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Wall and Boundary Free Energies

I. Ferromagnetic Scalar Spin Systems

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Abstract. The existence of wall or boundary free energies is discussed generally and analyzed explicitly for general lattice systems with scalar (real-valued) spin variables. For systems with ferromagnetic (positive) spin interaction potentials, K, in the bulk and W, for the walls, correlation inequalities and appropriate stability and tempering conditions are used to establish the existence and uniqueness of the limiting free energy per unit area, $f_{\times}(K, W)$, of an infinite planar wall.

Contents

0. Introduction

In the statistical mechanics of macroscopic systems, a mechanical system contained in a spatial domain Ω is specified by a Hamiltonian $\mathscr{H}(\Omega)$ depending on $N(\Omega)$ microscopic variables or "degrees of freedom". Thence the partition function, $Z(\Omega)=Z[\mathscr{H}(\Omega)]$ and total free energy $F(\Omega)=F[\mathscr{H}(\Omega)]$ are defined by

$$e^{\bar{F}(\Omega)}=Z(\Omega)=\mathrm{Tr}_{\Omega}\{e^{\bar{\mathscr{H}}(\Omega)}\}, \tag{0.1}$$

where, with T denoting the temperature, we have

$$\bar{F}(\Omega)=-F(\Omega)/k_B T, \qquad \bar{\mathscr{H}}(\Omega)=-\mathscr{H}(\Omega)/k_B T, \tag{0.2}$$

while Tr_{Ω} represents the appropriate trace or integration over the $N(\Omega)$ microscopic variables. Provided the interaction potentials entering $\mathscr{H}$ are physically reasonable it is then expected that $F(\Omega)$ should become asymptotically proportional to the size of the system as measured, for example, by the volume $V(\Omega)=|\Omega|$ or by the number of degrees of freedom, $N(\Omega)$, assuming that these have some asymptotic density, say, $\varrho \approx N/V$. Formally the thermodynamic limit may be defined in terms of the free energy density

$$f(\Omega)=\bar{F}(\Omega)/V(\Omega)=-F(\Omega)/Vk_B T, \tag{0.3}$$

by

$$f_{\infty}=\lim_{\Omega\to\infty} f(\Omega), \tag{0.4}$$

where the limit is taken through a sequence of domains $\{\Omega_k\}$ with $V(\Omega)\to\infty$. As a function of the thermodynamic variables, such as temperature, magnetic field, etc., the limiting free energy (density), f_{∞}, should possess certain important properties such as continuity, differentiability and convexity. The last of these implies thermodynamic stability and such explicit results as the positivity of compressibilities, susceptibilities, and specific heats. Furthermore, one anticipates that in the limit of an infinitely large system these properties, and f_{∞} itself, should be independent of the detailed *shape* of the domains, Ω, bounding the system and independent of the particular boundary conditions or wall potentials acting at the boundary, $\partial\Omega$, of Ω.

The mathematical problem of the existence of the thermodynamic limit was initially studied by Van Hove [1] for classical particle systems in the canonical ensemble. Yang and Lee [2] considered the grand canonical ensemble. More recently, Ruelle and Fisher [3–6] have rigorously established the existence of the thermodynamic limit for classical and quantal particle systems and proved certain crucial properties including continuity, almost-everywhere differentiability, and convexity, subject to suitable restrictions on the interaction potentials and domain shapes. (The *tempering conditions*, which play a vital role in the proofs, entail sufficiently rapid decay of the interaction potentials at large separations, which excludes Coulomb forces. However, the existence of the thermodynamic limit for neutral Coulomb systems has been settled by the work of Dyson and Lenard [7], Lieb and Lebowitz [8].) A proof of the existence of the thermodynamic limit for systems of Ising spins on a lattice has been carried through by Griffiths [9] (see also Ruelle [6]).

It is of both theoretical and practical interest to enquire more closely into the *rate* at which the thermodynamic limit is approached for particular sequences of domains, $\{\Omega_k\}$, and into how this rate is determined by the interactions in the bulk of a system and, especially, by the nature of the wall or boundary conditions. A first step in this direction was taken by Fisher and Lebowitz [10] who considered rectangular, or box domains Λ, on which *periodic boundary conditions* were imposed, thus converting the domain into a torus, Π. Subject to mild restrictions beyond the usual tempering and stability conditions [3–6], they showed that the limiting free energy densities $f_\infty(\Pi)$ and $f_\infty(\Lambda)$ were identical. (For the boxes, Λ, they assumed "hard wall" or free boundary conditions.)

More generally for sufficiently regular domains Ω of volume $V(\Omega)$ and surface or boundary area $A(\Omega)$ (taking V und A with appropriate meanings in d-dimensional Euclidean space), thermodynamics suggests that the free energy should vary as

$$\bar{F}(\Omega) \equiv V(\Omega) f(\Omega) = V(\Omega) f_\infty + A(\Omega) f^\times + o[A(\Omega)], \tag{0.5}$$

when $V(\Omega)$, $A(\Omega) \to \infty$, where $f^\times$ is the *boundary* or *wall free energy* (per unit area) which should, like f_∞, be independent of the shape of Ω but must, presumably, depend explicitly not only on the bulk interaction potentials but also on the nature of the wall potentials and on any fields acting only near the boundaries. Since a torus, Π (periodic boundary conditions), has no boundary, $A(\Pi) \equiv 0$, this leads to the problem of whether the difference between the free energy, $F(\Lambda)$, of a box Λ and the free energy, $F(\Pi)$, of the corresponding torus, is asymptotically proportional to the surface area $A(\Lambda)$. In fact, Lebowitz and Fisher [10] were able to prove that if the pair interaction potentials decrease sufficiently rapidly (roughly speaking, one power of distance faster than required for the existence of the limiting bulk free energy) then the difference $F(\Lambda) - F(\Pi)$ for free or hard wall conditions, is at most of the order of $A(\Lambda)$. More precisely, however, one would like to establish the existence and, as far as possible, the uniqueness of the limit

$$f^\times = \lim_{\Omega \to \infty} \frac{F(\Lambda) - F(\Pi)}{A(\Lambda)}. \tag{0.6}$$

However, other definitions of the boundary free energy, $f^\times$, easily suggest themselves and the equivalence of such different definitions should also be considered.

In this and subsequent papers we address these issues. Our present results are for *lattice spin systems* such as Ising-like models with continuous, scalar spins $s_i \in \mathbb{R}$ at the lattice sites i. A following paper will establish conditions sufficient to prove (0.6) and analogues involving partially periodic (e.g. cylinder) boundary conditions. In this paper we first discuss the creation of a pair of walls or boundaries by dividing a d-dimensional lattice domain into two subdomains and severing all interactions between them. The change in total free energy associated with this process provides a working definition of the boundary free energy for "free" boundaries (in a finite system) which plays a central role in our analysis. Change of the potentials near the boundaries in each subdomain yield different types of wall. Certain properties of the boundary free energy will follow directly from this formalism—in particular, the *convexity* of $f^\times$ as a function of the boundary or surface variables (such as magnetic fields acting only on the boundary spins or exchange couplings between surface spins and those in adjacent layers). The dependance on the bulk variables, such as the overall temperature, is more complex. Some monotonicity and positivity properties will be established; however, several counterexamples indicate the limits on possible results. In particular, the *nonuniqueness* of the expansion (0.5) under thermodynamic conditions allowing two-phase coexistence must be anticipated (see Section 2.7).

By specializing to box domains, Λ, the existence and uniqueness of the limiting boundary free energy will be proved for Ising-like spins interacting through ferromagnetic (i.e., positive) potentials. Incidentally, the existence and uniqueness of the free energy of a "grain boundary" or an interfacial "seam" of altered interactions, is established. Our basic tools are the Griffiths inequalities [11, 12] and their generalizations [13], in particular, those due to Kelly and Sherman [13, see also 14]. In a following paper we will consider more general domain shapes and more general boundary conditions. We will also consider "extended" boundaries (e.g. on *all* external boundaries of a box domain) and demonstrate that the boundary free energy is unaltered under reasonable conditions. For these latter results stronger restrictions are required on the decay of the interactions, and we assume thermodynamic conditions for which the decay of the bulk correlation functions can be controlled. (In the present paper the decay of the correlation functions is *not* invoked.)

Our analysis for scalar or Ising-like spins has been extended to planar or two-component, XY-like spins ($\vec{s}_i \in \mathbb{R}^2$ with $|\vec{s}_i| = 1$). The results are almost identical but the detailed proofs will be described separately.

It should be remarked that results bearing directly on (0.5) and (0.6) have been obtained for various two-dimensional lattice systems by exact, explicit analysis of closed form expressions for the partition functions. Thus Fisher [15] established the existence and value of the surface free energy for an $m \times n$ rectangular lattice filled with hard dimers. Ferdinand [16], in a more detailed analysis, showed explicitly that the boundary contribution to the total free energy vanished for a torus, and he evaluated explicitly the $o(A)$ terms in (0.5) for both torus and box [finding constant terms, $O(1)$, depending on the shape factor, m/n, and on the parity of m and n]. Likewise Fisher and Ferdinand [17, 18] calculated the boundary (and also grain boundary or seam) free energies for square and triangular Ising lattices with nearest-neighbor interactions in zero magnetic field. McCoy and Wu [19] evaluated the boundary free energy more generally for the case where a magnetic field is imposed on the boundary spins. In fact, McCoy and Wu considered a cylinder (with periodic boundary conditions imposed in one direction). The $o(A)$ terms were examined in detail by Au-Yang and Fisher [20] for the case of an infinite strip ($m \to \infty, n \gg 1$) especially as the critical temperature, T_c, is approached. These calculations serve, incidentally, to demonstrate that the boundary free energy, $f^{\times}(T)$, cannot in general be convex in $1/T$, the inverse bulk temperature; specifically the boundary specific heat, $C^{\times}(T)$, varies as $1/(T-T_c)$ as $T \to T_c\pm$. Similarly, the boundary energy, $U^{\times}(T) \propto \partial f^{\times}/\partial T$ varies as $\ln|T-T_c|$ and is unbounded.

In the area of rigorous (but nonexplicit) results Lenard and Newman [21] have proved asymptotic results for the two-dimensional, polynomial scalar field theory, $P(\phi)_2$, with Dirichlet boundary conditions and in circumstances where the mass is nonzero, which are analogous to (0.5). In view of the connection between the $P(\phi)_2$

field theory and scalar lattice spin systems with polynomial spin weights and nearest neighbor interactions [22], one can probably prove results by similar methods for such spin systems under appropriate boundary conditions and for states in which the correlations are *known* to decay exponentially. However, no assumptions regarding the decay of spin correlations are employed in this paper.

An outline of this paper is as follows [see also the Contents list presented above]: In Section 1 we set out definitions for lattice spin systems including, in particular, a specification of the lattice structure which allows for a finite number of spins per cell. The basic spin correlation inequalities for the systems under consideration are discussed in Subsection 1.3, while in Subsection 1.4 we characterize "acceptable" boundary conditions (which leave the limiting bulk free energy invariant). Definitions of planar walls and boundaries and of the corresponding free energies are presented in Section 2, in terms of the dissection of a domain Ω into two disjoint subdomains, Ω_1 and Ω_2, by a corrugated plane. The boundary free energy so defined is reexpressed in terms of spin correlation functions, using a coupling parameter device, in Section 3. Thence various properties are established including convexity, boundedness, and basic inequalities relating to decomposition of Ω into subdomains. Finally in Section 4 the central results of subadditivity and monotonicity for box domains are established and the existence of the limiting wall or boundary free energy per unit area of an infinite planar wall is thence proved for arbitrary sequences of box domains. Partial results are established concerning the uniqueness of the limiting wall free energy under variations of the "associated boundary conditions" (imposed on the original boundaries of Ω). The asymptotic analysis uses lemmas on multiply subadditive, monotonic functions which may be useful in other contexts.

1. Lattice Spin Systems

1.1. Lattice Geometry

Because of the appreciable calculational interest in lattice models of various structures we treat lattices more general than the customary d-dimensional hypercubic lattices, $\mathbb{Z}^d$. We thus define a *lattice*, $\mathscr{L}$, in d-dimensional Euclidean space as an infinite set of *lattice sites* arranged in a translationally invariant array of identical *cells* each containing q sites. The cells are indexed by integer vectors $\boldsymbol{n}=(n_\alpha)\in\mathbb{Z}^d$ and the *cell corners* are specified by the *lattice vectors*

$$\boldsymbol{R}=\sum_{\alpha=1}^{d} n_\alpha \boldsymbol{a}_\alpha, \tag{1.1.1}$$

where the d linearly independent vectors $\boldsymbol{a}_\alpha$ ($\alpha=1,2,\ldots,d$) represent the edges of the origin cell ($\boldsymbol{n}=\boldsymbol{0}$). Individual sites will be labelled $i,j,\ldots$ with sites $i=1,2,\ldots,q$ located in the origin cell $\boldsymbol{n}=\boldsymbol{0}$. Each site belongs to a unique cell $\boldsymbol{n}_i$. Translation by any lattice vector $\boldsymbol{R}$ transforms $\mathscr{L}$ into itself.

A (lattice) *domain*, $\Omega, \Lambda, \Gamma, \ldots$ of $\mathscr{L}$ is a finite set of $|\Omega|, |\Lambda|, |\Gamma|, \ldots$ distinct sites. The (lattice) *boundary* or *perimeter*, $\partial\Omega$, of a domain Ω is the set of sites in Ω which belong to cells of Ω which either contain sites not in Ω or adjoin (i.e., have a cell face in common with) cells containing sites not in Ω. Unless explicitly stated we will consider only domains, Ω, which are *cell-connected* in the sense that any two sites in Ω can be joined by a continuous curve lying wholly within cells containing sites of Ω.

A *collection*, A, of sites from a domain Ω, is a finite selection of sites drawn, *with repeats allowed*, from the set Ω; we will write $A \subsetneq \Omega$. (Sylvester [23] uses the term *family* in place of collection.) The number of *distinct* sites in a collection will be written $|A|$ but $\|A\|$ will denote the total number of sites in a collection *counting repeats*.

A domain Ω, a plane $\mathscr{P}$, or a collection of sites A, translated by a lattice vector will be written $\Omega + \boldsymbol{R}$, $\mathscr{P} + \boldsymbol{R}$, and $A + \boldsymbol{R}$ respectively. Reflection and rotation operations on the lattice will be denoted $\mathscr{R}$, and $\mathscr{R}\Omega$ and $\mathscr{R}A$ will describe domains and collections transformed by $\mathscr{R}$. By an obvious extension of the notation we may write $\mathscr{L} + \boldsymbol{R} = \mathscr{L}$ and $\mathscr{R}\mathscr{L} = \mathscr{L}$. In defining planar walls or boundaries we will consider only lattices which have certain minimal elements of reflection or rotation symmetry: the specific restrictions will be stated in Section 2.2 below (Condition **D**).

A collection of sites *couples* (or links) a set of (sitewise) disjoint domains if it contains sites from each domain. We will take $\Omega_1 \cdot \Omega_2 \cdot \ldots \cdot \Omega_m$ to denote the set of all collections of sites coupling the domains $\Omega_1, \Omega_2, \ldots, \Omega_m$ and drawn from $\bigcup_{k=1}^{m} \Omega_k$.

The *separation* or *distance* between any pair of sites, collections of sites, domains, or other sets of sites, $\mathscr{S}$, will be denoted $r(i,j)$, $r(i,A)$, $r(A,B)$, $r(A,\Omega)$, $r(\Omega_1,\Omega_2)$, $r(i,\mathscr{S})$, etc., and will, in each case, denote the minimum (or infimum) distance between sites in the respective collections, domains, etc. Likewise, the *diameter*, $d(\Omega)$, $d(A)$, ... of a domain, collection of sites, etc., is defined by

$$d(\Omega) = \max_{i,j \subset \Omega} \{r(i,j)\}, \tag{1.1.2}$$

and so on. The notation $d_\perp(A)$, etc., will be used to denote the *caliper diameter* measured in a direction normal to a given plane $\mathscr{P}$.

1.2. Spins and Interactions

In specifying the spin systems to be discussed we aim for reasonable generality as regards the many-point and long range character of the interactions. However, we do not strive to cover all possible systems. Our main tools will be bounds and inequalities for the correlation functions; the range of validity of such results will yield the most significant restrictions on the analysis. A very useful discussion of continuous scalar spin systems has been given by Sylvester [23] and we mainly follow his formulation.

With each site i we associate a real-valued spin variable $s_i \in \mathbb{R}$ subject to a spin weighting σ which is an even probability measure which decays sufficiently rapidly at infinity that

$$\mathrm{Tr}_i\{e^{J|s_i|^p}\} = \int \exp(J|s_i|^p) d\sigma(s_i) < \infty, \qquad \text{for all } J. \tag{1.2.1}$$

Here p is a positive integer specifying the maximum size $\|A\|$ of any collections of spins, A, on which nonzero interactions will be defined. In other words p will be the polynomial degree of the Hamiltonian (see below). In case interactions involve many-point interactions of unbounded order or spin-multiplicities of unbounded degree (1.2.1) must hold with $|s_i|^p$ replaced by an appropriate limiting function increasing more rapidly as $|s_i|\to\infty$. Ordinary Ising, spin $\frac{1}{2}$ variables are, of course, specified by

$$d\sigma(s)=\tfrac{1}{2}[\delta(s-1)+\delta(s+1)]ds. \tag{1.2.2}$$

If the support of the measure σ extends only to $|s|\leqq\|s\|$ we say the spins are *saturating* with *spin modulus* $\|s\|$. (Of course one could rescale so that $\|s\|=1$ but it is more informative to leave the spin modulus in evidence.) More generally $\|s\|$ will denote an effective spin modulus: see Section 1.4 below.

A set of values $\{s_i\}_\Omega$ for $s_i\subset\Omega$ will specify a *spin configuration* in Ω. The product, with repeats, of all spins in a collection A is defined by

$$s_A=\prod_{i\in A}s_i. \tag{1.2.3}$$

For saturating spins we have $|s_A|\leqq\|s_A\|=\|s\|^{\|A\|}$.

A *set of (reduced) interaction potentials* $K=\{K_A\}=-\Phi/k_BT$ *of degree* p is a real-valued function on the collections of sites $A\subsetneqq\mathscr{L}$ with $\|A\|\leqq p$, which respects the lattice symmetries so that

$$K_{A+\boldsymbol{R}}=K_A \quad\text{and}\quad K_{\mathscr{R}A}=K_A. \tag{1.2.4}$$

A potential acting on a single site, $A=\{i\}$, is called a field $h_i=K_i$. When convenient we will write $K_A=K(A)$.

Finite range potentials are those for which the *range*

$$R^\infty=\max_{A,K_A\neq 0}\{d(A)\} \tag{1.2.5}$$

is bounded.

A set of *potentials*, K^Ω, *for a domain* Ω, is defined similarly on all collections $A\subsetneqq\Omega$. In general these potentials will not have the lattice symmetries as defined above. [However, we could require that (1.1.5) hold *within* Ω i.e., whenever A, $A+\boldsymbol{R}$, and $\mathscr{R}A$ are drawn from Ω.]

The correlation inequalities on which our analysis rests (at this stage) have been established for:

Definition 1.2. Purely ferromagnetic interactions in a domain Ω or a lattice $\mathscr{L}$, are those for which

$$K_A^\Omega\geqq 0 \quad\text{or}\quad K_A\geqq 0, \tag{1.2.6}$$

for all A drawn from Ω or from $\mathscr{L}$, respectively.

Our strategy of proof could also be based on systems for which the Fortuin-Kasteleyn-Ginibre [14] sets of inequalities apply, such as lattice gases described by two-valued occupation variables $\varrho_i=0,1$, and with positive interaction potentials. When reexpressed in terms of Ising spins, $s_i=\pm1$, the FKG conditions admit spin interactions which are not purely ferromagnetic. However, we have not carried through the details of this analysis.

A (reduced) *Hamiltonian* on a domain Ω is defined by

$$\bar{\mathscr{H}}(\Omega) = -\mathscr{H}(\Omega)/k_B T = \sum_{A \subseteq \Omega} K_A^\Omega s_A\,, \tag{1.2.7}$$

and the corresponding partition function is

$$Z(K,\Omega) = Z[\mathscr{H}(\Omega)] = \mathrm{Tr}_\Omega\{e^{\bar{\mathscr{H}}(\Omega)}\}\,, \tag{1.2.8}$$

where $\mathrm{Tr}_\Omega = \prod_{i \in \Omega} \mathrm{Tr}_i$. The *total free energy*, $F(K,\Omega)$, of the domain, and the free energy per site, f, are defined by

$$f(K,\Omega) = |\Omega|^{-1} F(K,\Omega) = |\Omega|^{-1} \ln Z[\mathscr{H}(\Omega)]\,. \tag{1.2.9}$$

Note that by well known methods [3–6, 24] one can show that $f(K,\Omega)$ is a *convex downward* (or *concave*) function on each K_A^Ω and on all the K_A^Ω together.

