

Wall and Boundary Free Energies

II. General Domains and Complete Boundaries

Gunduz Caginalp* and Michael E. Fisher

Baker Laboratory, Cornell University, Ithaca, New York 14853, USA

Abstract. The asymptotic free energy of a planar wall with potentials W , cut in scalar spin systems, with ferromagnetic interactions K , enclosed in general domains subject to reasonable shape conditions, is shown (under conditions used in Part I) to exist and to be equal to the unique limiting wall free energy, $f_{\times}(K, W)$, of simple rectangular or box domains. Similar results are found for sets of walls forming the complete boundaries of domains; for “subfree” walls the total free energy of a box domain is proved to be asymptotically equal to a bulk plus a uniquely-defined surface term. Some limited results for periodic boundary conditions are reported.

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* Now at Rockefeller University, New York, New York 10021, USA

1 This paper is written as a direct continuation of Part I [Fisher, M. E., Caginalp, G.: Commun. math. Phys. 56, 11–56 (1977)]. Accordingly the numbering of sections, equations, and figures runs straight on from Part I [which contained Sects. 0 to 4, Eqs. (0.1) to (4.4.23), and Figs. 1 to 9]

5. Recapitulation and Summary

In the first part of this paper [1], to be referred to below as I, we discussed the definition and properties of wall or boundary free energies in a general way and initiated a program to establish the existence and, as far as possible uniqueness of wall free energies in lattice spin systems. Our overall strategy entailed the following main steps: (i) the *free energy per unit area*, $f_\times(K, W, \tilde{W}, \Omega)$, of a finite planar wall characterized by *wall potentials* W , in a system with *bulk interaction potentials* K , is defined in terms of the incremental free energy produced by cutting the reference domain, Ω , containing the system in d -dimensional Euclidean space, by a $d' = (d - 1)$ -dimensional plane into two subdomains, Ω_1 and Ω_2 , so forming a pair of matching walls; the additional potentials, \tilde{W} , represent the *associated wall potentials* imposed on those boundaries of Ω (and, correspondingly, of Ω_1 and Ω_2) which do not form part of the wall: see Fig. 2 in I. (ii) For a standard sequence of domains $\{A_{(k)}\}_{k \rightarrow \infty}$, specifically rectangular or box domains, $A_{\mathbf{L}, N_1 + N_2}$, in which the dimensions, $L_1^{(k)}, L_2^{(k)}, \dots, L_{d'}^{(k)}$ of the wall faces or cross-sections, \mathbf{L} , and the subbox lengths, $N_1^{(k)}$ and $N_2^{(k)}$, become infinite, the existence of a limiting wall free energy, $f_\times(K, W)$, is to be established; the resulting standard wall free energy, $f_\times(K, W)$, should be independent of the associated wall potentials, \tilde{W} . (iii) The existence of the limiting wall free energy for a planar wall cut in a *general* sequence of domains, is then to be proved; the result should be independent of the shapes of the reference domains Ω (subject only to reasonable geometric conditions) and equal to the standard value, $f_\times(K, W)$. (iv) The total wall free energy of *multiple* planar walls cut in large domains is to be shown, asymptotically, to equal simply the appropriately weighted sum of the standard wall free energies for the corresponding single, isolated walls; i.e. interference terms between different walls are negligible. Finally, (v) for a large domain Ω of volume $V(\Omega)$, bounded by planar faces of areas $A_\alpha(\Omega)$ ($\alpha = 1, 2, \dots$), the total (reduced) free energy should have the form

$$\bar{F}(\Omega) \equiv V(\Omega)f(\Omega) = V(\Omega)f_\infty(K) + \sum_\alpha A_\alpha(\Omega)f_\times(K, W_{(\alpha)}) + o(A_\alpha), \quad (5.1)$$

in which $f_\infty(K)$ is the limiting bulk free energy per unit volume, while $W_{(\alpha)}$ denotes the wall potentials of the wall α and $f_\times(K, W_{(\alpha)})$ is the corresponding standard wall free energy [compare with (0.5) of I]. Note that in this expression the total external perimeter or boundary of Ω is involved: there are no associated wall potentials and the walls are *not* cut into a reference domain.

In addition, as observed in I, it is of interest to go on (vi) to consider walls cut in a reference torus, Π (or box A with periodic boundary conditions) and (vii) to show that the total free energy of a torus, Π , satisfies (5.1) with all the wall areas, $A_\alpha(\Pi)$, set identically to zero. From this one may, alternatively, define the asymptotic wall free energy via

$$\lim_{A \rightarrow \infty} \frac{\bar{F}(K, W, A) - \bar{F}(K, \Pi)}{A(A)} = f_\times(K, W), \quad (5.2)$$

that is, in terms of the difference between the free energy of the torus and the corresponding box. [For simplicity in writing (5.2), we have assumed appropriate lattice symmetries, supposed $W_{(\alpha)} \equiv W$ (all α), and set $\sum_\alpha A_\alpha(A) = A(A)$.]

In I this strategy was implemented for systems with scalar, or Ising-like spin variables, interacting through *ferromagnetic* (or positive) potentials K , subject to the usual stability and tempering conditions [2, 3]; however, somewhat stronger conditions of spatial decrease of the bulk potentials and, similarly, of the wall potentials, W , are essential to ensure the boundedness of the limiting wall free energy [see conditions **B**, **D**, and **F** of I]. The definition of step (i) was transformed to yield an expression for $f_\times(\Omega)$ in terms of spin correlation functions. The assumed ferromagnetic character of the interactions then enabled us to use the correlation inequalities of Griffiths, Kelly and Sherman [4, 5] as the principal tool of analysis. In step (ii), results were thereby obtained for arbitrary bulk interaction K , including those allowing the possibility of coexisting phases, and for arbitrary wall potentials W [respecting the overall ferromagnetic character; see (2.3.6)].

However, a technical limitation on the results of I, arising from this approach, concerns the dependence on the associated wall potentials \tilde{W} ; these must be predominantly either: (a) *subfree* – formed by removing or weakening the bulk ferromagnetic interaction potentials [see (2.3.7)]; or, for bulk interactions of strictly finite range, (b) *superferromagnetic* – corresponding to the imposition of positively infinite boundary magnetic fields and strengthened ferromagnetic interactions near the boundary. These two situations yield standard, limiting free energies, $f_\times^0(K, W)$ and $f_\times^*(K, W)$, respectively, which, although both independent of the details of the associated wall potentials, \tilde{W} , cannot be proved to be equal. Indeed, it was argued in Sect. 2.7 (of I), that complete independence of \tilde{W} *cannot* be expected in situations in which more than one thermodynamic phase might be present. Nevertheless, for ‘most’ interactions K , we expect the equality $f_\times^0 \equiv f_\times^*$, for reasonable \tilde{W} respecting the ferromagnetic character. This can in fact be proved on the basis of further assumptions which imply that only one phase can exist – specifically the decay of correlations with distance [6]. Indeed correlation decay assumptions enable one to deal with arbitrary boundary conditions and even to dispense with the restriction to ferromagnetic interactions. For the present, however, we refrain from invoking such comparatively strong assumptions; thus the distinction between subfree and superferromagnetic associated boundary conditions must be retained, and some of our results below will be restricted correspondingly.

As regards step (iii), the consideration of walls in domains of general shape, some progress was made in I since it was proved that the limiting wall free energy for box domains $\mathcal{A}_{\mathbf{L}, N}$ (defined explicitly in Sect. 4.2 of I) was unique and independent of the way in which the dimensions $\{L_\beta\}$, N_1 and N_2 became infinite. The full task, however, is taken up here in the following section (Sect. 6). First, we consider cylinders, $\Gamma_{\mathbf{L}, N}$, of general cross-section, \mathbf{L} , so that the faces of the corresponding walls have general shapes. Subject to appropriate restrictions on these shapes, analogous to those used in proving the shape-independence of the bulk thermodynamic limit [2], we establish in Theorems 6.2.1 and 6.2.2, the existence and uniqueness of the corresponding wall free energies. In the statement of these and other theorems we utilize the decomposition

$$f_\times(\Omega) = f_\times^+(\Omega) - f_\times^-(\Omega), \quad (5.3)$$

of the total surface free energy into positive terms, f_x^+ and f_x^- , associated with the positive and negative parts of the wall potentials (see Sect. 3.1); in all cases both f_x^+ and f_x^- separately achieve thermodynamic limits.

To allow for more general shapes of domain Ω , as well as of wall face \mathbf{L} , we introduce in Sect. 6.3, doubly conical domains, $\Delta_{\mathbf{L},N}$, or, for short, *cones*, and doubled frustrated cones, $\Xi_{\mathbf{L},N}$, or *frustrums* (see Fig. 10 below). A wide class of sequences of domains, $\{\Omega_k\}_{k \rightarrow \infty}$, can be filled efficiently with cones which becomes indefinitely large, and can be contained within minimal frustrums (satisfying modest conditions). On this basis, Theorems 6.5.1 and 6.5.2 establish the existence and uniqueness of the wall free energies for general domains.

The question of multiple walls cut in a domain Ω , step (iv) above, is addressed in Sect. 7. The desired results, however, are achieved only for wall potentials, W , which are subfree (although otherwise general): see Theorem 7.2. The crucial expression for the asymptotic behavior of the total surface free energy [step (v)], namely (5.1) above, is established for box (or parallelepiped) domains with, likewise, subfree wall potentials, in Theorem 7.3. Some observations concerning wall potentials which are truncated at a finite range R are present in Sect. 7.4. (Note it is not feasible to truncate the bulk interactions, as in [7, 8] since one must normalize by the boundary area rather than by the volume.)

Lastly, in Sect. 8, walls cut in a torus, Π , or *partial torus* or *tube*, Π^t , (with periodic boundary conditions imposed only for some directions) are discussed. Owing to the geometrical properties of a tube or torus the correlation inequality technique is not very effective: some limited results are embodied in Propositions 8.2.1 to 8.2.4. Specifically the free energy $f_x^{\Pi}(K, W)$, of a subfree wall defined on a sequence of tori is bounded above by $f_x^0(K, W)$ and below by $f_x^*(K, W)$. When $f_x^0 = f_x^*$, as generally expected, walls in a torus have the standard limiting free energy and, furthermore, Proposition 8.2.5 then shows that the total free energy of a torus satisfies (5.1) with $A_x \equiv 0$ (all α). As indicated above, more powerful results can be established on the basis of decay of correlation assumptions [6]. It is hoped to present these, and extensions to vector spins with two components [6], in a future publication.

The proofs of the various lemmas, propositions and theorems given below rely heavily on the techniques developed in I; likewise, we utilize in full the various definitions and basic inequalities on compound domains, Propositions 3.3.1 and 3.3.2, etc. presented in I. For this reason the present paper is written as a direct continuation of I. Thus Figs. 1 to 9, Sects. 0 to 4, and Eqs. (0.1) to (4.4.23) are to be found in I; only the references are numbered afresh here. In addition we have suppressed details of various proofs that follow closely analyses presented fully in I.

6. The Boundary Free Energy for General Domains

We are interested in establishing existence and uniqueness theorems for the boundary free energies defined on general sequences of domains Ω_k subject to free, and more general associated boundary conditions. In Sect. 2.2 we showed how a given d -dimensional lattice \mathcal{L} can be decomposed relative to a chosen lattice plane \mathcal{P} , into disjoint blocks $\mathbf{l} = (l_0, l_1, \dots, l_d)$ with $d' = d - 1$, which specify translations by

block vectors \mathbf{R}_l with components $\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_d$. Recall that blocks with $l_0=0$ lie adjacent to the wall on the \mathcal{L}_1 side of \mathcal{P} ; blocks with $l_0 = -1$ lie adjacent to the wall on the \mathcal{L}_2 side. The area of the wall, $|\mathbf{L}_1|$ or $|\mathbf{L}_2|$ with $|\mathbf{L}| \equiv \frac{1}{2}(|\mathbf{L}_1| + |\mathbf{L}_2|)$, is defined (see Sect. 2.2) as the number of blocks in $\Omega_1 \equiv \Omega \cap \mathcal{L}_1$ or $\Omega_2 \equiv \Omega \cap \mathcal{L}_2$ which are adjacent to the wall. In I we proved various theorems about box (or rectangular) domains, $A_{\mathbf{L}, N_1 + N_2}$, with cross-sectional area $|\mathbf{L}| = L_1 L_2 \dots L_d$, and length $N = N_1 + N_2$, where N_1 is the length in \mathcal{L}_1 and N_2 in \mathcal{L}_2 . Using the results for box domains, we will here show that a rather general class of shapes yield the same thermodynamic limit for the boundary free energy.

6.1. Thermodynamic Limit for Cylindrical Domains

As a first step in considering more general domain shapes, we generalize the notion of a box domain by relaxing the restriction that the blocks be assembled in a rectangular array. The cross-section \mathbf{L} relative to the plane \mathcal{P} is then allowed to assume a general d' -dimensional shape while the array still extends N_1 and N_2 blocks in the directions of \mathbf{b}_\perp and $-\mathbf{b}_\perp$ respectively. Thus we introduce:

Definition 6.1.1. A cylindrical domain $\Gamma_{\mathbf{L}, N} (\equiv \Gamma_{\mathbf{L}, N_1 + N_2}, N_1 + N_2 = N)$ of cross-sectional area $|\mathbf{L}|$ and length N is a set of $|\mathbf{L}|N$ blocks satisfying $0 < l_0 \leq N$, while labels l_β for $1 \leq \beta \leq d'$, are specified so that the set of cell vectors $\mathbf{R}_l = \sum_{\beta=1}^{d'} l_\beta \mathbf{b}_\beta$ consists of all cell corners of a connected d' -dimensional domain \mathbf{L} with origin $\mathbf{O}_\mathbf{L}$.

