then it also belongs to the Banach space $\mathcal{B}_r^{\rm op}$. Conversely, if an interaction Φ belongs to a Banach space $\mathcal{B}_{r'}^{\rm op}$ for some $r' > 0$, then it also belongs to the Banach space $\mathcal{B}_r$ with r defined through eqn.(4.13). Given the above equivalence of norms and the relation between the corresponding Banach spaces, we prefer to use the Hilbert-Schmidt norm in our treatment of lattice systems since this makes the analysis simpler.

In the sequel we have to consider a particular class of interactions: the *classical* interactions. Let I be an index set and $\{e_j\}_{j\in I}$ be an orthonormal basis of $\mathcal{H}$. Then for $X \subset \mathbb{Z}^\nu$,

$$\mathcal{E}_X := \{\otimes_{x\in X} e^x_{j_x}\}\,, \quad \text{with } \; e^x_{j_x} = \phi_x^{-1}\, e_j \;, \tag{4.14}$$

is an orthonormal basis of $\mathcal{H}_X$. We denote by $\mathcal{C}(\mathcal{E}_X)$ the abelian subalgebra of $\mathcal{A}_X$ consisting of all operators which are diagonal in the basis $\mathcal{E}_X$.

An interaction Φ is called *classical*, if there exists a basis $\{e_j\}_{j\in I}$ of $\mathcal{H}$ such that

$$\Phi_X \in \mathcal{C}(\mathcal{E}_X), \quad \text{for all } \; X \subset \mathbb{Z}^\nu \;. \tag{4.15}$$

The *set*, Ω_X, of configurations in X is defined as the set of all assignments $\{j_x\}_{\{x\in X\}}$ of an element $j_x \in I$ to each x. A *configuration* ω_X is an element in Ω_X. If $Y \subset X$ then ω_Y denotes the restriction of the configuration ω_X to the subset Y. There is a one-to-one correspondence between basis vectors $\otimes_{x\in X} e^x_{j_x}$ of $\mathcal{H}_X$ and configurations on X:

$$\bigotimes_{x\in X} e^x_{j_x} \longleftrightarrow \omega_X \equiv \{j_x\}_{x\in X} \;. \tag{4.16}$$

In the sequel we shall use the notation e_{ω_X} to denote the basis vector defined by the configuration ω_X via the correspondence (4.16).
Since a classical interaction Φ only depends on the numbers

$$\Phi_X(\omega_X) \;:=\; \langle e_{\omega_X}|\Phi_X|e_{\omega_X}\rangle \tag{4.17}$$

we may view Φ_X as a (real-valued) function on the set of configurations. Similarly the algebra $\mathcal{C}(\mathcal{E}_X)$ may be viewed as the $*$-algebra of complex-valued functions on the set of configurations Ω_X.

We will consider Gibbs states on the field algebra $\mathcal{F}$. They may be specified in terms of interactions or in terms of (finite-volume) Hamiltonians.

Given an interaction, the Hamiltonian associated with a finite subset Λ of the lattice takes the form

$$H_\Lambda \;=\; \sum_{X\subset\Lambda} \Phi_X \;. \tag{4.18}$$

More generally, for a configuration σ, and finite regions $\Gamma \supset \Lambda$, the Hamiltonian "with boundary condition" σ is the operator

$$H_\Lambda^{\sigma_\Gamma} \;=\; \sum_{X\cap\Lambda\neq\emptyset} P^\sigma_{\Gamma\setminus\Lambda}\Phi_X P^\sigma_{\Gamma\setminus\Lambda} \;, \tag{4.19}$$

where $P^{\sigma}_{\Gamma\setminus\Lambda} := |\sigma_{\Gamma\setminus\Lambda}\rangle\langle\sigma_{\Gamma\setminus\Lambda}|$. The *Gibbs state* in the finite volume Λ for an interaction Φ, boundary condition σ and inverse temperature β is the positive linear functional on $\mathcal{F}_\Lambda$ defined by

$$\mathcal{F}_\Lambda \ni A \;\mapsto\; \lim_{\Gamma\to\mathbb{Z}^\nu} \frac{\mathrm{Tr} A\, \exp\left(-\beta H_\Lambda^{\sigma_\Gamma}\right)}{\mathrm{Tr}\exp\left(-\beta H_\Lambda^{\sigma_\Gamma}\right)}\;. \tag{4.20}$$

The infinite-volume limits of these functionals determine the phase diagram of the system.

EXAMPLES:

(i) *Spin–p quantum spin system*: Each lattice site is occupied by a particle of spin p. The Hilbert space at each site is isomorphic to $\mathcal{H} = \mathbb{C}^{2p+1}$. The field algebra and the observable algebra coincide,

$$\mathcal{A}_X \;=\; \mathcal{F}_X \;:=\; \mathcal{L}(\mathcal{H}_X)\;, \tag{4.21}$$

where $\mathcal{L}(\mathcal{H}_X)$ denotes the algebra of bounded operators on $\mathcal{H}_X$. The algebra $\mathcal{A}$ for the infinite system is a C^*-algebra.

(ii) *Quantum lattice-gas of spin* $1/2$*-fermions*: Each lattice site can be empty, occupied by a single particle or by two particles of opposite spin. Let us consider the Hilbert space $\mathcal{H} = \mathbb{C}^2\otimes\mathbb{C}^2 \simeq \mathbb{C}^4$ with the basis

$$\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix},\;\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix},\;\begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\;\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix}, \tag{4.22}$$

and the following representations of the Lie-algebra of $SU(2)$ on $\mathcal{H}$

$$\begin{aligned}
\sigma_1^+ &= \begin{pmatrix}0&1\\0&0\end{pmatrix}\otimes\mathbf{1}\,, & \sigma_2^+ &= \mathbf{1}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix},\\
\sigma_1^- &= \left(\sigma_1^+\right)^*\,, & \sigma_2^- &= \left(\sigma_2^+\right)^*,\\
\sigma_1^3 &= \begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes\mathbf{1}\,, & \sigma_2^3 &= \mathbf{1}\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}.
\end{aligned} \tag{4.23}$$

We have

$$\mathcal{H}_x = \phi_x^{-1}\mathcal{H}\;, \tag{4.24}$$

and thus we set

$$\begin{aligned}
\sigma^{\pm}_{x,i} &= \phi_x^{-1}\sigma_i^{\pm}\phi_x\;, \quad i=1,2\;,\\
\sigma^{3}_{x,i} &= \phi_x^{-1}\sigma_i^{3}\phi_x\;, \quad i=1,2\;.
\end{aligned} \tag{4.25}$$

We recall that we have chosen a total (spiral) ordering ($\preceq$) on $\mathbb{Z}^\nu$. We complement this ordering with the convention that in each factor $\mathcal{H}_x \simeq \mathbb{C}^2\otimes\mathbb{C}^2$ the first factor $\mathbb{C}^2$ is smaller than the second one, i.e., $(x,i)\prec(y,j)$ if $x\prec y$, $i,j=1,2$ and

$(x, 1) \prec (x, 2)$. With these conventions we define the fermion creation and annihilation operators at site x by the following Klein-Jordan-Wigner transformation:

$$c^*_{x\uparrow} = \bigotimes_{y \prec x} \left(\sigma^3_{y1} \otimes \sigma^3_{y2} \right) \bigotimes \sigma^+_{x1} \tag{4.26}$$

$$c^*_{x\downarrow} = \bigotimes_{y \prec x} \left(\sigma^3_{y1} \otimes \sigma^3_{y2} \right) \bigotimes \sigma^3_{x1} \otimes \sigma^+_{x2} \tag{4.27}$$

$$c_{x\uparrow} = \left(c^*_{x\uparrow} \right)^* \tag{4.28}$$

$$c_{x\downarrow} = \left(c^*_{x\downarrow} \right)^* . \tag{4.29}$$

It is straightforward to check that these creation- and annihilation operators satisfy the canonical anticommutation relations

$$\{c_{x\sigma}, c^*_{x'\sigma'}\} = \delta_{x\,x'} \delta_{\sigma\sigma'} , \tag{4.30}$$

$$\{c_{x\sigma}, c_{x'\sigma'}\} = 0 = \{c^*_{x\sigma}, c^*_{x'\sigma'}\} , \tag{4.31}$$

for $\sigma, \sigma' \in \{\uparrow, \downarrow\}$. The field algebra $\mathcal{F}_X$ is the algebra generated by the creation and annihilations operators:

$$\mathcal{F}_X := \langle\ c_{x\sigma}\ ,\ c^*_{x'\sigma'}\ |\ x, x' \in X;\ \sigma, \sigma' \in \{\uparrow, \downarrow\}\ \rangle\ . \tag{4.32}$$

The observable algebra $\mathcal{A}_X$ is the even part of $\mathcal{F}_X$, i.e., the algebra generated by the products of two annihilation or creation operators:

$$\mathcal{A}_X := \langle\ c_{x\sigma} c_{x'\sigma'}\ ,\ c^*_{x\sigma} c^*_{x'\sigma'}\ ,\ c^*_{x\sigma} c_{x'\sigma'}\ ,\ c_{x\sigma} c^*_{x'\sigma'}\ |\ x, x' \in X;\ \sigma, \sigma' \in \{\uparrow, \downarrow\}\ \rangle\ . \tag{4.33}$$

We have

$$\mathcal{A}_X \subset \mathcal{F}_X \subset \mathcal{L}(\mathcal{H}_{\overline{X}}) , \tag{4.34}$$

By using the identity

$$[A, BC] = \{A, B\}\, C - B\{C, A\} , \tag{4.35}$$

one checks easily that the commutativity condition (4.5) is satisfied. For the infinite system, both $\mathcal{A}$ and $\mathcal{F}$ are C^*-algebras. ¿From a physical point of view, it may appear more natural to choose $\mathcal{A}_X$ as the algebra of gauge-invariant operators. However, our definition of $\mathcal{A}_X$ is sufficient to ensure the condition of statistical independence of disjoint contours in the contour expansion of Section 5.2.

A similar construction holds for quantum lattice gases of fermions with arbitrary spin.

(iii) *Quantum lattice gas of scalar bosons*: Each lattice site can be occupied by an arbitrary number of particles. The Hilbert space at each site is $\mathcal{H} = l^2(IN)$. The field algebra $\mathcal{F}_X$ is generated by the creation and annihilation operators satisfying the canonical commutation relations.

$$[c^*_x, c_{x'}] = \delta_{x\,x'} , \tag{4.36}$$

$$[c_x, c_{x'}] = 0 = [c_x^*, c_{x'}^*] \tag{4.37}$$

for $x, x' \in X$.

The observable algebra $\mathcal{A}_X$ may be chosen as $\mathcal{A}_X := \mathcal{F}_X$. Since creation and annihilation operators for bosonic particles are unbounded operators, $\mathcal{A}_X$ and $\mathcal{F}_X$ are $*$-algebras of unbounded operators.

¿From a physical point of view it is more natural to choose $\mathcal{A}_X$ as the even part of $\mathcal{F}_X$ (as for fermions) or even as the algebra consisting of gauge-invariant operators. However, we will not need such assumptions in the sequel.

Our contour expansion methods of Section 5.2 do not apply to bosonic systems where an arbitrary large number of particles can be on some lattice site. We must restrict our attention to states satisfying a condition of regularity. Let $n_x = c_x^* c_x$ denote the particle number operator at site x. We will call a state, ρ, for a bosonic lattice gas *regular* if the following holds: For arbitrary $X \subset \mathbb{Z}^\nu$

$$\rho\left(e^{t \sum_{x \in X} n_x}\right) < e^{a(t) \mathrm{s}(X)} , \quad \text{for all} \quad |t| < \infty \tag{4.38}$$

for some function $a(t)$. For Gibbs states such a condition will follow by imposing a suitable hardcore condition.

A similar construction holds for quantum lattice gases of bosons with arbitrary spins.

4.3 Equivalence of interactions

In this section we begin to discuss the first component of our theory, namely the development of a block-diagonalization scheme analogous to that of Section 3, but suited to lattice systems. It would be of little use to directly apply the expressions of Section 3 to partially block-diagonalize each (finite-volume) Hamiltonian of a lattice system, because the convergence radius of the block-diagonalization procedure tends to zero in the volume of the region. Indeed, the information of interest refers to the thermodynamic limit, hence the procedure must, in some sense, partially block-diagonalize *all* finite-volume Hamiltonians at the *same time*. This is accomplished by requiring that each partially block-diagonalized Hamiltonian also be a sum of *local* operators. In other words, the objective is to partially block-diagonalize *interactions*, up to small error terms, rather than Hamiltonians.

A Hamiltonian and its partially block-diagonalized form must be equivalent, in the sense that they lead to the same quantum mechanics. We also need a notion of equivalence of interactions. Let us consider a *family* of unitary transformations $\{U_\Lambda\}$, labelled by the finite regions $\Lambda \subset \mathbb{Z}^\nu$, satisfying the following requirements:

(E1) The family of unitary operators $\{U_\Lambda\}$ determines a map between interactions

$$\Phi \in \mathcal{B}_r \longmapsto \widetilde{\Phi} \in \mathcal{B}_{\widetilde{r}} \tag{4.39}$$

for some $r, \widetilde{r} > 0$, i.e., if H_Λ are the Hamiltonians corresponding to the interaction $\Phi \in \mathcal{B}_r$, then the transformed Hamiltonians

$$U_\Lambda \, H_\Lambda \, U_\Lambda^{-1} \;=\; \widetilde{H}_\Lambda \;, \tag{4.40}$$

correspond to the interaction $\widetilde{\Phi} \in \mathcal{B}_{\widetilde{r}}$.

(E2) The transformations preserve *quasilocality*:

$$\begin{aligned} A \in \mathcal{A}_X \quad &\Longrightarrow \quad \lim_{\Lambda \to \mathbb{Z}^\nu} U_\Lambda A U_\Lambda^{-1} \in \mathcal{A} \\ A \in \mathcal{F}_X \quad &\Longrightarrow \quad \lim_{\Lambda \to \mathbb{Z}^\nu} U_\Lambda A U_\Lambda^{-1} \in \mathcal{F} \end{aligned} \tag{4.41}$$

(the limit taken through an increasing sequence of volumes).

The interactions Φ and $\widetilde{\Phi}$ related by such transformations constitute equivalent descriptions of the same physical system. Indeed, Condition **(E1)** implies that equivalent interactions have the same partition functions

$$\mathrm{Tr}\Big(e^{-\beta \widetilde{H}_\Lambda}\Big) \;=\; \mathrm{Tr}\Big(e^{-\beta H_\Lambda}\Big) \,. \tag{4.42}$$

and the same free energy, while condition **(E2)** implies that observables are transformed into observables with transformation law

$$\mathrm{Tr}\Big(A\, e^{-\beta \widetilde{H}_\Lambda}\Big) \;=\; \mathrm{Tr}\Big(U_\Lambda^{-1}\, A\, U_\Lambda\, e^{-\beta H_\Lambda}\Big) \,. \tag{4.43}$$

This shows that Φ and $\widetilde{\Phi}$ lead to the same statistical mechanics.

A fairly general way of satisfying both requirements **(E1)** and **(E2)** is by defining the transformations $U_\Lambda := \exp[S^\Lambda]$ as the exponential of a sum of *local* operators. We adopt this as our definition of equivalence. Given a translation-invariant family of anti-selfadjoint operators $\mathcal{S} = \{S_Y\}$, $S_Y \in \mathcal{A}_Y$, with $\mathcal{S} \in \mathcal{B}_r$, for some $r > 0$, we shall say that an interaction $\widetilde{\Phi}$ is $\mathcal{S}$*-related* to an interaction Φ if **(E1)** and **(E2)** are satisfied with

$$U_\Lambda \;=\; \exp\Big[S^\Lambda\Big] \;=\; \exp\Big[\sum_{Y \subset \Lambda} S_Y\Big] \,. \tag{4.44}$$

Corollary 4.2 below shows that in such a situation **(E2)** is satisfied. Corollary 4.4 shows that **(E1)** is satisfied as well. In particular, the family U_Λ preserves the exponential decay of interactions, although at a possibly slower rate.

More generally, two interactions Φ and $\widetilde{\Phi}$ are said to be *equivalent* if there exist families of anti-selfadjoint operators $\mathcal{S}_1, \ldots, \mathcal{S}_n$, with $\mathcal{S}_i \in \mathcal{B}_{r_i}$ for some $r_1, \ldots, r_n > 0$, and interactions $\Phi_0 \equiv \Phi, \Phi_1, \ldots, \Phi_n \equiv \widetilde{\Phi}$ such that Φ_i is $\mathcal{S}_i$-related to Φ_{i-1} for $1 \le i \le n$. This definition does indeed establish equivalence relations between classes of interactions representing the same physical system. Equivalent interactions are all exponentially decaying, albeit not necessarily at the same rate.

Before stating our results we introduce some notation: By the commutativity condition (4.5), for each $A_X \in \mathcal{A}_X$, (resp. in $\mathcal{F}_X$), there exist operators $C_Z^{(j)}(A_X) \in \mathcal{A}_Z$, (resp. in $\mathcal{F}_Z$), such that

$$\frac{1}{j!}\mathrm{ad}^j S^\Lambda(A_X) \ = \ \sum_{Z\subset\Lambda} C_Z^{(j)}(A_X)\ . \tag{4.45}$$

Moreover, if the operators S_Y (in (4.44)) are anti-selfadjoint, then

$$A_X \text{ selfadjoint} \quad \Longrightarrow \quad C_Z^{(j)}(A_X) \text{ selfadjoint}\ , \tag{4.46}$$

for each $Z \in \mathbb{Z}^\nu$, $j \geq 0$.

Indeed, due to the commutativity of operators localized in disjoint subsets of the lattice, we have that

$$\mathrm{ad}^j \sum_{Y\subset\Lambda} S_Y\,(A_X) \ = \ \sum_{\substack{Y_1,\ldots,Y_j\subset\Lambda\\ X-\text{c.s.}}} \mathrm{ad}S_{Y_j}(\cdots(\mathrm{ad}S_{Y_1}(A_X))\cdots)\ , \tag{4.47}$$

where "$X-$c.s." (X-connected subsequences) stands for the constraint

$$Y_1\cap X \ \neq \ \emptyset\,, Y_2\cap(Y_1\cup X) \ \neq \ \emptyset\,,\cdots\,, Y_n\cap(Y_{n-1}\cup\cdots\cup Y_1\cup X) \ \neq \ \emptyset\,. \tag{4.48}$$

We now resum all terms on the RHS of eqn.(4.47) with the same $Y_n\cup\cdots\cup Y_1\cup X = Z$. We obtain

$$\frac{1}{j!}\mathrm{ad}^j \sum_{Y\subset\Lambda} S_Y\,(A_X) \ = \ \sum_{\substack{Z\subset\Lambda\\ Z\supseteq X}} C_Z^{(j)}(A_X)\ , \tag{4.49}$$

with

$$C_Z^{(j)}(A_X) \ = \ \frac{1}{j!} \sum_{\substack{Y_1,\ldots,Y_j\subset\Lambda\\ X-\text{c.s.}\\ X\cup Y_1\cup\cdots\cup Y_j=Z}} \mathrm{ad}S_{Y_j}(\cdots(\mathrm{ad}S_{Y_1}(A_X))\cdots)\ . \tag{4.50}$$

This expression appears in (4.45).

We have the following result:

Lemma 4.1 *Let $\mathcal{S} = \{S_Y\}$ be a translation-invariant family of operators, $S_Y \in \mathcal{A}_Y$ with $\|\mathcal{S}\|_r < \infty$. Then for each $A_X \in \mathcal{A}_X$, (resp. in $\mathcal{F}_X$), we have that*

$$\sum_{Z\subset\Lambda} \|C_Z^{(j)}(A_X)\| \ \leq \ \|A_X\|\Big(\frac{2e^{-r}}{r}\|\mathcal{S}\|_r\Big)^j\ , \tag{4.51}$$

uniformly in Λ.

Using the Lie-Schwinger series, and noting that the RHS of (4.51) is independent of Λ, we obtain the following corollary.

Corollary 4.2 *Let $\mathcal{S} = \{S_Y\}$ be a translation-invariant family of operators, $S_Y \in \mathcal{A}_Y$. If*

$$\frac{2e^{-r}}{r}\|\mathcal{S}\|_r < 1, \tag{4.52}$$

then for each operator $A_X \in \mathcal{A}_X$, (resp. in $\mathcal{F}_X$), the limit $\lim_{\Lambda\to\mathbb{Z}^\nu} U_\Lambda A_X U_\Lambda^{-1}$ exists and defines an operator in $\mathcal{A}$, (resp. in $\mathcal{F}$).

