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PHASE AND ANTI-PHASE BOUNDARIES IN BINARY DISCRETE SYSTEMS: A VARIATIONAL VIEWPOINT

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Abstract. We provide a variational description of nearest-neighbours and next-to-nearest neighbours binary lattice systems. By studying the Γ-limit of proper scaling of the energies of the systems, we highlight phase and anti-phase boundary phenomena and show how they depend on the geometry of the lattice.

1. **Introduction.** In this paper we present a simple variational description of the overall properties of binary lattice systems; *i.e.*, systems driven by energies defined on functions parameterized on a lattice and that may only take two values (which is not restrictive to suppose the real numbers $+1$ and -1). These two values may have a physical interpretation as 'spins' or as parameterizing two types of atoms in a binary alloy. Our scope is not to compare our results with the enormous literature on those subjects (see for example [5, 16, 17, 20] and the references therein), but only to interpret some of those from the standpoint of variational convergence. This viewpoint has been shared recently in many papers dealing with the variational description of different discrete models (see *e.g.* [4, 8, 9, 10, 11, 12, 13, 14, 18, 19]).

Here, our main goal is to show how phase and anti-phase boundaries in binary lattice systems arise from minimization arguments, and can be conveniently described by computing some Γ-limits. To this end we will limit our analysis mainly to cubic lattices, and to nearest and next-to-nearest interactions, for which the energy densities of the limit surface energies can be explicitly and easily computed.

The simplest situation is when only nearest-neighbours are taken into account. If we denote by $u^i \in \{-1, 1\}$ the value taken by the function u at the point parameterized by the integer N-tuple $i = (i_1, \dots, i_N)$ then, up to affine changes of

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variables that do not affect the overall behaviour of the system, the energy density between neighbouring u^i and u^j (*i.e.*, with $|i-j|=1$) can only be of one of the following two forms

$$f_{\rm ferro}(u^i,u^j)=-u^iu^j \qquad \text{(ferromagnetic)}$$
$$f_{\rm anti}(u^i,u^j)=u^iu^j \qquad \text{(anti-ferromagnetic)},$$

their labeling coming from the physical literature. Clearly, minimizing ferromagnetic energies favour uniform states $u^i\equiv 1$ and $u^i\equiv -1$, while anti-ferromagnetic energies favour neighbours with alternating signs.

A Γ-limit analysis of these energies can be performed by approximation with an energy on the continuum. To this end we fix a bounded open subset $\Omega\subset\mathbf{R}^N$ and consider the scaled energies

$$E_\varepsilon^{\rm ferro}(u)=\sum_{\rm n.n.}\varepsilon^N f_{\rm ferro}(u^i,u^j),\qquad E_\varepsilon^{\rm anti}(u)=\sum_{\rm n.n.}\varepsilon^N f_{\rm anti}(u^i,u^j), \tag{1.1}$$

where the sum is performed over nearest neighbours (n.n.) $i,j\in\mathbf{Z}^N$ such that $\varepsilon i,\varepsilon j\in\Omega$. In this way the array $\{u^i\}$ can be viewed as a function defined on $\Omega\cap\varepsilon\mathbf{Z}^N$. Upon identifying such functions with their piecewise-constant interpolations the energies $E_\varepsilon^{\rm ferro}$, $E_\varepsilon^{\rm anti}$ can be interpreted as defined on (a subset of) $L^1(\Omega)$, and can therefore undergo a process of Γ-limit in that framework.

The Γ-limit $E_{\rm ferro}$ of $E_\varepsilon^{\rm ferro}$ is particularly simple, only giving the trivial constraint $|u|\le 1$, and the constant (minimum) value $-|\Omega|$ (corresponding to the uniform states) on all such functions. This summarizes the fact that a sequence (u_ε) can arbitrarily mix the uniform states -1 and 1 at a mesoscopic scale with a negligible variation from the value of the uniform states as $\varepsilon\to 0$. Note that the absolute minimum value at scale ε is precisely given by $c_\varepsilon=-\sum_{\rm n.n.}\varepsilon^N$.

We can examine sequences that realize the minimum value with a sharper precision; *i.e.*, such that

$$E_\varepsilon^{\rm ferro}(u_\varepsilon)=c_\varepsilon+O(\varepsilon).$$

For such functions the limit states u will take the values ± 1 only, and the scaled Γ-limit will be an interfacial energy of the form

$$E^{(1)}_{\rm ferro}(u)=\int_{S(u)}\|\nu\|_1\,d\mathcal{H}^{N-1},$$

where $S(u)$ denotes the (essential) interface between the sets $\{u=1\}$ and $\{u=-1\}$ and the interfacial energy density $\|\nu\|_1=\sum_{i=1}^N|\nu_i|$ depending on the normal to $S(u)$ reflects the symmetries of the lattice.

In the anti-ferromagnetic case the first Γ-limit is itself not trivial, being given by the bulk energy

$$E_{\rm anti}(u)=\int_\Omega(2|u|-1)\,dx \qquad |u|\le 1 \text{ a.e.}$$

The form of the Γ-limit reflects that minimum values are given by the alternating state, whose average is 0 (the minimum point of $2|u|-1$), and gives a quantitative estimate of the energy of a deviation from the minimal state. Note that the states not constantly equal to 0 or ± 1 are best approximated again by 'mixing' constant and alternating states at a mesoscopic level.

The analysis at higher order for anti-ferromagnetic energies is seemingly useless since the unique minimizer for E_{anti} is the constant 0. Nevertheless, the change of variables

$$v^i = (-1)^{i_1+i_2+\cdots+i_N} u^i \tag{1.2}$$

allows us to repeat the analysis above, since

$$E_\varepsilon^{\text{ferro}}(v) = E_\varepsilon^{\text{anti}}(u).$$

The previous analysis can be read as follows: sequences (u_ε) with $E_\varepsilon^{\text{anti}}(u_\varepsilon) = c_\varepsilon + O(\varepsilon)$ in the limit as $\varepsilon \to 0$ determine a partition into two sets (corresponding to $\{v = 1\}$ and $\{v = -1\}$, where v is the limit of the corresponding v_ε) in which u_ε take the alternating states $u_0 := (-1)^{i_1+i_2+\cdots+i_N}$ and $u_1 = -u_0$. The interface $S(v)$ between these sets is an anti-phase boundary that is energetically described again by $E^{(1)}_{\text{ferro}}(v)$. Note that the appearance of anti-phase boundaries depends on the geometry of the lattice. Indeed we provide an example of an hexagonal lattice which does not exhibit such a phenomenon.

In the simple case above we have obtained the description of anti-phase boundaries by the simple change of parameter (1.2). This is no longer possible if longer-range interactions are taken into account, as in that case minimum states may possess less symmetries. To exemplify this fact, limiting our analysis to square lattices in dimension 2, we consider a next-to-nearest neighbour system, with energy

$$E_\varepsilon(u) = c_1 \sum_{n.n.} \varepsilon^2 u^i u^j + c_2 \sum_{n.n.n.} \varepsilon^2 u^i u^j,$$

where now n.n.n. (next-to-nearest neighbours) are those such that $|i - j| = \sqrt{2}$ (corresponding to the diagonals of the squares of the lattice).

The first order Γ-limit can be again computed for all c_1, c_2 giving a non-trivial bulk energy. We are interested in the case

$$0 < 2c_2 < c_1, \tag{1.3}$$

that is the one bringing new features to the problem. In this case alternating next-to-nearest neighbours give the minimal energy. This implies that

1) again the minimum of the bulk energy is obtained by $u = 0$;

2) locally minimizing configurations can be viewed as 2-periodic functions on the lattice taking alternatingly values 1 and -1 on rows or on columns. It is suggestive to identify these four possible states as follows: with e_1 in the case $u^i = -(-1)^{i_1}$ (*i.e.*, when the value 1 is taken on even columns), with e_2 if $u^i = -(-1)^{i_2}$ (*i.e.*, when the value 1 is taken on even rows), and with $-e_1$, $-e_2$ in the cases with exchanged signs.

