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Rigidity of interfaces in the Falicov-Kimball model

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Dedicated to the memory of Roland Dobrushin

Abstract

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.

Keywords: 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 [34]. 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 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 [7, 8] 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 [42, 21], 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 [26] 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., [24, 19, 29, 22, 20, 18, 32, 27]) and, recently, convenient perturbation expansions have been developed for it [32, 11, 23]. 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 [26, 31].

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. [29, 32]). 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 [25]. 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 [40]). In the FK model this degeneracy is lifted. In this sense, this is an example of the phenomenon of "ground state selection" [21] by quantum fluctuations. We refer to Section 2.2 for a detailed discussion of the 111 interface configurations.

In [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 [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 [15] (see also [3, 4]) 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 [38, 39, 46, 7] to treat this situation, along the lines of [12] and [36], 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 the Appendix. 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 [16] is a lattice model of spin-polarized electrons and classical particles (ions) [16]. The electrons and ions interact via a purely on-site interaction. The electrons can hop between nearest neighbour sites of the lattice, 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 μ_i and μ_e denote the chemical potentials of the ions and electrons respectively. Let $\mathcal{Z}^3$ 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 $\Lambda \subset \mathcal{Z}^3$ is given by

$$\mathcal{H}_\Lambda(t, U) = \mathcal{H}_{0\Lambda}(U) + tV_\Lambda, \tag{2.1}$$

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

$$\mathcal{H}_{0\Lambda}(U) \quad = \quad 2U \sum_{x\in\Lambda} W(x) n_x - \mu_e \sum_{x\in\Lambda} n_x - \mu_i \sum_{x\in\Lambda} W(x),$$

$$:= \sum_{x\in\Lambda} \Phi_{0x} \tag{2.2}$$

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

$$\begin{aligned} V_\Lambda &= -t \sum_{<xy>\subset\Lambda} (c_x^\dagger c_y + c_y^\dagger c_x), \\ &=: \sum_{X=<xy>\subset\Lambda} V_X, \end{aligned} \tag{2.3}$$

Here $< xy >$ 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 [24]. 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

$$\mu_i = \mu_e = U, \tag{2.4}$$

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 the average number of ions, both being equal to half the number of lattice sites (half-filling).

The model described by the Hamiltonian $\mathcal{H}_\Lambda(t,U)$ for $U < 0$, is mathematically equivalent to the model with $U > 0$ (see [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 $U >> |t|$, and hence consider the hopping term tV_Λ to be a perturbation to the Hamiltonian $\mathcal{H}_{0\Lambda}(U)$. It is convenient to renormalize the hopping amplitude t to unity. This amounts to the following rescaling:

$$\begin{aligned} U/t &\longrightarrow U \\ \beta t &\longrightarrow \beta, \end{aligned} \tag{2.5}$$

where $\beta = 1/k_BT$ (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 $\mathcal{H}_{0\Lambda}(U)$ in the plane of chemical potentials can be easily obtained [18]. To obtain the ground states of $\mathcal{H}_{0\Lambda}(U)$, for any given set of values the chemical potentials μ_i and μ_e, we only need to find the single-site configuration which minimizes Φ_{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 (μ_i-μ_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.

It has been proved in [29, 32] that for $U > 6\,c\,|t|$, where c is a small positive constant, the ionic subsystem of the FK model defined on a finite cubic lattice Λ can be described by an effective classical Hamiltonian, when the values of the chemical potentials are close to U (in particular, when $\mu_i = \mu_e = U$). This effective classical Hamiltonian is given by

$$\mathcal{H}_\Lambda^{\mathrm{eff}}(U) = h \sum_{x\in\Lambda} s'_x + \frac{1}{4U} \sum_{<xy>\in\Lambda} s'_x s'_y + \mathcal{R}_\Lambda(U), \tag{2.6}$$

where

$$s'_x := 2W(x) - 1 \tag{2.7}$$

and

$$h := \mu_i - \mu_e. \tag{2.8}$$

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.

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 $\mathcal{R}_\Lambda(U)$. This remainder is expressible in terms of local classical interactions $\{R_B(U)\}$:

$$\mathcal{R}_\Lambda(U) = \sum_{\substack{B\cap\Lambda\neq\emptyset \\ |B|\geq 2}} R_B(U) \tag{2.9}$$

Here B denotes a *connected* set of lattice sites, i.e., if $x,\ y \in B$ then there exists a sequence of sites $x_0 = x,\, x_1, \ldots, x_n = y$ such that $x_i \in B$ and $|x_i - x_{i+1}| = 1$ for all $i = 0, \ldots, n-1$. 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 Λ. For each bond B appearing in the above sum (2.9), the interaction $R_B(U)$ can be expressed as a product of two or more on-site spin variables s'_x with $x \in B$.