In taking the thermodynamic limit $\lim_{k \rightarrow \infty} \Gamma_k$, where $\Gamma_k \equiv \Gamma_{\mathbf{L}_k, N_k}$, the d' -dimensional cross-sections or faces, $\{\mathbf{L}_k\}$, must satisfy shape conditions of the sort required for d -dimensional domains (see Sect. 1.4) if the boundary free energy is to be unique. Such conditions will be listed explicitly below after we have established the essential inequalities for the partial boundary free energies of arbitrary domains. Consider first *subfree associated boundary conditions*. As a direct application of Proposition 3.3.1 (compare with the proof of Lemma 4.2.1) we have:

Lemma 6.1.1. *The partial boundary free energies $f_\times^\pm(\Gamma_{\mathbf{L}, N}) \equiv f_\times^\pm(\mathbf{L}; N_1, N_2)$ for cylinders with (a) subfree associated wall potentials [see (2.3.7), (2.4.5)] and (b) ferromagnetic bulk and wall potentials, K and W , satisfy the inequalities*

$$(i) (|\mathbf{L}'| + |\mathbf{L}''|) f_\times^\pm(\mathbf{L}' \cup \mathbf{L}'') \geq |\mathbf{L}'| f_\times^\pm(\mathbf{L}') + |\mathbf{L}''| f_\times^\pm(\mathbf{L}''), \tag{6.1.1}$$

where \mathbf{L}' and \mathbf{L}'' are disjoint cross-sections, and

$$(ii) f_\times^\pm(\mathbf{L}; N_1 + N'_1, N_2) \geq f_\times^\pm(\mathbf{L}; N_1, N_2), \\ f_\times^\pm(\mathbf{L}; N_1, N_2 + N'_2) \geq f_\times^\pm(\mathbf{L}; N_1, N_2). \tag{6.1.2}$$

The corresponding result for superferromagnetic associated wall potentials is:

Lemma 6.1.2. *The partial boundary free energies $f_\times^\pm(\Gamma_{\mathbf{L}, N}) \equiv f_\times^\pm(\mathbf{L}; N_1, N_2)$ for cylinders in saturating spin systems with (a) superferromagnetic associated boundary conditions satisfying $R^0 \geq \frac{1}{2} \max \{R^\infty, R^\times\}$ (see Proposition 3.3.2) and (b) fer-*

romagnetic bulk and wall potentials of finite range and finite degree p , satisfy

$$(i) (|\mathbf{L}'| + |\mathbf{L}''|)f_{\times}^{\pm}(\mathbf{L}' \cup \mathbf{L}'') \leq |\mathbf{L}'|f_{\times}^{\pm}(\mathbf{L}') + |\mathbf{L}''|f_{\times}^{\pm}(\mathbf{L}'') + c_0 P(\mathbf{L}', \mathbf{L}''), \tag{6.1.3}$$

where \mathbf{L}' and \mathbf{L}'' are disjoint and where $P(\mathbf{L}', \mathbf{L}'')$ is the block length of the common perimeter of \mathbf{L}' and \mathbf{L}'' along \mathcal{P} , i.e. the mean of the number of blocks in \mathbf{L}' adjacent to blocks in \mathbf{L}'' and vice versa; furthermore

$$(ii) f_{\times}^{\pm}(\mathbf{L}; N_1 + N'_1, N_2) \leq f_{\times}^{\pm}(\mathbf{L}; N_1, N_2),$$

$$f_{\times}^{\pm}(\mathbf{L}; N_1, N_2 + N'_2) \leq f_{\times}^{\pm}(\mathbf{L}; N_1, N_2). \tag{6.1.4}$$

Proof. With the obvious decomposition of $\Gamma_{\mathbf{L}, N}$, application of Proposition 3.3.2 yields

$$(|\mathbf{L}'| + |\mathbf{L}''|)f_{\times}^{\pm}(\mathbf{L}' \cup \mathbf{L}'') \leq |\mathbf{L}'|f_{\times}^{\pm}(\mathbf{L}') + |\mathbf{L}''|f_{\times}^{\pm}(\mathbf{L}'')$$

$$+ Y_1^{\pm}(\Gamma_{\mathbf{L}', N}, \Gamma_{\mathbf{L}'', N}) + Y_2^{\pm}(\Gamma_{\mathbf{L}', N}, \Gamma_{\mathbf{L}'', N}), \tag{6.1.5}$$

where Y_1^{\pm} and Y_2^{\pm} are given by (3.3.8) and (3.3.9). A bound on $|Y_1^{\pm}|$ is easily established by writing, with the notation of Fig. 6 (of I)

$$|Y_1^{\pm}| = \left| \frac{1}{2} \left(\sum_{\Gamma_1', \Gamma_1''} + \sum_{\Gamma_2', \Gamma_2''} \right) W_A^{\pm} \|s_A\| \right|$$

$$\leq c_1 P(\mathbf{L}', \mathbf{L}'') \sum_{B \in \llbracket B \rrbracket^1} |W_B^{\pm}| \|s\|^{|B|}$$

$$\leq c_1 P(\mathbf{L}'; \mathbf{L}'') \|W\|_1 = \bar{c}_1 P(\mathbf{L}', \mathbf{L}''). \tag{6.1.6}$$

Here $\llbracket B \rrbracket^1$ is the set of all collections $B \subseteq \mathcal{L}_1$ which are inequivalent under translations \mathbf{R}_l^1 , parallel to the wall, and the final step follows by condition **F(ii)**. Similarly we have

$$|Y_2^{\pm}| = \frac{1}{2} \sum_{A \in \Gamma^*} \Delta W_A^{\pm} \|s_A\| \leq \bar{c}_2 P(\mathbf{L}', \mathbf{L}''), \tag{6.1.7}$$

where Γ^* denotes the set of collections linking at least three of $\Gamma_1', \Gamma_2', \Gamma_1''$ and Γ_2'' while $\Delta W_A \equiv W_A - \tilde{W}_A$. This establishes (6.1.3) with $c_0 = \bar{c}_1 + \bar{c}_2$. The inequalities (6.1.4) follow directly from Proposition 3.3.2 as in the proof of Lemma 4.2.3. \square

We must now introduce shape conditions that will suffice to ensure the uniqueness of the boundary free energy. Although we are dealing with a lattice system of discrete sites, it will be helpful, in discussing the geometry, to use a language appropriate to a continuum. Accordingly, we associate with each site a unit volume (so that a cell has a volume q), and the *volume of a domain* Ω is then $V(\Omega) = |\Omega|$ (see Sect. 1.1). With no loss of generality we will also suppose that the Euclidean space within which the lattice \mathcal{L} resides has been subjected to an affine transformation so that the block edge vectors $\mathbf{b}_0, \mathbf{b}_1, \dots, \mathbf{b}_d$ have become mutually orthogonal vectors of unit length $|\mathbf{b}_\beta| = 1$. Then each block is a *cube* and larger cubes may be assembled from blocks. Following [2], we now introduce the surface volume of a general domain through:

Definition 6.1.2. The *surface volume* $V_\sigma(h; \Omega)$ is the number of sites which lie within a distance h of any boundary site of Ω and which are in Ω if $h > 0$ but outside Ω if $h < 0$. (Recall, from Sect. 1.1, that the boundary $\partial\Omega$ consists of all sites in Ω which belong to cells which either contain, or are adjacent to cells containing sites not in Ω ; furthermore Ω is always supposed to be cell-connected.)

It is then convenient, again after [2], to describe the shape of a large domain via :

Definition 6.1.3. The *shape function* $\sigma(\alpha, \Omega)$ is the fraction of the volume within a distance $h = \alpha[V(\Omega)]^{1/d}$ of $\partial\Omega$, explicitly,

$$\sigma(h/H; \Omega) = V_\sigma(h; \Omega)/V(\Omega) \quad \text{with} \quad H^d = V(\Omega). \tag{6.1.8}$$

In taking the thermodynamic limit through a sequence of domains, $\{\Omega_k\}_{k \rightarrow \infty}$, we will finally require :

J. *Asymptotic shape regularity*

(i) Given $\{\Omega_k\}$ with $|\Omega_k| \rightarrow \infty$ as $k \rightarrow \infty$, there exists a fixed α' and a shape function $\sigma_0(\alpha) \rightarrow 0$ as $|\alpha| \rightarrow 0$, such that for all $k = 1, 2, 3 \dots$ and $\alpha \leq \alpha'$ we have

$$\sigma(\alpha; \Omega_k) \leq \sigma_0(\alpha). \tag{6.1.9}$$

(ii) If A_k^* is the smallest box domain containing Ω_k , then there is a $\delta > 0$ such that

$$V(\Omega_k)/V(A_k^*) \geq \delta, \quad \text{all } k. \tag{6.1.10}$$

The first condition merely ensures a vanishing surface-to-volume ratio in the limit $k \rightarrow \infty$. The second condition is not best possible but suffices for all practical purposes; it rules out certain filamentary domains that fail to fill out some d -dimensional volume. These conditions are modeled closely on Fisher's analysis [2] for particle systems and we may use his various packing lemmas, namely :

Lemma 6.1.3. *If a domain Ω is maximally filled with disjoint cubes A of side l (blocks along an edge) which are entirely contained in Ω , then the volume, $\Delta V^+(\Omega)$, remaining is less than $V_\sigma(d^{1/2}l; \Omega)$.*

Lemma 6.1.4. *If a domain Ω is contained in a cube A_0 , the difference domain $A_0 \setminus \Omega$ may be filled with cubes A of edge l in such a way that the unfilled volume, $\Delta V^-(\Omega)$, adjacent to Ω is less than $V_\sigma(-d^{1/2}l; \Omega)$.*

Lemma 6.1.5. *With no loss in generality the smallest box A_k^* in **J(ii)** may be taken to be a cube.*

Now if $\{\mathbf{L}_k\}$ is the sequence (of pairs) of plane wall faces corresponding to $\{\Omega_k\}$ and a given plane \mathcal{P} , it is clear that to discuss the limiting wall free energy and to control the edge free energies associated with the wall perimeters $\partial\mathbf{L}_k$, one requires appropriate shape restrictions on the domains \mathbf{L}_k , which may be regarded as $d' = (d - 1)$ -dimensional. We may, in fact, utilize precisely the same Conditions **J**

but in one lower dimension. Thus, we replace Ω by \mathbf{L} , d by d' , δ by δ' , d -dimensional cubes by *square plaques* of thickness one block, and $V(\Omega)$ and $V_\sigma(h; \Omega)$ by $A(\mathbf{L}) = |\mathbf{L}|$ and $A_\sigma(h; \mathbf{L})$, respectively, where A_σ is defined in appropriate analogy to Definition 6.1.2. With this understanding we will suppose that both sequences $\{\mathbf{L}_k\}$ and $\{\Omega_k\}$ satisfy **J**. We may now state and prove the simplest theorem for cylinder domains.

Theorem 6.1.1. *Cylinders with free associated wall potentials. Let $\{\Gamma_k\} = \{\Gamma_{\mathbf{L}_k; N_{1k}, N_{2k}}\}$ be a sequence of cylindrical domains with wall faces $\{\mathbf{L}_k\}$, both sequences satisfying the shape Conditions **J** as $k, N_{1k}, N_{2k} \rightarrow \infty$. If the $\{\Gamma_k\}$ are subject to (a) free associated wall potentials, $\tilde{W} \equiv 0$, and (b) ferromagnetic bulk and wall potentials, K and W , which satisfy the defining Conditions **D** and **E** (Sects. 2.2 and 2.3) and the boundedness Conditions **A** and **F** (Sects. 1.4 and 2.3), then the boundary free energies verify*

$$\lim_{k \rightarrow \infty} f_\times(\mathbf{K}, W, \tilde{W} \equiv 0; \Gamma_k) = f_\times^0(\mathbf{K}, W), \tag{6.1.11}$$

where $f_\times^0(\mathbf{K}, W)$ is the standard boundary free energy for box domains with free associated boundary conditions as defined in Theorem 4.4.1, and similarly for the partial boundary free energies.

Proof. We present only a sketch of the proof, as the method involves a maximal filling of the d' -dimensional region \mathbf{L}_k with square plaques of side l , in direct analogy with Fisher's proof of the shape independence of the bulk free energy [2]. On each plaque of side l , we may construct a box domain $A_{l,k} = A(l^{d'}, N_{1k}, N_{2k})$, and the union of these box domains forms the filling cylinder $\Gamma'_k = \Gamma_{\mathbf{L}_k; N_{1k}, N_{2k}} \subset \Gamma_k$. The cylinder domains $\Gamma_k, \Gamma'_k, \Delta_k = \Gamma_k \setminus \Gamma'_k$, and $A_{l,k}$ satisfy the conditions of Lemma 6.1.1. Hence, if we consider corresponding systems with the specified bulk and wall potentials, K and W , and free associated walls, $\tilde{W} \equiv 0$, we have the inequality

$$|\mathbf{L}_k| f_\times^\pm(\Gamma_k) \geq |\mathbf{L}'_k| f_\times^\pm(\Gamma'_k) + |\mathbf{L}_k \setminus \mathbf{L}'_k| f_\times^\pm(\Delta_k), \tag{6.1.12}$$

for the partial boundary free energies. The last term is non-negative, so that discarding it preserves the inequality, which, with $A(\mathbf{L}_k) = |\mathbf{L}_k|$, etc., we can write as

$$f_\times^\pm(\Gamma_k) \geq [A(\mathbf{L}'_k)/A(\mathbf{L}_k)] f_\times^\pm(\Gamma'_k). \tag{6.1.13}$$

Since Γ'_k consists of box domains $A_{l,k}$, we can apply Lemma 6.1.3 and, again, Lemma 6.1.1 repeatedly to obtain

$$f_\times^\pm(\Gamma_k) \geq R_{l,k} f_\times^\pm(\Gamma'_k) \geq R_{l,k} f_\times^\pm(A_{l,k}), \tag{6.1.14}$$

where the face filling ratio is

$$R_{l,k} = 1 - A_\sigma(d'^{1/2}l; \mathbf{L}_k)/A(\mathbf{L}_k). \tag{6.1.15}$$

On taking the limit $k \rightarrow \infty$ at fixed l , we see from **J(i)** (in d' dimensions) that $R_{l,k} \rightarrow 1$. Thus, on following this with the limit $l \rightarrow \infty$ we obtain, through Theorem 4.4.1, a lower bound

$$\liminf_{k \rightarrow \infty} f_\times^\pm(\Gamma_k) \geq f_\times^{0\pm}(\mathbf{K}, W). \tag{6.1.16}$$

To obtain the complementary inequality, let $A_k^* \equiv A(\mathbf{L}_k^*; N_{1k}, N_{2k})$ be the smallest box domain containing Γ_k . By Lemma 6.1.5, we may assume that its face \mathbf{L}_k^* is a square plaque. Applying Lemma 6.1.1 to the domains A_k^* , Γ_k , and $A_k^* = A_k^* \setminus \Gamma_k$, we find

$$f_{\times}^{\pm}(\Gamma_k) \leq \frac{A(\mathbf{L}_k^*)}{A(\mathbf{L}_k)} f_{\times}^{\pm}(A_k^*) - \frac{A(\mathbf{L}_k^* \setminus \mathbf{L}_k)}{A(\mathbf{L}_k)} f_{\times}^{\pm}(A_k^*). \tag{6.1.17}$$

Now we may fill A_k^* with the standard box domains $A_{l,k}$ to obtain

$$f_{\times}^{\pm}(A_k^*) \geq \frac{A(\mathbf{L}_k^* \setminus \mathbf{L}_k) - A_{\sigma}(-d^{l/2}l; \mathbf{L}_k)}{A(\mathbf{L}_k^* \setminus \mathbf{L}_k)} f_{\times}^{\pm}(A_{l,k}). \tag{6.1.18}$$

Then we may rewrite (6.1.17) as

$$\begin{aligned} f_{\times}^{\pm}(\Gamma_k) &\leq f_{\times}^{\pm}(A_k^*) + \frac{A(\mathbf{L}_k^* \setminus \mathbf{L}_k)}{A(\mathbf{L}_k)} [f_{\times}^{\pm}(A_k^*) - f_{\times}^{\pm}(A_k^*)], \\ &\leq f_{\times}^{\pm}(A_k^*) + \frac{1 - \delta'}{\delta'} [f_{\times}^{\pm}(A_k^*) - f_{\times}^{\pm}(A_{l,k})] \\ &\quad + [A_{\sigma}(-d^{l/2}l; \mathbf{L}_k)/A(\mathbf{L}_k)] f_{\times}^{\pm}(A_{l,k}), \end{aligned} \tag{6.1.19}$$

where condition **J(ii)** has been used to bound $A(\mathbf{L}_k^* \setminus \mathbf{L}_k)/A(\mathbf{L}_k)$. Now we may take $k \rightarrow \infty$ at fixed l , whereupon the last term on the second line vanishes by **J(i)** and $f_{\times}^{\pm}(A_k^*) \rightarrow f_{\times}^0(K, W)$ while $f_{\times}^{\pm}(A_{l,k}) \rightarrow f_{\times}^{\pm}(A_{l,\infty})$. Finally on taking $l \rightarrow \infty$ we have, by Theorem 4.4.1, $f_{\times}^{\pm}(A_{l,\infty}) \rightarrow f_{\times}^0(K, W)$ so that

$$\limsup_{k \rightarrow \infty} f_{\times}^{\pm}(\Gamma_k) \leq f_{\times}^0(K, W), \tag{6.1.20}$$

which, with (6.1.16) proves the theorem. \square

The corresponding result for systems with superferromagnetic conditions on the associated walls is:

Theorem 6.1.2. *Cylinders with simple superferromagnetic associated potentials. Let $\{\Gamma_k\}$ be a sequence of cylindrical domains with wall faces $\{\mathbf{L}_k\}$ as in Theorem 6.1.1. For a system of saturating spins of modulus $\|s\|$ and ferromagnetic bulk and wall potentials of finite ranges, R^{∞} and R^{\times} , respectively, of finite degree p , and subject to simple ferromagnetic boundary conditions, \tilde{W}^* [see Sect. 2.3], of range R^0 , the boundary free energy verifies*

$$\lim_{k \rightarrow \infty} f_{\times}(K, W, \tilde{W}^*; \Gamma_k) = f_{\times}^*(K, W), \tag{6.1.21}$$

where $f_{\times}^*(K, W)$ is the limiting boundary free energy for box domains with simple superferromagnetic associated wall conditions [see Theorem 4.4.3], and similarly for the partial boundary free energies.