Lemma 4.1 is a well-known result in the theory of quantum lattice systems [26, 22] [23, Lemma 7.6.1], [24, Lemma IV.3.4].

Concerning Condition **(E2)** we have the following result:

Lemma 4.3 *Let $\mathcal{S} = \{S_Y\}$ be a translation-invariant family of operators, $S_Y \in \mathcal{A}_Y$ with $\|\mathcal{S}\|_r < \infty$. Then for each $\widetilde{r} < r$*

$$\sum_{Z\ni 0}\sum_X \|C_Z^{(j)}(\Phi_X)\| e^{\widetilde{r}s(Z)} \;\le\; \|\Phi\|_r \frac{j+1}{r-\widetilde{r}}\Big(\frac{2e^{-(r-\widetilde{r})}}{r-\widetilde{r}}\|\mathcal{S}\|_r\Big)^j . \tag{4.53}$$

The transformed interaction $\widetilde{\Phi} = \{\widetilde{\Phi}_Z\}$ is given by

$$\widetilde{\Phi}_Z \;=\; \sum_{j\ge 0} t^j \sum_{X\subseteq Z} C_Z^{(j)}(\Phi_X) \tag{4.54}$$

Thus, combining Lemma (4.3) with the Lie-Schwinger series we obtain

Corollary 4.4 *Let $\mathcal{S} = \{S_Y\}$ be a family of anti-selfadjoint operators, $S_Y \in \mathcal{A}_Y$ with $\|\mathcal{S}\|_r < \infty$. Then, for each $\widetilde{r}$ satisfying*

$$\frac{2e^{-(r-\widetilde{r})}}{r-\widetilde{r}}\|\mathcal{S}\|_r \;<\; 1 , \tag{4.55}$$

the following holds: For each $\Phi \in \mathcal{B}_r$ there exists a $\mathcal{S}$-equivalent interaction $\widetilde{\Phi} \in \mathcal{B}_{\widetilde{r}}$. Moreover, $\widetilde{\Phi}$ satisfies

$$\|\widetilde{\Phi}\|_{\widetilde{r}} \;\le\; \|\Phi\|_r \sum_{n\ge 0} \frac{n+1}{r-\widetilde{r}}\Big(\frac{2e^{-(r-\widetilde{r})}}{r-\widetilde{r}}\|\mathcal{S}\|_r\Big)^n \;=\; \frac{\|\Phi\|_r}{r-\widetilde{r}}\left[1-\left(\frac{2e^{-(r-\widetilde{r})}}{r-\widetilde{r}}\|\mathcal{S}\|_r\right)^2\right]^{-1} . \tag{4.56}$$

Proof of Lemma 4.3:
The proof of this lemma is a slight variation of the proof of Lemma 4.1.

We have

$$C_Z^{(j)}(\Phi_X) \;=\; \frac{1}{j!} \sum_{\substack{Y_1,\ldots,Y_j\subset\Lambda \\ X-\text{c.s.} \\ X\cup Y_1\cup\cdots\cup Y_j = Z}} \mathrm{ad}S_{Y_j}(\cdots(\mathrm{ad}S_{Y_1}(\Phi_X))\cdots) , \tag{4.57}$$

where Z is a fixed finite subset of the lattice. To obtain (4.53), we start with the bounds

$$\|\mathrm{ad}A(B)\| \leq 2\|A\|\|B\| \,, \tag{4.58}$$

and

$$\mathrm{s}(Z) \;\leq\; \mathrm{s}(X) + \mathrm{s}(Y_1) + \cdots + \mathrm{s}(Y_j) \tag{4.59}$$

to get

$$\sum_{Z\ni 0}\sum_{X} \|C_Z^{(j)}(\Phi_X)\|\, e^{\widetilde{r}\,\mathrm{s}(Z)} \;\leq\; \frac{2^j}{j!} \sum_{\substack{X,Y_1,\ldots,Y_j\ X-\text{c.s.}\\ X\cup Y_1\cup\cdots\cup Y_j\ni 0}} \|\Phi_X\|\, e^{\widetilde{r}\,\mathrm{s}(X)}\, \|S_{Y_1}\| e^{\widetilde{r}\,\mathrm{s}(Y_1)} \cdots \|S_{Y_j}\|\, e^{\widetilde{r}\,\mathrm{s}(Y_j)} \,. \tag{4.60}$$

To bound the sum on the RHS we start with the following two steps:

(i) We bound the sum over X-c.s. containing the fixed site 0 by a sum over *pinned* X-c.s. These are X-c.s. with a fixed "initial" point, for instance, such that 0 is the *first* site of X in lexicographic order. The contribution of each pinned X-c.s. must be multiplied by the number of translations containing the origin, that is by the cardinality of the resulting set:

$$|X\cup Y_1\cup\cdots\cup Y_j| \;\leq\; \mathrm{s}(X) + \mathrm{s}(Y_1) - 1 + \ldots + \mathrm{s}(Y_j) - 1 \tag{4.61}$$

(the factors of "-1" arise from the requirement that each additional Y_l must have at least one point in common with the pre-existing sequence).

(ii) The pinned sequence $X, Y_1, \ldots, Y_j$ is constructed by taking a pinned X-connected subsequence $X, Y_1, \ldots, Y_{j-1}$ and adding to it an intersecting set Y_j. This in turn is accomplished by picking a site $z_{j-1} \in X\cup Y_1\cup\cdots\cup Y_{j-1}$ and a set $Y_j \ni z_{j-1}$.

These two steps yield:

$$\sum_{Z\ni 0}\sum_{X} \|C_Z^{(j)}(\Phi_X)\|\, e^{\widetilde{r}\,\mathrm{s}(Z)} \;\leq\; \frac{2^j}{j!} \sum_{\substack{X,Y_1,\ldots,Y_{j-1}\\ \text{pinned } X-\text{c.s.}}} \|\Phi_X\|\, e^{\widetilde{r}\,\mathrm{s}(X)} \cdots \|S_{Y_{j-1}}\|\, e^{\widetilde{r}\,\mathrm{s}(Y_{j-1})} \times N(X, Y_1, \cdots, Y_{j-1}) \,, \tag{4.62}$$

with

$$N(X, Y_1, \cdots, Y_{j-1}) \;:=\; \sum_{z_{j-1}\in X\cup Y_1\cup\cdots\cup Y_{j-1}} \times \sum_{Y_j\ni z_{j-1}} [\mathrm{s}(X) + \mathrm{s}(Y_1) - 1 + \ldots + \mathrm{s}(Y_j) - 1]\; \|S_{Y_j}\|\, e^{\widetilde{r}\,\mathrm{s}(Y_j)} \,. \tag{4.63}$$

As the sum over Y_j is independent of the chosen site z_{j-1}, we can use (4.61) to bound

$$\begin{aligned} N(X, Y_1, \cdots, Y_{j-1}) \;\; &\leq \;\; [\mathrm{s}(X) + \mathrm{s}(Y_1) - 1 + \ldots + \mathrm{s}(Y_{j-1}) - 1] \\ &\times \sum_{k_j \geq 1} [\mathrm{s}(X) + \mathrm{s}(Y_1) - 1 + \ldots + \mathrm{s}(Y_{j-1}) - 1 + k_j - 1] \\ &\quad \times \sum_{\substack{Y_j \ni 0 \\ \mathrm{s}(Y_j) = k_j}} \|S_{Y_j}\| \, e^{\widetilde{r}\, \mathrm{s}(Y_j)} \;. \end{aligned} \tag{4.64}$$

We now iterate step (ii) above: We construct the pinned sequence $X, Y_1, \ldots, Y_{j-1}$ by taking a pinned X-connected subsequence $X, Y_1, \ldots, Y_{j-2}$, a site $z_{j-2} \in X \cup Y_1 \cup \cdots \cup Y_{j-2}$ and a set $Y_{j-1} \ni z_{j-2}$. This leads to another factor $[\mathrm{s}(X) + \mathrm{s}(Y_1) - 1 + \ldots + \mathrm{s}(Y_{j-2}) - 1]$ in the bound analogous to (4.64). Continuing in this way we arrive at

$$\begin{aligned} \sum_{Z \ni 0} \sum_{X} \|C_Z^{(j)}(\Phi_X)\| e^{\widetilde{r}\, \mathrm{s}(Z)} \;\; &\leq \;\; \frac{2^j}{j!} \sum_{k \geq 1} \sum_{k_1 \geq 1} \cdots \sum_{k_j \geq 1} \prod_{i=1}^{j+1} \Big[k + \sum_{\ell=0}^{i-1} (k_\ell - 1)\Big] \\ &\quad \times \Big\{ \Big[\sum_{\substack{X \ni 0 \\ \mathrm{s}(X) = k}} \|\Phi_X\| e^{\widetilde{r}\, \mathrm{s}(X)} \Big] \prod_{i=1}^{j} \Big[\sum_{\substack{Y \ni 0 \\ \mathrm{s}(Y) = k_i}} \|S_Y\| e^{\widetilde{r}\, k_i} \Big] \Big\} \end{aligned} \tag{4.65}$$

with the convention $\mathrm{s}(Y_0) = 1$.

We now use the bound

$$x^n \;\leq\; \frac{n! \, \exp\big[(r - \widetilde{r}) x\big]}{[(r - \widetilde{r})]^n}, \tag{4.66}$$

which holds for all $\widetilde{r} < r$, to obtain

$$\begin{aligned} \prod_{i=1}^{j+1} \Big[\mathrm{s}(X) + \sum_{l=0}^{i-1} (\mathrm{s}(Y_l) - 1)\Big] \;\; &\leq \;\; \Big[\mathrm{s}(X) + \sum_{l=0}^{j} (\mathrm{s}(Y_l) - 1)\Big]^{j+1} \\ &\leq \;\; (j+1)! \, \frac{e^{(r - \widetilde{r})\, \mathrm{s}(X)}}{\big[(r - \widetilde{r})\big]^{j+1}} \prod_{l=0}^{j} \exp\big[(r - \widetilde{r})(\mathrm{s}(Y_l) - 1)\big] \;. \end{aligned} \tag{4.67}$$

¿From (4.65) and (4.67) we finally obtain

$$\begin{aligned} \sum_{Z \ni 0} \sum_{X \subseteq Z} \|C_Z^{(j)}(\Phi_X)\| e^{\widetilde{r}\, \mathrm{s}(Z)} \;\; &\leq \;\; \frac{(j+1) 2^j}{\big[(r - \widetilde{r})\big]^{j+1}} \Big[\sum_{X \ni 0} \|\Phi_X\| e^{r\, \mathrm{s}(X)} \Big] \\ &\quad \times \prod_{i=1}^{j} \Big[e^{-(r - \widetilde{r})} \sum_{Y \ni 0} \|S_Y\| \, e^{r\, \mathrm{s}(Y)} \Big] \\ &= \;\; \frac{(j+1)}{(r - \widetilde{r})} \|\Phi\|_r \left(\frac{2 \, e^{-(r - \widetilde{r})}}{r - \widetilde{r}} \, \|\mathcal{S}\|_r \right)^j \;. \;\blacksquare \end{aligned} \tag{4.68}$$

Of course there is a large amount of freedom left in defining the transformed interactions. Trivial manipulations like grouping terms or adding constants yield different interactions with the same physical content, but which may have very different norms [27]. In particular, when applying the Pirogov-Sinai theory to fermionic systems, one considers interactions that are given by sums of monomials of even degree in creation and annihilation operators. For these interactions the bound (4.56) holds if the operators in the family $\mathcal{S}$ (and hence too the transformed interactions $\widetilde{\Phi}$) are also given in terms of such monomials.

Therefore, the plan for this sequel is to adapt the formalism of Section 3 so as to produce families of anti-selfadjoint operators $t\mathcal{S}_1, \cdots t^n\mathcal{S}_n$ leading to equivalent interactions $\Phi^{(n)}(t)$ that are "block-diagonal" up to order n in t. We concentrate our attention on groundstates and on low-temperature phase diagrams. Our partial "block-diagonalization" scheme is designed to be combined with the Pirogov-Sinai theory of Section 5, more precisely with Theorem 5.2. It is therefore sufficient to analyze the bottom of the spectrum of the Hamiltonians: The scheme will not be required to remove, to the pre-established order, all off-diagonal terms, but *only* those terms which conspire against the smallness of the parameters listed in (5.22). As we shall see, successive $\mathcal{S}_n$ will diagonalize terms involving up to n bonds at a time: $\mathcal{S}_1$ diagonalizes —to second order— terms involving only one bond, $\mathcal{S}_2$ deals with the simultaneous action of two neighbouring bonds, and so on.

4.4 Local groundstates and excitations

Our starting point is a selfadjoint interaction of the form

$$\Phi(t) = \Phi_0 + tQ \ , \tag{4.69}$$

We shall denote by $H_0 = \sum_{X\subset\Lambda} \Phi_{0X}$ and $V = \sum_{X\subset\Lambda} Q_X$ the corresponding finite-volume (unperturbed) Hamiltonians and perturbations . (For simplicity we omit the Λ-dependence in the sequel.) We assume that the unperturbed interaction Φ_0 and the perturbation interaction Q satisfy the following properties:

(P1) The interaction Φ_0 is classical, i.e., there is a basis of $\mathcal{H}$ such that $\Phi_{0X} \in \mathcal{C}(\mathcal{E}_X)$, for arbitrary X, and of range $R < \infty$. Moreover, we assume that Φ_0 is given by a translation-invariant m-potential [15]. This last condition means that we can assume (if necessary by passing to a physically equivalent interaction) that there exists at least one configuration ω minimizing all Φ_{0X}, i.e.,

$$\Phi_{0X}(\omega) = \min_{\omega'} \Phi_{0X}(\omega') \ , \tag{4.70}$$

for all X. For any m-potential, the set of all configurations for which eqn.(4.70) holds are groundstate configurations of Φ_0. To simplify the notation, we normalize the m-potential by making the replacement

$$\Phi_{0X}(\omega) \longrightarrow \{\Phi_{0X}(\omega) - \min_{\omega'} \Phi_{0X}(\omega')\} . \tag{4.71}$$

Thus, we shall assume that

$$\Phi_{0X}(\omega) \geq 0 \quad \text{and} \quad \min_{\omega'} \Phi_{0X}(\omega') = 0 . \tag{4.72}$$

(P2) The perturbation interaction Q is in some space Banach space $\mathcal{B}_r$:

$$\|Q\|_r := \sum_{X \ni 0} \|Q_X\| e^{rs(X)} < \infty \tag{4.73}$$

for $r > 0$.

Let us first introduce some definitions related only to the "classical" Hamiltonian H_0. Because of our normalization of the m-potential (4.71), the groundstate energy of H_0 is equal to zero. We define the set of groundstate configurations of H_0 associated with a subset Y of Λ as follows:

$$\Omega_Y^0 = \{\omega_Y : \Phi_{0X}(\omega_Y) = 0 \text{ for any } X \subseteq Y\} . \tag{4.74}$$

We define P_Y^0 to be the projection operator onto the subspace $\mathcal{H}_Y^0$

$$\mathcal{H}_Y^0 := \{\psi \in \mathcal{H}_Y : \psi = \sum_{\omega_Y \in \Omega_Y^0} c_{\omega_Y} e_{\omega_Y}\}, \tag{4.75}$$

i.e., onto the subspace of $\mathcal{H}_Y$ spanned by the local groundstates in Y.

To deal properly with the local character of the different operators we define, for any $x \in \mathbb{Z}^\nu$, the *R-plaquette centered at* x (recall that R is the range of H_0):

$$W_x := \{y \in \Lambda : |y_i - x_i| \leq R, \text{ for } 1 \leq i \leq \nu\} . \tag{4.76}$$

For any set $X \subset \mathbb{Z}^\nu$, its coverings by R-plaquettes is denoted by

$$B_X := \bigcup_{x \in X} W_x . \tag{4.77}$$

We introduce some special projection operators on $\mathcal{H}_{B_X}$, the space generated by the vectors $e_{\omega_{B_X}}$ with $\omega_{B_X} \in \Omega_{B_X}$:

(1) The orthogonal projection onto the space of states which fail to be groundstates in a region $X \subset B_X$:
$$P_{B_X}^1 := P_{B_X \setminus X}^0 - P_{B_X}^0 . \tag{4.78}$$
The set $B_X \setminus X$ acts as a "protection zone" or "security corridor", introduced to ensure the additivity of excitation energies (Lemma 4.6 below).

(2) The projection onto states with excitations in the "protection zone" $B_X \setminus X$:

$$P^2_{B_X} := \mathbf{1}_{B_X} - P^1_{B_X} - P^0_{B_X} \;, \tag{4.79}$$

where $\mathbf{1}_{B_X}$ is the identity operator in $\mathcal{A}_{B_X}$.

We have that

$$\mathcal{H}^0_{B_X} \;=\; P^0_{B_X}\mathcal{H}_{B_X} \;. \tag{4.80}$$

We also define the space

$$\mathcal{H}^{\rm ex}_{B_X} \;:=\; (P^1_{B_X} + P^0_{B_X})\mathcal{H}_{B_X} \;, \tag{4.81}$$

whose elements we call *excitations with support* X. We see that

$$\mathcal{H}_{B_X} \supset \mathcal{H}^{\rm ex}_{B_X} \supset \mathcal{H}^0_{B_X} \;. \tag{4.82}$$

The set of operators that leave $\mathcal{H}^{\rm ex}_{B_X}$ invariant:

$$\mathcal{A}^{\rm ex}_{B_X} \;:=\; \Big\{A \in \mathcal{A}_{B_X} \colon A\mathcal{H}^{\rm ex}_{B_X} \subset \mathcal{H}^{\rm ex}_{B_X}\Big\} \tag{4.83}$$

will play a special role in the sequel. To define the most conspicuous example of such an operator, we decompose the Hamiltonian H_0 in the following way, for each $X \subset \mathbb{Z}^\nu$:

$$H_0 \;=\; \overline{H}_{0B^c_X} \;+\; \overline{H}_{0X} \;+\; H_{0(B_X\setminus X)} \tag{4.84}$$

where for any subset A of the lattice

$$\overline{H}_{0A} \;=\; \sum_{Y:Y\cap A\neq\emptyset} \Phi_{0Y} \;, \tag{4.85}$$

$$H_{0A} \;=\; \sum_{Y:Y\subset A} \Phi_{0Y} \;. \tag{4.86}$$

We have the following important facts.

Proposition 4.5 *For any (finite) set $X \subset \mathbb{Z}^\nu$:*

(a) $\mathcal{A}^{\rm ex}_{B_X}$ is an algebra:

$$A, B \in \mathcal{A}^{\rm ex}_{B_X} \implies AB \in \mathcal{A}^{\rm ex}_{B_X} \;. \tag{4.87}$$

(b) $\mathcal{A}_X \subset \mathcal{A}^{\rm ex}_{B_X}$.

(c) $\overline{H}_{0X} \in \mathcal{A}^{\rm ex}_{B_X}$. Hence we can write $P^1_{B_X} + P^0_{B_X}$ as a sum of orthogonal projections onto the eigenstates of $\overline{H}_{0X}$.

(d) If A is an off-diagonal operator [in the sense of (2.17)] with respect to the spectral decomposition of $\overline{H}_{0X}$, then

$$A \in \mathcal{A}^{\rm ex}_{B_X} \implies {\rm ad}^{-1}\overline{H}_{0X}(A) \in \mathcal{A}^{\rm ex}_{B_X} \;. \tag{4.88}$$

The proofs of these properties are immediate; in particular (d) follows from (c).

We say that two excitations are *disconnected* if their supports X_1, X_2 satisfy $X_2 \subset B^{\rm c}_{X_1} := \Lambda \setminus B_{X_1}$. In the estimations below, we make a crucial use of the following additivity property.

Lemma 4.6 *If $\psi \in \mathcal{H}^{\rm ex}_{B_X}$, then*

$$H_0 \psi = \overline{H}_{0 B^{\rm c}_X} \psi \, + \, \overline{H}_{0X} \psi \, . \tag{4.89}$$

As a consequence, the unperturbed energies of disconnected excitations are additive.