If the domain potentials K_A^Ω are equal to those for the infinite lattice the corresponding Hamiltonian is denoted

$$\bar{\mathscr{H}}^0(\Omega) = \sum_{A \subseteq \Omega} K_A s_A\,, \tag{1.2.10}$$

and is said to be the Hamiltonian of the domain Ω with *free boundary conditions.* The corresponding free energy per site will likewise be called $f^0(K,\Omega)$. Note that the free boundary conditions defined here differ from the boundary conditions typically used in field theoretic polynomial spin models [22] and also from "hard wall" conditions in the lattice gas interpretation of the standard Ising model.

The expectation value of a function Q of spins in Ω is defined as usual by

$$\langle Q \rangle_\Omega = \mathrm{Tr}_\Omega\{Q e^{\bar{\mathscr{H}}(\Omega)}\}/Z[\bar{\mathscr{H}}(\Omega)]\,. \tag{1.2.11}$$

When the spins are saturating, one or more fields h_j^Ω may be allowed to approach $\pm\infty$ in the calculation of expectation values. The same results can be achieved with a modified Hamiltonian $\bar{\mathscr{H}}^\dagger$, derived from $\bar{\mathscr{H}}$ by (i) deleting the infinite terms $h_j^\Omega s_j$, and (ii) replacing the "frozen" spin variables s_j by $\pm\|s\|$ (as $h_j^\Omega \to \pm\infty$) in all other interaction terms, and (iii) dropping any constant contributions involving only frozen spin terms. The residual trace operations over the frozen (or saturated) spins may be dropped.

1.3. Spin Correlation Inequalities

For *purely ferromagnetic interactions* in a domain Ω spin correlation inequalities of the Griffiths-Kelly-Sherman type [11–13] are valid and will be important for our analysis. For polynomial spin interactions of the type discussed above, Sylvester [23] has presented rather transparent proofs. Under the conditions stated by Sylvester [23], and presumably with even greater generality, we have the GKS inequalities

$$\langle s_A \rangle \geqq 0\,, \tag{1.3.1}$$

$$\langle s_A s_B \rangle - \langle s_A \rangle \langle s_B \rangle \geqq 0\,. \tag{1.3.2}$$

These inequalities yield an elementary but most useful result:

Lemma 1.3. *If $\langle\cdot\rangle^\zeta$ denotes an expectation value taken with the Hamiltonian $\mathscr{H}^\zeta(\Omega) = \mathscr{H}_0(\Omega) + \zeta\mathscr{H}_1(\Omega)$ in which $\mathscr{H}_0$ and $\mathscr{H}_1$ are purely ferromagnetic then $\langle s_A\rangle^\zeta$ is monotonic nondecreasing in ζ and, in particular,*

$$\langle s_A\rangle^{\zeta=1} \geqq \langle s_A\rangle^{\zeta=0}. \tag{1.3.3}$$

Proof. Since $\mathscr{H}_1$ is purely ferromagnetic we may write $\bar{\mathscr{H}}_1 = \sum_{B\subseteq\Omega} K_B'^\Omega s_B$ with $K_B'^\Omega \geqq 0$. Then we have

$$\langle s_A\rangle^{\zeta=1} - \langle s_A\rangle^{\zeta=0} = \int_0^1 d\zeta \frac{d\langle s_A\rangle^\zeta}{d\zeta},$$

with

$$\frac{d}{d\zeta}\langle s_A\rangle^\zeta = \sum_{B\subseteq\Omega} K_B'^\Omega[\langle s_A s_B\rangle^\zeta - \langle s_A\rangle^\zeta \langle s_B\rangle^\zeta], \tag{1.3.4}$$

from which the lemma follows by (1.3.2) and the nonnegativity of $K_B'^\Omega$. □

1.4. Thermodynamic Limit and Acceptable Boundary Conditions

Our interest will be restricted to sets of interactions K for which the thermodynamic limit exists and is unique for reasonable sequences of domains. In addition, to establish the finiteness of the boundary free energy, $f^\times$, we will need bounds on the spin correlation functions $\langle s_A\rangle_\Omega$ (uniform in Ω). In the case of *saturating spins* the trivial

A. *Uniform correlation bound*

$$|\langle s_A\rangle_\Omega| \leqq \|s\|^{\|A\|}, \quad (\text{all } \Omega), \tag{1.4.1}$$

will suffice. In the same circumstances a proof of the thermodynamic limit along well established lines [3–6] follows from the

B. *Stability condition*

$$\begin{aligned}\|K\| &= \sum_{i=1}^{q} \sum_{A\ni i} \frac{|K_A|}{|A|} \|s\|^{\|A\|}, \\ &= \sum_{A\subset[\![A]\!]} |K_A| \, \|s\|^{\|A\|} < \infty, \end{aligned}\tag{1.4.2}$$

in which $[\![A]\!]$ denotes a complete set of collections A which are *translationally inequivalent* on $\mathscr{L}$. Finite range potentials of finite degree, p, certainly satisfy ***B***. For pair potentials [$K_A = 0$ unless $A = \{i, j\}$] decreasing with separation as $[r(i,j)]^{-d-\sigma}$, one requires $\sigma > 0$ for stability; similar sufficient power-law decay conditions can be stated for many-site interactions [4].

More generally, however, in the case of unbounded or nonsaturating spins the available results are more restricted. Sylvester [23] has discussed the situation recently and has stated and proved various theorems for potentials of finite range, for pair potentials, etc. Lebowitz and Presutti [25] have extended the discussion to

Hamiltonians more general than the spin polynomials (1.2.7). (See also Ruelle [26, 27].) Rather than enter into these questions we will merely restrict attention to systems and to thermodynamic states for which bounds of the form $\boldsymbol{A}$ may be established with some appropriate assigned value of $\|s\|$, which is then an *effective spin modulus*. For such systems the condition $\boldsymbol{B}$ should, perhaps with some slight strengthening, suffice to ensure the existence and uniqueness of the thermodynamic limit for free boundary conditions, namely,

$$f_\infty(K) = \lim_{\Omega\to\infty} f^0(K,\Omega), \tag{1.4.3}$$

provided the sequences $\{\Omega_k\}_{k\to\infty}$ used in taking the limit $\Omega\to\infty$ satisfy various standard shape conditions [3–6] which, in particular, will imply that $|\partial\Omega|/|\Omega|\to 0$. Henceforth the notation $\Omega\to\infty$ will always imply a suitably restricted sequence of domains. The most obvious example [4] is a

Definition 1.4. Simple sequence of domains:

$$\Omega_k = \{i; i\in \xi_k^d\tilde{\Omega}_0\}, \qquad \xi_k\to\infty, \tag{1.4.4}$$

where $\tilde{\Omega}_0$ denotes a compact, simply connected continuum domain which is isotropically expanded by factors ξ_k to form the continuum domain $\xi_k^d\tilde{\Omega}_0$.

Further concrete examples will occur below in considering walls explicity. We remark that proof of the thermodynamic limit for purely ferromagnetic interactions is particularly straightforward if Lemma 1.3 is utilized.

Now consider a general sequence of domains for which $K_A^\Omega\to K_A$ as $\Omega\to\infty$ and define the *deviation Hamiltonian* by

$$\Delta\bar{\mathscr{H}}(\Omega) = \bar{\mathscr{H}}(\Omega) - \bar{\mathscr{H}}^0(\Omega) = \sum_{A\subseteq\Omega} \Delta K_A^\Omega s_A, \qquad \Delta K_A^\Omega = K_A^\Omega - K_A. \tag{1.4.5}$$

This clearly isolates any special boundary conditions incorporated in K^Ω as well as including terms which might, physically, be rather regarded as changes in bulk fields or interactions. Now the simple inequality $1/\langle e^{-Q}\rangle \leqq e^{\langle Q\rangle} \leqq \langle e^Q\rangle$, yields

$$f(\Omega) - f^0(\Omega) = \ln\langle e^{\Delta\bar{\mathscr{H}}}\rangle_\Omega^0/|\Omega| \geqq \langle\Delta\bar{\mathscr{H}}\rangle_\Omega^0/|\Omega|, \tag{1.4.6}$$

where the superscript zero denotes an expectation taken with free boundary conditions, and

$$f(\Omega) - f^0(\Omega) = -\ln\langle e^{-\Delta\bar{\mathscr{H}}}\rangle_\Omega/|\Omega| \leqq \langle\Delta\bar{\mathscr{H}}\rangle_\Omega/|\Omega|. \tag{1.4.7}$$

If we accept the correlation bound $\boldsymbol{A}$ for K and K^Ω, the right hand sides of these inequalities may be bounded in terms of

$$S(K,\Omega) = \sum_{A\subseteq\Omega} |\Delta K_A^\Omega|\, \|s_A\|^{\|A\|}. \tag{1.4.8}$$

Then the assumption of

C. *Acceptable boundary conditions*

$$S(K,\Omega)/|\Omega| \to 0 \quad \text{as} \quad \Omega\to\infty, \tag{1.4.9}$$

is sufficient to ensure that the thermodynamic limit exists and is independent of the boundary conditions; explicitly that is

$$\lim_{\Omega \to \infty} f(K, \Omega) = f_\infty(K). \tag{1.4.10}$$

We shall consider only such acceptable boundary conditions but it is instructive to characterize them in more concrete fashion. Accordingly let us first introduce a surface range, and corresponding finite-range boundary conditions.

Finite range boundary conditions are specified by a *surface range*

$$R^\times = \max_{A \subseteq \Omega, \Delta K_A^\Omega \neq 0} \{d(A), r(A, \partial\Omega)\}, \tag{1.4.11}$$

which is bounded (uniformly in Ω). Since the deviation potentials ΔK_A^Ω are nonzero only within distances $2R^\times$ of the perimeter of Ω we clearly have:

Lemma 1.4.1. *Finite range boundary conditions of finite degree p, are acceptable (i.e., C holds) and, furthermore,* $|f(K,\Omega) - f^0(K,\Omega)|$ *is of order* $|\partial\Omega|/|\Omega|$ *as* $\Omega \to \infty$, *that is, bounded by a surface term.*

Note that the bulk potentials K may be of long range ($R^\infty = \infty$) even if $R^\times < \infty$. In that case $f(K,\Omega)$ may differ from the limiting free energy, $f_\infty(K)$, by something asymptotically *greater* than a surface term (see below). More generally, to allow for long-range boundary conditions we introduce:

$\boldsymbol{C}_\tau$ *Tempered boundary conditions of exponent* τ are defined by the condition

$$S_i(K,\Omega) \equiv \sum_{i \subset A \subseteq \Omega} \frac{|\Delta K_A^\Omega|}{|A|} \|s\|^{\|A\|} \leqq \frac{C}{[a + r(i, \partial\Omega)]^\tau}, \tag{1.4.12}$$

where C, and a are fixed positive constants. To use this definition note that

$$S(K,\Omega) = \sum_{i \subset \Omega} S_i(K,\Omega) \leqq \sum_{i \subset \Omega} C/\varrho_i^\tau, \tag{1.4.13}$$

where $\varrho_i = a + r(i, \partial\Omega)$ measure the distance of i from the boundary of Ω. Now the number of sites at distance r from a given site increases as r^{d-1}. Hence the number of sites, $v_n(\Omega)$, in Ω with $(n-1)a \leqq \varrho_i < na$ is certainly bounded by $c_1 n^{d-1}|\partial\Omega|$ for suitable c_1. From this we can conclude:

Lemma 1.4.2. *Tempered boundary conditions of exponent* $\tau > d$ *are acceptable and* $|f(K,\Omega) - f^0(K,\Omega)|$ *is bounded by a surface term.*

Again, long-range bulk potentials may prevent $|f(K,\Omega) - f_\infty(K)|$ being also bounded by a surface term. This tempering result can be greatly strengthened if attention is restricted to simple sequences of domains, (1.4.4). In that case as $k \to \infty$ we have, on dimensional grounds, $v_n(\Omega_k) \approx \xi_k^{d-1} g_0(n/\xi_k)$, where $g_0(x)$ is a fixed function depending on the shape of the original continuum domain $\tilde{\Omega}_0$. On estimating $S(K, \Omega_k)$ by an integral we find $S(\Omega_k) = O(\xi_k^{d-\tau}) = o(|\Omega|)$, for $\tau < 1$ but $S(\Omega_k) = O(\xi_k^{d-1}) = O(|\partial\Omega_k|)$ for $\tau > 1$. On the boundary $\tau = 1$ a factor $\ln \xi_k$ is needed. Thus we can establish:

Lemma 1.4.3. *For a simple sequence of domains [Definition 1.4] tempered boundary conditions are acceptable if* $\tau > 0$. *Furthermore, if* $\tau > 1$ *then* $|f(K, \Omega_k) - f^0(K, \Omega_k)|$ *is bounded by a surface term.*

It is clear that these results are essentially best possible. Finally, to show more explicitly what is entailed in the tempering condition, consider pair interactions [$\Delta K_A^\Omega = 0$ unless $A = \{i, j\}$] bounded by power law decays. It is then not hard to prove:

Lemma 1.4.4. *Pair interaction potentials satisfying*

$$\Delta K_{\{i,j\}}^\Omega < C_1 / \varrho_{ij}^\tau r_{ij}^{d+\sigma}, \qquad (\text{all } \Omega), \tag{1.4.14}$$

where, with a fixed positive constant a,

$$\varrho_{ij} = a + \min\{r(i, \partial\Omega),\ r(j, \partial\Omega)\},\ r_{ij} = r(i, j), \tag{1.4.15}$$

represent tempered boundary conditions of exponent τ *provided* $\sigma \geqq \tau$.

2. Walls and Boundaries of Domains

2.1. Motivation

If the bulk interaction potentials K_A decay sufficiently rapidly with distance, i.e. as $d(A) \to \infty$, and if the deviation potentials ΔK_A^Ω are sufficiently small away from the boundaries of Ω (as discussed above), we expect $F(K, \Omega)$ and $|\Omega| f_\infty(K)$ to differ only by a term of order $|\partial\Omega|$. It is then reasonable to hope that the limit

$$f^\times(K) = \lim_{\Omega \to \infty} \frac{|\Omega|}{|\partial\Omega|} [f(K, \Omega) - \mathrm{f}_\infty(K)], \tag{2.1.1}$$

exists and represents the boundary free energy per boundary site. However it is clear (i) that the sequence of domains $\{\Omega_k\}$ should now satisfy additional regularity conditions, (ii) that $f^\times$ will depend explicitly on the shape and orientation of the limiting Ω_k with respect to the axes of the lattice $\mathscr{L}$, etc., and (iii) that $f^\times$ will also depend directly on the detailed properties of $\mathscr{H}(\Omega)$ in as far as these specify both bulk and wall potentials.

These considerations show that a more precise specification of the walls or boundaries of interest is imperative. Ideally the wall potentials should be defined relative to some hypothetical null boundary with zero boundary free energy. Free boundary conditions are not satisfactory in this sense since they certainly give rise to a nonzero boundary free energy of their own. For these reasons we define walls and boundaries by creating (or "cutting") a pair of conjugate walls of definite structure in an otherwise spatially uniform system, as indicated schematically in Figure 1. Since it is impossible to create only a single wall without, at the same time, making a bulk change in free energy (by removing a half-lattice or half domain), we will assume that the lattice $\mathscr{L}$, the potentials K, and the *wall potentials* W (to be defined explicitly below) have *minimal symmetry* such that both walls in a conjugate pair have identical boundary free energy (in the thermodynamic limit).

Now an ideal, translationally invariant planar wall can reside only in the infinite lattice (Fig. 1). To define the free energy of such a wall we will first cut out a finite

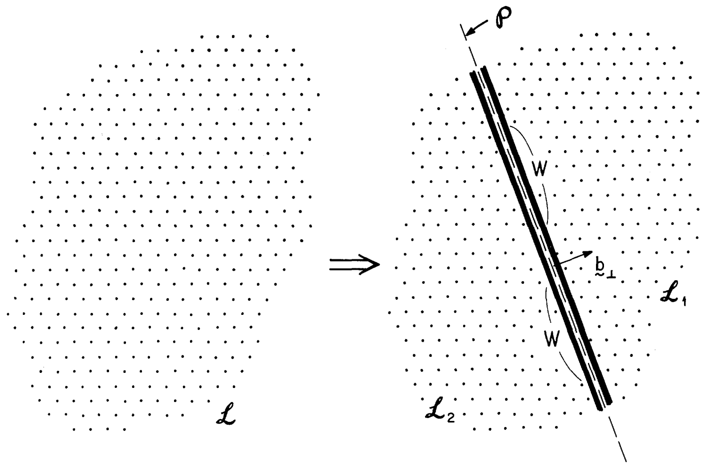

Fig. 1. The creation of a wall (or pair of boundaries) with potentials W by cutting an infinite lattice $\mathscr{L}$ by a plane $\mathscr{P}$ with perpendicular $\boldsymbol{b}_\perp$

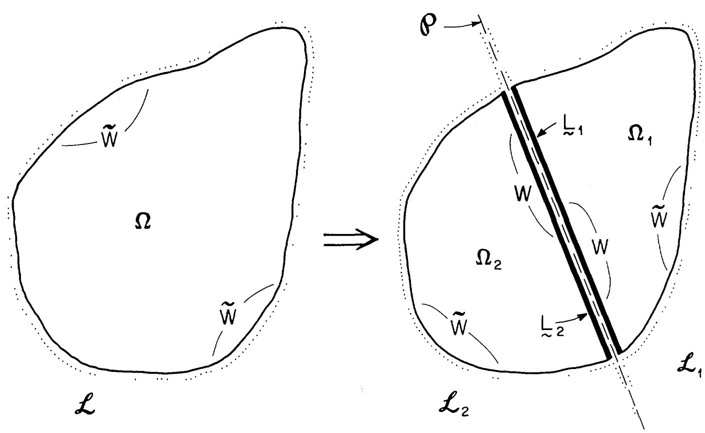

Fig. 2. Illustration of the intersection of a wall with a finite domain Ω which is decomposed into two disjoint domains, Ω_1 and Ω_2. The faces of the finite wall in Ω are labelled $\boldsymbol{L}_1$ and $\boldsymbol{L}_2$ and their area will be denoted $|\boldsymbol{L}|$. The symbol $\tilde{W}$ indicates the "associated wall potentials" involved in the domain Ω (see below)

domain Ω which is divided by the wall into disjoint domains Ω_1 and Ω_2 with $\Omega = \Omega_1 \cup \Omega_2$, as indicated in Figure 2. Comparison of the free energy $F(\Omega)$ with the total free energy, $F(\Omega_1) + F(\Omega_2)$, of the two subdomains yields a difference which may be associated with the *finite wall*, with faces $\boldsymbol{L}_1$ and $\boldsymbol{L}_2$, of total size (or "area") $2|\boldsymbol{L}|$, which have been created. (The *area*, $|\boldsymbol{L}|$, of a finite wall will be defined precisely below.) Thence the wall or boundary free energy, $f_\times$, of the finite wall may be defined by

Definition 2.1.

$$\begin{aligned} f_\times(K, W, \Omega) &= \tfrac{1}{2}|\boldsymbol{L}|^{-1}[F(K, \Omega_1) + F(K, \Omega_2) - F(K, \Omega)]\,, \\ &= (|\Omega|/2|\boldsymbol{L}|)\,[f(K, \Omega_1) + f(K, \Omega_2) - f(K, \Omega)]\,. \end{aligned} \tag{2.1.2}$$

The factor $\frac{1}{2}$ is included so that $f_\times$ may be regarded as the free energy for a single face. We use the notation $f_\times$ in place of $f^\times$ because both normalization, "per unit area", used here and the basis for comparison differs from that utilized in (2.1.1). As above, W denotes the set of wall potentials describing the cuts, etc., made in constructing the wall. It must be noted, however, that $F(\Omega)$, $F(\Omega_1)$, and $F(\Omega_2)$ also depend explicitly on the nature of the *associated wall potentials*, $\tilde{W}$, imposed on the original boundaries of Ω and on the remaining parts of those boundaries in Ω_1 and Ω_2, i.e., on the ΔK_A^Ω.

We now introduce various definitions that will enable us to make the construction of walls precise.