Proof. We will not present the details since they follow closely those of Theorem 6.1.1. However, allowance must be made for the common perimeter term, $c_0 P(\mathbf{L}', \mathbf{L}'')$, which enters the basic inequality in Lemma 6.1.2. The resulting

contributions to the boundary free energy inequalities, however, vary as $|\partial\mathbf{L}_k|/|\mathbf{L}_k|$ which vanishes as $k \rightarrow \infty$ by **J(i)**, or, for the wall faces of the standard boxes $A_{l,k}$, as $1/l$ which vanishes when one finally takes $l \rightarrow \infty$. \square

6.2. Uniqueness for Cylindrical Domains

Having established the thermodynamic limit of the boundary free energy for cylinders of general cross-section but subject only to free (or simple superferromagnetic) associated wall potentials we now consider more general boundary conditions. As for box domains, it is fairly straightforward to prove that cylinders with subfree associated boundary conditions satisfying the tempering Condition C_τ have the same limiting boundary free energy as those with free associated walls; the analogous result holds also for general superferromagnetic associated conditions. Specifically we have:

Theorem 6.2.1. *Cylinders with subfree associated walls. For a sequence of cylinders, $\{\Gamma_{\mathbf{L}_k, N_{1k}, N_{2k}}\}$ with ferromagnetic bulk and wall potentials satisfying the conditions of Theorem 6.1.1 and with subfree associated wall potentials \tilde{W} which satisfy the tempering condition C_τ [Sect. 1.4] with $\tau > 0$, the limiting boundary free energy and partial boundary free energies, as k, N_{1k} and N_{2k} approach ∞ in any way, exist and are equal to $f_\times^0(K, W)$, and $f_\times^{0\pm}(K, W)$, respectively [Theorem 4.4.1].*

Proof. Aside from geometric considerations, the proof is essentially the same as in Theorem 4.4.2 for box domains; hence we discuss only those points arising from the geometric aspects. We compare the partial boundary free energies, $f_\times^\pm(K, W, \tilde{W}; \Gamma_{\mathbf{L}, N_1, N_2})$, with those of the corresponding cylinder with free associated walls. As in the case of box domains, we immediately have

$$\limsup_{k \rightarrow \infty} f_\times^\pm(K, W, \tilde{W}; \Gamma_k) \leq f_\times^{0\pm}(K, W). \tag{6.2.1}$$

Corresponding to the reduced box domains, $A' = A_{\mathbf{L}', N'_1, N'_2}$, we now define the reduced cylinders, $\Gamma' = \Gamma_{\mathbf{L}', N'_1, N'_2}$, where

$$N'_1 + R \leq N_1 \quad \text{and} \quad N'_2 + R \leq N_2, \tag{6.2.2}$$

and $\mathbf{L}' \subset \mathbf{L}$ is the maximal face such that

$$d(i, \partial\mathbf{L}) > R, \quad \text{for} \quad i \in \mathbf{L}'. \tag{6.2.3}$$

Note that for $i \in \mathbf{L} \setminus \mathbf{L}'$ one has $d(i, \partial\mathbf{L}) \leq R$ so that $|\mathbf{L} \setminus \mathbf{L}'| = A_\sigma(R, \Gamma)$ and $|\mathbf{L}'|/|\mathbf{L}| = 1 - A_\sigma(R, \Gamma)/A(\Gamma)$. For associated boundary potentials \tilde{W} of finite range, $\tilde{R}^\times < R$, we have

$$f_\times^\pm(K, W, \tilde{W}, \Gamma) \geq (|\mathbf{L}'|/|\mathbf{L}|) f_\times^\pm(K, W, \tilde{W} = 0, \Gamma'), \tag{6.2.4}$$

so that **J(i)** implies $|\mathbf{L}'|/|\mathbf{L}| \rightarrow 1$ as $k \rightarrow \infty$ and we again obtain the complementary inequality to (6.2.1), which proves the theorem.

As regards associated potentials of infinite range the remainder of the proof of Theorem 4.4.2 applies, mutatis mutandi, for cylinders. If $f_\times^\dagger(\Gamma)$ denotes the boundary free energy with the associated wall potentials truncated to $\Gamma \setminus \Gamma'$ the

final estimate obtained with the aid of Lemma 4.4.1 and Condition C_τ is

$$|f_x^\dagger(\Gamma) - f_x(\Gamma)| \leq \frac{|\Gamma|C}{|\mathbf{L}|R^\tau} = \frac{C(N'_1 + N'_2)}{R^\tau} \frac{|\mathbf{L}'|}{|\mathbf{L}|}. \tag{6.2.5}$$

Taking the limits $\mathbf{L}, N_1, N_2 \rightarrow \infty$, so that $|\mathbf{L}'|/|\mathbf{L}| \rightarrow 1$, followed by $R \rightarrow \infty$ yields $|f_x^\dagger - f_x| \rightarrow 0$ for all N'_1 and N'_2 . Letting $N'_1, N'_2 \rightarrow \infty$ proves

$$\liminf_{k \rightarrow \infty} f_x^\pm(K, W, \tilde{W}, \Gamma_k) \geq f_x^{0\pm}(K, W) \tag{6.2.6}$$

and completes the theorem. \square

Likewise, in close analogy to Theorem 4.4.4 we have:

Theorem 6.2.2. *Cylinders with superferromagnetic associated walls. For a sequence of cylinders $\{\Gamma_{\mathbf{L}k, N_{1k}, N_{2k}}\}$ with ferromagnetic bulk and wall potentials satisfying the conditions of Theorem 6.1.2 with saturating spins and superferromagnetic associated wall potentials \tilde{W} [see Sect. 2.3] of finite range \tilde{R}^* , the limiting boundary free energy and partial boundary free energies, as $k, N_{1k}, N_{2k} \rightarrow \infty$, in any way, exists and are equal to $f_x^*(K, W)$ and $f_x^{*\pm}(K, W)$, respectively [Theorem 4.4.3].*

Proof. Except for geometrical considerations, the proof is the same as for Theorem 4.4.4. Specifically the shape Condition **J** is used to show $|\mathbf{L}'|/|\mathbf{L}| \rightarrow 1$, $|\mathbf{L}|\mathbf{L}' \rightarrow 0$, and $|\partial\mathbf{L}'|/|\mathbf{L}| \rightarrow 0$ as $k, N_{1k}, N_{2k} \rightarrow \infty$ where \mathbf{L}' is the face of an appropriate reduced cylinder. \square

6.3. Cones and Frustrums with Subfree Conditions

In pursuit of our desire to establish the existence and uniqueness of the boundary free energy for walls in a large class of domains we now introduce two further auxiliary types of domains, namely, *cones* and *frustrums* (actually doubled cones and doubled frustrated cones, see Fig. 10). The results for these domains parallel those for boxes and for cylinders, so that attention will be focussed on the geometrical considerations. Our result allowing greatest generality of shape will be stated in terms of cones and frustrums.

In defining these domains it will be convenient to extend the continuum language somewhat: For appropriate Ω in \mathcal{L} we define $\tilde{\Omega} \subset \mathbb{R}^d$ as the continuum domain which is a compact, simply connected subset of \mathbb{R}^d consisting of the continuum cells of Ω . With a face \mathbf{L} formed of one layer of blocks on a wall plane \mathcal{P} , we associate in the same way, a continuum set $\tilde{\mathbf{L}} \subset \mathbb{R}^d$ on the plane \mathcal{P} . As before, $\xi^d \tilde{\Omega}$ and $\xi^{d'} \tilde{\mathbf{L}}$ will denote isotropic expansions by linear factors ξ of $\tilde{\Omega}$ and $\tilde{\mathbf{L}}$ in \mathbb{R}^d and $\mathbb{R}^{d'}$ respectively, but we will explicitly assume that the origin of the expansion lies in $\tilde{\Omega}$ (or $\tilde{\mathbf{L}}$) so that $\xi^d \tilde{\Omega} \supset \tilde{\Omega}$ and $\xi^{d'} \tilde{\mathbf{L}} \supset \tilde{\mathbf{L}}$ for $\xi > 1$. Recall also that $\Omega + \mathbf{R}, \tilde{\mathbf{L}} + \mathbf{R}$, etc. denote translations of $\Omega, \tilde{\mathbf{L}}$, etc. by a vector \mathbf{R} . Then, as illustrated in Fig. 10, we introduce formally:

Definition 6.3.1. A doubly conical domain or cone, $\Delta = \Delta_{\mathbf{L}, N}(v)$, is the set of blocks with cell corners contained in the two continuum cones $\tilde{\Delta}_1$ and $\tilde{\Delta}_2$ formed with base $\tilde{\mathbf{L}}$ on \mathcal{P} and vertices $v_1 = v + N\mathbf{b}_0$ and $v_2 = v - N\mathbf{b}_0$, respectively, where v is a point in $\tilde{\mathbf{L}}$.

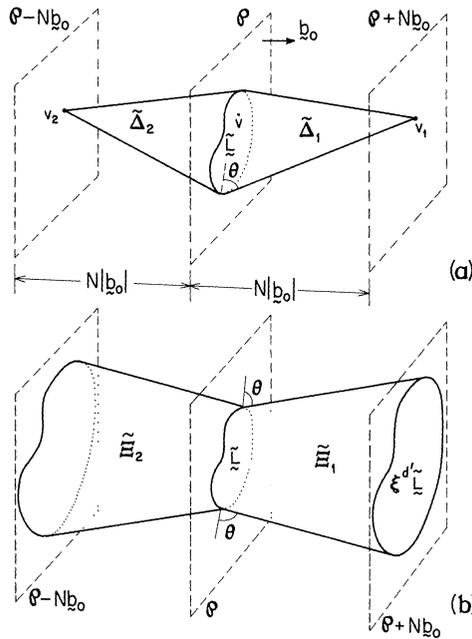


Fig. 10a and b. Illustrating (a) a doubly conical domain or *cone*, $\Delta_{L,N}(v)$, and (b) a doubled frustrated conical domain or *frustrum*, $\Xi_{L,N}(\xi)$, with base L on a plane \mathcal{P} . The cone vertices v_1 and v_2 are translates of v through $\pm N\mathbf{b}_0$; the frustrum expansion factor is $\xi > 1$; the contact angles are θ

Definition 6.3.2. A *doubled frustrated conical domain* or *frustrum* $\Xi \equiv \Xi_{L,N}(\xi)$, is the set of blocks with cell corners contained in the two continuum frustrums $\tilde{\Xi}_1$ and $\tilde{\Xi}_2$ formed with top \tilde{L} on \mathcal{P} and bases $\xi^d \tilde{L}$ on $\mathcal{P} + N\mathbf{b}_0$ and $\mathcal{P} - N\mathbf{b}_0$, respectively, with $\xi > 1$.

Remark 6.3.1. We could readily consider nonsymmetric cones with vertices v_1 and v_2 in $\tilde{L} + N_1\mathbf{b}_0$ and $\tilde{L} - N_2\mathbf{b}_0$ and, similarly, more general frustrums with bases not simple expansions of \tilde{L} . However, such domains will be covered by the theorem to be proved for general shapes.

Remark 6.3.2. It is clear from the definitions and Fig. 10, that the *contact angles*, θ , between the sides of frustrum (or a cone) and the wall-defining planes \mathcal{P} , are bounded by 0 and $\frac{1}{2}\pi$. In an infinite sequence of frustrums, $\{\Xi_k\}$, however, the limits $\theta=0$ may be approached indefinitely closely. In such circumstances the situation of the walls becomes pathological and the integrity condition **H** [of Sect. 2.4] is violated. To avoid this, we will consider only sequences $\{\Xi_k\}$ for which ξ_k is uniformly bounded above: then condition **H** is satisfied. Weaker conditions, such as $\xi_k \leq \xi_0 N_k$, might be contemplated but the proof of boundedness (Proposition 3.2.2) and other proofs would pose further difficulties and might demand stronger restrictions on the decay of interactions needed to ensure a finite wall free energy.

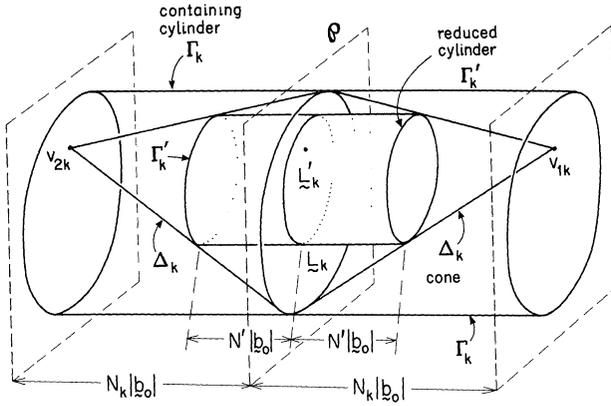


Fig. 11. Illustration of a cone, $\Delta_k = \Delta_{\mathbf{L}_k, N_k}$, contained in a cylinder, $\Gamma_k = \Gamma_{\mathbf{L}_k, N_k, N_k}$, on the same base \mathbf{L}_k and containing a reduced cylinder $\Gamma'_k = \Gamma_{\mathbf{L}'_k, N', N'}$ of maximal base \mathbf{L}'_k

Proposition 6.3.1. *Subfree cones. Let $\{\Delta_k\} \equiv \{\Delta_{\mathbf{L}_k, N_k}(v_k)\}$ be a sequence of cones with faces $\{\mathbf{L}_k\}$ satisfying the shape Conditions **J**, as $k, N_k \rightarrow \infty$, and subject to subfree associated boundary conditions, \tilde{W} , satisfying the tempering condition **C $_{\tau}$** with $\tau > 0$, and ferromagnetic bulk and wall potentials, K and W , satisfying the conditions of Theorem 6.1.1. Then the boundary free energies of the cones satisfy*

$$\lim_{k \rightarrow \infty} f_{\times}(K, W, \tilde{W}; \Delta_k) = f_{\times}^0(K, W). \tag{6.3.1}$$

and similarly for the partial boundary free energies.

Proof. The first step is simply to note (see Fig. 11) that the cone $\Delta_{\mathbf{L}, N}$ is contained within the cylinder, $\Gamma_{\mathbf{L}, N, N}$ on the same base. Application of Proposition 3.3.1 and Theorem 6.1.1 for free boundary conditions then yields

$$\limsup_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Delta_k) \leq f_{\times}^0(K, W). \tag{6.3.2}$$

To prove the complementary inequality consider (see Fig. 11) a reduced cylinder $\Gamma'_k \equiv \Gamma_{\mathbf{L}'_k, N', N'}$ contained in the cone Δ_k , and hence with $N' \leq N_k$, whose base, \mathbf{L}'_k , is of maximal area (for fixed N'). If Γ'_k is subject to the same potentials as Δ_k (i.e., $K_A^{\Gamma'_k} \equiv K_A^{\Delta_k}$ for all $A \in \Gamma'_k$) then by Proposition 3.3.1 we have

$$f_{\times}^{\pm}(K, W, \tilde{W}; \Delta_k) \geq (|\mathbf{L}'_k|/|\mathbf{L}_k|) f_{\times}^{\pm}(K, W, \tilde{W}; \Gamma'_k). \tag{6.3.3}$$

Furthermore, the potentials acting on Γ'_k satisfy the subfree conditions of Theorem 6.2.1; specifically it is easy to check that the potentials restricted to Γ'_k still verify **C $_{\tau}$** with $\tau > 0$.