Proof:

$$\begin{aligned} H_0 \psi &= H_0 P^0_{B_X \setminus X} \psi \\ &= \{ \overline{H}_{0 B^{\rm c}_X} + H_{0(B_X \setminus X)} + \overline{H}_{0X} \} P^0_{B_X \setminus X} \psi \\ &= \{ \overline{H}_{0 B^{\rm c}_X} + \overline{H}_{0X} \} P^0_{B_X \setminus X} \psi \\ &= \{ \overline{H}_{0 B^{\rm c}_X} + \overline{H}_{0X} \} \psi \, , \end{aligned} \tag{4.90}$$

since $\psi \in \mathcal{H}^{\rm ex}_{B_X}$ and $H_{0(B_X \setminus X)} P^0_{B_X \setminus X} \psi = 0$, due to the normalization of the m-potential. ∎

4.5 First order perturbation theory

The first step in our perturbation scheme consists of a partial block-diagonalization, to order t^2, of the interaction $\{Q_X\}$. To this end, it is convenient to write Q_X as

$$\begin{aligned} Q_X = \mathbf{1}_{B_X} Q_X \mathbf{1}_{B_X} &= (P^0_{B_X} + P^1_{B_X} + P^2_{B_X}) \, Q_X \, (P^0_{B_X} + P^1_{B_X} + P^2_{B_X}) \\ &= (P^0_{B_X} + P^1_{B_X}) \, Q_X \, (P^0_{B_X} + P^1_{B_X}) + P^2_{B_X} Q_X P^2_{B_X} \end{aligned} \tag{4.91}$$

since $Q_X \in \mathcal{A}^{\rm ex}_{B_X}$. We regroup the terms as follows:

$$Q_X = Q^{00}_{B_X} + Q^{01}_{B_X} + Q^{R}_{B_X} \, , \tag{4.92}$$

where $Q^{00}_{B_X}$ are "diagonal" operators defined as

$$Q^{00}_{B_X} \; := \; P^0_{B_X} Q_X P^0_{B_X} \, , \tag{4.93}$$

$Q^{01}_{B_X}$ the "off-diagonal" operators

$$Q^{01}_{B_X} \; := \; P^0_{B_X} Q_X P^1_{B_X} + P^1_{B_X} Q_X P^0_{B_X} \, , \tag{4.94}$$

and

$$Q^{R}_{B_X} = P^1_{B_X} Q_X P^1_{B_X} + P^2_{B_X} Q_X P^2_{B_X} \, . \tag{4.95}$$

Note that writing Q_X as $\mathbf{1}_{B_X} Q_X \mathbf{1}_{B_X}$ changes the norm of the interaction Q. Nevertheless, if $Q = \{Q_X\}$ belongs to $\mathcal{B}_r$, then $Q = \{\mathbf{1}_{B_X} Q_X \mathbf{1}_{B_X}\}$ belongs to $\mathcal{B}_{\widehat{r}}$ with

$$\widehat{r} \;=\; \frac{r}{[(2R+1)^\nu - 1]} \;. \tag{4.96}$$

Indeed, we have

$$\sum_{B_X \ni 0} \|\mathbf{1}_{B_X} Q_X \mathbf{1}_{B_X}\| e^{\widehat{r}\,\mathrm{s}(B_X)} \;\leq\; [(2R+1)^\nu - 1] \sum_{X \ni 0} \|Q_X\| e^{r\,\mathrm{s}(X)} \;, \tag{4.97}$$

where we have used that $\|Q_{B_X}\| = \|Q_X\|$ and that $\mathrm{s}(B_X) \leq [(2R+1)^\nu - 1]\,\mathrm{s}(X)$, [Each site in in X gives rise to at most $(2R+1)^\nu$ sites in B_X, but neighbouring R-plaquettes intersect, hence the factor "-1"]. The factor $[(2R+1)^\nu - 1]$ on the RHS of (4.97) arises from the fact that each site $x \in X$ can give rise to at most $[\mathrm{s}(W_x) - 1]$ additional sites in $B_X \setminus X$. ¿From now on, we assume that $Q = \{\mathbf{1}_{B_X} Q_X \mathbf{1}_{B_X}\}$ with $\|Q\|_{\widehat{r}} < \infty$.

Following the guidelines explained above, we search to eliminate the first-order off-diagonal terms $Q^{01}_{B_X}$, through a unitary transformation $U^{(1)}(t) = \exp(tS_1)$, with S_1 being a sum of local operators:

$$S_1 \;:=\; \sum_X S_{1B_X} \;. \tag{4.98}$$

By (3.3), the unitary operator $U^{(1)}(t)$ generates the transformed Hamiltonian

$$\begin{aligned} H^{(1)}(t) \;&:=\; e^{tS_1}\, H(t)\, e^{-tS_1} \\ &=\; H_0 + tV^{00} + tV^{01} + tV^R \\ &\qquad + \sum_{n \geq 1} \frac{t^n}{n!} \mathrm{ad}^n S_1 (H_0 + tV^{00} + tV^{01} + tV^R) \end{aligned} \tag{4.99}$$

where $V^{00} := \sum_X Q^{00}_{B_X}$, and similarly for V^{01} and V^R. This leads to the condition

$$\sum_X \mathrm{ad} H_0 (S_{1B_X}) \;=\; \sum_X Q^{01}_{B_X}. \tag{4.100}$$

However, as a consequence of Lemma 4.6, we have

$$\mathrm{ad}^{-1} H_0 \left(Q^{01}_{B_X} \right) \;=\; \mathrm{ad}^{-1} \overline{H}_{0X} \left(Q^{01}_{B_X} \right) \tag{4.101}$$

and, hence, (4.100) is satisfied if we choose

$$S_{1B_X} \;:=\; \mathrm{ad}^{-1} \overline{H}_{0X} \left(Q^{01}_{B_X} \right) \;. \tag{4.102}$$

[Note that the selfadjointness of $\overline{H}_{0X}$ and Q_{B_X} implies the anti-selfadjointness of S_{1B_X}.] Identity (4.101) is therefore the key that allows us to define S_1 as a sum of local terms. Its validity is one of the justifications for the use of "protection zones" $B_X \setminus X$.

Next we show that the above defined family of operators $\mathcal{S}_1 := \{S_{1B_X}\}$ belongs to $\mathcal{B}_{\widehat{r}}$, with $\widehat{r}$ given by (4.96). Indeed, the fact that Φ_0 is given by an m-potential implies that for each $X \subset \Lambda$ the operator $\overline{H}_{0X}$ has a gap, D_X, between its groundstate energy and the rest of its spectrum. This gap makes each operator S_{1B_X} well-defined because, in analogy with eqn.(2.35) of Sect. 2, the operator norm of $\mathrm{ad}^{-1}\overline{H}_{0X}$ on

$$\mathcal{O}_{B_X} := \{A^{01}_{B_X} := P^0_{B_X} A_X P^1_{B_X} + P^1_{B_X} A_X P^0_{B_X} : A_X \in \mathcal{A}_X\} \tag{4.103}$$

is bounded in the form:

$$||\mathrm{ad}^{-1}\overline{H}_{0X}\,|_{\mathcal{O}_{B_X}}\,||_{\mathrm{op}} \leq \frac{1}{D_X} \;\leq\; \frac{1}{\Delta}\;, \tag{4.104}$$

where

$$\Delta \;:=\; \min_X D_X\;. \tag{4.105}$$

Therefore,

$$\begin{aligned} \|\mathcal{S}_1\|_{\widehat{r}} \;&\leq\; t \sum_{B_X \ni 0} \frac{\|Q^{01}_{B_X}\|}{D_X} e^{\widehat{r}\,s(B_X)} \\ &\leq\; \frac{t}{\Delta}\|Q\|_{\widehat{r}}\;. \end{aligned} \tag{4.106}$$

where we have used that $\|Q^{01}_{B_X}\| \leq \|Q_{B_X}\|$.

Our choice of $\mathcal{S}_1$ yields a transformed Hamiltonian of the form

$$\begin{aligned} H^{(1)}(t) \;&=\; H_0 + tV^{00} + tV^R \\ &\quad + \sum_{n\geq 1} t^{n+1}\mathrm{ad}^n S_1\Big(\frac{1}{n!}V^{00} + \frac{1}{n!}V^R + \frac{n}{n+1!}V^{01}\Big)\;. \end{aligned} \tag{4.107}$$

¿From (4.106) and Corollary 4.4 we have that $H^{(1)}(t)$ corresponds to an interaction $\Phi^{(1)}(t)$ with

$$\|\Phi^{(1)}(t)\|_{r_1} \;\leq\; \|\Phi(t)\|_{\widehat{r}} \sum_{n\geq 0} \frac{(n+1)}{\widehat{r}-r_1}\Big(\frac{t}{\Delta}\,\frac{2e^{-(\widehat{r}-r_1)}}{\widehat{r}-r_1}\|Q\|_{\widehat{r}}\Big)^n\;, \tag{4.108}$$

for any $r_1 < \widehat{r}$, as long as t/Δ is so small that

$$\frac{t}{\Delta}\,\frac{2e^{-(\widehat{r}-r_1)}}{\widehat{r}-r_1}\|Q\|_{\widehat{r}} \;<\; 1\;. \tag{4.109}$$

Notice that one can choose $r_1 = r_1(r)$ such that $r_1 \to \infty$ if $r \to \infty$. Moreover, if we order the terms of $\Phi^{(1)}(t)$ according to the degree of t,

$$\Phi^{(1)}(t) \;=\; \Phi_0 \;+\; \sum_{j\geq 1} t^j\,\Phi^{(1)}_j\;, \tag{4.110}$$

we see that the transformed interaction $\Phi^{(1)}(t)$ also satisfies the hypotheses **(P1)** and **(P2)** above and, therefore, it is amenable to an iteration of our procedure. We shall make use of this fact below. Moreover we see, from (4.53) and (4.99) , that

$$\|t^j \Phi_j^{(1)}\|_{r_1} \;\le\; t\,\|Q\|_{\widehat{r}}\,\frac{j}{\widehat{r}-r_1}\Big(\frac{t}{\Delta}\,\frac{2e^{-(\widehat{r}-r_1)}}{\widehat{r}-r_1}\|Q\|_{\widehat{r}}\Big)^{j-1}\,. \qquad (4.111)$$

As our choice of $\mathcal{S}_1$ has made $P_Y^0\Phi_{1Y}^{(1)}(\mathbf{1}_Y - P_Y^0) = 0$ for each $Y \subset \mathbb{Z}^\nu$, we conclude that

$$\sum_{Y\ni 0}\Big\|P_Y^0\Phi_Y^{(1)01}(\mathbf{1}_Y - P_Y^0)\Big\|\,e^{r_1\,s(Y)} \;=\; \mathrm{O}\Big(t^2/\Delta\Big)\,. \qquad (4.112)$$

¿From (4.107) we see that the diagonal part of $\Phi^{(1)}$ is of the form

$$\Phi^{(1)00} \;=\; \Phi_0^{00} + tQ^{00} + t^2\Phi_2^{(1)00} + \mathrm{O}(t^3)\,, \qquad (4.113)$$

where

$$\Phi_2^{(1)00} \;=\; \Big\{\Phi_{2B_{X\cup X'}}^{(1)00} \,:\, X'\cap B_X \neq \emptyset\Big\}\,, \qquad (4.114)$$

with

$$\begin{aligned}\Phi_{2B_{X\cup X'}}^{(1)00} \;&=\; \int \frac{dP_{\overline{E}_X}\,P_{B_X}^0\,Q_X\,P_{B_X}^1\,dP_{\overline{E'}_X}}{E-E'}\,P_{B_{X'}}^1\,Q_{X'}\,P_{B_{X'}}^0 \\ &\quad -P_{B_{X'}}^0\,Q_{X'}\,P_{B_{X'}}^1\int \frac{dP_{\overline{E}_X}\,P_{B_X}^1\,Q_X\,P_{B_X}^0\,dP_{\overline{E'}_X}}{E-E'} \end{aligned} \qquad (4.115)$$

($dP_{\overline{E}_X}$ is the spectral decomposition of $\overline{H}_{0X}$).

Hence, this second-order correction corresponds to excitation–de-excitation processes, or in the example of hopping perturbations, to "two-bond excursions" of the hopping particle. Each term corresponds to the action of some quantum operator $Q_{X'}$ which produces an excitation which is subsequently removed by the action of a second operator Q_X.

4.6 Higher order perturbation theory

Let us now extend the partial block-diagonalization procedure to an arbitrary (but finite!) order n. The resulting algorithm is an adaptation to interactions of what was done in Lemma 3.1 for Hamiltonians. As in Section 3, we have two possible choices for the block-diagonalizing transformation:

$$U^{(n)}(t) \;=\; e^{tS_1+\cdots+t^nS_n} \qquad (4.116)$$

(Section 3.2), or

$$U^{(n)}(t) \;=\; e^{t^nS_n}\cdots e^{tS_1} \qquad (4.117)$$

(Section 3.4). The studies based on these two choices are similar, but (4.117) generates less terms in the expansion and, hence, is more convenient for computations. The following theorem holds for either choice of transformation.

Theorem 4.7 *Consider an interaction of the form*

$$\Phi(t) \;=\; \Phi_0 + tQ \tag{4.118}$$

where Φ_0 satisfies Condition **(P1)** *and Q satisfies Condition* **(P2)**. *Then, there exists a strictly decreasing sequence*

$$\widehat{r} > r_1 > r_2 > \cdots > r_n > \cdots \tag{4.119}$$

and a non-increasing sequence

$$t_0(1) \geq t_0(2) \geq \cdots \geq t_0(n) \geq \cdots \tag{4.120}$$

of numbers with r_i, $t_0(i) > 0$ ($\widehat{r}$ is defined in eqn. (4.96)) such that the following holds. For each $n > 0$, there exists an interaction of the form

$$\Phi^{(n)}(t) = \Phi_0 + \sum_{j\geq 1} t^j \Phi_j^{(n)} \;, \tag{4.121}$$

defined for $t < t_0(n)$, with the following properties:

(a) $\Phi^{(n)}(t)$ *is equivalent to* $\Phi(t)$.

(b) $\Phi^{(n)}(t) \in \mathcal{B}_{r_n}$.

(c) $\Phi_j^{(n)}$ *is independent of n, for $1 \leq j \leq n$.*

(d) If $\Phi_j^{(n)} = \{\Phi_{jY}^{(n)}\}$, *then*

$$\Phi_{jY}^{(n)} \;=\; 0 \quad \textit{if } Y \neq B_X \textit{ for all finite } X, \tag{4.122}$$

for all $j \geq 1$, and

$$\Phi_{jB_X}^{(n)01} \;=\; 0 \;. \tag{4.123}$$

for all finite $X \subset \Lambda$, and $1 \leq j \leq n$.

(e) The off-diagonal part, $\Phi^{(n)01}(t)$, of the interaction $\Phi^{(n)}(t)$ satisfies the summability condition:

$$\|\Phi^{(n)01}(t)\|_{r_n} \;=\; \mathrm{O}(t^{n+1}/\Delta^n) \;. \tag{4.124}$$

where Δ is given by (4.105) and

$$\|\Phi^{(n)01}(t)\|_{r_n} := \sum_{Y\ni 0} \sum_{j\geq 1} t^j \|\Phi_{jY}^{(n)01}\| e^{r_n\, \mathrm{s}(Y)} \tag{4.125}$$

The definition of the interaction $\Phi^{(n)}(t)$ is given in the proof [steps (A) and (B) below]. The values of r_n and $t_0(n)$ are constrained by eqn. (4.158) or (4.159).

Proof:

1) Motivation.

Let us first give a motivation for the method of the proof and the definitions used in it. Our intention is to block-diagonalize the interactions to any given finite order $n > 1$. More precisely, we want to construct an equivalent interaction such that, to order n in the perturbation parameter t, the matrix elements of the interaction between a state corresponding to a local groundstate and a state with a localized excitation vanishes. We would like to proceed, as in Sections 3.2 or 3.4, and start with the following unitary transformation.

$$
\begin{aligned}
&U^{(n)}(t)\,(H_0 + tV)\,U^{(n)}(t)^{-1} \\
&= H_0 + \sum_{j=1}^{n} t^j\,[\mathrm{ad}S_j(H_0) + V_j] + \sum_{j\geq n+1} t^j\,V_j,
\end{aligned}
\tag{4.126}
$$

where $V_1 = V$ and V_j is given by (3.22) or (3.51) for $j \geq 2$. The operators in this identity belong to the observable algebra $\mathcal{A}_\Lambda$, where Λ is a finite subset of the lattice. Since we want results valid in the thermodynamic limit, we require each of the operators S_j and V_j to be given by sums of local operators. Consequently we need to show that V_j is of the form $V_j = \sum_Y Q^{(n)}_{jY}$ with

$$
Q^{(n)}_{jY} = 0 \quad \text{if } Y \neq B_X \text{ for some finite } X,
\tag{4.127}
$$

and to find operators $S_j = \sum_X S_{j\,B_X}$ for which

$$
\left(\mathrm{ad}S_{jB_X}(H_0) + Q^{(n)}_{jB_X}\right)^{01} = 0, \quad \text{for} \quad \mathrm{j} = 1, \cdots, \mathrm{n}.
\tag{4.128}
$$

More precisely, we require that

$$
V_j \;=\; \sum_{X\subset\Lambda} Q^{(n)}_{jB_X}\;,
\tag{4.129}
$$

with the property

$$
Q^{(n)01}_{jB_X} \in \mathcal{A}^{\mathrm{ex}}_{B_X}\;.
\tag{4.130}
$$

If this is true, then Lemma 4.6 states that

$$
\mathrm{ad}^{-1}H_0\left(Q^{(n)01}_{jB_X}\right) \;=\; \mathrm{ad}^{-1}\overline{H}_{0X}\left(Q^{(n)01}_{jB_X}\right)
\tag{4.131}
$$

and hence we can satisfy the criterion (4.128) with operators

$$
\begin{aligned}
S_j \;&:=\; \sum_X \mathrm{ad}^{-1}\overline{H}_{0X}\left(Q^{(n)01}_{jB_X}\right) \\
&:=\; \sum_X S_{jB_X}
\end{aligned}
\tag{4.132}
$$

which are sums of local operators.

Assuming the validity of eqns. (4.129)–(4.130), and hence of (4.131), we can expand (3.2) or (3.4) using the multilinearity (2.23) to obtain

$$Q_{jY}^{(n)} = \sum_{\substack{p\geq 2\,,(k_1,\ldots,k_p):\\ 1\leq k_1,\cdots,k_p\leq n\\ k_1+\cdots+k_p=j}} c_p(k_1,\cdots,k_p) \sum_{\substack{X_1,\ldots,X_p:\\ B-\text{c.s.}\\ B_{X_1}\cup\cdots B_{X_p}=Y}} \mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_1B_{X_1}}\big(\overline{H}_{0X_1}\big)\cdots\Big)$$
$$+ \sum_{\substack{p\geq 1\,,(k_1,\ldots,k_p):\\ 1\leq k_1,\cdots,k_p\leq n\\ k_1+\cdots+k_p=j-1}} c_p(k_1,\cdots,k_p) \sum_{\substack{X,X_1,\ldots,X_p:\\ B-\text{c.s.}\\ B_X\cup B_{X_1}\cup\cdots B_{X_p}=Y}} \mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_1B_{X_1}}\big(Q_{B_X}\big)\cdots\Big)\,, \tag{4.133}$$

where we have abbreviated

$$c_p(k_1,\cdots,k_p) \;:=\; \begin{cases} \dfrac{1}{p!} & \text{for the choice (4.116)}\\ \dfrac{\chi(k_p\geq\cdots\geq k_1)}{\prod_{i=1}^{n}(\mathrm{card}\{l\colon k_l=i\})!} & \text{for the choice (4.117)} \end{cases} \tag{4.134}$$

($\chi(\cdot)$ is the characteristic function), and the notation "$B-$c.s." (B-connected subsequences), for a family $Y_1,\ldots,Y_m$, stands for the constraint

$$Y_2\cap B_{Y_1}\;\neq\;\emptyset\,,Y_3\cap B_{Y_2\cup Y_1}\;\neq\;\emptyset\,,\cdots\,,Y_m\cap B_{Y_{m-1}\cup\cdots\cup Y_1}\;\neq\;\emptyset\,. \tag{4.135}$$

On the first line on the RHS of (4.133) we have made use of the identity

$$\sum_X \mathrm{ad}S_{kB_X}(H_0) = \sum_X \mathrm{ad}S_{kB_X}(\overline{H}_{0X}), \tag{4.136}$$

which follows from Lemma 4.6. We immediately notice that the RHS of (4.133) is independent of n for $j\leq n$. This allows us to simplify the notation by defining

$$Q_{jB_X} \;:=\; Q_{jB_X}^{(n)}\,,\quad \text{for}\quad j=1,\ldots,n. \tag{4.137}$$

2) Recursive Definitions.