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

It can be shown [32] that for $|B| = 2$

$$|R_B(U)| \le \tilde{c}_2 \Big(\frac{c_1}{U}\Big)^3 \tag{2.10}$$

for all $U > c_1$, with c_1 and $\tilde{c}_2$ being positive (dimension-dependent) constants. For $|B| \ge 3$

$$|R_B(U)| \le \tilde{c}_2 \Big(\frac{c_1}{U}\Big)^{g(B)} \tag{2.11}$$

where

$$g(B) := n(B) - 1, \tag{2.12}$$

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. This implies that there exists a constant $r > 0$ such that

$$\sum_{B \ni 0} |R_B(U)| e^{rg(B)} < \infty \tag{2.13}$$

and hence the interaction $\{R_B(U)\}$ decays exponentially. Using the bound (2.10), the effective Hamiltonian (2.6) can be written as follows

$$\mathcal{H}^{\rm eff}_{\Lambda}(U) = \mathcal{H}^{(2)}_{0\Lambda}(U) + \mathcal{R}^{\ge 3}_{\Lambda}(U) \tag{2.14}$$

with

$$\begin{aligned} \mathcal{H}^{(2)}_{0\Lambda}(U) &= h \sum_{x \in \Lambda} s'_x + \frac{1}{4U} \sum_{<xy> \subset \Lambda} s'_x s'_y + \sum_{\substack{B \cap \Lambda \neq \emptyset \\ |B| = 2}} R_B(U) \\ &= h \sum_{x \in \Lambda} s'_x + J(U) \sum_{<xy> \in \Lambda} s'_x s'_y \end{aligned} \tag{2.15}$$

where

$$J(U) \simeq \frac{1}{4U} + \text{h.o.} > 0, \tag{2.16}$$

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 an infinite series of additional terms which are bounded by a positive constant times the next odd power of U^{-1}. We define

$$\mathcal{R}^{\ge 3}_{\Lambda}(U) := \sum_{\substack{B \cap \Lambda \neq \emptyset \\ |B| > 2}} R_B(U) \tag{2.17}$$

The leading part $\mathcal{H}^{(2)}_{0\Lambda}(U)$ 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.

In this paper we restrict our attention to the half-filled band of the Falicov Kimball model [(2.4)], which corresponds to the choice $h = 0$. In this case, the Hamiltonian $\mathcal{H}_\Lambda^{\rm eff}(U)$ (2.14) is invariant under "spin-flip", i.e., under the transformation $s'_x \longrightarrow -s'_x$, for all $x \in \Lambda$ [29, 32, 20].

For the choice $h = 0$, the leading part, $\mathcal{H}_{0\Lambda}^{(2)}(U)$ [(2.15)], 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 $\mathcal{H}_{0\Lambda}(U)$ (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 $\mathcal{H}_{0\Lambda}(U)$. This phenomenon in which the quantum perturbation lifts the infinite degeneracy of the classical ground states is known as "ground state selection" [42, 21]. Moreover, for low enough temperatures, the characteristic long range order of the Néel states persists under the action of the remainder $\mathcal{R}_\Lambda^{\geq 3}$ [11]. 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

$$s'_x \longrightarrow s_x = (-1)^{2\,|x|} s'_x \quad \text{for all} \quad x = (x_1, x_2, x_3) \in \Lambda, \tag{2.18}$$

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:

$$\mathcal{H}_\Lambda^{\rm ferro}(U) = -J(U) \sum_{<xy>\in\Lambda} s_x s_y, \tag{2.19}$$

where $J(U)$ is given by (2.16). Let us denote $s_x = 1$ by the symbol "$+$" and $s_x = -1$ by the symbol "$-$". The two ground states of $\mathcal{H}_\Lambda^{\rm ferro}(U)$ 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 $\Lambda \subset \mathcal{Z}^3$, the boundary conditions defined

$$\begin{aligned} \text{either by } s_x &= +1 \quad \text{for all } x \in \mathcal{Z}^3 \setminus \Lambda, \\ \text{or by } s_x &= -1 \quad \text{for all } x \in \mathcal{Z}^3 \setminus \Lambda. \end{aligned} \tag{2.20}$$

are referred to as *homogeneous b.c.*

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 [15] (see eqs.(2.21) and (2.22) below).

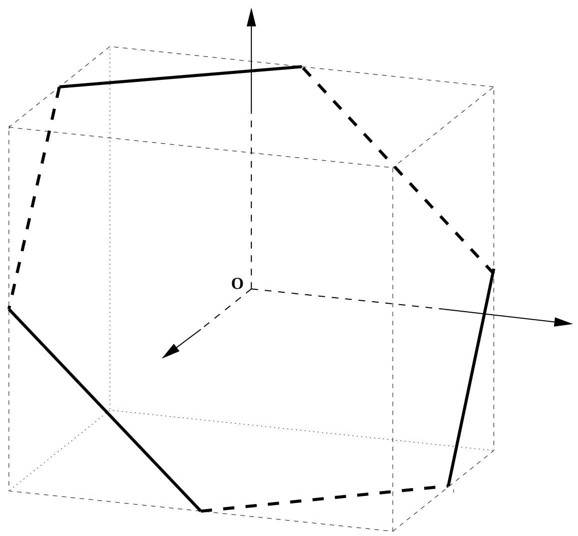

Figure 1: The intersection of a finite cubic lattice $\Lambda \subset \mathcal{Z}^3$ centered at the origin, with a plane passing through the origin and orthogonal to the vector $\mathbf{n} = (1, 1, 1)$.