Now by the geometry of a cone we have, as $k \rightarrow \infty$,

$$\frac{|\mathbf{L}'_k|}{|\mathbf{L}_k|} = \left(\frac{N_k - N'}{N_k}\right)^{d'} \left\{ 1 + O\left(\frac{|\partial \mathbf{L}'_k|}{|\mathbf{L}'_k|}\right) \right\}, \tag{6.3.4}$$

where the correction term arises from the discrete block structure. We may now take the limit $k \rightarrow \infty$ at fixed N' which yields $|\mathbf{L}'_k|/|\mathbf{L}_k| \rightarrow 1$. Then Theorem 6.2.1 and the limit $N' \rightarrow \infty$ yield

$$\liminf_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Delta_k) \geq f^{0\pm}(K, W), \tag{6.3.5}$$

which establishes the theorem. \square

Remark 6.3.3. The proof of Proposition 6.3.1 applies equally to a domain Ω_k which is the union of a disjoint set of m conical domains $\Delta_k^{(j)}$ with bases $\mathbf{L}_k^{(j)}$ on the same plane \mathcal{P} , provided each cone satisfies the conditions stated. We may further allow the total number, m_k , of such cones to vary with k and even approach infinity, provided, to state a clearly sufficient condition, each cone $\Delta_k^{(j)}$ is, up to a translation, drawn from a finite set of standard sequences of cones $\{\tilde{\Delta}_k^{(\alpha)}\}_{\alpha=1, \dots, n}$ separately satisfying the conditions of the proposition.

Remark 6.3.4. For the following proof for frustrums it is important to observe that Proposition 6.3.1 applies with an essentially identical proof to *complementary conical domains*, $\Theta_{\mathbf{L}, N}(\xi)$, defined via:

Definition 6.3.3. A *complementary conical domain* or *comcone*, $\Theta = \Theta_{\mathbf{L}, N}(\xi)$, is the set of blocks contained in the cylinder $\Gamma_{\xi^{d'} \mathbf{L}, N, N}$ but which are not in the corresponding frustrum $\Xi_{\mathbf{L}, N}(\xi)$, i.e., $\Theta_{\mathbf{L}, N}(\xi) = \Gamma_{\xi^{d'} \mathbf{L}, N, N} \setminus \Xi_{\mathbf{L}, N}(\xi)$. Note that for $d=2$ a comcone is, in general, a disconnected domain (of two triangles).

Now we can establish:

Proposition 6.3.2. *Subfree frustrums.* Let $\{\Xi_k\} \equiv \{\Xi_{\mathbf{L}_k, N_k}(\xi_k)\}$ be a sequence of frustrums satisfying $\xi_k \leq \xi_0$ (all k) and the shape Condition **J** as $k, N_k \rightarrow \infty$, and subject to subfree associated wall potentials, \tilde{W} , and ferromagnetic bulk and wall potentials, K and W , satisfying the conditions of Proposition 6.3.1. Then the limiting, full and partial boundary free energies exist and are equal to $f^0(K, W)$ and $f^{0\pm}(K, W)$, respectively.

Proof. As in the proof of Proposition 6.3.1, we note that Ξ_k contains a cylinder $\Gamma_k = \Gamma_{\mathbf{L}_k, N_k, N_k}$, on which the same potentials may be imposed as on Ξ_k (i.e., $K_A^{\Gamma} \equiv K_A^{\Xi}$ for all $A \in \Xi$). The subfree conditions of Theorem 6.2.1 then apply and we conclude

$$\liminf_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Xi_k) \geq f_{\times}^{0\pm}(K, W). \tag{6.3.6}$$

To obtain the opposite inequality, consider the expanded cylinder $\Gamma_k^+ \equiv \Gamma_{\xi_k^{d'} \mathbf{L}_k, N_k, N_k}$ with free associated boundary conditions, which can be decomposed into the frustrum Ξ_k , with the given subfree associated conditions, and the comcone $\Theta_k \equiv \Theta_{\mathbf{L}_k, N_k}(\xi_k)$, with free associated conditions. Application of Proposition 3.3.1 then yields

$$|\xi_k^{d'} \mathbf{L}_k| f_{\times}^{\pm}(\Gamma_k^+) \geq |\mathbf{L}_k| f_{\times}^{\pm}(\Xi_k) + |\xi_k^{d'} \mathbf{L}_k \setminus \mathbf{L}_k| f_{\times}^{\pm}(\Theta_k), \tag{6.3.7}$$

or, on rewriting and decomposing $|\xi^{d'} \mathbf{L} \setminus \mathbf{L}|$,

$$f_{\times}^{\pm}(\Xi) \leq f_{\times}^{\pm}(\Gamma^+) - X(\xi, \mathbf{L}) [f_{\times}^{\pm}(\Theta) - f_{\times}^{\pm}(\Gamma^+)], \tag{6.3.8}$$

where the subscripts k have been dropped for simplicity, and

$$X(\xi, \mathbf{L}) = |\xi^{d'} \mathbf{L}| / |\mathbf{L}| - 1 \leq \xi^{d'}. \tag{6.3.9}$$

Since, by hypothesis, $\xi_k^{d'}$ is uniformly bounded, we may take the limit $k \rightarrow \infty$ and use Theorem 6.1.1 and Proposition 6.3.1 with Remark 6.3.4 to conclude

$$\limsup_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Xi_k) \leq f_{\times}^{0 \pm}(K, W), \tag{6.3.10}$$

which proves the theorem. \square

6.4. Superferromagnetic Conditions on Cones and Frustrums

The propositions for cones and frustrums may be extended fairly straightforwardly to cover superferromagnetic associated boundary conditions when the interactions are of finite range. For completeness we state the results and indicate the proofs.

Proposition 6.4.1. *Superferromagnetic cones.* Let $\{\Delta_k\} = \{\Delta_{\mathbf{L}_k, N_k}(v_k)\}$ be a sequence of cones as in Proposition 6.3.1, subject to superferromagnetic associated boundary conditions with potentials \tilde{W} of finite range \tilde{R}^* , and ferromagnetic bulk and wall potentials, K and W , satisfying the conditions of Theorem 6.1.2. Then the limiting boundary free energy and partial free energies exist and are equal to $f_{\times}^*(K, W)$ and $f_{\times}^{*\pm}(K, W)$, respectively [Theorem 4.4.3].

Proof. As for subfree conditions, we first compare the cone $\Delta_{\mathbf{L}, N}$ with the containing cylinder $\Gamma_{\mathbf{L}, N, N}$. If we set $\Omega'' \equiv \Gamma \setminus \Delta$ and subject all three domains to superferromagnetic associated boundary conditions we can use Proposition 3.3.2 to conclude

$$|\mathbf{L}| f_{\times}^{\pm}(\tilde{W}, \Gamma) \leq |\mathbf{L}| f_{\times}^{\pm}(\tilde{W}, \Delta) + \frac{1}{2} \left(\sum_{\Delta_1, \Omega_1''} + \sum_{\Delta_2, \Omega_2''} \right) W_A^{\pm} \|s_A\| + \frac{1}{2} \sum^* \Delta W_A^{\pm} \|s_A\|, \tag{6.4.1}$$

where $\Delta W_A^{\pm} \equiv W_A^{\pm} - \tilde{W}_A^{\pm}$ and $\Delta_1 = \Delta \cap \mathcal{L}_1$, etc. [see Sect. 2.2] while \sum^* indicates a sum over collections linking at least three of $\Delta_1, \Delta_2, \Omega_1'', \Omega_2''$. Since, by the conditions of Theorem 6.1.2, the potentials are of finite range and degree, the last two terms in (6.4.1) can be bounded by $c_1 |\partial \mathbf{L}| + c_2$ for suitable constants. In taking the thermodynamic limit, subject to the shape Condition **J**, we have $|\partial \mathbf{L}| / |\mathbf{L}| \rightarrow 0$ and hence

$$\liminf_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Delta_k) \geq f_{\times}^{*\pm}(K, W). \tag{6.4.2}$$

Now, as in Proposition 6.3.1, consider the reduced cylinder $\Gamma'_k \equiv \Gamma_{\mathbf{L}_k, N', N'}$ maximally contained in Δ_k , and subject to superferromagnetic associated conditions consistent with those in Δ_k (in the sense of Proposition 3.3.2). A further application of Proposition 3.3.2 and use of the finite range and degree conditions and Theorem 6.1.2, yields the complementary inequality and completes the proof. \square

Proposition 6.4.2. *Superferromagnetic frustrums.* Let $\{\Xi_k\} \equiv \{\Xi_{\mathbf{L}_k, N_k}(\xi_k)\}$ be a sequence of frustrums satisfying $\xi_k \leq \xi_0$ (all k) and the shape Condition **J** as $k, N_k \rightarrow \infty$,

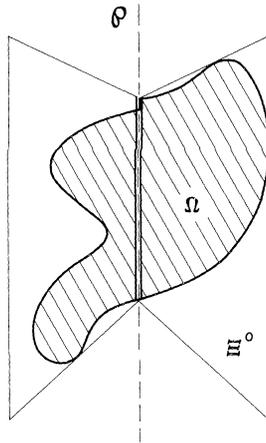


Fig. 12. A minimal frustrum, Ξ^0 , enclosing a general, ($d=2$)-dimensional domain, Ω , intersected by a plane \mathcal{P}

and subject to superferromagnetic wall conditions, W , of finite range \tilde{R}^\times . If the remaining conditions of Theorem 6.1.2 are satisfied the limiting boundary free energy and partial boundary free energies exist and are equal to $f_\times^*(K, W)$, respectively.

Proof. Following the proof of Proposition 6.3.2 the frustrum Ξ_k is compared with the inscribed cylinder $\Gamma_k = \Gamma_{\mathbf{L}_k, N_k, N_k}$ and with the expanded, escribed cylinder $\Gamma_k^+ \equiv \Gamma_{\xi_k^d \mathbf{L}_k, N_k, N_k}$. Use of Proposition 3.3.2 and Theorem 6.1.2 as in the proof for cones yields the required upper and lower bounds. \square

6.5. General Domains

We may now use the propositions established to prove the existence and uniqueness of the boundary free energy, $f_\times(K, W)$, for a rather general sequence of domains – essentially for all domains that can be contained within a limiting sequence of frustrums and be filled, sufficiently well, by a sequence of sets of cones. The shape conditions we will utilise are certainly not as weak as possible: however, they encompass a wide range of possibilities and relaxation of the conditions allows counterexamples to uniqueness to be constructed (see e.g. Remark 6.3.2).

Consider a general domain Ω intersected by a plane \mathcal{P} which forms faces \mathbf{L}_1 and \mathbf{L}_2 on Ω_1 and Ω_2 . For any Ω there is a corresponding enclosing frustrum $\Xi^0 \equiv \Xi_{\mathbf{L}^0, N^0}(\xi^0)$ on the same plane \mathcal{P} which, as illustrated in Fig. 12 is a

Definition 6.5.1. Minimal frustrum in the sense: (i) that the (matching) faces \mathbf{L}_1^0 and \mathbf{L}_2^0 of Ξ^0 just contain \mathbf{L}_1 and \mathbf{L}_2 ; this can be written more explicitly (but less transparently) as

$$\mathbf{L}_1^0 = \mathbf{L}_1 \cup (\mathbf{L}_2 + \mathbf{b}_0) \equiv (\mathbf{L}_1 - \mathbf{b}_0) \cup \mathbf{L}_2 + \mathbf{b}_0 = \mathbf{L}_2^0 + \mathbf{b}_0; \tag{6.5.1}$$

(ii) Ω cannot be contained in any frustrum of half-height $N^0 - 1$; (iii) no frustrum $\Xi_{\mathbf{L}^0, N^0}(\xi)$ with ξ less than ξ^0 can contain Ω .

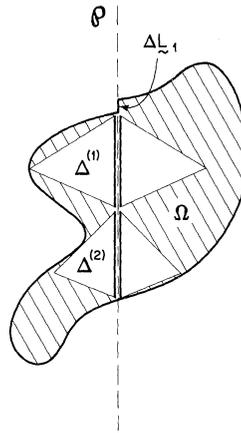


Fig. 13. A filling of a general, ($d=2$)-dimensional domain, Ω , by cones $\Delta^{(1)}$ and $\Delta^{(2)}$. Note the unfilled part, ΔL_1 , of the face L_1 (compare with Fig. 12)

In normal cases $|L_1|$, $|L_2|$, and $|L|$ will be close in magnitude and, in particular, in the thermodynamic limit we must have $|L_1|/|L|, |L_2|/|L| \rightarrow 1$ for our definition of wall free energy to make proper sense.

A general domain Ω with intersecting plane \mathcal{P} may also be filled with one or more cones $\Delta^{(1)}, \Delta^{(2)}, \dots, \Delta^{(m)}$, with disjoint bases $L_1^{(1)}, L_1^{(2)}, \dots$, and $L_2^{(1)}, L_2^{(2)}, \dots, L_2^{(m)}$ contained in L_1 and L_2 , as illustrated in Fig. 13. There is no special merit in defining a maximal filling by cones but we will require fillings which are *efficient* in the sense that the unfilled face ratios, $|\Delta L_1|/|L|$ and $|\Delta L_2|/|L|$, where

$$\Delta L_1 = L_1 \setminus \bigcup_{j=1}^m L_1^{(j)}, \quad \Delta L_2 = L_2 \setminus \bigcup_{j=1}^m L_2^{(j)}, \tag{6.5.2}$$

are small and, in particular, vanish in the thermodynamic limit. The number of cones used to fill Ω may grow indefinitely in the thermodynamic limit but some uniformity condition on their shape and size is required in accord with Remark 6.3.3. The following condition seems more than adequate for all practical purposes and suffices for our proof.

K. An asymptotically efficient filling of a sequence of domains $\{\Omega_k\}$ intersecting a plane \mathcal{P} and forming a wall of area $|L_k|$, is a sequence of sets of cones $\{\Delta_k^{(j)}\}_{j=1, \dots, m_k}$ constructed on \mathcal{P} and satisfying the conditions:

- (i) each cone $\Delta_k^{(j)}$ is, up to a translation, identical with a standard cone, $\bar{\Delta}_k^{(\alpha)}$, in a finite set of sequences $\{\bar{\Delta}_k^{(\alpha)}\}_{\alpha=1, \dots, n}$;
- (ii) The cones are disjoint, i.e. $\Delta_k^{(j)} \cap \Delta_k^{(j')} = \emptyset$ ($j \neq j'$, all k), and $\Delta_k^{(j)} \subset \Omega_k$ (all j, k);
- (iii) the unfilled parts, ΔL_{1k} and ΔL_{2k} , of the faces, L_{1k} and L_{2k} , of Ω_k [see (6.5.2)] satisfy

$$|\Delta L_{1k}|/|L_k|, \quad |\Delta L_{2k}|/|L_k| \rightarrow 0 \quad \text{as } k \rightarrow \infty; \tag{6.5.3}$$

- (iv) the standard cones, $\bar{\Delta}_k^{(\alpha)} \equiv \Delta_{L_k^{(\alpha)}, N_k^{(\alpha)}}(v_k^{(\alpha)})$, satisfy the shape Conditions **J** and $L_k^{(\alpha)} \rightarrow \infty, N_k^{(\alpha)} \rightarrow \infty$ as $k \rightarrow \infty$ for all $\alpha = 1, 2, \dots, n$.

$$\tag{6.5.4}$$

Now we can state the main theorem for subfree associated conditions.

