

# Rigidity of Interfaces in the Falicov–Kimball Model

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We analyze the thermodynamic properties of interfaces in the three-dimensional Falicov–Kimball model, which can be viewed as a primitive quantum lattice model of crystalline matter. In the strong coupling limit, the ionic subsystem of this model is governed by the Hamiltonian of an effective classical spin model whose leading part is the Ising Hamiltonian. We prove that the 100 interface in this model, at half-filling, is rigid, as in the three-dimensional Ising model. However, despite the above similarities with the Ising model, the thermodynamic properties of its 111 interface are very different. We prove that even though this interface is expected to be unstable for the Ising model, it is stable for the Falicov–Kimball model at sufficiently low temperatures. This rigidity results from a phenomenon of “ground-state selection” and is a consequence of the Fermi statistics of the electrons in the model.

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**KEY WORDS:** Falicov–Kimball model; ground-state selection; rigidity of interfaces; 100 and 111 interfaces.

## 1. INTRODUCTION

Domain boundaries can have important effects on the transport properties of condensed matter materials. In some cases, transport is believed to occur mainly or exclusively along domain boundaries.<sup>(35)</sup> This is related to the drastic effect the presence of a domain wall, or interface, can have on the low-lying excitations of the system. Therefore, it is important to study non-periodic equilibrium states, in particular interface states, in statistical

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Dedicated to the memory of Roland Dobrushin.

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mechanics, and to understand their stability, fluctuations, and low-lying excitations.

Many phenomena in condensed matter physics, which are of current interest, are intrinsically quantum mechanical in origin. Quantum effects also play a crucial role in the properties of interfaces. There are, however, very few rigorous results on interface states in quantum statistical mechanics. In refs. 2 and 3 a general perturbation theory was developed, which, under certain assumptions, shows that a small quantum perturbation does not destroy an existing interface Gibbs state of a classical discrete spin model (the so-called Dobrushin states).

In this paper we consider the opposite situation, namely, one in which quantum fluctuations stabilize the interface against thermal fluctuations, while the classical limit does *not* have a stable interface. We demonstrate the occurrence of such an “order by disorder” effect,<sup>(21, 43)</sup> in a simple quantum lattice model—the three-dimensional Falicov Kimball (FK) model [See Section 2 for a description of the model]. We are motivated by recent work<sup>(26)</sup> which demonstrates that, at zero temperature, in the two-dimensional ferromagnetic XXZ Heisenberg model with Ising-like anisotropy the quantum fluctuations stabilize the 11-interface (i.e., an interface in the diagonal direction). In the present work we prove such an effect at finite temperature for two interfaces in the FK model.

The FK model was chosen because its statistical mechanical properties have been studied extensively (see, e.g., refs. 18–20, 22, 24, 27, 29, 33) and, recently, convenient perturbation expansions have been developed for it.<sup>(11, 23, 32, 33)</sup> We expect that the XXZ model in three dimensions also has a stable 111 interface at sufficiently low temperatures. Its analysis is, however, more involved due to the presence of gapless excitations in the interface.<sup>(26, 31)</sup>

Our main result is that, in three dimensions, the FK model has a stable 111 interface at sufficiently low temperatures. This should be compared with the three-dimensional Ising model since, in the strong coupling limit, the FK model can be considered as a perturbation of the Ising model (see e.g., refs. 29, 32, 33). Dobrushin showed that the Ising model has 100-interface states, but its 111-interfaces are expected to be *unstable at any finite temperature*. It has been proved recently that in the zero-temperature limit of the three-dimensional Ising model the 111 interface fluctuates.<sup>(25)</sup> This is related to the degeneracy of the ground states with a 111-interface which grows exponentially with the volume (the rate of exponential growth may depend on the boundary conditions however! See ref. 41). In the FK model this degeneracy is lifted. In this sense, this is an example of the phenomenon of “ground state selection”<sup>(21)</sup> by quantum fluctuations. We refer to Section 2.2 for a detailed discussion of the 111 interface configurations.

In ref. 24 Lieb and Kennedy showed how to study the FK model in terms of an Ising-type model for the Ising configurations that is obtained by taking the trace over the electron states for any given ion configuration. The Hamiltonian for the ions can be explicitly computed to any order in perturbation theory together with a bound on the sum of the higher order terms [see Appendix A and ref. 32]. For the study of the 100-interface one needs the explicit form of this Hamiltonian up to second order. For the 111-interface fourth order perturbation theory is needed. In principle, our method could be used to study interfaces with more general orientations, but higher order terms in the perturbation series will be needed; e.g., the 112 interface is infinitely degenerate at fourth order, but we expect it to be stabilized at sufficiently low temperatures by the sixth order terms. Therefore, one should expect that the Falicov–Kimball model has an infinite number of interface phase transitions.

We follow Dobrushin<sup>(15)</sup> (see also refs. 5 and 6) in proving the existence of an interface by considering an effective two-dimensional model for the interface. Although, this two-dimensional model turns out to be quite complicated, and involves many-body interactions of arbitrarily long range, we can analyze it with a Peierls-type argument. It is probably possible to develop a general Pirogov–Sinai theory<sup>(2, 39, 40, 48)</sup> to treat this situation, along the lines of refs. 12 and 37, but we found it more convenient to make efficient use of simpler methods. The result is a more transparent and relatively short proof.

Our main results are stated at the end of the next section. Our main technical tool is the convergence of certain cluster expansions proved in Appendix B. Appendix A contains the proof of a bound on the remainder term in the expansion of the effective Hamiltonians for the ions. In Section 4 we discuss the rigidity of a 100-interface, which is much simpler than the case of the 111-interface treated in Section 5.

## 2. THE FK MODEL AND EFFECTIVE HAMILTONIANS

The Falicov Kimball (FK) model<sup>(16)</sup> is a lattice model of spin-polarized electrons and classical particles (ions).<sup>(16)</sup> The electrons and ions interact via a purely on-site interaction. The electrons can hop between nearest neighbour sites of the lattices, but the ions are static. There is a hard-core repulsion between the ions, which prevents more than one ion from occupying a single lattice site. The presence or absence of an ion at a lattice site  $x$  is described by a classical variable,  $W(x)$ , which is equal to unity if there is an ion at the site  $x$  and is zero otherwise. Let the number operator of an electron at the site  $x$  be given by  $n = c_x^\dagger c_x$ , where  $c_x^\dagger$  and  $c_x$  are the creation and annihilation operators of the electron at the site  $x$ . Let

$\mu_i$  and  $\mu_e$  denote the chemical potentials of the ions and electrons respectively. Let  $\mathcal{L}^3$  denote an infinite cubic lattice, with unit lattice spacing, such that the coordinates of the sites are given by half-integers. For notational simplicity in our description of the interface, it is more convenient to consider this lattice instead of  $\mathbb{Z}^3$ . The Hamiltonian of the model defined on a finite lattice  $A \subset \mathcal{L}^3$  is given by

$$\mathcal{H}_A(t, U) = \mathcal{H}_{0A}(U) + tV_A \quad (2.1)$$

where  $\mathcal{H}_{0A}(U)$  is a Hamiltonian which is given entirely in terms of an on-site interaction as follows:

$$\begin{aligned} \mathcal{H}_{0A}(U) &= 2U \sum_{x \in A} W(x) n_x - \mu_e \sum_{x \in A} n_x - \mu_i \sum_{x \in A} W(x) \\ &:= \sum_{x \in A} \Phi_{0x} \end{aligned} \quad (2.2)$$

The operator  $V_A$  causes electrons to hop between nearest neighbour sites of the lattice:

$$\begin{aligned} V_A &= -t \sum_{\langle xy \rangle \subset A} (c_x^\dagger c_y + c_y^\dagger c_x) \\ &=: \sum_{X = \langle xy \rangle \subset A} V_X \end{aligned} \quad (2.3)$$

Here  $\langle xy \rangle$  denotes a pair of nearest neighbour sites in the lattice. The hopping amplitude of the electrons is denoted by  $t \in \mathbb{R}$ . The first rigorous study of the above model was done by Kennedy and Lieb.<sup>(24)</sup> They considered the classical particles to be nuclei and the on-site interaction to be the Coulomb attraction between nuclei and electrons. In accordance with this interpretation, they chose the coupling constant  $U$  to be negative. They proved that the ground states of this model display perfect crystalline ordering for the choice

$$\mu_i = \mu_e = U \quad (2.4)$$

the ions being arranged in a checkerboard configuration. The choice (2.4) corresponds to a neutral model: the average number of electrons in the lattice is equal to the average number of ions, both being equal to half the number of lattice sites (half-filling).

The model described by the Hamiltonian  $\mathcal{H}_A(t, U)$  for  $U < 0$ , is mathematically equivalent to the model with  $U > 0$  (see ref. 24) and there is a

simple relation between the properties of the attractive model,  $U < 0$ , and the repulsive one,  $U > 0$ . In this paper we work with  $U > 0$ .

We study the FK model in the strong-coupling limit i.e., for  $U \gg |t|$ , and hence consider the hopping term  $tV_A$  to be a perturbation to the Hamiltonian  $\mathcal{H}_{0A}(U)$ . It is convenient to renormalize the hopping amplitude  $t$  to unity. This amounts to the following rescaling:

$$\begin{aligned} U/t &\rightarrow U \\ \beta t &\rightarrow \beta \end{aligned} \quad (2.5)$$

where  $\beta = 1/k_B T$  ( $k_B$  being the Boltzmann constant and  $T$  the absolute temperature). In our expansions  $U^{-1}$  plays the role of a small parameter.

For a fixed value of the coupling constant  $U$ , the zero temperature phase diagram of the unperturbed Hamiltonian  $\mathcal{H}_{0A}(U)$  in the plane of chemical potentials can be easily obtained.<sup>(18)</sup> To obtain the ground states of  $\mathcal{H}_{0A}(U)$ , for any given set of values the chemical potentials  $\mu_i$  and  $\mu_e$ , we only need to find the single-site configuration which minimizes  $\Phi_{0x}$  (2.2). When both the chemical potentials are negative, the ground state corresponds to all sites of the lattice being empty. In the rest of the  $(\mu_i - \mu_e)$  plane, it is found that for values of the chemical potentials such that  $\mu_e < 2U$  and/or  $\mu_i < 2U$ , there is no doubly occupied site at zero temperature. For these values of the chemical potentials, the ground state corresponds to an all-ion configuration if  $\mu_i > \mu_e$  with  $\mu_i > 0$ , and to an all-electron configuration if  $\mu_e > \mu_i$  with  $\mu_e > 0$ . For  $0 < \mu_i = \mu_e < 2U$  all singly occupied configurations are equally likely and hence the ground state is infinitely degenerate. The origin and the point  $\mu_i = \mu_e = 2U$  also correspond to infinitely many ground states. At the origin, each site is either empty or singly occupied, whereas at the point  $(2U, 2U)$  each site is either singly- or doubly occupied. At zero temperature, for  $\mu_i > 2U$  and  $\mu_e > 2U$ , every site is doubly occupied by an electron-ion pair.

As in refs. 29, 32, and 33, we will rely on the fact that for  $U > c|t|$ , where  $c$  is a positive constant, the ionic subsystem of the FK model defined on a finite cubic lattice  $A$  can be described by an effective classical Hamiltonian. We will study only the *neutral* model at *half-filling*, i.e.,  $\mu_i = \mu_e = U$ . Then, it follows from the circuit representation of ref. 33 and the bounds proved in Appendix A that the equilibrium states of the ions are described by an effective classical Hamiltonian of the form

$$\mathcal{H}_A^{\text{eff}}(U) = \frac{1}{4U} \sum_{\langle xy \rangle \in A} s'_x s'_y + \mathcal{R}_A(\beta, U) \quad (2.6)$$

where

$$s'_x := 2W(x) - 1 \quad (2.7)$$

The variable  $s'_x$  can be interpreted as an on-site spin variable since  $s'_x = 1$  if there is an ion at  $x$  and  $s'_x = -1$  otherwise. Note that  $\mathcal{H}_A^{\text{eff}}(U)$  depends on  $\beta$  through the remainder term  $\mathcal{R}_A(\beta, U)$ . This is unavoidable if one wants an exact correspondence between the correlation functions of the ions in the Falicov–Kimball model and the same correlation functions of the effective classical spin model. In particular, if one writes  $\mathcal{R}_A(\beta, U)$  as a sum of products of the  $s'_x$  variables, one sees that it still contains a nearest neighbour contribution with a coefficient that tends to zero exponentially fast as  $\beta \rightarrow \infty$ . As all our results are for  $\beta$  and  $U$  sufficiently large, this temperature dependence will be of no consequence however. Similarly, as we will do later on (2.34) and (2.35), one can extract from  $\mathcal{R}_A(\beta, U)$  the leading contributions for the next-nearest neighbour and plaquette interactions, which are independent of  $\beta$ , and estimate the temperature dependent corrections with the bounds proved in Appendix A.

All terms of higher orders in the perturbation parameter  $U^{-1}$ , i.e., all terms of order  $U^{-n}$ , with  $n \geq 3$ , are contained in the remainder  $\mathcal{R}_A(\beta, U)$ , which, just as the leading term, depends on  $\beta$  in an inessential way. Hence we simply write it as  $\mathcal{R}_A(U)$ . This remainder is expressible in terms of local classical interactions  $\{R_B(U)\}$ :

$$\mathcal{R}_A(U) = \sum_{\substack{B \cap A \neq \emptyset \\ |B| \geq 2}} R_B(U) \quad (2.8)$$

Here  $B$  denotes a *connected* set of lattice sites, i.e., if  $x, y \in B$  then there exists a sequence of sites  $x_0 = x, x_1, \dots, x_n = y$  such that  $x_i \in B$  and  $|x_i - x_{i+1}| = 1$  for all  $i = 0, \dots, n-1$ . The number of sites in  $B$  is denoted by  $|B|$ . We refer to such a set  $B$  as a *bond*. A bond can be represented by a graph, the vertices being the sites and the lines of the graph representing nearest neighbour bonds between pairs adjacent sites. Let  $\mathcal{B}$  denote the set of *all* bonds in the lattice  $A$ . For each bond  $B$  appearing in the above sum (2.8), the interaction  $R_B(U)$  can be expressed as a product of two or more on-site spin variables  $s'_x$  with  $x \in B$ .

Note that, for us, a *bond* is, by definition, a *connected set*. This is convenient in combinatorial arguments and a natural choice in view of the way perturbation theory produces long-range and multi-body interactions as a composition of nearest neighbour hoppings. It does not exclude the presence of terms of the form  $s'_x s'_y$ , with  $|x - y| \geq 2$ , in the effective Hamiltonian. Such terms *are included* in connected bonds  $B$  containing  $x$  and  $y$ .

A configuration on  $\mathcal{L}^3$ , denoted by  $\omega$ , is therefore given by a set of assignments  $\{s'_x\}_{x \in \mathcal{L}^3}$  of  $s'_x \in \{-1, 1\}$  to each  $x \in \mathcal{L}^3$ . For any finite subset  $Y \subset \mathcal{L}^3$ , let  $\omega_Y$  denote the restriction of the configuration  $\omega$  to the subset  $Y$ . A boundary condition (b.c.) will be specified by a configuration  $\bar{\omega}$ , meaning that for any finite volume  $\Lambda \subset \mathcal{L}^3$ , the system is considered with a fixed value for the spins on each  $x \in \mathcal{L}^3 \setminus \Lambda$ , determined by  $\bar{\omega}$ .

From Lemma 19 of Appendix A (in particular (A.75)) it follows that for  $\beta$  and  $U$  large enough, there exist positive constants,  $c_1$  and  $\tilde{c}_2$  (with  $c_1/U < 1$ ) such that:

- for  $|B| \geq 3$

$$|R_B(U)| \leq \tilde{c}_2 \left(\frac{c_1}{U}\right)^{g(B)} \quad (2.9)$$

where

$$g(B) := n(B) - 1 \quad (2.10)$$

with  $n(B)$  being defined as the minimum length (in units of lattice spacing) of a closed path which passes through all sites of  $B$ .

- while, for  $|B| = 2$ ,

$$|R_B(U)| \leq \tilde{c}_2 \left(\frac{c_1}{U}\right)^3 \quad (2.11)$$

The latter bound (2.11) results from the following fact: We have that  $g(B) = 1$  for  $|B| = 2$ ; however, the term in the effective Hamiltonian of order  $U^{-1}$ , has been extracted and is given by the first term on the RHS of (2.6). The contribution from electron hoppings between nearest neighbour sites, to the remainder term, are therefore of order  $U^{-3}$ , as even powers of  $U^{-1}$  do not occur in the expansion.

The above bounds imply that there exists a constant  $r > 0$  such that

$$\sum_{B \ni 0} |R_B(U)| e^{rg(B)} < \infty \quad (2.12)$$

and hence the interaction  $\{R_B(U)\}$  decays exponentially. Using the bound (2.11), the effective Hamiltonian (2.6) can be written as follows

$$\mathcal{H}_A^{\text{eff}}(U) = \mathcal{H}_{0A}^{(2)}(U) + \mathcal{R}_A^{\geq 3}(U) \quad (2.13)$$

with

$$\begin{aligned} \mathcal{H}_{0A}^{(2)}(U) &= \frac{1}{4U} \sum_{\langle xy \rangle \subset A} s'_x s'_y + \sum_{\substack{B \cap A \neq \emptyset \\ |B|=2}} R_B(\beta, U) \\ &= J(U) \sum_{\langle xy \rangle \in A} s'_x s'_y \end{aligned} \quad (2.14)$$

where

$$J(U) := J(\beta, U) \simeq \frac{1}{4U} + \text{h.o.} > 0 \quad (2.15)$$

the symbol ‘‘h.o.’’ denoting terms of higher orders in  $U^{-1}$  which are bounded by  $aU^{-3}$ , for some constant  $a > 0$ . Throughout the rest of the paper, whenever the symbol h.o. appears in a sum involving powers of  $U^{-1}$ , it will denote the presence of a correction term which is bounded by a positive constant times the next odd power of  $U^{-1}$ . The correction term is an infinite series that can be computed order by order in perturbation theory, and that has a dependence on  $\beta$ . This temperature dependence is inessential and we will routinely omit it from the notations. We will only use that, for  $\beta U$  sufficiently large, a bound of the form (2.9) holds. We refer to Appendix A for the proofs of the bounds. A more general class of models as well as a detailed discussion of the temperature dependence of the effective Hamiltonian is contained in ref. 32.

We define

$$\mathcal{R}_A^{\geq 3}(U) := \sum_{\substack{B \cap A \neq \emptyset \\ |B| > 2}} R_B(U) \quad (2.16)$$

The leading part  $\mathcal{H}_{0A}^{(2)}(U)$  of the effective Hamiltonian is identical to the Hamiltonian of an antiferromagnetic Ising model with nearest neighbour interactions of strength  $J(U)$  in the presence of a magnetic field of strength  $h$ .

The fact that the Hamiltonian  $\mathcal{H}_A^{\text{eff}}(U)$  (2.13) is invariant under ‘‘spin-flip,’’ is a consequence of half-filling. The leading part,  $\mathcal{H}_{0A}^{(2)}(U)$  (2.14), of the effective Hamiltonian has two ground states in each of which the  $+$ ’s and  $-$ ’s occupy alternate sites of the lattice, i.e., the antiferromagnetic Néel states. Thus, to order  $U^{-1}$ , the effective Hamiltonian governing the ionic subsystem has a two-fold degenerate ground state, while for the original unperturbed Hamiltonian  $\mathcal{H}_{0A}(U)$  (given by (2.2)) the ground state energy is independent of the ion configuration. Hence, as far as the ionic subsystem is concerned, the effect of the quantum perturbation  $tV$  is to *select*



two ground state configurations from the infinitely many ground states of  $\mathcal{H}_{0A}(U)$ . This phenomenon in which the quantum perturbation lifts the infinite degeneracy of the classical ground states is known as “ground state selection.”<sup>(21, 43)</sup> Moreover, for low enough temperatures, the characteristic long range order of the Néel states persists under the action of the remainder  $\mathcal{R}_A^{\geq 3}$ .<sup>(11)</sup> The main purpose of this paper is to prove that a similar phenomenon of ground state selection occurs for the 111 interface of the FK model and that the selected interfaces are *rigid*, i.e., the interfaces persist in the thermodynamic limit at finite but non-zero temperature. See Section 5.

It will be more convenient for us to perform the transformation

$$s'_x \rightarrow s_x = (-1)^{2|x|} s'_x \quad \text{for all } x = (x_1, x_2, x_3) \in A \quad (2.17)$$

where  $|x| = x_1 + x_2 + x_3$ . The above transformation yields an equivalent Hamiltonian with the leading part given by the *ferromagnetic* Ising model:

$$\mathcal{H}_A^{\text{ferro}}(U) = -J(U) \sum_{\langle xy \rangle \in A} s_x s_y \quad (2.18)$$

where  $J(U)$  is given by (2.15). Let us denote  $s_x = 1$  by the symbol “+” and  $s_x = -1$  by the symbol “−.” The two ground states of  $\mathcal{H}_A^{\text{ferro}}(U)$  are denoted by  $s_+$  and  $s_-$  and correspond to each site in the lattice being occupied by a + and a − respectively. We refer to these two ground state configurations and their low-temperature analogues as *homogeneous phases*. For a finite volume  $A \subset \mathcal{L}^3$ , the boundary conditions defined

$$\begin{aligned} &\text{either by } s_x = +1 && \text{for all } x \in \mathcal{L}^3 \setminus A \\ &\text{or by } s_x = -1 && \text{for all } x \in \mathcal{L}^3 \setminus A \end{aligned} \quad (2.19)$$

are referred to as *homogeneous b.c.*

It is an interesting question what boundary configuration of the effective spin system correspond to bona fide boundary conditions for the original Falicov–Kimball model *without* introducing special boundary interaction terms. It is not hard to see from the derivation of the effective Hamiltonian in ref. 32, that the homogeneous b.c. discussed above, as well as the boundary conditions employed later in this paper to construct interface Gibbs states, can be achieved by imposing Dirichlet boundary conditions for the electrons on a volume with includes the first boundary layer. On the effective Hamiltonian, this has the effect of truncating the interactions across the boundary to nearest neighbour interactions only, which is inconsequential. This simple correspondence between boundary conditions,

however, is only possible because we are considering spin-less fermions, at half-filling and with nearest neighbour hopping only.

In more general situations natural boundary conditions in the original system will lead to modified boundary interactions in the effective spin system. The general strategy adopted in ref. 32 to address this problem is to trace over all possible configurations of static fermions outside the volume  $\mathcal{A}$  under consideration. Due to the Pauli principle, each such configuration of spinless fermions simply defines an excluded volume. This means that the effective Hamiltonian describes a weighted average of Gibbs states obtained with different Dirichlet-type boundary conditions for the fermions. As the fermions can wander across the boundary of  $\mathcal{A}$ , the effective Hamiltonians thus obtained will have interaction terms of arbitrary range across the boundary. As is clear from our analysis here, this kind of “averaged” boundary conditions can equally well be used to demonstrate existence of Gibbs states with interfaces.

As mentioned before, the purpose of this paper is to study the thermodynamic properties of the 100 and 111 interfaces of the three-dimensional FK model. In finite volume, the presence of an interface can be enforced by a suitable choice of *mixed* boundary conditions in the standard way<sup>(15)</sup> (see Eqs. (2.20) and (2.21) below).

To construct the 100 interface Gibbs state we consider  $\mathcal{A} \subset \mathcal{Z}^3$  to be a parallelepiped centered at the origin. The 100 interface is orthogonal to the vector  $\mathbf{n} = (0, 0, 1)$ . The boundary condition which leads to a 100 interface (which we shall refer to as “b.c. 1”) is given as the configuration  $\{s_x\}$  on the sites  $x = (x_1, x_2, x_3) \in \mathcal{A}^c := \mathcal{Z}^3 \setminus \mathcal{A}$  defined by

$$s_x = \begin{cases} +1 & \text{if } x_3 \geq 1/2 \\ -1 & \text{if } x_3 \leq -1/2 \end{cases} \quad (2.20)$$

For an analysis of the 111 interface consider the intersection of a plane passing through the origin and orthogonal to the vector  $\mathbf{n} = (1, 1, 1)$  with a cube  $\mathcal{A} \subset \mathcal{Z}^3$ . This intersection yields a plane bounded by a hexagon (as shown in Fig. 1) which divides  $\mathcal{A}$  into two equal volumes. To obtain a 111 interface we consider the spin variables  $s_x$  (2.17) to have opposite values on the two sides of this dividing plane.

More precisely, the boundary condition that leads to a 111 interface (which we shall refer to as “b.c. 2”) is given as the configuration  $\{s_x\}$  on the sites  $x = (x_1, x_2, x_3) \in \mathcal{A}^c \equiv \mathcal{Z}^3 \setminus \mathcal{A}$  defined by

$$s_x = \begin{cases} +1 & \text{if } x_1 + x_2 + x_3 \geq 1/2 \\ -1 & \text{if } x_1 + x_2 + x_3 \leq -1/2 \end{cases} \quad (2.21)$$

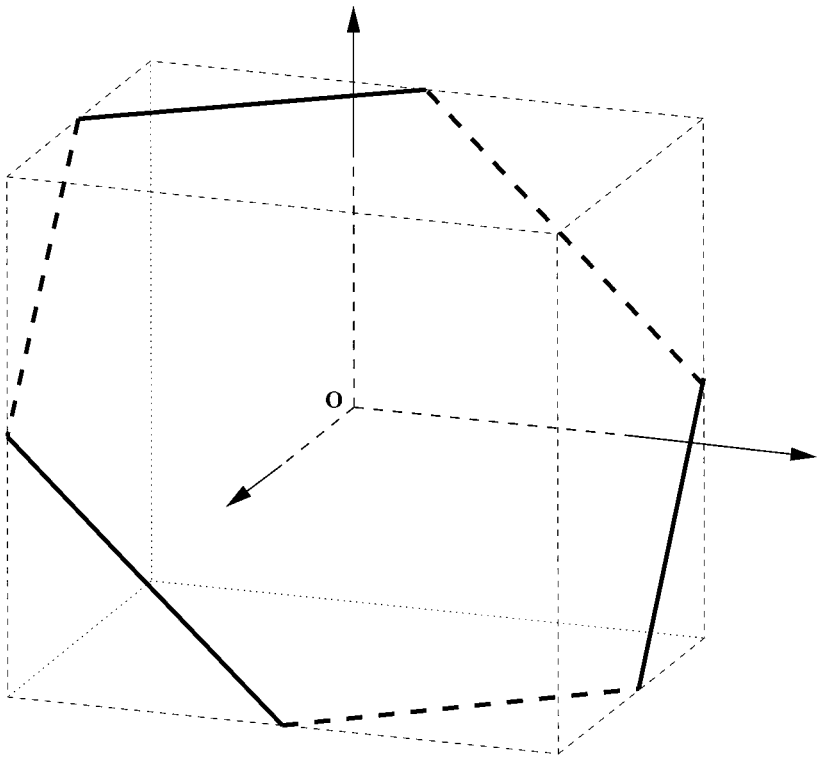


Fig. 1. The intersection of a finite cubic lattice  $\Lambda \subset \mathcal{L}^3$  centered at the origin, with a plane passing through the origin and orthogonal to the vector  $\mathbf{n} = (1, 1, 1)$ .

Each of these boundary conditions divide the volume  $\Lambda$  into two subvolumes (the configuration in the latter being given by the two homogeneous phases  $s_+$  and  $s_-$ ) and enforce the occurrence of an interface (domain wall) pinned to the boundary of the volume. The residual free energy per unit area of this interface is its surface tension and is denoted by the symbol  $\tau^{\text{mixed b.c.}}$ . It is defined by taking the difference of the free energy of the system in the volume  $\Lambda$  under mixed b.c. and the free energy corresponding to the homogeneous b.c.

$$\tau^{\text{mixed b.c.}} = \lim_{\Lambda \nearrow \mathcal{L}^3} -\frac{1}{\beta |I_\Lambda|} \log \left( \frac{\mathcal{E}_\Lambda^{\text{mixed}}}{\mathcal{E}_\Lambda^{\text{hom}}} \right) \quad (2.22)$$

where  $\mathcal{E}_\Lambda^{\text{mixed}}$  and  $\mathcal{E}_\Lambda^{\text{hom}}$  are the partition functions of the system in the finite volume  $\Lambda$  w.r.t. mixed b.c. and homogeneous b.c. respectively (see Section 3). The symbol  $|I_\Lambda|$  denotes the area of the portion of the ground

state interface which is contained in the volume  $\mathcal{A}$ . Such a definition is justified<sup>(34)</sup> since the volume contributions proportional to the free energies of the coexisting phases, as well as the boundary effects, cancel and only the contributions to the free energy of the interface are left.

The limit  $\lim_{\mathcal{A} \nearrow \mathcal{D}^3}$  is taken in a definite order: e.g., if the ground state interface lies in a plane  $P_{\mathbf{n}}$ , passing through the origin, which is orthogonal to a non-zero vector  $\mathbf{n}$ , then the dimensions of the lattice perpendicular to the plane  $P_{\mathbf{n}}$  are taken to infinity before the dimensions parallel to it are taken to infinity. The symbol  $|I_{\mathcal{A}}|$  denotes the area of the portion of the interface which is contained in the volume  $\mathcal{A}$ .

It will be convenient to consider the *relative Hamiltonian* defined with respect to the homogeneous phases  $s_+$  and  $s_-$ . For any configuration  $s = \{s_x\}_{x \in \mathcal{D}^3}$  the relative Hamiltonian is given by

$$\begin{aligned} H_{\mathcal{A}}(s) &:= -J(U) \sum_{\langle xy \rangle \in \mathcal{A}} (s_x s_y - 1) + \sum_{\substack{B \cap \mathcal{A} \neq \emptyset \\ |B| \geq 3}} \Phi_B(s) \\ &:= H_{0\mathcal{A}}^{(2)}(s) + R_{\mathcal{A}}^{\geq 3}(s) \end{aligned} \quad (2.23)$$

where

$$\Phi_B(s) := R_B(s) - R_B(s_+) = R_B(s) - R_B(s_-) \quad (2.24)$$

and  $J(U)$  is given by (2.15). Here are henceforth the explicit  $U$ -dependences of the relative Hamiltonian and its components have been suppressed for notational simplicity.

Each configuration in a finite volume  $\mathcal{A}$ , with respect to fixed boundary conditions (homogeneous or mixed) can be geometrically described by specifying the Ising contours which are defined as follows:<sup>(34)</sup> We define a *face* to be a unit square which bisects a nearest neighbour bond of the lattice perpendicularly. To each nearest neighbour bond we can associate a face. A face  $f$  belongs to  $\mathcal{A}$  if at least one site of the corresponding nearest neighbour bond is in  $\mathcal{A}$ . Given a configuration  $\omega_{\mathcal{A}}$  on a finite lattice  $\mathcal{A}$ , with b.c.  $\bar{\omega}$ , let  $\mathcal{S}^{\bar{\omega}}(\omega_{\mathcal{A}})$  be the set of faces associated with nearest neighbour bonds between opposite spins. Decompose  $\mathcal{S}^{\bar{\omega}}(\omega_{\mathcal{A}})$  into maximally connected pairwise disjoint components. Each such component is referred to as an *Ising contour* (or simply *contour*, if confusion is not likely) and is denoted by the symbol  $\gamma$ . For homogeneous b.c. the contours are closed surfaces lying entirely within the volume  $\mathcal{A}$ . However, for mixed b.c. there is necessarily one (and only one) contour which is pinned to the boundary of the volume  $\mathcal{A}$ . This is the only infinite maximally connected component of the set  $\mathcal{S}^{\bar{\omega}}(\omega_{\mathcal{A}})$  and is referred to as the interface.