To construct the 100 interface Gibbs state we consider $\Lambda \subset \mathcal{Z}^3$ 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 $x = (x_1, x_2, x_3,) \in \Lambda^c := \mathcal{Z}^3 \setminus \Lambda$ defined by

$$s_x = \begin{cases} +1 & \text{if } x_3 \geq 1/2 \\ -1 & \text{if } x_3 \leq -1/2 \end{cases} \tag{2.21}$$

For an analysis of the 111 interface consider the intersection of a a plane passing through the origin and orthogonal to the vector $\mathbf{n} = (1, 1, 1)$ with a cube $\Lambda \subset \mathcal{Z}^3$. This intersection yields a plane bounded by a hexagon (as shown in Figure 1) which divides Λ into two equal volumes. To obtain a 111 interface we consider the spin variables s_x [(2.18)] 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 $x = (x_1, x_2, x_3,) \in \Lambda^c \equiv \mathcal{Z}^3 \setminus \Lambda$ defined by

$$s_x = \begin{cases} +1 & \text{if } x_1 + x_2 + x_3 \geq 1/2 \\ -1 & \text{if } x_1 + x_2 + x_3 \leq -1/2 \end{cases} \tag{2.22}$$

Each of these boundary conditions divide the volume Λ 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 Λ under mixed b.c. and the free energy corresponding to the homogeneous b.c.

$$\tau^{\text{mixed b.c.}} = \lim_{\Lambda \nearrow \mathcal{Z}^3} -\frac{1}{\beta |I_\Lambda|} \log\Big(\frac{\Xi_\Lambda^{\text{mixed}}}{\Xi_\Lambda^{\text{hom}}}\Big) \tag{2.23}$$

where $\Xi_\Lambda^{\text{mixed}}$ and Ξ_Λ^{hom} are the partition functions of the system in the finite volume Λ 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 Λ. Such a definition is justified [33] 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 $\lim_{\Lambda \nearrow \mathcal{Z}^3}$ 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 $|I_\Lambda|$ denotes the area of the portion of the interface which is contained in the volume Λ.

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

$$\begin{aligned} H_\Lambda(s) &:= -J(U) \sum_{<xy>\in\Lambda} (s_x s_y - 1) + \sum_{\substack{B\cap\Lambda\neq\emptyset \\ |B|\geq 3}} \Phi_B(s) \\ &:= H_{0\Lambda}^{(2)}(s) + R_\Lambda^{\geq 3}(s) \end{aligned} \tag{2.24}$$

where

$$\Phi_B(s) := R_B(s) - R_B(s_+) = R_B(s) - R_B(s_-), \tag{2.25}$$

and $J(U)$ is given by (2.16). Here and henceforth the explicit U-dependences of the relative Hamiltonian and its components have been suppressed for notational simplicity.

Each configuration in a finite volume Λ, with respect to fixed boundary conditions (homogeneous or mixed) can be geometrically described by specifying the Ising contours which are defined as follows [33]: 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 Λ if at least one site of the corresponding nearest neighbour bond is in Λ. Given a configuration ω_Λ on a finite lattice Λ, with b.c. $\bar{\omega}$, let $\mathcal{S}^{\bar{\omega}}(\omega_\Lambda)$ be the set of faces associated with nearest neighbour bonds between opposite spins. Decompose $\mathcal{S}^{\bar{\omega}}(\omega_\Lambda)$ 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 γ. For homogeneous b.c. the contours are closed surfaces lying entirely within the volume Λ. However, for mixed b.c. there is necessarily one (and only one) contour which is pinned to the boundary of the volume Λ. This is the only infinite maximally connected component of the set $\mathcal{S}^{\bar{\omega}}(\omega_\Lambda)$ 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 $\Gamma = \{\gamma\}$: $\omega_\Lambda = \omega_\Lambda(\Gamma)$. We shall refer to such families as *compatible* families of contours. In the sequel we shall use the symbol γ to denote both the contour and its support. The number of faces in a contour γ is denoted by $|\gamma|$ and satisfies the bound $|\gamma| \geq 6$, since the lattice is three-dimensional. The energy of a contour γ is given by

$$E(\gamma) := H^{(2)}_{0\Lambda}(\Gamma' \cup \{\gamma\}) - H^{(2)}_{0\Lambda}(\Gamma'). \tag{2.26}$$

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

It follows from (2.24) that the relative energy of a configuration $\omega_\Lambda(\Gamma)$ is given by

$$H_\Lambda(\Gamma) = H^{(2)}_{0\Lambda}(\Gamma) + R^{\geq 3}_\Lambda(\Gamma) \tag{2.27}$$

with

$$H^{(2)}_{0\Lambda}(\Gamma) = \sum_{\gamma \in \Gamma} E(\gamma), \tag{2.28}$$

where

$$E(\gamma) = 2J(U) = \Big(\frac{1}{2U} + \text{h.o.}\Big)|\gamma| =: J_1(U)|\gamma| \tag{2.29}$$

and

$$R^{\geq 3}_\Lambda(\Gamma) = \sum_{\substack{B \cap \Gamma \neq \emptyset \\ |B| \geq 3}} \Phi_B(\Gamma). \tag{2.30}$$

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 γ w.r.t. $H^{(2)}_{0\Lambda}$. Its definition (2.29) implies that, for sufficiently large U, the Hamiltonian $H^{(2)}_{0\Lambda}$ satisfies the Peierls condition:

$$E(\gamma) \;\geq\; \mathcal{J}|\gamma|\,, \tag{2.31}$$

with a Peierls constant

$$\mathcal{J} = c_0 U^{-1}, \tag{2.32}$$

where c_0 is a positive constant. Moreover, from the definition (2.25) and the bound (2.11) it follows that for $|B| \geq 3$

$$|\Phi_B| \leq c_2 \Big(\frac{c_1}{U}\Big)^{g(B)}, \tag{2.33}$$

with $c_2 = 2\tilde{c}_2$. The effect of the term $R^{\geq 3}_\Lambda(U)$ 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 (2.22), the leading part $H^{(2)}_{0\Lambda}$