Theorem 6.5.1. *Existence for general domains with subfree conditions. Let $\{\Omega_k\}$ be a sequence of domains intersecting a plane \mathcal{P} such that (i) there is a corresponding sequence of enclosing minimal frustrums, $\{\Xi_k^0\} \equiv \{\Xi_{\mathbf{L}_k^0, N_k^0}(\xi_k^0)\}$, satisfying $\xi_k^0 \leq \xi_0$ (all k) and the shape Condition **J** as $k, N_k^0 \rightarrow \infty$, (ii) the mismatch in the faces \mathbf{L}_{1k} and \mathbf{L}_{2k} of Ω_k , namely,*

$$\Delta L_k^0 = \frac{1}{2}|\mathbf{L}_{1k}^0 \setminus \mathbf{L}_{1k}| + \frac{1}{2}|\mathbf{L}_{2k}^0 \setminus \mathbf{L}_{2k}|, \tag{6.5.5}$$

*satisfies $\Delta L_k^0/|\mathbf{L}_k| \rightarrow 0$ as $k \rightarrow \infty$, and (iii) $\{\Omega_k\}$ possesses an asymptotically efficient filling by cones, $\{\Delta_k^{(j)}\}$, as specified by Condition **K**. Then if the $\{\Omega_k\}$ are subject to (a) subferromagnetic associated boundary conditions with potentials \tilde{W} satisfying the tempering Condition **C τ** (Sect. 1.4) with $\tau > 0$, (b) ferromagnetic bulk and wall potentials, K and W , which satisfy the defining Conditions **D** and **E** (Sect. 2.2 and 2.3) and the boundedness Conditions **A** and **F** (Sect. 1.4 and 2.3), the boundary free energies satisfy*

$$\lim_{k \rightarrow \infty} f_{\times}(K, W, \tilde{W}; \Omega_k) = f_{\times}^0(K, W), \tag{6.5.6}$$

where $f_{\times}^0(K, W)$ is the standard free energy for box domains with free associated boundary conditions (Theorem 4.4.1), and similarly for the partial boundary free energies.

Proof. With the apparatus assembled the proof is straightforward. (Some detail contained in earlier proofs will be omitted.) By application of Proposition 3.3.1 and the fact that Ω_k is contained in a minimal frustrum Ξ_k^0 on which we may impose consistent subfree associated wall potentials, \tilde{W}^0 , we have

$$|\mathbf{L}_k| f_{\times}^{\pm}(K, W, \tilde{W}; \Omega_k) \leq |\mathbf{L}_k^0| f_{\times}^{\pm}(K, W, \tilde{W}_k^0; \Xi_k^0). \tag{6.5.7}$$

On noting, with the aid of (6.5.1), that $|\mathbf{L}_k^0| = |\mathbf{L}_k| + \Delta L_k^0$ and using the Condition (ii), which states that the facial mismatch is asymptotically negligible, we can obtain from Proposition 6.3.2, for subfree frustrums, the bound

$$\liminf_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Omega_k) \leq f_{\times}^{0\pm}(K, W). \tag{6.5.8}$$

The complementary inequality follows from the existence, by (iii), of the efficient filling by cones $\{\Delta_k^{(j)}\}$ on which we can impose subfree boundary conditions, $\tilde{W}_k^{(j)}$, consistent with K, W , and \tilde{W} . Specifically, by Proposition 3.3.1 we then have

$$|\mathbf{L}_k| f_{\times}(K, W, \tilde{W}; \Omega_k) \geq \sum_j |\mathbf{L}_k^{(j)}| f_{\times}^{\pm}(K, W, \tilde{W}_k^{(j)}; \Delta_k^{(j)}). \tag{6.5.9}$$

Now we may use Proposition 6.3.1 for subfree cones, and the Condition **K(iii)**, for efficient filling of the faces \mathbf{L}_{1k} and \mathbf{L}_{2k} by the cones to bound $\limsup_{k \rightarrow \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Omega_k)$ by $f_{\times}^{0\pm}(K, W)$, and thence complete the proof. \square

The parallel theorem for superferromagnetic associated boundary conditions may be proved along precisely the same lines with adaptations already well exposed in the proofs of the corresponding propositions. Thus we will give only the statement:

Theorem 6.5.2. *Existence for general domains with superferromagnetic conditions. Let $\{\Omega_k\}$ be a sequence of domains intersecting a plane \mathcal{P} and satisfying Conditions (i), (ii), and (iii) of Theorem 6.5.1. For a system of saturating spins subject to (a) superferromagnetic associated wall potentials, \tilde{W} , of finite range \tilde{R}^\times , and (b) ferromagnetic bulk and wall potentials, K and W , of finite range, R° and R^\times , respectively, of finite degree, and satisfying Conditions **A** (Sect. 1.4), **D** (Sect. 2.2), **E** and **F** (Sect. 2.3), the boundary free energies have a limit*

$$\lim_{k \rightarrow \infty} f_\times(K, W, \tilde{W}; \Omega_k) = f_\times^*(K, W), \tag{6.5.10}$$

where $f_\times^*(K, W)$ is the standard free energy for box domains with simple superferromagnetic associated potentials (Theorem 4.4.3).

Remark 6.5.1. These two theorems for arbitrary domains are evidently restricted to subferromagnetic or to superferromagnetic associated wall potentials (in saturating spin systems). However, along the lines of Theorem 4.4.5 we may allow arbitrary associated wall potentials over regions of the boundaries of the Ω_k provided the contribution to the total free energy of these regions is asymptotically negligible compared to the wall area $|\mathbf{L}_k|$. In the simplest case this leaves us at liberty to impose arbitrary associated conditions on a “strip” extending a fixed distance, say $M\mathbf{b}_0$, on either side of the wall plane \mathcal{P} while maintaining, say, subferromagnetic conditions on the boundaries further removed from \mathcal{P} .

7. Multiple Walls and Complete Boundaries

In the foregoing we have proved existence and uniqueness theorems for the thermodynamic limit of the free energies of planar walls constructed by cutting a domain Ω_k , drawn from a sequence $\{\Omega_k\}$ of domains of general shape, by a plane \mathcal{P} into subdomains $\Omega_{k,1}$ and $\Omega_{k,2}$. Granted ferromagnetic bulk interactions, K , we were able to handle general wall potentials, W , although, in proving uniqueness, we had to restrict the associated wall potentials, \tilde{W} , to be either predominantly subfree or, for interactions of finite range, to be predominantly superferromagnetic. Furthermore, we have been unable to establish the general equality of the two corresponding limiting free energies, $f_\times^0(K, W)$ and $f_\times^*(K, W)$ for subfree and superferromagnetic associated wall potentials, respectively. For the reasons explained in Sect. 2.7 one may, in fact, anticipate circumstances in which f_\times^0 and f_\times^* would not be equal; further conditions are then essential to exclude such situations.

Now we turn to more general definitions of the boundary free energy applicable to systems in which a number of planar walls are present. In particular, the case in which the set of walls form the *complete boundary* of a domain is of principal interest. In fact it will suffice for most practical purposes to restrict attention to the boundaries of parallelepipeds or, (after a suitable affine transformation of space as discussed in Sect. 6.1), simple rectangular or box domains, \mathcal{A} . Two concrete cases we will analyze are illustrated in Figs. 14 and 15; the latter case, in which one large box is subdivided into many smaller but identical boxes, will enable us to isolate the total boundary free energy of a *single* box domain, and

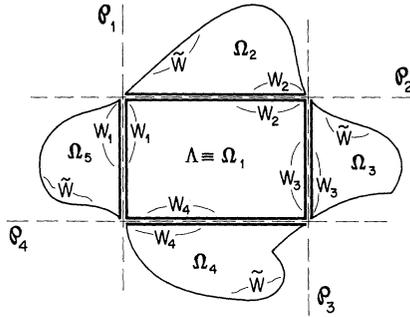


Fig. 14. A domain, Ω , in $d=2$ dimensions, intersected by four wall planes to form a box, $\Lambda \equiv \Omega_1$, whose complete boundary free energy is of interest, and four further subdomains, Ω_n ($n=2, \dots, 5$)

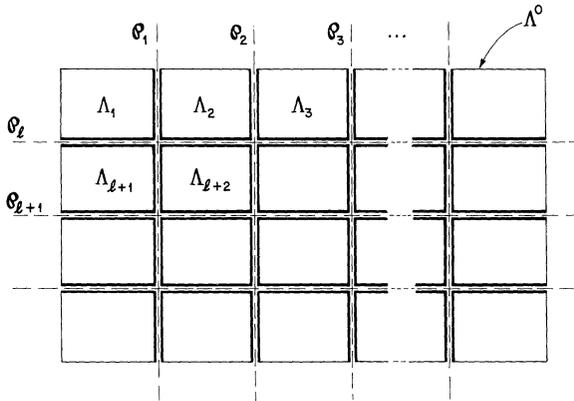


Fig. 15. A large box domain, $\Omega \equiv \Lambda^0$, divided by wall planes into many smaller, isomorphic box domains, $\Lambda_n \equiv \Omega_n$

hence to address the question originally posed in Eq. (0.5) and rephrased in Eq. (5.1).

As we will show, it is possible to prove that the total boundary free energy in such multiple-wall situations is, asymptotically, just equal to the sum of the constituent boundary free energies defined for the corresponding single planar walls. However, in parallel to the difficulty of proving complete independence of the associated wall potentials [specifically, the equality of $f_{\times}^0(K, W)$ and $f_{\times}^*(K, W)$], we pay the price of treating only wall potentials, W , which are *subfree*. This restriction is regrettable but, in the absence of other conditions, is probably necessary for reasons of the sort explained in Sect. 2.7. Nevertheless, subfree wall potentials do include the most important case of free walls constructed merely by removing all bulk interactions K_A which couple the domains separated by the walls.

The techniques involved in our proofs for multiple-wall situations are the same as those developed and applied in the previous sections. Accordingly we will explain the main ideas involved but omit many of the technical details.

7.1. Definitions for Multiple Walls

The overall boundary free energy of a system with multiple walls formed by planes $\mathcal{P}_1, \dots, \mathcal{P}_l, \dots$, which divide a domain Ω up into subdomains $\Omega_1, \dots, \Omega_n, \dots$ (as illustrated in Fig. 14 and 15) may be defined in obvious analogy to previous definitions (see e.g. Sect. 2.1) by:

Definition 7.1. The overall or mean boundary free energy is

$$\bar{f}_x(K, W, \tilde{W}, \Omega) = \frac{1}{2} |\mathbf{L}_\Omega|^{-1} \left[\sum_n F(K, \Omega_n) - F(K, \Omega) \right], \tag{7.1.1}$$

where $|\mathbf{L}_\Omega|$ is the total wall area generated by the intersection of the planes \mathcal{P}_l with Ω , while $F(K, \Omega_n) = |\Omega_n| f(K, \Omega_n)$ is the total reduced free energy of the subdomain Ω_n [see (1.2.9)]; this depends on the bulk potentials, K , on the overall wall potential, W , and on the associated wall potentials, \tilde{W} , originally imposed on Ω . The total wall area, $|\mathbf{L}_\Omega|$ may be defined precisely in terms of the number of complete blocks lying adjacent to the set of planes $\{\mathcal{P}_l\}$, in complete analogy to (2.2.6).

We would clearly like to regard the overall wall potential, W , as composed of a set of independently assigned, translationally invariant planar wall potentials, that is

$$W = \{W_{(l)}\} \tag{7.1.2}$$

where $W_{(l)}$ is defined in association with the plane \mathcal{P}_l , as in Sect. 2.3, and satisfies the bounds \mathbf{F} , etc. To make this concept precise, however, it is necessary to accept some convention as to the meaning of a specific wall interaction term, W_A , for a set of spins A when A lies near the intersection of two or more planes W_A so is nominally specified by a number of $W_{(l)}$. (The analog of this question was faced in Sect. 2.4 when associated wall potentials were defined explicitly.) The convention must clearly satisfy (i) the *separation condition*, $\mathbf{E}(\mathbf{i})$, i.e. $K_A + W_A \equiv 0$ whenever A links distinct subdomains Ω_n . For our methods of proof to go through, it must also respect (ii) the ferromagnetic character of W , i.e. $K_A + W_A \geq 0$ all A ; see (2.3.6). Both these ends are met by the local averaging convention:

Definition 7.2. Multiple wall potentials $W \equiv \{W_{(l)}\}$, where $W_{(l)} = \{W_{(l)A}\}$, imply, for a domain Ω intersected by planes $\mathcal{P}_1, \mathcal{P}_2, \dots$, the explicit interactions

$$W_A^\Omega \equiv K_A^\Omega - K_A = \sum_l \mu_{A,l}(W; \Omega) W_{(l)A}, \tag{7.1.3}$$

where the weights $\mu_{A,l}$ are given by:

(i) if $A \in \mathcal{L}_{l',1} \cdot \mathcal{L}_{l',2}$ for some l' (i.e. A links the half-lattices $\mathcal{L}_{l',1}$ and $\mathcal{L}_{l',2}$ separated by $\mathcal{P}_{l'}$; see Sect. 2.2)

$$\begin{aligned} \mu_{A,l}(W; \Omega) &= 0, & \text{if } A \notin \mathcal{L}_{l,1} \cdot \mathcal{L}_{l,2}, \\ &= 1/v_A(W; \Omega), & \text{otherwise,} \end{aligned}$$

where $v_A(W, \Omega)$ is the number of planes \mathcal{P}_l whose half-lattices are linked by A ; and

(ii) if $A \subseteq \Omega_n$ for some n (and hence A does not link subdomains)

$$\begin{aligned} \mu_{A,l}(W; \Omega) &= 0, & \text{if } \mathcal{P}_l \text{ does not bound } \Omega_n, \\ &= 1/\tilde{v}_A(W; \Omega), & \text{otherwise,} \end{aligned}$$

where $\tilde{v}_A(W; \Omega)$ is the number of planes, \mathcal{P}_l , bounding Ω_n for which $W_{(l)} \neq 0$.

In strict analogy with (2.4.8) we may define the *total wall Hamiltonian* via

$$\tilde{\mathcal{H}}(\Omega) + \mathcal{W}(\Omega) = \sum_n \tilde{\mathcal{H}}(\Omega_n), \tag{7.1.4}$$

and decompose it explicitly into disjoint contributions from the individual planes \mathcal{P}_l as

$$\mathcal{W}(\Omega) = \sum_l \mathcal{W}_l(\Omega). \tag{7.1.5}$$

On using (7.1.3) we can, in analogy to (2.4.9), write

$$\mathcal{W}_l(\Omega) = \sum_{A \subseteq \Omega} [v_A(W)]^{-1} W_{(l)A} s_A - \sum_{B(l)} \tilde{W}_B^\Omega s_B, \tag{7.1.6}$$

in which the sum in the second, associated wall interference term runs over all sets B linking subdomains separated by \mathcal{P}_l . Strictly, we require a convention here, like (7.1.3), to avoid overcounting; however, we will ignore this complication: we always assume the associated wall potentials \tilde{W} maintain the ferromagnetic character [see (2.4.5)] and satisfy the boundedness Conditions **G**.

For large domains we expect that the mean boundary free energy can be written as a sum of independent contributions from the separate walls, namely,

$$\tilde{f}_\times(K, W, \tilde{W}, \Omega) \approx \sum_l \lambda_l(\Omega) f_\times(K, W_{(l)}), \tag{7.1.7}$$

where $f_\times(K, W)$ is the limiting boundary free energy for a single planar wall (for appropriate associated boundary conditions, say, subfree). The weighting coefficients should simply be ratios of wall areas, namely,

$$\lambda_l(\Omega) = |\mathbf{L}_{(l)}|/|\mathbf{L}_\Omega|, \tag{7.1.8}$$

where the areas of the plane \mathcal{P}_l in Ω may be defined just as in (2.2.6).

Having disposed of these preliminaries, let us turn directly to the question of proving (7.1.7) in the thermodynamic limit for the situations illustrated in Figs. 14 and 15.

7.2. Overall Free Energy for Multiple Walls

Consider a situation, such as shown in Fig. 14, in which a domain A is bounded by walls formed by planes intersecting a domain Ω , on which subfree associated boundary conditions have been imposed. To estimate the overall boundary free energy, $\tilde{f}_\times(K, W, \tilde{W}; \Omega)$ defined by (7.1.1), our strategy, as in previous cases, is to attempt to construct upper and lower bounds to the partial boundary free energies, $f_\times^\pm(K, W, \tilde{W}; \Omega)$, in terms of the standard limiting partial free energies $f_\times^{0\pm}(K, W)$ defined originally on boxes, by using Proposition 3.3.1, the basic comparison theorem for compound domains.