There is a one-to-one correspondence between spin configurations on the lattice and non-intersecting families of contours  $\Gamma = \{\gamma\} : \omega_{\mathcal{A}} = \omega_{\mathcal{A}}(\Gamma)$ .

We shall refer to such families as *compatible* families of contours. In the sequel we shall use the symbol  $\gamma$  to denote both the contour and its support. The number of faces in a contour  $\gamma$  is denoted by  $|\gamma|$  and satisfies the bound  $|\gamma| \geq 6$ , since the lattice is three-dimensional. The energy of a contour  $\gamma$  is given by

$$E(\gamma) := H_{0A}^{(2)}(\Gamma' \cup \{\gamma\}) - H_{0A}^{(2)}(\Gamma') \quad (2.25)$$

for any set,  $\Gamma'$ , of non-intersecting contours, not containing  $\gamma$ , such that  $\Gamma' \cup \{\gamma\}$  is again a family of non-intersecting contours.

It follows from (2.23) that the relative energy of a configuration  $\omega_A(\Gamma)$  is given by

$$H_A(\Gamma) = H_{0A}^{(2)}(\Gamma) + R_A^{\geq 3}(\Gamma) \quad (2.26)$$

with

$$H_{0A}^{(2)}(\Gamma) = \sum_{\gamma \in \Gamma} E(\gamma) \quad (2.27)$$

where

$$E(\gamma) = 2J(U) = \left( \frac{1}{2U} + \text{h.o.} \right) |\gamma| =: J_1(U) |\gamma| \quad (2.28)$$

and

$$R_A^{\geq 3}(\Gamma) = \sum_{\substack{B \cap \Gamma \neq \emptyset \\ |B| \geq 3}} \Phi_B(\Gamma) \quad (2.29)$$

The condition  $B \cap \Gamma \neq \emptyset$  denotes that the above sum runs over all bonds  $B$  such that  $B \cap \gamma \neq \emptyset$  for some  $\gamma \in \Gamma$ , i.e., the bond  $B$  intersects at least one face of a contour  $\gamma \in \Gamma$ . The quantity  $E(\gamma)$  is the self-energy of the contour  $\gamma$  w.r.t.  $H_{0A}^{(2)}$ . Its definition (2.28) implies that, for sufficiently large  $U$ , the Hamiltonian  $H_{0A}^{(2)}$  satisfies the Peierls condition:

$$E(\gamma) \geq \mathcal{J} |\gamma| \quad (2.30)$$

with a Peierls constant

$$\mathcal{J} = c_0 U^{-1} \quad (2.31)$$

where  $c_0$  is a positive constant. Moreover, from the definition (2.24) and the bound (2.9) it follows that for  $|B| \geq 3$

$$|\Phi_B| \leq c_2 \left( \frac{c_1}{U} \right)^{g(B)} \quad (2.32)$$

with  $c_2 = 2\tilde{c}_2$ . The effect of the term  $R_A^{\geq 3}(U)$  is to modify the self-energy of the contours and also to introduce interactions between the contours. Hence the spin model is reformulated as a model of interacting contours.

This contour Hamiltonian can be used to prove the rigidity of the 100 interface. However, we show in Section 2.3 that, under the boundary condition b.c.2 (2.21), the leading part  $H_{0A}^{(2)}$  of the Hamiltonian yields infinitely many ground state interfaces in the thermodynamic limit. These interfaces are characterized by the fact that they all have minimal area. We refer to such interfaces as *minimal area interfaces*. Hence, to prove the rigidity of the 111 interface we consider a more detailed decomposition of the relative Hamiltonian in which all the terms up to order  $U^{-3}$  of the perturbation series are computed explicitly and retained in its leading part  $H_{0A}^{(4)}$ :

$$H_A = H_{0A}^{(4)} + R_A^{\geq 5} \quad (2.33)$$

where

$$\begin{aligned} H_{0A}^{(4)} = & - \left( \frac{1}{4U} - \frac{11}{16U^3} + \text{h.o.} \right) \sum_{\langle xy \rangle \subset A} (s_x s_y - 1) \\ & + \left( \frac{3}{16U^3} + \text{h.o.} \right) \sum_{\substack{x, y \in A \\ |x-y|=\sqrt{2}}} (s_x s_y - 1) \\ & + \left( \frac{1}{8U^3} + \text{h.o.} \right) \sum_{\substack{x, y \in A \\ |x-y|=2}} (s_x s_y - 1) \\ & + \left( \frac{5}{16U^3} + \text{h.o.} \right) \sum_{x, y, z, t \in P(A)} (s_x s_y s_z s_t - 1) \end{aligned} \quad (2.34)$$

where  $P(A)$  is the set of *plaquettes*, each plaquette consisting of four lattice sites forming a unit square.

The remainder  $R_A^{\geq 5}$  is obtained from the series (2.29) defining  $R_A^{\geq 3}$  by subtracting all terms which depend on  $U^{-n}$  with  $n \leq 3$ . It is given by

$$R_A^{\geq 5} = \sum_{\substack{B \cap A \neq \emptyset \\ |B| > 3}} \tilde{\Phi}_B \quad (2.35)$$

with the potentials  $\tilde{\Phi}_B$  satisfying the bound

$$|\tilde{\Phi}_B| \leq c_2 \left(\frac{c_1}{U}\right)^{m(B)} \tag{2.36}$$

where

$$m(B) := \max(5, g(B)) \tag{2.37}$$

In the expression for the relative Hamiltonian  $H_{0A}^{(2)}$  (2.23) the terms up to order  $U^{-1}$  are computed explicitly by second order perturbation theory, while the terms of order  $U^{-3}$  in  $H_{0A}^{(4)}$  (2.34) are obtained by fourth order perturbation theory. We shall refer to (2.23) as the second order decomposition of the relative Hamiltonian, and (2.33) as its fourth order decomposition.

In Section 5 we prove that from the infinite set of minimal area interfaces, and up to translations, a unique interface configuration is selected (i.e., attributed minimal energy) by  $H_0^{(4)}$ . This interface and its translations are referred to as *ground state interfaces* of the three-dimensional FK model under the boundary condition b.c.2 (2.21). Hence the 111 interface exhibits ground state selection. Further, we prove that the selected interface is rigid in the sense that it persists under the action of the remainder  $R_A^{\geq 5}(U)$  at sufficiently low temperatures, in the thermodynamic limit.

Our main results are that, for sufficiently large  $U$ , and at sufficiently low temperatures, the Gibbs states obtained in the thermodynamic limit  $A \nearrow \mathcal{Z}^3$  with the boundary conditions b.c.1 and b.c.2, describe rigid interfaces in the 100- and 111 directions respectively. For a precise statement of our main results we introduce the following notations: Let  $\langle \cdot \rangle_{[b.c.1]}$  and  $\langle \cdot \rangle_{[b.c.2]}$  denote the expectation values in the (infinite-volume) Gibbs states with the mixed boundary condition b.c.1 (2.20) and b.c.2 (2.21) respectively. Further, we recall that for a site  $x = (x_1, x_2, x_3)$  in the lattice,  $s_x$  denotes the on-site spin variable defined through (2.7) and (2.17). Using these notations and definitions, we state our main results through the following theorems:

**Theorem 1.** There exist positive constants  $U_0$  and  $D_0$  such that for all  $U > U_0$ , and  $\beta/U > D_0$ , the following bounds are satisfied:

$$\langle s_x \rangle_{[b.c.1]} \geq 1 - 2C_0 e^{-c'\beta/U} \quad \text{for } x_3 \geq 1/2 \tag{2.38}$$

and

$$\langle s_x \rangle_{[b.c.1]} \leq -1 + 2C_0 e^{-c'\beta/U} \quad \text{for } x_3 \leq -1/2 \tag{2.39}$$

where  $C_0$  and  $c'$  are positive constants given in terms of  $U_0$  and  $D_0$ .

**Theorem 2.** There exist positive constants  $\tilde{U}_0$ ,  $\tilde{D}_0$  and  $\tilde{D}'_0$  such that for all  $U > \tilde{U}_0$ ,  $\beta/U > \tilde{D}_0$  and  $\beta/U^3 > \tilde{D}'_0$ , the following bounds are satisfied:

$$\langle s_x \rangle_{[\text{b.c.2}]} \geq 1 - 2\{\tilde{C}_0 e^{-c''\beta/U^3} + \tilde{C}_1 e^{-c'_1\beta/U}\} \quad \text{for } x_1 + x_2 + x_3 \geq 1/2 \quad (2.40)$$

and

$$\langle s_x \rangle_{[\text{b.c.2}]} \leq -1 + 2\{\tilde{C}_0 e^{-c''\beta/U^3} + \tilde{C}_1 e^{-c'_1\beta/U}\} \quad \text{for } x_1 + x_2 + x_3 \leq -1/2 \quad (2.41)$$

where  $\tilde{C}_0$ ,  $c''$ ,  $\tilde{C}_1$  and  $c'_1$  are positive constants given in terms of  $\tilde{U}_0$ ,  $\tilde{D}_0$  and  $\tilde{D}'_0$ .

To prove these results we follow the method introduced by Dobrushin<sup>(15)</sup> and consider effective two-dimensional models of the 100- and 111 interfaces, obtained by projecting the interfaces on the planes defined by  $x_3 = 0$  and  $x_1 + x_2 + x_3 = 0$  respectively [see Section 1 and 2.2 for details] The rigidity of the interfaces follows from an analysis of the low-temperature properties of these effective two-dimensional models.

## 2.1. The Geometry of 100 Interfaces

The geometry of the 100 interfaces of the FK model is the same as the geometry of the 100 interfaces described by Dobrushin for the three dimensional Ising model. Hence we refer to ref. 15 for the definitions of geometrical objects which describe the interfaces and their significances as configurations of a two dimensional (contour) model: the *ceilings* (which project on to ground states of the two dimensional model), the *walls* (which project on to the contours), and the *standard walls* (which project on to the external contours).

## 2.2. The Geometry of 111 Interfaces

The geometry of the 111 interfaces of the FK model is much more involved. Let  $\tilde{\mathcal{F}}$  denote the family of interfaces under the b.c.2 (2.21) and  $\tilde{I}$  denote its typical element. Such an interface is pinned at the boundary of  $A$  on the curve defined by

$$\partial A \cap \{(x, y, z) \in \mathbb{Z}^3 \mid x + y + z = 0\} \quad (2.42)$$



In this section we describe the underlying geometrical structure necessary for the definition and study of the effective two-dimensional model for such an interface.

For each integer  $n$  we define planes  $P_n \subset \mathbb{Z}^3 \subset \mathbb{R}^3$  orthogonal to the vector  $\hat{n} = (1, 1, 1)$ , by  $P_n = \{(x, y, z) \in \mathbb{Z}^3 \mid x + y + z = n\}$ . Let  $\mathbb{P}$  denote the plane in  $\mathbb{R}^3$  which contains  $P_0$ . Let  $\mathcal{P}$  denote the orthogonal projection onto  $\mathbb{P}$  and let  $\mathbb{P}_A$  denote the portion of the plane  $\mathbb{P}$  which is contained in the volume  $A$ .

An effective two-dimensional model for the 111 interface is obtained by an orthogonal projection of the interface  $\tilde{I}$  onto  $\mathbb{P}$ . Its complete description requires the following ingredients:

1. A set of *vertices*  $\mathcal{V} = \mathcal{V}_0 \cup \mathcal{V}_1 \cup \mathcal{V}_2$ , where  $\mathcal{V}_{n \bmod 3} \equiv \mathcal{P}(P_n)$ ,  $n \in \mathbb{Z}$ , is a triangular lattice in  $\mathbb{P}$  with lattice constant  $\sqrt{2}$ . The set  $\mathcal{V}$  also forms a triangular lattice, but with lattice constant  $\sqrt{2/3}$ .
2. A set of *edges*  $\mathcal{E} = \mathcal{E}_{01} \cup \mathcal{E}_{12} \cup \mathcal{E}_{20}$ , where  $\mathcal{E}_{ij}$  is the set of nearest neighbour edges in the lattice  $\mathcal{V}_i \cup \mathcal{V}_j$ . All edges have Euclidean length  $\sqrt{2/3}$ .
3. A set of *triangles*  $\mathcal{T}$  consisting of all elementary triangles in  $\mathcal{V}$ .
4. A set of *rhombi*  $\mathcal{R} = \mathcal{R}_0 \cup \mathcal{R}_1 \cup \mathcal{R}_2$ , where  $\mathcal{R}_i$  is the set of all rhombi formed by two triangles in  $\mathcal{T}$  that share an edge  $e \in \mathcal{E}_{\{012\} \setminus \{i\}}$ ,  $i = 0, 1, 2$ .

The set of vertices  $\mathcal{V}$  is the projection of the vertices in  $\mathbb{Z}^3$ , and  $\mathcal{P}((x, y, z)) \in \mathcal{V}_i$  if and only if  $i = (x + y + z) \bmod 3$ .

The set of edges  $\mathcal{E}$  is the projection of the set of nearest neighbour bonds in  $\mathbb{Z}^3$ . They are the edges of a triangular lattice with lattice constant  $\sqrt{2/3}$ . For each pair of distinct  $i, j \in \{0, 1, 2\}$ , the set of vertices  $\mathcal{V}_i \cup \mathcal{V}_j$  forms a triangular lattice  $\mathcal{H}_{ij}$  (also with lattice constant  $\sqrt{2/3}$ ), and with edges  $\mathcal{E}_{ij}$ . Together the three  $\mathcal{H}_{ij}$  cover  $\mathcal{V}$  twice.

As before, to each nearest neighbour bond in the lattice  $\mathbb{Z}^3$  we associate a unit square (face) which bisects it perpendicularly. Recall that the vertices of such a face have integer coordinates. The rhombi in  $\mathcal{R}$  are the projections of these faces. Hence, an interface  $\tilde{I}$  in the lattice  $A$  projects onto a covering of the plane  $\mathbb{P}_A$  with rhombi in  $\mathcal{R}$ . We refer to such a rhombus covering as a *rhombus configuration* or, for brevity, as an *R-configuration* (to be distinguished from a configuration of Ising contours).

- A rhombus is said to be an *overlapping* one if it contains the projection of more than one face of the interface. Otherwise it is said to be *non-overlapping*. Each triangle  $t$  in an *R-configuration*  $\mathcal{C}_A$  necessarily belongs to the projection of an odd number of faces of the interface. To each such

triangle  $t$  we associate a number  $o(t)$  which we refer to as its *overlap number*, and define as follows:

$$o(t) := \left\{ \begin{array}{l} \text{the number of faces of the interface} \\ \text{whose projection contains } t \end{array} \right\} - 1 \quad (2.43)$$

A triangle with a non-zero overlap number is referred to as an overlapping triangle. It is evident that each overlapping triangle has an even overlap number.

- Two non-overlapping rhombi which share an edge are said to form a *good pair* if the angle enclosed by them is  $2\pi/3$ , i.e., if up to translations and rotations the pair is as shown in Fig. 2. The edge shared by such a pair is referred to as a *good edge*. We consider the good pairs as open complexes. This means that a good pair is composed of an open edge together with the two adjacent open rhombi. Two good pairs are connected if their intersection is an open rhombus.

- We define the *type* of a rhombus  $r$ ,  $\tau(r)$ , to be  $j$  if  $r \in \mathcal{R}_j$ , with  $j \in \{0, 1, 2\}$ .

Let a *tiling* of the plane  $\mathbb{P}$  be defined as a complete covering of  $\mathbb{P}$  with non-overlapping rhombi in  $\mathcal{R}$ . For each pair of distinct  $i, j \in \{0, 1, 2\}$  the set of edges  $\mathcal{E} \setminus \mathcal{E}_{ij}$  drawn in the plane  $\mathbb{P}$  yield a tiling of  $\mathbb{P}$  with the rhombi in  $\mathcal{R}_{\{012\} \setminus \{ij\}}$ . Minimal area interfaces and ground state interfaces have simple geometric descriptions in terms of tilings (see Section 2.3).

The mixed boundary condition b.c.2 translates into a boundary condition for the  $R$ -configuration in  $\mathbb{P}_A$ . It is given by a tiling of  $\mathbb{P} \setminus \mathbb{P}_A$  with rhombi of a single type, say  $\mathcal{R}_0$ . We call this the *standard b.c.* for the rhombus model.

### 2.3. The Minimal Area Interfaces

An interface  $\tilde{I}$  is of minimal area if and only if its projection  $\mathcal{P}(\tilde{I})$  is a tiling of  $\mathbb{P}$ . Equivalently each such tiling is in one-to-one correspondence

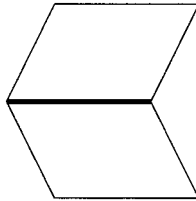


Fig. 2. A pair of rhombi in *good position*. The edge shared by the two rhombi is referred to as a *good edge*.

with a dimer covering of the hexagonal lattice dual to the triangular lattice  $\mathcal{V}$ , i.e., of the lattice with set of sites given by the centers of the triangles in  $\mathcal{T}$ . It is less obvious, although also a well-known fact in enumerative combinatorics,<sup>(28, 45)</sup> that all tilings of  $\mathbb{P}$  with rhombi in  $\mathcal{R}$  correspond to a unique minimal area interface. This is shown in the following proposition. The proof is constructive, i.e., it provides an algorithm for obtaining the interface from the tiling and vice versa.

**Proposition 3.** The tilings of the plane  $\mathbb{P}$  with rhombi in  $\mathcal{R}$  under standard b.c. are in one-to-one correspondence with the minimal area interfaces in the volume  $A$  under the mixed boundary condition b.c.2 (2.21).

*Proof.* As noted above it is obvious that each minimal area interface under the boundary condition b.c.2 (2.21) projects onto a tiling of  $\mathbb{P}_A$  with rhombi in  $\mathcal{R}$ . Hence, we only need to show that to each tiling there corresponds exactly one interface that has that tiling as its projection. The interface will automatically be minimal. This amounts to associating a unique face of  $\mathbb{Z}^3$  to each rhombus in the tiling such that the resulting set of faces form a connected set which is pinned at the boundary of  $A$  along the curve defined by (2.42). The projection of the set of faces constituting an interface  $\tilde{I}$  yields a set of rhombi in  $\mathcal{R}$  that covers  $\mathbb{P}_A$ . For each face  $f$  we can number its vertices  $a_1, a_2, a_3, a_4$  in such a way that there is a unique integer  $n(f)$  for which

$$a_1 \in P_{n(f)-1}, \quad a_2 \in P_{n(f)}, \quad a_3 \in P_{n(f)+1}, \quad a_4 \in P_{n(f)}$$

It is easy to see that if  $\mathcal{P}(f) = r \in \mathcal{R}_i, i = 0, 1, 2$ , then  $i = n(f) \bmod 3$ , and that  $\mathcal{P}(f)$  and  $n(f)$  uniquely determine  $f$ .

For any tiling with standard boundary conditions we will construct a unique *height function*  $h: \mathcal{V} \rightarrow \mathbb{Z}$  with the property that for each rhombus  $r$  in the tiling the heights of its vertices, when ordered appropriately, and such that  $\{v_i, v_{i+1}\}$  are edges of  $r$ , are given by

$$h(v_1) = n - 1, \quad h(v_2) = n, \quad h(v_3) = n + 1, \quad h(v_4) = n$$

for some integer  $n$  satisfying  $i = n \bmod 3$  iff  $r \in \mathcal{R}_i$ . It follows that  $h$  satisfies  $|h(v) - h(w)| = 1$  for each edge  $\{v, w\}$  of a rhombus in the tiling. A minimal area interface in  $A$  under the b.c.2 (2.21) is an interface whose projection on the plane  $\mathbb{P}_A$  is a tiling. It consists of all faces  $\{f\}$  in  $A$  for which:

1.  $\mathcal{P}(f)$  is a rhombus in the tiling, and
2. the vertices  $v_i$  of  $\mathcal{P}(f)$  satisfy  $\{h(v_i) \mid 1 \leq i \leq 4\} = \{n(f) - 1, n(f), n(f) + 1\}$ .

It remains to construct the *height function*  $h$  and to verify that it is the unique function with the stated properties. Let us denote by  $\vec{e}_1, \dots, \vec{e}_6$  the vectors of minimal length ( $=\sqrt{2/3}$ ), emanating from a single point of the triangular lattice (spanned by the edges in  $\mathcal{E}$ ) such that the tips of these vectors are the vertices of a hexagon. See Fig. 3. For any two vertices  $v, w \in \mathcal{V}$  for which  $\{v, w\}$  is an edge in a tiling of  $\mathbb{P}$ ,  $\vec{w} - \vec{v}$  is one of  $\vec{e}_i$ . Let us denote by  $\theta(\vec{e}_i, \vec{e}_j)$  the angle between  $\vec{e}_i$  to  $\vec{e}_j$ , which is a multiple of  $\pi/3$ . We claim that for each tiling there is a unique height function  $h$  satisfying

$$h(w) - h(v) = \begin{cases} +1 & \text{if } \theta(\vec{e}_1, \vec{w} - \vec{v}) \text{ is an even multiple of } \pi/3 \\ -1 & \text{if } \theta(\vec{e}_1, \vec{w} - \vec{v}) \text{ is an odd multiple of } \pi/3 \end{cases}$$

for each edge  $\{v, w\}$  of a rhombus in the tiling. The height function  $h$  must then be obtained by summing up the above differences along edges, starting from a convenient reference value on the boundary of  $\mathbb{P}_A$ . Consistency of this definition follows from the elementary observations that

1. any two paths connecting the same pair of vertices and consisting of edges in the tiling, together enclose a bounded subset of the plane tiled with rhombi, and
2. for any rhombus the differences  $h(w) - h(v)$  along the four edges of a rhombi sum up to zero because the rhombus has two angles of  $\pi/3$  and two of  $2\pi/3$ .

Then the uniqueness of  $h$  is also obvious.

Note that the height function  $h$  has been defined such that the height of any vertex in the tiling is equal to the sum of the coordinates of the point in the interface of which it is the projection. ■

**Proposition 4.** The number of minimal interfaces  $N_A$  grows exponentially with the area of the interface and satisfies the bounds:

$$2^{|I_A|/3} \leq N_A \leq 2^{2|I_A|}$$

where  $|I_A|$  is the area of the minimal area interfaces in the volume  $A$ .

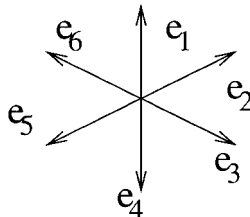


Fig. 3. The labeling of the six unit vectors emanating from a site of the triangular lattice.

*Proof.* Consider the interface defined by the  $\mathcal{R}_0$  tiling, and pick one of the three hexagonal sublattices of the vertices. Note that, independently of each other, each hexagon can be tiled in two ways with three rhombi. This proves the lower bound.

The upper bound is obtained by considering the hexagonal lattice dual to the triangular lattice. Since every tiling is in one-to-one correspondence with a dimer covering of this hexagonal lattice, it is also in one-to-one correspondence with a path covering of the hexagonal lattice, restricted by the condition that at each site the incidence of the path is two. The upper bound is just the straightforward bound on the number of paths given by

$$2^l \quad \text{where } l \text{ is the length of the path}$$

As the path is covering, the length of the path equals the number of bonds in the hexagonal lattice which equals twice the number of rhombi needed to tile the region, i.e., twice the area. ■

Note that the exact rate of exponential growth of the degeneracy depends on the shape of the finite volumes.<sup>(41)</sup>

From Proposition 4 it follows that in the limit  $A \nearrow \mathcal{L}^3$  there are infinitely many minimal area interfaces.

### 3. THE RELEVANT PARTITION FUNCTIONS

We shall define the partition functions of the FK model in terms of the second- and fourth order decompositions of the relative Hamiltonian. These are defined through (2.23)–(2.24) and (2.33)–(2.35) respectively. Such definitions are justified because the quantity relevant for the study of an interface is not a solitary partition function but rather the quotient of two partition functions, namely, a partition function corresponding to mixed b.c. and one corresponding to homogeneous b.c. (see (2.22)). The use of relative Hamiltonians in the definition of the partition functions corresponds to the simultaneous subtraction of the energy of a homogeneous phase from the Hamiltonians appearing in the numerator and denominator of the quotient and hence keeps the quotient unchanged.

Let  $\mathcal{E}_A^+$  and  $\mathcal{E}_A^-$  be the partition functions in  $A \subset \mathcal{L}^3$  w.r.t. the homogeneous boundary conditions defined by (2.19). The spin-flip symmetry of the effective Hamiltonian  $\mathcal{H}_A^{\text{eff}}(U)$  (2.13), for the choice  $h = 0$ , implies that

$$\mathcal{E}_A^+ = \mathcal{E}_A^- := \mathcal{E}_A^{\text{hom}} \quad (3.1)$$

Let  $\mathcal{E}_A^{100}$  and  $\mathcal{E}_A^{111}$  be the corresponding partition functions under the mixed boundary conditions b.c.1 (2.20) and b.c.2 (2.21) respectively.

A mixed b.c. (b.c.1 (2.20) or b.c.2 (2.21)) leads to the appearance of an interface  $I$  which divides the volume  $A$  into two subvolumes  $A_I^a$  and  $A_I^b$  which are, respectively, the regions above and below  $I$ . The configuration in these subvolumes are defined by finite sets of compatible contours  $\Gamma^a := \{\gamma_1^a, \dots, \gamma_p^a\}$  and  $\Gamma^b = \{\gamma_1^b, \dots, \gamma_q^b\}$  respectively. We define  $\Gamma := \Gamma^a \cup \Gamma^b$  and denote a configuration on the lattice by  $(I \cup \Gamma)$ . Let  $\mathcal{I}$  and  $\tilde{\mathcal{I}}$  denote the families of interfaces resulting from b.c.1 and b.c.2 respectively. Let  $I$  and  $\tilde{I}$  denote their typical elements.

In terms of the second order decomposition (2.26) of the relative Hamiltonian  $H_A$ , the partition function for homogeneous b.c. is given by

$$\Xi_A^{\text{hom}} = \sum_{\Gamma = \{\gamma_1, \dots, \gamma_n\} \subset A} \prod_{i=1}^n e^{-\beta J_1(U) |\gamma_i|} \prod_{\substack{|B| > 2 \\ B \cap \Gamma \neq \emptyset}} e^{-\beta \Phi_B(\Gamma)} \quad (3.2)$$

where  $J_1(U) \simeq (1/2U) + \text{h.o.}$ . The partition function relevant for the mixed boundary condition b.c.1 (2.20) is also obtained by using Eqs. (2.26)–(2.29). It is given by

$$\Xi_A^{100} = \sum_{I \in \mathcal{I}} \sum_{\Gamma := \Gamma^a \cup \Gamma^b} e^{-\beta \mathcal{E}_1(I \cup \Gamma)} \quad (3.3)$$

where  $\mathcal{E}_1(I \cup \Gamma)$  is the energy of the configuration  $(I \cup \Gamma)$ . It is the value that the relative Hamiltonian  $H_A$  takes on the configuration  $(I \cup \Gamma)$ :

$$\begin{aligned} \mathcal{E}_1(I \cup \Gamma) &= \sum_{\gamma^a \in \Gamma^a} J_1(U) |\gamma^a| + \sum_{\gamma^b \in \Gamma^b} J_1(U) |\gamma^b| + J_1(U) |I| \\ &+ \sum_{\substack{B: |B| \geq 3 \\ B \cap (I \cup \Gamma) \neq \emptyset}} \Phi_B(I \cup \Gamma) \end{aligned} \quad (3.4)$$

The first three terms on the r.h.s. of (3.4) are the energies of the contours in the configuration  $(I \cup \Gamma)$  as defined through (2.25). The third term is the energy of interaction among these contours and arises from the long-range tail potential  $R_A^{\geq 3}$  (2.29) of the relative Hamiltonian  $H_A$ .

Let  $(I \cup \emptyset)$  denote a configuration which consists only of the interface  $I$  and no other contours. The energy of such a configuration can be interpreted as the “bare” energy of the interface, i.e., the energy of the interface in the absence of any other contour. Let us denote this energy by  $E_1^{\text{bare}}(I)$ . It is given by

$$E_1^{\text{bare}}(I) := J_1(U) |I| + \sum_{\substack{B: |B| \geq 3 \\ B \cap I \neq \emptyset}} \Phi_B(I \cup \emptyset) \quad (3.5)$$

From (2.28) and (2.32) it follows that for sufficiently large  $U$ , the energy  $E_1^{\text{bare}}(I)$  satisfies the bound

$$|E_1^{\text{bare}}(I)| \leq \text{const.} \frac{1}{U} |I| \quad (3.6)$$

It is convenient to isolate the “bare” energy of the interface from the remaining terms in the expression (3.4) for  $\mathcal{E}_1(I \cup \Gamma)$ . From (3.4) and (3.5) it follows that

$$\mathcal{E}_1(I \cup \Gamma) = \sum_{\gamma \in \Gamma} E(\gamma) + E_1^{\text{bare}}(I) + \tilde{E}_1(I \cup \Gamma) \quad (3.7)$$

with

$$\begin{aligned} \tilde{E}_1(I \cup \Gamma) &= \sum_{\substack{B: |B| \geq 3 \\ B \cap (I \cup \Gamma) \neq \emptyset}} \Phi_B(I \cup \Gamma) - \sum_{\substack{B: |B| \geq 3 \\ B \cap I \neq \emptyset}} \Phi_B(I \cup \emptyset) \\ &= \sum_{\substack{B: |B| \geq 3 \\ B \cap (I \cup \Gamma) \neq \emptyset}} \{ \Phi_B(I \cup \Gamma) - \chi(B \cap I \neq \emptyset) \Phi_B(I \cup \emptyset) \} \\ &:= \sum_{\substack{B: |B| \geq 3 \\ B \cap (I \cup \Gamma) \neq \emptyset}} \Phi'_B(I \cup \Gamma) \end{aligned} \quad (3.8)$$

where  $\chi(\cdot)$  denotes the characteristic function. Note that

$$\Phi'_B(I \cup \emptyset) = 0 \quad \text{if } B \cap \Gamma = \emptyset \quad (3.9)$$

Hence, the functions  $\Phi'_B$  for which  $B$  intersects *only* the interface, do not contribute to the energy  $\tilde{E}_1(I \cup \Gamma)$ . The contributions of such bonds is included in the “bare” energy  $E_1^{\text{bare}}(I)$  of the interface.