2.2. Lattice Planes, Blocks, and Symmetry

A set $\{\boldsymbol{b}_\beta\}$, of $d' = d-1$ linearly independent lattice vectors $\boldsymbol{b}_\beta$ $(\beta = 1, 2, \ldots, d')$, specifies a d'-dimensional plane, $\mathscr{P}$, a *lattice plane*, containing the corners of the cells at

$$\boldsymbol{R}_l^{||} = \sum_{\beta=1}^{d'} l_\beta \boldsymbol{b}_\beta \quad \text{for} \quad \boldsymbol{l} = (l_\beta) \in \mathbb{Z}^{d'} . \tag{2.2.1}$$

Translation of the lattice by any $\boldsymbol{R}_l^{||}$ leaves both lattice $\mathscr{L}$ and plane $\mathscr{P}$ invariant. If the set $\{\boldsymbol{b}_\beta\}$ consists of the set of cell edge vectors $\{\boldsymbol{a}_\alpha\}$ with one vector, say $\boldsymbol{a}_\gamma$, removed we say $\mathscr{P}$ is a *cleavage plane* conjugate to $\boldsymbol{a}_\gamma$.

Now let $\boldsymbol{b}_\perp$ denote a formal vector, possibly of zero magnitude $|\boldsymbol{b}_\perp|$, which specifies a directed normal to $\mathscr{P}$ and consider a division of the lattice into two semi-infinite *half-lattices*, $\mathscr{L}_1$ and $\mathscr{L}_2$, satisfying:

D(i) *Separation*

$$\mathscr{L}_1 \cup \mathscr{L}_2 = \mathscr{L} \quad \text{and} \quad \mathscr{L}_1 \cap \mathscr{L}_2 = \emptyset \, ; \tag{2.2.2}$$

(ii) *Translational invariance*

The half-lattices $\mathscr{L}_1$ and $\mathscr{L}_2$ are invariant under translations parallel to $\mathscr{P}$, explicitly,

$$\mathscr{L}_1 + \boldsymbol{b}_\beta = \mathscr{L}_1 , \quad \mathscr{L}_2 + \boldsymbol{b}_\beta = \mathscr{L}_2 , \quad (\beta = 1, 2, \ldots, d') \, ; \tag{2.2.3}$$

(iii) *Minimal symmetry*

There is a symmetry operation $\mathscr{R}_\mathscr{P}$ of the lattice, $\mathscr{L}$, satisfying

$$\mathscr{R}_\mathscr{P}\mathscr{P} = \mathscr{P} , \quad \mathscr{R}_\mathscr{P}\mathscr{L}_1 = \mathscr{L}_2 , \quad \mathscr{R}_\mathscr{P}\mathscr{L}_2 = \mathscr{L}_1 . \tag{2.2.4}$$

(iv) *Limited corrugation*

All sites on the positive side of $\mathscr{P}$ (in the sense determined by $\boldsymbol{b}_\perp$) for which $r(i, \mathscr{P}) > |\boldsymbol{b}_\perp| \geqq 0$ belong to $\mathscr{L}_1$ and vice versa for $\mathscr{L}_2$; we will assume that $\boldsymbol{b}_\perp$ is the shortest vector for which this is true.

A *simple cleavage wall* is defined on a cleavage plane by $|\boldsymbol{b}_\perp| = 0$; the two half lattices then simply contain all cells with indices $\boldsymbol{n}$ satisfying $n_\gamma \geqq 0$ and $n_\gamma < 0$, respectively, for appropriate γ.

The significance of these statements can be appreciated from Figure 3. The first condition merely states the separating property of a wall. The translational

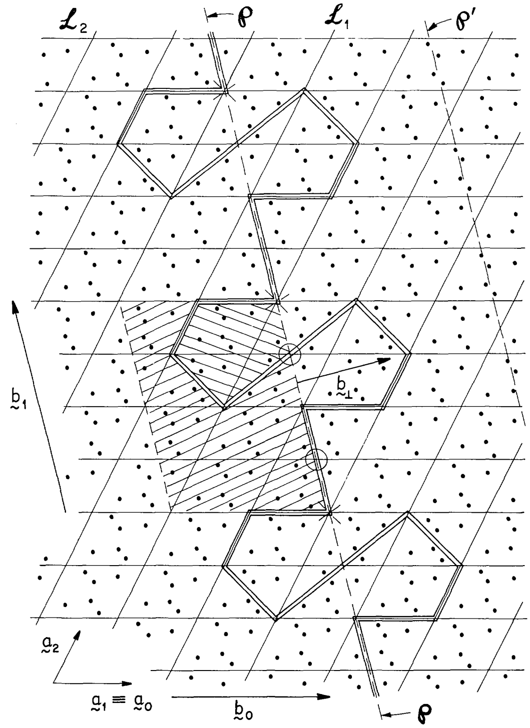

Fig. 3. Example of the detailed construction of a wall in a two-dimensional lattice $\mathscr{L}$ with cell vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ and $q=6$ sites per cell. Note the defining lattice plane $\mathscr{P}$ (dashed line), the normal vector $\boldsymbol{b}_\perp$ limiting the corrugations of the wall, the plane vector $\boldsymbol{b}_1$, which specifies the translational invariance of the wall, and the block edge vector $\boldsymbol{b}_0 = 2\boldsymbol{a}_0$ with $\boldsymbol{a}_0 = \boldsymbol{a}_1$. A block adjoining $\mathscr{P}$ is shaded. The division of $\mathscr{L}$ into $\mathscr{L}_1$ and $\mathscr{L}_2$ by the wall is fixed by the zig-zag parallel pairs of lines. The open circles are centered on points about which a rotation, $\mathscr{R}_{\mathscr{P}}$, through an angle π carries $\mathscr{L}_1$ into $\mathscr{L}_2$, and $\mathscr{P}$ into itself (although the cell corners on $\mathscr{P}$, marked by crosses, are carried into those not marked). By redefinition of the cells with respect to the sites, a wall could be built on planes like $\mathscr{P}'$ not containing cell corners (in this realization of the cells)

invariance along a wall, necessary for the existence of a limiting boundary free energy, is embodied in **D(ii)**. Condition **D(iv)** allows for finite corrugations of the wall, or face of a half-lattice, of maximum depth or height $|\boldsymbol{b}_\perp|$. Finally, **D(iii)** specifies the minimal lattice symmetry with respect to the plane $\mathscr{P}$, needed to ensure that the two faces of the half-lattices are physically identical. Note that $\mathscr{R}_{\mathscr{P}}$ need not necessarily carry the cell corners on $\mathscr{P}$ specified by (2.2.1) into themselves: see Figure 3.

In constructing walls it should also be borne in mind that the placing of sites in the cells of a lattice may be changed by adding an arbitrary vector to the position vectors of all sites, without altering the statistical mechanics of the situation. For example, in Figure 3 a shift $\boldsymbol{r}_0 = \frac{1}{2}(\boldsymbol{a}_1 + \boldsymbol{a}_2)$ would effectively bring the cell corners to the cell centers so that a plane (line) like $\mathscr{P}'$ in Figure 3 could equally be the basis for constructing a wall (even though it contains no cell corners).

The intersection of a domain Ω with a wall decomposes Ω into two disjoint subdomains, $\Omega_1 = \Omega \cap \mathscr{L}_1$ and $\Omega_2 = \Omega \cap \mathscr{L}_2$, as illustrated in Figure 2. The domains formed of the sites in cells of Ω_1 adjacent to cells containing sites of Ω_2 may be called the face, Γ_1, of the wall in Ω_1. The area of a wall face in Ω could then be defined simply in terms of the cell contents $|\Gamma_1|$ and $|\Gamma_2|$. However, it proves more convenient to define area in a way which explicitly recognizes the translational invariance of a wall. Accordingly, in place of cells we introduce *blocks* by the following definition:

Definition 2.2. A *block*, with edge $\boldsymbol{a}_0$ and faces parallel to a wall with plane $\mathscr{P}$ and defining vectors $\boldsymbol{b}_\beta$ $(\beta=1,2,\ldots,d')$, is a set of sites contained *either* in the parallelepiped defined by edge vectors $\boldsymbol{b}_0, \boldsymbol{b}_1, \ldots, \boldsymbol{b}_{d'}$, with $\boldsymbol{b}_0 = k\boldsymbol{a}_0$, where $\boldsymbol{a}_0$ is a cell vector not parallel to $\mathscr{P}$ and k is the smallest positive integer such that $\boldsymbol{b}_0 \cdot \boldsymbol{b}_\perp > |\boldsymbol{b}_\perp|^2$, *or* in a parallelepiped equivalent under translations by the *block vectors*

$$\boldsymbol{R}_{\boldsymbol{l}} = \sum_{\beta=0}^{d'} l_\beta \boldsymbol{b}_\beta, \qquad \boldsymbol{l} = (l_\beta) \in \mathbb{Z}^d. \tag{2.2.5}$$

Any sites lying *on* the plane $\mathscr{P}$ or on the translates $\mathscr{P} + l_0\boldsymbol{b}_0$, are assigned to a block or its adjoining neighbor in accord with the assignment implied by the wall construction.

A block, adjacent to the wall plane $\mathscr{P}$ and constructed with the selection $\boldsymbol{a}_0 = \boldsymbol{a}_1$, is shown shaded in Figure 3. The condition specifying the integer k is chosen (for convenience) so that only blocks adjoining the wall plane $\mathscr{P}$ can contain sites from both $\mathscr{L}_1$ and $\mathscr{L}_2$. (See Figure 3 where $k=2$.) It is easy to see that for simple cleavage walls, blocks are identical to cells. Blocks are indexed by the integer vector $\boldsymbol{l}$.

The *faces* of a wall intersecting a domain Ω are now redefined as the sets, $\boldsymbol{L}_1$, and $\boldsymbol{L}_2$, of *complete* blocks adjacent to $\mathscr{P}$ and contained in Ω_1 or Ω_2, respectively. The *area*, $|\boldsymbol{L}_1|$, *of the face*, $\boldsymbol{L}_1$, is defined as the number of blocks in $\boldsymbol{L}_1$ and similarly for $|\boldsymbol{L}_2|$. We define the *area of the wall* in Ω as

$$|\boldsymbol{L}| = \tfrac{1}{2}(|\boldsymbol{L}_1| + |\boldsymbol{L}_2|), \tag{2.2.6}$$

although in practice we will be mainly interested in situations where $|\boldsymbol{L}_1| = |\boldsymbol{L}_2| \equiv |\boldsymbol{L}|$.

The *perimeter* $\partial\boldsymbol{L}_1$, of *the face* $\boldsymbol{L}_1$ is the set of $|\partial\boldsymbol{L}_1|$ blocks in $\boldsymbol{L}_1$ which adjoin blocks not completely contained in Ω.

2.3. Wall and Boundary Potentials

An infinite planar wall, W, is specified by a lattice plane $\mathscr{P}$, with defining vectors $\boldsymbol{b}_\beta$ $(\beta=0,1,\ldots,d')$, normal $\boldsymbol{b}_\perp$, and minimal symmetry operation $\mathscr{R}_{\mathscr{P}}$, and by a set of *wall potentials*, $\{W_B\}$, such that the total potentials of interaction in the presence of a wall are given by

$$K_A^W = K_A + W_A. \tag{2.3.1}$$

The wall potentials should be of the same degree p as the bulk potentials K and, furthermore, must satisfy the conditions

E(i) *Separation (or decoupling)*

$$K_B + W_B = 0 \quad \text{all} \quad B \in \mathscr{L}_1 \cdot \mathscr{L}_2. \tag{2.3.2}$$

(ii) *Translational invariance*

$$W_{B+\boldsymbol{b}_\beta} = W_B, \qquad (\beta = 1, 2, \ldots, d'). \tag{2.3.3}$$

(iii) *Minimal symmetry*

$$W_{\mathcal{R}_{\mathcal{P}}B} = W_B\,. \tag{2.3.4}$$

In **E(i)**, recall that $\mathcal{L}_1 \cdot \mathcal{L}_2$ denotes the set of all collections of sites with nonempty intersections with both $\mathcal{L}_1$ and $\mathcal{L}_2$. Evidently this condition enables one to decompose the formal lattice Hamiltonian $\bar{\mathcal{H}}_W^\infty = \sum_A (K_A + W_A)s_A$ into a sum of two parts, $\bar{\mathcal{H}}_1^\infty$ and $\bar{\mathcal{H}}_2^\infty$, which are independent, or *uncoupled*, in that they have no spin variables in common. If this decoupling property is dropped we would be discussing *grain boundaries* or *seams*. Many of our arguments, however, would go through unaltered.

A *free boundary wall*, corresponding to free boundary conditions is specified, in accordance with the definition (1.2.10), by

$$\begin{aligned} W_B &= -K_B \quad \text{for all} \quad B \in \mathcal{L}_1 \cdot \mathcal{L}_2 \\ &= 0 \quad , \quad \text{otherwise}. \end{aligned} \tag{2.3.5}$$

A *ferromagnetic wall* (in practise in a purely ferromagnetic system) satisfies the condition

$$W_B \geqq -|K_B| \quad \text{for all } B\,. \tag{2.3.6}$$

Such a wall retains the purely ferromagnetic character of the system *with* a wall. Note that it includes free boundary conditions.

A *subfree wall* (in a purely ferromagnetic system) is specified by potentials satisfying

$$0 \geqq W_B \geqq -|K_B|\,, \quad \text{for all } B\,. \tag{2.3.7}$$

The significance of these conditions is that after removing the bulk interactions K coupling $\mathcal{L}_1$ and $\mathcal{L}_2$, the internal interactions near the wall are also weakened. Clearly subfree walls are also ferromagnetic.

A *superferromagnetic wall* in a saturating spin system, may be regarded, from the perspective of one half-lattice as obtained (a) by imposing an infinite field on all the spins in the complementary half-lattice and vice-versa, and (b) by increasing the internal interactions remaining in the two half-lattices. Apart from their intrinsic interest there are various more specific reasons for considering such walls, as will emerge below. On applying the rules for handling infinite fields, the corresponding wall potentials may be written

$$\begin{aligned} W_B &= -K_B \quad \text{for} \quad B \in \mathcal{L}_1 \cdot \mathcal{L}_2 \\ &= W_B^0 + \sum_{A \supset B}{}^{\cdot}\, K_A \|s_A\| / \|s_B\|\,, \quad \text{for} \quad B \subsetneqq \mathcal{L}_1 \end{aligned}$$

or

$$B \subsetneqq \mathcal{L}_2\,, \quad \text{with} \quad W_B^0 \geqq 0\,, \tag{2.3.8}$$

where the superscript dot indicates that the sum runs only over A in $\mathcal{L}_1 \cdot \mathcal{L}_2$. Evidently superferromagnetic walls are ferromagnetic (in a purely ferromagnetic system). If $W_B^0 = 0$ the wall is *simple superferromagnetic.*

For bulk interactions of finite range ($R^\infty < \infty$) superferromagnetic walls can also be realized by imposing infinite fields, $h_i = +\infty$, on all spins i in a "channel" which extends to a distance $R^0 > \frac{1}{2} R^\infty$ on both sides of $\mathscr{P}$. One may then remove the contribution to the free energy due to frozen spin terms of the form $K_C\|s_C\|$. This construction indicates a certain fundamental arbitrariness in any definition of boundary free energy which will be demonstrated more explicitly below.

We will need suitable *norms for wall potentials* in order to bound the surface free energy. Accordingly, consider first, free boundary conditions. A particular nonzero interaction potential K_A will contribute to the wall free energy under all translations $A \Rightarrow A' = A + \boldsymbol{R}$ for which $A' \in \mathscr{L}_1 \cdot \mathscr{L}_2$. The number of such translations, which are also distinct under translations $\boldsymbol{R}_l^{\|}$ parallel to the wall, is easily seen to be bounded by $c_0[d_\perp(A) + 2|\boldsymbol{b}_\perp|]$, where c_0 is an appropriate geometrical constant (involving the orientation of the wall, the number of cells in a block, etc.). Since $|\boldsymbol{b}_\perp|$ is fixed and finite we accordingly define bounded free wall potentials by

$$\textbf{F(i)} \qquad \|W\|_0 = \sum_{A \subset [\![A]\!]} d_\perp(A)\,|K_A|\,\|s\|^{\|A\|} < \infty\,, \tag{2.3.9}$$

where the sum runs over all translationally inequaivalent collections A, while the wall plane $\mathscr{P}$ specifies the direction for the caliper diameter $d_\perp(\cdot)$.

For long range forces this condition is clearly more restrictive than the bulk stability Condition **B** [(1.4.2)]. Thus, if pair potentials decrease as $1/r_{ij}^{d+\sigma}$, $\sigma > 0$ suffices to satisfy **B** but $\sigma > 1$ is necessary for **F(i)**. The need for such a stronger condition was already observed by Fisher and Lebowitz [10]. However, for finite range potentials K the Condition **F(i)** is implied by **B**.

For the remaining or *internal wall potentials*, W_B which do not link $\mathscr{L}_1$ and $\mathscr{L}_2$, it suffices to require the *boundedness condition*

$$\textbf{F(ii)} \qquad \|W\|_1 = \sum_{B \subset [\![B]\!]^{\|}} |W_B|\,\|s\|^{\|B\|} < \infty\,, \tag{2.3.10}$$

where $[\![B]\!]^{\|}$ is the set of all collections $B \subsetneq \mathscr{L}_1$ which are inequivalent under translations $\boldsymbol{R}_l^{\|}$, parallel to the wall. [Note we use **E(iii)** to restrict B to $\mathscr{L}_1$.]

The import of this condition can be appreciated by relating it to the previous discussion in Section 1.4 concerning acceptable boundary conditions. In the first place the Definition (1.4.11) of finite range boundary conditions extends trivially to wall potentials by replacing Ω by $\mathscr{L}_1$ and ΔK_A^Ω by W_A. Then in parallel to Lemma 1.4.1 we have

Lemma 2.3.1. *Finite range wall conditions of finite degree p, satisfy the condition* **F(ii)**.

Likewise the tempering exponent τ can be defined for wall potentials by making the corresponding replacement $\Omega \Rightarrow \mathscr{L}_1$, $\Delta K_A^\Omega \Rightarrow W_A$ in (1.4.12). With this understanding it is easy to prove

Lemma 2.3.2. *Tempered wall potentials W of exponent $\tau > 1$ satisfy the condition* **F(ii)**.

This should be compared with Lemma 1.4.3. It follows from Lemma 1.4.4. that pair potentials bounded by $C_1/\varrho_{ij}^\tau r_{ij}^{d+\sigma}$. [where ϱ_{ij} is defined in (1.4.15)] verify the wall bound **F(ii)** for $\sigma \geqq \tau > 1$. Note this is compatible with the requirement $\sigma > 1$ on the bulk potentials which is needed for **F(i)**. However, the tempering condition is primarily a restriction on decay perpendicular to the wall; the partial sums $S_i(K, \mathscr{L}_1)$ [see (1.4.12)] will remain bounded with much slower decay laws *parallel*. In particular, if the pair potentials decay as $1/r_{ij}^{d+\sigma^{||}}$ for $\varrho_{ij} < R_0$, one needs only $\sigma^{||} > -1$ (and finite degree p) for **F(ii)**.

2.4. Finite Walls and Associated Boundary Conditions

In order to approach the infinite walls introduced above through a suitable sequence of finite domains we first make precise the concept of a *finite wall* with potentials W in a domain Ω. To recapitulate and extend the notation we write

$$\bar{\mathscr{H}}(\Omega) = \bar{\mathscr{H}}(K, \tilde{W}, \Omega) = \sum_{A \subsetneq \Omega} K_A^{\Omega} s_A = \bar{\mathscr{H}}^0(K, \Omega) + \Delta\bar{\mathscr{H}}(\tilde{W}, \Omega), \tag{2.4.1}$$

with, as before,

$$\bar{\mathscr{H}}^0(K, \Omega) = \sum_{A \subsetneq \Omega} K_A s_A, \tag{2.4.2}$$

and, now,

$$\Delta\bar{\mathscr{H}}(\tilde{W}, \Omega) = \sum_{B \subsetneq \Omega} \tilde{W}_B^{\Omega} s_B = \tilde{\mathscr{W}}(\Omega), \tag{2.4.3}$$

where the *associated wall potentials*, $\tilde{W} = \{W_A^{\Omega}\}$, are defined on all domains Ω via

$$\tilde{W}_B^{\Omega} = K_B^{\Omega} - K_B, \quad \text{all} \quad B \subsetneq \Omega, \tag{2.4.4}$$

and are taken to be of the same degree, p, as the bulk potentials K. Note that the associated wall potentials are defined only for B drawn from Ω; since we will not investigate the free energies of the (associated) boundaries described by $\tilde{W}$, we do not need to worry about decoupling properties. However, the associated walls must be acceptable (in the sense of Condition **C**) and will have to satisfy certain further conditions which limit their influence on the wall W.