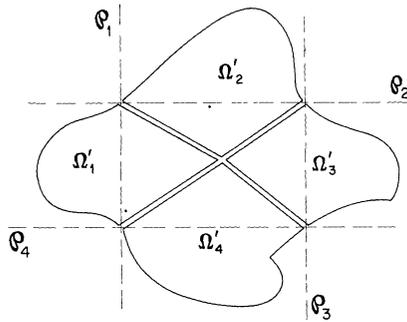


Fig. 16. A decomposition of the domain Ω , illustrated in Fig. 14, into disjoint subdomains, Ω'_l , each intersecting with only a single plane \mathcal{P}_l ($l = 1, \dots, 4$)

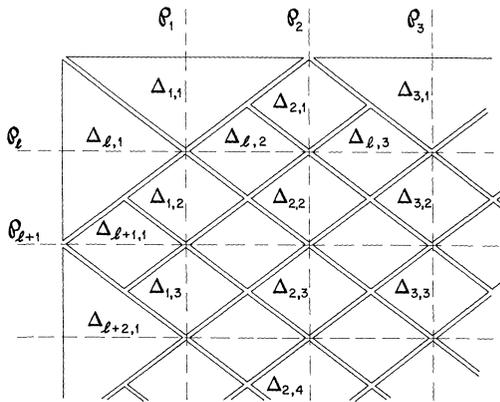


Fig. 17. A decomposition of the box domain $\Omega \equiv A^0$, shown in Fig. 15, into disjoint subdomains, in this case all cones $\Omega'_{l,m} \equiv \Delta_{l,m}$, and containing only a single segment m of the wall planes \mathcal{P}_l

In fact, lower bounds for the partial free energies are easy to obtain: consider a decomposition of Ω into disjoint subdomains $\Omega'_1, \Omega'_2, \dots$, such that each subdomain intersects only with a single plane. For the case illustrated in Fig. 14, a suitable decomposition is shown in Fig. 16; in this instance a decomposition with a single subdomain Ω'_l for each plane \mathcal{P}_l suffices. More generally, if the planes cross within Ω , as in Fig. 15, separate subdomains, $\Omega'_{l,m}$, are needed for each distinct segment, m , of a wall plane \mathcal{P}_l , as illustrated in Fig. 17. On each such subdomain, $\Omega'_{l,m}$, let free boundary conditions be imposed on the newly created boundaries.

Now the total partial boundary free energies, $|\mathbf{L}_\Omega| \tilde{f}_\times^\pm$, can be expressed as integrals over the expectations $\langle \mathcal{W}_\pm \rangle_\Omega^\zeta$ for partially coupled domains with coupling parameter ζ as in (3.1.8). However, the integrands are sums of ferromagnetic correlation functions, (see Proposition 3.3.1), and hence can be bounded below by the corresponding integrals in the decomposed domain, $\Omega' \equiv \{\Omega'_{l,m}\}$. Via the plane decomposition (7.1.5), these latter integrals entail the uncoupled expectations $\langle \mathcal{W}_{(l)\pm} \rangle_{\Omega'_{l,m}}^\zeta \equiv \langle \mathcal{W}_{(l)\pm} \rangle_{\Omega'_{l,m}}^\zeta$, which, in turn, are essentially just the integrands that would arise if the free energies $|\mathbf{L}_{(l,m)}| \tilde{f}_\times^\pm(K, W_{(l)}, \tilde{W}_{(l,m)}; \Omega'_{l,m})$

were computed directly. (Here $\tilde{W}_{(l,m)}$ denotes associated boundary conditions which are free on the new boundaries of $\Omega'_{l,m}$ but agree with \tilde{W} on the boundaries in common with Ω .) The “essentially” in the previous assertion occurs because of the interference terms arising along the perimeters where two walls intersect as a result of the convention (7.1.3). However, such interference terms will, for wall potentials $W_{(l)}$ and \tilde{W} respecting the bounds \mathbf{F} and \mathbf{G} , respectively, give rise to asymptotically negligible corrections to $f_x^\pm(K, W_{(l)}, \tilde{W}_{(l,m)}; \Omega'_{l,m})$ if the thermodynamic limit is taken in a reasonable way. Specifically, we may suppose that $\Omega, \Lambda, \Omega_m, \Omega'_{l,m}$ become infinite in such a way that the domains $\Omega'_{l,m}$ satisfy the shape conditions enunciated in Sect. 6 (see Theorem 6.5.1). Then

$$f_x^\pm(K, W_{(l)}, \tilde{W}_{(l,m)}; \Omega'_{l,m}) \rightarrow f_x^{0\pm}(K, W_{(l)})$$

and the surface area ratios satisfy

$$\sum_m |\mathbf{L}_{l,m}|/|\mathbf{L}_\Omega| \rightarrow \lim_{\Omega \rightarrow \infty} |\mathbf{L}_l|/|\mathbf{L}_\Omega| = \lambda_l^\infty, \tag{7.2.1}$$

where the limit may be identically zero. The appropriate shape restrictions will certainly be met if the limit is taken through a simple sequence of intersected domains $\Omega_k \equiv \{\Omega_{k,n}\}$ defined [see (1.4.4)] by expanding an initial configuration such as in Fig. 14. Our arguments show how to prove the following lemma:

Lemma 7.2.1. *Lower bound for multiple walls. The overall partial boundary free energies for a multiple-wall situation, defined in analogy to (7.1.1), for ferromagnetic bulk and wall potentials, K and W , and for subfree associated wall conditions \tilde{W} , satisfy*

$$\liminf_{\Omega \rightarrow \infty} \tilde{f}_x^\pm(K, W, \tilde{W}; \Omega) \geq \sum_l \lambda_l^\infty f_x^{0\pm}(K, W_{(l)}), \tag{7.2.2}$$

where the limiting wall area ratios, λ_l^∞ , are defined in (7.2.1), and the limit is taken through a simple (or other sufficiently regular) sequence of intersected domains $\Omega \equiv \{\Omega_n\}$. \square

Remark 7.2.1. This lemma applies to multiple boundaries with distinct wall potentials $W_{(l)}$ which are quite general provided only they respect the ferromagnetic conditions $W_B \geq |K_B|$ (all B).

Remark 7.2.2. Although we have focussed attention on the case where the walls form the complete boundary of a box Λ , it is clear that Λ may be replaced by a more general domain bounded by planar walls. Furthermore, no specially singled-out, completely bounded subdomain like Λ need be present; e.g. the domain Ω might simply be divided by two planes, \mathcal{P}_1 and \mathcal{P}_2 into four subdomains, each sharing part of their boundary with Ω . Likewise, the configuration of Fig. 15 is covered.

For later convenience, we state explicitly the complementary upper bound for superferromagnetic associated boundary conditions:

Lemma 7.2.2. *Bounds for superferromagnetic multiple walls. Under the conditions stated in Lemma 7.2.1, but with superferromagnetic associated wall conditions, \tilde{W} , and the additional restrictions that the spins are saturating, and that K and W are of finite range and finite degree (in accord with the conditions of Theorem 4.4.3), one*

has

$$\limsup_{\Omega \rightarrow \infty} \bar{f}_x^\pm(K, W, \tilde{W}; \Omega) \leq \sum_l \lambda_l^\infty f_x^{*\pm}(K, W_{(l)}). \tag{7.2.3}$$

Proof. This follows along the same lines used for Lemma 7.2.1, with appropriate modifications as in the proofs of Theorems 4.4.3, 4.4.4, 6.5.2, etc. \square

To obtain the required upper bound for subfree associated conditions corresponding to (7.2.2), a new argument is needed: certainly we cannot embed Ω usefully in larger domains of standard shapes with each one including only one wall segment. Instead, let us generalize the previous coupling integration method embodied in (3.1.2) and (3.1.3) by defining,

$$\bar{\mathcal{H}}^{\zeta_1, \zeta_2, \dots}(\Omega) = \bar{\mathcal{H}}(\Omega) + \sum_l \zeta_l \mathcal{W}_l(\Omega), \tag{7.2.4}$$

where the separate wall Hamiltonians are defined by (7.1.6). Now consider the sequential introduction of the walls $W_{(1)}, W_{(2)}, \dots$ by successive coupling integrations: $\int_0^1 d\zeta_1$ with $\zeta_2 = \zeta_3 = \dots = 0$; $\int_0^1 d\zeta_2$ with $\zeta_1 = 1, \zeta_3 = \dots = 0$; etc. In place of the original result (3.1.8), we finally obtain

$$2|\mathbf{L}_\Omega| \bar{f}_x^\pm(\Omega) = \sum_l \int_0^1 d\zeta_l \langle \mathcal{W}_{(l)\pm} \rangle_\Omega^{\zeta(l)}, \tag{7.2.5}$$

where the superscript $\zeta(l)$ means $\zeta_1 = \dots = \zeta_{l-1} = 1, \zeta_{l+1} = \dots = 0$, while ζ_l varies.

Consider the first step at which the wall Hamiltonian $\mathcal{W}_{(1)}(\Omega)$ is coupled in. If in (7.1.6) we had $\mu_{A,l}(W; \Omega) = 1$ for all A (with non-vanishing $W_{(1)A}$) and, if we neglect overcounting questions in the associated wall interference term, the contribution to the overall partial boundary free energies, $|\mathbf{L}_\Omega| \bar{f}_x^\pm$, would be just

$$|L_{(1)}| f_x^\pm(K, W_{(1)}, \tilde{W}; \Omega). \tag{7.2.6}$$

The corrections to this arising from the cases where $\mu_{A,l}(W; \Omega) < 1$ will be proportional to the total perimeters of the wall segments on plane \mathcal{P}_1 as defined by the intersection with the other planes $\mathcal{P}_l (l \neq 1)$. (Likewise, the associated boundary terms are of order $|\partial L_{(1)}|$.) For simple sequences of intersected domains, or for other regular sequences, such corrections will be asymptotically negligible.

This last assertion assumes, of course, that the wall potentials $W_{(l)}$ (and the associated potentials W) satisfy the boundedness Conditions **F** (and **G**, respectively) and, say, tempering \mathbf{C}_τ with $\tau > 1$ (see Lemma 2.3.2). In making the detailed estimates of the interference terms, however, it is easier to assume that the wall (and associated wall) potentials are of finite range R^\times (and \tilde{R}^\times). If the bulk potentials K are of infinite range, the corresponding ‘‘walls’’ will actually be ‘‘seams’’, since the subdomains will not be fully decoupled. However, we will show later (in Sect. 7.4) that the corresponding limiting free energies, $f_x(K, W)$, are *continuous* in the wall or seam potentials W , provided these remain bounded within the norms specified by **F** or \mathbf{C}_τ . Hence, the simplification of assuming finite ranges R^\times (and \tilde{R}^\times) is not restrictive.

At the next stage, consider the introduction of the *second wall* with Hamiltonian $\mathcal{W}_{(2)}(\Omega)$. In the *absence* of the first wall, this would, by the argument

already given, contribute to the overall boundary free energies, $|\mathbf{L}_\Omega|\bar{f}_x^\pm$, a term asymptotically equal to

$$|\mathbf{L}_{(2)}|f_x^\pm(K, W_{(2)}, \tilde{W}; \Omega). \tag{7.2.7}$$

However, in the *presence* of the first wall the actual contribution may differ from this in an uncontrollable way. The essence of the difficulty can be seen by reexamining the proofs of Propositions 3.3.1 and 3.3.2 on compound domains. The first wall represents, from the viewpoint of the second wall, a set of additional associated walls, with potentials \tilde{W}' , $\tilde{W}'' \equiv W_{(1)}$, whose effects can be controlled *only* if they are *either* subfree (Proposition 3.3.1) *or* superferromagnetic (Proposition 3.3.2). Since we are here desirous of an upper bound on the partial free energy contribution, we are forced to *restrict the original wall potentials $W_{(1)}$ to be subfree*, (but see Remark 7.2.3 for the converse situation). In that case the expression (7.2.7) represents, asymptotically, an upper bound to the contribution of $\mathcal{W}_{(2)}$ to the overall boundary free energies $|\mathbf{L}_\Omega|\bar{f}_x^\pm$.

At the third stage, we may similarly obtain an upper bound to the contribution arising from $W_{(3)}$ if we assume that $W_{(1)}$ and $W_{(2)}$ are both subfree. On continuing the argument for successive walls, we are forced to assume that all but the last (or, equivalently, the first) wall are subfree. This finally establishes a complementary upper bound to that embodied in Lemma 7.2.1: the result for fixed Ω may be stated as:

Lemma 7.2.3. *Upper bound for multiple walls. For a multiple-wall configuration as defined in (7.1.1), with ferromagnetic bulk and wall potentials, K and $W \equiv \{W_{(l)}\}$, satisfying Conditions **A**, **D**, **E**, **F**, and **C $_\tau$** with $\tau = 1$ and with subfree associated wall potentials, \tilde{W} , satisfying **G(i)** and **C $_\tau$** with $\tau > 0$, the overall partial boundary free energies obey*

$$|\mathbf{L}_\Omega|\bar{f}_x^\pm(K, W, \tilde{W}; \Omega) \leq \sum_l |\mathbf{L}_{(l)}|f_x^\pm(K, W_{(l)}, \tilde{W}; \Omega) + C(K, W, \tilde{W}) \left[\sum_l |\partial\mathbf{L}_{(l)}| + \sum_{(l,l')} |\partial\mathbf{L}_{(l,l')}| \right], \tag{7.2.8}$$

where the coefficient $C(K, W, \tilde{W})$ is independent of Ω and $\{\mathcal{P}_l\}$, provided the separate wall potentials $W_{(l)}$ are subfree for $l \geq 2$; in the last term $\partial\mathbf{L}_{(l)}$ denotes the outer perimeter of the face $\mathbf{L}_{(l)}$ of \mathcal{P}_l in Ω while $\partial\mathbf{L}_{(l,l')}$ denotes the mutual perimeter of the faces $\mathbf{L}_{(l)}$ and $\mathbf{L}_{(l')}$. \square

The two lemmas may be combined to prove the main result:

Theorem 7.2. *Multiple walls. In a multiple wall configuration as defined in (7.1.1), with ferromagnetic bulk and wall potentials, K and $W \equiv \{W_{(l)}\}$, satisfying the conditions stated in Lemma 7.2.3, the overall boundary free energy has the thermodynamic limit*

$$\lim_{\Omega \rightarrow \infty} \bar{f}_x(K, W, \tilde{W}; \Omega) = \sum_l \lambda_l^\infty f_x^0(K, W_{(l)}), \tag{7.2.9}$$

where the limiting wall area ratios, λ_l^∞ , are defined in (7.2.1), provided the separate wall potentials $W_{(l)}$ are subfree for $l \geq 2$ and that the limit is taken through a simple (or other sufficiently regular) sequence of domains $\Omega \equiv \{\Omega_n\}$ intersected by a finite number of planes \mathcal{P}_l .

Proof. Lemma 7.2.1 provides a lower bound to the partial boundary free energies of the appropriate form. An equal upper bound follows from Lemma 7.2.3 for a sufficiently regular sequence of domains because the perimeter-to-area ratios, $|\partial\mathbf{L}_{(l)}|/|\mathbf{L}_{\Omega}|$ and $|\partial\mathbf{L}_{(l,l')}|/|\mathbf{L}_{\Omega}|$, vanish as $\Omega \rightarrow \infty$. \square

Remark 7.2.4. As remarked after Lemma 7.2.1, the configuration of the multiple walls can be quite general; specifically, both Figs. 14 and 15 are covered by the theorem. It is also clear that, if the defining planes, \mathcal{P}_l , and wall potentials, $W_{(l)}$, are equivalent under the symmetry operations of the lattice \mathcal{L} , then (7.2.9) may be written simply as $\bar{f}_x(K, W) = f_x^0(K, W)$.