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 $H_{0\Lambda}^{(4)}$:

$$H_\Lambda = H_{0\Lambda}^{(4)} + R_{\Lambda}^{\geq 5} \tag{2.34}$$

where

$$\begin{aligned} H_{0\Lambda}^{(4)} \;&=\; -\Big(\frac{1}{4U} - \frac{11}{16U^3} + \text{h.o.}\Big) \sum_{<xy>\subset\Lambda} (s_x s_y - 1) + \Big(\frac{3}{16U^3} + \text{h.o.}\Big) \sum_{\substack{x,y\in\Lambda \\ |x-y|=\sqrt{2}}} (s_x s_y - 1) \\ &\quad + \Big(\frac{1}{8U^3} + \text{h.o.}\Big) \sum_{\substack{x,y\in\Lambda \\ |x-y|=2}} (s_x s_y - 1) + \Big(\frac{5}{16U^3} + \text{h.o.}\Big) \sum_{x,y,z,t\subset P(\Lambda)} (s_x s_y s_z s_t - 1) \end{aligned} \tag{2.35}$$

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

The remainder $R_{\Lambda}^{\geq 5}$ is obtained from the series (2.30) defining $R_{\Lambda}^{\geq 3}$ by subtracting all terms which depend on U^{-n} with $n \leq 3$. It is given by

$$R_{\Lambda}^{\geq 5} = \sum_{\substack{B\cap\Lambda\neq\emptyset \\ |B|>3}} \tilde{\Phi}_B, \tag{2.36}$$

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

$$|\tilde{\Phi}_B| \leq c_2 \left(\frac{c_1}{U}\right)^{m(B)}, \tag{2.37}$$

where

$$m(B) := \max(5, g(B)). \tag{2.38}$$

In the expression for the relative Hamiltonian $H_{0\Lambda}^{(2)}$ (2.24) the terms up to order U^{-1} are computed explicitly by second order perturbation theory, while the terms of order U^{-3} in $H_{0\Lambda}^{(4)}$ (2.35) are obtained by fourth order perturbation theory. We shall refer to (2.24) as the second order decomposition of the relative Hamiltonian, and (2.34) 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 (2.22). 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 $R_{\Lambda}^{\geq 5}(U)$ 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 $\Lambda \nearrow \mathcal{Z}^3$ 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 $<>_{[\text{b.c.1}]}$ and $<>_{[\text{b.c.2}]}$ denote the expectation values in the (infinite–volume) Gibbs states with the mixed boundary condition b.c.1 (2.21) and b.c.2 (2.22) 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 (2.18). 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:*

$$< s_x >_{[\text{b.c.1}]} \geq 1 - 2C_0 e^{-c'\beta/U} \qquad \text{for } x_3 \geq 1/2, \tag{2.39}$$

and

$$< s_x >_{[\text{b.c.1}]} \leq -1 + 2C_0 e^{-c'\beta/U} \qquad \text{for } x_3 \leq -1/2,, \tag{2.40}$$

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:*

$$< s_x >_{[\text{b.c.2}]} \geq 1 - 2\Big\{\tilde{C}_0 e^{-c''\beta/U^3} + \tilde{C}_1 e^{-c_1''\beta/U}\Big\} \qquad \text{for } x_1 + x_2 + x_3 \geq 1/2, \tag{2.41}$$

and

$$< s_x >_{[\text{b.c.2}]} \leq -1 + 2\Big\{\tilde{C}_0 e^{-c''\beta/U^3} + \tilde{C}_1 e^{-c_1''\beta/U}\Big\} \qquad \text{for } x_1 + x_2 + x_3 \leq -1/2, \tag{2.42}$$

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 [15] 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 [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 $\tilde{\mathcal{I}}$ denote the family of interfaces under the b.c.2 (2.22) and $\tilde{I}$ denote its typical element. Such an interface is pinned at the boundary of Λ on the curve defined by

$$\partial\Lambda \cap \{(x,y,z) \in \mathbb{Z}^3 \mid x+y+z=0\} \tag{2.43}$$

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 $\mathbb{P}_\Lambda$ denote the portion of the plane $\mathbb{P}$ which is contained in the volume Λ.

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 $\mathcal{V}_{\mathrm{n \bmod 3}} \equiv \mathcal{P}(P_n)$, $n \in \mathbb{Z}$, 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 $\mathcal{Z}^3$ 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 Λ projects onto a covering of the plane $\mathbb{P}_\Lambda$ 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).

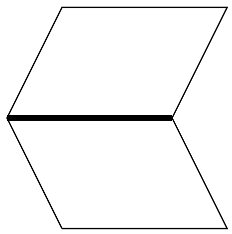

Figure 2: A pair of rhombi in *good position*. The edge shared by the two rhombi is referred to as a *good edge*.