A non-zero  $\Phi'_B(I \cup \emptyset)$  arises only from those bonds  $B$  which intersect at least one contour in  $\Gamma$ . This observation allows us to write  $\tilde{E}_1(I \cup \Gamma)$  as follows.

$$\tilde{E}_1(I \cup \Gamma) = \sum_{\substack{B: |B| \geq 3 \\ B \cap \Gamma \neq \emptyset}} \Phi'_B(I \cup \Gamma) \quad (3.10)$$

Further, it follows from (2.32) that  $\Phi'_B(I \cup \Gamma)$  satisfies the bound

$$|\Phi'_B(I \cup \Gamma)| \leq |\Phi_B(I \cup \Gamma)| + |\Phi_B(I \cup \emptyset)| < 2c_2 \left(\frac{c_1}{U}\right)^{g(B)} \tag{3.11}$$

for  $|B| \geq 3$ . For bonds  $B$  which do not intersect the interface  $I$ ,

$$\Phi'_B(I \cup \Gamma) = \Phi_B(I \cup \Gamma) \tag{3.12}$$

The partition function for the boundary condition b.c.1, defined by (3.3) is hence given by

$$\begin{aligned} \Xi_A^{100} &= \sum_{I \in \mathcal{F}} e^{-\beta E_1^{\text{bare}}(I)} \times \sum_{\Gamma^a = \{\gamma_1^a, \dots, \gamma_p^a\} = A_I^a} \sum_{\Gamma^b = \{\gamma_1^b, \dots, \gamma_q^b\} = A_I^b} e^{-\beta \tilde{E}_1(I \cup \Gamma)} \\ &\times \prod_{j=1}^p e^{-\beta J_1(U) |\gamma_j^a|} \times \prod_{k=1}^q e^{-\beta J_1(U) |\gamma_k^b|} \end{aligned} \tag{3.13}$$

with  $E_1^{\text{bare}}(I)$  and  $\tilde{E}_1(I \cup \Gamma)$  being defined through (3.5) and (3.10) respectively. The partition function for the boundary condition b.c.2 (2.21) can be similarly written as

$$\Xi_A^{111} = \sum_{\tilde{I} \in \tilde{\mathcal{F}}} \sum_{\Gamma := \Gamma^a \cup \Gamma^b} e^{-\beta \mathcal{E}_2(\tilde{I} \cup \Gamma)} \tag{3.14}$$

where  $\mathcal{E}_2(\tilde{I} \cup \Gamma)$  is the energy of the configuration  $(\tilde{I} \cup \Gamma)$ . In order to determine whether the 111 interface is rigid, it is necessary to use the fourth order decomposition [Eqs. (2.33)–(2.35)] of the relative Hamiltonian  $H_A$ , for computing the contribution of the interface  $\tilde{I}$  to the energy  $\mathcal{E}_2(\tilde{I} \cup \Gamma)$ . However, it is sufficient to consider the second order decomposition [Eqs. (2.26)–(2.29)] for evaluating the corresponding contribution of the contours in  $\Gamma$ . We first introduce some notations which are useful in evaluating  $\mathcal{E}_2(\tilde{I} \cup \Gamma)$ .

- Let  $P_{\tilde{I}} \subset P(\mathcal{A})$  denote the set of plaquettes in  $\mathcal{Z}^3$  which are intersected by the faces of  $\tilde{I}$ . Let  $p$  denote a typical element in this set.
- Let  $B_{\tilde{I}}^2 \subset \mathcal{Z}^3$  denote the set consisting of pairs of next nearest neighbour sites,

$$\{\{x, z\} \in \mathcal{Z}^3 \mid |x - z| = 2\} \tag{3.15}$$

such that the line joining each pair is intersected by a face in  $\tilde{I}$ .



From (2.33)–(2.35), it follows that the energy  $\mathcal{E}_2(\tilde{\Gamma} \cup \Gamma)$  is given by

$$\begin{aligned}
 \mathcal{E}_2(\tilde{\Gamma} \cup \Gamma) &= J_2(U) |\tilde{\Gamma}| + \left( \frac{1}{8U^3} + \text{h.o.} \right) \sum_{\{x, z\} \in B_{\tilde{\Gamma}}^2} h_{\{x, z\}}(\tilde{\Gamma}) \\
 &+ \left( \frac{1}{16U^3} + \text{h.o.} \right) \sum_{p=\{x, y, z, t\} \in P_{\tilde{\Gamma}}} h_p(\tilde{\Gamma}) \\
 &+ \sum_{\substack{B: |B| > 3 \\ B \cap \tilde{\Gamma} \neq \emptyset}} \tilde{\Phi}_B(\tilde{\Gamma} \cup \Gamma) + \sum_{\gamma^a \in \Gamma^a} J_1(U) |\gamma^a| \\
 &+ \sum_{\gamma^b \in \Gamma^b} J_1(U) |\gamma^b| + \sum_{\substack{B: |B| > 2 \\ B \cap \Gamma \neq \emptyset \\ B \cap \tilde{\Gamma} = \emptyset}} \Phi_B(\tilde{\Gamma} \cup \Gamma) \quad (3.16)
 \end{aligned}$$

where

$$h_p := 5(s_x s_y s_z s_t - 1) + 3(s_x s_z + s_y s_t - 2) \quad (3.17)$$

for each  $p = \{x, y, z, t\} \in P_{\tilde{\Gamma}}$ ,

$$h_{\{x, z\}} := s_x s_z - 1 \quad (3.18)$$

for each  $\{x, z\} \in B_{\tilde{\Gamma}}^2$ , and

$$J_2(U) \simeq \frac{1}{2U} - \frac{11}{8U^3} + \text{h.o.} \quad (3.19)$$

Let  $(\tilde{\Gamma} \cup \emptyset)$  denote a configuration which has the interface  $\tilde{\Gamma}$  as its only contour. We denote the corresponding “bare” energy of the interface by  $E_2^{\text{bare}}(\tilde{\Gamma})$ . It is defined as follows.

$$\begin{aligned}
 E_2^{\text{bare}}(\tilde{\Gamma}) &:= J_2(U) |\tilde{\Gamma}| + \left( \frac{1}{8U^3} + \text{h.o.} \right) \sum_{\{x, z\} \in B_{\tilde{\Gamma}}^2} h_{\{x, z\}}(\tilde{\Gamma}) \\
 &+ \left( \frac{1}{16U^3} + \text{h.o.} \right) \sum_{p=\{x, y, z, t\} \in P_{\tilde{\Gamma}}} h_p(\tilde{\Gamma}) \\
 &+ \sum_{\substack{B: |B| > 3 \\ B \cap \tilde{\Gamma} \neq \emptyset}} \tilde{\Phi}_B(\tilde{\Gamma} \cup \emptyset) \quad (3.20)
 \end{aligned}$$

The partition function for the boundary condition b.c.2 can be expressed as follows:

$$\begin{aligned} \Xi_A^{111} &= \sum_{\tilde{I} \in \mathcal{F}} e^{-\beta E_2^{\text{bare}}(\tilde{I})} \times \sum_{\Gamma^a = \{\gamma_1^a, \dots, \gamma_p^a\} \subset A_{\tilde{I}}^a} \sum_{\Gamma^b = \{\gamma_1^b, \dots, \gamma_q^b\} \subset A_{\tilde{I}}^b} e^{-\beta \tilde{E}_2(\tilde{I} \cup \Gamma)} \\ &\quad \times \prod_{j=1}^p e^{-\beta J_1(U) |\gamma_j^a|} \times \prod_{k=1}^q e^{-\beta J_1(U) |\gamma_k^b|} \end{aligned} \tag{3.21}$$

where

$$\begin{aligned} \tilde{E}_2(\tilde{I} \cup \Gamma) &:= \sum_{\substack{B: |B| \geq 3 \\ B \cap \Gamma \neq \emptyset \\ B \cap \tilde{I} = \emptyset}} \Phi_B(\tilde{I} \cup \Gamma) + \sum_{\substack{B: |B| > 3 \\ B \cap \tilde{I} \neq \emptyset}} \tilde{\Phi}_B(\tilde{I} \cup \Gamma) \\ &\quad - \sum_{\substack{B: |B| > 3 \\ B \cap \tilde{I} \neq \emptyset}} \tilde{\Phi}_B(\tilde{I} \cup \emptyset) \\ &= \sum_{\substack{B: |B| \geq 3 \\ B \cap \Gamma \neq \emptyset \\ B \cap \tilde{I} = \emptyset}} \Phi_B(\tilde{I} \cup \Gamma) + \sum_{\substack{B: |B| > 3 \\ B \cap \Gamma \neq \emptyset}} (\tilde{\Phi}_B(\tilde{I} \cup \Gamma) - \tilde{\Phi}_B(\tilde{I} \cup \emptyset)) \\ &= \sum_{\substack{B: |B| \geq 3 \\ B \cap \Gamma \neq \emptyset \\ B \cap \tilde{I} = \emptyset}} \Phi_B(\tilde{I} \cup \Gamma) + \sum_{\substack{B: |B| > 3 \\ B \cap \Gamma \neq \emptyset}} \tilde{\Phi}'_B(\tilde{I} \cup \Gamma) \end{aligned} \tag{3.22}$$

where we have defined the quantity

$$\tilde{\Phi}'_B(\tilde{I} \cup \Gamma) := \tilde{\Phi}_B(\tilde{I} \cup \Gamma) - \tilde{\Phi}_B(\tilde{I} \cup \emptyset) \tag{3.23}$$

It satisfies the bound

$$|\tilde{\Phi}'_B(\tilde{I} \cup \Gamma)| \leq 2c_2 \left(\frac{c_1}{U}\right)^{m(B)} \tag{3.24}$$

where  $m(B)$  is defined through (2.37).

We prove in Sections 4 and 5 that the 100 and 111 interfaces are rigid at low temperatures. The term dependent on the area of the interface, in the expression (3.5) for the “bare” energy  $E_1^{\text{bare}}(I)$  of the interface, is responsible for the rigidity of the 100 interface. However, for the 111 interface, the corresponding area-dependent term in the expression for the “bare” energy  $E_2^{\text{bare}}(I)$  of the interface is not sufficient for stabilizing it against thermal fluctuations. The rigidity at low temperatures results instead from the geometry-dependent contribution of the plaquette potential  $h_p(\tilde{I} \cup \emptyset)$  to the energy of the interface (i.e., the third term on the RHS of (3.20)).

The proofs of these results involve an analysis of the convergence properties of the partition functions  $\Xi_A^{\text{hom}}$ ,  $\Xi_A^{100}$  and  $\Xi_A^{111}$  in the limit  $A \nearrow \mathcal{Z}^3$ . A direct application of the method of cluster expansion requires the contours to be non-interacting. This means that the energy of a configuration is given by a sum of terms, each depending on only one contour in the corresponding compatible family. This is not true for the FK model, because the long range interactions in its effective Hamiltonian induce interactions among the contours. We overcome this technical difficulty by rewriting the partition functions in terms of configurations of non-interacting but more complicated contours called *decorated contours*. In the next section we define the decorated contours and derive expressions for the partition functions in terms of them.

### 3.1. Decorated Contours

Let us first explain how we express the partition function of a system under homogeneous boundary conditions (2.19) in terms of decorated contours. The partition function for homogeneous b.c. is given by (3.2), which we repeat here for convenience.

$$\Xi_A^{\text{hom}} = \sum_{\Gamma = \{\gamma_1, \dots, \gamma_n\} \subset A} \prod_{i=1}^n e^{-\beta J_1(U) |\gamma_i|} \prod_{\substack{|B| > 2 \\ B \cap \Gamma \neq \emptyset}} e^{-\beta \Phi_B(\Gamma)} \quad (3.25)$$

By convention we treat empty products as unity. The idea is to analyze the effect of the dominant part  $H_{0A}^{(2)}(U)$  of the relative Hamiltonian (2.23) by a low temperature expansion in terms of its contours  $\gamma$ , while treating the contribution of the long range tail,  $R_A^{\geq 3}$ , by a high temperature expansion.<sup>(12, 37)</sup> Hence, we write

$$\begin{aligned} \Xi_A^{\text{hom}} &= \sum_{\Gamma \subset A} \prod_{\gamma \in \Gamma} e^{-\beta J_1(U) |\gamma|} \prod_{\substack{B \cap \Gamma \neq \emptyset \\ |B| \geq 3}} [(e^{-\beta \Phi_B} - 1) + 1] \\ &= \sum_{\Gamma \subset A} \prod_{\gamma \in \Gamma} e^{-\beta J_1(U) |\gamma|} \\ &\quad \times \left[ 1 + \sum_{n \geq 1} \sum_{\substack{B_1, \dots, B_n \\ B_i \cap \Gamma \neq \emptyset \\ |B_i| > 2; (i = 1 \dots n)}} \prod_{i=1}^n (e^{-\beta \Phi_{B_i}} - 1) \right] \end{aligned} \quad (3.26)$$

To each term on the RHS of (3.26) we can associate a finite set of compatible contours and a set of bonds, each bond intersecting the support of

at least one contour in the set. More precisely, a *decorated contour* is defined by the pair

$$D = (\Gamma_D, \mathcal{B}_D) \quad (3.27)$$

where  $\Gamma_D \subset \Gamma$  is a finite set of compatible contours and  $\mathcal{B}_D := \{B_1, \dots, B_n\}$  is a finite set of bonds such that for each  $B_i$ ,  $1 \leq i \leq n$ , there is a  $\gamma \in \Gamma_D$  with  $B_i \cap \gamma \neq \emptyset$  and

$$\text{supp } D := \left( \bigcup_{\gamma \in \Gamma_D} \gamma \right) \cup \left( \bigcup_{B \in \mathcal{B}_D} B \right) \quad (3.28)$$

is a connected set. In (3.28)  $\text{supp } D$  denotes the support of a decorated contour  $D$ . In the sequel we shall use the symbol  $D$  for both a decorated contour and its support. Moreover,

$$|D| := \sum_{\gamma \in D} |\gamma| + \sum_{B \in D} g(B) \quad (3.29)$$

Decorated contours have the following properties:

- The interiors of any two distinct closed Ising contours, which belong to a decorated contour  $D$ , do not intersect.

- Each bond  $B$  in a decorated contour intersects at least one contour in  $D$ .

- Any two contours in a decorated contour  $D$  are connected through bonds and other contours in  $D$ , i.e., for each pair of Ising contours  $\gamma, \gamma'$  in  $D$ , there are contours  $\gamma_1, \dots, \gamma_k$  in  $D$  such that  $\gamma \sim \gamma_1, \gamma_1 \sim \gamma_2, \dots, \gamma_k \sim \gamma'$ , with the understanding that two contours  $\gamma_1$  and  $\gamma_2$  are connected, denoted by  $\gamma_1 \sim \gamma_2$ , if one of the following holds:

- there is a bond  $B$  in  $D$  such that  $B$  intersects both  $\gamma_1$  and  $\gamma_2$

- there are two bonds  $B_1$  and  $B_2$  in  $D$  such that  $B_1 \cap B_2 \neq \emptyset$ ,  $B_1$  intersects  $\gamma_1$  and  $B_2$  intersects  $\gamma_2$ .

To each decorated contour  $D = (\Gamma_D, \mathcal{B}_D)$  we can associate a weight  $W(D)$  as follows:

$$W(D) := \prod_{\gamma \in D} e^{-\beta J_1(U) |\gamma_i|} \prod_{\substack{B \in D \\ |B| \geq 3}} (e^{-\beta \Phi_B} - 1) \quad (3.30)$$

Let  $\mathcal{D}$  denote a finite family of compatible decorated contours, i.e., a finite set of mutually non-intersecting contours. Then the partition function can be expressed as follows.

$$\Xi_A^{\text{hom}} = \sum_{\mathcal{D} \subset A \neq \emptyset} \prod_{D \in \mathcal{D}} W(D) \quad (3.31)$$

where  $|W(D)| \leq W_0(D)$  for all  $D \in \mathcal{D}$ , with

$$W_0(D) := \prod_{\gamma \in \Gamma_D} e^{-\beta c_0 U^{-1} |\gamma|} \prod_{B \in \mathcal{B}_D} \left[ \exp \left( \beta c_2 \left( \frac{c_1}{U} \right)^{g(B)} \right) - 1 \right] \quad (3.32)$$

The above bound follows from the Peierls bound (2.30) and the exponential decay (2.32). In (3.31) the partition function for the lattice model under homogeneous boundary conditions has been expressed in terms of a gas of *non-interacting*, pairwise disjoint, decorated contours. The methods of cluster expansion can now be applied to analyze its convergence properties.

The partition functions corresponding to mixed boundary conditions (2.20)–(2.21) can be expressed in terms of decorated contours in a similar manner. However, under these boundary conditions there is a contour—the interface—which is pinned to the boundary of the volume  $A$ . In our definition of decorated contours the interface is treated differently from the remaining Ising contours in the volume  $A$ . It is not considered to be a part of a decorated contour. Consequently, in the expressions for the partition functions under mixed boundary conditions, there is an additional sum over all possible interfaces. As described in Section 2, an interface  $I$  divides the volume  $A$  into two subvolumes  $A_I^a$  and  $A_I^b$ . For each interface, the set of non-interacting decorated contours, corresponding to a mixed boundary condition, can be decomposed into three subfamilies which consists, respectively, of contours which intersect  $I$ , which are above  $I$  and which are below  $I$ . Hence, for a given interface  $I$ , under the boundary condition b.c.1 (2.20), we define the following compatible families of decorated contours.

$$\begin{aligned} \mathcal{D}_I &:= \{ \{ D_{l_1} \cdots D_{l_p} \mid D_{l_i} \cap I \neq \emptyset, 1 \leq i \leq p, l_i \in \mathbb{Z} \} \} \\ \mathcal{D}_I^a &:= \{ \{ D_{m_1} \cdots D_{m_q} \mid D_{m_i} \cap \Gamma^a \neq \emptyset, D_{m_i} \cap I = \emptyset, 1 \leq i \leq q, m_i \in \mathbb{Z} \} \} \\ \mathcal{D}_I^b &:= \{ \{ D_{n_1} \cdots D_{n_r} \mid D_{n_i} \cap \Gamma^b \neq \emptyset, D_{n_i} \cap I = \emptyset, 1 \leq i \leq r, n_i \in \mathbb{Z} \} \} \end{aligned} \quad (3.33)$$

where  $\Gamma^a$  and  $\Gamma^b$  are the subfamilies of compatible (Ising) contours which lie entirely in the subvolumes  $A_I^a$  and  $A_I^b$  respectively. For a given interface  $\tilde{I}$ ,

under the boundary condition b.c.2 (2.21), the corresponding families of compatible decorated contours are denoted by  $\mathcal{D}_{\bar{I}}$ ,  $\mathcal{D}_{\bar{I}}^a$  and  $\mathcal{D}_{\bar{I}}^b$ .

From (3.13), (3.8) and (3.12) it follows that

$$\begin{aligned} \Xi_A^{100} &= \sum_{I \in \mathcal{I}} e^{-\beta E_1^{\text{bare}}(I)} \left( \sum_{\mathcal{D}_I \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_I} W_I(D) \right) \\ &\quad \times \left( \sum_{\mathcal{D}_I^a \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_I^a} W(D) \right) \left( \sum_{\mathcal{D}_I^b \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_I^b} W(D) \right) \end{aligned} \quad (3.34)$$

where  $W(D)$  is defined through (3.30) and satisfies the bound  $|W(D)| \leq W_0(D)$ , with  $W_0(D)$  being defined through (3.32).

For  $D \in \mathcal{D}_I$

$$W_I(D) := \prod_{\gamma \in D} e^{-\beta J_1(U) |\gamma|} \prod_{\substack{B \in D \\ |B| \geq 3}} (e^{-\beta \Phi'_B} - 1) \quad (3.35)$$

From the Peierls bound (2.30) and the estimate (3.11) it follows that  $|W_I(D)| \leq W_I^0$  where

$$W_I^0(D) := \prod_{\gamma \in D} e^{-\beta c_0 U^{-1} |\gamma|} \prod_{\substack{B \in D \\ |B| \geq 3}} \left[ \exp \left( 2\beta c_2 \left( \frac{c_1}{U} \right)^{g(B)} \right) - 1 \right] \quad (3.36)$$

Similarly the partition function  $\Xi_A^{111}$ , defined through (3.21)–(3.22), can be written as

$$\begin{aligned} \Xi_A^{111} &= \sum_{\bar{I} \in \bar{\mathcal{I}}} e^{-\beta E_2^{\text{bare}}(\bar{I})} \left( \sum_{\mathcal{D}_{\bar{I}} \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_{\bar{I}}} W_{\bar{I}}(D) \right) \\ &\quad \times \left( \sum_{\mathcal{D}_{\bar{I}}^a \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_{\bar{I}}^a} W(D) \right) \left( \sum_{\mathcal{D}_{\bar{I}}^b \cap A \neq \emptyset} \prod_{D \in \mathcal{D}_{\bar{I}}^b} W(D) \right) \end{aligned} \quad (3.37)$$

where for  $D \in \mathcal{D}_{\bar{I}}$

$$W_{\bar{I}}(D) := \prod_{\gamma \in D} e^{-\beta J_1(U) |\gamma|} \prod_{\substack{B \in D \\ |B| \geq 3}} (e^{-\beta \bar{\Phi}'_B} - 1) \quad (3.38)$$

The bounds (2.30) and (3.24) imply that  $|W_{\bar{I}}(D)| \leq W_{\bar{I}}^0$  where

$$W_{\bar{I}}^0(D) := \prod_{\gamma \in D} e^{-\beta c_0 U^{-1} |\gamma|} \prod_{\substack{B \in D \\ |B| > 3}} \left[ \exp \left( 2\beta c_2 \left( \frac{c_1}{U} \right)^{m(B)} \right) - 1 \right] \quad (3.39)$$

where  $m(B)$  is defined through (2.37).

In order to proceed we need to analyze the convergence properties of series of the form

$$S_A := \sum_{\mathcal{D} \cap A \neq \emptyset} \prod_{D \in \mathcal{D}} W(D) \quad (3.40)$$

where  $\mathcal{D}$  is a finite set of compatible decorated contours with weights given by

$$W(D) := \prod_{\gamma \in D} e^{-\beta E(\gamma)} \prod_{B \in D} (e^{-\beta G_B} - 1) \quad (3.41)$$

where the function  $G_B$  is given by  $\Phi_B$  (2.24) for the homogeneous boundary conditions (2.19) and by the functions  $\Phi'_B$  (3.8) and  $\tilde{\Phi}'_B$  (3.23) for the mixed boundary conditions (2.20) and (2.21) respectively. The bounds satisfied by these functions are respectively given by (2.32), (3.11) and (3.24). Since the series in (3.40) is expressed as a sum over compatible families of non-interacting decorated contours, its convergence properties can be studied by the method of cluster expansions. The convergence of the above series (for  $G_B = \Phi_B$  and  $G_B = \Phi'_B$ ) follows from Lemma 5 given below.

**Lemma 5.** Consider the series

$$S_A := \sum_{\mathcal{D} \cap A \neq \emptyset} \prod_{D \in \mathcal{D}} W(D) \quad (3.42)$$

where

$$W(D) := \prod_{\gamma \in D} e^{-\beta E(\gamma)} \prod_{B \in D} (e^{-\beta G_B} - 1) \quad (3.43)$$

and assume that there exists positive constants  $C_1$  and  $C_2$  such that

$$E(\gamma) \geq C_1 \lambda |\gamma| \quad (3.44)$$

and

$$|G_B| \leq C_2 \lambda^{g(B)} \quad (3.45)$$

where  $g(B)$  is defined through (2.10) and  $\lambda < 1$ . Then there exists constants  $b_0, \lambda_0 > 0$  such that for  $\beta\lambda > b_0$  and  $\lambda < \lambda_0$ , the series  $S_A$  has a convergent cluster expansion, i.e.,

$$\log S_A = \sum_{N \geq 1} \frac{1}{N!} \sum_{D_1 \cap A \neq \emptyset} \cdots \sum_{D_N \cap A \neq \emptyset} \Psi^T(\{D_1, \dots, D_N\}) \quad (3.46)$$

(the *cluster expansion*), where  $\Psi^T$  is a function on families of decorated contours with the property that

$$\Psi^T(\{D_1, \dots, D_N\}) = 0 \quad \text{if } \{D_1, \dots, D_N\} \text{ is not a cluster} \quad (3.47)$$

i.e., if  $D_1 \cup \dots \cup D_N$  is not a connected set. It satisfies the bound

$$\sum_{\{D_1, \dots, D_N\} \ni 0} \frac{|\Psi^T(D_1, \dots, D_N)|}{|D_1 \cup \dots \cup D_N|} \leq s_N \quad (3.48)$$

where  $s_N$  is a constant of the order of

$$\sup \prod_{i=1}^N |W(D_i)|$$

the supremum being taken over all sets of  $N$  decorated contours (not necessarily pairwise disjoint).

The above lemma is proved in Appendix B. The proof of the convergence of the series  $S_A$  (3.40) for  $G_B = \tilde{\Phi}_B$  is analogous to the proof of the above lemma and is hence not included. The only difference is the replacement of the bound (3.45) by the bound

$$|G_B| \leq C_2 \lambda^{m(B)} \quad (3.49)$$

where  $m(B) := \max(5, g(B))$ .

Let  $P$  denote a cluster of decorated contours. It is a connected set of intersecting decorated contours. A single decorated contour can occur several times in a cluster. Further we define

$$|P| := \sum_{D \in P} |D| = \sum_{D \in P} \left( \sum_{\gamma \in D} |\gamma| + \sum_{B \in D} g(B) \right) \quad (3.50)$$



Let  $\Psi^T(P)$ ,  $\Psi_I^T(P)$  and  $\Psi_{\bar{I}}^T(P)$  denote truncated functions, defined on the cluster  $P$ , which satisfy the following bounds.

$$\sum_{P \ni 0} \frac{|\Psi^T(P)|}{|P|} \leq \sup \prod |W(D)| \tag{3.51}$$

$$\sum_{P \ni 0} \frac{|\Psi_I^T(P)|}{|P|} \leq \sup \prod |W_I(D)| \tag{3.52}$$

and

$$\sum_{P \ni 0} \frac{|\Psi_{\bar{I}}^T(P)|}{|P|} \leq \sup \prod |W_{\bar{I}}(D)| \tag{3.53}$$

If the cluster  $P$  consists of  $N$  decorated contours then the product is over a set of  $N$  decorated contours and the supremum in the above estimates is taken over all such of  $N$  decorated contours.

To determine whether the 100 and 111 interfaces are rigid, we need to analyze the following quotients.

$$\mathbf{Z}_A^{100} = \frac{\Xi_A^{100}}{\Xi_A^+} \quad \text{and} \quad \mathbf{Z}_A^{111} = \frac{\Xi_A^{111}}{\Xi_A^+} \tag{3.54}$$

Using the results of cluster expansions (see, e.g., ref. 34) we can express these quantities in terms of the truncated functions defined above.

**Proposition 6.** There exist three constants  $U_0$ ,  $B_1$ , and  $B_2$  independent of the volume  $A$ , such that for all  $U > U_0$  and  $\beta/U > B_1$ , the quotient  $\mathbf{Z}_A^{100}$  can be written as follows:

$$\mathbf{Z}_A^{100} = \sum_{I \in \mathcal{I}} e^{-\beta E_1^{\text{bare}}(I)} \times \exp \left\{ \sum_{\substack{P: \\ P \cap I \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_I^T(P) - \sum_{\substack{P: \\ P \cap \bar{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^T(P) \right\} \tag{3.55}$$

For all  $U > U_0$  and  $\beta/U^3 > B_2$ , the quotient  $\mathbf{Z}_A^{111}$  can be written as follows:

$$\mathbf{Z}_A^{111} = \sum_{\bar{I} \in \bar{\mathcal{I}}} e^{-\beta E_2^{\text{bare}}(\bar{I})} \times \exp \left\{ \sum_{\substack{P: \\ P \cap \bar{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_{\bar{I}}^T(P) - \sum_{\substack{P: \\ P \cap \bar{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^T(P) \right\} \tag{3.56}$$

*Proof.* The proof is standard. We expand the partition functions appearing in the numerator and in the denominator of  $\mathbf{Z}_A^{100}$  and of  $\mathbf{Z}_A^{111}$  by

the cluster expansion performed in the Appendix B. The truncated functions which are left are precisely those defined on the clusters which intersect the interface. ■

Alternatively  $Z_A^{111}$  can be written as

$$Z_A^{111} = \sum_{\tilde{I} \in \tilde{\mathcal{F}}} e^{-\beta E_2^{\text{dec}}(\tilde{I})} \quad (3.57)$$

where  $E_2^{\text{dec}}(\tilde{I})$  denotes the energy of the interface in the presence of the decorated contours and is defined as follows.

$$E_2^{\text{dec}}(\tilde{I}) := E_2^{\text{bare}}(\tilde{I}) - \frac{1}{\beta} \left[ \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_I^T(P) - \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^T(P) \right] \quad (3.58)$$

We shall refer to  $E_2^{\text{dec}}(\tilde{I})$  as the energy of the decorated interface.

#### 4. RIGIDITY OF THE 100 INTERFACE

The study of the 100 interface requires the second order decomposition of the effective Hamiltonian of the FK model, in which the second order truncated Hamiltonian  $\mathcal{H}_0^{(2)}(U)$  is the Ising Hamiltonian, with coupling constant  $J_1(U)$ . We point out that the Hamiltonian  $\mathcal{H}_0^{(2)}(U)$  is generated by the second order quantum fluctuations, this means that the rigidity of the 100 interface of the FK model is of quantum nature. The proof of the rigidity of the 100 interface of the three-dimensional FK model is a generalization of Dobrushin's proof of the rigidity of this interface in the three-dimensional Ising model at sufficiently low temperatures.<sup>(15)</sup>

*Proof of Theorem 1.* Let  $\text{Prob}_A(I)$  denote the probability of occurrence of an interface  $I$  in the FK model, defined on a finite cubic lattice  $A$ , under the boundary condition b.c.1 (2.20). It is defined as follows:

$$\begin{aligned} \text{Prob}_A(I) &= \frac{1}{Z_A^{100}} \exp\{-\beta E_1^{\text{bare}}(I)\} \\ &\times \exp\left\{ \sum_{\substack{P: \\ P \cap I \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_I^T(P) - \sum_{\substack{P: \\ P \cap I \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^T(P) \right\} \quad (4.1) \end{aligned}$$

To determine whether the 100 interface is rigid, we need to analyze the properties of this quantity in the thermodynamic limit.

We notice that the above expression (4.1) is similar to the corresponding probability of a 100 interface in the Ising model. This is because the leading term in the “bare” energy,  $E_1^{\text{bare}}(I)$  (3.5), of an interface  $I$  is exactly equal to the energy of an interface  $I$  for an Ising model with coupling constant  $J_1(U)$ . We point out that this similarity results from the fact that we have expressed the probability  $\text{Prob}_A(I)$  directly in terms of an actual interface  $I$ , separating the two coexisting phases, instead of expressing it in terms of a *decorated interface*. (The latter is given by a *connected set*  $(I, \mathcal{B}_I, \Gamma_I)$ , where  $\mathcal{B}_I$  is a finite set of bonds and  $\Gamma_I$  is a finite set of Ising contours; [see ref. 34 and references therein].) This leads to a considerable simplification in the calculations since an actual interface between two coexisting phases, under the boundary condition b.c. 1, reduces to a flat interface orthogonal to  $\mathbf{n} = (0, 0, 1)$  at zero temperature. This property is, however, not satisfied by a decorated interface.

Let us describe the minor differences which arise in the description of the 100 interface of the FK model with respect to that of the Ising model.

- The first difference lies in the contributions of the truncated functions. For the FK model these functions are defined on sets of decorated contours, whereas for the Ising model they are defined on sets of Ising contours. However, there exists a positive constant  $U_0$  for such that for all  $U > U_0$ , the contribution of the truncated functions is exponentially small for the FK model, as in the case for the Ising model. Difference arises from the fact that the “bare” energy,  $E_1^{\text{bare}}(I)$  (3.5), of the interface consists of terms in addition to the leading Ising-like term  $J_1(U) |I|$ . These terms are, however, small for  $U > U_0$ , where  $U_0$  is a positive constant. Hence they are treated in the same way as the truncated functions.