The preceding considerations motivate the following definitions with which we start our formal proof. For each $1\leq j\leq n$:

(A) We define a family of operators $\mathcal{S}_j$, recursively, in the following way.

(A.1) For each j, operators Q_{jY} are defined through the RHS of (4.133) (which is independent of n for the range of j's considered). We start by defining the operators for the index $j = 1$:

$$Q_{1Y} = \begin{cases} Q_{B_X} & \text{if } Y = B_X \text{ for some finite } X \\ 0 & \text{otherwise.} \end{cases} \tag{4.138}$$

(A.2) For each j, we define a family of operators $\mathcal{S}_j = \{S_{jY}\}$ as follows.

$$S_{jY} := \begin{cases} \mathrm{ad}^{-1}\overline{H}_{0X}\left(Q^{01}_{jB_X}\right) & \text{if } Y = B_X \text{ for some finite } X \\ 0 & \text{otherwise.} \end{cases} \tag{4.139}$$

(B) For each j, we define interactions $\Phi^{(n)}_j = \{\Phi^{(n)}_{jY}\}$, as follows.

$$\Phi^{(n)}_{jY} = 0 \quad \text{if } Y \neq B_X \text{ for all finite } X \tag{4.140}$$

and

$$\Phi^{(n)}_{jB_X} = \begin{cases} Q^{(n)}_{jB_X} & \text{if } j \geq n+1 \\ \mathrm{ad}S_{jB_X}(\overline{H}_{0X}) + Q^{(n)}_{jB_X} = \mathrm{ad}S_{jB_X}(\overline{H}_{0X}) + Q_{jB_X} & \text{if } 1 \leq j \leq n\ , \end{cases} \tag{4.141}$$

where $Q^{(n)}_{jY}$ is defined through (4.133).

3) Proof of properties (a)–(e).

Our definitions automatically satisfy property (d) of the theorem. We first prove (a), (b) and (c), leaving the verification of (e) for the end. The proof requires the following steps, (I) and (II), for all $1 \leq j \leq n$.

(I) We need to show that equation (4.133) implies that

$$Q^{(n)}_{jY} = 0 \quad \text{unless } Y = B_X \text{ for some finite } X\ , \tag{4.142}$$

and to prove the validity of the property (4.130).

These would in turn imply the following: (i) Eqn. (4.131) holds and and the criterion (4.128) is satisfied. (ii) Each of the operators V_j appearing on the RHS of (4.126) is given by a sum (4.129) of local operators, which are defined through eqn. (4.133).

(II) We need to show that the operators in the family $\mathcal{S}_j$ belong to the Banach space $\mathcal{B}_{r_{j-1}}$ for $j = 1, \ldots n$, with $\hat{r} =: r_0 > \cdots > r_{n-1} > 0$. (Note our choice of subscripts: $\mathcal{S}_n \in \mathcal{B}_{r_{n-1}}$ so that $\Phi^{(n)} \in \mathcal{B}_{r_n}$. This shift of indices is an unavoidable consequence of our recursive construction.)

Then, Corollary 4.4 would imply that there exists a positive number $t_0(n)$ such that for $t < t_0(n)$ the operator $U^{(n)}(t)$ —defined either by (4.116) or (4.117)— determines a map from the interaction $\Phi(t)$, to an equivalent interaction which belongs to $\mathcal{B}_{r_n}$ for some $r_n < r_{n-1}$. Given (I), it follows from the above calculations that such an interaction is precisely $\Phi^{(n)}(t)$.

To show (I) we first use (4.139) to rewrite (4.133) in the form

$$
\begin{aligned}
Q^{(n)}_{jY} = & \\
& \sum_{\substack{p\geq 2\,,(k_1,\dots,k_p):\\ 1\leq k_1,\cdots,k_p\leq n\\ k_1+\cdots+k_p=j}} c_p(k_1,\cdots,k_p) \sum_{\substack{X_1,\dots,X_p:\\ B-\text{c.s.}\\ B_{X_1}\cup\cdots B_{X_p}=Y}} \mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_2B_{X_2}}\Big(-Q^{01}_{k_1B_{X_1}}\big)\cdots\Big) \\
& + \sum_{\substack{p\geq 1\,,(k_1,\dots,k_p):\\ 1\leq k_1,\cdots,k_p\leq n\\ k_1+\cdots+k_p=j-1}} c_p(k_1,\cdots,k_p) \sum_{\substack{X,X_1,\dots,X_p:\\ B-\text{c.s.}\\ B_X\cup B_{X_1}\cup\cdots B_{X_p}=Y}} \mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_1B_{X_1}}\Big(Q_{1B_X}\Big)\cdots\Big).
\end{aligned}
\tag{4.143}
$$

[On the RHS we have used the notation of (4.137).] This proves (4.142), since $B_{X_1}\cup\cdots\cup B_{X_p} = B_{X_1\cup\cdots\cup X_p}$. We prove (4.130) by an induction in j. For $j=1$ it is obviously valid. To prove it for an arbitrary j, assuming it to be true for all indices up to $j-1$, we decompose Q_{1B_X} as in Section 4.5 (see (4.92)):

$$
Q_{1B_X} = Q^{00}_{1B_X} + Q^{01}_{1B_X} + Q^{R}_{1B_X}\ . \tag{4.144}
$$

Each term in (4.143) which does not contain $Q^R_{1B_X}$ is a product of operators satisfying (4.130) with supports $B_{X_1},\cdots,B_{X_p}$ [inductive hypothesis alongwith eqn. (4.88)] and hence the products also satisfy (4.130) with support $B_{X_1\cup\cdots\cup X_p}$. For the terms which contain $Q^R_{1B_X} = P^1_{B_X}Q_{1X}P^1_{B_X} + P^2_{B_X}Q_{1X}P^2_{B_X}$ the verification of (4.130) is less immediate, since, in general, $Q^R_{1B_X} \notin \mathcal{A}^{\text{ex}}_{B_X}$. However, the operators Q^{01}_{jY} only involve products of the form

$$
P^0_{B_{X\cup X_1\cup\cdots\cup X_p}}\mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_1B_{X_1}}\Big(Q^R_{1B_X}\Big)\Big)\cdots\Big)P^1_{B_{X\cup X_1\cup\cdots\cup X_p}} \tag{4.145}
$$

or

$$
P^1_{B_{X\cup X_1\cup\cdots\cup X_p}}\mathrm{ad}S_{k_pB_{X_p}}\Big(\cdots\Big(\mathrm{ad}S_{k_1B_{X_1}}\Big(Q^R_{1B_X}\Big)\Big)\cdots\Big)P^0_{B_{X\cup X_1\cup\cdots\cup X_p}} \tag{4.146}
$$

which vanish when applied to a state with an excitation in $B_{X_1\cup\cdots\cup X_p}\setminus X_1\cup\cdots\cup X_p$. Hence (4.130) is valid.

To prove (II) we start with the bound

$$\|\mathcal{S}_j\|_{r_{j-1}} \;\le\; \frac{1}{\Delta}\sum_{B_X\ni 0}\|Q^{01}_{jB_X}\|\,e^{r_{j-1}\mathrm{s}(B_X)} \;\le\; \frac{1}{\Delta}\|Q_j\|_{r_{j-1}}\;, \tag{4.147}$$

which follows from (4.139) and (4.104) $[\|Q_{j-1}\|_{r_{j-1}} := \sum_{B_X\ni 0}\|Q_{jB_X}\|e^{r_{j-1}\mathrm{s}(B_X)}]$. This bound shows that it is sufficient to prove that there are positive numbers r_{j-1}, for $1\le j\le n$, such that

$$\|Q_j\|_{r_{j-1}} < \infty\;. \tag{4.148}$$

In Section 4.5 we found that for $j=1$ the bound (4.148) holds, with $r_0=\widehat{r}$, (see (4.106)). Let us assume that we have found $r_1>\ldots>r_{j-1}$ such that

$$\|Q_l\|_{r_{l-1}} < \infty \quad \text{for} \quad 1\le l\le j-1\;. \tag{4.149}$$

To prove (4.148) we follow the method of the proof of Lemma 4.3, and show that for any $r_{j-1}<r_{j-2}$, $\|Q_j\|_{r_{j-1}}<\infty$. We do the following steps.

(i) We multiply both sides of (4.143) by $e^{r_{j-1}\mathrm{s}(Y)}$ and sum over all $Y\ni 0$. On the RHS we partition $\mathrm{s}(Y)$ into positive numbers $\mathrm{s}(B_X),\mathrm{s}(B_{X_1}),\cdots,\mathrm{s}(B_{X_p})$ such that $\mathrm{s}(Y)\le \mathrm{s}(B_X)+\mathrm{s}(B_{X_1})+\cdots+\mathrm{s}(B_{X_p})$.

(ii) We bound the commutators by 2^p times the product of the norms of the operators.

(iii) We use the bound $\|S_{k_iB_{X_i}}\|\le\|Q_{k_iB_{X_i}}\|/\Delta$.

(iv) We use the bound

$$\sum_{\substack{(k_1,\ldots,k_p):\\ k_1,\cdots,k_p\ge 1\\ k_1+\cdots+k_p=j}} c_p(k_1,\cdots,k_p)(\cdot) \;\le\; \frac{1}{p!}\sum_{\substack{(k_1,\ldots,k_p):\\ k_1,\cdots,k_p\ge 1\\ k_1+\cdots+k_p=j}}(\cdot)\;. \tag{4.150}$$

In this way we obtain [recall that $j\le n$]

$$\begin{aligned}\|Q_j\|_{r_{j-1}} \;\le\;& \\ &\sum_{\substack{p\ge 2,\,(k_1,\ldots,k_p):\\ 1\le k_1,\cdots,k_p\\ k_1+\cdots+k_p=j}}\frac{2^{p-1}}{p!\Delta^{p-1}}\sum_{\substack{X_1,\ldots,X_p:\\ B-\text{c.s.}\\ B_{X_1}\cup\cdots B_{X_p}\ni 0}}\|Q^{01}_{k_pB_{X_p}}\|\,e^{r_{j-1}\mathrm{s}(B_{X_p})}\cdots\|Q^{01}_{k_1B_{X_1}}\|\,e^{r_{j-1}\mathrm{s}(B_{X_1})}\\ &+\sum_{\substack{p\ge 1,\,(k_1,\ldots,k_p):\\ 1\le k_1,\cdots,k_p\\ k_1+\cdots+k_p=j-1}}\frac{2^{p}}{p!\Delta^{p}}\sum_{\substack{X,X_1,\ldots,X_p:\\ B-\text{c.s.}\\ B_X\cup B_{X_1}\cup\cdots B_{X_p}\ni 0}}\|Q^{01}_{k_pB_{X_p}}\|\,e^{r_{j-1}\mathrm{s}(B_{X_p})}\cdots\|Q_{B_X}\|\,e^{r_{j-1}\mathrm{s}(B_X)}\end{aligned}$$

$$(4.151)$$

In the first sum on the RHS of (4.151) we have terms of the form

$$\sum_{\substack{X_1,\ldots,X_p: \\ B-\text{c.s.} \\ B_{X_1}\cup\cdots B_{X_p}\ni 0}} \|Q^{01}_{k_p B_{X_p}}\| \, e^{r_{j-1}\mathrm{s}(B_{X_p})} \cdots \|Q^{01}_{k_1 B_{X_1}}\| \, e^{r_{j-1}\mathrm{s}(B_{X_1})} \;, \tag{4.152}$$

which may be estimated following the lines of the proof of Lemma 4.1. The result is

$$(4.152) \;\leq\; p! \, \frac{\left(e^{-(r_{j-2}-r_{j-1})}\right)^{p-1}}{(r_{j-2}-r_{j-1})^p} \, \|Q_{k_p}\|_{r_{j-2}} \cdots \|Q_{k_1}\|_{r_{j-2}} \;. \tag{4.153}$$

A similar result holds for each term in the second sum on the RHS of (4.151) and we finally obtain

$$\begin{aligned} \|Q_j\|_{r_{j-1}} \;\; \leq & \sum_{\substack{p\geq 2\,,\,(k_1,\ldots,k_p): \\ 1\leq k_1,\cdots,k_p \\ k_1+\cdots+k_p=j}} \frac{2^p}{\Delta^{p-1}} \, \frac{\left(e^{-(r_{j-2}-r_{j-1})}\right)^{p-1}}{(r_{j-2}-r_{j-1})^p} \, \|Q_{k_p}\|_{r_{j-2}} \cdots \|Q_{k_1}\|_{r_{j-2}} \\ & + \sum_{\substack{p\geq 1\,,\,(k_1,\ldots,k_p): \\ 1\leq k_1,\cdots,k_p \\ k_1+\cdots+k_p=j-1}} \frac{(p+1)\,2^p}{\Delta^p} \, \frac{\left(e^{-(r_{j-2}-r_{j-1})}\right)^{p}}{(r_{j-2}-r_{j-1})^{p+1}} \, \|Q_{k_p}\|_{r_{j-2}} \cdots \|Q_{k_1}\|_{r_{j-2}} \;. \end{aligned} \tag{4.154}$$

By the inductive hypothesis, $\|Q_l\|_{r_{j-2}} < \|Q_l\|_{r_{l-1}} < \infty$, for $1 \leq l \leq j-1$. Hence, it follows from (4.154) that

$$\|Q_j\|_{r_{j-1}} < \infty \;. \tag{4.155}$$

This concludes the proof of (II).

We remark that by Corollary 4.4 we have that

$$\|\Phi^{(n)}\|_{r_n} \;\leq\; \sum_{k\geq 0} \frac{k+1}{r_{n-1}-r_n} \left(\frac{2e^{-(r_{n-1}-r_n)}}{r_{n-1}-r_n} \sum_{j=1}^{n} t^j \, \|\mathcal{S}_j\|_{r_{n-1}} \right)^k \|\Phi\|_{r_{n-1}}, \tag{4.156}$$

for any $r_n > r_{n-1}$, for the choice (4.116) of transformations, and

$$\|\Phi^{(n)}\|_{r_n} \;\leq\; \prod_{j=1}^{n} \left(\sum_{n_j\geq 0} \frac{n_j+1}{r_{j-1}-r_j} \left(\frac{2e^{-(r_{j-1}-r_j)}}{r_{j-1}-r_j} \, \|t^j \mathcal{S}_j\|_{r_{j-1}} \right)^{n_j} \right) \, \|\Phi\|_{r_0} \tag{4.157}$$

for the choice (4.117). Hence, it is enough to choose $t_0 = t_0(n)$ so that

$$\frac{2e^{-(r_{n-1}-r_n)}}{r_{n-1}-r_n} \sum_{j=1}^{n} t_0^j \, \|\mathcal{S}_j\|_{r_{n-1}} \;=\; 1 \tag{4.158}$$

or

$$\max_{1\le j\le n} \frac{2e^{-(r_{j-1}-r_j)}}{r_{j-1}-r_j} \|t_0^j \mathcal{S}_j\|_{r_{j-1}} \;=\; 1\;. \tag{4.159}$$

Note that from (4.147) and (4.161) below

$$\|\mathcal{S}_j\|_{r_{j-1}} \;\le\; \mathrm{O}\left(\frac{1}{\Delta^{j-1}}\right)\;. \tag{4.160}$$

Finally we turn to the proof of property (e). We again apply steps (i)–(iv) above to (4.143) but for unrestricted j. We obtain a formula similar to (4.151), but with $Q_j^{(n)}$ instead of Q_j on the LHS and the constraint $k_1,\ldots,k_p \le n$ in both the sums on the RHS. With such an expression we can immediately show, by induction, that

$$\|\Phi_j^{(n)}\|_{r_n} \;\le\; \mathrm{O}\left(\frac{1}{\Delta^{j-1}}\right)\;. \tag{4.161}$$

This bound, alongwith property (d), implies the property (e). ∎

4.7 Diagonalization with respect to a low-lying band

In order to obtain better convergence properties of the diagonalization procedure one may wish, in the same spirit as in Section 3, to define $P^0_{B_X}$ not as a projection operator onto the groundstates of the restriction of H_0 to B_X but on some band of low-energy states of the restriction of H_0 to B_X. However, by doing so, one loses Lemma 4.6 which permits one to define the unitary transformations as exponentials of sums of local operators. A way to circumvent this problem is the following one.

We define a projection operator $P_Y^{\rm low}$ on a subspace $\mathcal{H}_Y^{\rm low}$ of $\mathcal{H}_Y$ which corresponds to the set of configurations $\Omega^{\rm low}$

$$\Omega^{\rm low} \;=\; \{\omega_Y : 0 \le \Phi_{0X}(\omega_Y) \le D\} \tag{4.162}$$

$$\mathcal{H}_Y^{\rm low} \;=\; \{\psi \in \mathcal{H}_Y : \psi = \sum_{\omega_Y \in \Omega_Y^{\rm low}} c_{\omega_Y} e_{\omega_Y}\} \tag{4.163}$$

and we assume that the energies of the configurations in $\Omega^{\rm low}$ are separated from the energies of the other configurations by a gap Δ

$$\min_{X:\Phi_X^0\neq 0} \; \min_{\substack{\omega_X^h \notin \Omega^{\rm low} \\ \omega_X^l \in \Omega^{\rm low}}} \left(\Phi_X^0(\omega_X^h) \;-\; \Phi_X^0(\omega_X^l)\right) \ge \Delta \tag{4.164}$$

We split the interaction Φ_0 into $\widetilde{\Phi}_0 + \delta\Phi_0$ by assigning to each configuration belonging to $\Omega^{\rm low}$ the same energy 0, i.e.,

$$\widetilde{\Phi}_{0X} \;:=\; \left(\mathbf{1}_X - P_X^{\rm low}\right)\Phi_{0X}\left(\mathbf{1}_X - P_X^{\rm low}\right) \tag{4.165}$$

$$\delta\Phi_{0X} \;:=\; P_X^{\rm low}\Phi_{0X}P_X^{\rm low} \tag{4.166}$$

Now we may apply our diagonalization procedure to the interaction

$$\widetilde{\Phi}_0 + (\delta\Phi_0 + tQ) \tag{4.167}$$

by using projection operators $\widetilde{P}^0_{B_X} \left(= P^{\mathrm{low}}_{B_X}\right)$, $\widetilde{P}^1_{B_X}$ and $\widetilde{P}^2_{B_X}$ and treating $\delta\Phi_0$ as a part of the perturbation.

This procedure makes sense if we assume that D/Δ is small enough such that the unitarily transformed interaction is exponentially decaying.

5 Phase diagrams at low-temperatures

5.1 The Peierls condition

We now turn to a quick review of phase-diagram technology. For the rest of this section, our interactions will be of the form

$$\Phi = \Phi^{\mathrm{cl}} + Q\ , \tag{5.1}$$

where Φ^{cl} is a classical finite-range interaction, i.e., there is a tensor product basis such that $\Phi^{\mathrm{cl}}_X \in \mathcal{C}(\mathcal{E}_X)$, for all X, and the interaction Q is an exponentially decaying "quantum" perturbation, i.e., $Q \in \mathcal{B}_r$ for some r.