Remark 7.2.5. By recalling Remark 7.2.3 and the argument following (7.2.4) above we can see that a complementary theorem can be proved in terms of $f_x^*(K, W)$ for superferromagnetic associated boundary conditions \bar{W} , provided all the separate wall potentials $W_{(l)}$ for $l \geq 2$ are also superferromagnetic, and, as usual, that the spins saturate and that K and W are of finite range and degree.

7.3. Free Energy of a Single Box Domain

Up to this point, our analysis of the free energy associated with a wall has always dealt with *pairs* of walls created by the intersection of a plane with a domain. Thus, in Fig. 14, for example, the overall boundary free energy computed in Theorem 7.2 is that associated with the boundaries of the box domain A , *plus* that of the adjacent walls of the four domains $\Omega_2, \Omega_3, \Omega_4$, and Ω_5 . Of course, we expect that, in the limit of large A , the sum of these wall free energies will asymptotically equal the total wall free energy of A ; however, even a symmetry assumption such as **D(iii)** is not sufficient to guarantee this. Nevertheless, we may use Lemma 7.2.3, with a multiple wall configuration such as that illustrated in Fig. 15, to establish the asymptotic behavior of the total free energy of a *single* box domain. Explicitly for *subfree wall potentials* $W \equiv \{W_{(\alpha)}\}$, with $\alpha = 1, 2, \dots, d$, we can prove

$$\begin{aligned} F(K, \{W_{(\alpha)}\}, A) &= \ln Z[\mathcal{H}(A)], \\ &= |A| f_\infty(K) + A_A \sum_\gamma \lambda_\gamma^\infty f_x^0(K, W_{(\gamma)}) + o(A_A), \end{aligned} \tag{7.3.1}$$

where A_A is the overall area of the box A , λ_γ^∞ is the relative area of the face $\gamma (= 1, 2, \dots, 2d)$, and $A \rightarrow \infty$ in any way. This expression enunciates the fundamental expectation of thermodynamics regarding the independent existence of the wall free energies for the distinct (planar) boundaries of a large domain in the shape of a parallelepiped.

To make this statement more precise and then embody it in a theorem, a few points require further explication. First, following Definition 4.1 for a box domain with one distinguished axis, we will adopt the convention that

$$A_{\mathbf{L}} \equiv A_{\mathbf{L}, N=L_d} \tag{7.3.2}$$

denotes a box domain of $L_1 \times L_2 \times \dots \times L_{d-1} \times L_d$ blocks. Second, note that the minimal symmetry restrictions **D(iii)** and **E(iii)** will *not* be invoked, so that two opposite faces of $A_{\mathbf{L}}$, say $\mathbf{L}_{\alpha,+}$ and $\mathbf{L}_{\alpha,-}$, parallel to the plane \mathcal{P}_α , need not be of similar lattice structure; neither need the specific wall interactions associated with these faces be related. However, the set of wall interactions $\bar{W}_{(\alpha,+A)}$ and $\bar{W}_{(\alpha,-)A}$

may be associated with the first and second sides of \mathcal{P}_α , and, taken together with the set of decoupling potentials, $W_{(\alpha)B} = -K_B$ for $B \in \mathcal{L}_{\alpha,1} \cdot \mathcal{L}_{\alpha,2}$, then clearly are sufficient to specify a wall potential set $W_{(\alpha)}$ in the sense of (7.2.1). Conversely, if we again accept the convention embodied in Definition 7.2, regarding the interference between walls in a multiple wall configuration, a given set $\{W_{(\alpha)}\}$ of wall potentials yields an explicit specification of the wall potentials in a box domain $A_{\mathbf{L}}$ via an indefinitely large array of the sort illustrated in Fig. 15. (Note that the numbers v_A and \tilde{v}_A entering in Definition 7.2 are finite for all bounded A , even if an infinite array of boxes is contemplated as necessary in the case of long range interactions.) The standard boundary free energy $f_\infty^0(K, W_{(\alpha)})$ then represents the average of the limiting free energies per unit area associated with the opposite faces $\mathbf{L}_{\alpha,+}$ and $\mathbf{L}_{\alpha,-}$.

Having disposed of these preliminaries, we may state the main result:

Theorem 7.3. *Single box domain.* For a box domain, $A_{\mathbf{L}}$, of sides L_1, L_2, \dots, L_d blocks in length, with ferromagnetic bulk potentials, K , satisfying condition **A**, and ferromagnetic wall potentials, $W \equiv \{W_{(\alpha)}\}$, which are subfree and satisfy Conditions **D**, **E**, **F**, and **C $_\tau$** with $\tau > 1$, but do not necessarily respect the minimal symmetry requirements **D(iii)** and **E(iii)**, the total (reduced) free energy, $F(A_{\mathbf{L}}) \equiv F(K, \{W_{(\alpha)}\}, A_{\mathbf{L}})$, verifies

$$\lim_{\mathbf{L} \rightarrow \infty} [F(A_{\mathbf{L}}) - |A_{\mathbf{L}}| f_\infty(K)] / 2A_{\mathbf{L}} = \sum_{\alpha=1}^d \lambda_\alpha^\infty f_\infty^0(K, W_{(\alpha)}), \tag{7.3.3}$$

where the limit $\mathbf{L} = (L_1, L_2, \dots, L_d) \rightarrow \infty$ may be taken in any way, while $f_\infty(K)$ is the limiting bulk free energy, the total wall or boundary area is

$$A_{\mathbf{L}} = \sum_{\gamma=1}^{2d} |\mathbf{L}_{(\gamma)}| \quad \text{with} \quad |\mathbf{L}_{(\alpha)}| = \sum_{\beta \neq \alpha}^d L_\beta, \tag{7.3.4}$$

and the limiting wall ratios are given by

$$\lambda_\alpha^\infty = \lim_{\mathbf{L} \rightarrow \infty} (|\mathbf{L}_{(\alpha)}| / A_{\mathbf{L}}) = \lim_{\mathbf{L} \rightarrow \infty} \left[2L_\alpha \sum_{\beta=1}^d (1/L_\beta) \right]^{-1}. \tag{7.3.5}$$

Proof. We present only the main steps which utilise a multiple-wall configuration of the sort shown in Fig. 15, consisting of a d -dimensional array of $N \times N \times N \dots \times N = N^d = \mathcal{N}$ replicas of the box $A_{\mathbf{L}}$ forming a compound box domain $\Omega = A_{\mathbf{L}}^{\mathcal{N}}$. By appropriate choice of subfree associated wall potentials, \tilde{W} , on the compound domain, the Hamiltonian and hence the free energy for each box domain can be made isomorphic. Thus the overall wall free energy for $A_{\mathbf{L}}^{\mathcal{N}}$ may be written

$$\begin{aligned} F_\times &\equiv 2|\mathbf{L}_{A_{\mathbf{L}}^{\mathcal{N}}}| \bar{f}_\times(A_{\mathbf{L}}^{\mathcal{N}}) = \mathcal{N} F(K, W, A_{\mathbf{L}}) - F(K, W, A_{\mathbf{L}}^{\mathcal{N}}), \\ &= \mathcal{N} \{ [F(A_{\mathbf{L}}) - |A_{\mathbf{L}}| f_\infty(K)] - |A_{\mathbf{L}}| \Delta f_{\mathcal{N}} \}, \end{aligned} \tag{7.3.6}$$

where, by the existence theorems for the bulk thermodynamic limit,

$$\Delta f_{\mathcal{N}}(K, W) \equiv F(K, W, A_{\mathbf{L}}^{\mathcal{N}}) / |A_{\mathbf{L}}^{\mathcal{N}}| - f_\infty(K) \rightarrow 0, \tag{7.3.7}$$

as $\mathcal{N} \rightarrow \infty$ (at fixed \mathbf{L}).

Now a lower bound to the corresponding partial boundary free energy can be found, as in Lemma 7.2.1, by using a decomposition of $A_{\mathbf{L}}^{\mathcal{N}}$ into subdomains as shown in Fig. 17, and appealing to the basic inequality, Proposition 3.3.1. Since all walls are subfree one has $f_{\times}^{-} \equiv -f_{\times}$ and so, in terms of the intersecting planes \mathcal{P}_l , one obtains the upper bound

$$F_{\times} \leq \sum_{l,m} |\mathbf{L}_{(l)m}^{\mathcal{N}}| f_{\times}(K, W_{(l)}, \tilde{W}; \Delta_{l,m}) \tag{7.3.8}$$

where the subdomains are cones, $\Delta_{l,m}$ with faces $\mathbf{L}_{(l)m}^{\mathcal{N}}$ while the subfree conditions \tilde{W} may be chosen to take account of the perimeter interference terms. Except for surface corrections at the boundary of the compound box $A_{\mathbf{L}}^{\mathcal{N}}$, the cones can be chosen to be replicas of a set of d cones $\Delta_{\mathbf{L},\alpha}$ with bases \mathbf{L}_{α} ($\alpha = 1, \dots, d$) corresponding to the faces of a single box (see Fig. 17). Thus one can conclude

$$F_{\times} \leq \mathcal{N} \sum_{\alpha=1}^d 2|\mathbf{L}_{(\alpha)}| f_{\times}(K, W_{(\alpha)}, \tilde{W}; \Delta_{\mathbf{L},\alpha}) + N^{d-1} A_{\mathbf{L}} g(K, W, \tilde{W}), \tag{7.3.9}$$

where the area $|\mathbf{L}_{(\alpha)}|$ is given explicitly in (7.3.4), while $g(K, W, \tilde{W})$ is a coefficient of order unity which looks after the special surface cones.

A complementary bound follows directly from Lemma 7.2.3 which (on again changing f_{\times}^{-} to $-f_{\times}$) yields

$$F_{\times} \geq \sum_l |\mathbf{L}_{(l)}^{\mathcal{N}}| f_{\times}(K, W_{(l)}, \tilde{W}; A_{\mathbf{L}}^{\mathcal{N}}) - C(K, W, \tilde{W}) \mathcal{N} P_{\mathbf{L}}^{\mathcal{N}}, \tag{7.3.10}$$

where the superscripts \mathcal{N} merely serve as a reminder that the compound domain $A_{\mathbf{L}}^{\mathcal{N}}$ is involved. The coefficient $C(K, W, \tilde{W})$ is defined in the lemma and the total perimeter is likewise given by

$$\begin{aligned} \mathcal{N} P_{\mathbf{L}}^{\mathcal{N}} &= \sum_l |\partial \mathbf{L}_{(l)}^{\mathcal{N}}| + \sum_{(l,l')} |\partial \mathbf{L}_{(l,l')}^{\mathcal{N}}|, \\ &= \mathcal{N} \sum_{(\gamma,\gamma')}^{2d} |\partial \mathbf{L}_{(\gamma,\gamma')}|, \end{aligned} \tag{7.3.11}$$

where $\partial \mathbf{L}_{(\gamma,\gamma')}$ is the common perimeter (or ‘‘edge’’) of the faces $\mathbf{L}_{(\gamma)}$ and $\mathbf{L}_{(\gamma')}$ of $A_{\mathbf{L}}$. Apart from ‘corner’ effects where perimeters meet, one then has

$$\begin{aligned} P_{\mathbf{L}}^{\mathcal{N}} &= \left[\prod_{\alpha=1}^d L_{\alpha} \right] \sum_{(\gamma,\gamma')}^{2d} (1/L_{\gamma} L_{\gamma'}), \\ &\leq \frac{1}{2} \left[\prod_{\alpha=1}^d L_{\alpha} \right] \left[2 \sum_{\alpha=1}^d (1/L_{\alpha}) \right]^2 = A_{\mathbf{L}} \sum_{\alpha=1}^d (1/L_{\alpha}), \end{aligned} \tag{7.3.12}$$

where $A_{\mathbf{L}}$ is the total area of $A_{\mathbf{L}}$ as defined in (7.3.4).

Now the total wall area of each plane \mathcal{P}_l in $A_{\mathbf{L}}^{\mathcal{N}}$ is $|\mathbf{L}_{(l)}^{\mathcal{N}}| = N^{d-1} |\mathbf{L}_{(\alpha)}|$, for appropriate α , and there are $(N-1)$ parallel walls with essentially the same wall free energy [since when the L_{α} are large the location of \mathcal{P}_l in $A_{\mathbf{L}}^{\mathcal{N}}$ has only an asymptotically negligible effect on $f_{\times}(W_{(l)})$]. From (7.3.10) we thus obtain the bound

$$F_{\times} \geq \mathcal{N}(1 - N^{-1}) \sum_{\alpha=1}^d 2|\mathbf{L}_{(\alpha)}| f_{\times}(K, W_{(\alpha)}, \tilde{W}; A_{\mathbf{L}}^{\mathcal{N}}) - \mathcal{N} C P_{\mathbf{L}}^{\mathcal{N}}. \tag{7.3.13}$$

Now we may combine this result with (7.3.9) and (7.3.6), divide through by \mathcal{N} , and take the limit $N \rightarrow \infty$. On using (7.3.7) and dividing by $2A_{\mathbf{L}}$ one obtains the bounds

$$\begin{aligned}
 [F(A_{\mathbf{L}}) - |A_{\mathbf{L}}|f_{\infty}] / 2A_{\mathbf{L}} &\leq \sum_{\alpha=1}^d \lambda_{\alpha} f_{\times}(K, W_{(\alpha)}, \tilde{W}; A_{\mathbf{L}, \alpha}), \\
 &\geq \sum_{\alpha=1}^d \lambda_{\alpha} f_{\times}^0(K, W_{(\alpha)}) - CP_{\mathbf{L}}^{\mathcal{M}} / A_{\mathbf{L}},
 \end{aligned}
 \tag{7.3.14}$$

where $\lambda_{\alpha} = |L_{(\alpha)}| / A_{\mathbf{L}}$. Finally we may take $\mathbf{L} \rightarrow \infty$ in any way and use Proposition 6.3.1 for cones and (7.3.12) for the perimeter. This establishes (7.3.3) with (7.3.5). \square

7.4. Truncated Wall Potentials

To obtain the detailed estimates required for some of the proofs in the previous section, it is a considerable simplification, as remarked, to suppose that the wall and associated wall potentials, W and \tilde{W} , have finite ranges R^{\times} and \tilde{R}^{\times} . If the bulk potentials are actually of infinite range, this means that one is restricted to considering “seams” or “grain boundaries”, since some (long range) couplings will remain present after introduction of W . It is thus natural to enquire into *truncated* potentials of a range R which is afterwards allowed to become infinite. A convenient, although somewhat arbitrary, definition is provided by:

Definition 7.4.1. Truncated potentials. Given wall potentials, $W \equiv \{\tilde{W}_A\}$, and associated wall potentials $\tilde{W} \equiv \{\tilde{W}_A\}$ in a domain Ω , the corresponding potentials, $W^{(R)} \equiv \{W_A^{(R)}\}$ and $\tilde{W}^{(R)} \equiv \{\tilde{W}_A^{(R)}\}$, truncated at range R are defined by

$$\begin{aligned}
 W_A^{(R)} &= W_A, \quad \text{if } d(A) \leq R, \\
 &= 0, \quad \text{otherwise;}
 \end{aligned}
 \tag{7.4.1}$$

$$\begin{aligned}
 \tilde{W}_A^{(R)} &= \tilde{W}_A, \quad \text{if } d(A) \leq R \quad \text{and} \quad d(i, \partial\Omega) \leq R \quad \text{for all } i \in A \\
 &= 0, \quad \text{otherwise.}
 \end{aligned}
 \tag{7.4.2}$$

It is then possible to prove a number of propositions allowing one to interchange the limit $R \rightarrow \infty$ with the thermodynamic limit. These results amount, essentially, to continuity of the boundary free energy in the wall potentials under the norms defined in condition **F**. The simplest situation is covered by:

Proposition 7.4.1. Truncated wall potentials. *Under the conditions required for the uniform boundedness of the free energy (Proposition 3.2.2), namely Conditions **F**, **A**, **G(i)**, and **H**, we have*

$$\lim_{\Omega \rightarrow \infty} f_{\times}(K, W, \tilde{W}; \Omega) = \lim_{R \rightarrow \infty} \left[\lim_{\Omega \rightarrow \infty} f_{\times}(K, W^{(R)}, \tilde{W}^{(R)}; \Omega) \right].
 \tag{7.4.3}$$

Proof. We may employ Lemma 4.4.1 to compare the wall free energies of two Hamiltonians describing different walls in a domain Ω in terms of the difference Hamiltonian $\mathcal{Q} = \mathcal{W} - \mathcal{W}^{(R)}$. This yields

$$|f_{\times}(K, W, \tilde{W}; \Omega) - f_{\times}(K, W^{(R)}, \tilde{W}^{(R)}; \Omega)| \leq 2 \langle\langle \mathcal{W} - \mathcal{W}^{(R)} \rangle\rangle / |\mathbf{L}|;
 \tag{7.4.4}$$

where $\langle\langle \cdot \rangle\rangle$ denotes the maximum modulus of the expectation within the various ensembles (with and without the walls). Evidently, one has

$$\begin{aligned} \langle\langle \mathcal{W} - \mathcal{W}^{(R)} \rangle\rangle &\leq \sum_{A \subset \Omega} |W_A - W_A^{(R)}| \|s\|^{|A|}, \\ &\leq |\mathbf{L}| (\|W - W^{(R)}\|_0 + \|W - W^{(R)}\|_1), \end{aligned} \tag{7.4.5}$$

where in the second step the norms introduced in **F(i)** and **F(ii)** have been used to bound (i) the wall interactions coupling the subdomains Ω_1 and Ω_2 (created by the wall), and (ii) the wall terms within the separate subdomains, respectively. On substitution in (7.4.4), the wall area $|\mathbf{L}|$ cancels and the limit $\Omega \rightarrow \infty$ may be taken. Finally, the boundedness of $\|W\|_0$ and $\|W\|_1$ ensures that the right hand side then vanishes as $R \rightarrow \infty$, and this proves (7.4.3).