The proof of the rigidity of the 100 interface of the FK model is similar to Dobrushin’s proof of the rigidity of the 100 interface of the three-dimensional Ising model.<sup>(15)</sup> The proof of the rigidity can be converted into the study of a two-dimensional contour model, which resembles an Ising model with long range interactions, in which the ground states are the projections of the *ceilings* on the 100 plane and the contours are the corresponding projections of the *walls*. The rigidity of the 100 interface at low temperatures follows from a Peierls argument on the contours (walls).<sup>(15)</sup> Taking into account the small modifications described above, we deduce that there exists positive constants  $U_0$  and  $D_0$  such that, for all  $U > U_0$  and  $\beta/U > D_0$ , the assertions of Theorem 1 (see Section 2) are true. ■

We would like to remark that Theorem 1, stated for the FK model, is in general valid for a wide class of lattice Hamiltonians, namely, those which can be expressed as a sum of two terms: a dominant nearest

neighbour Ising Hamiltonian, and a remainder consisting of long-range many-body interactions satisfying exponential decay (2.12).

## 5. RIGIDITY OF THE 111 INTERFACE

The case of the 111 interface can be treated by using the ideas of Dobrushin but the situation is more involved. The main difference between the 111 interface and the 100 interface is that the second order decomposition of the effective Hamiltonian (2.27) does not lead to the existence of a unique ground state interface in the 111 direction. The energy of a 111 interface w.r.t. the leading part,  $H_0^{(2)}(U)$ , of the relative Hamiltonian, is proportional to the area of the 111 interface. Hence, the ground state interface has minimal area. However, there are infinitely many such interfaces in the infinite volume limit (Proposition 4 of Section 2.3). Hence, the *ground state* of the 111 interface has an *infinite degeneracy*. Thus, to prove the rigidity of the 111 interface we require a more refined decomposition of the effective Hamiltonian, namely, the fourth-order decomposition. In this section we prove that the degeneracy of the 111 ground state interface is lifted by the fourth-order truncated effective Hamiltonian,  $H_0^{(4)}(U)$ , which takes into account the fourth-order quantum fluctuations. The study of the properties of the 111 interface can be reduced to the analysis of a model defined on a two-dimensional triangular lattice which is obtained by projecting the interface onto a fixed plane (see Sections 2.2 and 5.1 for details). We refer to this model as the *rhombus model*. The rigidity of the 111 interface at sufficiently low temperatures can be deduced from the low temperature behaviour of the rhombus model.

We first define the main quantity required in our proof of the rigidity of the 111 interface: the probability of occurrence of an interface  $\tilde{I}$ , in the volume  $A$ , under the boundary condition b.c.2 (2.21):

$$\begin{aligned} \text{Prob}_A(\tilde{I}) &= \frac{1}{Z_A^{111}} \exp\{-\beta E_2^{\text{bare}}(\tilde{I})\} \\ &\times \exp\left\{ \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_{\tilde{I}}^T(P) - \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^T(P) \right\} \end{aligned} \quad (5.1)$$

### 5.1. Description of the Rhombus Configurations

As we have seen, the projection of each face of the interface  $\tilde{I}$ , onto the plane  $\mathbb{P}$  yields a rhombus of one of the three types, i.e., belonging to  $\mathcal{R}_0$ ,  $\mathcal{R}_1$  or  $\mathcal{R}_2$ . An interface  $\tilde{I}$  is projected onto a covering of  $\mathbb{P}$  with rhombi,

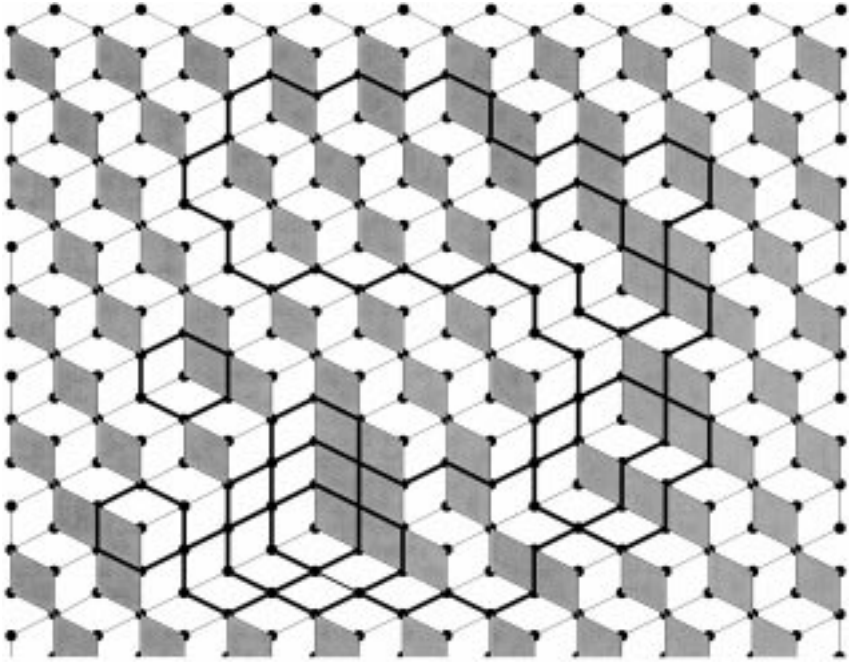


Fig. 4. A minimal area interface with its  $\delta$ -edges (given by the dark lines). The only purpose of the shading is to guide the eye.

which we refer to as in  $R$ -configuration (see Section 2.2). In general, this rhombus covering is not a tiling. Moreover, many interfaces are represented by the same  $R$  configuration. Let  $\mathcal{C}_A$  denote an  $R$  configuration on  $\mathbb{P}_A$ .

The correspondence between the relative positions of the rhombi in an  $R$ -configuration and the local geometry of the corresponding interface (as determined by the spin configurations on the plaquettes of  $P_{\bar{I}}$ , and the bonds of  $B_{\bar{I}}^2$ ) is given as follows:

$$\begin{aligned}
 \text{local spin configuration on } \mathcal{L}^3 &\leftrightarrow \text{rhombus configuration on } \mathbb{P} \\
 \begin{matrix} + & + \\ + & - \end{matrix} &\leftrightarrow \begin{matrix} \text{two adjacent rhombi of the same type} \\ \text{i.e., a good pair of rhombi} \end{matrix} \tag{5.2}
 \end{aligned}$$

$$\begin{aligned}
 \begin{matrix} + & - \\ + & - \end{matrix} &\leftrightarrow \begin{matrix} \text{two adjacent rhombi of different types;} \\ \text{the common edge is then called} \\ \text{a } \delta\text{-edge. See Fig. 4} \end{matrix} \tag{5.3}
 \end{aligned}$$

$$\begin{aligned}
 \begin{matrix} + & - \\ - & + \end{matrix} &\leftrightarrow \begin{matrix} \text{four overlapping rhombi sharing an} \\ \text{edge: the common edge is then called} \\ \text{an } \omega\text{-edge} \end{matrix} \tag{5.4}
 \end{aligned}$$

$$\begin{array}{l}
 + \quad - \quad + \quad \leftrightarrow \\
 \text{two parallel rhombi sharing a vertex,} \\
 \text{with one of them being necessarily} \\
 \text{overlapping: the two rhombi are said to} \\
 \text{be connected by a } \lambda\text{-link (see below)} \\
 \end{array} \tag{5.5}$$

and the same correspondences for spin configurations obtained by a spin flip transformation or by rotations of the ones above.

*Definition of a  $\lambda$ -link.* Consider a pair of parallel faces of an interface, which are a unit distance apart. Consider a line segment which connects the centers of these faces and is perpendicular to them. The projection of such a line segment on the plane  $\mathbb{P}$  is referred to as a  $\lambda$ -link. A single  $\lambda$ -link can be the projection of several such line segments. Hence, each  $\lambda$ -link has a multiplicity,  $m$ , which counts the number of line segments which project onto it.

### 5.2. The Energy of a Rhombus Configuration

To order  $U^{-3}$ , the bare energy  $E_2^{\text{bare}}(\tilde{I})$  of an interface  $\tilde{I}$ , defined by (3.20), is a function of the local geometry of the interface, and hence is a function of the  $R$ -configuration. The plaquette potential  $h_p$ , (given by (3.17)), as well as the next nearest neighbour interaction  $h_{\{x, z\}}$  with  $|x - z| = 2$ , (given by (3.18)), play crucial roles in determining this energy. Their contributions to the energy for different spin configurations are given as follows:

$$h_p \begin{pmatrix} + & + \\ + & - \end{pmatrix} = -16 \tag{5.6}$$

$$h_p \begin{pmatrix} + & - \\ + & - \end{pmatrix} = -12 \tag{5.7}$$

$$h_p \begin{pmatrix} + & - \\ - & + \end{pmatrix} = 0 \tag{5.8}$$

$$h_{\{x, z\}}(+ \quad - \quad +) = 0 \tag{5.9}$$

$$h_{\{x, z\}}(+ \quad - \quad -) = h_{\{x, z\}}(- \quad - \quad +) = -2 \tag{5.10}$$

The plaquette and next nearest neighbour configurations which correspond to the lowest energy for these potentials are those given in (5.6) and (5.10) respectively. Moreover, from (5.2) it follows that the plaquette configuration with lowest energy corresponds to a good pair of rhombi. Hence, a connected set of faces of the interface whose projection on the plane  $\mathbb{P}_A$

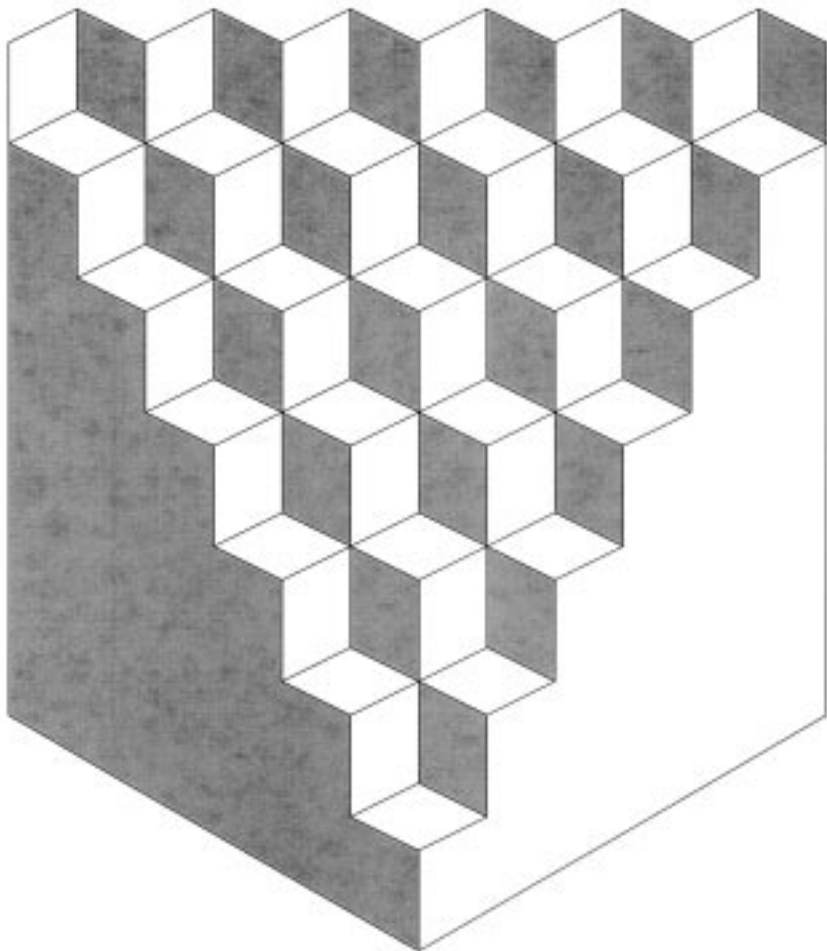


Fig. 5. The “perfect staircase” structure of the interface  $\tilde{I}_{\mathcal{R}_0}$ .

consists entirely of good pairs of rhombi defines a *local ground state configuration* of the interface with respect to the truncated Hamiltonian  $H_0^{(4)}$  (2.34). Since two rhombi that form a good pair are necessarily of the same type, it follows that there are three such local ground state configurations corresponding to rhombi in the families  $\mathcal{R}_0$ ,  $\mathcal{R}_1$  and  $\mathcal{R}_2$  respectively.

We conclude from the above that those minimal area interfaces whose projections on the plane  $\mathbb{P}$  are tilings with rhombi belonging to a single family have minimum energy with respect to  $H_0^{(4)}$  (2.34) and are hence referred to as *ground state interfaces*. Since we have chosen the standard b.c. for the  $R$ -configuration to be given by a tiling of the plane  $\mathbb{P} \setminus \mathbb{P}_A$  with

rhombi in the family  $\mathcal{R}_0$  [see Section 2.2], it follows that a ground state interface projects onto a tiling of  $\mathbb{P}_A$  with rhombi in the family  $\mathcal{R}_0$ . We hence denote a ground state interface as  $\tilde{I}_{\mathcal{R}_0}$ . It is easy to see that  $\tilde{I}_{\mathcal{R}_0}$  has a *perfect staircase structure* (see Fig. 5). Thus, under the boundary condition b.c.2 (2.21), the geometry-dependent contribution of the plaquette potential  $h_p$  leads to the selection of a unique ground state interface (up to translations) from the infinitely many minimal area interfaces.

For any interface  $\tilde{I}$  the connected components of the set  $\tilde{I} \setminus \tilde{I}_{\mathcal{R}_0}$  are referred to as *pyramids*. They represent the local distortions of the interface from a perfect staircase structure.

We would like to point out that the above mentioned phenomenon of ground state selection is a consequence of the Fermi statistics of the electrons in the model. The anticommutation relations for the electron creation and annihilation operators play a crucial role in determining the exact expressions for the potentials  $h_p$  (3.17) and  $h_{\{x,z\}}$  (3.18) which are responsible for lifting the infinite degeneracy. If instead of fermions we consider bosons, then the corresponding commutation rules for the creation and annihilation operators yield the following expression for the plaquette potential:

$$\tilde{h}_p = 1 - s_x s_y s_z s_w + 5(s_x s_z + s_y s_w - 2) \quad (5.11)$$

where  $w, x, y$  and  $z$  are four sites forming a plaquette. It is easy to see that

$$\tilde{h}_p \begin{pmatrix} + & + \\ + & - \end{pmatrix} > \tilde{h}_p \begin{pmatrix} + & - \\ + & - \end{pmatrix} \quad (5.12)$$

and hence, in the bosonic case, the perfect staircase configuration is not favoured by the plaquette potential in fourth order of perturbation theory.

### 5.3. The Energy of a Ground State Interface

The energy of the ground state interface  $\tilde{I}_{\mathcal{R}_0}$  is given by

$$E_2^{\text{dec}}(\tilde{I}_{\mathcal{R}_0}) := E_2^{\text{bare}}(\tilde{I}_{\mathcal{R}_0}) - \frac{1}{\beta} \left[ \sum_{\substack{P: \\ P \cap \tilde{I}_{\mathcal{R}_0} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi_{\tilde{I}_{\mathcal{R}_0}}^{\text{T}}(P) - \sum_{\substack{P: \\ P \cap \tilde{I}_{\mathcal{R}_0} \neq \emptyset \\ P \cap A \neq \emptyset}} \Psi^{\text{T}}(P) \right] \quad (5.13)$$

where,

$$E_2^{\text{bare}}(\tilde{I}_{\mathcal{R}_0}) = \left( J_2(U) - \frac{1}{4U^3} \right) |\tilde{I}_{\mathcal{R}_0}| - \left( \frac{1}{U^3} + \text{h.o.} \right) N_1(\tilde{I}_{\mathcal{R}_0}) \\ + \sum_{\{B: |B| > 3; B \cap \tilde{I}_{\mathcal{R}_0} \neq \emptyset\}} \tilde{\Phi}_B(\tilde{I}_{\mathcal{R}_0} \cup \emptyset) \quad (5.14)$$



Here  $|\tilde{I}_{\mathcal{R}_0}|$  is the total number of faces in the interface  $\tilde{I}_{\mathcal{R}_0}$ , which is equal to the number of rhombi in the corresponding tiling of  $\mathbb{P}_A$ , and  $N_1(\tilde{I}_{\mathcal{R}_0})$  is the total number of shared edges of rhombi in the tiling. The above expression (5.14) follows from (3.20). It is obvious that  $E_2^{\text{bare}}(\tilde{I}_{\mathcal{R}_i})$ , is the same for  $i = 0, 1$  and  $2$ . Hence, we can define the relative energy of an interface  $\tilde{I}$  as follows.

$$\varepsilon_2^{\text{dec}}(\tilde{I}) := E_2^{\text{dec}}(\tilde{I}) - E_2^{\text{dec}}(\tilde{I}_{\mathcal{R}_0}) \quad (5.15)$$

## 5.4. The Components of an $R$ -Configuration

An  $R$ -configuration can be decomposed into *bases*—which are local ground state configurations of  $H_0^{(4)}$  (2.34), and  *$R$ -contours*—which represent the excitations.

*Bases:* A base of a given  $R$  configuration is a maximally connected set of good pairs of rhombi. As each base is the union of open sets, it is an open set, and by definition distinct bases do not intersect. Denote by  $\{C_1, \dots, C_p\}$  the family of bases of a given  $R$  configuration. The type of a base  $C_i$  is defined as follows:  $\tau(C_i) = j$ , if the rhombi it consists of belong to  $\mathcal{R}_j$ . Due to the mixed boundary conditions one of the bases is connected to the boundary and hence becomes infinite in the thermodynamic limit. Let  $C_1$  denote this base. Since the standard b.c. is chosen to be a tiling of  $\mathbb{P} \setminus \mathbb{P}_A$  with rhombi in  $\mathcal{R}_0$ , we have  $\tau(C_1) = 0$ .

*$R$ -contours:* The maximally connected components of the complements of the bases, i.e., of  $\mathbb{P}_A \setminus \bigcup_{i=1}^p C_i$ , are called the  $R$ -contours. Isolated vertices are not considered to be  $R$ -contours. Each  $R$ -contour is a closed complex and is denoted by the symbol  $Y$ .

An  $R$ -contour  $Y$  is defined by a pair

$$Y = (\text{supp } Y, \Theta_Y) \quad (5.16)$$

where

- $\text{supp } Y$  denotes the geometric support of the  $R$ -contour and is a connected subset of the plane  $\mathbb{P}$ ,
- $\Theta_Y$  denotes the configuration on this support. It is defined in terms of overlapping rhombi,  $\delta$ - and  $\omega$ - lines and  $\lambda$ -links that span  $\text{supp } Y$ .

For notational simplicity we shall often use the symbol  $Y$  to denote both the  $R$ -contour and its geometric support  $\text{supp } Y$ .

An  $R$ -configuration, under standard boundary conditions, is given by a compatible family of  $R$ -contours,  $\mathcal{C}_A := \{Y_1, \dots, Y_n\}$ , i.e., a finite set of non-intersecting, closed  $R$ -contours, along with a specification of the types of the bases separating the  $R$ -contours. To avoid complicated notations, the types of the bases will be specified only when required. Those  $R$ -contours whose supports are not in the interiors of any other  $R$ -contours in  $\mathcal{C}_A$  are referred to as the external contours of  $\mathcal{C}_A$ .

## 5.5. The Structure of the $R$ -Contours

Each  $R$ -contour  $Y$  has a detailed structure. It can be decomposed into two families of subcontours, one of which can be empty.

- The *overlapping  $R$ -subcontours*  $\{Y_1^{ov}, \dots, Y_p^{ov}\}$  are the maximally connected sets of overlapping rhombi contained in  $Y$ . Each overlapping  $R$ -subcontour is a closed complex.
- The complement of the overlapping  $R$ -subcontours in  $Y$ , i.e.,  $Y \setminus \bigcup_{i=1}^p Y_i^{ov}$  is considered as an open complex, whose elements  $\{Y_1^{st}, \dots, Y_q^{st}\}$  are maximally connected open complexes. They are called the *standard  $R$ -subcontours*. We refer to an  $R$ -contour as a standard  $R$ -contour if it has no overlapping components.

Hence, an  $R$  contour  $Y$  has the following decomposition:

$$Y := Y(p, q) = \left\{ \bigcup_{i=1}^p Y_i^{ov} \right\} \cup \left\{ \bigcup_{k=1}^q Y_k^{st} \right\} \quad (5.17)$$

Let us describe the detailed structure of the different  $R$ -subcontours. A standard  $R$ -subcontour  $Y_k^{st}$  is uniquely specified by a configuration  $A_k^{st}$  of  $\delta$ -lines. We refer to such  $\delta$ -lines as *standard  $\delta$ -lines*. An overlapping  $R$ -subcontour  $Y_i^{ov}$  is characterized by four families of configurations.

- A *configuration of overlapping triangles*  $\mathcal{T}_i^{ov}$ . It is easy to see that each overlapping triangle in the projection of an interface has an even overlap number and each rhombus in  $Y_i^{ov}$  contains at least one overlapping triangle. Let  $|\mathcal{T}_i^{ov}|$  denote the sum of the overlap number of all the overlapping triangles contained in  $Y_i^{ov}$ , i.e.,

$$|\mathcal{T}_i^{ov}| := \sum_{t \in \mathcal{T}_i^{ov}} o(t) \quad (5.18)$$

Let  $a_i^{ov}$  denote the number of extra faces of an interface (in comparison with the number of faces of a minimal area interface) which project on to the support  $\text{supp } Y_i^{ov}$ . It is given by

$$a_i^{ov} = \frac{|\mathcal{F}_i^{ov}|}{2} \quad (5.19)$$

Since  $|\mathcal{F}_i^{ov}|$  is even,  $a_i^{ov}$  is an integer.

- A configuration  $\Delta_i^{ov}$  of  $\delta$  lines. The total length of the  $\delta$  lines in  $Y_i^{ov}$  is denoted by  $|\Delta_i^{ov}|$ .
- A configuration  $\Omega_i^{ov}$  of  $\omega$  lines. The total length of the  $\omega$  lines in  $Y_i^{ov}$  is denoted by  $|\Omega_i^{ov}|$ .
- A configuration  $\Lambda_i^{ov}$  of  $\lambda$  links. The total length of the  $\lambda$  links of  $Y_i^{ov}$  is denoted by  $|\Lambda_i^{ov}|$ .

The number of rhombi spanning  $\text{supp } Y_i^{ov}$  is bounded above by  $a_i^{ov}$ , since each rhombus in  $\text{supp } Y_i^{ov}$  is an overlapping one. Each of these rhombi contribute at most three distinct sites to  $\text{supp } Y_i^{ov}$  since the latter is a connected set. The number of sites in the  $R$  contour  $Y(p, q)$  (defined through (5.17)) hence satisfies the bound

$$\begin{aligned} |Y| &\leq \sum_{i=1}^p \{3 |a_i^{ov}| + (|\Delta_i^{ov}| + 1) + (|\Lambda_i^{ov}| + 1) + (|\Omega_i^{ov}| + 1)\} \\ &\quad + \sum_{k=1}^q (|\Delta_k^{st}| + 1) \end{aligned} \quad (5.20)$$

The relative energy of the interface  $\tilde{I}$  can be expressed in terms of the energy of the corresponding  $R$  configuration  $\mathcal{C}_A = \{Y_1, \dots, Y_n\}$ . It is given by

$$\begin{aligned} \varepsilon_2^{\text{dec}}(\tilde{I}) &\equiv \varepsilon_2^{\text{dec}}(\{Y_1, \dots, Y_n\}) \\ &:= \sum_{i=1}^{i=n} F(Y_i) + W(\{Y_1, \dots, Y_n\}) \end{aligned} \quad (5.21)$$

where  $F(Y_i)$  is the energy of the  $R$ -contour  $Y_i$  computed with the fourth order truncated relative Hamiltonian  $H_{0A}^{(4)}$  defined in (2.34), and  $W(\{Y_1, \dots, Y_n\})$  is the contribution to the energy of the  $R$  configuration arising from the long-range tail  $R_A^{\geq 5}$  defined in (2.35). The latter consists of higher order corrections to the energy of each individual contour, as well as interaction energies between the different  $R$  contours in the compatible family. From (5.15), (3.20) and (3.58) it follows that

$$\begin{aligned}
\sum_{i=1}^n F(Y_i) &= J_2(U)(|\tilde{I}| - |\tilde{I}_{\mathcal{A}_0}|) + \left(\frac{1}{8U^3} + \text{h.o.}\right) \\
&\times \left[ \sum_{\{x,z\} \in B_{\tilde{I}}^2} h_{\{x,z\}}(\tilde{I}) - \sum_{\{s,z\} \in B_{\tilde{I}_{\mathcal{A}_0}}^2} h_{\{x,z\}}(\tilde{I}_{\mathcal{A}_0}) \right] \\
&+ \left(\frac{1}{16U^3} + \text{h.o.}\right) \\
&\times \left[ \sum_{p=\{x,y,z,t\} \in P_{\tilde{I}}} h_p(\tilde{I}) - \sum_{p=\{x,y,z,t\} \in P_{\tilde{I}_{\mathcal{A}_0}}} h_p(\tilde{I}_{\mathcal{A}_0}) \right] \quad (5.22)
\end{aligned}$$

and

$$\begin{aligned}
W(\{Y_1, \dots, Y_n\}) &= \left\{ \sum_{\substack{B: |B| > 3 \\ B \cap \tilde{I} \neq \emptyset}} \tilde{\Phi}_B(\tilde{I} \cup \emptyset) - \sum_{\substack{B: |B| > 3; \\ B \cap \tilde{I}_{\mathcal{A}_0} \neq \emptyset}} \tilde{\Phi}_B(\tilde{I}_{\mathcal{A}_0} \cup \emptyset) \right\} \\
&- \frac{1}{\beta} \left\{ \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap \Lambda \neq \emptyset}} \Psi_{\tilde{I}}^T(P) - \sum_{\substack{P: \\ P \cap \tilde{I}_{\mathcal{A}_0} \neq \emptyset \\ P \cap \Lambda \neq \emptyset}} \Psi_{\tilde{I}_{\mathcal{A}_0}}^T(P) \right\} \\
&+ \frac{1}{\beta} \left\{ \sum_{\substack{P: \\ P \cap \tilde{I} \neq \emptyset \\ P \cap \Lambda \neq \emptyset}} \Psi^T(P) - \sum_{\substack{P: \\ P \cap \tilde{I}_{\mathcal{A}_0} \neq \emptyset \\ P \cap \Lambda \neq \emptyset}} \Psi^T(P) \right\} \quad (5.23)
\end{aligned}$$

**Lemma 7.** Let  $Y$  be an  $R$ -contour defined through (5.17) and let  $\mathcal{C}_A$  denote an  $R$ -configuration. The energies  $F(Y)$  and  $W(\mathcal{C}_A)$ , defined through (5.22) and (5.23) respectively, are given by the following expressions:

$$\begin{aligned}
F(Y) &= J_2(U) \sum_{i=1}^{i=p} a_i^{ov} + K_2(U) \left( \sum_{k=1}^{k=q} |A_k^{st}| + \sum_{i=1}^{i=p} |A_i^{ov}| \right) \\
&+ \left(\frac{1}{U^3} + \text{h.o.}\right) \sum_{i=1}^{i=p} |\Omega_i^{ov}| + \left(\frac{1}{4U^3} + \text{h.o.}\right) \sum_{i=1}^{i=p} |A_i^{ov}| \quad (5.24)
\end{aligned}$$

where

$$J_2(U) = \frac{1}{2U} - \frac{11}{8U^3} + \text{h.o.} \quad (5.25)$$

$$K_2(U) = \frac{1}{4U^3} + \text{h.o.} \quad (5.26)$$

and

$$W(\mathcal{C}_A) = \sum_{\substack{B: |B| > 3 \\ B_{\mathbb{P}} \cap \mathcal{C}_A \neq \emptyset}} \widehat{\Phi}_B(\mathcal{C}_A) - \frac{1}{\beta} \left\{ \sum_{\substack{P: \\ P_{\mathbb{P}} \cap \mathcal{C}_A \neq \emptyset}} \Psi_{\tilde{I}}^T(P) - \sum_{\substack{P: \\ P_{\mathbb{P}} \cap \mathcal{C}_A \neq \emptyset}} \Psi^T(P) \right\} \quad (5.27)$$

where

$$\widehat{\Phi}_B(\mathcal{C}_A) := \tilde{\Phi}_B(\tilde{I} \cup \emptyset) - \tilde{\Phi}_B(\tilde{I}_{\mathcal{R}_0} \cup \emptyset) \quad (5.28)$$

and  $B_{\mathbb{P}}$  is the projection of the bond  $B$  on the plane  $\mathbb{P}$ . The notation  $B_{\mathbb{P}} \cap \mathcal{C}_A \neq \emptyset$  is used to denote the condition that  $B_{\mathbb{P}}$  intersects either of the following in the  $R$  configuration: an overlapping triangle, a  $\delta$ -line, an  $\omega$ -line, or a  $\lambda$ -link. Similarly,  $P_{\mathbb{P}}$  denotes the projection of the cluster  $P$  of decorated contours, on the plane  $\mathbb{P}$ .

*Proof.* We use (5.6)–(5.10) and the definition of the different components of an  $R$ -contour to obtain the expression for the energy  $F(Y)$  from (5.22). It is a sum of the energies of the overlapping- and standard  $R$ -subcontours in  $Y$ . The energy of an overlapping  $R$ -subcontour is given in terms of the number of overlapping triangles,  $\delta$ -lines,  $\omega$ -lines, and  $\lambda$ -links which constitute it. The energy of a standard  $R$ -subcontour is proportional to the number of  $\delta$ -lines in it.

The expression (5.27) follows from the definition (5.23), since the only terms which survive in each of the three parenthesis on the RHS of (5.23) are those in which the projections of the bonds  $B$  or the clusters  $P$  on the plane  $\mathbb{P}$ , intersect at least one  $R$ -contour in the compatible family  $\mathcal{C}_A$ . This concludes the proof.

In the definition (5.28) we have made use of the fact that while the interface  $\tilde{I}$  corresponds to the  $R$ -configuration  $\mathcal{C}_A$ , containing the  $R$ -contour  $Y$ , the projection of the ground state interface  $\tilde{I}_{\mathcal{R}_0}$  contains no  $R$ -contours.  $\blacksquare$

More generally, the energy of an  $R$ -configuration  $\mathcal{C}_A$  can be expressed as follows:

$$\varepsilon_2^{\text{dec}}(\mathcal{C}_A) = \sum_{Y \in \mathcal{C}_A} \varepsilon(Y | \mathcal{C}_A) \quad (5.29)$$

where  $\varepsilon(Y | \mathcal{C}_A)$  denotes the total energy of an  $R$ -contour  $Y$  belonging to the  $R$ -configuration  $\mathcal{C}_A$ . It is defined as follows:

$$\varepsilon(Y | \mathcal{C}_A) := F(Y) + W(Y | \mathcal{C}_A) \quad (5.30)$$

where  $F(Y)$  is given by (5.24) and  $W(Y | \mathcal{C}_A)$  is given by

$$\begin{aligned} W(Y | \mathcal{C}_A) = & \sum_{\substack{B: |B| > 3 \\ B_p \cap Y \neq \emptyset}} \widehat{\Phi}_B(\mathcal{C}_A) \\ & - \frac{1}{\beta} \left\{ \sum_{\substack{P: \\ P_p \cap Y \neq \emptyset}} \Psi_{\tilde{I}}^T(P) - \sum_{\substack{P: \\ P_p \cap Y \neq \emptyset}} \Psi^T(P) \right\} \end{aligned} \quad (5.31)$$

## 5.6. The Relevant Probabilities

The probability of occurrence of an interface  $\tilde{I}$  in the volume  $A$  can be identified with the probability of the corresponding compatible family of  $R$ -contours  $\mathcal{C}_A \equiv \{Y_1, \dots, Y_n\}$  in the rhombus model.

$$\begin{aligned} \text{Prob}_A(\tilde{I}) &= \text{Prob}_A(\{Y_1, \dots, Y_n\}) \\ &= \frac{e^{-\beta \varepsilon_2^{\text{dec}}(\{Y_1, \dots, Y_n\})}}{\sum_{\{Y_1, \dots, Y_n\} \in \mathbb{P}_A} e^{-\beta \varepsilon_2^{\text{dec}}(\{Y_1, \dots, Y_2\})}} \end{aligned} \quad (5.32)$$

Further, let  $\text{Prob}_A Y$  denote the probability of occurrence of an  $R$ -contour  $Y$ . It is given by

$$\text{Prob}_A Y = \frac{\sum' e^{-\varepsilon_2^{\text{dec}}(\mathcal{C}_A)}}{\sum e^{-\varepsilon_2^{\text{dec}}(\mathcal{C}_A)}} \quad (5.33)$$

where the sum in the numerator is over all  $R$ -configurations which contain the given  $R$ -contour  $Y$ , while the denominator has an unrestricted sum over all  $R$ -configurations.