Associated wall potentials describing *free*, *ferromagnetic*, *subfree* and *superferromagnetic* conditions may be defined in analogy with the corresponding definitions for infinite planar walls in Section 2.3. However, linking conditions like the first part of (2.3.5), are not needed since $\tilde{W}_B$ is defined only for $B \subsetneq \Omega$. As in the infinite wall case, simple superferromagnetic associated wall potentials are realized by imposing infinite fields, $h_i = +\infty$, on all spins i within a distance $R^0 > \frac{1}{2}R^{\infty}$ of the perimeter, $\partial\Omega$, of Ω. The condition needed in all cases to maintain the necessary *ferromagnetic character*, in a purely ferromagnetic system with a ferromagnetic wall, is

$$\tilde{W}_B^{\Omega} \geqq -K_B - W_B, \quad \text{all} \quad B \subsetneq \Omega. \tag{2.4.5}$$

Note that free associated boundary conditions ($\tilde{W}_B^{\Omega} = 0$ for $B \subsetneq \Omega$) are automatically of ferromagnetic character when $W_B \geqq -K_B$.

We now assume that Ω is separated by a planar wall with given potentials W, into two subdomains Ω_1 and Ω_2 as described above. (See also Fig. 2.) We define the separate, uncoupled Hamiltonians for the subdomains by

$$\bar{\mathscr{H}}_1 = \bar{\mathscr{H}}(K, W, \tilde{W}, \Omega_1) = \sum_{A \subsetneq \Omega_1} (K_A^{\Omega} + W_A) s_A, \tag{2.4.6}$$

and similarly for $\bar{\mathscr{H}}_2$. Note this is equivalent to taking $\mathscr{H}_1 = \mathscr{H}(\Omega_1)$ with potentials

$$K_A^{\Omega_1} = K_A + \tilde{W}_A^{\Omega} + W_A, \quad \text{for} \quad A \subsetneq \Omega_1, \tag{2.4.7}$$

and similarly for $K_A^{\Omega_2}$.

The total (reduced) *wall Hamiltonian*, $\mathscr{W}(\Omega)$, for the finite wall in the domain Ω may now be defined via

$$\bar{\mathscr{H}}_1 + \bar{\mathscr{H}}_2 = \bar{\mathscr{H}}(\Omega) + \mathscr{W}(\Omega). \tag{2.4.8}$$

After some algebra this yields the basic relation

$$\mathscr{W}(\Omega) = \sum_{A \subsetneq \Omega} W_A s_A - \sum_{B \in \Omega_1 \cdot \Omega_2} \tilde{W}_B^{\Omega} s_B. \tag{2.4.9}$$

The first term here is merely the expected contribution in Ω of the potentials W describing the infinite wall in $\mathscr{L}$. The second term is bounded by

$$U(W, \tilde{W}, \Omega) = \sum_{B \in \Omega_1 \cdot \Omega_2} |\tilde{W}_B^{\Omega}| \, \|s\|^{\|B\|}, \tag{2.4.10}$$

and represents a "corner" or perimeter effect arising from interference between the wall potentials, W, and the independently assigned associated boundary potentials acting on Ω. By (2.4.4) this term vanishes identically if the associated boundary conditions are free. More generally, however, we will need:

G. *Associated boundary acceptability*

(i) $u(W, \tilde{W}, \Omega) = U(W, \tilde{W}, \Omega)/|\boldsymbol{L}| \leqq u_0(\tilde{W}) < \infty$, (2.4.11)

where u_0 is independent of Ω and of the wall potentials; and

(ii) $u(W, \tilde{W}, \Omega) \to 0, \quad \text{as} \quad \Omega \to \infty$. (2.4.12)

The first part of this condition will yield a uniform bound on the contribution the interference term can make to $f_\times$; the second part ensures that the interference actually vanishes in the thermodynamic limit. If the range, $\tilde{R}^\times$, of the associated boundary potentials $\tilde{W}$, is defined as in (1.4.11) with $\Delta K_A^{\Omega} \equiv \tilde{W}_A^{\Omega}$, and if Ω is of reasonable shape relative to W it is easy to prove

Lemma 2.4.1. *Associated boundary potentials of finite range* ($\tilde{R}^\times < \infty$) *and finite degree satisfy*

$$u(W, \tilde{W}, \Omega) \leqq c_3(|\partial \boldsymbol{L}_1| + |\partial \boldsymbol{L}_2|)/|\boldsymbol{L}|, \tag{2.4.13}$$

provided $|\Gamma| \leqq c_4(|\partial \boldsymbol{L}_1| + |\partial \boldsymbol{L}_2|)$ *where* $\Gamma = \{i \subset \partial\Omega;\ r(i, \mathscr{P}) < 2\tilde{R}^\times\}$ *and* c_3 *and* c_4 *are constants independent of* W *and* Ω.

The condition involving Γ simply asserts that the boundary of Ω stays away from the wall except near the perimeters $\partial \boldsymbol{L}_1$ and $\partial \boldsymbol{L}_2$. If the perimeter-to-area ratio, $(|\partial \boldsymbol{L}_1| + |\partial \boldsymbol{L}_2|)/|\boldsymbol{L}|$, of the wall approaches zero as $\Omega \to \infty$, as will be the case for simple sequences (1.4.4), we see that finite range associated boundary potentials satisfy **G**. However, the previous tempering conditions for long-range boundary potentials are not sufficient to imply **G** because they permit slow decay parallel to the boundaries of Ω. Rather than introduce further tempering conditions analogous to

(1.4.12) we will merely state:

Lemma 2.4.2. *If the associated wall potentials $\tilde{W}$ contain only pair potentials subject to*

$$\tilde{W}^{\Omega}_{\{i,j\}} < C_1/\varrho_{ij}^{\tau} r_{ij}^{d+\sigma}, \tag{2.4.14}$$

with ϱ_{ij} defined by (1.4.15), *then the acceptability Condition* **G** *is satisfied for simple sequences*, (1.4.4), *provided $\tau > 0$ and $\sigma > 1$.*

Proof. We sketch a proof along the lines used for Lemma 1.4.3. For large $k \to \infty$ (in the sequence $\{\Omega_k\}$) we have formally, from (2.4.10) and (2.4.14),

$$u = U/|\boldsymbol{L}_k| < C_2 |\boldsymbol{L}_k|^{-1} \int d\varrho \int r^{d-1} dr\, \omega_k(\varrho, r) \varrho^{-\tau} r^{-d-\sigma}, \tag{2.4.15}$$

where $\omega_k(\varrho, r)$ is the density of pairs of sites i and j in Ω_k in which i and j lie on opposite sides of the wall plane $\mathscr{P}$ and at a separation r, while the site i is at a distance ϱ from the boundary, $\partial\Omega_k$, and the site j is not closer to $\partial\Omega_k$. On dimensional grounds we have $|\boldsymbol{L}_k| \propto \xi_k^{d-1}$ and $\omega_k(\varrho, r) \approx \xi_k^{d-2} r g_1(\varrho/\xi_k)$ where the shape function $g_1(x)$ depends on the original continuum domain $\tilde{\Omega}_0$. Substitution in (2.4.15) yields a bound on u of the form $\xi_k^{-\tau} \int g_1(x) x^{-\tau} dx \int dr/r^{\sigma}$. Provided $\sigma > 1$ and $\tau > 0$, this vanishes when $k \to \infty$. □

Notice that the restriction $\sigma > 1$ is expected in the light of earlier surface results but $\tau > 0$ is weaker than might have been anticipated. The weaker condition suffices since the associated boundary conditions only play an interfering role for regions near the wall. When one has $\tau > 1$ the contribution of $\tilde{W}$ will amount only to a perimeter correction satisfying (2.4.1).

Finally, for the sequence of domains $\{\Omega\}$ and the walls in them, we need a shape condition which maintains the "integrity" of the wall and ensures that the total strength of the wall potential term, $\sum_{A \subseteq \Omega} W_A s_A$ in (2.4.9), is asymptotically no greater than a multiple of the wall area, $|\boldsymbol{L}(\Omega)|$, as defined in (2.2.6). Specifically we need to exclude pathological situations in which the lattice plane, $\mathscr{P}$, intersects Ω only in a "small" region, of wall area $|\boldsymbol{L}|$, but "grazes" Ω over an indefinitely greater area in the vicinity of which, by the Definition (2.4.6), wall potentials are introduced into one or both subdomains Ω_1 and Ω_2. If the subdomains themselves form simple sequences this cannot occur; more generally we will require:

H. *Wall integrity*

For all (allowable) $\mathscr{P}$ and Ω there is a vector $\boldsymbol{b}^{\dagger}(\Omega)$, not parallel to $\mathscr{P}$, and a pair of *extended wall faces* $\boldsymbol{L}_1^{\dagger}$ and $\boldsymbol{L}_2^{\dagger}$, i.e. a set of $|\boldsymbol{L}_1^{\dagger}| + |\boldsymbol{L}_2^{\dagger}|$ blocks adjacent to $\mathscr{P}$, satisfying

$$|\boldsymbol{L}(\Omega)|/(|\boldsymbol{L}_1^{\dagger}| + |\boldsymbol{L}_2^{\dagger}|) \geqq \delta > 0, \tag{2.4.16}$$

for fixed δ, and such that for each $i \in \Omega$ there is a translation parallel to $\boldsymbol{b}^{\dagger}(\Omega)$ which carries i into a cell belonging to the extended faces.

In effect this condition asserts that Ω lies within a cylinder of a cross section which does not exceed some uniformly bounded multiple of $|\boldsymbol{L}(\Omega)|$.

2.5. *Definition of Boundary Free Energy*

Finally we define explicitly the boundary free energy per block of a finite wall, W, in a domain Ω with associated wall potentials $\tilde{W}$, cut from a lattice with bulk potentials K, by

$$f_\times(K, W, \tilde{W}, \Omega) = \tfrac{1}{2}|\boldsymbol{L}|^{-1}[F(\Omega_1) + F(\Omega_2) - F(\Omega)], \qquad (2.5.1)$$

where $|\boldsymbol{L}|$ is the area of the wall in Ω as defined in (2.2.6). If we use (1.2.9) this may be rewritten as

$$\exp[2|\boldsymbol{L}| f_\times(K, W, \tilde{W}, \Omega)] = Z[\bar{\mathscr{H}} + \mathscr{W}]/Z[\mathscr{H}]. \qquad (2.5.2)$$

with $\bar{\mathscr{H}}$ and $\mathscr{W}$ defined in (2.4.8) and (2.4.9). More generally if the decoupling property **E(i)** is violated this definition would stand as the definition of a grain boundary or seam specified by W.

If either of the minimal symmetry conditions **D(iii)** and **E(iii)** are violated $f_\times$ must be interpreted as the *mean boundary free* energy of a conjugate pair of wall faces in Ω_1 and Ω_2, respectively. The special case of *free associated boundary conditions* ($\tilde{W}_B \equiv 0$) will be denoted by $f^0_\times(K, W, \Omega)$.

Interest now focuses on the existence and properties of $f_\times$ in the limit $\Omega \to \infty$ with $\Omega_1, \Omega_2 \to \infty$ and $|\boldsymbol{L}| \to \infty$. We expect the limit, when it exists, to depend on K and W but, at least under suitable restrictions, *not* on the associated wall potentials $\tilde{W}$ or on the sequences $\{\Omega_k\}$.

2.6. *Arbitrariness of Boundary Free Energy*

We must point out that in the Definition (2.5.1), there is a concealed physical ambiguity in the process of cutting the domain Ω into subdomains. Mathematically, the prescription is quite unique and corresponds physically to an infinitely thin "barrier" being placed between Ω_1 and Ω_2 which "screens out" all interactions between the two subdomains. To approximate this physically, however, we would need to employ a barrier of finite thickness, say an "empty channel" of width $2R^0 > R^\infty$ and uniform crossection in which all interactions are removed, as illustrated in Figure 4 where box domains Λ, Λ_1, and Λ_2 are shown. This latter situation is the same physically as that in which we reduce the length of each of the two subdomains Λ_1 and Λ_2 by R^0, thus creating reduced subdomains Λ_1' and Λ_2' shown in Figure 4(b). By translation these can be derived from a reduced total domain, Λ' [Fig. 4(c)]. For large enough systems, the boundary free energy derived from Λ' differs from that derived from Λ by a multiple of the bulk free energy $f_\infty(K)$. Specifically we will find

$$f_\times(\Lambda) \approx f_\times(\Lambda') - c_5 R^0 f_\infty, \quad \text{as} \quad \Lambda, \Lambda' \to \infty, \qquad (2.6.1)$$

where c_5 is a geometrical factor depending on the orientation of the walls, and details of the lattice. This ambiguity arises in a similar way with fully ferromagnetic walls.

We conclude that in real physical terms, boundary free energies are defined *only up to the addition of a multiple* (positive or negative) *of the bulk free energy*. It follows immediately that properties such as definite convexity or monotonicity in

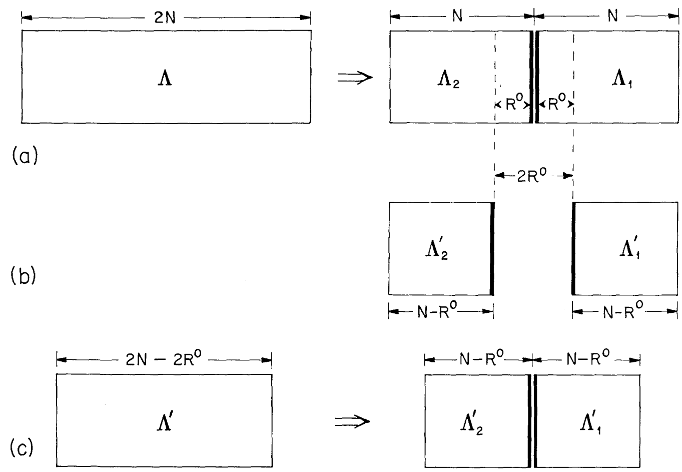

Fig. 4 a—c. Definition of surface free energy to a system with bulk potentials of finite range, R^{∞}, illustrating an ambiguity in the definition of $f_{\times}$. In **a** a free wall is defined in Λ in accord with the general definition (involving decoupling potentials). In **b** an expanded free wall is constructed by deleting all spin interactions in a channel of width $R^0 > \frac{1}{2}R^{\infty}$. Finally in **c** this expanded wall is reassembled into a free wall in a reduced domain Λ'

the bulk fields and potentials, which might have been conjectured for $f_{\times}(K, W)$, cannot in fact hold generally if this kind of ambiguity is considered. Note, however, that this does not apply to properties defined only with respect to the wall potentials, W. Indeed, the convexity of $f_{\times}(K, W, \tilde{W}, \Omega)$ with respect to the wall potentials follows directly from the Definition (2.5.2) as will be recorded again below.

2.7. Dependence on Associated Wall Conditions

In a subsequent article we will establish, under sufficiently strong conditions, that the limiting boundary free energy $f_{\times}$ is actually independent of the associated wall potentials $\tilde{W}$. To see that this cannot be the case in general, however, consider the situations illustrated in Figures 5(a) and (b). Suppose the system is a two-dimensional ferromagnet in zero bulk field and at a temperature T lower than T_c; it could be a nearest-neighbor, spin $\frac{1}{2}$ Ising model. Consider a box domain (or rectangle) Λ of dimensions $2N \times L$ which is then divided by a wall of length L into two subdomains Λ_1 and Λ_2 each of dimensions $N \times L$. Suppose the wall is of ferromagnetic character in the sense that W involves large fields which freeze the boundary spins in a "plus" or "up" orientation. In the first instance, (a), consider associated wall potentials $\tilde{W}_a$ which similarly freeze the spins in an up orientation. Equivalently one may think of the spins being fixed as plus along the boundary of Λ and along the corresponding boundaries of Λ_1 and Λ_2: see Figure 5(a). The spins in the bulk, both with and without the wall present, will then tend to favor the plus or up direction as indicated in the figure. Compare this now with the second situation, Figure 5(b), in which the associated boundary potentials, $\tilde{W}_b$, are similar except that the sign of the field imposed on the boundary is *reversed* on all except the central length of $2M$ of the $2N$ spins on each side, with $M < L$. In this situation the spins in

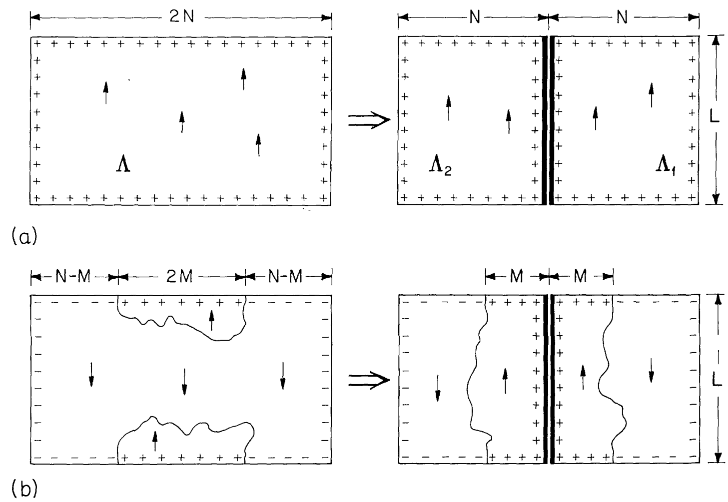

Fig. 5 a and b. Illustrating the effects of the associated boundary conditions on the definition of a boundary free energy under conditions allowing two-phase coexistence, specifically a two-dimensional ferromagnet in zero field beneath T_c. In **a** the boundary spins are all held plus (or up) by large boundary fields. In **b** the boundary fields have been reversed on parts of the boundary leading to the appearance of interfaces which contribute differently to the free energy with or without a central wall

the bulk will tend to assume radically different configurations. When the wall is present the free energy will be minimized by the appearance of two *interfaces* separating up phases from down phases. If Σ is the *interfacial free energy* per unit length, the free energy will be higher by an amount of order $2\Sigma L$. (Abraham [28] has performed rigorous calculations for the square Ising model establishing the existence of this incremental free energy.) On the other hand, before the wall is inserted the free energy will be minimized by two interfaces, of length about M, which more or less cling to the boundaries, as illustrated in Figure 5(b). When the boundary free energy of the central wall is computed according to the Definition (2.5.1) we will thus find the difference

$$\Delta f_\times = f_\times(K, W, \tilde{W}_b, \Lambda) - f_\times(K, W, \tilde{W}_a, \Lambda), \approx (2L\Sigma - 2M\Sigma)/2L = [1-(M/L)]\Sigma . \tag{2.7.1}$$

Hence, if the limit $\Lambda, \Lambda_1, \Lambda_2 \to \infty$ is taken in any way *other than with* $M/L \to 1$, there will remain a *non zero difference* between the boundary free energies for the two different associated boundary conditions. (Note this will be true even if $M \to \infty$ provided $M < L$, as assumed originally.) In this case the source of the problem is easy to grasp; but it is evident that it will be harder to control the interfaces for more complex shapes and more elaborate associated boundary conditions.

3. Correlation Expressions and Basic Inequalities

3.1. Correlation Function Formulations

The basic Definition (2.5.2) of the boundary free energy can be rewritten as

$$\exp[2|L| f_\times(K, W, \tilde{W}, \Omega)] = \frac{\mathrm{Tr}_\Omega\{e^{\mathscr{H}+\mathscr{W}}\}}{\mathrm{Tr}_\Omega\{e^{\mathscr{H}}\}} = \langle e^{\mathscr{W}} \rangle_\Omega , \tag{3.1.1}$$

that is, as an expectation value in the wall-free domain Ω. This reveals the potential utility of correlation function inequalities. It is more effective, however, to linearize the exponential by writing (as in Lemma 1.3)

$$\mathscr{H}^{\zeta}(\Omega)=\bar{\mathscr{H}}(\Omega)+\zeta\mathscr{W}(\Omega). \tag{3.1.2}$$

Then, the expectation values being well defined, we have

$$2|\boldsymbol{L}|f_{\times}(K,W,\tilde{W},\Omega)=\int_0^1 d\zeta\langle\mathscr{W}\rangle_{\Omega}^{\zeta}, \tag{3.1.3}$$

where $\langle\cdot\rangle_{\Omega}^{\zeta}$ denotes an expectation computed with $\mathscr{H}^{\zeta}(\Omega)$. Through (2.4.9) this expresses $f_{\times}$ directly in terms of spin correlation functions $\langle s_A\rangle$.