Note that these are not all the states corresponding to $u = 0$, the alternating function $u^i = -(-1)^{i_1+i_2}$ having this same average. This choice entails a homogenization process. We have chosen condition (1.3) precisely to avoid the alternating situation already considered.

With this description of the new limit parameter $v \in \{\pm e_1, \pm e_2\}$ we can prove a Γ-limit result for the scaled energies, showing that the limit behaviour is now described by an energy of the form

$$F^{(1)}(v) = \int_{S(v)} \varphi(v^+, v^-, \nu) d\mathcal{H}^1.$$

Again this formula describes a limit partition into sets $\{v = \pm e_j\}$, of which $S(v)$ describes the interfaces. The energy density now not only depends on the normal

ν to $S(v)$, but also on the traces $v^{\pm}$ on both sides of $S(v)$. The form of φ can be explicitly computed, and also takes into account, beside the anisotropy of the lattice, that at a discrete level the interface can be 'sharp' (*i.e.* concentrated on one cell) or 'diffuse' (*i.e.* concentrated on more cells). The various possibilities for interfaces are summarized in Figure 1 where black dots stand for 1 and white for -1.

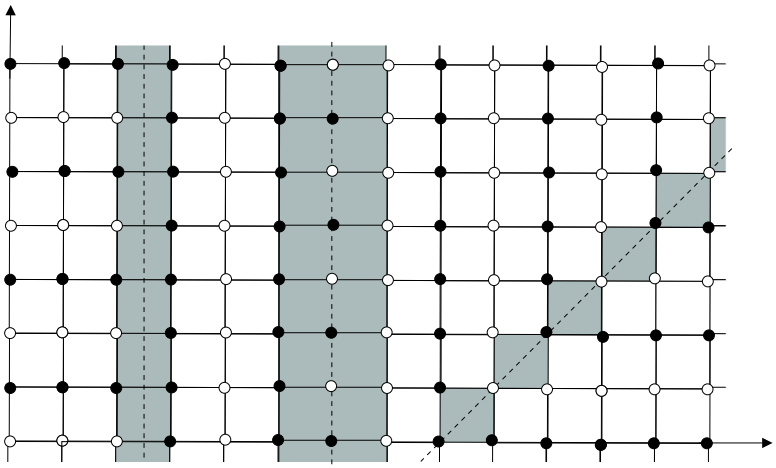

FIGURE 1. a figure showing microscopical transitions between four different phases; namely, from left to right e_2, e_1, $-e_1$ and $-e_2$ in the notation introduced above. The shaded regions represent the cells contributing to the interface energies, which concentrate on the dotted lines in the limit.

A technical point must be mentioned here: next-to-nearest neighbour interactions bring a non trivial boundary layer term (see [8]), whose contribution is not negligible in the computation of the Γ-limit, but is anyhow concentrated on the boundary of Ω. Since we do not want to concentrate on this term, we limit our analysis to Ω a torus (*i.e.*, to periodic u). Equivalently, our analysis can be stated to arbitrary Ω, but in that case $F^{(1)}$ represents the energy not concentrating on the boundary. Note however that boundary conditions cannot be neglected in general, and the boundary term can affect the form of the minimizers..

The paper is organized as follows: in Section 2 we fix some notation and we give a preliminary Γ-convergence result for binary systems in an elementary case. Moreover we recall some basic definitions and results about BV functions with values in a finite set. In Section 3 we deal with nearest-neighbour binary systems by studying the Γ-convergence of the energies in (1.1). In Section 4 we compute the Γ-limit of a proper scaling of the energies in (1.1), thus providing a sharper description of the model. Section 5 is devoted to next-to-nearest neighbour binary systems.

2. **Notation and preliminary results.** In what follows $\Omega \subset \mathbf{R}^N$ will be a bounded open set with Lipschitz boundary. Given $\varepsilon > 0$, for all $u : \varepsilon\mathbf{Z}^N \cap \Omega \to \mathbf{R}$ we set $u^i = u(\varepsilon i)$ and define $\mathbf{Z}_\varepsilon(\Omega) =: \{i \in \mathbf{Z}^N : \ \varepsilon i \in \Omega \cap \varepsilon\mathbf{Z}^N\}$.

2.1. **Almost trivial systems: uncoupled energies.** The 'almost-trivial' case of discrete system is when its total energy is simply obtained by the sum of the uncoupled energies of the single values. Given $n \in \mathbf{N}$ and $K = \{a_1, a_2, \dots, a_n\} \subset \mathbf{R}$ with $a_1 < a_2 < \cdots < a_n$,

$$E_\varepsilon(u) = \sum_{i \in \mathbf{Z}_\varepsilon(\Omega)} \varepsilon^N f(u^i),$$

where $u : \varepsilon\mathbf{Z}^N \cap \Omega \to K$ and $f : K \to \mathbf{R}$. Here the normalization factor ε^N is necessary to have $E_\varepsilon(u)$ bounded and not infinitesimal as $\varepsilon \to 0$. More precisely, upon identifying each function u with a piecewise-constant interpolation by defining the set

$$C_\varepsilon(\Omega; K) := \{u : \mathbf{R}^N \to K : u(x) = u^i \ \forall x \in \{i + Q_\varepsilon\} \cap \Omega\}, \tag{2.4}$$

where

$$Q_\varepsilon = \varepsilon\Big[-\frac{1}{2}, \frac{1}{2}\Big)^N,$$

it is possible to rewrite the energy $E_\varepsilon : C_\varepsilon(\Omega; K) \to \mathbf{R}$ as follows:

$$E_\varepsilon(u) = \int_\Omega f(u(x))\, dx + r_\varepsilon$$

where the reminder term r_ε comes from the fact that a portion of the cubes $\varepsilon i + Q_\varepsilon$ may not be completely contained in Ω. It is easy to see that $r_\varepsilon = o(1)$.

In order to set the problem in the framework of Γ-convergence it is useful to extend our functionals to be defined in L^∞. Then let $E_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ be defined as

$$E_\varepsilon(u) = \begin{cases} \displaystyle\int_\Omega f(u(x))\, dx + r_\varepsilon & \text{if } u \in C_\varepsilon(\Omega; K) \\ +\infty & \text{otherwise,} \end{cases} \tag{2.5}$$

then, by standard Γ-convergence results (see [7] for a simple introduction to the subject), the following Theorem holds true:

Theorem 1. *Let $E_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ be defined as in (2.5), then E_ε Γ-converges with respect to the w^*-topology of $L^\infty(\Omega)$ to the functional $E : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ defined as*

$$E(u) = \begin{cases} \displaystyle\int_\Omega f^{**}(u(x))\, dx & \text{if } u \in L^\infty(\Omega; \overline{K}) \\ +\infty & \text{otherwise,} \end{cases}$$

where f^{**} is the lower semicontinuous and convex envelope of $\tilde{f} : \mathbf{R} \to \mathbf{R}$ defined as

$$\tilde{f}(z) = \begin{cases} f(z) & \text{if } z \in K \\ +\infty & \text{otherwise} \end{cases}$$

and $\overline{K} = [a_1, a_n]$

In what follows we will use the previous theorem with $K = \{-1, 0, 1\}$ or $K = \{-1, -\frac{1}{2}, 0, \frac{1}{2}, 1\}$. We will denote by $C_\varepsilon(\Omega)$ the set $C_\varepsilon(\Omega; \{-1, 1\})$.