To prove the rigidity of the 111 interface, we need to find an upper bound to the probability  $\text{Prob}_A Y$  defined in (5.33). This is given in the following proposition.

**Proposition 8.** There exists positive constants  $U_0$  and  $b_0$ , such that for all  $U > U_0$  and  $\beta/U > b_0$ , the probability,  $\text{Prob}_A(Y(p, q))$ , of

occurrence of an  $R$ -contour  $Y(p, q)$  (defined through (5.17)) satisfies the following bound:

$$\text{Prob}_{\mathcal{A}}(Y(p, q)) \leq \prod_{i=1}^{i=p} \{e^{-\beta J_3(U) a_i^{ov}}\} \times \prod_{k=1}^{k=q} \{e^{-\beta K_3(U) |A_k^{st}|}\} \quad (5.34)$$

where

$$\begin{aligned} J_3(U) &= J_2(U) - A_1 U^{-5} - \frac{2}{\beta} e^{-6\beta A_2 U^{-1}} \\ K_3(U) &= K_2(U) - A_1 U^{-5} - \frac{2}{\beta} e^{-6\beta A_2 U^{-1}} \end{aligned} \quad (5.35)$$

and  $A_1$  and  $A_2$  are positive constants depending on  $c_1$ ,  $c_2$  and  $U_0$ . The constants  $J_2(U)$  and  $K_2(U)$  are defined through (5.25) and (5.26) respectively.

The proof of this proposition requires two steps. The first is to obtain a lower bound on the total energy,  $\varepsilon(Y | \mathcal{C}_{\mathcal{A}})$ , of an  $R$ -contour  $Y$  which belongs to an  $R$  configuration  $\mathcal{C}_{\mathcal{A}}$ . This energy is defined through (5.30).

The second step is a generalization of the Peierls argument analogous to Dobrushin's treatment of the antiferromagnetic Ising model.<sup>(14)</sup> A unique specification of an  $R$  configuration requires the specification of not only a compatible family of  $R$ -contours, but also the type of the bases adjacent to the inner and outer boundaries of each  $R$ -contour. In other words contours in the  $R$  configuration are not only required to be pairwise disjoint, but there is the additional requirement of matching of boundary conditions. One way of analyzing such contour expansions would be to use the Pirogov–Sinai theory extended to interacting contours.<sup>(12, 37)</sup> However, instead of doing this we resort to a much simpler method. We use a recipe for removing a contour from a compatible family which is a generalization of the one introduced by Dobrushin in the study of the antiferromagnetic Ising model. The idea is to map a configuration of  $R$ -contours  $\{Y_1, \dots, Y_p\}$  to a new one  $\{Y'_2, \dots, Y'_p\}$  with one contour less, where  $Y_r$  and  $Y'_r$  are either the same, or related to each other by a simple geometric transformation. The transformation preserves the energy of the  $R$ -contour, at least to order  $U^{-3}$ . By using this generalization of Dobrushin's construction we avoid using the Pirogov–Sinai theory.

**Step 1. A lower bound to the total energy of an  $R$ -contour.** The following lemma is necessary to determine a lower bound to the total energy  $\varepsilon(Y | \mathcal{C}_{\mathcal{A}})$ , [defined through (5.30)].

**Lemma 9.** There exist positive constants  $U_0, b_0$ , such that for all  $U > U_0$  and  $\beta/U > b_0$  the following bound is satisfied:

$$|W(Y | \mathcal{C}_A)| \leq W_0(Y | \mathcal{C}_A) \quad (5.36)$$

where

$$W_0(Y | \mathcal{C}_A) := |Y| \left\{ a_1 U^{-5} + \frac{c}{\beta} e^{-6\beta a_2 U^{-1}} \right\} \quad (5.37)$$

with  $c, a_1$  and  $a_2$  being positive constants depending on  $c_1, c_2, U_0$  and  $b_0$ .

*Proof.* From the definition (5.31) of  $W(Y | \mathcal{C}_A)$  it follows that

$$\begin{aligned} |W(Y | \mathcal{C}_A)| &\leq \sum_{\substack{B: |B| > 3 \\ B_{\mathbb{P}} \cap Y \neq \emptyset}} |\widehat{\Phi}_B(\mathcal{C}_A)| \\ &\quad + \frac{1}{\beta} \left\{ \sum_{\substack{P: \\ P_{\mathbb{P}} \cap Y \neq \emptyset}} |\Psi_I^T(P)| + \sum_{\substack{P: \\ P_{\mathbb{P}} \cap Y \neq \emptyset}} |\Phi^T(P)| \right\} \\ &\leq \sum_{x^* \in Y} \sum_{\substack{B: |B| > 3 \\ B \ni x}} \frac{|\widehat{\Phi}_B(\mathcal{C}_A)|}{|B|} \\ &\quad + \sum_{x^* \in Y} \frac{1}{\beta} \left\{ \sum_{P \ni x} \frac{|\Psi_I^T(P)|}{|P|} + \sum_{P \ni x} \frac{|\Psi^T(P)|}{|P|} \right\} \end{aligned} \quad (5.38)$$

where  $x^*$  is the projection of the site  $x$  of the lattice on the plane  $\mathbb{P}$ . From the definition (5.28) of  $\widehat{\Phi}_B$  and the bound (2.36) it follows that for all  $U > c_d c_1$ ,

$$\sum_{x^* \in Y} \left\{ \sum_{\substack{B: |B| > 3 \\ B \ni x}} \frac{|\widehat{\Phi}_B(\mathcal{C}_A)|}{|B|} \right\} \leq a_1 |Y| U^{-5} \quad (5.39)$$

where  $a_1$  is a positive constant depending on  $U_0, c_1$  and  $c_2$ . Further, using the bounds (3.51) and (3.53), and the definitions (3.32) and (3.39), we obtain the following bound:

$$\frac{1}{\beta} \sum_{x^* \in Y} \left\{ \sum_{P \ni x} \frac{|\Psi_I^T(P)|}{|P|} + \sum_{P \ni x} \frac{|\Psi^T(P)|}{|P|} \right\} \leq \frac{c |Y|}{\beta} e^{-6\beta a_2 U^{-2}} \quad (5.40)$$



where  $c$  and  $a_2$  denote positive constants depending on  $c_1, c_2, U_0$  and  $b_0$ . The factor of six in the exponent arises from the fact that the smallest Ising contour has six faces. ■

The lower bound to  $\varepsilon(Y | \mathcal{C}_A)$  is given by the following corollary.

**Corollary 10.** There exist positive constants  $U_0$  and  $b_0$ , such that for all  $U > U_0$  and  $\beta/U > b_0$ , the total energy  $\varepsilon(Y | \mathcal{C}_A)$  (5.30), of an  $R$ -contour  $Y$  (defined through (5.17)) which belongs to an  $R$ -configuration  $\mathcal{C}_A$ , satisfies the following bound:

$$|\varepsilon(Y | \mathcal{C}_A)| \geq J_3(U) \sum_{i=1}^p a_i^{ov} + K_3(U) \sum_{k=1}^q |A_k^{st}| \tag{5.41}$$

where

$$J_3(U) = J_2(U) - 6a_1 U^{-5} - \frac{6c}{\beta} e^{-6\beta a_2 U^{-1}} \tag{5.42}$$

$$K_3(U) = K_2(U) - 2a_1 U^{-5} - \frac{2c}{\beta} e^{-6\beta a_2 U^{-1}} \tag{5.43}$$

and  $c, a_1$  and  $a_2$  are the positive constants of Lemma 9. The constants  $J_2(U)$  and  $K_2(U)$  are defined through (5.25) and (5.26) respectively.

*Proof.* From the definition (5.30) of  $\varepsilon(Y | \mathcal{C}_A)$  it follows that

$$|\varepsilon(Y | \mathcal{C}_A)| \geq F_0(Y) - W_0(Y | \mathcal{C}_A)$$

where  $F_0(Y)$  is a lower bound to  $F(Y)$ , and  $W_0(Y | \mathcal{C}_A)$  is an upper bound to  $W(Y | \mathcal{C}_A)$ . Obtaining  $F_0(Y)$  from (5.24), using Lemma 9 and the bound (5.20) yields the bound (5.41). The leading contributions to the energy of the overlapping  $R$  subcontours  $Y_i^{ov}$  of the  $R$ -contour  $Y$  stem from the *overlapping triangles*  $\mathcal{T}_i^{ov}$  of  $Y_i^{ov}$ . An edge of an overlapping triangle can in general coincide with either one of the following—a  $\delta$ -edge, an  $\omega$ -edge, or a  $\lambda$ -link. A uniform lower bound to the energy  $\varepsilon(Y | \mathcal{C}_A)$  is obtained by omitting the positive energies of these additional edges. ■

**Step 2. A generalized Dobrushin’s transformation.** Consider an  $R$ -configuration  $\mathcal{C}_A$  defined by the  $R$ -contours  $Y_1, \dots, Y_l$ . Let  $Y_1$  be the contour we want to remove;  $Y_1^c = \mathbb{P} \setminus Y_1$  is an open set, which has maximally connected components  $\{O_0, \dots, O_r\}$ , where  $O_0$  is its exterior and

$\{O_1, \dots, O_r\}$  are the components of its interior. As  $Y_1$  is a maximally connected component of the complement of the bases, any  $R$ -contour in  $O_i$  is not connected to  $Y_1$ . Therefore, we can uniquely define a type  $\tau(O_i)$  of each interior, according to the type of base that separates  $Y_1$  and the contours in the interior of  $O_i$ . For simplicity assume that  $\tau(O_0) = 0$ . We would like to lift  $Y_1$  out of the  $R$ -configuration and fill the gap thus created with bases of type 0. This can be done only if  $\tau(O_i) = 0$  for every  $i$ , which is not the case in general. The extension of Dobrushin's trick<sup>(14)</sup> is first to apply a translation  $S_i$  to  $O_i$  such that

$$\tau(S_i[O_i]) = 0, \quad i = 1, \dots, r \quad (5.44)$$

It is easy to see that such translations  $S_i$  over one lattice spacing exists; e.g., we can use vertical translations over one lattice unit in the upward downward direction. Let us denote these translations by  $S$  and  $S^{-1}$ , respectively. Then the following relation holds for a base  $C_0$  of type 0:

$$\tau(S^n[C_0]) = -n \pmod{3} \quad (5.45)$$

Now we will apply  $S$  to each  $O_i$  of type 1, and  $S^{-1}$  to each  $O_i$  of type 2. Let  $n_i = 0, \pm 1$  be the exponent such that:

$$\tau(S^{n_i}[O_i]) = 0, \quad i = 1, \dots, r \quad (5.46)$$

In general the translations of the different  $O_i$  can now overlap, i.e.,

$$S^{n_i}[O_i] \cap S^{n_j}[O_j] \neq \emptyset \quad (5.47)$$

As long as all intersections are bases of type 0, there is no problem, and a new configuration with the contour  $Y_1$  removed can be defined. This corresponds to the situation in which the  $R$ -contours in  $S^{n_i}[O_i]$  and  $S^{n_j}[O_j]$  do not intersect each other. We now prove that this is indeed the case. Denote the inner  $R$ -contours in  $O_i$  by  $Y_{i,1}, \dots, Y_{i,q_i}$ . Then we have the following property of the interiors.

**Lemma 11.** For every  $R$ -contour  $Y_{i,j}$  in the interior  $O_i$  we have:

$$S^{n_i}[Y_{i,j}] \subset \bar{O}_i; \quad j = 1, \dots, q_i \quad (5.48)$$

where  $\bar{O}_i$  denotes the closure of  $O_i$ , and where  $n_i$  is an integer such that  $\tau(S^{n_i}[O_i]) = 0$ .

*Proof.* As  $O_i$  is a simply-connected set, and  $Y_{i,j}$  is closed, it is enough to show that, for every edge  $e \subset Y_{i,j}$  we have  $S^{n_i}(e) \subset \bar{O}_i$ . Let  $P_e$  be

the union of all closed triangles intersecting  $e$  either with an edge or a vertex. Then we have

$$P_e \subset \bar{O}_i, \quad \text{for all } e \in Y_{i,j} \tag{5.49}$$

because otherwise  $Y_{i,j}$  would be connected to  $O_i^c$ . It is then obvious that

$$S^{n_i}[e] \subset P_e \subset \bar{O}_i \quad \blacksquare \tag{5.50}$$

**Lemma 12.** For any pair of  $R$ -contours  $Y_{i_1, j_1}$  and  $Y_{i_2, j_2}$ , the following is true:

$$S^{n_{i_1}}[Y_{i_1, j_1}] \cap S^{n_{i_2}}Y_{i_2, j_2} = \emptyset, \tag{5.51}$$

for all  $i_1 \neq i_2; \quad 1 \leq j_1 \leq q_{i_1}; \quad 1 \leq j_2 \leq q_{i_2}$

*Proof.* As the  $R$ -contours  $Y_{i_1, j_1}$  and  $Y_{i_2, j_2}$  are closed complexes in two distinct interiors  $O_{i_1}$  and  $O_{i_2}$ , we have

$$d(Y_{i_1, j_1}, Y_{i_1}) \geq 1 \tag{5.52}$$

Hence we have

$$d(Y_{i_1, j_1}, Y_{i_2, j_2}) \geq 2 \tag{5.53}$$

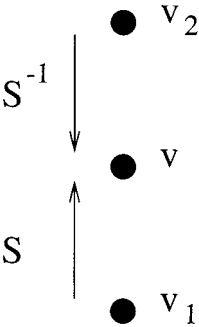


Fig. 6. The relative positions of  $v, v_1$  and  $v_2$  used in the proof of Lemma 12.

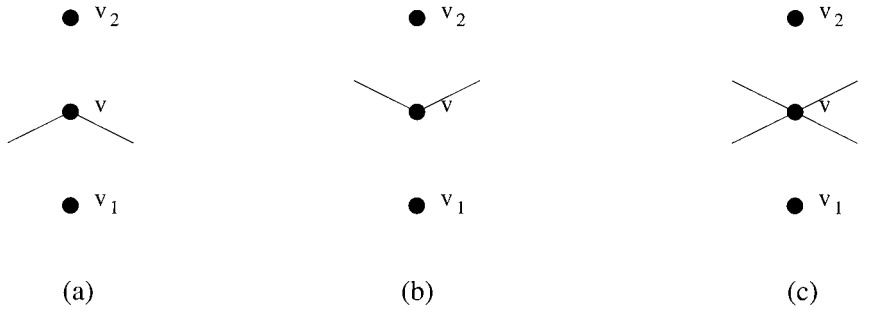


Fig. 7. The three cases used in the proof of Lemma 12.

As  $S^{n_{i_1}}$  and  $S^{n_{i_2}}$  are both translations over one lattice unit, it is clear that

$$S^{n_{i_1}}[Y_{i_1, j_1}] \cap S^{n_{i_2}}[Y_{i_2, j_2}] = \emptyset \tag{5.54}$$

whenever  $d(Y_{i_1, j_1}, Y_{i_2, j_2}) \geq 3$ . Hence the only case that we need to investigate is

$$d(Y_{i_1, j_1}, Y_{i_2, j_2}) = 2$$

Let us suppose that

$$S^{n_{i_1}}[Y_{i_1, j_1}] \cap S^{n_{i_2}}[Y_{i_2, j_2}] \neq \emptyset \tag{5.55}$$

Then there should exist a vertex  $v$  such that

$$v \in Y_1, \quad v \in S^{n_{i_1}}[Y_{i_1, j_1}], \quad v \in S^{n_{i_2}}[Y_{i_2, j_2}] \tag{5.56}$$

- If  $n_{i_1} = n_{i_2}$ , then we conclude that  $Y_{i_1, j_1}$  and  $Y_{i_2, j_2}$  have to intersect, which is excluded by hypothesis.
- Hence, we must have  $n_{i_1} = 1$  and  $n_{i_2} = -1$  (or  $n_{i_1} = -1$  and  $n_{i_2} = 1$ ). This means that there is  $v \in Y_1$ ,  $v_1 \in Y_{i_1, j_1}$  and  $v_2 \in Y_{i_2, j_2}$  as Fig. 6.

The points  $v$ ,  $v_1$  and  $v_2$  are related:  $S(v_1) = v = S^{-1}(v_2)$ . As the three vertices belong to non-intersecting  $R$ -contours, there are only the three possibilities shown in Fig. 7. Using the fact that the contour boundaries

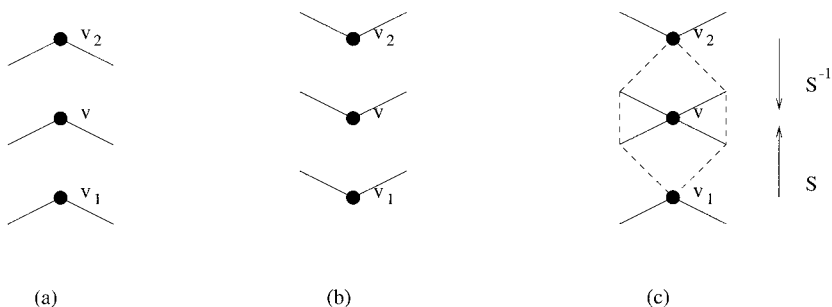


Fig. 8. The assignment of edges corresponding to the three cases shown in Fig. 7.

cannot subtend angles of  $\pi/3$  when the  $R$ -contours do not intersect, we complete these diagrams as shown in Fig. 8. In each case we can show that this leads to contradicting assignment of types to the rhombi containing the vertex  $v$ . For example, in the case (a) we are forced to assign the types of the rhombi as shown in Fig. 9. This contradicts the fact that  $S^{-1}[2] = 0$  and  $S(1) = 0$ , and hence is not allowed. We exclude the case (b) in the same way. For case (c), consider the dotted hexagon. It is easy to see that all rhombi with diagonals that are edges of the same hexagon must be of the same type. This implies that:  $\tau(O_{i_1}) = \tau(O_{i_2})$  contradicting the condition  $n_{i_1} = -n_{i_2}$ . ■

Now we can complete the Dobrushin argument and the proof of Proposition 8. We have shown that any  $R$ -contour  $Y$  can be removed, meaning that the following operations were performed to obtain a new configuration of non-overlapping  $R$ -contours.

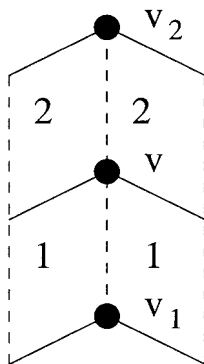


Fig. 9. The assignment of types to the rhombi of Fig. 8(a).

- Erase  $Y$
- Translate the interior  $O_i$  by  $S^{n_i}$  such that

$$\tau(S^{n_i}[O_i]) = \tau(O_0) = 0 \quad (5.57)$$

where  $O_0$  is the exterior of  $Y$ . After the translations have been performed some parts of the bases, which are now all of the type 0, will overlap.

- Fill up the gaps that were left with the base of type 0

The essential point of this construction is that the  $R$  contours which lie in the interiors of  $Y_1$  have been translated without intersecting each other. The effect of the translation is to modify only the energies corresponding to the potentials of range greater than two, which are corrections to the leading terms. This concludes the proof of Proposition 8.

## 5.7. The Peierls Conditions for the Geometric $R$ -Contours

There may be many  $R$ -contours which have the same support. Different  $R$ -contours whose supports coincide differ from each other in the configuration of their constituent overlapping  $R$ -subcontours, e.g., in the overlap numbers of the overlapping triangles, the multiplicity of the  $\lambda$ -links etc.

It is convenient to group the  $R$ -contours into equivalence classes depending on their support. This allows us to obtain bounds on relative probabilities entirely in terms of the supports of the  $R$ -contours. We define *equivalent contours* as follows.

Two  $R$ -contours

$$Y := \left( \bigcup_{i=1}^{i=p} Y_i^{ov} \right) \cup \left( \bigcup_{k=1}^{k=q} Y_k^{st} \right)$$

and

$$Y' := \left( \bigcup_{i=1}^{i=p} Y_i'^{ov} \right) \cup \left( \bigcup_{k=1}^{k=q} Y_k'^{st} \right)$$

are said to be *equivalent* iff they fulfill the following conditions:

- The standard subcontour  $Y_k^{st} \in Y$  is identical to the standard subcontour  $Y_k'^{st} \in Y'$  for  $k = 1, \dots, q$ . Each standard  $R$ -subcontour is given by a unique configuration of  $\delta$ -lines.

- The overlapping  $R$ -subcontour  $Y_i^{ov} \in Y$  and the overlapping  $R$ -subcontour  $Y_i^{ov} \in Y'$  have the same support, denoted by  $\text{supp}(\bar{Y}_i^{ov})$ , for  $i = 1, \dots, p$ .

A *geometric contour*  $\bar{Y} \equiv \bar{Y}(p, q)$  is an equivalence class of  $R$ -contours, i.e.

$$\begin{aligned} \bar{Y}(p, q) \equiv \bar{Y} &:= \left\{ Y_\alpha = \left( \bigcup_{i=1}^{i=p} Y_{\alpha i}^{ov} \right) \cup \left( \bigcup_{k=1}^{k=q} Y_k^{st} \right) \middle| \text{supp } Y_{\alpha i}^{ov} \right. \\ &= \left. \text{supp } \bar{Y}_i^{ov} \text{ for } 1 \leq i \leq p \right\} \end{aligned} \tag{5.58}$$

where the subscript  $\alpha$  is used to label the different  $R$ -contours which have overlapping subcontours of identical support. Like an  $R$ -contour, a geometric contour can also be decomposed into overlapping and standard subcontours:

$$\begin{aligned} \bar{Y}(p, q) &= \left( \bigcup_{i=1}^{i=p} \bar{Y}_i^{ov} \right) \cup \left( \bigcup_{k=1}^{k=q} Y_k^{st} \right) \\ &=: \bar{Y}^{ov} \cup \bar{Y}^{st} \end{aligned} \tag{5.59}$$

where the symbol  $\bar{Y}_i^{ov}$  denotes the  $i$ th overlapping geometric subcontour. It follows from (5.58) that all  $R$ -contours constituting a geometric contour have the same support.

We can associate a unique number  $r_i^{ov}$  to the support  $\text{supp}(\bar{Y}_i^{ov})$  which is defined as follows:

$$\begin{aligned} r_i^{ov} &:= \text{minimum number of (distinct) rhombi in which} \\ &\text{supp } \bar{Y}_i^{ov} \text{ can be decomposed} \end{aligned} \tag{5.60}$$

For simplicity we shall often use the symbol  $\bar{Y}$  to denote both the geometric contour and its support.

Each overlapping  $R$ -subcontour  $Y_{\alpha i}^{ov}$  is characterized by a configuration of overlapping triangles, each of which is labeled by an even overlap number. The  $R$ -subcontours belonging to a given geometric subcontour  $\bar{Y}_i^{ov}$  differ from each other in the distribution and overlap numbers of their overlapping triangles. Since each of these  $r_i^{ov}$  rhombi is an overlapping rhombus, the following bound is satisfied:

$$a_{\alpha i}^{ov} \geq r_i^{ov} \tag{5.61}$$

where  $a_{\alpha i}^{ov}$  is defined through (5.19), the subscript  $\alpha$  labelling the different  $R$ -subcontours belonging to  $\bar{Y}_i^{ov}$ . Let  $\text{Prob}_A \bar{Y}$  denote the probability of occurrence of an  $R$ -contour with support  $\text{supp } \bar{Y}$ , with support through (5.58) in  $\mathbb{P}_A$ . To compute this probability we need to sum over all possible  $R$ -contours which belong to  $\bar{Y}$ .

**Proposition 13.** There exist positive constants  $U_0, d_0$  and  $d_1$  such that, for all  $U > U_0, \beta/U > d_0$  and  $\beta/U^3 > d_1$ , the probability  $\text{Prob}_A(\bar{Y}(p, q))$  satisfies the bound

$$\text{Prob}_A(\bar{Y}(p, q)) \leq \prod_{i=1}^{i=p} e^{-\beta U^{-1} D_1 r_i^{ov}} \times \prod_{k=1}^{k=q} e^{-\beta U^{-3} D_2 |A_k^{st}|} \tag{5.62}$$

where  $D_1$  and  $D_2$  are positive constants depending on  $U_0, d_0$  and  $d_1$ .

*Proof.* The probability  $\text{Prob}_A(\bar{Y}(p, q))$  can be expressed in terms of the probability  $\text{Prob}_A(Y(p, q))$  that an  $R$ -contour  $Y(p, q)$  occurs in a given  $R$ -configuration. Using Proposition 8 we obtain the following bound.

$$\begin{aligned} \text{Prob}_A(\bar{Y}(p, q)) &= \sum_{\{Y \in \bar{Y}\}} \text{Prob}_A(Y(p, q)) \\ &\leq \prod_{i=1}^{i=p} \left( \sum_{\substack{\alpha \geq 1: \\ Y_{\alpha i}^{ov} \in \bar{Y}_i^{ov}}} e^{(-\beta J_3(U) a_{\alpha i}^{ov})} \right) \times \prod_{k=1}^{k=q} e^{(-\beta K_3(U) |A_k^{st}|)} \end{aligned} \tag{5.63}$$

Next we need to estimate the sum over  $\alpha$  in the last line of (5.63). Each overlapping subcontour with a given support is obtained by the projection of a set of faces (not necessarily connected) of an interface. The number of faces of an interface which projects onto the overlapping  $R$ -subcontour  $Y_i^{ov}$  is equal to  $(a_{\alpha i}^{ov} + r_i^{ov})$ . Since all the overlapping  $R$ -subcontours in  $\bar{Y}_i^{ov}$  have the same support, it is possible to find an edge, which belongs either to a base or to a standard  $R$ -subcontour, such that it intersects all these overlapping  $R$ -subcontours at a fixed vertex. (The choice of such an edge is, however, not unique). From these considerations it follows that we can replace the sum over  $\alpha$  by a sum over the variables  $a_i$ , which take integer values and correspond to the distinct sets of faces (each set belonging to an interface  $\tilde{I}$ ) which satisfy the following properties:

- (1) The projection of the (disjoint) union of the faces in each such set is connected to a fixed end of a fixed edge in the triangular lattice spanning the plane  $\mathbb{P}$ .
- (2) Each set has  $a_i + r_i^{ov}$  faces with  $a_i \geq r_i^{ov}$ .



Since the projection of each such set of faces is a connected set of rhombi, at least one vertex of each rhombus is shared by another rhombus. Hence each rhombus has at most three vertices to which the fixed edge can be attached. The number of ways of placing  $a_i + r_i^{ov}$  rhombi on the supp  $\bar{Y}_i^{ov}$ , which is connected to a fixed end of a fixed edge in the triangular lattice spanning  $\mathbb{P}$ , is bounded by the number of ways of constructing a connected set which consists of  $a_i + r_i^{ov}$  rhombi and is connected to this fixed vertex. This latter number, which we denote by  $N^{ov}(a_i)$ , is easily seen to satisfy the bound

$$N^{ov}(a_i) \leq m^{a_i + r_i^{ov}} \tag{5.64}$$

with  $m = 36$ , by the Königsberg Bridge Lemma.<sup>(44)</sup> Hence,

$$\begin{aligned} \text{Prob}_A(\bar{Y}(p, q)) &\leq \sum_{a_1 \geq r_1^{ov}, \dots, a_p \geq r_p^{ov}} m^{a_1 + r_1^{ov} + \dots + a_p + r_p^{ov}} \\ &\quad \times e^{-\beta(a_1 + \dots + a_p) J_3(U)} \times \prod_{k=1}^{k=q} e^{-\beta K_3(U) \times |A_k^{st}|} \\ &\leq \prod_{i=1}^{i=p} m^{2r_i^{ov}} e^{-\beta r_i^{ov} J_3(U)} \left( \sum_{a_i \geq 0} m^{a_i} e^{-\beta a_i J_3(U)} \right) \\ &\quad \times \prod_{k=1}^{k=q} e^{-\beta K_3(U) \times |A_k^{st}|} \end{aligned} \tag{5.65}$$

It is easy to see that there exists positive constants  $U_0, d_0$ , such that for all  $U > U_0$  and  $\beta/U > d_0$ , the geometric series in parenthesis (on RHS of (5.65)) converges. Hence, using the definitions (5.42) and (5.43) of  $J_3(U)$  and  $K_3(U)$  we find that for all  $U > U_0, \beta/U > d_0$  and  $\beta/U^3 > d_1$  (where  $d_1$  is a positive constant) the following bound holds

$$\text{Prob}_A(\bar{Y}(p, q)) \leq \prod_{i=1}^{i=p} e^{-\beta U^{-1} D_1 r_i^{ov}} \times \prod_{k=1}^{k=q} e^{-\beta U^{-3} D_2 |A_k^{st}|} \tag{5.66}$$

where  $D_1$  and  $D_2$  are positive constants depending on  $U_0, d_0$  and  $d_1$ . ■

### 5.8. Proof of the Rigidity of the 111 Interface

The rigidity of the 111 interface can be expressed in terms of the probability,  $\text{Prob}_A(s_{x_0} = -1 \mid \text{b.c.2})$ , that a lattice site  $x_0 = (x_1, x_2, x_3)$ , such

that  $x_1 + x_2 + x_3 \geq 1/2$ , is occupied by a “-” spin under the boundary condition b.c.2 (2.21). To have  $s_{x_0} = -1$ , the site  $x_0$  must be enclosed either by a pyramid of the interface or by a least one Ising contour. As a result we have that

$$\text{Prob}_A(s_{x_0} = -1 \mid \text{b.c.2}) \leq \sum_{\bar{Y} \ni x_0^*} \text{Prob}_A \bar{Y} + \sum_{\gamma \ni x_0} \text{Prob}_A \gamma \quad (5.67)$$

where  $x_0^*$  denotes the projection of the site  $x_0$  on the plane  $\mathbb{P}_A$ . The first term on the RHS of (5.67) arises when the interface has at least one pyramid whose projection on  $\mathbb{P}_A$  encloses the point  $x_0^*$ . The second term arises when the “-” spin at  $x_0$  is enclosed by one or more Ising contours, whose presence does not lead to a distortion of the interface from its perfect staircase structure around the site  $x_0$ . The above bound (5.67) is also satisfied by the probability  $\text{Prob}_A(s_{\tilde{x}_0} = 1 \mid \text{b.c.2})$ , for  $\tilde{x}_0 = (x_1, x_2, x_3)$  with  $x_1 + x_2 + x_3 \leq -1/2$ .