Since our analysis well use positivity and associated monotonicity properties, it is convenient to decompose the wall Hamiltonian as

$$\mathscr{W}=\mathscr{W}_{+}-\mathscr{W}_{-}, \tag{3.1.4}$$

where $\mathscr{W}_{+}$ and $\mathscr{W}_{-}$ are purely ferromagnetic Hamiltonians. Explicitly we can write

$$\mathscr{W}_{\pm}(\Omega)=\sum_{A\subseteq\Omega_1}W_A^{\pm}s_A+\sum_{A\subseteq\Omega_2}W_A^{\pm}s_A+\sum_{B\in\Omega_1\cdot\Omega_2}\Delta W_B^{\pm}s_B, \tag{3.1.5}$$

with the notation

$$X^{\pm}=\tfrac{1}{2}(|X|\pm X)\geqq 0, \quad \text{and} \quad \Delta W_B=W_B-\tilde{W}_B. \tag{3.1.6}$$

The boundary free energy may then be decomposed as

$$f_{\times}(\Omega)=f_{\times}^{+}(\Omega)-f_{\times}^{-}(\Omega), \tag{3.1.7}$$

where the partial boundary free energies,

$$f_{\times}^{\pm}(\Omega)=\tfrac{1}{2}|\boldsymbol{L}|^{-1}\int_0^1 d\zeta\langle\mathscr{W}_{\pm}\rangle_{\Omega}^{\zeta}, \tag{3.1.8}$$

entail only expectation values of ferromagnetic (nonnegative) interactions. These expressions will provide the basis for all further analysis.

It may be worth noting that this decomposition can also be achieved in nonlinear form, for example via

$$\exp(2|\boldsymbol{L}|f_{\times}^{\pm})=\langle e^{\mathscr{W}_{\pm}}\rangle_{\Omega}^{-}, \tag{3.1.9}$$

where $\langle\cdot\rangle_{\Omega}^{-}$ denotes an expectation computed with $\mathscr{H}^{-}(\Omega)=\bar{\mathscr{H}}(\Omega)-\mathscr{W}_{-}(\Omega)$. (If $\mathscr{H}$ is restricted to be purely ferromagnetic, $\mathscr{H}^{-}$ might reasonably also be so restricted.)

3.2. Properties of Boundary Free Energy

At this point we may record certain properties of the boundary free energy which hold uniformly over the domains Ω, Ω_1, and Ω_2 and will hence be inherited by any thermodynamic limit.

Proposition 3.2.1. *Boundary convexity. The boundary free energy $f_{\times}(K,W,\tilde{W},\Omega)$ is a convex downward (or concave) function of any wall potential W_B, and of all the wall potentials together.*

Proof. As already remarked, this follows by well known results on convexity (see e.g. [24]), from the Definition (2.5.2) and from the fact that no W_B enters, as such, into the Hamiltonian $\mathscr{H}(\Omega)$ defined in (2.4.1). □

Remark 3.2.1. Note that (i) continuity, (ii) differentiability almost everywhere, (iii) one-sided differentiability everywhere, and (iv) monotonicity of the derivative of $f_\times(W)$ with respect to any combination of the W_B, all follow from convexity by standard arguments [29].

The proposition applies equally to potentials W_A where A is a collection coupling Ω_1 and Ω_2, provided the separation condition **E(i)**, $W_A = -K_A$, is not imposed as an identity. In applications, however, convexity in the interactions decoupling Ω is not of much interest.

Remark 3.2.2. Counterexamples to a conjecture of concavity (or convexity) in the bulk potentials K, may be found in the linear chain ($d=1$) spin $\frac{1}{2}$ Ising model with nearest-neighbor pair interactions of strength K_2 and wall potentials vanishing except for $W_{\{-1,0\}} = -K_2$ and $W_{\{-2,-1\}} = W_{\{0,1\}} = W_2$ where $-2, -1, 0$, and 1 label sites in linear order. The boundary free energy (for any sufficiently long chain) is easily found to be

$$f_\times(K, W) = \ln\cosh(K_2 + W_2) - \tfrac{3}{2}\ln\cosh K_2 . \tag{3.2.1}$$

By examining the derivative with respect to K_2 for large $|W_2|$, this is seen to be neither convex nor concave in K_2. (Note we have imposed the separation condition $W_{\{-1,0\}} = -K_2$ as an identity; however, this does not alter the conclusion.)

Proposition 3.2.2. *Boundedness. Under Conditions* **F** *(Section 2.3),* **A** *(Section 1.4),* **G(i)** *and* **H** *(Section 2.4), there is a bound*

$$|f_\times(K, W, \tilde{W}, \Omega)| < C_\times(K, W, \tilde{W}), \tag{3.2.2}$$

independent of Ω, *and likewise for* $f_\times^{\pm}(K, W, \tilde{W}, \Omega)$.

Proof. The first step is to use the linearized correlation relation (3.1.3), the basic expression (2.4.9) for $\mathscr{W}(\Omega)$, the spin correlation bound (1.4.1) [Condition **A**], the wall integrity [Condition **H** for fixed $\delta > 0$], and the finiteness of the norms $\|W\|_0$ and $\|W\|_1$ in (2.3.9) and (2.3.10) [Condition **F**], to bound terms $W_A s_A$ which couple or do not couple the subdomains, respectively. The associated wall terms in (3.1.3) are then bounded via (2.4.10) and (2.4.11) [Condition **G(i)**]. □

Remark 3.2.3. The significance of this result lies, of course, in the sufficient conditions on the bulk potentials, wall potentials, and associated wall potentials discussed in Sections 1.4, 2.3, and 2.4 in connection with the Conditions **C, F,** and **G.** Recall, in particular, Lemmas 1.4.4, 2.3.1, and 2.4.2 which relate to pair interactions bounded by power law decays of the form $1/\varrho_{ij}^{\tau} r_{ij}^{d+\sigma}$.

Now, when the bulk potentials K are *purely ferromagnetic*, the Griffiths inequalities (Section 1.3) lead to various positivity and monotonicity properties of the boundary free energy. However, since, in general, $\mathscr{W}$ contains both positive and negative potentials, conditions must also be imposed on the boundary conditions.

Proposition 3.2.3. *Negativity and monotonicity. If the bulk potentials K are purely ferromagnetic, the associated wall potentials $\tilde{W}$ are ferromagnetic* [*see* (2.4.5)], *and* *the finite wall Hamiltonian is nonpositive in the sense* $\mathscr{W}_+ = 0$, *then* $f_\times(K, W, \tilde{W}, \Omega)$ *is* (i) *negative and* (ii) *monotonic nonincreasing in* K_B *for any* B.

Corollary. *The negativity and monotonicity of* $f_\times(K)$ *hold for subfree wall conditions* $[0 \leqq -W_A \leqq K_A$; *see* (2.3.6)] *and free or ferromagnetic associated wall conditions,* $\tilde{W}_A \geqq 0$ *all* $A \subset \Omega$.

Proof. The conditions on K and $\tilde{W}$ stated in the proposition ensure that $\bar{\mathscr{H}}(\Omega)$ is purely ferromagnetic. Furthermore, $-\mathscr{W} \equiv \mathscr{W}_-$ is also purely ferromagnetic by assumption and hence, by (3.1.2) and (3.1.5), so is $\bar{\mathscr{H}}^\zeta(\Omega)$ for $0 \leqq \zeta \leqq 1$. Negativity and monotonicity then follows from (3.1.3) by using (1.3.1), which implies $\langle s_A \rangle^\zeta \geqq 0$, and Lemma 1.3. The corollary follows from (3.1.5) since the conditions stated yield $\mathscr{W}_+ = 0$. □

Remark 3.2.4. When the wall contains positive, ferromagnetic interactions ($W_B > 0$) the Hamiltonian $\mathscr{W}$ is no longer of definite sign, and negativity and monotonicity are in doubt even when K is purely ferromagnetic. In fact, it is easy to find counterexamples in one-dimensional Ising models. Furthermore, if the potentials K are ferromagnetic and nontrivial, in the sense that they couple Ω_1 and Ω_2, one cannot have $\mathscr{W}$ *purely* ferromagnetic since the decoupling condition **E(i)** would be violated. Thus, no simple positivity results can be expected either.

Remark 3.2.5. Finally, note that monotonicity in the bulk potentials implies that $f_\times$ can be regarded as the *derivative* with respect to a bulk field h, or with respect to the overall inverse temperature, $\theta = 1/k_B T$, of a convex function of h or of θ. This fact partially answers the question of what the thermodynamic behavior of $f_\times(K, W)$ might be.

3.3. *Inequalities on Domains*

Except for the last proposition, our discussion to this point has allowed for potentials of arbitrary sign, i.e. ferromagnetic or antiferromagnetic in character. From this stage on, however, attention is restricted to systems with *purely ferromagnetic bulk interactions* in which, furthermore, the wall and associated wall potentials are also ferromagnetic so that all intermediate Hamiltonians are likewise fully ferromagnetic. For such systems we will give a proof of the existence of the thermodynamic limit for the boundary free energy. The basic tools will be two simple propositions which are based on the GKS inequalities, and which relate the boundary free energy for a compound domain to those defined on the subdomains. It is convenient to state and prove these propositions here. The first proposition concerns a basic inequality for domains in which the associated boundary conditions are *subfree* (Section 2.3). A parallel proposition will be established for *superferromagnetic* associated walls in saturating spin systems (Section 2.3) in which, in addition, the bulk interactions must be of finite range.

Proposition 3.3.1. *Compound domains. Let a domain* Ω *with associated wall potentials* $\tilde{W}$ *be intersected by a planar wall with potentials* W. *Suppose* Ω *is decomposed into two disjoint subdomains* Ω' *and* Ω'' *with associated wall potentials,* $\tilde{W}'$ *and* $\tilde{W}''$, *and let* Ω_1,

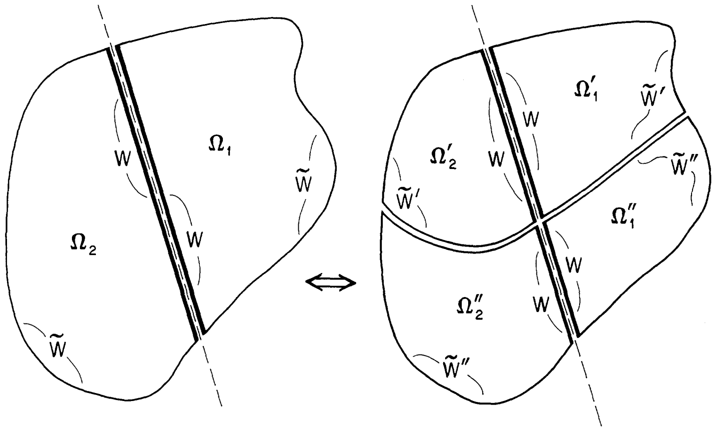

Fig. 6. A planar wall with potentials W, intersecting a compound domain Ω formed from two subdomains Ω' and Ω''

potentials W, $\tilde{W}$, $\tilde{W}'$, *and* $\tilde{W}''$, *are ferromagnetic* [*see* (2.3.6) *and* (2.4.5)], *and* (c) *the associated wall potentials satisfy the subfree consistency relations*

$$\tilde{W}'_B \leqq \tilde{W}_B \leqq 0 \quad \text{for} \quad B \subsetneq \Omega', \; \tilde{W}''_B \leqq \tilde{W}_B \leqq 0 \quad \text{for} \quad B \subsetneq \Omega'', \tag{3.3.1}$$

then the partial boundary free energies $f^+_\times$ *and* $f^-_\times$ *for given* K *and* W *satisfy the inequalities*

$$|\boldsymbol{L}|\, f^\pm_\times(\tilde{W}, \Omega) \geqq |\boldsymbol{L}'|\, f^\pm_\times(\tilde{W}', \Omega') + |\boldsymbol{L}''|\, f^\pm_\times(\tilde{W}'', \Omega''), \tag{3.3.2}$$

where $|\boldsymbol{L}|$, $|\boldsymbol{L}'|$, *and* $|\boldsymbol{L}''|$ *are the areas of the wall in* Ω, Ω', *and* Ω'', *respectively.*

Proof. The partial free energies entering the inequality to be proved can be expressed by (3.1.8) and (3.1.5) in terms of spin expectation values computed in partially coupled domains with Hamiltonians, $\bar{\mathscr{H}}(\zeta) = \bar{\mathscr{H}} + \zeta\mathscr{W}$, $\bar{\mathscr{H}}'(\zeta) = \bar{\mathscr{H}}' + \zeta\mathscr{W}'$, and $\bar{\mathscr{H}}''(\zeta) = \bar{\mathscr{H}}'' + \zeta\mathscr{W}''$, where $\bar{\mathscr{H}} = \bar{\mathscr{H}}(\Omega)$, $\bar{\mathscr{H}}' = \bar{\mathscr{H}}(\Omega')$, etc. The later two ζ-dependent Hamiltonians can be combined into a compound Hamiltonian, $\bar{\mathscr{H}}^\dagger(\zeta) = \bar{\mathscr{H}}'(\zeta) + \bar{\mathscr{H}}''(\zeta)$, for the compound domain $\Omega^\dagger = \Omega_1 \cup \Omega_2 = \Omega$. The Conditions (a) and (b) ensure that all these Hamiltonians are purely ferromagnetic for $0 \leqq \zeta \leqq 1$. The idea of the proof is simply that the difference $\Delta\bar{\mathscr{H}}(\zeta) = \bar{\mathscr{H}}(\zeta) - \bar{\mathscr{H}}^\dagger(\zeta)$ is also purely ferromagnetic so that, by appeal to the GKS inequalities as embodied in Lemma 1.3 [with $\mathscr{H}_0 = \mathscr{H}^\dagger(\zeta)$ and $\mathscr{H}_1 = \Delta\mathscr{H}(\zeta)$], one has $\langle s_A \rangle^\zeta \geqq \langle s_A \rangle^{\dagger\zeta}$ for any correlation function entering the partial free energy expressions. Provided the corresponding coefficients are non-negative, the inequality follows. Owing to the possibility of interference between the various wall potentials the algebraic details are a little complicated.

We first check the ferromagnetic character of $\Delta\bar{\mathscr{H}}(\zeta)$. The Definitions (2.4.1), (2.4.6), and (2.4.9) show that $\Delta\bar{\mathscr{H}}(\zeta)$ is a sum only of the following terms:

(i) $(K_B + \zeta W_B + \tilde{W}_B)\, s_B$, for all $B \in \Omega' \cdot \Omega''$,

(ii) $(\tilde{W}_B - \tilde{W}'_B)\, s_B$, for all $B \subsetneq \Omega'_1$ and $B \subsetneq \Omega'_2$,

(iii) $(1-\zeta)(\tilde{W}_B - \tilde{W}'_B)\, s_B$, for all $B \in \Omega'_1 \cdot \Omega'_2$, and similar terms with $\tilde{W}''_B$ replacing $\tilde{W}'_B$, etc., and, finally,

(iv) $-\zeta \tilde{W}_B s_B$, for all $B \in \Omega^{\bullet}$,

where $\Omega^{\bullet}$ denotes the set of all collections linking at least three of the subdomains $\Omega'_1, \Omega'_2, \Omega''_1$, and Ω''_2. The purely ferromagnetic nature of the terms (i) for $\zeta \leqq 1$ follows from the ferromagnetic character of W and $\tilde{W}$ [see (2.4.5)]. The consistency Conditions (3.3.1) ensure the ferromagnetic nature of the terms (ii) and (iii) for $\zeta \leqq 1$. Finally the subfree character of $\tilde{W}$ makes the terms (iv) ferromagnetic for $\zeta \geqq 0$. The use of Lemma 1.3 is thus justified.

To check the positivity of the coefficients of the correlation functions we use (3.1.5) to rewrite the difference of the two sides of the inequality as

$$\begin{aligned} |\boldsymbol{L}| \Delta f_{\times}^{\pm} = \tfrac{1}{2} \int_0^1 d\zeta \Bigg\{ & \left[\sum_{\Omega'_1} + \sum_{\Omega'_2} + \sum_{\Omega''_1} + \sum_{\Omega''_2} \right] W_A^{\pm} (\langle s_A \rangle^{\zeta} - \langle s_A \rangle^{\dagger\zeta}) \\ & + \left[\sum_{\Omega'_1 \cdot \Omega''_1} + \sum_{\Omega'_2 \cdot \Omega''_2} \right] W_A^{\pm} \langle s_A \rangle^{\zeta} + \sum_{\Omega^{\bullet}} \Delta W_B^{\pm} \langle s_B \rangle^{\zeta} \\ & + \sum_{\Omega'_1 \cdot \Omega'_2} [\Delta W_B'^{\pm} (\langle s_B \rangle^{\zeta} - \langle s_B \rangle^{\dagger\zeta}) + (\Delta W_B^{\pm} - \Delta W_B'^{\pm}) \langle s_B \rangle^{\zeta}] \\ & + \sum_{\Omega''_1 \cdot \Omega''_2} [\Delta W_B''^{\pm} (\langle s_B \rangle^{\zeta} - \langle s_B \rangle^{\dagger\zeta}) + (\Delta W_B^{\pm} - \Delta W_B''^{\pm}) \langle s_B \rangle^{\zeta}] \Bigg\}, \end{aligned} \tag{3.3.3}$$

where $\Delta W_B = W_B - \tilde{W}_B$, $\Delta W'_B = W_B - \tilde{W}'_B$, etc., while $\Omega^{\bullet}$ is defined as above. By the Definitions (3.1.6) the coefficients $W_A^{\pm}$, $\Delta W_B'^{\pm}$, and $\Delta W_B''^{\pm}$ are nonnegative. By Lemma 1.3.3, $(\langle s_A \rangle^{\zeta} - \langle s_A \rangle^{\dagger\zeta})$ is nonnegative for $0 \leqq \zeta \leqq 1$. Hence the first line in the formula for $\Delta f_{\times}^{\pm}$ is nonnegative. Since $\mathscr{H}(\zeta)$ is purely ferromagnetic the GKS inequality (1.3.1) implies $\langle s_A \rangle^{\zeta} \geqq 0$. This ensures the nonnegativity of the second line. Finally the separation Condition (2.3.2) gives $\Delta W_B = -K_B - \tilde{W}_B$, $\Delta W'_B = -K_B - \tilde{W}'_B$, etc., in the last two lines, which, combined with the subferromagnetic consistency relations (3.3.1), yields $\Delta W_B^{\pm} \geqq \Delta W_B''^{\pm}$. Thus each term in the expression is nonnegative and the proposition is proved. □

Remark 3.3.1. It is clear from the proof that the role of the consistency relations $\tilde{W}'_B \leqq \tilde{W}_B$ and $\tilde{W}''_B \leqq \tilde{W}_B$, is to ensure that no interactions in $\bar{\mathscr{H}}' + \bar{\mathscr{H}}''$ are stronger than in $\bar{\mathscr{H}}$. If the associated wall potentials are located only near the boundaries, and match on the common boundaries of Ω, Ω', and Ω'' the consistency relation has real effect only where the boundary between Ω' and Ω'' meets the boundary of Ω.

Remark 3.3.2. The proposition applies even if the wall fails to intersect one subdomain so that, say, Ω''_1 is empty. The resulting basic subferromagnetic inequalities then read

$$f_{\times}^{\pm}(K, W, \tilde{W}, \Omega) \geqq f_{\times}^{\pm}(K, W, \tilde{W}', \Omega'). \tag{3.3.4}$$

Furthermore, this inequality applies even when Ω'' itself is empty so that $\Omega' = \Omega$. In this trivial case the result is easily proved by direct appeal to Lemma 1.3.

Remark 3.3.3. Note that the main wall potentials, W, are *not* restricted to be subfree; all that is required is $W_A \geqq -K_A$ (all A) i.e., ferromagnetic character.

We turn now to the statement and proof of a somewhat more restricted basic inequality for superferromagnetic associated boundary conditions.