2.2. **Piecewise constant BV functions.** Next we recall some basic properties of BV functions with values in a finite set we will need in Sections 4 and 5 (see [1] and [2] for a general exposition of the subject). Let A be an open subset of $\mathbf{R}^N$ and let K be a finite subset of $\mathbf{R}^d$, $d \in \mathbf{N}$. We denote by $BV(A;K)$ the set of measurable function $u : A \to K$ whose distributional derivative Du is a measure with bounded total variation. Such a u can be written

$$u = \sum_1^{+\infty} a_i \chi_{E_i},$$

with $a_i \in K$ and E_i sets of finite perimeter. We denote by $S(u)$ the jump set of u. If $x \in S(u)$ we denote by $\nu_u(x)$ the unit normal to $S(u)$ and by $u^+(x)$, $u^-(x)$ the traces of u on $S(u)$. Then

$$Du = (u^+ - u^-) \otimes \nu_u \mathcal{H}^{N-1} \lfloor_{S(u)},$$

where $\mathcal{H}^{N-1}$ is the $N-1$-dimensional Hausdorff measure.

In the sequel we will use the following compactness and semicontinuity result (see [1, 2]).

Theorem 2. *Let $u_n \in BV(A;K)$ such that*

$$\sup_n \left(\int_A |u_n| \, dx + \mathcal{H}^{N-1}(S(u_n)) \right) < +\infty.$$

Then there exists a subsequence (not relabeled) and $u \in BV(A;K)$ such that $u_n \to u$ in the L^1 convergence. Moreover for every norm $\varphi : \mathbf{R}^N \to [0, +\infty)$

$$\liminf_n \int_{S(u_n)} \varphi(\nu_{u_n}) \, d\mathcal{H}^{N-1} \geq \int_{S(u)} \varphi(\nu_u) \, d\mathcal{H}^{N-1}.$$

If Q is a cube we will denote by $BV_\#(Q;K)$ the set of Q-periodic functions belonging to $BV_{\rm loc}(\mathbf{R}^N;K)$.

3. **Nearest-neighbour interactions: a dual lattice approach.** We now examine the case when non trivial pairwise interactions are taken into account. Let $f : \mathbf{R}^2 \to \mathbf{R}$ and let $E_\varepsilon : C_\varepsilon(\Omega) \to \mathbf{R}$ be defined as

$$E_\varepsilon(u) = \sum_{\substack{i,j \in \mathbf{Z}_\varepsilon(\Omega) \\ |i-j|=1}} \varepsilon^N f(u^i, u^j).$$

Upon rewriting

$$E_\varepsilon(u) = \sum_{\substack{i,j \in \mathbf{Z}_\varepsilon(\Omega) \\ |i-j|=1}} \varepsilon^N \frac{1}{2}(f(u^i,u^j) + f(u^j,u^i)) =: \sum_{\substack{i,j \in \mathbf{Z}_\varepsilon(\Omega) \\ |i-j|=1}} \varepsilon^N \tilde{f}(u^i,u^j),$$

we may suppose that f is symmetric: $f(u,v) = f(v,u)$. It is also not restrictive to suppose that $f(1,1) = f(-1,-1)$. In fact, if $g : \mathbf{R}^2 \to \mathbf{R}$ is such that

$$g(\pm 1, \pm 1) = f(\pm 1, \pm 1), \qquad g(-1,1) = g(1,-1) = \frac{1}{2}(f(1,1) + f(-1,-1)),$$

we can rewrite

$$\begin{aligned} E_\varepsilon(u) &= \sum_{\substack{i,j\in\mathbf{Z}_\varepsilon(\Omega)\\ |i-j|=1}} \varepsilon^N(f(u^i,u^j)-g(u^i,u^j)) + \sum_{\substack{i,j\in\mathbf{Z}_\varepsilon(\Omega)\\ |i-j|=1}} \varepsilon^N g(u^i,u^j) \\ &= \sum_{\substack{i,j\in\mathbf{Z}_\varepsilon(\Omega)\\ |i-j|=1}} \varepsilon^N(f(u^i,u^j)-g(u^i,u^j)) \\ &\quad + f(1,1)\#\{(i,j): u^i=u^j=1\} + f(-1,-1))\#\{(i,j): u^i=u^j=-1\} \\ &\quad + \frac{1}{2}(f(1,1)+f(-1,-1))\#\{(i,j): u^i=1, u^j=-1\} \\ &= \sum_{\substack{i,j\in\mathbf{Z}_\varepsilon(\Omega)\\ |i-j|=1}} \varepsilon^N(f(u^i,u^j)-g(u^i,u^j)) + \sum_{i\in\mathbf{Z}_\varepsilon(\Omega)} \varepsilon^N f(u^i,u^i). \end{aligned}$$

The last sum is an energy of the 'almost-trivial' form considered in the section above. Since in this case it coincides with (the restriction of) a linear functional, it is a continuous perturbation and hence it would just add a linear term to the limit energy. Hence, in the following sections, we will just drop it.

The behaviour of our energy will then be governed by the two values $f(1,1) = f(-1,-1)$ and $f(1,-1) = f(-1,1)$. Apart from the trivial case in which the two values are equal, we may always suppose that one of the two values is 1 and the other is -1 (this 'renormalization' amounts just to an affine change of the value of the energy). After these simplifications we are left with the two cases:

(i) $f(u,v) = -uv$ (*ferromagnetic type energies*) . In this case the minimization of E_ε will favour uniform states $u = v = 1$ or $u = v = -1$;

(ii) $f(u,v) = uv$ (*anti-ferromagnetic type energies*). In this case the minimization of E_ε will favour oscillating states $u = -v$, alternating 1 and -1.

Then, in order to study the asymptotic properties of the functionals $E_\varepsilon^\pm : L^\infty(\Omega) \to \mathbf{R}\cup\{+\infty\}$

$$E_\varepsilon^\pm(u) = \begin{cases} \pm \displaystyle\sum_{\substack{i,j\in\mathbf{Z}_\varepsilon(\Omega)\\ |i-j|=1}} \varepsilon^N u^i u^j & \text{if } u\in C_\varepsilon(\Omega) \\ +\infty & \text{otherwise} \end{cases} \tag{3.6}$$

we find it useful to perform a change of variables and describe the energies as defined on a 'dual lattice'. To this end we set

$$\mathcal{Z} = \Big\{\frac{i+j}{2} : i,j\in\mathbf{Z}^N, |i-j|=1\Big\},$$
$$\mathcal{Z}_\varepsilon(\Omega) = \Big\{\frac{i+j}{2} : i,j\in\mathbf{Z}_\varepsilon(\Omega), |i-j|=1\Big\}$$

and

$$C'_\varepsilon(\Omega) = \big\{w : \mathbf{R}^N \to \{-1,0,1\} : w(x) = w^k \ \forall x\in\{k+\varepsilon\mathcal{Q}\},\ k\in\mathcal{Z}_\varepsilon\big\}$$

where $\mathcal{Q}$ is the semi open reference cube of the dual lattice $\mathcal{Z}$ (see Fig. 2). For each

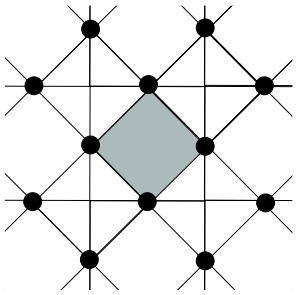

FIGURE 2. the dual lattice $\mathcal{Z}$ with its reference cube $\mathcal{Q}$ shaded.

$u \in C_\varepsilon(\Omega)$ we introduce an auxiliary function $w \in C'_\varepsilon(\Omega)$ defined as

$$w^k = \frac{u^i + u^j}{2}, \text{ where } k = \frac{i+j}{2},\ i,j \in \mathbf{Z}^N,\ |i-j| = 1.$$

Note that w takes the three values

$$w^k = \begin{cases} -1 & \text{if } u^i = u^j = -1 \\ 0 & \text{if } u^i = -u^j \\ 1 & \text{if } u^i = u^j = 1. \end{cases}$$

Then we have that

$$E^\pm_\varepsilon(u) = 2F^\pm_\varepsilon(w) \tag{3.7}$$

where $F^\pm_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ is defined as

$$F^\pm_\varepsilon(w) := \begin{cases} \pm \displaystyle\sum_{k \in \mathcal{Z}_\varepsilon(\Omega)} \varepsilon^N g(w^k_\varepsilon) & \text{if } w \in C'_\varepsilon(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

with $g : \{-1,0,1\} \to \mathbf{R}$

$$g(z) = \begin{cases} 1 & \text{if } z = \pm 1 \\ -1 & \text{if } z = 0. \end{cases}$$

Note that the factor 2 comes from the fact that each k corresponds to a pair (i,j) and the symmetric (j,i).