Hence, to prove the rigidity of the 111 interface we need to estimate the terms on the RHS of (5.67). An estimate of the first term is given by the following proposition.

**Proposition 14.** There exist positive constants  $U_0$  and  $b_1$  and  $b_2$ , such that for all  $U > U_0$   $\beta/U > b_1$  and  $\beta/U^3 > b_2$ , the following estimate is true:

$$\sum_{\bar{Y} \ni x_0^*} \text{Prob}_A \bar{Y} \leq \tilde{C}_0 e^{-c'' \beta U^{-3}} \quad (5.68)$$

where  $\tilde{C}_0$  and  $c''$  are positive constants depending on  $U_0$ ,  $b_1$  and  $b_2$ .

*Proof.* From Proposition 13 it follows that

$$\sum_{\substack{\bar{Y} \\ \bar{Y} \ni x_0^*}} \text{Prob}_A \bar{Y} \leq \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{ov} \cup \bar{Y}^{st}}} \prod_{\bar{Y}_i^{ov} \in \bar{Y}^{ov}} e^{-\beta U^{-1} D_1 r_i^{ov}} \prod_{\bar{Y}_k^{st} \in \bar{Y}^{st}} e^{-\beta U^{-3} D_2 |\Delta_k^{st}|} \quad (5.69)$$

where we have used the following notations:  $\bar{Y}_i^{ov}$  denotes an overlapping geometric subcontour (see (5.58)), while  $|\Delta_k^{st}|$  denotes the total number of  $\delta$ -lines in the standard geometric subcontour  $\bar{Y}_k^{st} \equiv Y_k^{st}$ . Further, an empty product is equal to unity.

$$\begin{aligned}
 \text{RHS of (5.69)} &= \sum_{\substack{\bar{Y} \ni x_0^* \\ Y := \bar{Y}^{ov} \cup \bar{Y}^{st} \\ \bar{Y}^{ov} \neq \emptyset}} \prod_{Y_i^{ov} \in \bar{Y}^{ov}} e^{-\beta U^{-1} D_1 r_i^{ov}} \times \prod_{Y_k^{st} \in \bar{Y}^{st}} e^{-\beta U^{-3} D_2 |A_k^{st}|} \\
 &+ \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{st} \\ \bar{Y}^{ov} = \emptyset}} e^{-\beta U^{-3} D_2 |A^{st}|} \\
 &= \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{ov} \cup \bar{Y}^{st} \\ \bar{Y}^{ov} \neq \emptyset}} \prod_{Y_i^{ov} \in \bar{Y}^{ov}} e^{-\beta U^{-1} D_1 r_i^{ov}} \\
 &\quad \times \left[ \prod_{Y_k^{st} \in \bar{Y}^{st}} \{ (e^{-\beta U^{-3} D_2 |A_k^{st}|} - 1) + 1 \} \right] + \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{st} \\ \bar{Y}^{ov} = \emptyset}} e^{-\beta U^{-3} D_2 |A^{st}|} \\
 &= \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{ov} \cup \bar{Y}^{st} \\ \bar{Y}^{ov} \neq \emptyset}} \prod_{Y_i^{ov} \in \bar{Y}^{ov}} e^{-\beta U^{-1} D_1 r_i^{ov}} \\
 &\quad \times \left\{ 1 + \sum_{n \geq 1} \sum_{\substack{Y_1^{st}, \dots, Y_n^{st} \\ Y_i^{st} \cap \bar{Y}^{ov} \neq \emptyset \\ (i=1, \dots, n)}} \prod_{k=1}^n (e^{-\beta U^{-3} D_2 |A_k^{st}|} - 1) \right\} \quad (5.70) \\
 &+ \sum_{\substack{\bar{Y} \ni x_0^* \\ \bar{Y} := \bar{Y}^{st} \\ \bar{Y}^{ov} = \emptyset}} e^{-\beta U^{-3} D_2 |A^{st}|} \quad (5.71)
 \end{aligned}$$

where  $|A^{st}|$  denotes the number of  $\delta$ -lines in the standard  $R$ -contour  $Y^{st}$ .

The term on the RHS of (5.70) is similar to (3.26) of Section 3.1. This allows us to prove the bound (5.68) by using a method analogous to the one used in that section. Each geometric contour  $\bar{Y}$  appearing in the sum on the RHS of (5.70) consists of a finite set of non-intersecting overlapping geometric subcontours and a finite set of standard geometric subcontours such that each standard geometric subcontour intersects at least one overlapping geometric subcontour in the set. We can alternatively express each such  $\bar{Y}$  as a connected set of auxiliary polymers, each polymer being a connected set consisting of only a *single* overlapping geometric subcontour and a finite set of standard geometric subcontours which intersect it. To each term on the RHS of (5.71) we can associate a standard geometric contour which is given by a standard  $R$ -contour. These considerations allow us to express the RHS of (5.69) in terms of the elements of a more general

polymer system, the polymers being referred to as *spider contours* (or  $S$  contours, for brevity) and defined as follows:

An  $S$  contour,  $\zeta$  is a finite connected set of geometric  $R$ -subcontours, containing at most one overlapping geometric  $R$ -subcontour. Hence, in general

$$\zeta := \bar{Y}^{ov} \cup \left\{ \bigcup_{i=1}^{i=s} \Upsilon_i^{st} \right\} \quad (5.72)$$

where  $\bar{Y}^{ov}$  denotes an overlapping geometric subcontour.

In particular, an  $S$  contour can reduce to a single overlapping  $R$ -contour (with no standard part) or to one standard  $R$ -contour. We refer to an  $S$  contour which has no overlapping part as a *standard*  $S$  contour and denote it by the symbol  $\zeta^{st}$ . The other  $S$  contours are said to be overlapping and are denoted by the symbol  $\zeta^{ov}$ . Every standard  $R$ -subcontour which belongs to an overlapping  $S$  contour, (defined through (5.72)), necessarily intersects the overlapping geometric subcontour  $\bar{Y}^{ov}$ .

A given geometric  $R$ -contour  $\bar{Y}$ , with support  $\text{supp } \bar{Y}$ , can be built from a finite family of intersecting  $S$  contours. For an  $S$  contour  $\zeta$  given by (5.72), we define

$$|\zeta| := r^{ov} + \sum_{i=1}^s |A_i^{st}| \quad (5.73)$$

where  $r^{ov}$  denotes the minimal number of rhombi needed to cover the support of  $\bar{Y}^{ov}$  (see (5.60)). For a standard  $S$ -contour  $\zeta^{st}$  we define

$$|\zeta^{st}| := |A^{st}| \quad (5.74)$$

which is the number of  $\delta$ -lines in it.

We define the weight  $\eta(\cdot)$  of an *overlapping*  $S$  contour  $\zeta^{ov}$  (defined through (5.72)) to be

$$\eta(\zeta^{ov}) := e^{-\beta U^{-1} D_1 r^{ov}} \times \prod_{\Upsilon_k^{st} \cap \bar{Y}^{ov} \neq \emptyset} e^{-\beta U^{-3} D_2 |A_k^{st}|} \quad (5.75)$$

In (5.75) we use the convention that an empty product is unity. Hence the case in which the  $S$  contour does not contain any standard part, is included in (5.75). The corresponding weight for a *standard*  $S$  contour  $\zeta^{st} \equiv \Upsilon^{st}$  is defined as

$$\eta(\zeta^{st}) := e^{-\beta U^{-3} D_2 |A^{st}|} \quad (5.76)$$

From (5.70), (5.71), (5.75) and (5.76) it follows that

$$\sum_{\substack{\bar{Y} \\ \bar{Y} \ni x_0^*}} \text{Prob}(\bar{Y}) \leq \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{\zeta_1, \dots, \zeta_n \\ \zeta_1 \cup \dots \cup \zeta_n = \bar{Y} \\ \bar{Y} \ni x_0^*, \text{ connected}}} \prod_{j=1}^n \eta(\zeta_j) \leq \sum_{n \geq 1} \frac{C^n}{n} \quad (5.77)$$

where

$$C := \sum_{\zeta \ni x_0^*} \eta(\zeta) e^{|\zeta|} \quad (5.78)$$

In obtaining the bound (5.77), we have made use of Lemma 3.5 of ref. 36 (as in (B.8) of the Appendix B). The proof of the bound (5.68) reduces to the proof of the following lemma. ■

**Lemma 15.** For each  $D' > 0$ , there exist positive constants  $b_1$  and  $b_2$  such that for all  $\beta/U > b_1$  and  $\beta/U^3 > b_2$  the following bound holds:

$$\sum_{\zeta \ni x_0^*} \eta(\zeta) e^{|\zeta|} \leq D' \quad (5.79)$$

*Proof.*

$$\text{LHS of (5.79)} = \sum_{\zeta^{ov} \ni x_0^*} \eta(\zeta^{ov}) e^{|\zeta^{ov}|} + \sum_{\zeta^{st} \ni x_0^*} \eta(\zeta^{st}) e^{|\zeta^{st}|} \quad (5.80)$$

Let us first evaluate the second term on the RHS of (5.80). To do this we use the fact that the smallest standard  $R$ -contour consists of six  $\delta$ -lines. Hence,

$$\sum_{\zeta^{st} \ni x_0^*} \eta(\zeta^{st}) e^{|\zeta^{st}|} \leq \sum_{k \geq 6} \sum_{\substack{\zeta^{st} \ni x_0^* \\ |\zeta^{st}| = k}} e^{-\beta U^{-3} D_2 k} e^k \quad (5.81)$$

Consider each standard  $S$  contour, appearing in the above sum, as a connected graph which contains a fixed vertex  $x_0^*$ . The maximum coordination number of each vertex in the graph is five, because a  $\delta$ -line which intersects a given  $\delta$ -line at a fixed end, can emerge in any one of five directions (in the triangular lattice spanning  $\mathbb{P}$ ). Then by the Königsberg Bridge Lemma<sup>(44)</sup>

$$\text{RHS of (5.81)} \leq 6 \sum_{k \geq 6} 5^{2k} e^{-\beta U^{-3} D_2 k} e^k \quad (5.82)$$

The factor of six arises from the fact that there can be at most six different  $\delta$ -lines in the rhombus model which contains the fixed site  $x_0^*$ . Let  $b > 0$  be a constant, such that for all  $\beta/U^3 > b$ , the geometric series in (5.82) converges. Then for all  $\beta/U^3 > b$ ,

$$\sum_{\zeta^{st} \ni x_0^*} \eta(\zeta^{st}) e^{|\zeta^{st}|} \leq e^{-6D_4\beta U^{-3}} \quad (5.83)$$

where  $D_4$  is a positive constant depending on  $b$ . Next we need to evaluate the first term on the RHS of (5.80). This term can be further decomposed into two sums, depending on whether the fixed site  $x_0^*$  belongs to the overlapping subcontour of an  $S$  contour or not. Using the definition (5.72) of an overlapping  $S$  contour, we can write

$$\sum_{\zeta^{ov} \ni x_0^*} \eta(\zeta^{ov}) e^{|\zeta^{ov}|} = \sum_{\substack{\zeta^{ov} \\ \bar{\gamma}^{ov} \ni x_0^*}} (\zeta^{ov}) e^{|\zeta^{ov}|} + \sum_{\substack{\zeta^{ov} \ni x_0^* \\ \bar{\gamma}^{ov} \ni x_0^*}} \eta(\zeta^{ov}) e^{|\zeta^{ov}|} \quad (5.84)$$

The second term on the RHS of (5.84) corresponds to the situation in which the fixed vertex is necessarily contained in a  $R$ -standard subcontour of the overlapping  $S$  contour.

**Evaluation of the First Term on the RHS of (5.84).** Let us construct  $\bar{\gamma}^{ov}$  starting from  $x_0^*$ . Once a rhombus which has  $x_0^*$  as one of its vertices is chosen, the next rhombus which intersects it can be placed in twenty four different ways; it can intersect the first rhombus either at any one of its four vertices or along any one of its four edges. Further, for intersection either along an edge, or at a vertex, there are three possible orientations of the pair of rhombi. This allows us to consider each rhombus as a vertex of a connected graph which contains a fixed vertex. The fixed vertex of the graph corresponds to the rhombus which contains the site  $x_0^*$ . There are twelve different rhombi in the triangular lattice spanning  $\mathbb{P}$  which contains a given site. Then, by the Königsberg Bridge Lemma<sup>(44)</sup> the number,  $N(\bar{\gamma}^{ov} | n; x_0^*)$ , of different ways of constructing an overlapping geometric contour  $\bar{\gamma}^{ov}$ , such that it contains a fixed site  $x_0^*$ , and has  $r^{ov} = n$ , satisfies the bound

$$N(\bar{\gamma}^{ov} | n; x_0^*) \leq 12d_1^{2n} \quad \text{with} \quad d_1 = 24 \quad (5.85)$$

The overlapping geometric contour  $\bar{\gamma}^{ov}$  has at most  $(3n+1)$  vertices at which a  $\delta$ -line can intersect it. Moreover, from each vertex of  $\bar{\gamma}^{ov}$  there can emerge at most four standard  $\delta$ -lines. Further, each such standard  $\delta$ -line

can correspond to either one of two different pairs of rhombi. These considerations yield the bound

$$\sum_{\substack{\zeta^{ov} \\ \bar{\gamma}^{ov} \ni x_0^*}} \eta(\zeta^{ov}) e^{|\zeta^{ov}|} \leq \sum_{n \geq 1} 12d_1^{2n} e^{-\beta U^{-1} D_1 n} \\ \times \left\{ 8 \times (3n + 1) \sum_{k \geq 1} 5^{2k} e^{-(\beta U^{-3} D_2 k)} e^{k} \right\} \quad (5.86)$$

Let  $b'_1$  and  $b'$  be positive constants such that for all  $\beta/U > b'_1$  and  $\beta/U^3 > b'$  the series in  $n$  and  $k$  converges. Then for such values of  $\beta$  and  $U$  the RHS of (5.86) satisfies the bound

$$\text{RHS of (5.86)} \leq e^{-\beta U^{-3} D_6} e^{-\beta U^{-1} D_5} \quad (5.87)$$

where  $D_5$  and  $D_6$  are positive constants depending on  $b'_1$  and  $b'$  respectively.

**Evaluation of the Second Term on the RHS of (5.84).** To evaluate this sum we make use of the fact that each standard  $R$ -subcontour in  $\zeta^{ov}$  intersects  $\bar{\gamma}^{ov}$ . We construct  $\zeta^{ov}$  starting from the site  $x_0^*$  which now belongs to a standard  $R$ -subcontour. If the standard  $R$ -subcontour which contains  $x_0^*$  has  $m$   $\delta$ -lines, then there are at most  $m + 1$  vertices at which  $\bar{\gamma}^{ov}$  can intersect it. Moreover, there can be at most four standard  $\delta$ -lines emerging from each of the  $(3r^{ov} + 1)$  vertices of  $\bar{\gamma}^{ov}$  and there are two possible orientations of each such pair of  $\delta$  lines. From these considerations we obtain

$$\sum_{\substack{\zeta^{ov} \ni x_0^* \\ \bar{\gamma}^{ov} \ni x_0^*}} \eta(\zeta^{ov}) e^{|\zeta^{ov}|} \\ \leq \sum_{m \geq 1} 5^{2m} e^m e^{-\beta U^{-3} D_2 m} \\ \times \left[ (m + 1) \sum_{n \geq 1} d_1^{2n} e^{-\beta U^{-1} n} \left\{ 8 \times (3n + 1) \sum_{k \geq 1} 5^{2k} e^k e^{-\beta U^{-3} D_2 k} \right\} \right] \quad (5.88)$$

Let  $b''_1$  and  $b''$  be positive constants such that for all  $\beta/U > b''_1$  and  $\beta/U^3 > b''$  the series on the RHS of (5.88) converges. Then, for such values of  $\beta$  and  $U$  the following bound is satisfied:

$$\text{RHS of (5.88)} \leq e^{-\beta U^{-3} D_8} e^{-\beta U^{-1} D_7} \quad (5.89)$$

where  $D_7$  and  $D_8$  are positive constants depending on  $b'_1$  and  $b''$  respectively. Let

$$b_1 := \max(b'_1, b''_1) \quad (5.90)$$

and

$$b_2 := \max(b, b', b'') \quad (5.91)$$

Then from (5.83), (5.87) and (5.89) it follows that for all  $\beta/U > b_1$  and  $\beta/U^3 > b_2$

$$\sum_{\zeta \ni x_0^*} \eta(\zeta) e^{|\zeta|} \leq C_0 e^{-c''/\beta/U^3} =: D' \quad (5.92)$$

where  $C_0$  and  $c''$  are positive constants depending on  $b_1$  and  $b_2$  respectively. Hence  $D'$  is a positive constant which can be made arbitrarily small by making  $b_1$  and  $b_2$  large enough. This concludes the proof. ■

To estimate the second term on the RHS of (5.67) we make use of the result of the cluster expansion given in Lemma 5. This yields the following proposition.

**Proposition 16.** There exist constants  $U_1, b_3 > 0$  such that for all  $U > U_1$  and  $\beta/U > b_3$  the following estimate is true:

$$\sum_{\gamma \ni x_0} \text{Prob}_A(\gamma) \leq \tilde{C}_1 e^{-c'_1 \beta U^{-1}} \quad (5.93)$$

where  $\tilde{C}_1, c'_1$  are positive constants depending on  $U_1$  and  $b_3$ .

*Proof.* We have that

$$\sum_{\gamma \ni x_0} \text{Prob}_A(\gamma) \leq \sum_{\substack{D: \\ \mathcal{D} \ni \gamma \\ \gamma \ni x_0}} \text{Prob}_A(D) \quad (5.94)$$

where  $\text{Prob}_A D$  denotes the probability of occurrence of a decorated contour  $D$  in  $A$ .

$$\text{RHS of (5.94)} \leq \frac{[\sum_{D: \mathcal{D} \ni \gamma, \gamma \ni x_0} W(D) \{\sum'_{\mathcal{D}} \prod_{D' \in \mathcal{D}} W(D')\}]}{[\sum_{\mathcal{D}} \prod_{D' \in \mathcal{D}} W(D')]} \quad (5.95)$$

The symbol  $\sum'_{\mathcal{D}}$  is used to denote a sum over all finite compatible sets  $\mathcal{D} = \{\mathcal{D}'\}$  of decorated contours which are *compatible* with  $D$ , the latter being a decorated contour which encloses the site  $x_0$ . In the denominator



we have an unrestricted sum. The result of the cluster expansion [Lemma 5] can be applied to both these sums to yield

RHS of (5.95)

$$\leq \sum_{\substack{D: \\ \mathcal{D} \ni \gamma \\ \gamma \ni x_0}} W_0(D) \exp \left\{ - \sum_{N \geq 1} \frac{1}{N!} \sum_{\substack{D_1, \dots, D_N \\ (i) \& (ii)}} \Psi^T(\{D_1, \dots, D_N\}) \right\} \quad (5.96)$$

where (i)&(ii) refer to the following conditions:

- (i)  $D_1 \cup \dots \cup D_N \equiv P$  is a connected set (a cluster),
- (ii)  $P \cap D \neq \emptyset$ .

We have made use of the fact that  $|W(D)| \leq W_0(D)$ , where  $W_0(D)$  is given by (3.32).

$$\text{RHS of (5.96)} \leq \sum_{\substack{D: \\ \mathcal{D} \ni \gamma \\ \gamma \ni x_0}} W_0(D) \exp \left\{ -|D| \sum_{N \geq 1} \frac{1}{N!} \sum_P^* \frac{|\Psi^T(P)|}{|P|} \right\} \quad (5.97)$$

where

$$|D| = \sum_{\gamma \in D} \left\{ |\gamma| + \sum_{B \cap \gamma \neq \emptyset} g(B) \right\}$$

and the symbol  $\sum_P^*$  denotes a sum over all clusters  $P$  which contain a fixed site. The bound (5.93) is then obtained by making use of (3.32) and the bound (3.51) on the RHS of (5.97). ■

From the Propositions 14 and 16 it follows that for  $x_0 = (x_1, x_2, x_3)$  such that  $x_1 + x_2 + x_3 \geq 1/2$ , we have the following upper bound on the probability  $\text{Prob}_A(s_{x_0} = -1)$ :

**Lemma 17.** There exist positive constants  $\tilde{U}_0$ ,  $\tilde{D}_0$  and  $\tilde{D}'_0$  such that for all  $U > \tilde{U}_0$ ,  $\beta/U > \tilde{D}_0$  and  $\beta/U^3 > \tilde{D}'_0$  the following bound is satisfied:

$$\begin{aligned} \text{Prob}_A(s_{x_0} = -1) &\leq \{ \tilde{C}_0 e^{-c''\beta/U^3} + \tilde{C}_1 e^{-c'_1\beta/U} \} \\ &\text{for } x_0 = (x_1, x_2, x_3) \text{ and } x_1 + x_2 + x_3 \geq 1/2 \end{aligned} \quad (5.98)$$

### 5.9. Proof of Theorem 2

We now have all the estimates necessary to prove our main result on the rigidity of the 111 interface, i.e., Theorem 2.

*Proof.* For  $x = (x_1, x_2, x_3)$  with  $x_1 + x_2 + x_3 \geq 1/2$ , we have that

$$\langle s_x \rangle_{[\text{b.c.2}]} = 1 - 2 \times \lim_{A \nearrow \mathbb{Z}^3} \text{Prob}_A(s_x = -1 \mid \text{b.c.2}) \quad (5.99)$$

where  $x^*$  denotes the projection of the site  $x$  on the plane  $\mathbb{P}$ .

Lemma 17 provides an upper bound to the probability  $\text{Prob}_A(s_x = -1 \mid \text{b.c.2})$  which is uniform in the volume  $A$ . Introducing this bound, (5.98), in (5.99) yields (2.40).

Similarly for  $x = (x_1, x_2, x_3)$  with  $x_1 + x_2 + x_3 \leq -1/2$ , we have that

$$\langle s_x \rangle_{[\text{b.c.2}]} = -1 + 2 \times \lim_{A \nearrow \mathbb{Z}^3} \text{Prob}_A(s_x = 1 \mid \text{b.c.2}) \quad (5.100)$$

which reduces to (2.41) by the analogue of Lemma 17 for  $\text{Prob}_A(s_x = 1 \mid \text{b.c.2})$  with  $x_1 + x_2 + x_3 \leq -1/2$ . ■

## APPENDIX A. BOUND ON THE REMAINDER TERM OF THE EFFECTIVE HAMILTONIAN

In this appendix we present a complete proof of a bound on the remainder term for the effective Hamiltonians derived from the circuit representation of ref. 33, which is missing in this reference. A proof of a similar bound for a more general class of Hamiltonians will be given in ref. 32. The bound is essential to control the temperature dependence of the effective Hamiltonians. Therefore, we present the proof here in considerable detail, although we certainly do not claim that the proof is new: the proof of Lemma 18 (given below) closely follows ideas of ref. 9, and, in general, our discussion follows the lines of ref. 33 and ref. 46.

### A.1. Definitions

The Hamiltonian defined on a finite lattice  $A \subset \mathbb{Z}^d$ ,  $d \geq 2$  is given by

$$H_A = H_0 + tV - \mu_e N_e - \mu_i N_i \quad (A.1)$$

where

$$H_0 = 2U \sum_{x \in A} W(x) c_x^\dagger c_x \quad (A.2)$$

and

$$V = - \sum_{\langle xy \rangle} c_x^\dagger c_y + \text{h.c.} \quad (A.3)$$

where  $\langle xy \rangle$  denotes a pair of nearest neighbour sites on the lattice. Let us restrict our attention to the *neutral case at half-filling*, i.e.,  $\mu_e = \mu_i = U$ . In order to make the origin of various terms in the series expansions more transparent, we do not set  $t = 1$  in this appendix, unlike in the main text.

The effective hamiltonian (for a given configuration  $S = \{s_x\}$  of ions) is defined through the relation

$$\exp[-\beta H_{\text{eff}}(\beta, S)] = \text{Tr}_{\mathcal{F}_e} \exp[-\beta H_A] \quad (\text{A.4})$$

where the trace is over the electronic Fock space (denoted by  $\mathcal{F}_e$ ).

Iterating Duhamel's formulas

$$e^{-\beta(H_0 + tV)} = e^{-\beta H_0} + \int_0^\beta d\tau e^{-(\beta-\tau)H_0} (-tV) e^{-\tau(H_0 + tV)} \quad (\text{A.5})$$

we obtain the Dyson series

$$\begin{aligned} e^{-\beta H_A} := & e^{\beta U(N_e + N_i)} \int_{n=0}^{\infty} \int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1 e^{(\beta-\tau_n)H_0} (-tV) \\ & \times e^{-(\tau_n-\tau_{n-1})H_0} (-tV) \cdots e^{-(\tau_2-\tau_1)H_0} (-tV) e^{-\tau_1 H_0} \end{aligned} \quad (\text{A.6})$$

Hence

$$\begin{aligned} e^{-\beta H_A} := & e^{\beta U(N_e + N_i)} \sum_{n=0}^{\infty} t^n \sum_{\langle x_1 y_1 \rangle, \dots, \langle x_n y_n \rangle} \int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1 \\ & \times e^{(\beta-\tau_n)H_0} c_{x_n}^\dagger c_{y_n} \cdots e^{-(\tau_2-\tau_1)H_0} c_{x_1}^\dagger c_{y_1} e^{-\tau_1 H_0} \end{aligned} \quad (\text{A.7})$$

As in ref. 33 we introduce the set  $\mathcal{C}(A)$  of (classical) configurations associated to the electron subsystem. An element  $X \in \mathcal{C}(A)$  is a finite sequence  $X = (x_1, \dots, x_m)$  of distinct sites in  $A$ . The state  $|X\rangle \in \mathcal{F}_e$ , associated to  $X \in \mathcal{C}(A)$  is defined as follows:

$$|X\rangle := [c^\dagger(x_1) \cdots c^\dagger(x_m)] \leqslant |0\rangle \quad (\text{A.8})$$

where  $|0\rangle \in \mathcal{C}(A)$  denotes the vacuum.

The symbol  $\leqslant$  denotes a total ordering of the sites in  $A$ , chosen to avoid ambiguities in the definition of the phase in (A.8). For convenience we choose the spiral order<sup>(9)</sup> for  $d=2$  and an analogous ordering for  $d \geqslant 3$ . This ordering is chosen to have the property that, for any finite set  $X \subset A$ , the set  $\{X'\} = \{x \in \mathbb{Z}^d; x \leqslant X\}$  of lattice sites which are smaller than  $X$ , or belong to  $X$ , is finite.

For a given sequence of pairs of nearest neighbour sites,  $(\langle x_1 y_1 \rangle, \dots, \langle x_n y_n \rangle)$ , let

$$\varepsilon_j |X_j\rangle = c_{x_j}^\dagger c_{y_j} |X_{j-1}\rangle \quad \text{for } 1 \leq j \leq n \quad (\text{A.9})$$

where each  $\varepsilon_j = \pm 1$ . [Note that  $|X_j| = |X_{j-1}|$  for  $j = 1, \dots, n$ .]

Setting  $\tau_0 = 0$ ,  $\tau_{n+1} = \beta$  and  $X_0 = X_n = X$  we obtain

$$\begin{aligned} \text{Tr}_{\mathcal{F}_e} e^{-\beta H_A} := & \sum_{x_0, \dots, x_n \in \mathcal{C}(A)} e^{\beta U(N_e + N_i)} \sum_{n=0}^{\infty} t^n \left\{ \prod_{j=0}^n \langle X_j | e^{-(\tau_{j+1} - \tau_j) H_0} | X_j \rangle \right\} \\ & \times \langle X | \left[ \prod_{j=0}^n c_{x_j}^\dagger c_{y_j} \right] \llcorner | X \rangle \end{aligned} \quad (\text{A.10})$$

Note that

$$H_0 |X_j\rangle = e(X_j) |X_j\rangle \quad (\text{A.11})$$

where

$$e(X_j) := 2U \times [\text{number of sites in } X_j \text{ for which } W(x) = 1, \text{ (i.e., } s_x = 1)] \quad (\text{A.12})$$

As in ref. 33, we introduce the notion of *trajectories*. Let  $\tau_i$  be a positive integer variable (with  $\tau_0 = 0$  and  $\tau_{n+1} = \beta$ ) which we refer to as the “time.” A trajectory  $\zeta = \zeta(\tau_i)$  is a sequence  $x(\tau_0), x(\tau_1), \dots, x(\tau_{n+1})$  of sites in  $A$  such that either

$$\tau_i \neq \tau_{i+1} \quad \text{with } x(\tau_i) = x(\tau_{i+1})$$

or

$$\tau_i = \tau_{i+1} \quad \text{with } x(\tau_i) \text{ and } x(\tau_{i+1}) \text{ being nearest neighbour sites on the lattice}$$

This last case we describe as a *jump*. Let

$$\mathcal{J}(\zeta) := \{ \langle x(\tau_i) x(\tau_{i+1}) \rangle \mid \tau_i = \tau_{i+1}; x(\tau_i), x(\tau_{i+1}) \in \zeta \} \quad (\text{A.13})$$

denote the set of jumps in the trajectory  $\zeta$ . Let  $\mathcal{T} = \{\zeta\}$  denote a set of non-intersecting trajectories. If  $g$  is a function on the trajectories, then we define a “sum” over sets of trajectories as follows:

$$\sum_{\zeta} g(\zeta) := 1 + \sum_{n \geq 1} \sum_{(B_1, \dots, B_n)} \sum_{\substack{(X_0, \dots, X_n) \\ X_j \in \mathcal{C}(A)}} \mathbb{I}[(i), (ii)] \int_0^\beta d\tau_n \cdots \int_0^{\tau_2} d\tau_1 g(\zeta) \quad (\text{A.14})$$

where  $\underline{B}_i = \{\langle x_i, y_i \rangle\}$  denotes a set of nearest neighbour sites on the lattice. By  $I[E]$  we mean the indicator function of the event  $E$ ; in particular,  $I[(i), (ii)]$  in (A.14) vanishes unless

- (i) the relation (A.9) holds
- (ii)  $X_0 = X_n$ .

Hence the RHS of (A.10) can be expressed as a “sum” over sets of non-intersecting trajectories:

$$\exp[-\beta H_{\text{eff}}(\beta, S)] = e^{\beta U N_i} \sum_{\mathcal{T}} e^{\beta U |\mathcal{T}|} \varepsilon(\mathcal{T}) \prod_{\zeta \in \mathcal{T}} e^{-2U |\zeta|} \left( \prod_{\langle xy \rangle \in \zeta} t \right) \quad (\text{A.15})$$

where  $|\mathcal{T}|$  is the number of trajectories in  $\mathcal{T}$ , and  $|\zeta|$  is defined as follows:

$$|\zeta| := (\text{vertical length of } \zeta) \cap (\{x: s_x = +1\} \times [0, \beta]) \quad (\text{A.16})$$

and

$$\varepsilon(\mathcal{T}) := \langle X | \mathbf{T} \prod_{\zeta \in \mathcal{T}} \left( \prod_{\langle x(\tau_i), x(\tau_{i+1}) \rangle \in \mathcal{F}(\zeta)} c_{x(\tau_{i+1})}^\dagger c_{x(\tau_i)} \right) | X \rangle = \pm 1 \quad (\text{A.17})$$

The symbol  $\mathbf{T}$  denotes that the product is “time-ordered”, and  $\varepsilon(\mathcal{T})$  denotes the sign of the permutation of the electrons under the action of  $\mathcal{T}$ .