The results of [10] require the validity of the *Peierls condition* for the *classical part* Φ^{cl}. In order to state it, we introduce the notion of *contours*. Let $\Omega^0_{\mathrm{per}} := \{\omega^0_i\}_{i=1}^k$ be the set of periodic groundstate configurations of Φ^{cl}, i.e., the set of periodic configurations for which $\Phi^{\mathrm{cl}}_X(\omega^0_i) = 0$, $X \subset \Lambda$ [see eqn.(4.70)]. We define *sampling plaquettes* $W(x)$ as

$$W(x) := \{y \in \Lambda : \mid x_i - y_i \mid \leq a \text{ for } 1 \leq i \leq \nu\}\ . \tag{5.2}$$

The constant a is chosen to be larger than the range of Φ^{cl} and the period of each of its periodic groundstate configurations. A contour is constructed out of sampling plaquettes on which the configuration does not coincide with any of the groundstate configurations of Φ^{cl}. The *defect set* $\partial\omega$ of a configuration $\omega \in \Omega_\Lambda$ is defined as

$$\partial\omega = \bigcup_{x\in\Lambda} \{W(x) : \omega_{W(x)} \neq (\omega^0_i)_{W(x)} \text{ for all } 1 \leq i \leq k\}\ . \tag{5.3}$$

A *contour* of a configuration ω is a pair $\gamma = (M, \omega_M)$, where M is a maximally connected (with respect to intersections) component of the defect set $\partial\omega$. The set M is the support of γ. Two contours γ, γ' are *disjoint* if no pair of sampling plaquettes, $W(x) \subset M$, $W(x') \subset M'$, intersect. Due to our choice of the size of the sampling plaquettes, we can set up a one-to-one correspondence between configurations and families of contours by associating to each configuration of the lattice the corresponding set of disjoint contours, with the restriction that the interiors and exteriors of nested contours match. The families of contours corresponding to a configuration are said to be *compatible*. The energy of a configuration is then expressible in terms of its contours. Each contour γ has a unique configuration ω^γ that has it as its only contour. The configuration in any connected component of the set $\Lambda \setminus M$ coincides with one of the groundstates. If the energy of the groundstates is normalized to zero then the energy of the configuration ω^γ is given by

$$\begin{aligned} H^{\rm cl}(\omega^\gamma) &= \sum_Y \frac{|Y \cap M|}{|Y|}\, \Phi^{\rm cl}_Y(\omega^\gamma) \\ &:= E(\gamma)\ . \end{aligned} \tag{5.4}$$

We can interpret $E(\gamma)$ as the energy of the contour γ. If a configuration ω corresponds to a family of *compatible* contours $\{\gamma_1, \ldots, \gamma_n\}$, then its energy is given by the sum of the energies of its contours, i.e.,

$$H^{\rm cl}(\omega) = \sum_{i=1}^{n} E(\gamma_i)\ . \tag{5.5}$$

This allows us to rewrite the partition function $Z(\Lambda)$ for $H^{\rm cl}$ as a sum over an ensemble of pairwise disjoint contours and use cluster expansion methods to find its low-temperature behaviour.

The *Peierls condition* demands that the energy of a contour be proportional to the total number of sampling plaquettes in the contour. More precisely, it requires that there exist a positive constant $\kappa > 0$ —the *Peierls constant*—, such that the energy $E(\gamma)$, of a contour γ, satisfies

$$E(\gamma) > \kappa\, {\rm s}(\gamma)\ , \tag{5.6}$$

where ${\rm s}(\gamma)$ coincides with the cardinality of the support of γ. (Strictly speaking, this is the Peierls condition at the point of maximal coexistence of a phase diagram. For other points, the Peierls condition must be stated with respect to a set of reference configurations, not all of which need to be groundstates. Formulas (5.4) and (5.5) then acquire other terms balancing the different energy densities of the reference configurations. Nevertheless, this more general Peierls condition follows if the parametrization of the interaction is smooth.)

5.2 Stability of phase diagrams

In this section we summarize the results on the stability of phase diagrams obtained in [10], and some (minor) extensions that will be necessary. We consider a classical part $\Phi^{\rm cl}_{\underline{\mu}} = \{\Phi^{\rm cl}_{\underline{\mu}X}\}$ parametrized by a finite family $\underline{\mu}$ of parameters with values in a certain (small) set $\mathcal{O}_\infty \in I\!R^{p-1}$. These parameters label the "coordinate axes" of the zero-temperature ($\beta = \infty$) classical phase diagram. The assumptions on $\Phi^{\rm cl}_{\underline{\mu}}$ are:

(i) The range of $\Phi^{\rm cl}_{\underline{\mu}}$ is some finite number R throughout the region $\mathcal{O}_\infty$, and its zero-temperature phase diagram involves a *finite degeneracy*. That is, the different periodic groundstates found in the region $\mathcal{O}_\infty$ constitute a finite family $\Omega^{\rm ref} = \{\sigma_1, \ldots, \sigma_p\}$. In the present situation, a periodic configuration σ is a groundstate for $\Phi^{\rm cl}_{\underline{\mu}X}$ if

$$e_{\underline{\mu}}(\sigma) \;=\; \min_{\tilde\sigma \text{ periodic}} e_{\underline{\mu}}(\tilde\sigma) \;, \tag{5.7}$$

where

$$e_{\underline{\mu}}(\sigma) \;:=\; \lim_{\Lambda \nearrow \mathbb{Z}^d} \frac{1}{|\Lambda|} \sum_{X\cap\Lambda\neq\emptyset} \Phi^{\rm cl}_{\underline{\mu}X}(\sigma) \;. \tag{5.8}$$

The symbol $|\Lambda|$ denotes the cardinality of the set Λ, and the limit is taken, for instance, via sequences of growing parallelepipeds.

(ii) The zero-temperature phase diagram is *regular*. Regularity means that the Gibbs phase rule is satisfied: There is exactly one point $\underline{\mu}_\infty \in \mathcal{O}_\infty$ where the p configurations of $\Omega^{\rm ref}$ are all the periodic groundstates of $\Phi^{\rm cl}_{\underline{\mu}_\infty}$, $p-1$ lines radiating from $\underline{\mu}_\infty$ where there are $p-1$ groundstates, given by the different $(p-1)$-subsets of $\Omega^{\rm ref}$, and so on.

(iii) The parametrization is smooth, in the sense that the maps $\mathcal{O}_\infty \ni \underline{\mu} \mapsto \Phi^{\rm cl}_{\underline{\mu}X}$ are differentiable. Furthermore, these maps and their derivatives are uniformly bounded. Often, the $\underline{\mu}$-dependence is linear, hence these conditions are automatically satisfied for bounded regions of the phase diagram. In addition, we need to assume that the determinant of the matrix of derivatives

$$\left(\frac{\partial}{\partial\mu_j}(e(\sigma_i) - e(\sigma_p))\right)_{1\le i,j\le p-1} \tag{5.9}$$

is uniformly bounded away from zero throughout $\mathcal{O}_\infty$. Models in which the degeneracy-breaking effects of the parameters $\underline{\mu}$ are due to orders higher than linear, present additional difficulties. In particular, these models fall outside the scope of the theory presented in [2, Section 6] from which our theory derives.

(iv) The interaction $\Phi^{\rm cl}_{\underline{\mu}_\infty}$ — where $\underline{\mu}_\infty$ is the point of maximal coexistence of the zero-temperature phase diagram— satisfies the Peierls condition, with some Peierls constant $\kappa > 0$.

By the continuity required in (iii), condition (iv) implies the validity of the Peierls condition [in the generalized sense mentioned parenthetically after (5.6)] for a neighbourhood of $\underline{\mu}_\infty$, with a slightly smaller Peierls constant.

In addition, we consider a quantum perturbation $Q_{\underline{\mu}}(\lambda)$ defined by operators $Q_{\underline{\mu}X}(\lambda) \in \mathcal{A}_X$ such that

(v) The maps $\mathcal{O}_\infty \ni \underline{\mu} \mapsto Q_{\underline{\mu}X}$ have the same smoothness properties of $\underline{\mu} \mapsto \Phi^{\rm cl}_{\underline{\mu}X}$ [assumption (iii) above];

(vi)

$$\sup_{\underline{\mu}\in\mathcal{O}_\infty} \left\{ \|Q_{\underline{\mu}X}\| + \sum_{i=1}^{p-1} \Big\| \frac{\partial}{\partial \mu_i} Q_{\underline{\mu}X} \Big\| \;\le\; \varepsilon\, |\lambda|^{{\rm s}(X)} \right\} , \tag{5.10}$$

with $\varepsilon > 0$, uniformly on $\mathcal{O}_\infty$. Usually, $\mathcal{O}_\infty$ is a bounded set, hence by continuity it is enough to check (5.10) at the maximal-coexistence point $\underline{\mu}_\infty$.

The basic result of [10, 3] can be stated as follows.

Theorem 5.1 (Quantum Pirogov-Sinai theory) *Consider interactions of the form $\Phi_{\underline{\mu}} = \Phi^{\rm cl}_{\underline{\mu}} + Q_{\underline{\mu}}$ satisfying hypotheses (i)–(vi) above. Then there exist constants $\overline{\kappa} = {\rm O}(\kappa)$ and ϵ_0, such that in the region*

$$\max\Big(e^{-\beta\overline{\kappa}} \,,\, \frac{\varepsilon\lambda}{\kappa}\Big) \;<\; \epsilon_0 \;, \tag{5.11}$$

there exists a non-empty open set $\mathcal{O}_{\beta\lambda} \in I\!R^{P-1}$ where the phase diagram is regular and is a smooth deformation of the zero-temperature phase diagram of $\Phi^{\rm cl}_{\underline{\mu}}$ in $\mathcal{O}$. In fact, if $\underline{\mu}_{\beta\lambda}$ are the coordinates of the maximal-coexistence point of the $\mathcal{O}_{\beta\lambda}$-diagram,

$$|\underline{\mu}_\infty - \underline{\mu}_{\beta\lambda}| \;=\; {\rm O}(\epsilon_{\beta\lambda}) \;, \tag{5.12}$$

with $\epsilon_{\beta\lambda}$ defined by the LHS of (5.11).

We point out that our definition of a phase diagram is based on the notion of *stable* phases adopted in [10]. A stable phase is a phase minimizing a certain truncated free energy (see Section 7.2 of [10]). It has the properties one would expect: Its truncated free energy coincides with the free energy of the system and its quantum expectations are analytic functions of the parameters and converge to the groundstate expectations when the temperature goes to zero (see Theorem 2.2 of [10]).

This theorem is proven by using a contour expansion in $\nu + 1$ dimensions obtained by iterating the Duhamel formula. The resulting contours [10] are piecewise-cylindrical surfaces in $\Lambda \times [0,\beta]$, where Λ is a finite subset of the lattice $\mathbb{Z}^\nu$. We refer to $[0,\beta]$ as the "time" axis. These contours are periodic in the "time"-direction and their ν-dimensional sections are the "classical" contours described in Section 5.1. The two terms on the LHS of (5.11) arise from two different types of contours. The factor $e^{-\beta\overline{\kappa}}$ is the leading order contribution of the "long contours" which extend from 0 to β and hence carry the thermal effects. The factor $\varepsilon\lambda/\kappa$ arises from the "short" contours, whose length in the "time"-direction is strictly less than β. Hence, this term can be interpreted as the leading order contribution of the quantum fluctuations.

By resorting to a finer classification of different types of quantum contours, one can obtain more detailed bounds tailored to particular models. We present one of these refinements needed in this paper.

We consider systems involving two levels of (local) excitations. The formal definition of such systems requires two ingredients:

- A family of reference configurations (which are groundstates at the point of maximal coexistence) $\Omega^{\rm ref} = \{\sigma_1, \ldots, \sigma_p\}$.
- A family of projection operators [“projections on low-lying (local) excitations”] $\{P^0_Y : Y \subset \mathbb{Z}^\nu \text{ finite }\}$, such that all the reference configurations σ_i belong to the range of each P^0_Y.

A plaquette $W(x)$ belongs to a *low-energy defect* of a configuration ω if

$$P^0_{W(x)}\omega = \omega \ , \ \text{but } \omega_{W(x)} \neq (\sigma_i)_{W(x)} \text{ for all } 1 \le i \le p \, . \tag{5.13}$$

A plaquette $W(x)$ belongs to a *high-energy defect* of a configuration ω if

$$P^0_{W(x)}\omega = 0 \tag{5.14}$$

(i.e., ω describes an excitation outside the range of $P^0_{W(x)}$). We then consider contours (=connected components of the defect set) as in Section 5.1, and for each contour γ we single out the set

$$\gamma^{\rm high} \ := \ \{\text{high-energy defects in } \gamma\} \, . \tag{5.15}$$

A two-level Peierls condition is a bound of the form

$$E(\gamma) \ > \ \kappa \, {\rm s}(\gamma) + D \, {\rm s}(\gamma^{\rm high}) \, . \tag{5.16}$$

To determine the range of applicability of a generalized form of the Pirogov-Sinai theory, we have to analyze the size of the matrix elements of interactions between configurations corresponding to low- and high- energy defects. Given an interaction $\Phi = \{\Phi_X\}$, let $\Phi^{\ell\ell}$, $\Phi^{\ell{\rm h}}$, $\Phi^{{\rm h}\ell}$ and $\Phi^{\rm hh}$ be the pieces defined by

$$\Phi^{\ell\ell}_X \ := \ P^0_X \, \Phi_X \, P^0_X \tag{5.17}$$

$$\Phi^{\ell{\rm h}}_X \ := \ (\mathbf{1}_X - P^0_X) \, \Phi_X \, P^0_X \tag{5.18}$$

$$\Phi^{{\rm h}\ell}_X \ := \ P^0_X \, \Phi_X \, (\mathbf{1}_X - P^0_X) \tag{5.19}$$

$$\Phi^{\rm hh}_X \ := \ (\mathbf{1}_X - P^0_X) \, \Phi_X \, (\mathbf{1}_X - P^0_X) \, . \tag{5.20}$$

These interaction pieces give rise to “low$\to$low” ($\ell\ell$), “low$\to$high” (ℓh), “high$\to$low” (hℓ) and “high$\to$high” (hh) transitions.

Theorem 5.2 *:*
[Quantum Pirogov-Sinai theory for systems with two levels of excitations]

Consider interactions of the form $\Phi_{\underline{\mu}} = \Phi^{\rm cl}_{\underline{\mu}} + Q_{\underline{\mu}}$*, and a family of local projections* $\{P^0_Y\}$*, such that*

(a) *The interaction $\Phi^{\rm cl}_{\underline{\mu}}$ satisfies hypotheses (i)–(iii) above, and condition (5.16) at the point of maximal coexistence, for some $\kappa > 0$, $D \geq 0$.*

(b) *The different pieces $Q^{\ell\ell}$, $Q^{\rm hh}$, $Q^{\ell \rm h}$ and $Q^{\rm h\ell}$, of the quantum perturbation Q satisfy hypotheses (v) and (vi) above, in particular*

$$\sup_{\underline{\mu}\in\mathcal{O}_\infty} \left\{ \|Q^{\alpha\delta}_{\underline{\mu}X}\| + \sum_{i=1}^{p-1} \left\| \frac{\partial}{\partial \mu_i} Q^{\alpha\delta}_{\underline{\mu}X} \right\| \;\leq\; \varepsilon_{\alpha\delta}\, \lambda^{{\rm s}(X)} \right\} , \tag{5.21}$$

for some $\lambda < 1$ and constants $\varepsilon_{\alpha\delta}$, for each $\alpha, \delta \in \{\ell\, \rm h\}$.

Then there exist constants $\overline{\kappa} = {\rm O}(\kappa)$ and ϵ_0 such that, in the region

$$\max\left(e^{-\beta\overline{\kappa}} , \frac{\varepsilon_{\ell\ell}\lambda}{\kappa} , \lambda\sqrt{\frac{\varepsilon_{\ell\rm h}\varepsilon_{\rm h\ell}}{\kappa(\kappa+D)}} , \frac{\varepsilon_{\rm hh}\lambda}{\kappa+D} , \frac{\varepsilon_{\rm h\ell}\lambda}{\kappa+D} , \frac{\varepsilon_{\ell\rm h}\lambda}{\kappa+D} \right) \;<\; \epsilon_0, \tag{5.22}$$

there exists a non-empty open set $\mathcal{O}_{\beta\lambda} \in I\!R^{P-1}$ where the phase diagram is regular and is a smooth deformation of the zero-temperature phase diagram of $\Phi^{\rm cl}_{\underline{\mu}}$ in $\mathcal{O}$. If $\underline{\mu}_{\beta\lambda}$ are the coordinates of the maximal-coexistence point of the $\mathcal{O}_{\beta\lambda}$-diagram,

$$|\underline{\mu}_\infty - \underline{\mu}_{\beta\lambda}| \;=\; {\rm O}(\epsilon_{\beta\lambda})\;. \tag{5.23}$$

where $\epsilon_{\beta\lambda}$ is defined by the LHS of (5.22).

Remarks:

(i) Of course, the zero-temperature phase diagram of $\Phi^{\rm cl}_{\underline{\mu}}$ involves only $\left(\Phi^{\ell\ell}_{\underline{\mu}}\right)^{\rm cl}$.

(ii) Usually, only the first three arguments in the LHS of (5.22) need to be looked at. In most cases their smallness implies that of the remaining two arguments.

This theorem is proven adapting the methods of [10]. The argument is sketched in Appendix A.

5.3 Pirogov-Sinai theory for transformed interactions

At low-temperatures, the Pirogov-Sinai theory summarized in the Section 5.2 yields precise information on the phase diagram. In particular, in the limit as $\beta \to \infty$, it gives a description of the groundstates of the full Hamiltonian. In this sense, it yields more information, and in a less cumbersome way, than standard diagonalization processes. With the help of the partial block-diagonalization procedure of Section 4 we can now investigate the following phenomenon: Suppose that the classical part of the interaction has infinitely degenerate groundstates but that the perturbation lifts this degeneracy and restores the Peierls condition. Then, using Theorem 5.2, we conclude that the long-range order characterizing the new groundstates survives at low-temperatures.

We consider interactions of the form $\Phi(t) = \Phi_0 + tQ$ where Φ_0 satisfies Condition (**P1**) of Section 4.4. In this section, we consider *finite-range* perturbations Q, but the discussion may easily be generalized to exponentially decaying interactions.

If the degeneracy of the groundstate of Φ_0 is lifted in order m in t, with $m = 2n$ or $2n+1$, then we consider the family of unitary transformations $U^{(n)}(t)$ defined in Section 4.6. This yields an equivalent interaction $\Phi^{(n)}(t) \in \mathcal{B}_{r_n}$ which we write as

$$\Phi^{(n)}(t) \;=\; \Phi_0 \;+\; \sum_{j\geq 1} t^j \Phi_j^{(n)} \;. \tag{5.24}$$

By inspection of the proof of Theorem 4.7, one easily sees that a finite-range perturbation Q implies that $\Phi_j^{(n)}$, for all $j \geq 1$, have finite range. In fact, for $1 \leq j \leq n$, the range of $\Phi_j^{(n)}$ is bounded by cjR, where R is the range of Q and c is a constant which depends on Φ_0. In the proof of Theorem 4.7 we have shown that $\Phi_j^{(n)}$ is of the form $\Phi_j^{(n)} = \{\Phi_{jB_X}^{(n)}\}$, for all $j \geq 1$. Thus, using the partition of unity $\mathbf{1}_{B_X} = P_{B_X}^0 + P_{B_X}^1 + P_{B_X}^2$ we may split the interaction as follows:

$$\Phi_{jB_X}^{(n)} \;=\; \Phi_{jB_X}^{(n)00} + \Phi_{jB_X}^{(n)01} + \Phi_{jB_X}^{(n)R} \;, \tag{5.25}$$

(see (4.93), (4.94) and (4.95)). We denote

$$\Phi_j^{(n)00} = \{\Phi_{jB_X}^{(n)00}\} \;, \tag{5.26}$$

and similarly $\Phi_j^{(n)01}$ and $\Phi_j^{(n)R}$.
By Theorem 4.7 we have that

$$\Phi_j^{(n)01} \;=\; 0, \;\text{ for }\; j \leq n = [m/2] \;, \tag{5.27}$$

where $[a]$ denotes the integer part of a. We now split $\Phi^{(n)}(t)$ into a new "classical" part and a new perturbation:

$$\Phi^{(n)}(t) \;:=\; \Phi_0^m(t) + Q^m(t) \;, \tag{5.28}$$

where

$$\Phi_0^m(t) \;:=\; \Phi_0 + \sum_{j=1}^{m} t^j \Phi_j^{(n)00} \tag{5.29}$$

is assumed to be a finite-range classical interaction, and

$$\begin{aligned} Q^m(t) \;&:=\; \sum_{j\geq m+1} t^j \Phi_j^{(n)00} + \sum_{j\geq [m/2]+1} t^j \Phi_j^{(n)01} + \sum_{j\geq 1} t^j \Phi_j^{(n)R} \\ &:=\; Q^{m00}(t) + Q^{m01}(t) + Q^{mR}(t). \end{aligned} \tag{5.30}$$

To make the connection with Pirogov-Sinai theory we define

$$Q^{m,\ell\ell}(t) \;:=\; Q^{m00}(t)\;, \tag{5.31}$$
$$Q^{m,\mathrm{hh}}(t) \;:=\; Q^{mR}(t)\;, \tag{5.32}$$

and

$$Q^{m,\ell\mathrm{h}}(t) + Q^{m,\mathrm{h}\ell}(t) := Q^{m01}(t)\;, \tag{5.33}$$

where $Q^{m,\ell\mathrm{h}}(t)$ contains all the terms of the form $P^0_{B_X}\Phi^{(n)}_{jB_X}P^1_{B_X}$ and $Q^{m,\mathrm{h}\ell}(t)$ all the terms of the form $P^1_{B_X}\Phi^{(n)}_{jB_X}P^0_{B_X}$.