Observe that the change of variables we made allows us to regard the non trivial case of ferromagnetic/antiferromagnetic type energies as being of the almost trivial type considered in the previous section. Then the following Theorem holds:

Theorem 3. *Let $E_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ be defined as in (3.6), then E_ε Γ-converges with respect to the w^*-topology of $L^\infty(\Omega)$ to the functional $E^\pm : L^\infty(\Omega) \to \mathbf{R} \cap \{+\infty\}$ defined as*

$$E^\pm(u) = \begin{cases} 2^N \displaystyle\int_\Omega \psi^\pm(u(x))\,dx & \text{if } u \in L^\infty(\Omega;[-1,1]) \\ +\infty & \text{otherwise} \end{cases}$$

where

$$\psi^-(z) = (-g(z))^{**} = \begin{cases} -1 & \text{if } |z| \le 1 \\ +\infty & \text{otherwise} \end{cases}$$

and

$$\psi^+(z) = (+g(z))^{**} = \begin{cases} 2|z| - 1 & \text{if } |z| \le 1 \\ +\infty & \text{otherwise.} \end{cases}$$

Proof. The proof follows by Theorem 1 taking into account (3.7) and that 2^{1-N} is the volume of the reference cube $\mathcal{Q}$ of $\mathcal{Z}$. □

4. **A higher-order description: phase transitions.** We now focus on the ferromagnetic case and consider the following minimum problem:

$$m_\varepsilon = \min\Big\{ E_\varepsilon^-(u) : \sum_i \varepsilon^N u^i = c_\varepsilon \Big\},$$

where c_ε are such that these minima are not $+\infty$ (for example one can take c_ε such that $c_\varepsilon \#\{i \in \mathbf{Z}^N : \varepsilon i \in \Omega\} \in \mathbf{N}$) and $c_\varepsilon \to c$. The condition $\sum_i \varepsilon^N u(\varepsilon i) = c_\varepsilon$ prescribes the number of i such that $u(\varepsilon i) = \pm 1$.

By the properties of Γ-convergence and by the results stated in Theorem 3, it is possible to show that the limit of these problems is the trivial problem

$$m^{(0)} = \min\Big\{ E^-(u) : \int_\Omega u\,dx = c \Big\} = -|\Omega|.$$

(the only consideration is to show that if $\int_\Omega u = c$ then we may construct the recovery sequence u_ε for u with $\sum_i \varepsilon^N u_\varepsilon^i = c_\varepsilon$, but this is easily done). Since $E^-(u) = -|\Omega|$ is a constant when $|u| \le 1$, the limit problem does not give much information on the form of minimizers.

The idea is then to look for finer properties of minimizers by considering a proper scaling of the energy, noting that if we consider constants r_ε and δ_ε then the minimizers of the problem above are the same as those of

$$m_\varepsilon^{(1)} = \min\Big\{ \frac{E_\varepsilon(u) - r_\varepsilon}{\delta_\varepsilon} : \sum_i \varepsilon^N u(\varepsilon i) = c_\varepsilon \Big\} = \frac{m_\varepsilon - r_\varepsilon}{\delta_\varepsilon}.$$

If we show that the new functionals

$$E_\varepsilon^{(1)}(u) = \frac{E_\varepsilon(u) - r_\varepsilon}{\delta_\varepsilon}$$

possess a Γ-limit $F^{(1)}$, so that the problems $m_\varepsilon^{(1)}$ converge to

$$m^{(1)} = \min\Big\{ E^{(1)}(u) : \int_\Omega u\,dx = c \Big\},$$

then we obtain that

$$\lim_{\varepsilon \to 0} \frac{m_\varepsilon - r_\varepsilon}{\delta_\varepsilon} = m^{(1)},$$

and the minimizers of m_ε (that are the same as those of $m_\varepsilon^{(1)}$!) converge to those of $m^{(1)}$. Clearly, this information is meaningful only if $\delta_\varepsilon \to 0$.

In our case we have a 'natural' choice of r_ε by choosing

$$r_\varepsilon = -\varepsilon^N \#\{\{i,j\} : \varepsilon i, \varepsilon j \in \Omega,\ |i-j| = 1\};$$

i.e., the number of pairs of nearest neighbours that intervene in the computation of the energy renormalized by the scaling factor $-\varepsilon^N$. This is nothing but $E_\varepsilon(1)$; *i.e.*, the energy of a configuration minimizing each interaction. Note that $r_\varepsilon \to -|\Omega|$.

We also choose $\delta_\varepsilon = \varepsilon$. In this way the energy $E^{(1)}_\varepsilon(u) : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ is rewritten

$$E^{(1)}_\varepsilon(u) = \begin{cases} \displaystyle\sum_{\substack{i,j \in \mathbf{Z}_\varepsilon(\Omega) \\ |i-j|=1}} \varepsilon^{N-1}(1 - u^i u^j) & \text{if } u \in C_\varepsilon(\Omega) \\ +\infty & \text{otherwise.} \end{cases}$$

One can show that sequences with equibounded energies are compact with respect to L^1-strong convergence. This justifies the choice of the convergence we make in studying the Γ-convergence of $E^{(1)}_\varepsilon$.

Theorem 4. *The functionals $E^{(1)}_\varepsilon : L^\infty(Q) \to \mathbf{R} \cup \{+\infty\}$ Γ-converge with respect to the L^1-topology to the functional $E^{(1)} : L^1(Q) \to \mathbf{R} \cup \{+\infty\}$ defined as*

$$E^{(1)}(u) = \begin{cases} 4 \displaystyle\int_{S(u)} \|\nu_u\|_1 d\mathcal{H}^{N-1} & u \in BV(\Omega; \{\pm 1\}) \\ +\infty & \textit{otherwise,} \end{cases}$$

where $\|\nu_u\|_1 = \sum_{i=1}^N |\nu_i|$.

Proof. Let $u_\varepsilon \to u$ in $L^1(\Omega)$ be such that $\sup_\varepsilon E^{(1)}_\varepsilon(u_\varepsilon) < +\infty$. Consider a term $\varepsilon^{N-1}(1 - u^i_\varepsilon u^j_\varepsilon))$. If $u^i_\varepsilon = u^j_\varepsilon$ then the value is 0; otherwise it is equal to $2\varepsilon^{N-1}$. Note that the value ε^{N-1} is exactly the $N-1$-dimensional measure of the common boundary between the two cubes $\varepsilon(i + [-\frac{1}{2}, \frac{1}{2})^N)$ and $\varepsilon(j + [-\frac{1}{2}, \frac{1}{2})^N)$. Hence we may write

$$E^{(1)}_\varepsilon(u_\varepsilon) = 4\mathcal{H}^{N-1}\big(S(u_\varepsilon) \cap \Omega\}\big) + o(1) \tag{4.8}$$

(an additional factor 2 comes from the fact that to each (i, j) there corresponds the symmetric (j, i)). The remainder term $o(1)$ comes from the fact that close to the boundary of Ω, the $N-1$-dimensional measure of the common boundary between the two cubes internal to Ω may be less than ε^{N-1}.