- 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 $\mathcal{C}_\Lambda$ 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:

$$o(t) := \{\text{the number of faces of the interface whose projection contains}\, t\} - 1 \quad (2.44)$$

  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 Figure 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 $\mathbb{P}_\Lambda$. It is given by a tiling of $\mathbb{P} \setminus \mathbb{P}_\Lambda$ 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 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 [28, 44], 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 Λ under the mixed boundary condition b.c.2 (2.22).*

Proof: As noted above it is obvious that each minimal area interface under the boundary condition b.c.2 (2.22) projects onto a tiling of $\mathbb{P}_\Lambda$ 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 Λ along the curve defined by (2.43). The projection of the set of faces constituting an interface $\tilde{I}$ yields a set of rhombi in $\mathcal{R}$ that covers $\mathbb{P}_\Lambda$. 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* $h : \mathcal{V} \to \mathbb{Z}$ 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 Λ under the b.c.2 (2.22) is an interface whose projection on the plane $\mathbb{P}_\Lambda$ is a tiling. It consists of all faces $\{f\}$ in Λ for which:

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

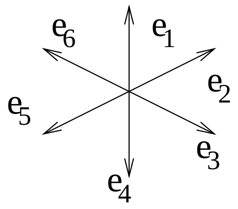

Figure 3: The labeling of the six unit vectors emanating from a site of the triangular lattice.

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 $\vec{e}_1, \ldots, \vec{e}_6$ the vectors of minimal length $(= \sqrt{\frac{2}{3}})$, 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 Figure 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 $\mathbb{P}_\Lambda$. 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_Λ grows exponentially with the area of the interface and satisfies the bounds:*

$$2^{\frac{|I_\Lambda|}{3}} \leq N_\Lambda \leq 2^{2|I_\Lambda|}$$

where $|I_\Lambda|$ is the area of the minimal area interfaces in the volume Λ.

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 [40].

From Proposition 4 it follows that in the limit $\Lambda \nearrow \mathcal{Z}^3$ 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 (2.24) - (2.25) and (2.34) - (2.36) 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 (2.23)). 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 Ξ_Λ^+ and Ξ_Λ^- be the partition functions in $\Lambda \subset \mathcal{Z}^3$ w.r.t the homogeneous boundary conditions defined by (2.20). The spin-flip symmetry of the effective Hamiltonian $\mathcal{H}_\Lambda^{\text{eff}}(U)$ (2.14), for the choice $h = 0$, implies that

$$\Xi_\Lambda^+ = \Xi_\Lambda^- := \Xi_\Lambda^{\text{hom}}. \tag{3.1}$$

Let Ξ_Λ^{100} and Ξ_Λ^{111} be the corresponding partition functions under the mixed boundary conditions b.c.1 (2.21) and b.c.2 (2.22) respectively.

A mixed b.c. (b.c.1 (2.21) or b.c.2 (2.22)) leads to the appearance of an interface I which divides the volume Λ into two subvolumes Λ_I^a and Λ_I^b which are, respectively, the regions above and below I. The configuration in these subvolumes are defined by finite sets of compatible contours $\Gamma^a := \{\gamma_1^a, \ldots, \gamma_p^a\}$ and $\Gamma^b = \{\gamma_1^b, \ldots, \gamma_q^b\}$ respectively. We define $\Gamma := \Gamma^a \cup \Gamma^b$ and denote a configuration on the lattice by $(I \cup \Gamma)$. Let $\mathcal{I}$ and $\widetilde{\mathcal{I}}$ 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 (2.27) of the relative Hamiltonian H_Λ, the partition function for homogeneous b.c. is given by

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

where $J_1(U) \simeq \frac{1}{2U} + \text{h.o.}$ The partition function relevant for the mixed boundary condition b.c.1 (2.21) is also obtained by using eqns.(2.27) - (2.30). It is given by

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

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_Λ takes on the configuration $(I\cup\Gamma)$:

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

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 (2.26). The third term is the energy of interaction among these contours and arises from the long-range tail potential $R_\Lambda^{\geq 3}$ (2.30) of the relative Hamiltonian H_Λ.

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

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

From (2.29) and (2.33) it follows that for sufficiently large U, the energy $E_1^{\text{bare}}(I)$ satisfies the bound

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

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

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

with

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

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

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

Hence, the functions Φ'_B for which B intersects *only* the interface, do not contribute to the energy $\widetilde{E}_1(I\cup\Gamma)$. 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 Γ. This observation allows us to write $\widetilde{E}_1(I\cup\Gamma)$ as follows.

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

Further, it follows from (2.33) that $\Phi'_B(I\cup\Gamma)$ satisfies the bound

$$\begin{aligned}
|\Phi'_B(I\cup\Gamma)| &\leq |\Phi_B(I\cup\Gamma)| + |\Phi_B(I\cup\emptyset)|\\
&< 2c_2\Big(\frac{c_1}{U}\Big)^{g(B),} \qquad (3.11)
\end{aligned}$$