This decomposition, combined with Theorem 4.7, leads to the following estimates:

1.
$$\|Q^{m,\ell\ell}(t)\|_{r_n} \;=\; \mathrm{O}(t^{m+1}/\Delta^m) \tag{5.34}$$

2.
$$\|Q^{m,\mathrm{hh}}(t)\|_{r_n} \;=\; \mathrm{O}(t) \tag{5.35}$$

3.
$$\|Q^{m,\ell\mathrm{h}}(t)\|_{r_n} \;=\; \mathrm{O}(t^{[m/2]+1}/\Delta^{[m/2]}) \;=\; \mathrm{O}(t^{n+1}/\Delta^n) \tag{5.36}$$
$$\|Q^{m,\mathrm{h}\ell}(t)\|_{r_n} \;=\; \mathrm{O}(t^{[m/2]+1}/\Delta^{[m/2]}) \;=\; \mathrm{O}(t^{n+1}/\Delta^n). \tag{5.37}$$

In this situation, the parameters required in Theorem 5.2 are given by

$$\lambda \;=\; \mathrm{O}(t) \tag{5.38}$$
$$\varepsilon_{\ell\ell} \;=\; \mathrm{O}(t^m) \tag{5.39}$$
$$\varepsilon_{\ell\mathrm{h}} \;=\; \mathrm{O}(t^{[m/2]}) \tag{5.40}$$
$$\varepsilon_{\mathrm{h}\ell} \;=\; \mathrm{O}(t^{[m/2]}) \tag{5.41}$$
$$\varepsilon_{\mathrm{hh}} \;=\; \mathrm{O}(1)\;. \tag{5.42}$$

In order to apply the contour expansion methods of Section 5.2, we have to further assume that $\Phi^m_0(t)$ can be written as a classical interaction satisfying Conditions (i), (ii) and (iii) of Section 5.2 and the generalized Peierls condition (5.17). This means that we assume the existence of a *tensor-product basis*, in which $\Phi^m_{0X}(t)$ is diagonal, for all X. This is not generally true: the interaction $\Phi^m_0(t)$ is *block-diagonal* in the tensor-product basis in which Φ_0 is diagonal, but it need not be a classical interaction. However, in many interesting models (see Section 6 and [11]) $\Phi^m_0(t)$ actually turns out to be a classical interaction. If, in addition, $\Phi^m_0(t)$ is an m-potential with a finite number of periodic groundstates, the Peierls condition follows. The spectrum of the finite-volume Hamiltonians $H^m_0(t)$ corresponding to the interaction $\Phi^m_0(t)$ then have the following stucture: there is a gap of order t^m between the groundstate of $H^m_0(t)$ and the low-energy excited states (i.e., states describing excitations in some subset X of the lattice that are in the range of P_X^1) and there is another gap of order 1, inherited from the gap of H_0, between the groundstate of $H_0^m(t)$ and states describing (local) excitations in X which are not in the range of P_X^0. In (5.16), the Peierls constant κ is of order t^m, and the constant D is of order 1:

$$\begin{aligned} \kappa &= \mathrm{O}(t^m) && (5.43)\\ D &= \mathrm{O}(1). && (5.44) \end{aligned}$$

In order to apply the full Pirogov-Sinai theory, one has to further check Condition (ii) (smoothness of the parametrization) and (iii) (Gibbs phase rule). Theorem 5.2 then describes the first-order phase transitions at low-temperatures when the parameters are varied. The reader may check that all the parameters in formula (5.22) of Theorem 5.2 scale properly as t goes to zero.

There are models for which the Peierls condition is valid but their zero-temperature phase diagrams do not satisfy the Gibbs phase rule. However, even for such a model, there may be regions in its phase diagram where we can apply a low-temperature expansion, in terms of compatible families of space-time contours [10], to study the stability of the corresponding phases. This can be done whenever the groundstates are related in a way such that the removal of any contour of a compatible family leads to another compatible family of contours. Usually, this property is a consequence of some symmetry relating the different groundstates. To abbreviate, let us refer to those values of the parameters for which this contour-removal property holds as the *symmetric-phase regime*. In particular, this includes regions for which there is a single groundstate (single-phase regime). For these regions we can use the low-temperature expansion method of [10, Section 6] to prove that the periodic groundstates "survive" at low-temperatures, i.e., give rise to stable phases. In fact, the low-temperature expansion for these symmetric-phase regimes is one of the main steps in the proof of Theorem 5.2 in [10] (see Sections 6 and 7 in this reference and Appendix A below).

To summarize, the block-diagonalization procedure of Section 4, combined with Theorem 5.2, yields the following result.

Corollary 5.3 *(i) If, for some fixed value of the parameters, the interaction $\Phi_0^m(t)$ is in the single-phase or symmetric-phase regime and satisfies the Peierls condition, then there exist $t_0 > 0$ and $\beta_0 = \beta_0(t)$ such that, for $0 < t < t_0$, the groundstates of $\Phi^{(n)}(t)$ (or of $\Phi(t)$) are small perturbations of the groundstates of $\Phi_0^m(t)$, and the long-range order of the groundstates persists for $\beta > \beta_0(t)$.*

(ii) If, for some open set in the parameter space, the interaction $\Phi_0^m(t)$ satisfies assumptions (i)–(iv) of Section 5.2 —i.e., it has a smooth parametrization with linear degeneracy-breaking, its zero-temperature phase diagram satisfies the Gibbs phase rule and involves only a finite degeneracy, and it satisfies the Peierls condition at the point of maximal coexistence— then there exist

$t_0 > 0$ and $\beta = \beta_0(t)$ such that, for $0 < t < t_0$ and $\beta > \beta_0(t)$, the phase diagram of $\Phi^{(n)}(t)$ is a smooth deformation of the phase diagram of $\Phi_0^m(t)$ at zero-temperature.

Next, we derive the explicit formulas for $\Phi_0^2(t)$ and $\Phi_0^4(t)$ which we will need in the examples. We denote by $H_0^m(t) := \sum_{X\subset\Lambda}\Phi_{0X}^m(t)$ the corresponding finite-volume Hamiltonians.

It is useful to recall the following notation: for finite subsets $X_1, \cdots X_n$ of $\mathbb{Z}^\nu$, $X_1, \cdots X_n$ $B-$c.s. stands for the constraint

$$X_2 \cap B_{X_1} \neq \emptyset\,, X_3 \cap B_{X_2\cup X_1} \neq \emptyset\,, \cdots, X_n \cap B_{X_{n-1}\cup\cdots\cup X_1} \neq \emptyset\,. \tag{5.45}$$

¿From (4.102) we obtain

$$H^{(1)}(t) = H_0 + tV^{00} + tV^R + t^2 \mathrm{ad}S_1\left(V^{00} + V^R + \frac{1}{2}V^{01}\right) + \mathrm{O}(t^3), \tag{5.46}$$

and hence

$$\begin{aligned} H_0^2(t) &= H_0 + tV^{00} + t^2\left(\mathrm{ad}S_1\left(V^{00}+V^R+\frac{1}{2}V^{01}\right)\right)^{00} \\ &= H_0 + tV^{00} + t^2\left(\mathrm{ad}S_1\left(\frac{1}{2}V^{01}\right)\right)^{00} \\ &= H_0 + t\sum_X V_{B_X}^{00} + t^2 \sum_{X_1,X_2 B-\mathrm{c.s.}}\left(\mathrm{ad}S_{1B_{X_2}}\left(\frac{1}{2}V_{B_{X_1}}^{01}\right)\right)^{00} \,. \end{aligned} \tag{5.47}$$

¿From the recursion relation (4.132) and from (5.46) we have that

$$\begin{aligned} S_2 &= \sum_{X_1,X_2 B-\mathrm{c.s.}} \mathrm{ad}^{-1}\overline{H}_{0X_1\cup X_2}\left(\left(\mathrm{ad}S_{1B_{X_2}}\left(Q_{B_{X_1}}^{00} + Q_{B_{X_1}}^R + \frac{1}{2}Q_{B_{X_1}}^{01}\right)\right)^{01}\right) \\ &:= \sum_{X_1,X_2 B-\mathrm{c.s.}} \mathrm{ad}^{-1}\overline{H}_{0X_1\cup X_2}\left(Q_{2B_{X_1\cup X_2}}^{01}\right)\,, \end{aligned} \tag{5.48}$$

and we obtain

$$\begin{aligned} H_0^4(t) &= H_0 + tV^{00} + t^2\left(\mathrm{ad}S_1\left(\frac{1}{2}V^{01}\right)\right)^{00} \\ &\quad + t^3\left(\mathrm{ad}^2S_1\left(\frac{1}{2!}V^{00} + \frac{1}{2!}V^R + \frac{2}{3!}V^{01}\right)\right)^{00} \\ &\quad + t^4\left(\mathrm{ad}^3S_1\left(\frac{1}{3!}V^{00} + \frac{1}{3!}V^R + \frac{3}{4!}V^{01}\right)\right)^{00} \\ &\quad + t^4\left(\mathrm{ad}S_2\left(V_2^{00} + V_2^R + \frac{1}{2}V_2^{01}\right)\right)^{00}\,, \end{aligned} \tag{5.49}$$

where

$$V_2 := \mathrm{ad}S_1\left(V^{00} + V^R + \frac{1}{2}V^{01}\right)\,. \tag{5.50}$$

The operator $H_0^4(t)$ may be written as a sum of local operators.

6 Examples: Quantum magnets

Consider a system of spin-$\frac{1}{2}$ fermions on a square lattice $\Lambda \subset \mathbb{Z}^2$ with a replusive interaction of strength U and an exchange interaction of strength J, between nearest neighbours. The system is described by the Hamiltonian

$$\begin{aligned} H(t) &= -t \sum_{\substack{<xy>\subset\Lambda \\ \sigma=\uparrow,\downarrow}} \{c^*_{x\sigma}c_{y\sigma} + c^*_{y\sigma}c_{x\sigma}\} + \frac{U}{2}\sum_{<xy>\subset\Lambda} n_x n_y \\ &+ \frac{J}{2}\sum_{<xy>\subset\Lambda} \sigma^{(3)}_x\sigma^{(3)}_y n_x n_y - \mu\sum_{x\subset\Lambda} n_x \ , \end{aligned} \tag{6.1}$$

where $c^*_{x\sigma}(c_{x\sigma})$ creates (annihilates) a fermion with spin σ at site x, and $n_x = \sum_{\sigma=\uparrow,\downarrow} c^*_{x\sigma}c_{x\sigma}$ is the particle number operator at site x; μ is the chemical potential and t the hopping amplitude. The sum $\langle xy\rangle$ is over a pair of nearest neighbour sites. In addition, we assume that there is an infinite on-site repulsion which forbids double occupancy. This assumption corresponds to restricting the Hilbert space of $H(t)$ to $\mathcal{H} = \bigotimes \mathbb{C}^3$. As a basis for $\mathbb{C}^3$ we choose $\{|\uparrow\rangle, |\downarrow\rangle, |\, e\rangle\}$, where e refers to an empty site.

We consider the strong coupling limit $U, J \gg t$ and treat the hopping term as a perturbation. Hence we write the Hamiltonian as

$$H(t) = H_0 + tV \ , \tag{6.2}$$

where

$$\begin{aligned} H_0 &= \frac{U}{2}\sum_{<xy>\subset\Lambda} n_x n_y + \frac{J}{2}\sum_{<xy>\subset\Lambda} \sigma^{(3)}_x\sigma^{(3)}_y n_x n_y \\ &\quad -\mu\sum_{x\subset\Lambda} n_x \ , \end{aligned} \tag{6.3}$$

and

$$V = -\sum_{\substack{<xy>\subset\Lambda \\ \sigma=\uparrow,\downarrow}} \{c^*_{x\sigma}c_{y\sigma} + c^*_{y\sigma}c_{x\sigma}\} := \sum_{X\subset\Lambda} Q_X \ . \tag{6.4}$$

In order to find the groundstates of the Hamiltonian H_0, we regroup the terms on the RHS of (6.3) so as to express H_0 in terms of an m-potential as follows:

$$H_0 = \sum_{M\subset\Lambda} \Phi_M, \tag{6.5}$$

where M is a set of four sites forming a unit square on the lattice and

$$\Phi_M = \sum_{<xy>\subset M} \frac{1}{4}\left[U n_x n_y + J\sigma^{(3)}_x\sigma^{(3)}_y n_x n_y\right] - \sum_{x\subset M}\frac{1}{4}\mu n_x \ . \tag{6.6}$$

The range r of the m-potential Φ_M, is one.

For $U > J > 0$ and $0 < \mu < 2(U-J)$ and for $U > -J > 0$ and $0 < \mu < 2(U+J)$, the configurations which minimize Φ_M, for all M, are those configurations in which two consecutive spins are separated by an empty site: they correspond to a half-filled lattice with a "checkerboard configuration". The groundstate energy density is given by

$$\frac{E_0}{|\Lambda|} = -\frac{\mu}{2}. \tag{6.7}$$

The corresponding groundstate of H_0 has a macroscopic degeneracy because the spins can have arbitrary orientation. The multiplicity of the groundstate is $2(2^{|\Lambda|/2})$ where $|\Lambda|$ is the number of sites in the lattice.

The support of each term of the perturbation V is a pair of nearest neighbour sites, $X = \langle xy \rangle$. We choose

$$B_X = W_x \cup W_y, \tag{6.8}$$

$$W_x = \{y \in \Lambda :| x_i - y_i | \leq 1 \text{ for } 1 \leq i \leq 2\}\ . \tag{6.9}$$

In this example the perturbation is decomposed as follows

$$Q_X \ = \ Q^{01}_{B_X} + Q^{R}_{B_X}\ , \tag{6.10}$$

where

$$Q^{01}_{B_X} \ = \ P^1_{B_X} Q_X P^0_{B_X} + P^0_{B_X} Q_X P^1_{B_X} \tag{6.11}$$

$$Q^{R}_{B_X} \ = \ P^2_{B_X} Q_X P^2_{B_X}. \tag{6.12}$$

The diagonal contributions $P^0_{B_X} Q_X P^0_{B_X}$ and $P^1_{B_X} Q_X P^1_{B_X}$ vanish.

Consider the transformed Hamiltonian

$$H^{(1)}(t) = U^{(1)}(t)\,[H_0 + tV]\,U^{(1)}(t)^{-1}. \tag{6.13}$$

We split $H^{(1)}(t)$ into $H^2_0(t)$ and $Q^2(t)$, as described at the end of Section 5.3. The Hamiltonian $Q^2(t)$ will be treated as the perturbation. In order to find the groundstates of $H^2_0(t)$, we have to diagonalize the operator

$$P_0 H^2_0(t) P_0, \tag{6.14}$$

where $P_0 = P^0_\Lambda$ and

$$H^2_0(t) \ = \ H_0 + \frac{t^2}{2}\sum_X P^0_{B_X}\,\mathrm{ad}S_{1B_X}\left(Q^{01}_{B_X}\right)P^0_{B_{X_1}}. \tag{6.15}$$

Let E_{1X} be the energy of the configuration resulting from the hopping of a single particle to a nearest neighbour site, and let

$$\epsilon_{1X} := E_{1X} - E_0. \tag{6.16}$$

The contribution to the groundstate energy *to order* t^2 is given by

$$\begin{aligned}
\sum_X \Delta_X &= P_0 \sum_X \{\mathrm{ad} S_{1B_X}(Q^{01}_{B_X})\} P_0 \\
&= P_0 \sum_X \Big[\mathrm{ad}^{-1}\overline{H}_{0X}(P^0_{B_X} Q_X P^1_{B_X}) Q_X P^0_{B_X} \\
&\quad - P^0_{B_X} Q_X \mathrm{ad}^{-1}\overline{H}_{0X}(P^1_{B_X} Q_X P^0_{B_X})\Big] P_0 \\
&= \sum_X -t^2 \frac{1}{\epsilon_{1X}} \,. \qquad (6.17)
\end{aligned}$$

The energy difference ϵ_{1X}, and hence Δ_X, takes different values depending on the alignment of the spins of the particles which are at distance one from the pair $X = \langle xy \rangle$, i.e., in B_X. In the figures below we list all the different cases (up to spin flip) and indicate the contribution Δ_X resulting from the hopping of the rightmost particle of the central nearest-neighbour bond to the hole to its left and back.

1. $\begin{array}{cccc} & + & \circ & \\ + & \circ & + & \circ \\ & + & \circ & \end{array} \qquad \Delta_X = -t^2 \frac{2}{3U+3J}$

2. $\begin{array}{cccc} & + & \circ & \\ + & \circ & - & \circ \\ & + & \circ & \end{array} \qquad \Delta_X = -t^2 \frac{2}{3U-3J}$

3. $\begin{array}{cccc} & + & \circ & \\ - & \circ & + & \circ \\ & + & \circ & \end{array} \qquad \Delta_X = -t^2 \frac{2}{3U+J}$

4. $\begin{array}{cccc} & + & \circ & \\ - & \circ & - & \circ \\ & + & \circ & \end{array} \qquad \Delta_X = -t^2 \frac{2}{3U-J}$

5. $\begin{array}{cccc} & + & \circ & \\ + & \circ & - & \circ \\ & - & \circ & \end{array} \qquad \Delta_X = -t^2 \frac{2}{3U-J}$

To determine the groundstates of $H_0^2(t)$ we consider a hole surrounded by four particles and add the contributions to the groundstate energy resulting from the hopping of the four particles to the hole and back. Summing over all the $|\Lambda|/2$ holes in the half-filled lattice gives the following results:

1. For the ferromagnetic case ($J < 0$), the four groundstates are *periodic*: a checkerboard configuration with all spins aligned. The energy density is

$$\frac{E}{|\Lambda|} = -\frac{\mu}{2} - t^2 \frac{4}{3U+3J} \,. \qquad (6.18)$$

The spectral gap between the groundstates and the first excited states (one spin misaligned) is given by

$$\Delta^f = -96t^2 \frac{J(3U-J)}{(3U+J)(3U+3J)(3U-3J)} \ . \tag{6.19}$$

2. For an antiferromagnetic coupling, $J > 0$, we have two cases:

   (a) For $U > \frac{5}{3}J$, the groundstates are such that around each hole the spins are oriented as shown in figure 4 or 5 above. In other words all spins are Néel ordered in one diagonal direction, but the spins can be flipped independently on each diagonal line. The energy density is

   $$\frac{E}{|\Lambda|} = -\frac{\mu}{2} - t^2 \frac{4}{3U-J} \ . \tag{6.20}$$

   The spectral gap is given by

   $$\Delta_1^{af} = 32t^2 \frac{J(3U-5J)}{(3U+J)(3U-J)(3U-3J)} \ . \tag{6.21}$$

   (b) For $U < \frac{5}{3}J$, the groundstates are such that around each hole the spins are oriented as shown in figure 2 or 3 above. The energy density is

   $$\frac{E}{|\Lambda|} = -\frac{\mu}{2} - t^2 \frac{4(3U-2J)}{(3U+J)(3U-3J)} \ . \tag{6.22}$$

   The spectral gap is

   $$\Delta_2^{af} = 32t^2 \frac{J(5J-3U)}{(3U+J)(3U-J)(3U-3J)} \ . \tag{6.23}$$

Thus we see that for $J > 0$ the groundstate of the Hamiltonian $H_0^2(t)$ has an infinite degeneracy. In order to arrive at a Hamiltonian which has a finite number of groundstates, we have to go to higher orders of our perturbation method. This is done below.