Then, by (4.8) and Theorem 2, we get that $u \in BV(\Omega; \{\pm 1\})$. Moreover note that, since ν_{u_ε} is parallel to the coordinate axes, we also have that

$$E^{(1)}_\varepsilon(u_\varepsilon) = 4 \int_{S(u_\varepsilon)} \|\nu_{u_\varepsilon}\|_1 \, d\mathcal{H}^{N-1} + o(1).$$

Then, again by Theorem 2 we get

$$\liminf_{\varepsilon \to 0} E^{(1)}_\varepsilon(u_\varepsilon) \geq E^{(1)}(u).$$

To conclude, for any $u \in BV(\Omega; \{\pm 1\})$, we have to construct a recovery sequence u_ε such that

$$\lim_{\varepsilon \to 0} E^{(1)}_\varepsilon(u_\varepsilon) = E^{(1)}(u).$$

By density it suffices to consider u such that $S(u)$ is a polyhedral set. Up to a localization argument we can further reduce to the case when $S(u)$ is an hyperplane, that is

$$u(x) = \begin{cases} 1 & \text{if } \langle x, \overline{\nu} \rangle \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

with $\overline{\nu}$ a fixed vector. In this case, it is easy to verify that

$$u_\varepsilon^i = \begin{cases} 1 & \text{if } \langle i, \overline{\nu}\rangle \geq 0 \\ -1 & \text{otherwise,} \end{cases} \qquad i \in \mathbf{Z}^N$$

defines such a u_ε. □

Remark 1. The argument of convergence of minimum problems outlined above then tells us that minimum points of m_ε converge to functions u minimizing

$$m^{(1)} = \min\Big\{4\int_{S(u)} \|\nu_u\|_1 \, d\mathcal{H}^{N-1} : \int_\Omega u = c\Big\}.$$

This means that, in order to minimize E_ε the values 1 and -1 will arrange in such a way as to minimize the' interface' between the two regions $\{u_\varepsilon = -1\}$ and $\{u_\varepsilon = 1\}$. In other words, the two 'phases' 1 and -1 will not mix and will give rise to a sharp interface in the limit.

Remark 2. (The anti-ferromagnetic case: anti-phase boundaries) We now consider the anti-ferromagnetic case, when the interaction energy favours the alternance of $+1$ and -1. This case can be reduced to the previous one by using a different variable, setting

$$v^i = (-1)^{i_1+i_2+\ldots+i_N} u^i.$$

In this way

$$E_\varepsilon^+(u) = \sum_{i,j} \varepsilon^{N-1} u^i u^j = -\sum_{i,j} \varepsilon^{N-1} v^i v^j = E_\varepsilon^-(v),$$

and the Γ-limit of the scaled energies

$$E_\varepsilon^{(1)}(v) = \sum_{i,j} \varepsilon^{N-1}(1 - v^i v^j) = \sum_{i,j} \varepsilon^{N-1}(1 + u^i u^j)$$

Γ-converges to $E^{(1)}(v) = 4\int_{S(v)} \|\nu_v\|_1 \, d\mathcal{H}^{N-1}$.

In terms of u this result can be read as follows: sequences of functions (u_ε) such that $E_\varepsilon^+(u_\varepsilon) = -|\Omega| + O(\varepsilon)$ will arrange in two regions where neighbouring values will alternate, but with a mismatch on the common boundary of these regions (anti-phase boundary). This mismatch may be forced by boundary conditions. The simplest case is in dimension 1 when we consider the minimum problem ($\varepsilon = 1/n$)

$$m_n = \min\Big\{\sum_{i=1}^n u\Big(\frac{i}{n}\Big) u\Big(\frac{i-1}{n}\Big) : |u| = 1, u(0) = 1, u(1) = -1\Big\}.$$

If n is even then the minimizers are given by

$$u\Big(\frac{i}{n}\Big) = \begin{cases} (-1)^i & \text{if } 0 \leq i < i_0 \\ (-1)^{i+1} & \text{if } i_0 \leq i \leq n, \end{cases}$$

where i_0 is any number in $\{1, \ldots, n\}$.

The anti phase boundary phenomenon is peculiar of a 'loose packed' lattice; *i.e.* a lattice that can be decomposed into two interpenetrating sublattices such that all the nearest neighbors of a spin on one sublattice belong to the other one. Thus an anti-ferromagnetic system can be decomposed into two ferromagnetic systems laying in two double interpenetrating lattices.

Remark 3. (Hexagonal lattices) We consider the two-dimensional case $N = 2$ and in place of $\mathbf{Z}^2$ we take the 'hexagonal' lattice $\mathcal{W}$, generated *e.g.* by the two vectors $(1, 0)$ and $(\frac{1}{2}, \frac{\sqrt{3}}{2})$. In this lattice each point possesses six nearest neighbours; *e.g.*, the nearest neighbours of 0 are $\pm(1, 0)$, $\pm(\frac{1}{2}, \frac{\sqrt{3}}{2})$, and $\pm(-\frac{1}{2}, \frac{\sqrt{3}}{2})$.

We then consider the energies

$$E_\varepsilon^{\pm}(u) = \pm \sum_{i,j} \varepsilon^2 u(\varepsilon i)u(\varepsilon j),$$

where now the sum runs on all pairs of nearest neighbours $i, j \in \mathcal{W}$ such that εi and εj belong to a fixed Ω.

We can extend each discrete function u to the piecewise-constant function that takes the same value on the rhombus with center εi and two sides parallel to the generators of the lattice and of length one. With this identification we can proceed in the computation of the Γ-limit.

It is not difficult to see that again the Γ-limit E^- of E_ε^- is finite only if $|u| \leq 1$ a.e. and on these functions its value is $-\frac{2}{\sqrt{3}}|\Omega|$ (the value $\frac{\sqrt{3}}{2}$ is simply the area of the unit rhombus, by which we have to divide). We may also proceed further to show the appearance of phase transitions: after normalizing and dividing by ε, we obtain another Γ-limit of the form $E^{(1)}$ as in Theorem (4) with a function φ with hexagonal symmetries in place of $\|\cdot\|_1$.

We focus on the limit of E_ε^+. It is convenient now to introduce a new variable: for each triplet $(i, j, k) \in \mathcal{W}^3$ identifying a minimal equilateral triangle; *i.e.*, such that each one of the three points is a nearest neighbour of the other two, we set

$$v(\varepsilon i, \varepsilon j, \varepsilon k) = \frac{1}{3}(u(\varepsilon i) + u(\varepsilon j) + u(\varepsilon k)).$$

Note that the functions v can be also regarded as defined in the 'dual lattice' consisting of all centers $\frac{\varepsilon}{2}(i + j + k)$ of all such triangles. We will not make this choice in order to not overburden the notation. Note moreover that with this normalization, if u_ε converges weakly to u then v_ε (extended with the constant value $v_\varepsilon(\varepsilon i, \varepsilon j, \varepsilon k)$ in the triangle with vertices $\varepsilon i, \varepsilon j, \varepsilon k$) still converges to u. We have the following correspondence:

$$\begin{aligned}
u(\varepsilon i) = u(\varepsilon j) = u(\varepsilon k) = \pm 1 \quad &\Longrightarrow \quad v(\varepsilon i, \varepsilon j, \varepsilon k) = \pm 1,\\
u(\varepsilon i) = u(\varepsilon j) = 1,\ u(\varepsilon k) = -1 \quad &\Longrightarrow \quad v(\varepsilon i, \varepsilon j, \varepsilon k) = \frac{1}{3},\\
u(\varepsilon i) = u(\varepsilon j) = -1,\ u(\varepsilon k) = 1 \quad &\Longrightarrow \quad v(\varepsilon i, \varepsilon j, \varepsilon k) = -\frac{1}{3}.
\end{aligned}$$

We then set

$$f(v) = \begin{cases} \frac{3}{2} & \text{if } v = \pm 1 \\ -\frac{1}{2} & \text{if } v = \pm\frac{1}{3}, \end{cases}$$

so that

$$f(v(\varepsilon i, \varepsilon j, \varepsilon k)) = \frac{1}{2}(u(\varepsilon i)u(\varepsilon j) + u(\varepsilon j)u(\varepsilon k) + u(\varepsilon k)u(\varepsilon i)).$$

The factor $\frac{1}{2}$ comes from the fact that each pair of such points belong to two different triangles. We can write

$$E_\varepsilon^+(u) = \sum_{(i,j,k)} \varepsilon^2 f(v(\varepsilon i, \varepsilon j, \varepsilon k)) + o(1),$$

where the sum runs over all triangles with vertices $\varepsilon i, \varepsilon j, \varepsilon k$ contained in Ω. Again, the term $o(1)$ is an error due to the fact that some triangles may intersect the boundary of Ω.