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

$$\Phi'_B(I\cup\Gamma) = \Phi_B(I\cup\Gamma) \qquad (3.12)$$

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

$$\begin{aligned}
\Xi_\Lambda^{100} &= \sum_{I\in\mathcal{I}} e^{-\beta E_1^{\text{bare}}(I)} \times \sum_{\Gamma^a=\{\gamma_1^a,\ldots,\gamma_p^a\}\subset\Lambda_I^a}\ \sum_{\Gamma^b=\{\gamma_1^b,\ldots,\gamma_q^b\}\subset\Lambda_I^b} e^{-\beta\widetilde{E}_1(I\cup\Gamma)}\\
&\quad \prod_{j=1}^{p} e^{-\beta J_1(U)|\gamma_j^a|} \times \prod_{k=1}^{q} e^{-\beta J_1(U)|\gamma_k^b|}, \qquad (3.13)
\end{aligned}$$

with $E_1^{\text{bare}}(I)$ and $\widetilde{E}_1(I\cup\Gamma)$ being defined through (3.5) and (3.10) respectively. The partition function for the boundary condition b.c.2 (2.22) can be similarly written as

$$\Xi_\Lambda^{111} = \sum_{\tilde{I}\in\widetilde{\mathcal{I}}}\ \sum_{\Gamma:=\Gamma^a\cup\Gamma^b} e^{-\beta\mathcal{E}_2(\tilde{I}\cup\Gamma)}, \qquad (3.14)$$

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 [eqns. (2.34) - (2.36)] of the relative Hamiltonian H_Λ, 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 [eqns. (2.27) - (2.30)] for evaluating the corresponding contribution of the contours in Γ. We first introduce some notations which are useful in evaluating $\mathcal{E}_2(\tilde{I} \cup \Gamma)$.

- Let $P_{\tilde{I}} \subset P(\Lambda)$ 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 $B^2_{\tilde{I}} \subset \mathcal{Z}^3$ denote the set consisting of pairs of next nearest neighbour sites,
$$\{\{x, z\} \in \mathcal{Z}^3 |\, |x - z| = 2\}, \tag{3.15}$$
such that the line joining each pair is intersected by a face in $\tilde{I}$.

From (2.34) - (2.36), it follows that the energy $\mathcal{E}_2(\tilde{I} \cup \Gamma)$ is given by

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

where
$$h_p := 5(s_x s_y s_z s_t - 1) + 3(s_x s_z + s_y s_t - 2) \tag{3.17}$$
for each $p = \{x, y, z, t\} \in P_{\tilde{I}}$,
$$h_{\{x,z\}} := s_x s_z - 1 \tag{3.18}$$
for each $\{x, z\} \in B^2_{\tilde{I}}$, and
$$J_2(U) \simeq \frac{1}{2U} - \frac{11}{8U^3} + \text{h.o.} \tag{3.19}$$
Let $(\tilde{I} \cup \emptyset)$ denote a configuration which has the interface $\tilde{I}$ as its only contour. We denote the corresponding "bare" energy of the interface by $E_2^{\text{bare}}(\tilde{I})$. It is defined as follows.

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

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

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

where

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

where we have defined the quantity

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

It satisfies the bound

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

where $m(B)$ is defined through (2.38).

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 $E_1^{\rm bare}(I)$ 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 $E_2^{\rm bare}(I)$ 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 $\Xi_\Lambda^{\rm hom}$, Ξ_Λ^{100} and Ξ_Λ^{111} in the limit $\Lambda\nearrow\mathcal{Z}^3$. 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 (2.20) in terms of decorated contours. The partition function for homogeneous b.c. is given by (3.2), which we repeat here for convenience.

$$\Xi_\Lambda^{\mathrm{hom}} = \sum_{\Gamma=\{\gamma_1,\ldots,\gamma_n\}\subset\Lambda} \prod_{i=1}^{n} e^{-\beta J_1(U)|\gamma_i|} \prod_{\substack{|B|>2\\ B\cap\Gamma\neq\emptyset}} e^{-\beta\Phi_B(\Gamma)}. \tag{3.25}$$

By convention we treat empty products as unity. The idea is to analyze the effect of the dominant part $H_{0\Lambda}^{(2)}(U)$ of the relative Hamiltonian (2.24) by a low temperature expansion in terms of its contours γ, while treating the contribution of the long range tail, $R_\Lambda^{\geq 3}$, by a high temperature expansion [36, 12]. Hence, we write

$$\begin{aligned}\Xi_\Lambda^{\mathrm{hom}} &= \sum_{\Gamma\subset\Lambda}\prod_{\gamma\in\Gamma} e^{-\beta J_1(U)|\gamma_i|} \prod_{\substack{B\cap\Gamma\neq\emptyset\\ |B|\geq 3}} \Big[(e^{-\beta\Phi_B}-1)+1\Big] \\ &= \sum_{\Gamma\subset\Lambda}\prod_{\gamma\in\Gamma} e^{-\beta J_1(U)|\gamma_i|}\Big[1+\sum_{n\geq 1}\sum_{\substack{B_1,\ldots,B_n\\ B_i\cap\Gamma\neq\emptyset\\ |B_i|>2\,;\,(i=1\ldots n)}}\prod_{i=1}^{n}(e^{-\beta\Phi_{B_i}}-1)\Big]\end{aligned} \tag{3.26}$$

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

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

where $\Gamma_D \subset \Gamma$ is a finite set of compatible contours and $\mathcal{B}_D := \{B_1, \ldots B_n\}$ 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

$$\mathrm{supp}D := \Big(\cup_{\gamma\in\Gamma_D}\gamma\Big) \cup \Big(\cup_{B\in\mathcal{B}_D} B\Big) \tag{3.28}$$

is a connected set. In (3.28) 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,

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

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 γ, γ' in D, there are contours $\gamma_1, \ldots \gamma_k$ in D such that $\gamma \sim \gamma_1$, $\gamma_1 \sim \gamma_2$, $\ldots$, $\gamma_k \sim \gamma'$, with the understanding that two contours γ_1 and γ_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 γ_1 and γ_2
  - there are two bonds B_1 and B_2 in D such that $B_1 \cap B_2 \neq \emptyset$, B_1 intersects γ_1 and B_2 intersects γ_2.