Proposition 3.3.2. *Compound domains with superferromagnetic walls. Consider, as in Proposition 3.3.1 (and Fig. 6), a domain Ω with associated wall potentials $\tilde{W}$ which is decomposed into disjoint subdomains Ω' and Ω'' with associated wall potentials $\tilde{W}'$ and $\tilde{W}''$. If* (a) *the spins are saturating with modulus $\|s\|$,* (b) *the bulk potentials, K, are purely ferromagnetic and of finite range, R^∞,* (c) *the wall potentials W are ferromagnetic* [*see* (2.3.6)] *and of finite range $R^\times$,* (d) *the associated wall potentials, $\tilde{W}$, $\tilde{W}'$, and $\tilde{W}''$ are superferromagnetic and formed by imposing fields $h_i = +\infty$ on each spin $i \in \Omega$ which satisfies $r(i, \partial\Omega) \leqq R^0$, (see Section 2.3) and similarly for Ω' and Ω'', where*

$$R^0 \geqq \tfrac{1}{2} \max\{R^\infty, R^\times\}, \tag{3.3.5}$$

and (e) *the associated wall potentials satisfy the superferromagnetic consistency conditions*

$$\tilde{W}'_B \geqq \tilde{W}_B \geqq 0 \quad \textit{for} \quad B \subsetneq \Omega', \qquad \tilde{W}''_B \geqq \tilde{W}_B \geqq 0 \quad \textit{for} \quad B \subsetneq \Omega'', \tag{3.3.6}$$

then the partial boundary free energies for given K and W satisfy the inequalities

$$\begin{aligned} |\mathbf{L}| f_\times^\pm(\tilde{W}, \Omega) \leqq{} & |\mathbf{L}'| f_\times^\pm(\tilde{W}', \Omega') + |\mathbf{L}''| f_\times^\pm(\tilde{W}'', \Omega'') \\ & + Y_1^\pm(\Omega', \Omega'') + Y_2^\pm(\tilde{W}; \Omega', \Omega''), \end{aligned} \tag{3.3.7}$$

where the boundary interference terms are

$$Y_1^\pm = \tfrac{1}{2}\Big(\sum_{\Omega'_1 \cdot \Omega''_1} + \sum_{\Omega'_2 \cdot \Omega''_2}\Big) W_A^\pm \|s_A\|, \tag{3.3.8}$$

$$Y_2^\pm = \tfrac{1}{2} \sum_{A \in \Omega^\bullet} \Delta W_A^\pm \|s_A\|, \quad \textit{with} \quad \Delta W_A = W_A - \tilde{W}_A, \tag{3.3.9}$$

in which, as before, $\Omega^\bullet$ denotes the set of collections linking at least three of Ω'_1, Ω'_2, Ω''_1, and Ω''_2.

Proof. The idea of the proof, as in Proposition 3.3.1, is to compare the spin expectations, computed in the two partially coupled domains with Hamiltonians $\bar{\mathscr{H}}(\zeta)$ and $\bar{\mathscr{H}}^\dagger(\zeta) = \bar{\mathscr{H}}'(\zeta) + \bar{\mathscr{H}}''(\zeta)$. Conditions (b), (c), and (d) ensure that these Hamiltonians are purely ferromagnetic for $0 \leqq \zeta \leqq 1$. The superferromagnetic boundary conditions will be used to show that the difference Hamiltonian $\bar{\mathscr{H}}^\dagger(\zeta) - \bar{\mathscr{H}}(\zeta)$ is also purely ferromagnetic if proper allowance is made for the terms coupling Ω' and Ω''. Hence Lemma 1.3 yields $\langle s_A \rangle^{\dagger\zeta} \geqq \langle s_A \rangle^\zeta$, so that, again allowing for coupling terms, the inequality (3.3.7) follows from the partial free energy expressions (3.1.8) and (3.1.5).

As a first step, note that in calculating $\langle s_A \rangle^{\dagger\zeta}$ we may add any constant term to $\bar{\mathscr{H}}^\dagger(\zeta)$ without changing expectation values. Hence consider the incremental Hamiltonian

$$\Delta\bar{\mathscr{H}}^\dagger(\zeta) = \bar{\mathscr{H}}^\dagger(\zeta) + \sum_{B \in \Omega' \cdot \Omega''} (K_B + \tilde{W}_B + \zeta W_B) \|s_B\| - \bar{\mathscr{H}}(\zeta), \tag{3.3.10}$$

in which the "interaction" term involves only the constant spin moduli $\|s_B\| = \|s\|^{\|B\|}$. Note, furthermore, that owing to the range Condition (3.3.5) any collection B for which $(K_A + \tilde{W}_A + \zeta W_A)$ is nonvanishing contain only spins that are fully frozen ($s_i = \|s\|$) by the infinite boundary fields, h_i, acting in the subdomains Ω' and Ω'' so that one may replace $\|s_B\|$ by s_B in this definition of $\Delta\bar{\mathscr{H}}^\dagger$. On using the

Definitions (2.4.1), (2.4.6), and (2.4.9) the only contributions to $\Delta\bar{\mathscr{H}}^{\dagger}(\zeta)$ are then found to be

(i) $(\tilde{W}'_B - \tilde{W}_B)s_B$, for all $B \subsetneq \Omega_1$ and $B \subsetneq \Omega_2$,

(ii) $(1-\zeta)(\tilde{W}'_B - \tilde{W}_B)s_B$, for all $B \in \Omega'_1 \cdot \Omega'_2$

and similarly for $B \in \Omega''_1 \cdot \Omega''_2$, with $\tilde{W}''_B$ replacing $\tilde{W}'_B$, and

(iii) $\zeta \tilde{W}_B s_B$, for all $B \in \Omega^{\cdot}$.

The superferromagnetic consistency Conditions (3.3.6), ensure that all these terms are ferromagnetic. This justifies an appeal to Lemma 1.3.

The second step is to calculate $\Delta f^{\pm}_{\times}$; this leads to the same expression (3.3.3) as before but the aim is now to prove that $|\boldsymbol{L}|\Delta f^{\pm}_{\times}$ is less that $Y^{\pm}_1 + Y^{\pm}_2$. Accordingly, note that the first line in (3.3.3) will now be nonpositive since $\langle s_A \rangle^{\zeta} \leqq \langle s_A \rangle^{\dagger\zeta}$. The terms in the second line are majorized by $Y^{\pm}_1$ and $Y^{\pm}_2$ as defined in (3.3.8) and (3.3.9), because $\langle s_A \rangle \leqq \|s_A\|$ (all ζ). In the third and fourth lines the correlation inequality ensures the nonpositivity of the terms involving $\Delta W'^{\pm}_B$ and $\Delta W''^{\pm}_B$. The remaining terms are nonpositive since $\langle s_B \rangle^{\zeta} \geqq 0$ by the ferromagnetic condition and because the separation condition (2.3.2) yields $\Delta W_B = -(K_B + \tilde{W}_B)$ and $\Delta W'_B = -(K_B + \tilde{W}'_B)$ so that superferromagnetic consistency, (3.3.6), gives $\Delta W^{\pm}_B \leqq \Delta W'^{\pm}_B$ and, likewise, $\Delta W^{\pm}_B \leqq \Delta W''^{\pm}_B$. This proves the inequality (3.3.7). □

Remark 3.3.4. The finite range Condition (3.3.5) can be relaxed significantly. Thus suppose, for concreteness, that the boundary separating Ω' and Ω'' can be regarded as a planar wall, W'''. Then R^{∞} and $R^{\times}$ can be replaced by the range of the bulk interactions, K, and of the original wall potentials, W, *normal* to this wall, i.e., with the diameter $d(A)$ of a collection A replaced with the caliper diameter $d_{\perp}(A)$ with respect to the defining plane $\mathscr{P}'''$ in the range definitions.

Remark 3.3.5. For finite range bulk and wall potentials satisfying $\boldsymbol{B}$ and $\boldsymbol{F}$ the boundary interference terms, $Y^{\pm}_1$ and $Y^{\pm}_2$, in (3.3.7) can be bounded by a constant, depending only on K and W, times the length. say $|\partial \boldsymbol{L}'''|$, of a suitably defined *common perimeter* of the faces $\boldsymbol{L}'_1$ and $\boldsymbol{L}''_1$ (or $\boldsymbol{L}_2$ and $\boldsymbol{L}'_2$). For simple sequences of domains $\{\Omega_k\}$, $\{\Omega'_k\}$, $\{\Omega''_k\}$, one will have $|\partial \boldsymbol{L}'''|/|\boldsymbol{L}| \to 0$ in the thermodynamic limit.

Remark 3.3.6. As in Proposition 3.3.1 the inequality (3.3.7) applies even when one subdomain fails to intersect the wall. Provided $r(\mathscr{P}, \Omega'') > 2R^0$ the sums defining $Y^{\pm}_1$ and $Y^{\pm}_2$ become empty. The basic superferromagnetic inequalities then reduce to

$$f^{\pm}_{\times}(K, W, \tilde{W}, \Omega) \leqq f^{\pm}_{\times}(K, W, \tilde{W}', \Omega'), \tag{3.3.11}$$

where, as before, the only restriction on K and W is their ferromagnetic character ($K_A \geqq 0$, $W_A \geqq -K_A$). Again the inequality remains valid with Ω' replaced by Ω.

4. Thermodynamic Limit for Box Domains

In this chapter we establish a variety of existence and uniqueness theorems for the boundary free energies defined on general sequences of *box domains*, $\Lambda_{\boldsymbol{L},N}$. First we define appropriate box domains. Then, using the propositions established in

Chapter 3 to compare different boxes, we prove basic subadditive inequalities for $f_{\times}^{+}(\Lambda)$ and $f_{\times}^{-}(\Lambda)$. Finally, the thermodynamic limit for $f_{\times}$ follows from subadditivity lemmas, and some uniqueness theorems follow from the propositions on comparing domains.

4.1. Definition of Box Domains

We are interested in establishing the existence of the thermodynamic limit of $f_{\times}(K, W, \Omega)$ for a set of wall potentials W corresponding to a definite lattice plane $\mathscr{P}$. In Section 2.2 we showed how the lattice could be decomposed relative to $\mathscr{P}$ into disjoint *blocks* labelled by an integer vector $\boldsymbol{l}=(l_0, l_1, \dots, l_{d'})$ with $d'=d-1$, which specifies translations by block vectors $\boldsymbol{R}_l$ with components $\boldsymbol{b}_0, \boldsymbol{b}_1, \dots \boldsymbol{b}_{d'}$ [see (2.2.5)]. Blocks with $l_0=0$ lie adjacent to the wall on the $\mathscr{L}_1$ side of $\mathscr{P}$; blocks with $l_0=-1$ lie adjacent to the wall on the opposite, $\mathscr{L}_2$ side. Recall also that the area of a wall in a finite domain Ω is defined [in (2.2.6)] in terms of the number of blocks in Ω adjacent to the wall. It is thus convenient to choose a collection of standard domains constructed by assembling sets of blocks into "rectangular" arrays. Accordingly we introduce:

Definition 4.1. A *box* or *box domain*, $\Lambda_{\boldsymbol{L},N}$ of crossectional area $|\boldsymbol{L}|$ and *length* N, is a set of $L_1 L_2 \dots L_{d'} N > 0$ blocks with labels satisfying

$$0 < l_\beta \leqq L_\beta \quad \text{for} \quad 1 \leqq \beta \leqq d', \quad \text{and} \quad 0 < l_0 \leqq N, \tag{4.1.1}$$

or a set of blocks equivalent under translation by a block vector.

Note that a box $\Lambda_{\boldsymbol{L},N}$ of length $N=N_1+N_2$ $(N_1,\ N_2>0)$ with first label satisfying $N_1 > l_0 \geqq -N_2$, is intersected by the wall W as illustrated in Figure 7(a). The wall area is

$$|\boldsymbol{L}| = L_1 L_2 \dots L_{d'}, \tag{4.1.2}$$

while N_1 and N_2 represent the length of the box on the two sides of the wall. The corresponding boundary free energy will be denoted

$$f_{\times}(K, W, \tilde{W}; \boldsymbol{L}; N_1, N_2) = f_{\times}(K, W, \tilde{W}, \Lambda_{\boldsymbol{L},N_1+N_2}), \tag{4.1.3}$$

and the partial free energies $f_{\times}^{+}(\Lambda)$ and $f_{\times}^{-}(\Lambda)$ will be written analogously.

4.2. Super- and Subadditive Inequalities

We now use the propositions of Section 3.3 to compare the partial boundary free energies for different boxes with free or simple superferromagnetic associated wall conditions. This leads to certain superadditive, subadditive, and monotonicity inequalities for the boundary free energy, $f_{\times}(L_1, \dots, L_d; N_1, N_2)$. We consider first *free associated boundary conditions* $(\tilde{W}=0)$.

Lemma 4.2.1. *Superadditivity. The partial boundary free energies for boxes* $\Lambda_{\boldsymbol{L},N_1+N_2}$ *with* (a) *free associated wall potentials and* (b) *ferromagnetic bulk and wall potentials, K and W* [*see* (2.3.6) *and* (2.4.15)], *satisfy for any* γ $(1 \leqq \gamma \leqq d')$ *the inequalities*

$$(L'_\gamma + L''_\gamma)\, f_{\times}^{\pm}(L'_\gamma + L''_\gamma) \geqq L'_\gamma f_{\times}^{\pm}(L'_\gamma) + L''_\gamma f_{\times}^{\pm}(L''_\gamma), \qquad (L'_\gamma, L''_\gamma > 0), \tag{4.2.1}$$

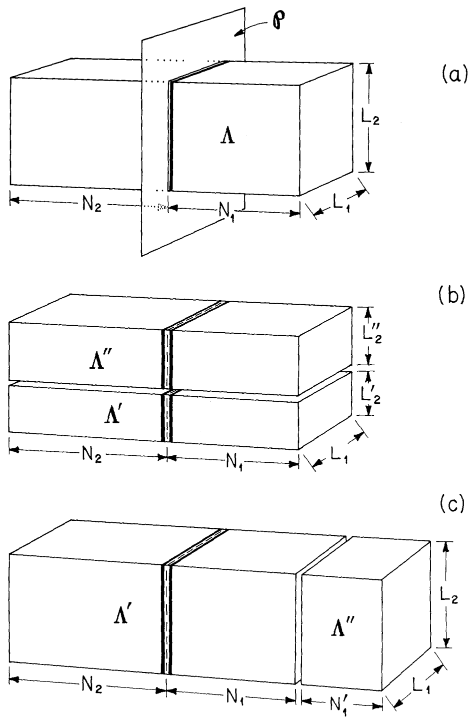

Fig. 7a—c. Schematic illustrations of a box domain Λ_{L,N_1+N_2} in $d=3$ dimensions showing **a** the intersection with a wall plane, $\mathscr{P}$, **b** decomposition into two box domains intersecting the walls, and **c** into two box domains, one not intersecting the wall. Note that box domains are not in general rectangular in the original Euclidean space

where the undisplayed arguments $L_1, \ldots, L_{\gamma-1}, \ldots, L_{d'}, N_1$, and N_2 are the same in all terms.

Proof. By the translational invariance of the wall potentials [Condition **E(ii)**] the box Λ with $L_\gamma = L'_\gamma + L''_\gamma$, can be regarded as decomposed into two similar boxes Λ' and Λ'' but with sides L'_γ and L''_γ, respectively [as illustrated in Fig. 7(a) and (b) for $\gamma=2, d=3$]. Then note that Conditions (a) and (b) of Proposition 3.3.1 are satisfied (ferromagnetic character). Furthermore, the free associated wall conditions on Λ and on Λ' and Λ'' satisfy the subferromagnetic consistency condition of Proposition 3.3.1. On using (4.1.2) the lemma follows immediately from the proposition. □

Lemma 4.2.2. *Monotonicity. The partial boundary free energies for boxes Λ_{L,N_1+N_2} with* (*a*) *free associated wall potentials and* (b) *ferromagnetic bulk and wall potentials, satisfy, for N'_1, $N'_2 \geqq 0$, the inequalities*

$$f_\times^\pm(L; N_1+N'_1, N_2) \geqq f_\times^\pm(L; N_1, N_2), \tag{4.2.2}$$

$$f_\times^\pm(L; N_1, N_2+N'_2) \geqq f_\times^\pm(L; N_1, N_2). \tag{4.2.3}$$

Proof. As illustrated in Figure 7(c), the domain Λ of the total length $N_1+N'_1+N_2$ can be decomposed into domains of length N_1+N_2 and N'_1. Application of Proposition 3.3.1 is justified as in the proof of Lemma 4.2.1, and, on recalling

Remark 3.3.1, this leads immediately to (4.2.2.). The second inequality follows likewise. □

Now we consider *simple superferromagnetic associated boundary conditions*, $\tilde{W}^*$, realized by taking $\tilde{W}_A=0$ except for the imposition of fields $h_i=+\infty$ on each (saturating) spin in Λ for which $r(i, \partial\Omega)\leqq R^0$ where, for finite range bulk and wall potentials, the channel width R^0 satisfies (3.3.5) of Proposition 3.3.2 [but see also Remark 3.3.4].

Lemma 4.2.3. *Subadditivity. The partial boundary free energies in saturating spin systems for boxes* Λ_{L,N_1+N_2} *with* (a) *simple superferromagnetic associated boundary conditions satisfying* (3.3.5), *and* (b) *ferromagnetic bulk and wall potentials of finite range and finite degree p, satisfy, for any* γ $(1\leqq\gamma\leqq d')$

$$(L'_\gamma+L''_\gamma)f_\times^\pm(L'_\gamma+L''_\gamma)\leqq L'_\gamma f_\times^\pm(L'_\gamma)+L''_\gamma f_\times^\pm(L''_\gamma)+Y_0(K,W), \tag{4.2.4}$$

where the undisplayed arguments K, W, $\tilde{W}^*$, $L_1,\ldots,L_{\gamma-1},L_{\gamma+1},\ldots,L_{d'}$, N_1, *and* N_2 *are the same in all terms, and* L'_γ, $L''_\gamma\geqq L_\gamma^0$ *where* L_γ^0 *is large enough to avoid triviality (i.e., no unfrozen spins in* Λ' *or* Λ''*), and* $Y_0(K,W)$ *is a finite constant independent of* N_1, N_2, *and* $\mathbf{L}$.

Proof. With a decomposition of Λ of the form illustrated in Figure 7(b), Conditions of (a), (b), (c), and (d) Proposition 3.3.2 are all met. Condition (e) of the proposition (consistency), follows since $W'_A=0$ except for the infinite fields on the boundary spins in which, by definition are also infinite in Λ' and Λ''. Application of the proposition together with (4.1.2) leads to the desired result but with Y_0 replaced by

$$|\mathbf{L}^\gamma|^{-1}(Y_1^\pm+Y_2^\pm)\leqq\tfrac{1}{2}|\mathbf{L}^\gamma|^{-1}\sum_{A\in\Lambda'\cdot\Lambda''}W_A^\pm\|s_A\|, \tag{4.2.5}$$

where the contact perimeter between Λ' and Λ'' is

$$|\mathbf{L}^\gamma|=\prod_{\beta\neq\gamma}^{d'}L_\beta. \tag{4.2.6}$$

On the right of (4.2.4) $\tilde{W}_A=0$ has been used in (3.3.9) which has then been combined with (3.3.8) and augmented by some nonnegative wall potentials $W_A^\pm$ (with A not in $\Lambda'_1\cdot\Lambda''_1$, $\Lambda'_2\cdot\Lambda''_2$, or $\Lambda^\bullet$). Now following the discussion of bounded wall potentials (Conditions **F** in Section 2.3), it is not hard to see that for bulk and wall potentials of finite range and degree that the sum in (4.2.5) can be bounded by $Y_0(K,W)|\mathbf{L}^\gamma|$ with finite Y_0. □

Lemma 4.2.4. *Monotonicity for superferromagnetic associated walls. Under the conditions of the previous lemma the partial boundary free energies satisfy*

$$f_\times^\pm(\mathbf{L};N_1+N'_1,N_2)\leqq f_\times^\pm(\mathbf{L};N_1,N_2), \tag{4.2.7}$$

for N_1 *sufficiently large and* $N'_1\geqq0$, *and likewise in terms of* N_2 *and* N'_2.

Proof. The decomposition of Λ shown in Figure 7(c) is used together with Proposition 3.3.2 and Remark 3.3.6. □

4.3. *Subadditive and Monotonic Functions*

In this section we prove some general lemmas concerning the limiting behavior for large arguments of *multiply* subadditive and monotonic functions. These results represent extensions of well known theorems for ordinary subadditive and monotonic functions and serve to show the existence of a limiting value which is *independent* of how the various arguments approach infinity.

A function $g(x)$ defined on $\mathbb{R}$ or $\mathbb{Z}$ is said to be subadditive [30] if it satisfies

$$g(x+y) \leqq g(x)+g(y). \tag{4.3.1}$$

Likewise a function $g(\boldsymbol{x})=g(x_1, \ldots, x_d)$ on $\mathbb{R}^d$ or $\mathbb{Z}^d$ will be called *multiply subadditive* if it satisfies

$$g(x_1, \ldots, x_{\gamma-1}, x'_\gamma + x''_\gamma, x_{\gamma+1}, \ldots, x_d) \leqq g(x_1, \ldots, x'_\gamma, \ldots, x_d) + g(x_1, \ldots, x''_\gamma, \ldots x_d), \quad \text{for all} \quad \gamma \; (1 \leqq \gamma \leqq d). \tag{4.3.2}$$

The close relation of the partial free energies $f^{\pm}_{\times}(\boldsymbol{L}; N_1, N_2)$ to such functions will be made explicit below. The following lemma, essential to our final results, generalizes the well known result for $d=1$ (proved e.g., by Hille [30]). However our definition of multiply subadditive is quite distinct from the "vector subadditivity" studied by Rosenbaum [31].