We may now repeat the argument in the computation of $E^{\pm}$ and show that the Γ-limit of E^{+}_{ε} is

$$E^{+}(u) = \frac{4}{\sqrt{3}} \int_{\Omega} \psi(u)\, dx,$$

where ψ is the convex envelope of f; i.e,

$$\psi(u) = \begin{cases} -\frac{1}{2} & \text{if } |u| \leq \frac{1}{3} \\ 3\Big(|u| - \frac{1}{2}\Big) & \text{if } \frac{1}{3} \leq |u| \leq 1. \end{cases}$$

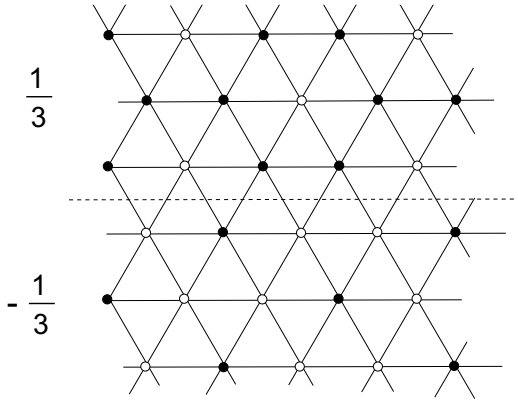

FIGURE 3. microscopical pattern for a transition with no interfacial energy

Now, even if we are considering the 'plus case', the limit energy density presents a flat part contrary to the square lattice case. It is interesting to note however that the hexagonal geometry now does not 'encourage' phase transitions. We may easily exhibit a configuration converging to $\frac{1}{3}$ in one region and to $-\frac{1}{3}$ in another region of the plane and such that no interfacial energy appears between the two regions. This is best illustrated by Figure 3 where a microscopical pattern is shown (black dots represent the value 1 and white dots the value -1) such that above the dotted line each triangle has two ones and one minus one in the vertices (corresponding to the value $1/3$ and the energy $-1/2$) and conversely below the dotted line each triangle has two minus ones and one one in the vertices (corresponding to the value $-1/3$ and always to the energy $-1/2$).

In this way each triangle has minimal energy, but, scaling this construction we will have a limit u on the continuum taking the value $1/3$ above the dotted line and $-1/3$ below. This construction can be repeated for all interfaces in the directions of the lattice, and then by approximation for all functions u with $|u| \leq 1/3$.

This lack of interfacial energy can be again described by studying the Γ-limit of the scaled energies

$$E_\varepsilon^{(1)}(v) = \sum_{(i,j,k)} \varepsilon\Big(f(v(\varepsilon i, \varepsilon j, \varepsilon k)) + \frac{1}{3}\Big).$$

In the case of Ω a cube and v satisfying periodic conditions the Γ-limit of $E_\varepsilon^{(1)}$ is 0 on all $|u| \le 1/3$ (by the construction above). If Ω is arbitrary then some contribution will appear from the lack of proper compatibility conditions between the geometry of the boundary and the construction made above.

5. **Next-to-nearest neighbour interactions.** We now study the more complex case when each point in a square lattice 'interacts' with its nearest and second-nearest neighbours. Again, the pattern that may appear to depend on the 'sign' of the interactions that may favour or disfavour oscillating configurations, but also on the balance between first and second-neighbour interactions. We treat the two-dimensional setting only, in the case that we consider the most interesting; *i.e.* when ground states possess less symmetries.

Our energy will be of the form

$$E_\varepsilon(u) = c_1 \sum_{n.n.} \varepsilon^2 u^i u^j + c_2 \sum_{n.n.n.} \varepsilon^2 u^i u^j, \quad u \in C_\varepsilon(\Omega)$$

where n.n. (nearest neighbours) entails that the sum is taken over all $i, j \in \mathbf{Z}^2$ such that $\varepsilon i, \varepsilon j \in \Omega$ and $|i - j| = 1$, while n.n.n. (next-to-nearest neighbours) are such that $|i - j| = \sqrt{2}$ (corresponding to the diagonals of the squares of the lattice). As usual we consider the extended energies $E_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ defined as

$$E_\varepsilon(u) = \begin{cases} c_1 \displaystyle\sum_{|i-j|=1} \varepsilon^2 u^i u^j + c_2 \sum_{|i-j|=\sqrt{2}} \varepsilon^2 u^i u^j & u \in C_\varepsilon(\Omega) \\ +\infty & \text{otherwise.} \end{cases} \tag{5.9}$$

It is convenient to rewrite the energy taking into account the local interactions in a fashion similar to that used for the hexagonal lattice. Indeed we may rewrite

$$E_\varepsilon(u) = \sum_{i,j,k,l} \varepsilon^2 \Big(\frac{1}{2} c_1 \big(u^i u^j + u^j u^k + u^k u^l + u^l u^i\big) + c_2 \big(u^i u^k + u^j u^l\big)\Big) + o(1)$$

where the sum is taken over all i, j, k, l vertices of a lattice square, ordered in such a way that $|i - j| = |j - k| = |k - l| = |l - i| = 1$ and $|i - k| = |j - l| = \sqrt{2}$. The factor $\frac{1}{2}$ comes from the fact that each pair of nearest neighbours belongs to two such lattice squares, and again the error $o(1)$ is due to the squares close to the boundary. Note that each cube is considered four times.

Note that indeed the sum above can be rewritten as parameterized on the centres of the cubes; *i.e.* on the points $m = \frac{1}{4}(i+j+k+l)$. As done in Section 3 we introduce equivalent energies of the simpler form

$$F_\varepsilon(v) = \sum_m \varepsilon^2 f(v^m),$$

where

$$v^m = \frac{1}{4}(u^i + u^j + u^k + u^l).$$

The possible values of v are

$$\begin{aligned} u^i = u^j = u^k = u^l = 1 &\implies v^m = 1 \\ u^i = u^j = u^k = u^l = -1 &\implies v^m = -1 \\ u^i = u^j = u^k = 1,\ = u^l = -1 &\implies v^m = \frac{1}{2} \\ u^i = u^j = u^k = -1,\ = u^l = 1 &\implies v^m = -\frac{1}{2} \\ u^i = u^j = -1\ u^k = u^l = 1 &\implies v^m = 0 \\ u^i = u^k = -1\ u^j = u^l = 1 &\implies v^m = 0. \end{aligned}$$

The list comprises all different cases (upon cyclical permutation of the indices).