In order to verify the Peierls condition for the ferromagnetic coupling ($J < 0$), we rewrite $H_0^2(t)$ as a sum over four by four blocks, M, consisting of sixteen lattice sites.

$$H_0^2(t) = \sum_{M \subset \Lambda} \Phi_M, \tag{6.24}$$

Each nearest neighbour bond $X = \langle xy \rangle$ is contained in twelve such different blocks, while each B_X, defined by eqn.(6.8), is contained in two different blocks. Hence

$$\begin{aligned} \Phi_M \ = \ & \frac{1}{24} \sum_{<xy> \subset M} \{U n_x n_y + J\sigma_x^{(3)}\sigma_y^{(3)} n_x n_y\} - \frac{\mu}{16} \sum_{x \subset M} n_x \\ & + \frac{t^2}{4} \sum_{\substack{B_X \subset M \\ X = <xy>}} P_{B_X}^0 \,\mathrm{ad}S_{1B_X}(V_X^{01})\, P_{B_X}^0 . \end{aligned} \tag{6.25}$$

We note that Φ_M is invariant under rotations and reflections of the block M. Since the degeneracy is completely lifted, Φ_M is easily seen to be an m-potential. Thus, by the criterion of [15], $H_0^2(t)$ satisfies the Peierls condition. One can alternatively check the Peierls condition directly for this model. Hence, by Corollary 5.3, we conclude that the groundstates of the Hamiltonian $H(t)$, for t strictly positive but sufficiently small, $J<0$, and $0<\mu<2(U-J)$, are a small perturbation of the checkerboard configuration with all spins aligned, and long-range order survives at sufficiently low-temperatures.

For the antiferromagnetic model the infinite degeneracy is only partially lifted to order t^2. We then consider the transformed interaction $\Phi^{(2)}(t)$ and decompose it as described in 5.3. The "classical" part, $H_0^4(t)$, of the transformed Hamiltonian is given by (5.49). We write it as a sum of local operators:

$$
\begin{aligned}
H_0^4(t) = H_0 + t^2 & \sum_{X_1,X_2 B-\text{c.s.}} \left(\mathrm{ad}S_{1B_{X_2}}\left(Q^{01}_{B_{X_2}} + \frac{1}{2}Q^{01}_{B_{X_1}}\right)\right)^{00} \\
+t^3 & \sum_{X_1,X_2,X_3 B-\text{c.s.}} \left(\mathrm{ad}S_{1B_{X_3}}(\mathrm{ad}S_{1B_{X_2}}\left(\frac{1}{2!}Q^{R}_{B_{X_1}} + \frac{2}{3!}Q^{01}_{B_{X_1}}\right)\right)^{00} \\
+t^4 & \sum_{X_1,X_2,X_3,X_4\, B-\text{c.s.}} \left(\mathrm{ad}S_{1B_{X_4}}(\mathrm{ad}S_{1B_{X_3}}(\mathrm{ad}S_{1B_{X_2}}\left(\frac{1}{3!}Q^{R}_{B_{X_1}} + \frac{3}{4!}Q^{01}_{B_{X_1}}\right)\right)^{00} \\
+t^4 & \sum_{\substack{X_1,X_2\, B-\text{c.s.}\,;\, X_3,X_4\, B-\text{c.s.} \\ X_1\cup X_2, X_3\cup X_4 B-\text{c.s.}}} \left(\mathrm{ad}S_{2B_{X_3\cup X_4}}\left(Q^{00}_{2B_{X_1\cup X_2}} + Q^{R}_{2B_{X_1\cup X_2}} + \frac{1}{2}Q^{01}_{2B_{X_1\cup X_2}}\right)\right)^{00}
\end{aligned}
\tag{6.26}
$$

The groundstates of $H_0^4(t)$ are obtained by diagonalizing the operator

$$
P_0 H_0^4(t) P_0 \ . \tag{6.27}
$$

In this model, the perturbation has no diagonal component in the groundstate and in the first excited states of H_0 ($P^0_{B_X}Q_X P^0_{B_X}$ and $P^1_{B_X}Q_X P^1_{B_X}$ vanish). Hence the contributions of order t and t^3 vanish.

Let ϵ_{1X} be as above (see (6.16)). Note that, for $U>\frac{5J}{3}$, ϵ_{1X} is independent of X and $\epsilon_{1X} := \epsilon_1 = \frac{1}{2}(3U-J)$. Let $E_{2X\cup Y}$ be the energy of two connected excitations and we set $\epsilon_{2X\cup Y} := (E_{2X\cup Y} - E_0)$. It can take the following values: $2U$, $2U-2J$, $\frac{1}{2}(5U-3J)$, $\frac{1}{2}(5U-J)$.

The contribution to the groundstate energy to order t^4 is the following:

$$
\begin{aligned}
& \sum_{\substack{X,Y \\ Y\cap B_X\neq\emptyset}} \left(\frac{1}{\epsilon_1}\right)^3 P^0_{B_X}Q_X P^1_{B_X}Q_X P^0_{B_X}P^0_{B_Y}Q_Y P^1_{B_Y}Q_Y P^0_{B_Y} \\
- & \sum_{\substack{X,Y,X' \\ Y\cap B_X\neq\emptyset X'\in\{X,Y\}}} \left(\frac{1}{\epsilon_1}\right)^2 \left(\frac{1}{\epsilon_{2X\cup Y}}\right) \times \\
& \times P^0_{B_X}Q_X P^1_{B_X}Q_Y P^1_{B_{X\cup Y}}Q_{X'}P^1_{B_{X\cup Y\setminus X'}}Q_{X\cup Y\setminus X'}P^0_{B_{X\cup Y\setminus X'}} \ .
\end{aligned}
\tag{6.28}
$$

To determine the groundstates to order t^4, we need to compute the energies $E_{2X\cup Y}$ for the different cases. We consider the following cells:

$$
\begin{array}{ccccccc}
 & & & + & & & \\
 & & + & \circ & - & & \\
 & + & \circ & - & \circ & + & \\
+ & \circ & - & \circ & + & \circ & - \\
 & - & \circ & + & \circ & - & \\
 & & + & \circ & - & & \\
 & & & - & & &
\end{array}
\qquad
\begin{array}{ccccccc}
 & & & - & & & \\
 & & + & \circ & + & & \\
 & + & \circ & - & \circ & - & \\
+ & \circ & - & \circ & + & \circ & + \\
 & - & \circ & + & \circ & - & \\
 & & + & \circ & - & & \\
 & & & - & & &
\end{array}
\qquad
\begin{array}{ccccccc}
 & & & - & & & \\
 & & + & \circ & + & & \\
 & + & \circ & - & \circ & - & \\
- & \circ & - & \circ & + & \circ & + \\
 & + & \circ & + & \circ & - & \\
 & & - & \circ & - & & \\
 & & & + & & &
\end{array}
$$

1 **2** **3**

$$
\begin{array}{ccccccc}
 & & & - & & & \\
 & & + & \circ & + & & \\
 & - & \circ & - & \circ & - & \\
+ & \circ & + & \circ & + & \circ & + \\
 & - & \circ & - & \circ & - & \\
 & & + & \circ & + & & \\
 & & & - & & &
\end{array}
\qquad
\begin{array}{ccccccc}
 & & & + & & & \\
 & & + & \circ & - & & \\
 & - & \circ & - & \circ & + & \\
+ & \circ & + & \circ & + & \circ & - \\
 & - & \circ & - & \circ & - & \\
 & & + & \circ & + & & \\
 & & & - & & &
\end{array}
\qquad
\begin{array}{ccccccc}
 & & & + & & & \\
 & & + & \circ & - & & \\
 & - & \circ & - & \circ & + & \\
- & \circ & + & \circ & + & \circ & - \\
 & + & \circ & - & \circ & - & \\
 & & - & \circ & + & & \\
 & & & + & & &
\end{array}
$$

4 **5** **6**

Up to spin flip and rotation by $\frac{\pi}{2}$ these are the only cells wich occur in the groundstates for $U > \frac{5J}{3}$.

We compute the energies of all the connected excitations with support in $X \cup Y$ such that X contains the central site of the cell and $Y \cap B_X \neq \emptyset$.

We use the following symmetry considerations:

- There are four choices of X. One can check that the number of excitations with a given energy does not depend on the choice of X.
- The cell **2** (resp. **5**) is obtained from the cell **1** (resp. **6**) by flipping all the spins on a diagonal line of the boundary of the cell. The cell **3** (resp. **6**) is obtained from the cell **1** (resp. **6**) by flipping all the spins on two diagonal lines of the boundary of the cell. It can be checked that such an operation does not change the number of excitations with a given energy.

Hence the cells **1**, **2** and **3** (resp. **4**, **5** and **6**) give the same contribution to (6.28).

Note that if a configuration contains a cell of type **2** or **3** it must necessarily contain a cell of type **5** or **6**. Therefore the groundstate configurations contain either only cells of type **1** or only cells of type **4**.

The corresponding energy densities are

$$\begin{aligned}\frac{E^{f-af}}{|\Lambda|} &= -\frac{\mu}{2} - t^2\frac{4}{3U-J} + t^4\frac{16}{(3U-J)^3} \\ &+ t^4\frac{8}{(3U-J)^2}\left(\frac{32}{3U-J} - \frac{40}{5U-J} - \frac{16}{5U-3J} - \frac{1}{U-J} - \frac{1}{U}\right)\end{aligned} \tag{6.29}$$

for the first case and

$$\begin{aligned}\frac{E^{af}}{|\Lambda|} &= -\frac{\mu}{2} - t^2\frac{4}{3U-J} + t^4\frac{16}{(3U-J)^3} \\ &+ t^4\frac{8}{(3U-J)^2}\left(\frac{32}{3U-J} - \frac{32}{5U-J} - \frac{24}{5U-3J} - \frac{2}{U}\right)\end{aligned} \tag{6.30}$$

for the second one. We have

$$\frac{E^{f-af}}{|\Lambda|} < \frac{E^{af}}{|\Lambda|}\ , \tag{6.31}$$

for $3J^2 + 9U^2 - 8JU > 0$, which is always true for $U > \frac{5}{3}J$. The 8 groundstate configurations of $H_0^4(t)$ are therefore those in which the spins are Néel ordered in one diagonal direction and aligned in the other diagonal direction.

In order to check the Peierls condition one may easily rewrite the interaction as an m-potential and use the criterion of [15], or one may check it explicitly.

A Proof of Theorem 5.2

The only difference between the proof of this theorem and that of the "basic Pirogov-Sinai" result of [10] (Theorem 5.1) pertains to the "key estimate" presented as Lemma 6.5 in [10]. We refer the reader to [10] for notation and general background.

The proof relies on a contour expansion in $\nu+1$ dimensions obtained by iterating the Duhamel formula. The resulting contours are piecewise-cylindrical surfaces in $\Lambda\times[0,\beta]$, where Λ is a finite subset of the lattice $\mathbb{Z}^\nu$. We refer to $[0,\beta]$ as the "time" axis. These contours are periodic in the "time"-direction and their ν-dimensional sections are the "classical" contours described in Section 5.1. Each cylindrical piece of "height" τ and section of size l, of which k plaquettes are high-energy defects, has a weight bounded by

$$e^{-(\kappa l + Dk)\,\tau}\ . \tag{A.1}$$

To avoid annoying factors a^ν in formulas like this one, in this appendix we measure section areas in units of plaquette areas, i.e., in multiples of a^ν. Thus the reader should bear in mind that the constants appearing in this appendix differ from the ones in the text according to the rules:

$$\kappa_{\text{app}} = a^\nu\,\kappa_{\text{text}}, \qquad D_{\text{app}} = a^\nu\,D_{\text{text}}, \qquad \lambda_{\text{app}} = (\lambda_{\text{text}})^{a^\nu}\ . \tag{A.2}$$

Contour sections can change only by the action of operators Q_X. For fermions, we need to decompose the operator Q_X further:

$$Q_X \;=\; \sum_{\underline{X}} Q_{\underline{X}} \;, \tag{A.3}$$

where each $Q_{\underline{X}}$ is an (even-degree) monomial in creation and annihilation operators. In addition, we decompose each operator $Q_{\underline{X}}$ into the terms defined in (5.17)–(5.20):

$$Q_{\underline{X}} \;=\; Q^{\ell\ell}_{\underline{X}} + Q^{\ell\mathrm{h}}_{\underline{X}} + Q^{\mathrm{h}\ell}_{\underline{X}} + Q^{\mathrm{hh}}_{\underline{X}} \;. \tag{A.4}$$

The sections of the contours can change only by the action of *one* operator $Q^{\alpha\delta}_{\underline{X}}$ at a "time". Each section change (= "transition"), therefore involves a factor of the form $\langle\Gamma|Q^{\alpha\delta}_{\underline{X}}|\Gamma'\rangle$ (for bosons $\underline{X} \to X$), where $|\Gamma\rangle$ denotes the basis vector labelled by the family of (classical) contours Γ and $\alpha, \delta \in \{\ell\,, \mathrm{h}\}$. By hypothesis (b), such a factor is bounded in the form

$$\Big|\langle\Gamma|Q^{\alpha\delta}_{\underline{X}}|\Gamma'\rangle\Big| \;\le\; \varepsilon_{\alpha\delta}\, \lambda^{\mathrm{s}(X)} \;, \tag{A.5}$$

according to which type of transition connects the configurations Γ and Γ'.

The "key estimate", from which the bound (5.22) follows, is an upper bound on the sum, S, of the weights of all (finite) contours containing the origin in its support. The nontrivial part is the contribution, $S^{>0}$, arising from contours which involve some quantum transition; (the straight cylinders, with no change of section, are bounded exactly as in the classical Peierls argument). In fact, the contour-expansion formalism involves some additional "entropy" contributions which, for each space-time contour ζ, is of the form $e^{\widehat{\kappa}_0|\zeta|}$, where $\widehat{\kappa}_0$ is a fixed, finite number. (Cf. formulas (6.13), (7.8), (7.27) and (7.39) in [10].) To compensate this contribution, a sufficiently fast damping is needed in (A.1). This is obtained, as in [10], via a rescaling based on the identity:

$$\beta(H^{\mathrm{cl}} + Q) \;=\; \frac{\beta}{\beta'}\,(\beta' H^{\mathrm{cl}} + \beta' Q) \;. \tag{A.6}$$

We define β' so that

$$\beta'\kappa \;:=\; \widehat{\kappa} \tag{A.7}$$

satisfies

$$\widehat{\kappa} \;>\; \widehat{\kappa}_0 \;. \tag{A.8}$$

The quotient β/β' plays the role of β; i.e., we rescale

$$\beta \to \frac{\beta\kappa}{\widehat{\kappa}} := \widehat{\beta} \tag{A.9}$$

and, as a consequence,

$$\varepsilon_{\alpha\delta} \;\;\to\;\; \frac{\varepsilon_{\alpha\delta}\widehat{\kappa}}{\kappa} := \widehat{\varepsilon}_{\alpha\delta} \tag{A.10}$$

$$D \;\;\to\;\; \frac{D\widehat{\kappa}}{\kappa} := \widehat{D} \;. \tag{A.11}$$

The contours contributing to $S^{>0}$ have a number $n \geq 1$ of section changes. As we must keep track of the type of transitions involved in each change, we introduce labels e_i which are ordered pairs $(\alpha\delta)$ with $\alpha, \delta \in \{\ell, \mathrm{h}\}$. Such a label e_i indicates that the transition from the $(i-1)$-th to the i-th section of the quantum contour is of type $\alpha \to \delta$, that is, due to the action of an operator $Q^{\alpha\delta}_{\underline{X}}$. We have (cf. formula (6.19) of [10]):

$$S^{>0} \;\leq\; \sum_{n\geq 1} \sum_{\substack{(j_1,\ldots,j_n)\\ j_i\geq 1}} \overline{\lambda}^{j_1+\cdots+j_n} \sum_{\substack{(l_1,\ldots,l_n)\\ |l_i-l_{i-1}|\leq j_i\ (l_0\equiv l_n)}} \sum_{\substack{(k_1,\ldots,k_n)\\ 0\leq k_i\leq l_i\\ |k_i-k_{i-1}|\leq j_i\ (k_0\equiv k_n)}} \sum_{\substack{(e_1,\ldots,e_n)\\ \in T(k_1,\ldots,k_n)}} \prod_{i=1}^{n} \widehat{\varepsilon}_{e_i}$$

$$\times\, N(j_1,e_1,l_1,k_1,\ldots,j_n,e_n,l_n,k_n)\; R(l_1,k_1,\ldots,l_n,k_n)\;, \tag{A.12}$$

where

(i) $T(k_1,\ldots,k_n)$ is the set of possible n-tuples $(e_1,\ldots,e_n)$ compatible with the areas $k_1,\ldots,k_n$ of high-energy defects and the periodicity requirement in the "time"-direction. (Of course, there is also a dependence on the j_i's and l_i's, but we shall not use it.)

(ii) $N(j_1,e_1,l_1,k_1,\ldots,j_n,e_n,l_n,k_n)$ is an "entropy factor" that bounds the number of ways of constructing contours through the action of n quantum bonds of sizes $j_1,\ldots,j_n$, such that the quantum bond of size j_i leads to a section of area l_i, of which k_i plaquettes are high-energy defects. More precisely,

$$N(j_1,e_1,l_1,k_1,\ldots,j_n,e_n,l_n,k_n) \;:=\; \mathrm{card}\Big\{(\Gamma_0,\ldots,\Gamma_n)\;:\;\text{(a), (b) and (c) below}\Big\} \tag{A.13}$$

(a) $|\Gamma_i| = l_i$, of which k_i plaquettes are high energy defects (h.e.d); $\Gamma_0 = \Gamma_n$.

(b) There exists a sequence $(\underline{X}_1,\ldots,\underline{X}_n)$ of quantum bonds with $\mathrm{s}(\underline{X}_i) = j_i$, such that there is a quantum contour, whose support contains the point $(\vec{0},0)$, formed by the sections Γ_i and the bonds $\underline{X}_i$.

(c) Γ_i differs from Γ_{i-1} by a transition of type e_i.

(iv) $R(l_1,k_1,\ldots,l_n,k_n)$ is an "energy factor" obtained by integrating the exponential damping arising from the cylindrical pieces:

$$R(l_1,k_1,\ldots,l_n,k_n) \;:=\; \int_0^{\widehat{\beta}} d\tau_1 \cdots \int_0^{\widehat{\beta}} d\tau_n\; \mathrm{I}\left[\widehat{\beta} \geq \textstyle\sum_{i=1}^n \tau_i\right]$$

$$\times \exp\Big\{-\sum_{i=0}^{n} (\widehat{\overline{\kappa}} l_i + \widehat{D} k_i)\,\tau_i\Big\}\;, \tag{A.14}$$

where

$$\tau_0 := \widehat{\beta} - \sum_{i=1}^{n} \tau_i \quad ; \quad \widehat{\overline{\kappa}} := \widehat{\kappa} - \widehat{\kappa}_0\;, \tag{A.15}$$

and $\kappa_0 := \kappa_n$; $l_0 := l_n$.

(v) $\overline{\lambda} := \lambda\, e^{\widehat{\kappa}_0}$ is the reduced quantum coupling produced by the above mentioned "entropy" contributions inherent to the combinatorics of the cluster expansion.

The bound on the energy factor is obtained as in [10] [see discussion between formulas (6.28) and (6.29) therein]. For each $\tau = \tau_1, \ldots, \tau_n$, $(\widehat{\beta} - \sum_{i=1}^{n} \tau_i)$, we use the bound

$$e^{-(\widehat{\overline{\kappa}}\, l_i + \widehat{D}\, k_i)\tau} \;\leq\; e^{-(\widehat{\overline{\kappa}}\, l_{\min} + \widehat{D}\, k_{\min})\tau/2}\, e^{-(\widehat{\overline{\kappa}}\, l_i + \widehat{D}\, k_i)\tau/2}, \tag{A.16}$$

with

$$l_{\min} := \min_i l_i \quad \text{and} \quad k_{\min} := \min_i k_i \;. \tag{A.17}$$

In this way we extract an overall factor

$$e^{-(\widehat{\overline{\kappa}}\, l_{\min} + \widehat{D}\, k_{\min})\,\widehat{\beta}/2} \;=\; e^{-(\overline{\kappa}\, l_{\min} + D\, k_{\min})\,\beta/2} \tag{A.18}$$

outside the integral on the RHS of (A.14). We have denoted

$$\overline{\kappa} \;:=\; \kappa\left(1 - \frac{\widehat{\kappa}_0}{\widehat{\kappa}}\right) . \tag{A.19}$$

The remaining integral is the same as the original one, but with $(\widehat{\overline{\kappa}}\, l_i + \widehat{D}\, k_i)$ replaced by $(\widehat{\overline{\kappa}}\, l_i + \widehat{D}\, k_i)/2$. By neglecting the indicator function and the term proportional to l_0 and k_0 in the exponent, and extending the limits of integration to infinity, we obtain

$$R(l_1, k_1, \ldots, l_n, k_n) \;\leq\; \left[\prod_{i=1}^{n} \frac{2}{\widehat{\overline{\kappa}}\widetilde{l}_i + \widehat{D} k_i}\right] e^{-\frac{\beta}{2}(\overline{\kappa} l_{\min} + D k_{\min})} \;, \tag{A.20}$$

where $\widetilde{l}_i := \max(l_i, 1)$. [The variables $\widetilde{l}_i$ are introduced to treat "long" and "short" contours simultaneously; $\widetilde{l}_i = 1$ —for only *one* i— for the short contours.]