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

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

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.

$$\Xi_\Lambda^{\mathrm{hom}} = \sum_{\mathcal{D} \cap \Lambda \neq \emptyset} \prod_{D \in \mathcal{D}} W(D). \tag{3.31}$$

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

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

The above bound follows from the Peierls bound (2.31) and the exponential decay (2.33). 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 (2.21)– (2.22) 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 Λ. In our definition of decorated contours the interface is treated differently from the remaining Ising contours in the volume Λ. 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 Λ into two subvolumes Λ_I^a and Λ_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 consist, 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 (2.21), we define the following compatible families of decorated contours.

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

where Γ^a and Γ^b are the subfamilies of compatible (Ising) contours which lie entirely in the subvolumes Λ_I^a and Λ_I^b respectively. For a given interface $\tilde{I}$, under the boundary condition b.c.2 (2.22), the corresponding families of compatible decorated contours are denoted by $\mathcal{D}_{\tilde{I}}$, $\mathcal{D}_{\tilde{I}}^a$ and $\mathcal{D}_{\tilde{I}}^b$.

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

$$\begin{aligned} \Xi_\Lambda^{100} &= \sum_{I\in\mathcal{I}} e^{-\beta E_1^{\mathrm{bare}}(I)} \Big(\sum_{\mathcal{D}_I\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_I} W_I(D)\Big) \\ &\times \Big(\sum_{\mathcal{D}_I^a\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_I^a} W(D)\Big)\Big(\sum_{\mathcal{D}_I^b\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_I^b} W(D)\Big) \end{aligned} \tag{3.34}$$

where $W(D)$ is defined through (3.30) and satisfies the bound $|W(D)|\le W_0(D)$, with $W_0(D)$ being defined through (3.32).
For $D\in\mathcal{D}_I$

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

From the Peierls bound (2.31) and the estimate (3.11) it follows that $|W_I(D)|\le W_I^0$ where

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

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

$$\begin{aligned} \Xi_\Lambda^{111} &= \sum_{\tilde{I}\in\tilde{\mathcal{I}}} e^{-\beta E_2^{\mathrm{bare}}(\tilde{I})} \Big(\sum_{\mathcal{D}_{\tilde{I}}\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_{\tilde{I}}} W_{\tilde{I}}(D)\Big) \\ &\times \Big(\sum_{\mathcal{D}_{\tilde{I}}^a\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_{\tilde{I}}^a} W(D)\Big)\Big(\sum_{\mathcal{D}_{\tilde{I}}^b\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}_{\tilde{I}}^b} W(D),\Big) \end{aligned} \tag{3.37}$$

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

$$W_{\tilde{I}}(D) := \prod_{\gamma\in D} e^{-\beta J_1(U)|\gamma_i|} \prod_{\substack{B\in D\\ |B|\ge 3}} (e^{-\beta\widetilde{\Phi}'_B}-1). \tag{3.38}$$

The bounds (2.31) and (3.24) imply that $|W_{\tilde{I}}(D)|\le W_{\tilde{I}}^0$ where

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

where $m(B)$ is defined through (2.38).

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

$$S_\Lambda := \sum_{\mathcal{D}\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}} W(D) \tag{3.40}$$

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

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

where the function G_B is given by Φ_B (2.25) for the homogeneous boundary conditions (2.20) and by the functions Φ'_B (3.8) and $\widetilde{\Phi}'_B$ (3.23) for the mixed boundary conditions (2.21) and (2.22) respectively. The bounds satisfied by these functions are respectively given by (2.33), (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*

$$S_\Lambda := \sum_{\mathcal{D}\cap\Lambda\neq\emptyset} \prod_{D\in\mathcal{D}} W(D), \tag{3.42}$$

where

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

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

$$E(\gamma) \geq C_1\lambda|\gamma| \tag{3.44}$$

and

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

where $g(B)$ is defined through (2.12) 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_Λ has a convergent cluster expansion, i.e.,

$$\log S_\Lambda \;=\; \sum_{N\geq 1} \frac{1}{N!} \sum_{D_1\cap\Lambda\neq\emptyset} \cdots \sum_{D_N\cap\Lambda\neq\emptyset} \Psi^{\mathrm{T}}(\{D_1,\ldots,D_N\}) \tag{3.46}$$

(the cluster expansion*), where Ψ^{T} is a function on families of decorated contours with the property that*

$$\Psi^{\mathrm{T}}(\{D_1,\cdots,D_N\}) \;=\; 0 \quad \textit{if} \quad \{D_1,\cdots,D_N\} \textit{ is not a cluster}\,, \tag{3.47}$$

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

$$\sum_{\{D_1,\ldots,D_N\}\ni 0} \frac{|\Psi^{\mathrm{T}}(D_1,\ldots,D_N)|}{|D_1 \cup \cdots \cup D_N|} \;\le\; s_N \tag{3.48}$$

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 the Appendix. The proof of the convergence of the series S_Λ (3.40) for $G_B = \widetilde{\Phi}_B$ 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

$$|G_B| \le C_2 \lambda^{m(B)}. \tag{3.49}$$

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

$$|P| := \sum_{D\in P} |D| = \sum_{D\in P} \Big(\sum_{\gamma\in D} |\gamma| + \sum_{B\in D} g(B) \Big) \tag{3.50}$$

Let $\Psi^{\mathrm{T}}(P)$, $\Psi^{\mathrm{T}}_I(P)$ and $\Psi^{\mathrm{T}}_{\tilde I}(P)$ denote truncated functions, defined on the cluster P, which satisfy the following bounds.