In defining f there is no ambiguity for $v = \pm 1$ and $v = \pm\frac{1}{2}$. In these cases

$$f(v^m) = \frac{1}{2}c_1\big(u^iu^j + u^ju^k + u^ku^l + u^lu^i\big) + c_2\big(u^iu^k + u^ju^l\big)$$

so that

$$f(v) = \begin{cases} 2c_1 + 2c_2 & \text{if } |v| = 1 \\ 0 & \text{if } |v| = \frac{1}{2}. \end{cases} \tag{5.10}$$

For $v = 0$ the definition must take into account the two values $-2c_2$, corresponding to the case $u^i = u^j = -1$ $u^k = u^l = 1$, and $-2c_1 + 2c_2$, corresponding to the case $u^i = u^k = -1$ $u^j = u^l = 1$. As dealing with Γ-convergence we are interested in minimum energy configurations, the 'natural' definition for $f(0)$ is then

$$f(0) = \min\{-2c_2,\ -2c_1 + 2c_2\}. \tag{5.11}$$

Theorem 5. *Let $E_\varepsilon : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ be defined as in* (5.9)*; then E_ε Γ-converges with respect to the w^*-topology of $L^\infty(\Omega)$ to the functional $E : L^\infty(\Omega) \to \mathbf{R} \cup \{+\infty\}$ defined as*

$$E(u) = \begin{cases} \displaystyle\int_\Omega f^{**}(u)\,dx & \text{if } u \in L^\infty(\Omega),\ |u| \le 1 \\ +\infty & \text{otherwise.} \end{cases}$$

where f^{**} is the lower semicontinuous and convex envelope of $\tilde f : \mathbf{R} \to \mathbf{R}$ defined as

$$\tilde f(z) = \begin{cases} f(z) & \text{if } z \in \{\pm 1, \pm\frac{1}{2}, 0\} \\ +\infty & \text{otherwise} \end{cases}$$

and f is given by (5.10) *and* (5.11)*.*

Proof. The proof is the same as in Theorem 3; the only care is in using the minimal configuration in the computation of $f(0)$. □

Note that two cases can occur, whether

$$-2c_2 \ge -2c_1 + 2c_2 \qquad (i.e.,\ 2c_2 \le c_1)$$

or not. In the first case, when $f(0) = -2c_1 + 2c_2$, the minimum configuration is the same alternating state as that we encountered in the 'plus case' for nearest neighbours.

The case $f(0) = -2c_2$ is more interesting since the minimizers have less symmetries. We will focus on this case.

The limit absolutely minimal state is now 0, as in the 'plus case' for nearest neighbours, where anti-phase boundaries appeared in the description of the second

Γ-limit. In that computation, a simple change of sign in the variables allowed us to use the computation for the 'minus case'. Here, this is not possible since the minimal configurations have symmetries.

We study the Γ-limit of the scaled functional

$$E_\varepsilon^{(1)}(u) = c_1 \sum_{n.n.} \varepsilon u^i u^j + c_2 \sum_{n.n.n.} \varepsilon(u^i u^j + 1). \tag{5.12}$$

Since we are not interested in boundary layer effects (see for example [8]) we assume that Ω is a torus that we may identify with the semi-open cube $Q := [0,1)^2$, $\varepsilon = \frac{1}{2n}$ and u is Q-periodic. We find it useful to describe our energies in terms of a four-dimensional parameter: for each $u : \mathbf{Z}^2 \to \{-1,1\}$ we define $w : \mathbf{Z}^2 \to \{-1,1\}^4$ as follows:

$$\begin{aligned} w(i_1,i_2) &= T(u)(i_1,i_2) \\ &= (u(p(i_1),p(i_2)), u(d(i_1),p(i_2)), u(d(i_1),d(i_2)), u(p(i_1),d(i_2))) \end{aligned}$$

where $p : \mathbf{N} \to \mathbf{N}$ and $d : \mathbf{N} \to \mathbf{N}$ are

$$p(i) = \begin{cases} i & i \text{ is even} \\ i+1 & i \text{ is odd,} \end{cases} \quad d(i) = \begin{cases} i+1 & i \text{ is even} \\ i & i \text{ is odd.} \end{cases}$$

Next we label all the possible configurations. After defining

$$\begin{aligned} e_1 &= (-1,1,1,-1) & e_2 &= (-1,-1,1,1) \\ e_3 &= (1,-1,1,-1) & e_4 &= (-1,1,-1,-1) \\ e_5 &= (-1,-1,1,-1) & e_6 &= (-1,-1,-1,1) \\ e_7 &= (1,-1,-1,-1) & e_8 &= (1,1,1,1), \end{aligned}$$

they are given by the set $\{\pm e_i,\ i = 1,2,\dots,8\}$. Note that the change of variables we performed is justified by the fact that minimal configuration is identified with those w which are constant and take values in $\{\pm e_1, \pm e_2\}$. From now on we use the notation $E_n^{(1)}$ in place of $E_{\frac{1}{2n}}^{(1)}$, $\mathbf{Z}_n(Q)$ in place of $\mathbf{Z}_{\frac{1}{2n}}(Q)$ and we set

$$C_n^\#(Q) = \{u \in C_{\frac{1}{2n}}(Q),\ u\ Q\text{-periodic}\}.$$

It is possible to rewrite the scaled energies as:

$$E_n^{(1)}(u) = F_n(w) = \sum_{i \in \mathbf{Z}_n(Q)} \frac{1}{2n} f(w^i), \quad u \in C_n^\#(Q)$$

where $w = T(u)$ and $f : \{-1,1\}^4 \to \mathbf{R}$ is defined as

$$f(w) = \begin{cases} 0 & w \in \{\pm e_1, \pm e_2\} \\ 4c_2 - 2c_1 & w = \pm e_3 \\ 2c_2 & w \in \{\pm e_4, \pm e_5, \pm e_6, \pm e_7\} \\ 2c_1 + 4c_2 & w = \pm e_8. \end{cases}$$

Set

$$D_n^\#(Q) = \left\{ w : \frac{1}{2n}\mathbf{Z}^2 \to \{-1,1\}^4 \text{ such that } \exists\ u \in C_n^\#(Q) : w = T(u) \right\}.$$

By identifying w with its piecewise-constant interpolation on the lattice cells, we may regard $D_n^\#(Q)$ as a subset of $L^\infty(Q)$ and reduce our analysis to the study of

the Γ-limit of the family of functionals $F_n : L^\infty(Q) \to \mathbf{R} \cup \{+\infty\}$ defined as

$$F_n(u) = \begin{cases} \displaystyle\sum_{i \in \mathbf{Z}_n(Q)} \frac{1}{2n} f(w^i) & w \in D_n^\#(Q) \\ +\infty & \text{otherwise.} \end{cases}$$

Theorem 6. *The functionals $F_n : L^\infty(Q) \to \mathbf{R} \cup \{+\infty\}$ Γ-converge with respect to the L^1-topology to the functional $F : L^1(Q) \to \mathbf{R} \cup \{+\infty\}$ defined as*

$$F(w) = \begin{cases} \displaystyle\int_{S(w)} \varphi(w^+, w^-, \nu_w) d\mathcal{H}^1 & w \in BV_\#(Q; \{\pm e_1, \pm e_2\}) \\ +\infty & \textit{otherwise,} \end{cases}$$

where $\varphi : \{\pm e_1, \pm e_2\} \times S^1 \to \mathbf{R}^+$ is defined as follows:

$$\begin{aligned} &\varphi(\pm e_1, \pm e_2, \nu) = 2c_2(|\nu_1| \vee |\nu_2|) \\ &\varphi(\pm e_1, \mp e_1, \nu) = 4c_2|\nu_1| + (4c_2 - 2c_1)(|\nu_2| - |\nu_1|)^+ \\ &\varphi(\pm e_2, \mp e_2, \nu) = 4c_2|\nu_2| + (4c_2 - 2c_1)(|\nu_1| - |\nu_2|)^+. \end{aligned}$$

Proposition 1. *We have*

$$\Gamma\text{-}\liminf_n F_n(w) \geq F(w).$$

Proof. It suffices to consider $w_n \to w$ such that $\liminf_n F(w_n) < +\infty$. Up to subsequences we may suppose that $\liminf_n F(w_n) = \lim_n F(w_n)$. Since w_n is Q-periodic then w is Q-periodic. Since

$$\sup_n \frac{1}{2n} \#\{i \in \mathbf{Z}_n(Q) : \ w_n \neq \pm e_1, \pm e_2\} < +\infty,$$

we deduce that $|\{w_n \neq \pm e_1, \pm e_2\}| \to 0$ and so $w(x) \in \{\pm e_1, \pm e_2\}$ for a.e. $x \in Q$. Moreover note that $S(w_n)$ is contained in the boundary of the cells of the lattice where $w_n \neq \pm e_1, \pm e_2$ and thus

$$\frac{1}{4}((4c_2 - 2c_1) \wedge 2c_2)\mathcal{H}^1(S(w_n)) \leq \frac{1}{2n} \#\{i \in \mathbf{Z}_n(Q) : \ w_n \neq \pm e_1, \pm e_2\} < C.$$

In particular, by Theorem 2, we deduce that $w \in BV_\#(Q; \{\pm e_1, \pm e_2\})$.