## A.2. Circuit Representation

To a given ion configuration  $S$  and a given set of trajectories  $\mathcal{T}$  we associate a set,  $\Omega$ , of oriented circuits as follows:

Vertical segments of trajectories located on sites  $x \in \mathcal{A}$  with  $s_x = +1$ , will be considered as up-oriented components of circuits; vertical segments of the complement of the set of trajectories in  $\mathcal{A} \times [0, \beta]$ , located on sites with  $s_x = -1$ , are considered as down-oriented components of circuits. On each horizontal bond at which a jump takes place, we draw a segment with an arrow in the direction of the jump. The vertical segments together with the horizontal jumps form oriented closed circuits. More precisely, an *oriented closed circuit*,  $\omega$ , is a maximally connected component of the oriented segments of the trajectories. Let  $\Omega = \{\omega_1 \cdots \omega_n\}$  denote a finite set of such circuits. The space of all circuits compatible with an ion configuration  $S$  is denoted by  $\mathcal{W}(S)$  [compatibility means that segment of circuits are oriented upwards if they are located on sites occupied by ions and are oriented downwards otherwise].

Let  $|\omega|$  be the total length of the vertical segments of a circuit  $\omega$ , and let  $p(\omega) \in \mathbb{Z}$  be the winding number of  $\omega$ . The latter can take positive or negative integer values, with negative values indicating that  $\omega$  winds around the “time”-axis  $[0, \beta]$  with a downward orientation.

The following two relations hold:

$$\sum_{\tau \in \mathcal{F}} |\zeta| = \frac{1}{2} \sum_{\omega \in \Omega} (|\omega| + \beta p(\omega)) \quad (\text{A.18})$$

$$|\mathcal{F}| = |\mathcal{A}| - N_i + \sum_{\omega \in \Omega} p(\omega) \quad (\text{A.19})$$

As we are concerned with the half-filled case, we always have that  $\sum_{\omega \in \Omega} p(\omega) = 0$ .

From (A.15), (A.18) and (A.19) we have that

$$e^{-\beta H_{\text{eff}}(\beta, S)} = e^{\beta U |\mathcal{A}|} \sum_{\Omega} \varepsilon(\Omega) \prod_{\omega \in \Omega} e^{-U |\omega|} \left( \prod_{\langle xy \rangle \in \omega} t \right) \quad (\text{A.20})$$

where  $\sum_{\Omega}$  denotes a “sum” over all sets,  $\Omega$ , of non-intersecting closed circuits (defined analogous to (1.14)) and  $\varepsilon(\Omega)$  is the sign of permutation of the electrons under the action of the circuits. The following lemma is crucial for the next step. Its proof closely follow ref. 9, and ideas from ref. 46.

**Lemma 18.** There exists a function  $\varepsilon(\omega)$  such that  $\forall \Omega$ :

$$\varepsilon(\Omega) = \prod_{\omega \in \Omega} \varepsilon(\omega)$$

So we can write

$$e^{-\beta H_{\text{eff}}(\beta, S)} = e^{\beta U |\mathcal{A}|} \sum_{\zeta} \prod_{\omega \in \Omega} z(\omega) \quad (\text{A.21})$$

with the *weight*,  $z(\omega)$ , of a circuit,  $\omega$ , defined as follows:

$$z(\omega) = \varepsilon(\omega) e^{-U |\omega|} t^{j(\omega)} \quad (\text{A.22})$$

where  $j(\omega)$  denotes the number of jumps in  $\omega$ .

*Proof of Lemma 18.* Let  $n_x(\tau_n)$  denote the number of electrons at the site  $x$  at the time  $\tau_n$ . Then the set of sites  $x \in \mathcal{A}$  for which

$$W(x) + n_x(\tau_n) \neq 1 \quad (\text{A.23})$$

is said to define the *defect set*,  $D_n(S)$ , for a given ion configuration  $S$ , at the time  $\tau_n$ .

The *section*,  $\Gamma_n(\omega)$ , of a circuit  $\omega$ , at a time  $\tau_n$ , is defined as follows:

$$\Gamma_n(\omega) := \{x \in [\omega \cap (\text{the plane } \tau = \tau_n)]\} \quad (\text{A.24})$$

In particular,  $\Gamma_0(\omega)$  is referred to as the initial (“time-zero”) section of the circuit  $\omega$ , since  $\tau_0 = 0$ . It is clear that each  $x \in \Gamma_n(\omega)$  belongs to the defect set  $D_n(S)$  (for  $n \geq 0$ ).

Let  $|\Gamma_n(\omega)\rangle$  denote the state in the electron Fock space,  $\mathcal{F}_e$ , defined as follows:

$$|\Gamma_n(\omega)\rangle := \left( \prod_{\substack{x \in \Gamma_n(\omega) \\ \text{s.t. } s_x = 1}} c_x^\dagger \right) |0\rangle \quad (\text{A.25})$$

where  $|0\rangle$  denotes the vacuum. More generally, for a set,  $\Omega$ , of circuits, we define the section at time  $\tau_n$  to be

$$\Gamma_n(\Omega) := \{x \in [\Omega \cap (\text{the plane } \tau = \tau_n)]\} \quad (\text{A.26})$$

and the corresponding state to be

$$|\Gamma_n(\Omega)\rangle := \left( \prod_{\substack{x \in \Gamma_n(\Omega) \\ \text{s.t. } s_x = 1}} c_x^\dagger \right) |0\rangle \quad (\text{A.27})$$

The following relations hold:

(a)

$$|\Gamma_i(\omega)\rangle = \Phi_{\underline{B}_i} |\Gamma_{i-1}(\omega)\rangle \quad \text{for } 1 \leq i \leq n \quad (\text{A.28})$$

where  $\underline{B}_i = \{\langle x_i y_i \rangle\}$  denotes a finite set of pairs of nearest neighbour sites, and  $\Phi_{\underline{B}_i}$  denotes the corresponding set of operators

$$\Phi_{\underline{B}_i} := \{c_{x_i}^\dagger c_{y_i}\} \quad (\text{A.29})$$

(b)

$$\Gamma_0(\omega) = \Gamma_n(\omega) \quad (\text{A.30})$$

The above relation is due to the periodicity in the “time” direction.

Each circuit  $\omega$  is uniquely determined by the following

- its initial section  $\Gamma_0(\omega)$  (and hence on the state  $|\Gamma_n(\omega)\rangle$ );

- a sequence of operators  $\Phi_{B_1}, \dots, \Phi_{B_n}$ ;
- a sequence of “times”  $\tau_1, \dots, \tau_n$  at which these operators act.

The sign  $\varepsilon(\omega)$  of a circuit  $\omega$  is given by

$$\begin{aligned} \varepsilon(\omega) &= \prod_{i=1}^n \langle \Gamma_i(\omega) | \Phi_{B_i} | \Gamma_{i-1}(\omega) \rangle \\ &= \langle \Gamma_0(\omega) | \Phi_{B_n} \cdots \Phi_{B_1} | \Gamma_0(\omega) \rangle \end{aligned} \quad (\text{A.31})$$

The second line follows from (a) and (b) above.

To prove the factorization property it is enough to consider a set,  $\Omega$ , of circuits (compatible with an ion configuration  $S$ ) that can be divided into two mutually non-intersecting (“time”-periodical) subsets, denoted by  $\omega_B$  and  $\omega_C$ . Each subset can be made up of several circuits. To each of  $\Omega$ ,  $\omega_B$  and  $\omega_C$  is associated a sign.

The sign of  $\omega_B$  is given by

$$\varepsilon(\omega_B) = \langle \Gamma_0(\omega_B) | \Phi_{B_n} \cdots \Phi_{B_1} | \Gamma_0(\omega_B) \rangle \quad (\text{A.32})$$

The sign,  $\varepsilon(\omega_C)$ , of the component  $\omega_C$  is defined in an analogous fashion, with the sequence of operators  $\Phi_{B_n} \cdots \Phi_{B_1}$  replaced by  $\Phi_{C_m} \cdots \Phi_{C_1}$ . The set  $\Omega$  is defined by an initial section  $\Gamma_{0D} (= \Gamma_0(\omega_D))$  and a sequence of operators  $\Phi_{D_1}, \dots, \Phi_{D_{n+m}}$ , which is a uniquely determined permutation of the sequence  $\Phi_{B_1}, \dots, \Phi_{B_n}, \Phi_{C_1}, \dots, \Phi_{C_m}$ . Its sign  $\varepsilon(\Omega)$  is also defined by (A.32) with the obvious changes. We need to show that the sign for  $\Omega$  factorizes, i.e.,

$$\varepsilon(\Omega) = \varepsilon(\omega_B) \varepsilon(\omega_C) \quad (\text{A.33})$$

By iteration of the argument we obtain the factorization into the signs of the individual circuits.

Let us first discuss the computation of the sign of a single component  $\omega_B$ . In terms of the vacuum  $|0\rangle$ , the expression of the sign  $\varepsilon(\omega_B)$  takes a very simple form. To obtain it, we observe that

$$\langle \Gamma_{0B} | \Phi_{B_n}^q \cdots \Phi_{B_1}^q | \Gamma_{0B} \rangle = \langle 0 | \mathbf{C}_{\Gamma_{0B}} \Phi_{B_n}^q \cdots \Phi_{B_1}^q \mathbf{C}_{\Gamma_{0B}}^* | 0 \rangle \quad (\text{A.34})$$

where  $\mathbf{C}_{\Gamma_{0B}}^*$  is a product of creation operators that creates the section  $\Gamma_{0B} (= \Gamma_0(\omega_B))$ , i.e.,

$$\mathbf{C}_{\gamma_{0B}}^* := \left( \prod_{\substack{x \in \Gamma_{0B} \\ \text{s.t. } s_x = 1}} c_x^\dagger \right) \ll \quad (\text{A.35})$$



The product

$$\mathbf{A}_B := \mathbf{C}_{r_{0B}} \Phi_{B_n} \cdots \Phi_{B_1} \mathbf{C}_{r_{0B}}^* \quad (\text{A.36})$$

is a monomial in creation and destruction operators that can be combined into *number* operators, because of the required periodicity,

$$\mathbf{A}_B |0\rangle = \varepsilon(\omega_B) |0\rangle \quad (\text{A.37})$$

of  $\omega_B$ . The factorization of signs is a consequence of the fact that this combination can be made in a well-defined fashion which is not affected by the presence of other (compatible) circuits.

We choose the following procedure which we refer to as *circuit collapsing*. Consider the string of operators appearing in the product  $\mathbf{A}_B$ . For brevity we shall refer to each appearance of a destruction or creation operator supported on a site  $x$  as an *occurrence* of  $x$ . We denote by  $\mathcal{S}(\mathbf{A}_B)$  (“shadow” of  $\mathbf{A}_B$ ) the set of sites  $x$  occurring in  $\mathbf{A}_B$ . We start with the leftmost operator in the product  $\mathbf{A}_B$  (A.36). In order to yield a non-zero contribution this has to be a destruction operator with support on some site  $x$ , i.e.,  $c_x$ . We now move this operator through the operators present to its right (i.e., downwards in time), using the anticommutation relations, until we encounter the next occurrence of the site  $x$  in the product (A.36). This is necessarily a creation operator,  $c_x^\dagger$ , since otherwise the successive actions of these two operators would yield zero. Hence we obtain a factor

$$\mathbf{c}_x \mathbf{c}_x^\dagger = \mathbf{1} - \mathbf{n}_x \quad (\text{A.38})$$

times a phase  $\alpha_x^{(1)}(\omega_B)$  ( $\mathbf{n}_x$  being the number operator for electrons at the site  $x$ ). This phase arises due to the anticommutation of the initial  $\mathbf{c}_x$  with intermediate operators. All the operators which appear to the left of this factor are *not* supported in  $x$  and, hence, we can move this factor to the leftmost end of the string to obtain

$$\mathbf{A}_B = \alpha_x^{(1)}(\omega_B) (\mathbf{1} - \mathbf{n}_x) \hat{\mathbf{A}}_B \quad (\text{A.39})$$

where  $\hat{\mathbf{A}}_B$  satisfies

$$\hat{\mathbf{A}}_B |0\rangle = \alpha_x^{(1)}(\omega_B) \varepsilon(\omega_B) |0\rangle \quad (\text{A.40})$$

and has two fewer occurrences of  $x$ .

Next, we repeat the above procedure for the string of operators defining  $\hat{\mathbf{A}}_B$  and continue pulling out, in the same way, successive phases and

factors  $\mathbf{1} - \mathbf{n}_x$ . Once all occurrences of  $x$  have been dealt with, we obtain a product of factors  $(\mathbf{1} - \mathbf{n}_x)^k = \mathbf{1} - \mathbf{n}_x$  and an overall phase  $\alpha_x(\omega_B)$ , so that

$$\mathbf{A}_B = \alpha_x(\omega_B)(\mathbf{1} - \mathbf{n}_x) \tilde{\mathbf{A}}_B \quad (\text{A.41})$$

where  $\tilde{\mathbf{A}}_B$  satisfies

$$\tilde{\mathbf{A}}_B |0\rangle = \alpha_x(\omega_B) \varepsilon(\omega_B) |0\rangle \quad (\text{A.42})$$

and has *no* occurrence of the site  $x$ :  $\mathcal{S}(\tilde{\mathbf{A}}_B) = \mathcal{S}(\mathbf{A}_B) \setminus \{x\}$ .

We then repeat the whole procedure for  $\tilde{\mathbf{A}}_B$ . At the end, once all the sites  $x$  in  $\mathcal{S}(\mathbf{A}_B)$  have been exhausted, one obtains that the whole of  $\mathbf{A}_B$  has “collapsed” into factors  $\mathbf{1} - \mathbf{n}_x$  times a numerical factor. A simple replacement in (A.37) shows that this factor must equal  $\eta(\omega_B)$ . That is,

$$\mathbf{A}_B = \varepsilon(\omega_B) \prod_{x \in \mathcal{S}(\omega_B)} (\mathbf{1} - \mathbf{n}_x) \quad (\text{A.43})$$

We are now ready to prove the factorization property that we need: Let  $\Omega$  be a family of circuits and let it be decomposed into two (“time-periodical”) subfamilies of circuits,  $\omega_B$  and  $\omega_C$ . Then

$$\varepsilon(\Omega) = \varepsilon(\Omega_B) \varepsilon(\Omega_C) \quad (\text{A.44})$$

We can write  $\omega_C$  via an operator

$$\mathbf{A}_C := \mathbf{C}_{\Gamma_{0C}} \Phi_{\underline{C}_m} \cdots \Phi_{\underline{C}_1} \mathbf{C}_{\Gamma_{0C}}^* \quad (\text{A.45})$$

[with  $\Gamma_{0C} = \Gamma_0(\omega_C)$ ], such that

$$\mathbf{A}_C |0\rangle = \varepsilon(\omega_C) |0\rangle \quad (\text{A.46})$$

We shall use the following two consequences of the compatibility (i.e., mutual non-intersection) of the two components  $\omega_B$  and  $\omega_C$ :

**(C1)** The monomials  $\mathbf{C}_{\Gamma_{0B}}^*$  and  $\mathbf{C}_{\Gamma_{0C}}^*$  have disjoint support, so that

$$|\Gamma_{0D}\rangle = \delta \mathbf{C}_{\Gamma_{0B}} \mathbf{C}_{\Gamma_{0C}}^* |0\rangle \quad (\text{A.47})$$

where  $\delta$  is a phase factor. Hence,

$$\varepsilon(\Omega) = \langle 0 | \mathbf{A}_D |0\rangle \quad (\text{A.48})$$

with

$$\mathbf{A}_D := \mathbf{C}_{\Gamma_{0C}} \mathbf{C}_{\Gamma_{0B}} \Phi_{\underline{D}_{n+1}} \cdots \Phi_{\underline{D}_1} \mathbf{C}_{\Gamma_{0B}}^* \mathbf{C}_{\Gamma_{0C}}^* \quad (\text{A.49})$$

(C2) The occurrence of a creation operator  $\mathbf{c}_x^\dagger$  in factors of  $\mathbf{A}_B$  implies that the site  $x$  becomes, or continues to be, part of the support of  $\omega_B$  at least until there is a further occurrence of a destruction operator  $\mathbf{c}_x$ . In particular since  $\omega_B$  and  $\omega_C$  do not intersect, we have the following property:

Between an occurrence of  $\mathbf{c}_x$  in factors of  $\mathbf{A}_B$  and the preceding (i.e. immediately to the right) occurrence of  $\mathbf{c}_x^\dagger$  in factors of  $\mathbf{A}_B$ , there cannot be an occurrence of  $x$  in factors of  $\mathbf{A}_C$  (A.50)

Moreover, as the whole set  $\Omega$  is periodic in the “time”-direction, we have that each occurrence of  $\mathbf{c}_x$  in  $\mathbf{A}_D$  must be preceded by an occurrence of  $\mathbf{c}_x^\dagger$ . Combining this observation with (C2) we obtain the last property needed:

(C3) Between an occurrence of  $\mathbf{c}_x^\dagger$  in factors of  $\mathbf{A}_B$  and the immediately preceding occurrence of  $\mathbf{c}_x$  in factors of  $\mathbf{A}_B$ , there is an even number of occurrences of  $x$  in factors of  $\mathbf{A}_C$ . Of course, these occurrences correspond to alternating creations and destructions. The same property holds after the last occurrence of  $\mathbf{c}_x$  in factors of  $\mathbf{A}_B$  and before the first occurrence of  $\mathbf{c}_x^\dagger$  in factors of  $\mathbf{A}_B$ .

From (C1)–(C3) we conclude that the “collapse” of  $\mathbf{A}_B$  gives exactly the same factor as in the absence of the component  $\omega_C$ . Indeed, the last occurrence of a site  $x$  in factors of  $\mathbf{A}_B$  is a destruction operator, that we can displace up to the previous occurrence to produce a factor  $\mathbf{1} - \mathbf{n}_x$ . Between these two occurrences there is no occurrence of  $x$  in factors of  $\mathbf{A}_C$  because of (C2). Hence  $\mathbf{c}_x$  commutes with all the operators  $\Phi_{C_i}$  encountered during the displacement (recall that such operators are monomials of even degree). Thus, the phase acquired during this displacement only depends on the operators in  $\mathbf{A}_B$  and hence it is the same phase  $\alpha_x^{(1)}(\omega_B)$  obtained when collapsing the component  $\omega_B$  in the absence of any other circuit. Moreover, by (C3) the operators in  $\mathbf{A}_D$  located to the left of the factor  $\mathbf{1} - \mathbf{n}_x$ , obtained in the above manner, involve an even number of creation and destruction operators supported in  $x$ . Therefore, we can freely move this factor  $\mathbf{1} - \mathbf{n}_x$  all the way to the left to obtain

$$\mathbf{A}_D = \alpha_x^{(1)}(\omega_B)(\mathbf{1} - \mathbf{n}_x) \hat{\mathbf{A}}_D \quad (\text{A.51})$$

where  $\hat{\mathbf{A}}_D$  has two fewer occurrences of  $x$  in factors of  $\mathbf{A}_B$  but otherwise satisfies (C1)–(C3). Iterating this process we collapse  $\mathbf{A}_B$  exactly as done in (A.39)–(A.43). We obtain

$$\mathbf{A}_D = \varepsilon(\omega_B) \prod_{x \in \mathcal{S}(\omega_B)} (\mathbf{1} - \mathbf{n}_x) \mathbf{A}_C \quad (\text{A.52})$$

Combining this expression with (A.48) and (A.46) we get the desired factorization (A.44). ■

### A.3. Cluster expansion

The logarithm of

$$\sum_{\Omega} \prod_{\omega \in \Omega} z(\omega)$$

can be developed in a cluster expansion. Adapting Theorem 3.1 of ref. 36 to our case (in which one variable, the “time,” is continuous) we have the following result:

$$\text{if } \sum_{\omega \in \mathcal{W}_j(S)} |z(\omega)| e^{|\omega|} \chi[(x, \tau) \in \omega] \leq C_j \quad \text{with } \sum_{j \geq 0} C_j < 1 \quad (\text{A.53})$$

(where  $\chi$  denotes the characteristic function) then we have an absolutely convergent cluster expansion given by

$$\sum_{\Omega} \prod_{\omega \in \Omega} z(\omega) = \exp \left\{ \sum_{n \geq 1} \frac{1}{n!} \sum_{\omega_1 \dots \omega_n} \varphi_n^T(\omega_1, \dots, \omega_n) \prod_{k=1}^n z(\omega_k) \right\} \quad (\text{A.54})$$

Here  $\mathcal{W}_j(S)$  is the space of circuits compatible with the ion configuration  $S$  and having  $j$  jumps, and  $\varphi_n^T(\omega_1, \dots, \omega_n)$  is a combinatoric function on families of circuits whose value is zero whenever  $\{\omega_1, \dots, \omega_n\}$  is not a *cluster* (i.e., whenever the support of the set of circuits  $\{\omega_1, \dots, \omega_n\}$  is not connected in  $\mathbf{R}^{d+1}$ ).

Furthermore, we shall use the following bound, (A.55), which is an extension of Lemma 3.5 of ref. 36:

$$\begin{aligned} & \sum_{\omega_1 \in \mathcal{W}_{j_1}(S)} \sum_{\omega_2 \in \mathcal{W}_{j_2}(S)} \cdots \sum_{\omega_n \in \mathcal{W}_{j_n}(S)} \chi[(x, \tau) \in \omega_1] \\ & \times |\varphi_n^T(\omega_1, \dots, \omega_n)| \prod_{k=1}^n |z(\omega_k)| \leq (n-1)! \prod_{k=1}^n C_{j_k} \end{aligned} \quad (\text{A.55})$$

We show that (A.53) holds in our case as follows. For  $j \neq 0$ , (i.e.,  $j \geq 2$ ) we have

$$\begin{aligned}
\sum_{\omega \in \mathcal{W}_j(S)}^{\dot{\int}} |z(\omega)| e^{|\omega|} \chi[(x, \tau) \in \omega] &\leq \sum_{\omega \in \mathcal{W}_j(S)}^{\dot{\int}} t^j e^{-(U-1)|\omega|} \chi[(x, \tau) \in \omega] \\
&\leq (2dt)^j \left[ \int_0^\beta d\tau e^{-(U-1)\tau} \right]^j \\
&\leq (2dt)^j \left( \frac{1 - e^{-\beta(U-1)}}{U-1} \right)^j \tag{A.56}
\end{aligned}$$

For  $U$  large enough,  $U-1 \geq cU$ , for some constant  $c$  with  $0 < c < 1$ . Hence

$$\text{RHS of (A.56)} \leq C_j \tag{A.57}$$

where we define

$$C_j := \left( \frac{2dt}{cU} \right)^j \quad \text{for } j \geq 2 \tag{A.58}$$

For  $j=0$  we find

$$C_0 = e^{-\beta cU} \tag{A.59}$$

From (A.58) and (A.59) it follows that the bound (A.53) is satisfied for  $U$  and  $\beta$  large enough.

Hence we obtain an expression for the effective hamiltonian:

$$H_{\text{eff}}(\beta, S) = -U|A| - \frac{1}{\beta} \sum_{n \geq 1} \frac{1}{n!} \sum_{\omega_1 \dots \omega_n}^{\dot{\int}} \varphi_n^T(\omega_1, \dots, \omega_n) \prod_{k=1}^n z(\omega_k) \tag{A.60}$$

We define the support,  $\text{supp } \omega$ , of a circuit  $\omega$ , to be its orthogonal projection onto the plane  $\tau=0$ . Hence  $\text{supp } \omega \subset A$ .

Let  $A \subset A$ . The potential  $\Omega_A(\beta, S_A)$  is introduced as follows:

$$\begin{aligned}
\Phi_A(\beta, S_A) &= -\frac{1}{\beta} \sum_{n \geq 1} \frac{1}{n!} \sum_{\omega_1 \dots \omega_n}^{\dot{\int}} \chi \left[ \bigcup_{k=1}^n \text{supp } \omega_k = A \right] \\
&\quad \times \varphi_n^T(\omega_1, \dots, \omega_n) \prod_{k=1}^n z(\omega_k) \tag{A.61}
\end{aligned}$$

where  $S_A$  denotes the restriction of the ion configuration  $S$  to  $A \subset A$ .

**Lemma 19.** There exists positive constants  $U_0 \gg t$  and  $\beta_0$ , such that for all  $U > U_0$  and  $\beta > \beta_0$

$$|\Phi_A(\beta, S_A)| \leq c_1 \frac{(c_2 t)^{n(A)}}{U^{n(A)-1}} \quad \text{for } |A| \geq 2 \tag{A.62}$$

for some constants  $c_1$  and  $c_2$ , with  $n(A)$  being the minimum length of a closed path which passes through all sites of  $A$ .

*Proof.* Let  $j_1, \dots, j_n$  denote the number of jumps for the circuits  $\omega_1, \dots, \omega_n$ , such that  $\{\omega_1, \dots, \omega_n\}$  forms a cluster with support equal to  $A$ .

If  $\bigcup_{k=1}^n \text{supp } \omega_k = A$  then  $\sum_{k=1}^n j_k \geq n(A)$  for any  $\omega_1, \dots, \omega_n$ , then

$$\begin{aligned} |\Phi_A(\beta, S_A)| &\leq \frac{1}{\beta} \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{j_1, \dots, j_n \geq 0 \\ \sum_k j_k \geq n(A)}} \prod_{\omega_1 \in \mathcal{W}_{j_1}(S)} \cdots \prod_{\omega_n \in \mathcal{W}_{j_n}(S)} \\ &\times \chi \left[ \bigcup_{k=1}^n \text{supp } \omega_k = A \right] |\varphi_n^T(\omega_1, \dots, \omega_n)| \prod_{k=1}^n |z(\omega_k)| \tag{A.63} \end{aligned}$$

Now,

$$\sum_{x \in A} \int_0^\beta d\tau \chi[(x, \tau) \in \omega_1] \frac{1}{|\omega_1|} = 1$$

for any  $\omega_1$  with  $\text{supp } \omega_1 \subset A$ . Introducing this identity into the above equation (A.63) yields

$$\begin{aligned} |\Phi_A(\beta, S_A)| &\leq \frac{1}{\beta} \sum_{x \in A} \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{j_1, \dots, j_n \geq 0 \\ \sum_k j_k \geq n(A)}} \int_0^\beta d\tau \\ &\times \prod_{\omega_1 \in \mathcal{W}_{j_1}(S)} \chi[(x, t) \in \omega_1] \frac{1}{|\omega_1|} \\ &\times \prod_{\omega_2 \in \mathcal{W}_{j_2}(S)} \cdots \prod_{\omega_n \in \mathcal{W}_{j_n}(S)} |\varphi_n^T(\omega_1, \dots, \omega_n)| \prod_{k=1}^n |z(\omega_k)| \tag{A.64} \end{aligned}$$

Note that  $|A| \geq 2$  implies that  $j_i \geq 2$  for at least one  $i \in \{1 \dots n\}$ . We have assumed that  $j_1 \geq 2$ .

Let us define  $z'(\omega, U)$  to be equal to the weight  $z(\omega)$ , but with explicit dependence on the coupling constant  $U$ . Let us define

$$\begin{aligned}
 F(U_1, \dots, U_n) &:= \sum_{\omega_1 \in \mathcal{W}_{j_1}(S)} \chi[(x, t) \in \omega_1] \frac{|z'(\omega_1, U_1)|}{|\omega_1|} \\
 &\times \sum_{\omega_2 \in \mathcal{W}_{j_2}(S)} \cdots \sum_{\omega_n \in \mathcal{W}_{j_n}(S)} \\
 &\times |\varphi_n^T(\omega_1, \dots, \omega_n)| \prod_{k=2}^n |z'(\omega_k, U_k)| \quad (\text{A.65})
 \end{aligned}$$

and obtain an upper bound for this function. Eventually, we shall set  $U_i = U$  for all  $i = 1 \dots n$ .

Note that  $F(\infty, \dots, U_n) = 0$ . Moreover,

$$\frac{\partial}{\partial U_1} |z'(\omega_1, U_1)| = -|\omega_1| |z'(\omega_1, U_1)|$$

Hence,

$$\begin{aligned}
 \left| \frac{\partial}{\partial U_1} F(U_1, \dots, U_n) \right| &\leq \sum_{\omega_1 \in \mathcal{W}_{j_1}(S)} \chi[(x, t) \in \omega_1] \sum_{\omega_2 \in \mathcal{W}_{j_2}(S)} \cdots \sum_{\omega_n \in \mathcal{W}_{j_n}(S)} \\
 &\times |\varphi_n^T(\omega_1, \dots, \omega_n)| \prod_{k=1}^n |z'(\omega_k, U_k)| \quad (\text{A.66})
 \end{aligned}$$

From (A.55) we have that

$$\left| \frac{\partial}{\partial U_1} f(U_1, \dots, U_n) \right| \leq (n-1)! \prod_{k=1}^n C'_{j_k}(U_k) \quad (\text{A.67})$$

where  $C'_{j_k}(U_k)$  is the same as  $C_{j_k}$ , except for the explicit dependence on  $U_k$ . Since

$$F(U_1, \dots, U_n) = - \int_{U_1}^{\infty} \frac{\partial}{\partial V} F(V, \dots, U_n) dV$$

we have that

$$\begin{aligned}
 F(U_1, \dots, U_n) &\leq \int_{U_1}^{\infty} \left| \frac{\partial}{\partial V} F(V, \dots, U_n) \right| dV \\
 &\leq (n-1)! \prod_{k=2}^n C'_{j_k}(U_k) \int_{U_1}^{\infty} C'_{j_1}(V) dV \quad (\text{A.68})
 \end{aligned}$$

From (A.58) we have that

$$\begin{aligned} \int_{U_1}^{\infty} C'_{j_1}(V) dV &\leq (2dt)^{j_1} \int_{U_1}^{\infty} (cV)^{-j_1} dV \\ &\leq \left[ \frac{2dt}{c} \right]^{j_1} \frac{1}{U_1^{j_1-1}} \end{aligned} \quad (\text{A.69})$$

(since  $j_1 \geq 2$ ). Hence,

$$\begin{aligned} |F(U_1, \dots, U_n)| \\ \leq (n-1)! \frac{2dt}{c} \left[ \frac{2dt}{cU_1} \right]^{j_1-1} \prod_{\substack{k=2 \\ j_k \neq 0}}^n \left[ \frac{2dt}{cU_k} \right]^{j_k} \prod_{\substack{k=2 \\ j_k=0}}^n C'_0(U_k) \end{aligned} \quad (\text{A.70})$$

Let  $i$  be the number of circuits without any jump. From (A.64) we have that

$$\begin{aligned} |\Phi_A(\beta, S_A)| &\leq \frac{1}{\beta} \sum_{x \in A} \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{j_1, \dots, j_n \geq 0 \\ \sum_k j_k \geq n(A)}} \int_0^\beta |F(U_1 \dots U_n)| \\ &\leq |A| \sum_{n \geq 1} \frac{1}{n} \sum_{i=0}^n \frac{n!}{(n-1)! i!} C_0^i \sum_{m=n(A)}^{\infty} \\ &\quad \times \sum_{\substack{j_1, \dots, j_{n-1} \geq 2 \\ \sum_k j_k = m}} (2dt/c) \left[ \frac{2dt}{cU} \right]^{m-1} \end{aligned} \quad (\text{A.71})$$

Further, we have that

$$\sum_{\substack{j_1, \dots, j_r \geq 2 \\ \sum_k j_k = m}} 1 \leq 2^{m-r} \quad (\text{A.72})$$

It is true for all  $j$  when  $m=1$ , and by induction

$$\begin{aligned} \sum_{\substack{j_1, \dots, j_{r+1} \geq 2 \\ \sum_k j_k = m}} 1 &= \sum_{j_{r+1} \geq 2} \sum_{\substack{j_1, \dots, j_r \geq 2 \\ \sum_k j_k = m - j_{r+1}}} 1 \\ &\geq 2^{m-r} \sum_{j_{r+1} \geq 2} 2^{-j_{r+1}} = 2^{m-(r+1)} \end{aligned}$$



Using the bound (A.72) on the RHS of (A.71), we obtain

$$\begin{aligned}
 |\Phi_A(\beta, S_A)| &\leq |A| \sum_{n \geq 1} \frac{1}{n} \sum_{i=0}^n \frac{n!}{(n-1)! i!} C_0^i 2^{-(n-1)} \sum_{m=n(A)}^{\infty} 2^m \frac{(2dt/c)^m}{U^{m-1}} \\
 &= |A| \left[ \sum_{n \geq 1} \frac{1}{n} \left( \frac{1}{2} + C_0 \right)^n \right] \sum_{m \geq n(A)} \frac{(4dt/c)^m}{U^{m-1}} \quad (\text{A.73})
 \end{aligned}$$

Now, since  $C_0 = e^{-\beta c U}$  (A.59), there exists positive constants  $U_0 \gg t$  and  $\beta_0$ , such that for all  $\beta > \beta_0$  and  $U > U_0$  the sums over  $n$  and  $m$  on RHS of (A.73) converge. Thus we obtain the bound (A.62) for some positive constants  $c_1$  and  $c_2$ . ■

**Remark.** For  $A \subset \Lambda$  we have that (2.10)

$$g(A) = n(A) - A \quad (\text{A.74})$$

Set  $t = 1$ . Then the bound (A.62) can be written as

$$|\Phi_A(\beta, S_A)| \leq C_1 \left( \frac{C_2}{U} \right)^{g(A)} \quad (\text{A.75})$$

for some positive constants  $C_1$  and  $C_2$ , with  $C_2/U < 1$ . This is our desired estimate.