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

$$\sum_{P\ni 0} \frac{|\Psi^{\mathrm{T}}_I(P)|}{|P|} \;\le\; \sup \prod |W_I(D)|, \tag{3.52}$$

and

$$\sum_{P\ni 0} \frac{|\Psi^{\mathrm{T}}_{\tilde I}(P)|}{|P|} \;\le\; \sup \prod |W_{\tilde I}(D)|. \tag{3.53}$$

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.

$$\mathbf{Z}^{100}_\Lambda = \frac{\Xi^{100}_\Lambda}{\Xi^{+}_\Lambda} \quad \text{and} \quad \mathbf{Z}^{111}_\Lambda = \frac{\Xi^{111}_\Lambda}{\Xi^{+}_\Lambda}. \tag{3.54}$$

Using the results of cluster expansions (see, e.g., [33]) 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 Λ, such that for all $U > U_0$ and and $\beta/U > B_1$, the quotient $\mathbf{Z}_\Lambda^{100}$ can be written as follows:*

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

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

$$\mathbf{Z}_\Lambda^{111} = \sum_{\tilde{I} \in \widetilde{\mathcal{I}}} e^{-\beta E_2^{\mathrm{bare}}(\tilde{I})} \times \exp\left\{ \sum_{\substack{P: \\ P\cap \tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi_{\tilde{I}}^{\mathrm{T}}(P) - \sum_{\substack{P: \\ P\cap \tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi^{\mathrm{T}}(P) \right\}. \tag{3.56}$$

Proof: The proof is standard. We expand the partition functions appearing in the numerator and in the denominator of $\mathbf{Z}_\Lambda^{100}$ and of $\mathbf{Z}_\Lambda^{111}$ by the cluster expansion performed in the the Appendix. The truncated functions which are left are precisely those defined on the clusters which intersect the interface. ■

Alternatively $\mathbf{Z}_\Lambda^{111}$ can be written as

$$\mathbf{Z}_\Lambda^{111} = \sum_{\tilde{I} \in \widetilde{\mathcal{I}}} e^{-\beta E_2^{\mathrm{dec}}(\tilde{I})} \tag{3.57}$$

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

$$E_2^{\mathrm{dec}}(\tilde{I}) := E_2^{\mathrm{bare}}(\tilde{I}) - \frac{1}{\beta}\Big[\sum_{\substack{P: \\ P\cap \tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi_{\tilde{I}}^{\mathrm{T}}(P) - \sum_{\substack{P: \\ P\cap \tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi^{\mathrm{T}}(P) \Big] \tag{3.58}$$

We shall refer to $E_2^{\mathrm{dec}}(\tilde{I})$ 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. [15].

Proof of Theorem 1:

Let $\mathrm{Prob}_\Lambda(I)$ denote the probability of occurrence of an interface I in the FK model, defined on a finite cubic lattice Λ, under the boundary condition b.c.1 (2.21). It is defined as follows:

$$\mathrm{Prob}_\Lambda(I) = \frac{1}{\mathbf{Z}_\Lambda^{100}} \exp\{-\beta E_1^{\mathrm{bare}}(I)\} \times \exp\left\{ \sum_{\substack{P: \\ P\cap I\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi_I^{\mathrm{T}}(P) - \sum_{\substack{P: \\ P\cap I\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi^{\mathrm{T}}(P) \right\} \qquad (4.1)$$

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, $E_1^{\mathrm{bare}}(I)$ (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 $\mathrm{Prob}_\Lambda(I)$ 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 Γ_I is a finite set of Ising contours; [see [33] 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 is the case for the Ising model. difference arises from the fact that the "bare" energy, $E_1^{\mathrm{bare}}(I)$ [(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 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 [15]. 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) [15]. 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. $\blacksquare$

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 (2.13).

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 (2.28) 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 Λ, under the boundary condition b.c.2 (2.22):

$$\mathrm{Prob}_\Lambda(\tilde{I}) = \frac{1}{\mathbf{Z}_\Lambda^{111}} \exp\{-\beta E_2^{\mathrm{bare}}(\tilde{I})\} \times \exp\left\{ \sum_{\substack{P:\\ P\cap\tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi^{\mathrm{T}}_{\tilde{I}}(P) - \sum_{\substack{P:\\ P\cap\tilde{I}\neq\emptyset \\ P\cap\Lambda\neq\emptyset}} \Psi^{\mathrm{T}}(P) \right\}. \tag{5.1}$$

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, which we refer to as an 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 $\mathcal{C}_\Lambda$ denote an R configuration on $\mathbb{P}_\Lambda$.