Lemma 4.3.1. *Subadditivity. Let $g(\boldsymbol{x})=g(x_1, \ldots, x_d)$ be multiply subadditive on $\mathbb{R}^d_+$ or $\mathbb{Z}^d_+$ (the subscript indicating $x_\beta > 0$ all β) and suppose*

$$\|\boldsymbol{x}\|^{-1} |g(\boldsymbol{x})| < j^+ < \infty, \tag{4.3.3}$$

where $\|\boldsymbol{x}\| = \prod_{\beta=1}^{d} x_\beta$. Then the limit

$$j_\infty = \lim_{\boldsymbol{x}\to\infty} \|\boldsymbol{x}\|^{-1} g(\boldsymbol{x}), \tag{4.3.4}$$

in which $x_1, x_2, \ldots, x_d$ approach infinity in any way, exists and equals

$$j^-_\infty = \liminf_{\boldsymbol{x}\to\infty} \|\boldsymbol{x}\|^{-1} g(\boldsymbol{x}). \tag{4.3.5}$$

Proof. For given $\varepsilon > 0$ there is an $\boldsymbol{x}=\boldsymbol{k}$ such that

$$\|\boldsymbol{k}\|^{-1} g(\boldsymbol{k}) < (1+\varepsilon) j^-_\infty. \tag{4.3.6}$$

For any arbitrary $\boldsymbol{x}$ satisfying $x_\beta \geqq k_\beta$ (all β) write

$$x_\beta = (n_\beta + 1) k_\beta + c_\beta \quad \text{with} \quad n_\beta \text{ integral and} \quad 0 < c_\beta < k_\beta. \tag{4.3.7}$$

Then to $g(\boldsymbol{x})=g(n_1 k_1 + k_1 c_1, \ldots, n_d k_d + k_d + c_d)$ we may apply the subadditive inequality (4.3.2) n_1 times with $\gamma=1$ to yield

$$g(\boldsymbol{x}) \leqq n_1 g(k_1, x_2, \ldots, x_d) + g(k_1 + c_1, x_2, \ldots, x_d), \tag{4.3.8}$$

and n_2 times with $\gamma=2$ to yield

$$g(\boldsymbol{x}) \leqq n_1 n_2 g(k_1, k_2, x_3, \ldots, x_d) + n_1 g(k_1, k_2 + c_2, x_3, \ldots, x_d) + n_2 g(k_1 + c_1, k_2, x_3, \ldots, x_d) + g(k_1 + c_1, k_2 + c_2, x_3, \ldots, x_d). \tag{4.3.9}$$

On repeating for the variables $x_3, x_4, \ldots, x_d$ we obtain

$$g(\boldsymbol{x}) \leqq n_1 n_2 \ldots n_d g(\boldsymbol{k}) + G(\boldsymbol{x}), \tag{4.3.10}$$

where the remainder is given by

$$G(\boldsymbol{x}) = \sum_{\boldsymbol{v}}{}' \prod_{\beta=1}^{d} [v_\beta(n_\beta - 1) + 1] g(k_1 + \bar{v}_1 c_1, k_2 + \bar{v}_2 c_2, \ldots, k_d + \bar{v}_d c_d), \tag{4.3.11}$$

in which $v_\beta = 1 - \bar{v}_\beta = 1$ or 0 and the primed sum runs over the $2^d - 1$ values of $\boldsymbol{v}$ for which *at least one* v_γ vanishes. Now on using (4.3.6) and the bound (4.3.3) we obtain

$$\frac{g(\boldsymbol{x})}{\|\boldsymbol{x}\|} \leqq (1+\varepsilon) j_\infty^- \prod_{\beta=1}^{d} \frac{n_\beta k_\beta}{(n_\beta k_\beta + k_\beta + c_\beta)} + j^+ \sum_{\boldsymbol{v}}{}' \prod_{\beta=1}^{d} \frac{(v_\beta n_\beta - v_\beta + 1)(k_\beta + \bar{v}_\beta c_\beta)}{(n_\beta k_\beta + k_\beta + c_\beta)}, \tag{4.3.12}$$

in which each product in the sum over $\boldsymbol{v}$ is of order $1/n_\gamma$ for some γ as $\boldsymbol{x} \to \infty$ (which implies $\boldsymbol{n} \to \infty$). On taking the limit in any way we hence obtain

$$\lim_{\boldsymbol{x} \to \infty} g(\boldsymbol{x}) / \|\boldsymbol{x}\| \leqq (1+\varepsilon) j_\infty^-, \tag{4.3.13}$$

which proves the lemma. □

We now consider monotonic functions. A function $h(\boldsymbol{y}) = h(y_1, y_2, \ldots, y_d)$ on $\mathbb{R}^d$ or $\mathbb{Z}^d$ is said to be *multiply monotonic nonincreasing* if

$$h(y_1, \ldots, y_{\gamma-1}, y_\gamma + y'_\gamma, y_{\gamma+1}, \ldots, y_d) \leqq h(\boldsymbol{y})$$
$$\text{for} \quad y'_\gamma \geqq 0 \quad \text{and all } \gamma \quad (1 \leqq \gamma \leqq d). \tag{4.3.14}$$

The basic result is:

Lemma 4.3.2. *Monotonicity. If $h(\boldsymbol{y})$ is a multiply monotonic nonincreasing function on $\mathbb{R}^d$ or $\mathbb{Z}^d$ which is bounded below by h^-, then the limit*

$$h_\infty = \lim_{\boldsymbol{y} \to \infty} h(y_1, y_2, \ldots, y_d) \geqq h^-, \tag{4.3.15}$$

exists and is independent of the way in which $y_1, \ldots, y_d$ approach $+\infty$.

Proof. Define $h^0(z) = h(z, z, \ldots, z)$. By repeated application of (4.3.14) this function is monotonic nonincreasing in z. Since it is bounded below by h^-, the limit

$$\lim_{z \to \infty} h^0(z) = h_\infty^0, \tag{4.3.16}$$

exists. Now for any $\boldsymbol{y}$ define $z_{\max} = \max_\beta \{y_\beta\}$ and $z_{\min} = \min_\beta \{y_\beta\}$. Repeated application of (4.3.14) then yields

$$h^0(z_{\max}) \leqq h(\boldsymbol{y}) \leqq h^0(z_{\min}). \tag{4.3.17}$$

When $\boldsymbol{y} \to \infty$ we have $z_{\max} \to \infty$ and $z_{\min} \to \infty$, and so by (4.3.16) the limit h_∞ exists (and equals h_∞^0). □

We now consider functions which are subadditive in some arguments and monotonic in others.

Lemma 4.3.3. *Subadditivity and monotonicity. Let* $g(\boldsymbol{x},\boldsymbol{y})=\|\boldsymbol{x}\|j(\boldsymbol{x},\boldsymbol{y})$ *with* $\|x\|=\prod_{\beta=1}^{d'} x_\beta$ *be a function which is subadditive on* $\boldsymbol{x}\in\mathbb{R}^{d'}$ *(or* $\mathbb{Z}^{d'}$*) and monotonic on* $\boldsymbol{y}\in\mathbb{R}^{d''}$ *(or* $\mathbb{Z}^{d''}$*) [in the senses (4.3.2) and (4.3.14)]. Then if* $|j(\boldsymbol{x},\boldsymbol{y})|$ *is bounded, the limit*

$$\lim_{\boldsymbol{x},\boldsymbol{y}\to\infty} j(\boldsymbol{x},\boldsymbol{y})=j_\infty\,, \tag{4.3.18}$$

exists and is independent of the way in which the variables $x_1,\dots,x_{d'}$, $y_1,\dots,y_{d''}$ *approach* $+\infty$.

Proof. First note that $g_1(\boldsymbol{x})=\lim_{\boldsymbol{y}\to\infty}\|x\|j(\boldsymbol{x},\boldsymbol{y})$ is subadditive in $\boldsymbol{x}$ so that

$$\lim_{\boldsymbol{x}\to\infty}\lim_{\boldsymbol{y}\to\infty} j(\boldsymbol{x},\boldsymbol{y})=j_{1,\infty}\,, \tag{4.3.19}$$

exists, where the notation $\boldsymbol{x}\to\infty$ means that the separate components, x_β, approach $+\infty$ in any way (and likewise for $\boldsymbol{y}\to\infty$). Conversely, $j_2(\boldsymbol{y})=\lim_{\boldsymbol{x}\to\infty} j(\boldsymbol{x},\boldsymbol{y})$ is monotonic in $\boldsymbol{y}$ so that the limit with reversed order, namely

$$\lim_{\boldsymbol{y}\to\infty}\lim_{\boldsymbol{x}\to\infty} j(\boldsymbol{x},\boldsymbol{y})=j_{2,\infty} \tag{4.3.20}$$

also exists. Secondly note that for fixed $\boldsymbol{x}$ and $\boldsymbol{y}_1$ we have

$$\lim_{\boldsymbol{y}\to\infty} j(\boldsymbol{x},\boldsymbol{y})\leqq j(\boldsymbol{x},\boldsymbol{y}_1)\,, \tag{4.3.21}$$

because $j(\boldsymbol{x},\boldsymbol{y})$ is monotonic on $\boldsymbol{y}$. Now suppose $\boldsymbol{y}_0(\cdot)$ is an arbitrary function except that $\boldsymbol{y}_0(\boldsymbol{x})\to\infty$ as $\boldsymbol{x}\to\infty$. By setting $\boldsymbol{y}_1=\boldsymbol{y}_0(\boldsymbol{x})$ and letting $\boldsymbol{x}\to\infty$ we conclude

$$j_{1,\infty}\leqq\liminf_{\boldsymbol{x}\to\infty\,\boldsymbol{y}_0} j(\boldsymbol{x},\boldsymbol{y}_0(x))=\liminf_{\boldsymbol{x},\boldsymbol{y}\to\infty} j(\boldsymbol{x},\boldsymbol{y})=j_\infty^-\,, \tag{4.3.22}$$

where, finally, the x_α and y_β approach $+\infty$ in any way. On the other hand we have similarly, by monotonicity for any fixed $\boldsymbol{y}_2$,

$$\begin{aligned} j_\infty^+ &=\limsup_{\boldsymbol{x},\boldsymbol{y}\to\infty} j(\boldsymbol{x},\boldsymbol{y})=\limsup_{\boldsymbol{x}\to\infty\,\boldsymbol{y}_0} j(\boldsymbol{x},\boldsymbol{y}_0(\boldsymbol{x}))\,,\\ &\leqq\lim_{\boldsymbol{x}\to\infty} j(\boldsymbol{x},\boldsymbol{y}_2)\,, \end{aligned} \tag{4.3.23}$$

which, on letting $\boldsymbol{y}_2\to\infty$, yields $j_\infty^+\leqq j_{2,\infty}$.

Lastly it remains to prove that $j_\infty^+=j_\infty^-$; this will be achieved by proving that $j_{1,\infty}=j_{2,\infty}$. To this end consider subsequences defined by $x_\beta=2^{n_\beta}$ $(1\leqq\beta\leqq d')$, where $\boldsymbol{n}=(n_\beta)$ is an integer vector, and set

$$j(2^{n_1},\dots,2^{n_{d'}},\boldsymbol{y})=\bar{j}(\boldsymbol{n};\boldsymbol{y})\,. \tag{4.3.24}$$

The existence of the limits in (4.3.19) and (4.3.20) means that any subsequence converges, so we have

$$\lim_{\boldsymbol{n}\to\infty}\lim_{\boldsymbol{y}\to\infty}\bar{j}(\boldsymbol{n};\boldsymbol{y})=j_{1,\infty}\quad\text{and}\quad\lim_{\boldsymbol{y}\to\infty}\lim_{\boldsymbol{n}\to\infty}\bar{j}(\boldsymbol{n};\boldsymbol{y})=j_{2,\infty}\,. \tag{4.3.25}$$

However, the subadditive inequality (4.3.2) yields

$$2^{n_\gamma+1}\bar{j}(n_1,\ldots,n_{\gamma-1},n_\gamma+1,n_{\gamma+1},\ldots,n_{d'};\boldsymbol{y})\leqq 2[2^{n_\gamma}\bar{j}(\boldsymbol{n};\boldsymbol{y})]$$
$$\text{for any } \gamma\ (1\leqq\gamma\leqq d'). \tag{4.3.26}$$

This means $\bar{j}(\boldsymbol{n};\boldsymbol{y})$ is a multiple monotonic function in the variables $\boldsymbol{n}$ and $\boldsymbol{y}$ together. It follows immediately from Lemma 4.3.2 that $\lim_{\boldsymbol{n},\boldsymbol{y}\to\infty}\bar{j}(\boldsymbol{n};\boldsymbol{y})$ exists and is independent of the order of limits. By (4.3.25) we thus have $j_{1,\infty}=j_{2,\infty}$ which completes the proof. □

We may now apply these lemmas to the inequalities found in Section 4.2 for the partial boundary free energies.

4.4. Existence Theorems

In this section we first establish the existence of the limiting boundary free energy, $f_\times^0(K,W)$ for arbitrary sequences of boxes with ferromagnetic interactions and free associated boundary conditions. Then boxes with general subfree associated boundary conditions, $\tilde{W}$, will be shown to yield the *same* limiting boundary free energy (independent of $\tilde{W}$). A parallel argument establishes the existence of a limiting boundary free energy $f_\times^*(K,W)$, for boxes with saturating spins, interactions of finite range, and simple superferromagnetic boundary conditions. Boxes with general superferromagnetic associated boundary conditions, $\tilde{W}$, are shown to yield the same limit $f_\times^*$, independent of $\tilde{W}$. However, the identify of $f_\times^0$ and $f_\times^*$ is *not* established here. (It will be proved in a following paper with the aid of correlation decay assumptions.) Nevertheless, some further uniqueness results, specifically for "flat" boxes, are established for more general associated boundary conditions.

Theorem 4.4.1. *Existence for free associated wall potentials. For a sequence of boxes* $\Lambda_{\boldsymbol{L},N_1+N_2}$ [see Fig. 7(a)] *with* (a) *free associated wall potentials* ($\tilde{W}\equiv 0$) *and* (b) *bulk potentials, K, and wall potentials, W, which are ferromagnetic [see* (1.2.6) *and* (2.3.6)*] and which satisfy the boundedness Conditions* **A** *(Section 1.4) and* **F** *(Section 2.3), and the defining Conditions* **D** *and* **E** *(Sections 2.2 and 2.3), the limiting boundary free energy*

$$f_\times^0(K,W)=\lim_{\boldsymbol{L},N_1,N_2\to\infty} f_\times(K,W,\tilde{W}\equiv 0;\boldsymbol{L},N_1,N_2), \tag{4.4.1}$$

exists and is independent of how the limits $L_1\to\infty,\ldots,L_{d'}\to\infty$, $N_1\to\infty$ and $N_2\to\infty$ are taken. Furthermore, $f_\times^0(K,W)$ is convex downward in the potentials W, and, if $W_A\leqq 0$ all A, negative and monotonic nonincreasing in the potentials K. The limits, $f_\times^{0\pm}(K,W)\geqq 0$, of the partial free energies $f_\times^\pm(K,W,\tilde{W}=0;\Lambda)$, are similarly uniquely defined.

Proof. We will use the decomposition (3.1.7), namely

$$f_\times(K,W,\tilde{W};\Lambda)=f_\times^+(K,W,\tilde{W};\Lambda)-f_\times^-(K,W,\tilde{W};\Lambda). \tag{4.4.2}$$

By hypothesis the conditions required by Lemmas 4.2.1 and 4.2.2 are satisfied so that the functions $j^\pm(\boldsymbol{L},\boldsymbol{N})\equiv -f_\times^\pm(L_1,\ldots,L_{d'};N_1,N_2)$ are multiply subadditive and monotonic in the sense of Lemma 4.3.3. Furthermore the uniform boundedness of

$|j^{\pm}(\boldsymbol{L}, \boldsymbol{N})|$ follows from Proposition 3.2.2 which is applicable by virtue of Conditions **A**, **F**, and $\tilde{W} \equiv 0$ (which implies **G**). The existence of the separate limits $f_{\times}^{0\pm} = \lim f_{\times}^{\pm}(\boldsymbol{L}, N_1, N_2)$ and their independence of the way $L_1, \ldots, N_2$ approach infinity, then follows, from Lemma 4.3.3, and this proves (4.4.1).

Finally the convexity in W, and the negativity and monotonicity in K when $W_A \leqq 0$ (all A) follow from Propositions 3.2.1 and 3.2.3. □

Remark 4.4.1. It is worth stressing that, apart from the ferromagnetic restriction $[W_A + K_A \geqq 0$ for $A \in \mathscr{L}_1 \cdot \mathscr{L}_2]$ and the boundedness of the norms $\|W\|_0$ and $\|W\|_1$ of Condition **F**, the wall potentials can be quite general both as regards sign, strength and range. Furthermore, in the case of saturating spins, superferromagnetic walls are also allowed [see (2.3.8) where, indeed, the condition $W_B^0 \geqq 0$ may also be relaxed]. Recall, however, that Condition **F(i)** [(2.3.9)] implies that the bulk potentials, K, decay in directions normal to the wall plane, $\mathscr{P}$, at a rate essentially one inverse power of distance faster than needed for bulk stability. Finally note that the wall separation Condition **E(i)** has not played a vital role in the existence proof. Thus the arguments also establish the existence of a limiting grain boundary or seam free energy.

We now consider associated boundary potentials which are subfree.

Theorem 4.4.2. *Uniqueness for subfree associated potentials. For a sequence of boxes with ferromagnetic bulk and wall potentials satisfying the conditions of Theorem 4.4.1, and with associated wall potentials, $\tilde{W}$, which are subfree* [(2.3.7) *and* (2.4.5)] *and satisfy the tempering condition $\boldsymbol{C}_\tau$ [(1.4.12)] with exponent $\tau > 0$, the limiting boundary free energy,*

$$\lim_{\boldsymbol{L}, N_1, N_2 \to \infty} f_{\times}(K, W, \tilde{W}; \boldsymbol{L}, N_1, N_2),$$

exists and is equal to $f_{\times}^0(K, W)$, the limit for free associated boundary conditions, independent of $\tilde{W}$ and of how the limit is taken.

Proof. Again the decomposition (4.4.2) will be employed. The first step is to compare the partial free energies $f_{\times}^{\pm}(\tilde{W}; \Lambda)$ with those for the same box Λ but with free associated wall potentials ($\tilde{W} \equiv 0$). Appeal to Proposition 3.3.1 [recalling Remark 3.3.2] yields an inequality from which, using Theorem 4.4.1, we conclude

$$\limsup_{\Lambda \to \infty} f_{\times}^{\pm}(K, W, \tilde{W}; \Lambda) \leqq f_{\times}^{0\pm}(K, W). \tag{4.4.3}$$

The second step is to compare the box $\Lambda \equiv \Lambda_{\boldsymbol{L}, N_1 + N_2}$ with a reduced box $\Lambda' \equiv \Lambda_{\boldsymbol{L}', N_1 + N_2}$, where, as illustrated in Figure 8,

$$\begin{aligned} &L'_\gamma + 2R = L_\gamma, \ (\gamma = 1, \ldots, d'), \\ &N'_1 + R \leqq N_1, \quad \text{and} \quad N'_2 + R \leqq N_2, \end{aligned} \tag{4.4.4}$$

on which free associated boundary conditions are imposed. If the associated wall potentials, $\tilde{W}$, are of *finite range*, $\tilde{R}^{\times}$, and we choose $R > \tilde{R}^{\times}$ it is easy to see that the subfree consistency relations (3.3.1) of Proposition 3.3.1 are satisfied. Noting that

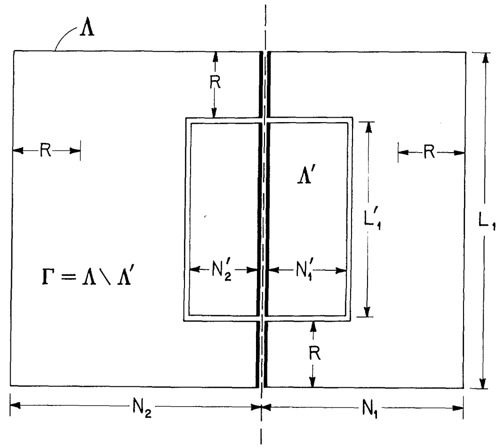

Fig. 8. Insertion of a reduced box Λ', with free associated boundary conditions, into a box Λ with more general associated boundary conditions

$f_\times^\pm(\Gamma)$ is nonnegative for the difference domain $\Gamma = \Lambda \backslash \Lambda'$ we then conclude from the proposition that

$$|\boldsymbol{L}| f_\times^\pm(\tilde{W};\, \boldsymbol{L}, N_1, N_2) \geqq |\boldsymbol{L}'| f_\times^\pm(\tilde{W} \equiv 0;\, \boldsymbol{L}', N_1', N_2'). \tag{4.4.5}$$

Now divide by $|\boldsymbol{L}|$ and (i) let $\boldsymbol{L}, N_1', N_2' \to \infty$ at fixed R so that $|\boldsymbol{L}'|/|\boldsymbol{L}| \to 1$, followed by (ii) $N_1', N_2' \to \infty$. Theorem 4.4.1 then yields

$$\liminf_{\Lambda \to \infty} f_\times^\pm(K, W, \tilde{W}; \Lambda) \geqq f_\times^{0\pm}(K, W), \tag{4.4.6}$$

from which, in combination with (4.4.3), the present theorem follows.