To bound the "entropy" contribution (A.13) we proceed exactly as in [10, Section 6.3]. We start with the inequality

$$\begin{aligned} &N(j_1, e_1, l_1, k_1, \ldots, j_n, e_n, l_n, k_n) \;\leq \\ &\qquad (l_{\max} + j_{\max})\, \widetilde{N}(j_1, e_1, l_1, k_1, \ldots, j_n, e_n, l_n, k_n) \;, \end{aligned} \tag{A.21}$$

where $l_{\max} = \max_i l_i$, $j_{\max} = \max_i j_i$, and $\widetilde{N}(j_1, e_1, l_1, k_1, \ldots, j_n, e_n, l_n, k_n)$ is the number of "pinned" contours, that is, contours with the given section and quantum bond sizes for which $(\vec{0}, 0)$ is the first point (e.g. in lexicographic order) of its support. To evaluate $\widetilde{N}$ we imagine that we "construct" the quantum contour by starting from a section with minimal size l_{min}:

$$\begin{aligned} &\widetilde{N}(j_1, e_1, l_1, k_1 \ldots, j_n, e_n, l_n, k_n) \;\leq \\ &\qquad \sum_{\Gamma \in \mathrm{CC}(l_{\min}, j_1, \ldots, j_n)} \mathcal{N}_{\Gamma \to \Gamma}(j_{i_{\min}+1}, e_{i_{\min}+1}, l_{i_{\min}+1}, k_{i_{\min}+1}, \ldots, \\ &\qquad\qquad j_{i_{\min}-1}, e_{i_{\min}-1} l_{i_{\min}-1}, k_{i_{\min}-1}, j_{i_{\min}}, e_{i_{\min}}, k_{i_{\min}}) \;. \end{aligned} \tag{A.22}$$

Here, $i_{\min}$ satisfies $l_{i_{\min}} = l_{\min}$,

$\mathrm{CC}(l, j_1, \ldots, j_n)$:= $\{\Gamma : |\Gamma| = l$, and Γ is a section of a quantum contour with n section changes produced by the action of operators $Q^{e_i}_{\underline{X}_i}$ with $\mathrm{s}(X_i) = j_i, i+1, \ldots, n\}$

and

$\mathcal{N}_{\Gamma_0\to\Gamma_n}(j_1, e_1, l_1, k_1 \ldots, j_{n-1}, e_{n-1}, l_{n-1}, k_{n-1}, j_n, e_n, l_n, k_n)$:= number of ways of choosing sections $\Gamma_1, \ldots, \Gamma_{n-1}$ of areas $l_1, \ldots, l_{n-1}$ having $k_1, \ldots, k_{n-1}$ high energy defects, such that the section Γ_i is obtained from the section Γ_{i-1} by the action of an operator $Q^{e_i}_{\underline{X}_i}$ with $\mathrm{s}(X_i) = j_i$.

A more careful account of the types of section changes involved, is embodied in the formula

$$\mathcal{N}_{\Gamma_0\to\Gamma_n}(j_1, e_1, l_1, k_1 \ldots, j_{n-1}, e_{n-1}, l_{n-1}, k_{n-1}, j_n, e_n, l_n, k_n) \quad \leq$$
$$(a^{2\nu})^n \prod_{i=1}^n j_i\, {c_\nu}^{j_i} \prod_{\substack{i\in\{1\ldots n\}\\ e_i=(\ell,\ell)}} (l_i + j_i) \prod_{\substack{i\in\{1\ldots n\}\\ e_i\neq(\ell\ell)}} (k_i + j_i) \tag{A.23}$$

[cf. eqn. (6.23) in [10]]. Here c_ν is a dimension-dependent constant. The proof of this inequality is given at the end of this appendix. Therefore,

$$\widetilde{N}(j_1, e_1, l_1, k_1, \ldots, j_n, e_n, l_n, k_n) \;\leq\; \mathrm{card}\Big(\mathrm{CC}(l_{\min}, j_1, \ldots, j_n)\Big)$$
$$\times\, (a^{2\nu})^n \prod_{i=1}^n j_i\, {c_\nu}^{j_i} \prod_{\substack{i\in\{1\ldots n\}\\ e_i=(\ell\ell)}} (l_i + j_i) \prod_{\substack{i\in\{1\ldots n\}\\ e_i\neq(\ell\ell)}} (k_i + j_i)\,. \tag{A.24}$$

As in [10], to find a bound on $\mathrm{card}\Big(\mathrm{CC}(l_{\min}, j_1, \ldots, j_n)\Big)$ we make use of the fact that for each $l_{\min}$ there is a connected set formed by no less than $l_{\min}$ and no more than $l_{\min} + j_1 + \cdots + j_n$ plaquettes. Thus, by the Königsberg bridge lemma, there exists a constant $c_\nu \geq 1$, depending only on the spatial dimension, such that

$$\begin{aligned}\mathrm{card}\Big(\mathrm{CC}(l_{\min}, j_1, e_1, k_1, , \ldots, j_n, e_n, k_n)\Big) &\leq c_\nu^{l_{\min}} + \cdots + c_\nu^{l_{\min}+j_1+\cdots+j_n}\\ &\leq (j_1 + \cdots + j_n + 1)\, c_\nu^{l_{\min}+j_1+\cdots+j_n}\,.\end{aligned} \tag{A.25}$$

Substituting (A.20), (A.21), (A.24) and (A.25) in (A.12) we obtain the bound

$$S^{>0} \;\leq\; \sum_{n\geq 1} (2a^{2\nu})^n \sum_{(j_1,\ldots,j_n)\,:\,j_i\geq 1} (j_1 + \cdots + j_n + 1) \Big(\prod_{i=1}^n j_i\Big)\, (c_\nu^2\, \overline{\lambda})^{j_1+\cdots+j_n}$$

$$\times \sum_{\substack{(l_1,\ldots,l_n):\, l_i\geq 1 \\ |l_i-l_{i-1}|\leq j_i\ (l_0\equiv l_n)}} (l_{\max}+j_{\max})\, c_\nu^{l_{\min}}\, e^{-\beta\overline{\kappa} l_{\min}/2}$$

$$\times \sum_{\substack{(k_1,\ldots,k_n) \\ 0\leq k_i\leq l_i \\ |k_i-k_{i-1}|\leq j_i\ (k_0\equiv k_n)}} e^{-\beta D k_{\min}/2}\, G_n(l_1,k_1,j_1,\ldots,l_n,k_n,j_n)\ , \tag{A.26}$$

where

$$G_n \ := \sum_{\substack{(e_1,\ldots,e_n) \\ \in T(k_1,\ldots,k_n)}} \left[\prod_{\substack{i\in\{1\ldots n\}: \\ e_i=(\ell\ell)}} \frac{\varepsilon_{\ell\ell}\,(l_i+j_i)}{\overline{\kappa}\widetilde{l}_i + Dk_i}\right]\left[\prod_{\substack{i\in\{1\ldots n\}: \\ e_i\neq(\ell\ell)}} \frac{\varepsilon_{e_i}\,(k_i+j_i)}{\overline{\kappa}\widetilde{l}_i + Dk_i}\right]. \tag{A.27}$$

To bound G_n we start with the inequalities

$$\begin{aligned} \frac{\varepsilon_{\ell\ell}\,(l_i+j_i)}{\overline{\kappa}\widetilde{l}_i + Dk_i} &\leq \frac{\varepsilon_{\ell\ell}\,(l_i+j_i)}{\overline{\kappa}\widetilde{l}_i} \\ &\leq \frac{\varepsilon_{\ell\ell}}{\overline{\kappa}}\,(1+j_i) \end{aligned} \tag{A.28}$$

and, for $e_i \neq (\ell\ell)$,

$$\frac{\varepsilon_{e_i}\,(k_i+j_i)}{\overline{\kappa}\widetilde{l}_i + Dk_i} \ \leq \ \begin{cases} \dfrac{\varepsilon_{e_i}\,(l_i+j_i)}{\overline{\kappa}\,\widetilde{l}_i} \leq \dfrac{\varepsilon_{e_i}}{\overline{\kappa}}\,(1+j_i) & \text{if } k_i=0 \\[2ex] \dfrac{\varepsilon_{e_i}\,(k_i+j_i)}{(\overline{\kappa}+D)k_i} \leq \dfrac{\varepsilon_{e_i}}{\overline{\kappa}+D}\,(1+j_i) & \text{if } k_i>0\ . \end{cases} \tag{A.29}$$

We point out that the first line on the RHS of (A.29) can only occur when $e_i = (\mathrm{h}\ell)$; all other transitions (different from $\ell \to \ell$) yield $k_i > 0$. These inequalities lead us to the bound

$$G_n \ \leq \ \left[\prod_{i=1}^{n}(1+j_i)\right] \sum_{\substack{(e_1,\ldots,e_n) \\ \in T(k_1,\ldots,k_n)}} \prod_{i=1}^{n} \widetilde{\varepsilon}_{e_i}\ , \tag{A.30}$$

with

$$\widetilde{\varepsilon}_{\ell\ell} = \frac{\varepsilon_{\ell\ell}}{\overline{\kappa}} \quad , \quad \widetilde{\varepsilon}_{\ell\mathrm{h}} = \frac{\varepsilon_{\ell\mathrm{h}}}{\overline{\kappa}+D} \quad , \quad \widetilde{\varepsilon}_{\mathrm{hh}} = \frac{\varepsilon_{\mathrm{hh}}}{\overline{\kappa}+D} \tag{A.31}$$

and

$$\widetilde{\varepsilon}_{\mathrm{h}\ell} \ = \ \begin{cases} \dfrac{\varepsilon_{\mathrm{h}\ell}}{\overline{\kappa}+D} & \text{if } k_i>0 \\[2ex] \dfrac{\varepsilon_{\mathrm{h}\ell}}{\overline{\kappa}} & \text{if } k_i=0\ . \end{cases} \tag{A.32}$$

Of these factors, the most dangerous one is $\widetilde{\varepsilon}_{\mathrm{h}\ell}$ when $k_i = 0$. Indeed, it is often the case that $\varepsilon_{\mathrm{h}\ell}$ is of *lower* order than $\overline{\kappa}$, hence this factor can in fact diverge as the strength of the quantum perturbation tends to zero. However, this factor *always* appears in combination with a factor $\widetilde{\varepsilon}_{\ell \mathrm{h}}$. This is because, for each transition $\mathrm{h} \to \ell$ leading to $k_i = 0$, i.e., to the destruction of the high-energy defects of the contour, there must exist another transition of the type $\ell \to \mathrm{h}$ at which these defects start to be created. Formally, this means that one can set up a one-to-one association between each i with $e_i = (\mathrm{h}\ell)$ and $k_i = 0$ and some $j(i)$ with $e_j = (\ell\mathrm{h})$. The dominant contribution of such a contour is given by a factor $\widetilde{\varepsilon}_{\ell \mathrm{h}}\, \widetilde{\varepsilon}_{\mathrm{h}\ell}$.

These considerations imply the bound

$$\begin{aligned} G_n \;&\le\; \prod_{i=1}^{n}(1+j_i) \sum_{\substack{n_1,n_2,n_3,n_4 \ge 0 \\ n_1+2n_2+n_3+n_4 = n}} \binom{n}{n_1\; 2n_2\; n_3\; n_4} \\ &\qquad \times \left(\frac{\varepsilon_{\ell\ell}}{\overline{\kappa}}\right)^{n_1} \left(\frac{\varepsilon_{\ell\mathrm{h}}\varepsilon_{\mathrm{h}\ell}}{\overline{\kappa}(\overline{\kappa}+D)}\right)^{n_2} \left(\frac{\varepsilon_{\mathrm{hh}}}{\overline{\kappa}+D}\right)^{n_3} \left(\frac{\max(\varepsilon_{\mathrm{h}\ell}\,,\,\varepsilon_{\ell\mathrm{h}})}{\overline{\kappa}+D}\right)^{n_4} \\ &\le\; (4\,\varepsilon)^n \prod_{i=1}^{n}(1+j_i)\;, \end{aligned} \tag{A.33}$$

where

$$\varepsilon \;:=\; \max\left(\frac{\varepsilon_{\ell\ell}}{\overline{\kappa}}\,,\, \sqrt{\frac{\varepsilon_{\ell\mathrm{h}}\varepsilon_{\mathrm{h}\ell}}{\overline{\kappa}(\overline{\kappa}+D)}}\,,\, \frac{\varepsilon_{\mathrm{hh}}}{\overline{\kappa}+D}\,,\, \frac{\varepsilon_{\mathrm{h}\ell}}{\overline{\kappa}+D}\,,\, \frac{\varepsilon_{\ell\mathrm{h}}}{\overline{\kappa}+D}\right)\,. \tag{A.34}$$

When (A.33) is inserted on the RHS of (A.26), we are left with no further dependence on the individual l_i and k_i, but only with a dependence on $l_{\min}$, $k_{\min}$ and $j_1,\ldots,j_n$. In such a situation, the sum over the l_i, $1 \le i \le n$ can be bounded by a sum over $l_{\min}$, times a factor $\prod_i (2j_i+1)$ arising from the fact that for each l_i there are only $2j_i+1$ possible values for l_{i+1}. By an analogous argument, the sum over the k_i, $1 \le i \le n$, can be bounded by a sum over $k_{\min}$ and a factor $\prod_i(2j_i+1)$. The maximum size, $l_{\max}$, of a section of the contour satisfies the bound

$$l_{\max} \;\le\; l_{\min} + j_1 + \cdots + j_n\;. \tag{A.35}$$

This is because the section of "area" $l_{\max}$ is obtained from the section of "area" $l_{\min}$ by the action of *at most* n quantum interactions, $Q^{e_1}_{\underline{X}_1},\ldots,Q^{e_n}_{\underline{X}_n}$, the latter corresponding to quantum bonds $\underline{X}_1,\ldots,\underline{X}_n$ of sizes $j_1,\cdots,j_n$. Also,

$$j_{\max} \;\le\; j_1 + \cdots + j_n\;. \tag{A.36}$$

With the bounds (A.33), (A.35) and (A.36), and the preceding considerations on the sums over l_i and k_i, inequality (A.26) implies that

$$\begin{aligned} S^{>0} \;&\le \\ &\sum_{n\ge 1}\left(8\,a^{2\nu}\right)^n \sum_{(j_1,\ldots,j_n)\,:\,j_i\ge 1} (j_1+\cdots+j_n+1)\Big[\prod_{i=1}^{n} j_i^2(1+j_i)^2(1+2j_i)\Big](c_\nu^2\,\varepsilon\,\overline{\lambda})^{j_1+\cdots+j_n} \\ &\times \sum_{l_{\min}} (l_{\min}+2j_1+\cdots+2j_n)\,\left(c_\nu\, e^{-\beta\overline{\kappa}/2}\right)^{l_{\min}} \sum_{k_{\min}=0}^{l_{\min}} e^{-\beta D\,k_{\min}/2}\;. \end{aligned} \tag{A.37}$$

The series on the RHS is convergent if

$$\max\Big(e^{-\beta\overline{\kappa}/2}\,,\,\varepsilon\overline{\lambda}\Big) \tag{A.38}$$

is small enough. This is precisely the condition (5.22). ∎

Remark: Within the region of convergence of the RHS of (A.37), the cluster expansion technology tells us that the dominant contributions to the thermodynamic potentials (Theorem 6.3 in [10]) and quantum expectations (Sections 5.2 and 6.5 in [10]) come from the leading terms of the series presented in this appendix. In particular, we have that:

(a) The "long" contours, that is the contours with $l_{\rm min} > 0$, have a contribution

$$\mathrm{O}(e^{-\beta\overline{\kappa}/2})\;. \tag{A.39}$$

Contours with "long" high-energy parts, i.e., $k_{\rm min} > 0$ have an even smaller contribution $\mathrm{O}(e^{-\beta(\overline{\kappa}+D)/2})$.

(b) The "short" contours, i.e., the contours with $l_{\rm min} = 0$, have a contribution

$$\mathrm{O}\left(\frac{\varepsilon_{\ell\ell}\lambda}{\overline{\kappa}}\right) \tag{A.40}$$

if they involve "low→low" transitions. This estimate covers the most general case in which long-range "classical" (=diagonal) terms are allowed in the quantum part. If $Q_{\underline{\mu}}$ had no diagonal terms then the minimal order would be the *square* of (A.40). This corresponds to a "vacuum fluctuation" in which a single low-energy defect is generated and then destroyed.

(c) The short contours without "low→low" transitions have a contribution

$$\mathrm{O}\left(\frac{\varepsilon_{\ell\mathrm{h}}\,\varepsilon_{\mathrm{h}\ell}\,\lambda}{\overline{\kappa}\,(\overline{\kappa}+D)}\right)\;. \tag{A.41}$$

The leading contribution corresponds to the creation and later destruction of a single high-energy defect.

Proof of the claim (A.23). The proof follows by induction in n. It is based on the identity

$$\begin{aligned}\mathcal{N}_{\Gamma_0\to\Gamma_n}(j_1,e_1,l_1,k_1\ldots,j_{n-1},e_{n-1},l_{n-1},k_{n-1},j_n,e_n,k_n) \;=\\ \sum_{\Gamma_{n-1}\in \mathrm{CC}_{l_{n-1},k_{n-1},j_n,e_n}(\Gamma_n)} \mathcal{N}_{\Gamma_0\to\Gamma_{n-1}}(j_1,e_1,l_1,k_1\ldots,j_{n-2},e_{n-2},l_{n-2},k_{n-2},\\ j_{n-1},e_{n-1},k_{n-1},)\;,\end{aligned} \tag{A.42}$$

where

$\mathrm{CC}_{l_{n-1},k_{n-1},j_n,e_n}(\Gamma_n) \;:=\; \{\Gamma \,:\, |\Gamma| = l_{n-1}$, of which k_{n-1} plaquettes are high energy defects, and Γ_n is obtained from Γ by the action of some $Q^{e_n}_{\underline{X}_n}$ with $|X_n| = j_n\}$.

The inductive step consists in showing that

$$\mathrm{card}\Big(\mathrm{CC}_{l_{n-1},k_{n-1},j_n,e_n}(\Gamma_n)\Big) \;\leq\; a^{2\nu}\, j_n\, c_\nu^{j_n} \times \begin{cases} l_n + j_n & \text{if } e_n = (\ell\ell) \\ k_n + j_n & \text{if } e_n \neq (\ell\ell) \end{cases} \tag{A.43}$$

The proof for the case $e_n = (\ell\ell)$ is identical to the proof of the analogous inequality in [10] [claim (6.23) therein]. We have to consider two cases:

(i) $l_{n-1} \geq l_n$. In this case, the bond X_n must intersect the support of Γ_{n-1}. The number of such possibilities is bounded by the product of the number of sites in Γ_{n-1} $(= l_{n-1}a^\nu)$, the number of sites in X_n $(= j_n a^\nu)$ and the number of bonds $\underline{X}_n$ with $|X_n| = j_n$. The latter is less than or equal to $c_\nu^{j_n}$, for some constant c_ν depending on the dimension d.

(ii) $l_{n-1} < l_n$. In this case, X_n must intersect the support of Γ_n. Hence we can use the preceding argument, with Γ_{n-1} replaced by Γ_n.

Therefore, in both cases,

$$\begin{aligned} \mathrm{card}\Big(\mathrm{CC}_{l_{n-1},j_n}(\Gamma_n)\Big) \;&\leq\; (a^\nu)^2 \max(l_{n-1}, l_n)\, j_n\, c_\nu^{j_n} \\ &\leq\; a^{2\nu}\,(l_n + j_n)\, j_n\, c_\nu^{j_n}\,, \end{aligned} \tag{A.44}$$

where we have used that $l_{n-1} \leq l_n + j_n$. This proves the first line of (A.43).

The proof for the case $e_n \neq (\ell\ell)$ is analogous, but with k_i replacing l_i in the previous argument. Indeed, the condition $e_n \neq (\ell\ell)$ implies that X_n intersects a high-energy defect either of Γ_{n-1} (if $k_{n-1} \geq k_n$) or of Γ_n. ∎

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