## APPENDIX B. PROOF OF LEMMA 5

From the standard results of cluster expansions<sup>(36, 42, 5, 6, 13)</sup> it follows that a sufficient condition for the convergence of the series given in (3.42) is given by

$$\sum_{D \ni 0} W(D) e^{|D|} < 1 \quad (\text{B.1})$$

Hence, the task of proving Lemma 5 amounts to proving that the condition (B.1) is satisfied. In order to do so, we consider an auxiliary polymer system whose elements (the *polymers*) are denoted by  $\varrho$  and defined as follows.

$$\varrho := (\gamma, M_\gamma) \quad (\text{B.2})$$

where  $\gamma$  is a contour and  $M_\gamma$  is a *decoration* of  $\gamma$ . A decoration of  $\gamma$  is a (possibly empty) set of bonds  $\{B_1, \dots, B_j\} \subset \mathcal{B}$ , such that each bond intersects  $\gamma$ , i.e.,  $B_i \cap \gamma \neq \emptyset$  for  $1 \leq i \leq j$ . Hence a polymer  $\varrho$  consists of a contour  $\gamma$  and a finite set of bonds which intersect its support. Let  $\mathcal{B}_\gamma$  denote the set of *all* bonds which intersect the contour  $\gamma$ . Then  $M_\gamma \subset \mathcal{B}_\gamma$ . For a polymer  $\varrho = (\gamma, M_\gamma)$ , we define

$$|\varrho| := |\gamma| + \sum_{B \in M_\gamma} g(B) \quad (\text{B.3})$$

The weight of a polymer is given by

$$w(\varrho) := e^{-\beta E(\gamma)} \prod_{B \in M_\gamma} (e^{-\beta G_B} - 1) \quad (\text{B.4})$$

and satisfies the bound  $|\omega(\varrho)| \leq \omega_0(\varrho)$  where

$$w_0(\varrho) := e^{-\beta C_1 \lambda |\gamma|} \prod_{B \in M_\gamma} (e^{\beta C_2 \lambda g(B)} - 1) \quad (\text{B.5})$$

Each decorated contour  $D$  can be considered to be the union of a finite number of intersecting polymers, i.e., a connected *cluster of polymers*. The weight of a decorated contour can then be expressed in terms of the weights of its constituent polymers. The decomposition of a decorated contour into polymers is however not unique. The condition (B.1) for the model of decorated contours can be transcribed into a condition for the auxiliary polymer system, by making use of the “tree-graph approximation” used in cluster expansions.<sup>(42, 36)</sup> We sketch the idea below, following ref. 36. We first bound the LHS of (B.1) in terms of a sum over polymers:

$$\sum_{D \ni 0} W(D) e^{|D|} \leq \sum_{n \geq 1} \frac{1}{n!} \sum_{\substack{\varrho_1, \dots, \varrho_n \\ \varrho_1 \cup \dots \cup \varrho_n = D \\ D \ni 0, \text{ connected}}} \prod_{j=1}^n w(\varrho_j) e^{|\varrho_j|} \quad (\text{B.6})$$

The fact that (B.6) is not an equality but only a bound is due to the non-uniqueness of decomposition of a decorated contour into polymers. A decorated contour  $D$  consisting of  $n$  polymers,  $\varrho_1, \dots, \varrho_n$ , can be represented by a connected, oriented graph, whose vertices are the polymers and the lines between pairs of vertices corresponding to intersecting polymers. The graph is oriented by introducing an ordering of the vertices. Let  $\mathcal{G}_n$  be the corresponding *complete graph*, i.e., the graph with  $n$  vertices, with a line between each pair of vertices. The sum over the polymers on the RHS of

(B.6) can be bounded by a sum over all tree graphs of the corresponding complete graph. Hence, we can write

$$\sum_{D \ni 0} W(D) e^{|D|} \leq \sum_{n \geq 1} \frac{1}{n!} \sum_{T \subset \mathcal{G}_n} \sum_{\varrho_1 \ni 0} \cdots \sum_{\varrho_n} \prod_{j=1}^n w(\varrho_j) e^{|\varrho_j|} \tag{B.7}$$

where  $T$  denotes a tree graph.

From Lemma 3.5 of ref. 36 it follows that

$$\sum_{T \subset \mathcal{G}_n} \sum_{\varrho_1 \ni 0} \cdots \sum_{\varrho_n} \prod_{j=1}^n w(\varrho_j) e^{|\varrho_j|} \leq (n-1)! C^n \tag{B.8}$$

where

$$C := \sum_{\varrho \ni 0} w_0(\varrho) e^{2|\varrho|} \tag{B.9}$$

with  $w_0(\varrho)$  being defined through (B.5). Hence,

$$\sum_{D \ni 0} W(D) e^{|D|} \leq \sum_{n \geq 1} \frac{C^n}{n} \tag{B.10}$$

The series on the RHS of (B.10) converges to  $C/(1-C)$  if  $C < 1$ , which is  $< 1$  if  $C < 1/2$ . Hence the proof of (B.1), and hence of Lemma 5, is completed by proving the following lemma.

**Lemma 20.** For each  $C' > 0$ , there exist constants  $\lambda_0$  and  $b_0$  such that for all  $\lambda < \lambda_0$  and  $\beta\lambda > b_0$  one has the bound

$$\sum_{\varrho \ni 0} w_0(\varrho) e^{2|\varrho|} \leq C' \tag{B.11}$$

where  $w_0(\varrho)$  is given by (B.5).

*Proof.* For convenience we consider the sum

$$Z_{\text{pol}} := \sum_{\varrho \ni 0} w_0(\varrho) e^{a|\varrho|} \leq C' \tag{B.12}$$

for a constant  $a > 0$ , and set  $a = 2$  at the end of the proof. Let  $k_0$  be the smallest positive integer for which

$$C_2 \beta (\lambda c_d e^a)^{k_0} \leq 1 \tag{B.13}$$

where  $c_d=36$ . We define

$$\alpha := C_2\beta(\lambda c_d e^\alpha)^{k_0} \tag{B.14}$$

Let  $x = C_2\beta\lambda^k$  and  $x_0 = C_2\beta\lambda^{k_0}$ . Then for  $k > k_0$  we use the bound  $e^x - 1 \leq xe^x$  and for  $k \leq k_0$  we use the bound  $e^x - 1 < e^x$ . It follows from (B.3), (B.5), and the above bounds, that

$$\begin{aligned} w_0(\varrho) e^{\alpha|\varrho|} &\leq e^{-\beta C_1 \lambda^{|\gamma|}} e^{\alpha|\gamma|} \times \left[ \prod_{\substack{B \in M_\gamma \\ g(B) \leq k_0}} e^{\beta C_2 \lambda^{g(B)}} e^{\alpha g(B)} \right] \\ &\times \left[ \prod_{\substack{B \in M_\gamma \\ g(B) > k_0}} \beta C_2 \lambda^{g(B)} e^{\beta C_2 \lambda^{g(B)}} e^{\alpha g(B)} \right] \end{aligned} \tag{B.15}$$

We have that

$$\begin{aligned} \sum_{B \in M_\gamma} \lambda^{g(B)} &\leq \sum_{B \cap \gamma \neq \emptyset} \lambda^{g(B)} \leq \sum_{x \in \gamma} \sum_{B \ni x} \frac{\lambda^{g(B)}}{|B|} \leq \sum_{x \in \gamma} \sum_{B \ni x} \frac{\lambda^{g(B)}}{2} \\ &\leq |\gamma| \sum_B^* \lambda^{g(B)} \leq |\gamma| \sum_{k \geq 3} \sum_{\substack{B: \\ g(B)=k}}^* \lambda^k \leq |\gamma| \sum_{k \geq 3} c_d^k \lambda^k \end{aligned} \tag{B.16}$$

The symbol  $\sum_{x \in \gamma}$  denotes the sum over all sites  $x \in \Lambda$  for which at least one nearest neighbour bond of the lattice, which contains the site  $x$ , is intersected by a face in  $\gamma$ . There are  $2|\gamma|$  such sites in the  $\Lambda$ . The symbol  $\sum_B^*$  denotes the sum over all  $B$ 's containing a fixed point. For the last inequality we used the Königsberg Bridge lemma [ref. 44, pp. 464–465], which gives  $c_d = (2d)^2$ ,  $d$  being the dimension of the lattice, i.e.,  $c_d = 36$ .

Hence, we obtain the uniform bound

$$\prod_{B \in M_\gamma} e^{\beta C_2 \lambda^{g(B)}} \leq e^{\beta C_3 \lambda^3 |\gamma|} \tag{B.17}$$

with

$$C_3 := \frac{C_2 c_d^3}{1 - c_d \lambda} \tag{B.18}$$

provided

$$c_d \lambda < 1 \tag{B.19}$$

For convenience we define

$$a_0 := \beta(C_1 \lambda - C_3 \lambda^3) - a \tag{B.20}$$

Then, if (B.19) is satisfied, we have that

$$w_0(\varrho) e^{a|\varrho|} \leq e^{-a_0|\gamma|} \times \left[ \prod_{\substack{B \in M_\gamma \\ g(B) \leq k_0}} e^{ag(B)} \right] \tag{B.21}$$

$$\times \left[ \prod_{\substack{B \in M_\gamma \\ g(B) > k_0}} \beta C_2 \lambda^{g(B)} e^{\beta C_2 \lambda^{g(B)}} e^{ag(B)} \right] \tag{B.22}$$

Hence,

$$\begin{aligned} \sum_{\varrho \ni 0} w_0(\varrho) e^{a|\varrho|} &\leq \sum_{j \geq 0} \frac{1}{j!} \sum_{\substack{\gamma, B_1, \dots, B_j \\ \gamma \cup B_1 \cup \dots \cup B_j \ni 0 \\ B_i \cap \gamma \neq \emptyset}} e^{-a_0|\gamma|} \left[ \prod_{\substack{1 \leq i \leq j \\ g(B) \leq k_0}} e^{ag(B)} \right] \\ &\times \left[ \prod_{\substack{1 \leq i \leq j \\ g(B) > k_0}} \beta C_2 \lambda^{g(B)} e^{\beta C_2 \lambda^{g(B)}} e^{ag(B)} \right] \end{aligned} \tag{B.23}$$

The sum on the LHS of (B.23) is over all polymers which contain the origin. For each terms in the sum on the RHS of (B.23), the origin can be contained either in the contour of a polymer and/or in one or more of the bonds intersecting it. This sum can be bound by a sum over all polymers for which the origin is contained in their respective contours. We refer to such a polymer as a *pinned polymer*. More precisely, a pinned polymer  $\varrho$  is defined by the connected sequences  $\gamma, B_1, \dots, B_j$  such that  $\gamma \ni 0$ . The contribution of each pinned polymer must be multiplied by the number of translations containing the origin. Since for all  $i, B_i \cap \gamma \neq \emptyset$ , this number is bounded by

$$\left| \bigcup_{1 \leq i \leq j} B_i \setminus \gamma \right| \leq \sum_{1 \leq i \leq j} |B_i| - 1 \leq \sum_{1 \leq i \leq j} (g(B_i) - 1) \tag{B.24}$$

since  $|B| \leq g(B)$ . The factors of “ $-1$ ” arise from the fact that each bond  $B$  must intersect the contour  $\gamma$ . Starting from a given contour  $\gamma$  containing the origin, a pinned polymer can be constructed by successively adding bonds which intersect it. For a given  $\gamma$ , the sum over decorations can be split into a sum over decorations with “small” bonds, i.e.,  $B$  with  $g(B) \leq k_0$ , and a

sum over decorations with “large” bonds, i.e.,  $B$  with  $g(B) > k_0$ . This gives the following estimate:

$$Z_{\text{pol}} \leq \sum_{\gamma \geq 0} e^{-a_0 |\gamma|} \sum_{\substack{j \geq 0, \{B_1, \dots, B_j\} \in \mathcal{B}_\gamma \\ g(B_i) \leq k_0}} \sum_{\substack{j' \geq 0, \{B'_1, \dots, B'_{j'}\} \in \mathcal{B}_\gamma \\ g(B'_i) > k_0}} \times \left[ \sum_{1 \leq i \leq j} (g(B_i) - 1) + \sum_{1 \leq i \leq j'} (g(B'_i) - 1) \right] \quad (\text{B.25})$$

$$\times \left[ \prod_{1 \leq i \leq j} e^{ag(B_i)} \right] \left[ \prod_{1 \leq i \leq j'} \beta C_2 \lambda^{g(B'_i)} e^{ag(B'_i)} \right] \quad (\text{B.26})$$

If both  $j \geq 1$  and  $j' \geq 1$  then (since  $g(B) \geq 3$ ) the sum of the two sums in parenthesis in (B.25) can be bounded by the product of the two sums, such that the first sum can be combined with the first factor of (B.26) and the second sum with the second factor. The result is

$$Z_{\text{pol}} \leq \sum_{\gamma \geq 0} e^{-a_0 |\gamma|} \left\{ 1 + \sum_{\substack{j \geq 1, \{B_1, \dots, B_j\} \in \mathcal{B}_\gamma \\ g(B_i) \leq k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \times \left[ \prod_{1 \leq i \leq j} e^{ag(B_i)} \right] \right\} \quad (\text{B.27})$$

$$\times \left\{ 1 + \sum_{\substack{j' \geq 1, \{B'_1, \dots, B'_{j'}\} \in \mathcal{B}_\gamma \\ g(B'_i) > k_0}} \left( \sum_{1 \leq i \leq j'} g(B'_i) - 1 \right) \times \left[ \prod_{1 \leq i \leq j'} \beta C_2 \lambda^{g(B'_i)} e^{ag(B'_i)} \right] \right\} \quad (\text{B.28})$$

The cases with  $j=0$  or  $j'=0$  have been incorporated by adding 1 to each factor. Next, we estimate the sums in (B.27).

The sum in (B.27) can be treated with a “reverse” high-temperature expansion, i.e., resummation, as follows.

$$\sum_{\substack{j \geq 1, \{B_1, \dots, B_j\} \in \mathcal{B}_\gamma \\ g(B_i) \leq k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \left[ \prod_{1 \leq i \leq j} e^{ag(B_i)} \right] \quad (\text{B.29})$$

$$\leq \sum_{\substack{j \geq 1, \{B_1, \dots, B_j\} \in \mathcal{B}_\gamma \\ g(B_i) \leq k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) \right) \left[ \prod_{1 \leq i \leq j} e^{ag(B_i)} \right] \quad (\text{B.30})$$

$$= \frac{d}{da} \sum_{j \geq 0, \{B_1, \dots, B_j\} \subset \mathcal{B}_\gamma} \left[ \prod_{1 \leq i \leq j} e^{ag(B_i)} \right] \quad (\text{B.31})$$

$$= \frac{d}{dt} \left[ \prod_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} (e^{ag(B)} + 1) \right] \quad (\text{B.32})$$

$$= \sum_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} g(B) \frac{e^{ag(B)}}{e^{ag(B)} + 1} \prod_{\substack{B' \in \mathcal{B}_\gamma \\ g(B') \leq k_0}} (e^{ag(B')} + 1) \quad (\text{B.33})$$

$$\leq \left[ \sum_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} g(B) \right] \prod_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} e^{a'g(B)} \quad (\text{B.34})$$

$$= \left[ \sum_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} g(B) \right] \exp \left( a' \sum_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} g(B) \right) \quad (\text{B.35})$$

with  $a' = a + (\log 2)/3$ , guaranteeing that for all  $g(B) \geq 3$ ,  $\exp(ag(B)) + 1 \leq \exp(a'g(B))$ . The estimate of the sum over “small” decorations can now be completed by using the bound

$$\begin{aligned} \sum_{\substack{B \in \mathcal{B}_\gamma \\ g(B) \leq k_0}} g(B) &= \sum_{x \in \gamma} \sum_{\substack{B \ni x \\ g(B) \leq k_0}} \frac{g(B)}{|B|} \leq |\gamma| \sum_{k=3}^{k_0} \sum_{\substack{B \\ g(B)=k}}^* k \\ &\leq |\gamma| \sum_{k=3}^{k_0} c_d^k k \leq C_4 |\gamma| \end{aligned} \quad (\text{B.36})$$

with

$$C_4 = (k_0 + 1)(c_d)^{k_0 + 1} \quad (\text{B.37})$$

At this point we have:

$$Z_{\text{pol}} \leq \sum_{\gamma \ni 0} e^{-a_0 |\gamma|} [1 + C_4 |\gamma| e^{C_4 a' |\gamma|}] \quad (\text{B.38})$$

$$\begin{aligned} &\times \left[ 1 + \left( \sum_{\substack{j' \geq 1, \{B'_1, \dots, B'_{j'}\} \subset \mathcal{B}_\gamma \\ g(B'_i) > k_0}} \left( \sum_{1 \leq i \leq j'} g(B'_i) - 1 \right) \right) \right. \\ &\left. \times \prod_{1 \leq i \leq j'} \beta C_2 U^{-g(B'_i)} e^{ag(B'_i)} \right] \end{aligned} \quad (\text{B.39})$$

The second term in (B.39) represents a sum over the “large” decorations. Let us denote this term by  $L$ , i.e.,

$$L := \sum_{\substack{j' \geq 1, \{B'_1, \dots, B'_{j'}\} \subset \mathcal{B}_\gamma \\ g(B'_i) > k_0}} \left( \sum_{1 \leq i \leq j'} g(B'_i) - 1 \right) \\ \times \prod_{1 \leq i \leq j'} \beta C_2 U^{-g(B'_i)} e^{ag(B'_i)} \quad (\text{B.40})$$

and find an upper bound for it. We first make some simplifying estimates. Using  $k_0 \geq 3$  and  $|\gamma| \geq 6$  one can see that

$$1 + C_4 |\gamma| e^{C_4 a' |\gamma|} \leq C_4 |\gamma| e^{C_4 a'' |\gamma|} \quad (\text{B.41})$$

with,

$$a'' = a + 1/4 \quad (\text{B.42})$$

For convenience we introduce the notations

$$\mathcal{B}_{\gamma, > k_0} = \{B \in \mathcal{B} \mid B \cap \gamma \neq \emptyset, g(B) > k_0\} \quad (\text{B.43})$$

and

$$\tilde{\beta} = \beta C_2, \quad z = \lambda e^a \quad (\text{B.44})$$

Using the trivial observation

$$\sum_{\{B_1, \dots, B_j\} \subset \mathcal{B}_{\gamma, > k_0}} (\cdot) \leq \frac{1}{j!} \sum_{B_1, \dots, B_j \in \mathcal{B}_{\gamma, > k_0}} (\cdot) \quad (\text{B.45})$$

we obtain

$$L \leq \sum_{j \geq 1} \frac{1}{j!} \sum_{B_1, \dots, B_j \in \mathcal{B}_{\gamma, > k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \prod_{1 \leq i \leq n} \tilde{\beta}_Z^{g(B_i)} \\ \leq \sum_{j \geq 1} \sum_{B_1 \in \mathcal{B}_{\gamma, > k_0}} \dots \sum_{B_{j-1} \in \mathcal{B}_{\gamma, > k_0}} \left[ \prod_{1 \leq i \leq j} \tilde{\beta}_Z^{g(B_i)} \right] \\ \times \sum_{B_j \in \mathcal{B}_{\gamma, > k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \tilde{\beta}_Z^{g(B_j)} \quad (\text{B.46})$$



We have that

$$\begin{aligned} & \sum_{B_j \in \mathcal{B}_{\gamma, >k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \tilde{\beta}_z^{g(B_j)} \\ & \leq \sum_{x \in \gamma} \sum_{\substack{B_j \ni x \\ g(B_j) > k_0}} \left( \sum_{1 \leq i \leq j} g(B_i) - 1 \right) \tilde{\beta}_z^{g(B_j)} \end{aligned} \tag{B.47}$$

The sum over  $B_j$  is independent of the choice of the point  $x$ . Hence

$$\begin{aligned} \text{RHS of (B.47)} & \leq 2 |\gamma| \sum_{k_j \geq k_0} [g(B_1) - 1 + \dots + g(B_{j-1}) - 1 + k_j - 1] \\ & \quad \times \sum_{\substack{B_j \\ g(B_j) = k_j}}^* \tilde{\beta}_z^{k_j} \end{aligned} \tag{B.48}$$

Iterating the above steps, we obtain the following upper bound to the contribution of the large decorations:

$$L \leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} \sum_{k_1 > k_0} \dots \sum_{k_j > k_0} \left[ \left( \sum_{i=1}^j k_i - 1 \right) \prod_{i=1}^j \left( \sum_{\substack{B_i \\ g(B_i) = k_i}}^* \tilde{\beta}_z^{k_i} \right) \right] \tag{B.49}$$

Since,  $k_i > k_0 \geq 3$ , we have that

$$\sum_{i=1}^j (k_i - 1) \leq \prod_{i=1}^j (k_i - 1) \tag{B.50}$$

Each factor of  $(k_i - 1)$  can be inserted into the sum over  $k_i$ . This yields

$$\begin{aligned} L & \leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} \prod_{i=1}^j \left( \sum_{k_i > k_0} (k_i - 1) \sum_{\substack{B_i \\ g(B_i) = k_i}}^* \tilde{\beta}_z^{k_i} \right) \\ & \leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} \prod_{i=1}^j \sum_{k_i > k_0} (k_i - 1) c_d^{k_i} \tilde{\beta}_z^{k_i} \\ & \leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} \tilde{\beta}_z^{k_0} (c_d z)^{k_0} \left[ \sum_{k \geq 1} k (c_d z)^k \right]^j \\ & \leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} k_0 [\tilde{\beta}(c_d z)^{k_0}] \left[ \frac{c_d z}{(1 - c_d z)^2} \right]^j \end{aligned} \tag{B.51}$$

provided

$$c_d z \equiv c_d e^{a\lambda} < 1 \quad (\text{B.52})$$

By definition ((B.13), (B.14)) we have that

$$\tilde{\beta}(c_d z)^{k_0} \equiv \beta C_2 (c_d e^{a\lambda})^{k_0} = \alpha < 1 \quad (\text{B.53})$$

Hence, if (B.52) holds, then

$$\begin{aligned} L &\leq \sum_{j \geq 1} \frac{|\gamma|^j}{j!} \left( \frac{k_0 c_d z}{(1 - c_d z)^2} \right)^j \\ &\leq \exp \left[ \frac{|\gamma| k_0 c_d z}{(1 - c_d z)^2} \right] \\ &:= \exp(a_1 |\gamma|) \end{aligned} \quad (\text{B.54})$$

with

$$a_1 := \frac{k_0 c_d z}{(1 - c_d z)^2} \quad (\text{B.55})$$

Hence from (B.39), (B.41) and (B.54) it follows that

$$\begin{aligned} Z_{\text{pol}} &\leq \sum_{\gamma \geq 0} e^{-a_0 |\gamma|} C_4 |\gamma| e^{C_4 a'' |\gamma|} [1 + e^{a_2 |\gamma|}] \\ &\leq \sum_{\gamma \geq 0} e^{-a_0 |\gamma|} 2C_4 |\gamma| e^{C_4 a'' |\gamma|} e^{a_1 |\gamma|} \end{aligned} \quad (\text{B.56})$$

since  $a_1 > 0$ . Defining

$$q := a_0 - \log c_d - a_1 - a'' C_4 \quad (\text{B.57})$$

we have that

$$Z_{\text{pol}} \leq \sum_{k \geq 6} 2C_4 k e^{-kq} \quad (\text{B.58})$$

$$\leq 2C_4 \frac{e^{-q}}{(1 - e^{-q})^2} \quad (\text{B.59})$$

provided

$$q > 0 \quad (\text{B.60})$$

Let us inspect the condition (B.60) in more detail. From the definitions, (B.20), (B.55), (B.42) and (B.37), of  $a_0$ ,  $a_1$ ,  $a''$  and  $C_4$ , and (B.60), it follows that (B.59) holds provided

$$\lambda\beta X(\lambda) > a + \log c_d + k_0 \frac{c_d \lambda e^a}{(1 - c_d \lambda e^a)^2} + \left(a + \frac{1}{4}\right) (k_0 + 1) c_d^{k_0 + 1} \quad (\text{B.61})$$

where

$$X(\lambda) := C_1 - \frac{C_2 c_d^3 \lambda^2}{1 - c_d \lambda} \quad (\text{B.62})$$

and  $k_0$  satisfied the bound (B.13). Before proceeding further, let us recall the conditions which have been imposed on  $\lambda$  in order to arrive at the form (B.59). These are given by (B.19) and (B.52). Moreover, for (B.61) to hold, it is necessary that  $X(\lambda) > 0$ . The inequalities (B.19) and (B.52) are satisfied if

$$\lambda < \lambda_1 := (c_d e^a)^{-1} \quad (\text{B.63})$$

Since  $X(\lambda)$  is monotone decreasing,  $X(\lambda) > 0$  can be satisfied by requiring  $\lambda$  to be smaller than the solution of  $X(\lambda) = 0$ , i.e.,

$$\lambda < \lambda_2 := \frac{2}{c_d \left(1 + \sqrt{1 + \frac{4c_d C_2}{C_1}}\right)} \quad (\text{B.64})$$

In order to satisfy (B.63) and (B.64) we choose  $\lambda > \lambda_0$  with

$$\lambda_0 := (B c_d^2 e^a)^{-1} \quad (\text{B.65})$$

where

$$B := \frac{1}{2} \left(1 + \sqrt{1 + \frac{4c_d C_2}{C_1}}\right) \quad (\text{B.66})$$

Note that  $B > 1$  since  $C_1$ ,  $C_2$  and  $c_d$  are positive.

The quantity  $q$  defined through (B.57) can be expressed as a function of  $\lambda$  and  $b := \beta\lambda$ . Next, let us determine  $b_0$  such that for all  $b > b_0$  and  $\lambda < \lambda_0$ , (B.60) is satisfied. On the RHS of (B.61),  $k_0$  (expressed as a function of  $\lambda$  and  $b$ ) has to satisfy

$$k_0 = k_0(\lambda, b) > 1 - \frac{\log(C_2 c_d e^{ab})}{\log(\lambda c_d e^a)} \quad (\text{B.67})$$

This follows from the defining relation (B.13) for  $k_0$ . For all  $\lambda < \lambda_0$  this can be achieved by choosing

$$\begin{aligned} k_0 = \bar{k}_0(b) &= 1 - \frac{\log(C_2 c_d e^{ab})}{\log(\lambda_0 c_d e^{a\lambda_0})} \\ &= 1 + \frac{\log(C_2 c_d e^{ab})}{\log(bc_d)} \end{aligned} \quad (\text{B.68})$$

where  $B$  is defined through (B.66). Let us denote the RHS of (B.61), with the above choice  $\bar{k}_0$ , by  $A(\lambda, b)$ , i.e.,

$$A(\lambda, b) = a + \log c_d + \frac{\bar{k}_0 \lambda e^a}{(1 - c_d \lambda e^a)^2} + c_d \left( a + \frac{1}{4} \right) (\bar{k}_0 + 1) c_d^{\bar{k}_0} \quad (\text{B.69})$$

Recall that  $X(\lambda)$  is monotone decreasing, and note that  $A(\lambda, b)$ , for a fixed value of  $b$ , is monotone increasing in  $\lambda$ . Hence, for all  $\lambda < \lambda_0$  we can satisfy (B.61) by requiring that

$$bX(\lambda_0) > A(\lambda_0, b) \quad (\text{B.70})$$

That (B.70) is satisfied for all  $b > b_0$ , for some  $b_0 > 0$ , follows from the fact that  $A(\lambda_0, b)$  increases strictly less than linearly in  $b$ . More precisely,

$$A(\lambda_0, b) = A_0 + A_1 \log(d_0 b) + A_2 (d_0 b)^r + A_3 (d_0 b)^r \log(d_0 b) \quad (\text{B.71})$$

where  $A_0, A_1, A_2, A_3$  and  $d_0$  depend on  $C_1, C_2, e^a$  and  $c_d$ , and  $r$  is given by

$$r = \frac{\log c_d}{\log B c_d} \quad (\text{B.72})$$

In particular,

$$d_0 = C_2 c_d e^a \quad (\text{B.73})$$

Since  $B > 1$  (see (B.66)), we have that  $r < 1$ . This proves the convergence of the series for  $Z_{\text{pol}}$  and the bound (B.59).

It is now easy to see that, in fact, the bound  $C'$  for  $Z_{\text{pol}}$  as in the statement of the lemma, can be made arbitrarily small by choosing  $b_0$  arbitrarily large. With  $k_0 = \bar{k}_0$ ,  $C'$  is given by

$$C'(b) 2c_d^2 \left[ 2 + \frac{\log(C_1 b)}{\log(Bc_d)} \right] (C_1 b)^r \times \frac{e^{-q(b)}}{(1 - e^{-q(b)})^2} \quad (\text{B.74})$$

where we have used the definitions of  $C_4$  (B.37) and  $\bar{k}_0$  (B.68). The constants  $d_0$  and  $B$  are defined in (B.73) and (B.66). The function  $q(b)$  is bounded below by  $bX(\lambda_0) - A(\lambda_0, b)$ , which increases linearly in  $b$ . Then again since  $r < 1$ ,  $C'(b) \rightarrow 0$  as  $b \rightarrow \infty$ . ■

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