Similar propositions may be proved in which the range of the associated potentials is held fixed until after the thermodynamic limit; however, in analogy, to the Condition **F** one needs \mathbf{C}_τ , with $\tau > 1$, and a simple, or other sufficiently regular sequence of domains Ω_k . Likewise, the overall free energies, $\tilde{f}_\times(K, W, \tilde{W}; \Omega)$, discussed above, may be dealt with.

8. Periodic Boundary Conditions

8.1. Introduction and Definitions

If one has a box domain $A_{\mathbf{L}}$ formed by pairs of parallel lattice planes, $\mathcal{P}_{\alpha+}$ and $\mathcal{P}_{\alpha-}$ for $\alpha = 1, 2, \dots, d$, one may identify pairs of opposite planes so that the box faces $\mathbf{L}_{(\beta)+}$ and $\mathbf{L}_{(\beta)-}$ become adjacent. If this is done for all d pairs, $(\mathcal{P}_{\alpha+}, \mathcal{P}_{\alpha-})$, one obtains a *box with periodic boundary conditions* or a *lattice torus*, $\Pi_{\mathbf{L}}$, of size $\mathbf{L} = (L_1, L_2, \dots, L_d)$ blocks. Such a torus has *no* boundaries. However, if one identifies only t pairs $(\mathcal{P}_{\beta+}, \mathcal{P}_{\beta-})$, for some $t < d$, one obtains a partial torus or tube, $\Pi_{\mathbf{L}}^t$. It is convenient to label the periodically identified planes $\beta = 1, 2, \dots, t$. Then a tube has a boundary of total area

$$A_{\mathbf{L}}^{(t)} = 2 \sum_{\beta=t+1}^d |\mathbf{L}_{(\beta)}|. \tag{8.1.1}$$

In the case $t = 1$, where only a single pair of box planes are identified, one may speak of a strip. If the lattice symmetry and the dimensions L_β for $\beta > 1$ permit, one may even introduce a twist before identifying the opposite planes \mathcal{P}_{1+} and \mathcal{P}_{1-} ; this yields a Möbius strip!

Now any wall constructed on a plane, say \mathcal{P}_0 parallel to one of the planes $\mathcal{P}_{\gamma\pm}$ and intersecting the underlying box, will, by the construction outlined, lead to the definition of a corresponding wall in the associated torus, $\Pi_{\mathbf{L}}$, or tube $\Pi_{\mathbf{L}}^t$. In view of the use of periodic boundary conditions in many exact or approximate theoretical computations (see e.g. the comments of Fisher and Lebowitz [9]), it is of interest to discuss the free energy of such a wall in a torus or tube. We may define the corresponding *periodic wall* free energy in the usual way, namely via

$$f_\times(K, W; \Pi_{\mathbf{L}}) = [F(K, W; \Pi_{\mathbf{L}}^{d-1}) - F(K; \Pi_{\mathbf{L}})] / 2|\mathbf{L}_{(\gamma)}|. \tag{8.1.2}$$

For tubes $\Pi_{\mathbf{L}}^t$ one must clearly specify the associated wall potentials \tilde{W} acting on the tubes' boundaries and the free energy $F(K, W, \tilde{W}; \Pi_{\mathbf{L}}^{t-1})$ also enters. Similarly,

multiple-wall periodic boundary free energies $\bar{f}_\times(K, W, \tilde{W}; \Pi_{\mathbf{L}}^t)$ may be defined. It is also of interest to discuss the asymptotic behavior of the total free energy, $F(K; \Pi_{\mathbf{L}})$, of a torus. Specifically, one would like to show that no term proportional to $A_{\mathbf{L}} (\equiv A_{\mathbf{L}}^{(0)})$, the area of the underlying box, appears in the asymptotic behavior.

To discuss these points, the meaning of $F(K; \Pi_{\mathbf{L}})$ and $F(K, \tilde{W}; \Pi_{\mathbf{L}}^t)$ must be specified more precisely: i.e. the significance of periodic boundary conditions for the interactions must be explained. For potentials K, W, \tilde{W} of finite ranges R, R^\times , and \tilde{R}^\times realized on $\Pi_{\mathbf{L}}$ or $\Pi_{\mathbf{L}}^t$, the issue is quite straightforward whenever $\min_\alpha \{L_\alpha\} > 2 \max \{R, R^\times, \tilde{R}^\times\}$ i.e. for large enough tori or tubes. More generally for long range interactions one may merely consider truncations of the potentials at a range $R = \frac{1}{2} \min_\alpha \{L_\alpha\}$; this serves to remove interference efforts around the torus. However, as discussed by Fisher and Lebowitz [9], it is more natural to define ‘‘periodized interactions’’, K^Π , acting on the underlying box $A_{\mathbf{L}}$, by considering the couplings of the spins in $A_{\mathbf{L}}$ with the corresponding spins in the periodically repeated images of $A_{\mathbf{L}}$. The explicit realization of this idea is straightforward and we will not present the details (but see [6]).

8.2. Thermodynamic Limits

It is clear from the definitions that a torus or tube cannot be embedded in a larger domain (periodic or otherwise) which has greater dimensions in the periodic directions. This simple geometrical fact presents a serious obstacle to the techniques based on the Griffiths inequalities which we have developed so far. However, some progress is possible and will be reported briefly here.

Uniform boundedness of the periodic wall free energies $f_\times(\Pi_{\mathbf{L}})$, $\bar{f}_\times(\Pi_{\mathbf{L}})$, etc., is equivalent to the statement that the total free energy of a box \mathcal{A} (or partial torus Π^t) differs from the total free energy of the corresponding torus Π by at most a surface term. For continuous particle systems with pair interactions such a result has been proved by Fisher and Lebowitz [9] using appropriate restriction (analogous to \mathbf{C}_τ with $\tau > 1$). For our lattice spin systems, more general results can be established using the methods of Sects. 1.4, 2.3 and Lemma 4.4.1. Without proof we quote:

Proposition 8.2.1. *Uniform boundedness. Under Conditions \mathbf{F} and \mathbf{A} , there are bounds*

$$|f_\times(K, W; \Pi_{\mathbf{L}})| \leq C_\times(K, W), \quad |\bar{f}_\times(K, W; \Pi_{\mathbf{L}})| \leq \bar{C}_\times(K, W), \tag{8.2.1}$$

independent of \mathbf{L} , and similarly for $f_\times(K, W, \tilde{W}; \Pi_{\mathbf{L}}^t)$, etc. \square

Although one cannot embed a torus or a tube in a larger domain, one can convert it to a box by cutting it by d or t ancillary walls. In general, one cannot control the effects of these ancillary walls by the previous techniques. However, consider a strip ($t=1$), which is long in the periodic direction, $\alpha=1$, so that the transverse cross-sectional area, $|\mathbf{L}_{(1)}| = \prod_{\alpha=2}^d L_\alpha$, is small compared to the areas, $|\mathbf{L}_{(\beta)}| (\beta > 1)$, of all lengthwise sections, by a factor of order $1/L_1$. Then, given interaction potentials K satisfying $\mathbf{F}(\mathbf{i})$, we may use Lemma 4.4.1 to compare the free energies of lengthwise walls in the strip and in the underlying box. Specifically,

one may show that the difference

$$|f_x(K, W, \tilde{W}; \Pi_{\mathbf{L}}^1) - f_x(K, W, \tilde{W}; A_{\mathbf{L}})|, \tag{8.2.2}$$

for a wall parallel to a plane $\mathcal{P}_{\gamma\pm}$ (with $\gamma \neq 1$) and with, say, subfree associated boundary potentials \tilde{W} , is at most of order

$$|\mathbf{L}_{(1)}|/|\mathbf{L}_{(\gamma)}| = L_\gamma/L_1. \tag{8.2.3}$$

If this ratio vanishes in the thermodynamic limit, corresponding to an infinitely long, thin strip, then the limiting wall free energy for the strip is equal to $f_x^0(K, W)$, the standard box free energy for subfree associated conditions.

This argument applies equally to a Möbius strip and further generalizes to any wall which is parallel to a free face (i.e. normal to a nonperiodic direction) of a tube, Π^t , which is “flat” in the sense that the area of the wall is asymptotically large compared with the areas of the ancillary walls needed to convert the tube to a box. Thus we have:

Proposition 8.2.2. *Flat tubes.* For a tube $\Pi_{\mathbf{L}}^t$ with ferromagnetic bulk and wall potentials, K and W , describing a wall parallel to the nonperiodic face $\mathbf{L}_{(d)}$, and subfree associated wall potentials, \tilde{W} , all meeting the conditions of Theorems 4.4.2 and 4.4.1, the wall free energy obeys

$$\lim_{\mathbf{L} \rightarrow \infty} f_x(K, W, \tilde{W}; \Pi_{\mathbf{L}}^t) = f_x^0(K, W), \tag{8.2.4}$$

provided the limit $\mathbf{L} \rightarrow \infty$ is taken in such a way that $L_\beta/L_d \rightarrow \infty$ for all $\beta = 1, 2, \dots, t$.

Although one cannot embed a torus or a tube in a larger nonperiodic domain, one can decompose a torus into tubes, and a tube into lower order tubes or boxes. Via Proposition 3.3.1 this leads to a series of lower bounds on the partial wall free energies for walls in a torus or tube, which in turn yield:

Proposition 8.2.3. *Subfree lower bounds.* For potentials, K and W , and subfree associated potentials, \tilde{W} , all meeting the conditions of Theorem 4.4.2, one has

$$\begin{aligned} \liminf_{\mathbf{L} \rightarrow \infty} f_x^\pm(K, W; \Pi_{\mathbf{L}}) &\geq \liminf_{\mathbf{L} \rightarrow \infty} f_x^\pm(K, W, \tilde{W}; \Pi_{\mathbf{L}}^t) \geq \\ &\geq \liminf_{\mathbf{L} \rightarrow \infty} f_x^\pm(K, W, \tilde{W}; \Pi_{\mathbf{L}}^t) \geq f_x^{\pm 0}(K, W), \end{aligned} \tag{8.2.5}$$

where $t \geq t'$, and similarly for multiple wall partial free energies for subfree W . \square

A precisely analogous series of *upper bounds* on the partial free energies for systems with saturating spins and potentials of finite range follows on a torus, or on tubes with superferromagnetic associated boundary conditions, from Proposition 3.3.2. We will not trouble to state these results formally but will discuss the special case of a free torus in further detail. Specifically, consider the overall boundary free energy of a box constructed by cutting d walls with subfree potentials $W = \{W_{(a)}\}$ in a torus, namely,

$$f_x^H(K, W; \mathbf{L}) = [F(K, W; A_{\mathbf{L}}) - F(K, \Pi_{\mathbf{L}})]/A_{\mathbf{L}}, \tag{8.2.6}$$

where $A_{\mathbf{L}} \equiv A_{\mathbf{L}}^{(0)}$ [see (8.1.1)] is the total surface area of the box $A_{\mathbf{L}}$. For simplicity we may suppose there is high lattice symmetry; then we have:

Proposition 8.2.4. *Torus wall free energy bounds.* For bulk interactions, K , and subfree wall potentials, W , meeting the conditions of Theorem 4.4.1, the overall torus

wall free energy [defined in (8.2.6)] satisfies

$$f_{\times}^0(K, W) \geq \limsup_{\mathbf{L} \rightarrow \infty} f_{\times}^{\mathbf{II}}(K, W; \mathbf{L}), \tag{8.2.7}$$

$$\liminf_{\mathbf{L} \rightarrow \infty} f_{\times}^{\mathbf{II}}(K, W; \mathbf{L}) \geq f_{\times}^*(K, W), \tag{8.2.8}$$

where in (8.2.8) saturating spins and finite range interactions are supposed. Furthermore, the lattice symmetries are assumed to allow the d -fold transformation of any box-defining lattice plane, \mathcal{P}_{∞} , into any other plane, $\mathcal{P} = \mathcal{R}_{\rho_{\mathcal{P}}}\mathcal{P}_{\infty}$, and the bulk and wall potentials are taken to respect these symmetries. \square

Now, under rather general conditions, we expect to have $f_{\times}^0(K, W) = f_{\times}^*(K, W)$. For the symmetric situation this then implies

$$\lim_{\mathbf{L} \rightarrow \infty} f_{\times}^{\mathbf{II}}(K, W; \mathbf{L}) = f_{\times}^{\mathbf{II}}(K, W; \infty) = f_{\times}^0(K, W). \tag{8.2.9}$$

More generally we expect this limiting equality to hold in many cases even for systems with nonsaturating spins or long range interactions (when f_{\times}^* is not defined). Indeed one may prove (8.2.9) on the basis of a correlation decay assumption [6]. When (8.2.9) is valid, we may use Theorem 7.3 to discuss the asymptotic behavior of the total free energy of a torus and show explicitly that a torus has no surface free energy!

Proposition 8.2.5. *Free energy of a torus. If the asymptotic equality (8.2.9) holds [where $f_{\times}^{\mathbf{II}}$ is defined in (8.2.6)] for subfree W and K satisfying the conditions of Theorem 7.3, one has*

$$F(K; \Pi_{\mathbf{L}}) \equiv F(K^{\mathbf{II}}; A_{\mathbf{L}}) = |A_{\mathbf{L}}|f_{\infty}(K) + o(A_{\mathbf{L}}). \tag{8.2.10}$$

(As in Proposition 8.2.4, a d -fold symmetry of the lattice and the potentials is assumed.)

Proof. A straightforward application of Theorem 7.3 to the definition (8.2.6) yields

$$F(K; \Pi_{\mathbf{L}}) \approx |A_{\mathbf{L}}|f_{\infty}(K) + A_{\mathbf{L}}[f_{\times}^0(K, W) - f_{\times}^{\mathbf{II}}(K, W; \mathbf{L})], \tag{8.2.11}$$

which, with (8.2.9) establishes the proposition. \square

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