However, for associated wall potentials of *infinite range* the subfree consistency relations (3.3.1) fail, so we first introduce the truncated associated wall potentials $\tilde{W}^\dagger$ defined, for given Λ, by

$$\begin{aligned} \tilde{W}_A^\dagger &= \tilde{W}_A, \quad \text{if} \quad A \cap \Lambda' = \emptyset, \\ &= 0, \quad \text{if } A \text{ contains sites in } \Lambda'. \end{aligned} \tag{4.4.7}$$

With these truncated potentials, the consistency relations are satisfied so Proposition 3.3.1 can be applied to obtain (4.4.5) but with $\tilde{W}$ replaced by $\tilde{W}^\dagger$. In order to compare $f_\times(K, W, \tilde{W}; \Lambda)$ and $f_\times(K, W, \tilde{W}^\dagger; \Lambda)$ we use the following crude but informative lemma:

Lemma 4.4.1. *If $f_\times$ and $f_\times^\dagger$ denote the wall free energies in a finite domain with Hamiltonians $\bar{\bar{\mathscr{H}}}$ and $\bar{\bar{\mathscr{H}}}^\dagger = \bar{\bar{\mathscr{H}}} + \mathscr{Q}$, respectively, then*

$$|f_\times^\dagger - f_\times| \leqq 2\langle\langle \mathscr{Q} \rangle\rangle / |\boldsymbol{L}|, \tag{4.4.8}$$

where $|\boldsymbol{L}|$ is the wall area and $\langle\langle \cdot \rangle\rangle$ denotes the maximum modulus of the expectation over the ensembles with total Hamiltonian $\bar{\mathscr{H}}, \bar{\mathscr{H}}^\dagger, \bar{\mathscr{H}} + \mathscr{W}$, and $\bar{\mathscr{H}}^\dagger + \mathscr{W}^\dagger$, in which $\mathscr{W}$ is the wall Hamiltonian, and $\mathscr{W}^\dagger - \mathscr{W} = \mathscr{Q}^\bullet$ represents the change in the wall-associated-wall interference term [see (2.4.9) *and* (3.1.5)*].*

Proof. By the Definition (3.1.1) and straightforward rearrangement we have

$$\begin{aligned}\exp[2|\boldsymbol{L}|(f_\times^\dagger - f_\times)] &= \frac{\mathrm{Tr}\{e^{\mathscr{H}^\dagger + \mathscr{W}^\dagger}\}\,\mathrm{Tr}\{e^{\mathscr{H}}\}}{\mathrm{Tr}\{e^{\mathscr{H}+\mathscr{W}}\}\,\mathrm{Tr}\{e^{\mathscr{H}^\dagger}\}},\\ &= \langle e^{\mathscr{Q}+\mathscr{Q}^\cdot}\rangle_{\mathscr{H}+\mathscr{W}}\langle e^{-\mathscr{Q}}\rangle_{\mathscr{H}^\dagger},\\ &= [\langle e^{-\mathscr{Q}-\mathscr{Q}^\cdot}\rangle_{\bar{\mathscr{H}}^\dagger+\mathscr{W}^\dagger}\langle e^{\mathscr{Q}}\rangle_{\bar{\mathscr{H}}}]^{-1},\end{aligned} \tag{4.4.9}$$

where the subscripts indicate the paricular ensemble involved. Repeated use of the inequality $\langle e^{\mathscr{Q}}\rangle \geqq e^{\langle\mathscr{Q}\rangle}$, the triangle inequality, and the relation $\langle\langle\mathscr{Q}^\cdot\rangle\rangle \leqq \langle\langle\mathscr{Q}\rangle\rangle$, proves the lemma. □

To use the estimate (4.4.8) we identify $\bar{\mathscr{H}}^\dagger - \bar{\mathscr{H}}$ in terms of the difference between $\tilde{W}$ and $\tilde{W}^\dagger$ as

$$\mathscr{Q}(\boldsymbol{L}, N_1, N_2; R, N_1', N_2') = \sum_{A \cap \Lambda' \neq \emptyset} \tilde{W}_A s_A . \tag{4.4.10}$$

Then the correlation bound $\boldsymbol{A}$ yields

$$\langle\langle\mathscr{Q}\rangle\rangle \leqq \sum_{i \subset \Lambda'} \tilde{S}_i(K, \tilde{W}, \Lambda), \tag{4.4.11}$$

where, for $i \subset \Lambda'$,

$$\tilde{S}_i = \sum_{i \subset A \subseteq \Lambda} |\tilde{W}_A|\, \|s\|^{|A|}/|A| \leqq C/R^\tau, \tag{4.4.12}$$

in which the last inequality follows from the tempering condition $\boldsymbol{C}_\tau$ and the specification (4.4.4) of Λ'. Finally the lemma yields

$$|f_\times^\dagger(\Lambda) - f_\times(\Lambda)| \leqq 2|\Lambda'|C/|\boldsymbol{L}|R^\tau = c_6(N_1' + N_2')|\boldsymbol{L}'|/|\boldsymbol{L}|R^\tau, \tag{4.4.13}$$

where c_6 is a constant. Now when, in (4.4.5) with $\tilde{W}^\dagger$ replacing $\tilde{W}$, we let $\boldsymbol{L}, N_1, N_2$, *and* R approach infinity at fixed N_1' and N_2' in such a way that $R/L_\gamma \to 0$ (all γ) we have $|\boldsymbol{L}'|/|\boldsymbol{L}| \to 1$ and, since $\tau > 0$ by hypothesis, $|f_\times^\dagger - f_\times| \to 0$. On finally allowing $N_1', N_2' \to \infty$ we recapture (4.4.6) for the full associated potentials $\tilde{W}$, and by (4.4.3) the theorem then follows.

Remark 4.4.3. It is clear that the power law tempering condition, $\boldsymbol{C}_\tau$, could be relaxed further; all that is required in the proof is that the contribution of the associated wall potentials vanishes as the distance, R, from the walls becomes infinite.

For saturating spin systems with interactions of finite range we now establish similar results for superferromagnetic associated boundary conditions.

Theorem 4.4.3. *Simple superferromagnetic associated potentials. For a sequence of boxes $\Lambda_{\boldsymbol{L}, N_1+N_2}$ in a system with saturating spins of modulus $\|s\|$, and ferromagnetic bulk and wall potentials, K and W, of finite range, R^∞ and $R^\times$, respectively, and of finite degree p, subject to simple superferromagnetic associated boundary conditions, $\tilde{W}^*$, imposed on a channel of width $R^0 \geqq \frac{1}{2}\max\{R^\infty, R^\times\}$ (see Proposition 3.3.2), the limiting boundary free energy*

$$f_\times^*(K, W) = \lim_{\boldsymbol{L}, N_1, N_2 \to \infty} f_\times(K, W, \tilde{W}^*; \boldsymbol{L}, N_1, N_2), \tag{4.4.14}$$

and the corresponding partial free energies, $f_\times^{*\pm}$, exist and are independent of R^0 and of how the limit is taken. Furthermore $f_\times^*(K, W)$ is convex downward in the wall potentials, W, and the partial free energies satisfy the inequalities

$$f_\times^{0+}(K, W) \leqq f_\times^{*+}(K, W), \quad f_\times^{0-}(K, W) \leqq f_\times^{*-}(K, W), \tag{4.4.15}$$

where the superscript 0 *denotes free associated boundary conditions (Theorem 4.4.1).*

Proof. The conditions stated ensure the validity of Lemmas 4.2.3 and 4.2.4 (subadditivity and monotonicity). The inequality (4.2.4) of Lemma 4.2.3 involves the additive constant $Y_0(K, W)$ but it is straightforward to check that

$$j^\pm(\boldsymbol{L};\boldsymbol{N}) = f_\times^\pm(K, W, W^*;\, \boldsymbol{L}; N_1, N_2) + Y_0(K, W) \sum_{\beta=1}^{d'} L_\beta^{-1}, \tag{4.4.16}$$

yields a multiply subadditive and monotonic function in the sense of Lemma 4.3.3. Furthermore, the finite range and degree conditions stated, imply, by Lemmas 2.3.1 and 2.4.1, Conditions **F** and **G(i)** which, in turn, by Proposition 3.2.2, means that $j^\pm$ is uniformly bounded. Consequently the limits $f_\times^{*\pm}$ and $f_\times^*$ exist and are unique. The convexity of $f^*(K, W)$ in W follows from Proposition 3.2.1. Finally, the inequalities (4.4.15) follow by using the GKS Lemma 1.3 and the correlation expressions (3.1.8) for $f_\times^\pm(K, W, \tilde{W}, \Lambda)$ to compare free associated boundary condition, $\tilde{W} \equiv 0$ with the simple superferromagnetic conditions, $\tilde{W}^*$, and using Theorem 4.4.1. □

Remark 4.4.4. The finite range restrictions on K and W can be relaxed significantly. Some range restrictions are required for Lemma 4.2.3 which in turn rests on Proposition 3.3.2 (decomposition of domains) but, as observed in Remark 3.3.4, it is only the finiteness of the ranges of K and W *normal* to the associated (or side) walls of the boxes that is needed. Thus the bulk and wall potentials could be of infinite range in the direction of the block vector $\boldsymbol{b}_0$. By utilizing saturated spin barriers of width R^0, which are allowed to increase sufficiently fast to ∞ in the limit $\Lambda \to \infty$, it should be possible to replace even these weaker finite range restrictions by a tempering condition.

Remark 4.4.5. The inequalities (4.4.15) provide a relation between the boundary free energies for superferromagnetic walls and for free walls. Proof of the reverse inequalities would, of course, establish $f_\times^0(K, W) = f_\times^*(K, W)$. There are good reasons to believe this equality and, indeed, in the following paper we shall present a proof under the assumption of correlation decay. The difficulty of a proof without such an assumption may be seen along the lines of the argument of Section 2.7. Specifically, if a first order transition occured as a function of field, h, at some non-zero h_σ, then the free and superferromagnetic boundary conditions would, for $h = h_\sigma$, yield distinct bulk phases with distinct wall free energies. In reality, for ferromagnetic systems, Yang-Lee theorems prove the absence of such phase transitions for $h_\sigma \neq 0$. However, this fact must be embodied in the argument in some definite way.

Theorem 4.4.4. *Superferromagnetic associated walls. Under the conditions of Theorem 4.4.3 the limiting boundary free energy for a sequence of boxes* Λ_{L,N_1+N_2} *with saturating spins and superferromagnetic associated wall potentials* $\tilde{W}$ $[\tilde{W}_A \geqq 0$, *see Section 2.3*$]$ *of finite range* $\tilde{R}^{\times}$, *exists and is equal to* $f^*_{\times}(K, W)$ *(Theorem 4.4.3) independently of* $\tilde{W}$, *and likewise for the partial boundary free energies.*

Proof. The first step is to compare simple, $\tilde{W}^*$, and general superferromagnetic boundary conditions, $\tilde{W}$, on the same box Λ. Using Proposition 3.3.2 in the form (3.3.11), and taking the limit yields

$$\liminf_{\Lambda\to\infty} f^{\pm}_{\times}(K, W, \tilde{W}; \boldsymbol{L}, N_1, N_2) \geqq f^{*\pm}_{\times}(K, W). \tag{4.4.17}$$

Following the proof of Theorem 4.4.2, the second step is to introduce the reduced box $\Lambda' \equiv \Lambda_{L', N_1+N_2}$ (Fig. 8) satisfying (4.4.4) with $R > \tilde{R}^{\times}$, on which only simple superferromagnetic associated conditions are imposed. The superferromagnetic consistency relations of Proposition 3.3.2 are then satisfied and we may conclude

$$\begin{aligned} |\boldsymbol{L}| f^{\pm}_{\times}(\tilde{W}, \Lambda) \leqq\, & |\boldsymbol{L}'| f^{\pm}_{\times}(\tilde{W}^*, \Lambda') + |\boldsymbol{L}''| f^{\pm}_{\times}(\tilde{W}'', \Gamma) \\ & + Y^{\pm}_1(\Lambda', \Gamma) + Y^{\pm}_2(\tilde{W}; \Lambda', \Gamma), \end{aligned} \tag{4.4.18}$$

in which $\Gamma = \Lambda \backslash \Lambda'$, with corresponding wall $\boldsymbol{L}''$ and associated wall potentials $\tilde{W}''$, while $Y^{\pm}_1$ and $Y^{\pm}_2$ are given in (3.3.8) and (3.3.9). Now, as in the proof of Theorem 4.4.3, the finite range and degree conditions imply that $f^{\pm}_{\times}(\tilde{W}'', \Gamma)$ is bounded independently of Γ. Likewise it is straightforward to show that $(Y^{\pm}_1 + Y^{\pm}_2)$ is of the same order as the common wall perimeter of Λ' and Γ, i.e., bounded by $c_7 |\boldsymbol{L}'| \sum_{\beta=1}^{d'} L_\beta^{-1}$. Thus, on (i) taking the limit $\boldsymbol{L}, N_1, N_2 \to \infty$ in (4.4.18) at fixed R, N'_1, and N'_2 so that $|\boldsymbol{L}'|/|\boldsymbol{L}| \to 1$ and $|\boldsymbol{L}''|/|\boldsymbol{L}| \to 0$, and then (ii) letting $N'_1, N'_2 \to \infty$, we conclude

$$\limsup_{\Lambda\to\infty} f^{\pm}_{\times}(K, W, \tilde{W}; \Lambda) \leqq f^{*\pm}_{\times}(K, W). \tag{4.4.19}$$

In combination with (4.4.17), this proves the theorem. □

Remark 4.4.6. As in the proof of Theorem 4.4.2 for subfree associated walls, the result could be extended to tempered superferromagnetic associated potentials of infinite range. However, this is not especially satisfying in light of the facts (a) that the finite range of K and W normal to the associated walls would still be needed and (b) that with the available tools we cannot prove the equality of $f^0_{\times}(K, W)$ and $f^*_{\times}(K, W)$.

Finally we prove a result for boxes with *arbitrary* associated potentials imposed on the side walls (namely those of lengths N_1 and N_2).

Theorem 4.4.5. *Arbitrary associated side wall potentials. Consider a sequence of boxes* Λ_{L,N_1+N_2} *with ferromagnetic bulk and wall potential satisfying the conditions of*

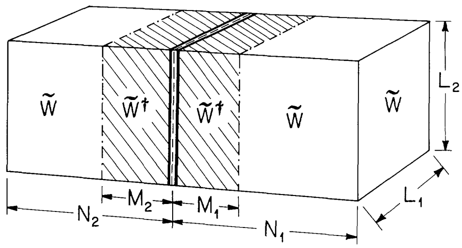

Fig. 9. Illustrating a box Λ_{L,N_1+N_2} with arbitrary additional associated wall potentials, $\tilde{W}^\dagger$, imposed over bands of width M_1 and M_2 on the side walls

Theorem 4.4.1 and subject to subfree associated wall potentials, $\tilde{W}$, except over bands of width $M_1 \leqq N_1$ and $M_2 \leqq N_2$ on the side walls (see Fig. 9) where arbitrary tempered additional wall potentials $\tilde{W}^\dagger$, of exponent $\tau > 0$ [see (1.4.12)] are imposed with the understanding that $\tilde{W}^\dagger_A$ vanishes except for $A \subsetneq \Lambda' \equiv \Lambda_{L,M_1+M_2}$. Then the corresponding limiting boundary free energy exists, is unique, and is equal to $f^0_\times(K, W)$ independent of $\tilde{W}$ and $\tilde{W}^\dagger$, provided $(M_1+M_2)/[L_\gamma]^\tau \to 0$ (all γ) as $\Lambda \to \infty$ where

$$\begin{aligned}[z]^\tau &= z^\tau, \quad \textit{for} \quad 0<\tau<1, \\ &= z/\ln z, \quad \textit{for} \quad \tau=1, \\ &= z, \quad \textit{for} \quad \tau>1. \end{aligned} \tag{4.4.20}$$

Proof. The theorem is a straightforward application of Lemma 4.4.1 to bound the difference between the free energies, $f^\dagger_\times(\Lambda)$ and $f_\times(\Lambda)$, with and without the additional potentials $\tilde{W}^\dagger$. To bound $\langle\langle \mathcal{Q} \rangle\rangle$ of the lemma, it suffices to estimate

$$\begin{aligned} S^\dagger(K,\Lambda') &= \sum_{i \subset \Lambda'} \sum_{i \subset A \subsetneq \Lambda'} |\tilde{W}^\dagger_A| \, \|s\|^{\|A\|}/|A|, \\ &\leqq \sum_{i \subset \Lambda'} C/(a+r_i)^\tau, \end{aligned} \tag{4.4.21}$$

where the inequality embodies the tempering condition $\boldsymbol{C}_\tau$ [see (1.4.12)] in which C and a are constants while r_i here denotes the distance from site i to the *side* walls of Λ [or, more formally, $r_i = r(i, \partial\Lambda_{L,\infty})$]. Now with $L_m \equiv L_{\gamma_m} = \min_\beta\{L_\beta\}$, note that r_i is bounded by $c_8 L_m$. By the geometry of the box Λ', the total density of sites distance r from the sides is bounded by $c_9(M_1+M_2)|\boldsymbol{L}|/L_m$, from the pair of opposite sides not involving L_m, plus

$$c_{10}(M_1+M_2) \sum_{\beta \neq \gamma_m} |\boldsymbol{L}|/L_\beta \leqq (d-2)c_{10}(M_1+M_2)|\boldsymbol{L}|/L_m, \tag{4.4.22}$$

from the remaining $(d-2)$ pairs of sides. Hence by Lemma 4.4.1 we have

$$|f^\dagger_\times - f_\times| \leqq c_{11} C(M_1+M_2) \int_a^{c_8 L_m} \frac{d\varrho}{L_m \varrho^\tau} = O((M_1+M_2)/[L_M]^\tau) \tag{4.4.23}$$

where $[z]^\tau$ is defined in (4.4.20). The proof is completed by taking $\Lambda \to \infty$ and using Theorem 4.4.2. □

Remark 4.4.7. The added wall potentials $\tilde{W}^{\dagger}$ may be quite arbitrary, subject to the tempering condition, and, in particular need *not* respect the ferromagnetic character of the remaining potentials K, W, and $\tilde{W}$ so that negative fields and antiferromagnetic couplings are allowed. Furthermore, they could be superferromagnetic (if the spins saturate).

Remark 4.4.8. The theorem applies with $M_1 = N_1$ and $M_2 = N_2$ so that for "flat" boxes, with $(N_1 + N_2)/[L_y]^{\tau} \to 0$ as $\boldsymbol{L}$, N_1, $N_2 \to \infty$, arbitrary associated wall potentials are allowed along the side walls.

Remark 4.4.9. It is clear from the proof that the bands of arbitrary added potentials, $\tilde{W}^{\dagger}$, need not be disposed just as shown in Figure 9. Indeed, the bands may be broken up in any way provided the total contribution to $S^{\dagger}(K, \Lambda')$ is asymptotically small relative to the wall area $|\boldsymbol{L}|$. However if arbitrary potentials are imposed on the "far walls" of Λ (of area $|\boldsymbol{L}|$) the proof of uniqueness fails since $S^{\dagger}$ always remains of order $|\boldsymbol{L}|$. Thus we cannot prove the identity of $f^0_{\times}(K, W)$ and $f^*_{\times}(K, W)$ this way.

Remark 4.4.10. A precisely analogous theorem may be proved if the subfree associated potentials $\tilde{W}$ are replaced by superferromagnetic potentials, provided, naturally, that $f^0_{\times}(K, W)$ is replaced by $f^*_{\times}(K, W)$.

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