Consider now the family of measures

$$\mu_n = \sum_{i \in \mathbf{Z}_n(Q)} \frac{1}{2n} f(w_n^i) \delta_i.$$

Note that $\sup_n \mu_n(Q) = \sup_n F_n(w_n) < +\infty$ and then, up to passing to a subsequence, we may suppose that there exists a positive finite measure μ such that $\mu_n \rightharpoonup \mu$. Now we use a blow-up argument. By the Radon-Nikodym Theorem, we may decompose μ into two mutually singular nonnegative measures:

$$\mu = \xi \mathcal{H}^1 \lfloor_{S(w)} + \mu_s.$$

Hence we complete the proof if we show that

$$\xi(x_0) \geq \varphi(w^+(x_0), w^-(x_0), \nu_w(x_0)) \quad \text{for } \mathcal{H}^1 \lfloor_{S(w)} \text{ a.e. } x_0 \in S(w).$$

By the properties of BV functions (see [3]) we know that for $\mathcal{H}^1 \lfloor_{S(w)}$ a.e. $x_0 \in S(w)$ it holds:

(i) $$\lim_{\rho \to 0^+} \frac{1}{\rho^2} \int_{x_0 + \rho Q^\pm_{\nu_w(x_0)}} |w(x) - w^\pm(x_0)| \, dx = 0,$$

(ii) $\lim_{\rho\to 0^+} \frac{1}{\rho}\mathcal{H}^1(S(w)\cap\{x_0+\rho Q_{\nu_w(x_0)}\}) = 1,$

(iii) $\xi(x_0) = \lim_{\rho\to 0^+} \frac{\mu(\{x_0+\rho Q_{\nu_w(x_0)}\})}{\mathcal{H}^1(S(w)\cap\{x_0+\rho Q_{\nu_w(x_0)}\})},$

where for any $\nu\in S^1$ we set

$$Q_\nu = \left(-\frac{|\nu_2|\vee|\nu_1|}{2}, \frac{|\nu_2|\vee|\nu_1|}{2}\right)^2.$$

Fix such a $x_0\in S(w)$ and let (ρ_m) be a sequence of positive numbers converging to zero such that $\mu(\partial\{x_0+\rho_m Q_{\nu_w(x_0)}\}) = 0$. By (ii) and (iii) we get

$$\begin{aligned}\xi(x_0) &= \lim_m \frac{\mu(\{x_0+\rho_m Q_{\nu_w(x_0)}\})}{\rho_m}\\ &= \lim_m \frac{1}{\rho_m}\lim_n \sum_{\substack{i\in\frac{1}{2n}\mathbf{Z}^2\\ i\in\{x_0+\rho_m Q_{\nu_w(x_0)}\}}} \frac{1}{2n} f(w_n^i) =: I\end{aligned}$$

Observe that, for any m and n we can find $\rho_{m,n}$ with $\lim_n \rho_{m,n} = \rho_m$ and $x_0^n\in\frac{1}{2n}\mathbf{Z}^2$ with $x_0^n\to x_0$, such that

$$\frac{1}{2n}\mathbf{Z}^2\cap(x_0^n+\rho_{m,n}Q_{\nu_w(x_0)}) = \frac{1}{2n}\mathbf{Z}^2\cap(x_0+\rho_m Q_{\nu_w(x_0)}).$$

Then

$$\begin{aligned} I &= \lim_m\lim_n \sum_{\substack{i\in\frac{1}{2n}\mathbf{Z}^2\\ i\in\{x_0^n+\rho_{m,n}Q_{\nu_w(x_0)}\}}} \frac{1}{2n\rho_{m,n}} f(w_n^i)\\ &= \lim_m\lim_n \sum_{\substack{j\in\frac{1}{2n\rho_{m,n}}\mathbf{Z}^2\\ j\in Q_{\nu_w(x_0)}}} \frac{1}{2n\rho_{m,n}} f(w_n(x_0^n+\rho_{m,n}j))\end{aligned}$$

For any $\varepsilon>0$ and $\nu\in S^1$ define

$$D_\varepsilon(Q_\nu) = \left\{w:\frac{1}{2n}\mathbf{Z}^2\to\{-1,1\}^4 \text{ such that } \exists\, u\in C_\varepsilon(Q_\nu): w = T(u)\right\}, \quad (5.13)$$

where $C_\varepsilon(Q_\nu)$ is defined as in (2.4) with Q_ν in place of Ω.

Then, the function $\tilde w_{m,n}$, defined as

$$\tilde w_{m,n}(j) = w_n(x_0^n+\rho_{m,n}j)\quad j\in\frac{1}{2n\rho_{m,n}}\mathbf{Z}^2\cap Q_{\nu_w(x_0)},$$

belongs to $D_{\frac{1}{2n\rho_{m,n}}}(Q_{\nu_w(x_0)})$. Set

$$w_0(x) = \begin{cases} w^+(x_0) & \text{if } \langle x,\nu_w(x_0)\rangle > 0\\ w^-(x_0) & \text{if } \langle x,\nu_w(x_0)\rangle \le 0.\end{cases}$$

Since $w_n\to w$ in $L^1(Q)$, by (i) we get

$$\lim_m\lim_n \int_{Q_{\nu_w(x_0)}} |\tilde w_{m,n}(x) - w_0(x)|\,dx = 0.$$

Hence, by using a standard diagonalization procedure we can find a sequence of positive numbers $\lambda_k \to 0$ and a sequence $w_k \in D_{\lambda_k}(Q_{\nu_w(x_0)})$ such that $w_k \to u_0$ in $L^1(Q_{\nu_w(x_0)})$ and

$$\xi(x_0) \geq \lim_k \sum_{j \in \lambda_k \mathbf{Z}^2 \cap Q_{\nu_w(x_0)}} \lambda_k f(w_k^j).$$

The conclusion follows by the next lemma. □

Given λ_k a sequence of positive numbers converging to 0, $\nu \in S^1$, set

$$F_k(w) = \sum_{j \in \lambda_k \mathbf{Z}^2 \cap Q_\nu} \lambda_k f(w^j), \quad w \in D_{\lambda_k}(Q_\nu),$$

where $D_{\lambda_k}(Q_\nu)$ has been defined in (5.13).

Given $a, b \in \{\pm e_1, \pm e_2\}$, set

$$w_{a,b,\nu}(x) = \begin{cases} a & \text{if } \langle x, \nu \rangle > 0 \\ b & \text{if } \langle x, \nu \rangle \leq 0. \end{cases} \tag{5.14}$$

Lemma 1. *Let $a, b \in \{\pm e_1, \pm e_2\}$, $\nu \in S^1$ and let $w_k \in D_{\lambda_k}(Q_\nu)$ be such that $w_k \to w_{a,b,\nu}$ in $L^1(Q_\nu)$. Then*

$$\liminf_k F_k(w_k) \geq \varphi(a, b, \nu).$$

Proof. Without loss of generality we may suppose that ν_1 and ν_2 are nonnegative. Set

$$I_k = \left\{ i_1 \in \left(-\frac{\nu_2}{2\lambda_k}, \frac{\nu_2}{2\lambda_k} \right) : \exists i_2^a, i_2^b \in \left(-\frac{\nu_1}{2\lambda_k}, \frac{\nu_1}{2\lambda_k} \right) : w_k(i_1, i_2^a) = a,\ w_k(i_1, i_2^b) = b \right\}$$

and

$$I_k^c = \left\{ -\left[\frac{\nu_2}{2\lambda_k} \right], \left[\frac{\nu_2}{2\lambda_k} \right] + 1, \ldots, \left[\frac{\nu_2}{2\lambda_k} \right] \right\} \setminus I_k.$$

We have that $\#(I_k)\lambda_k \to \nu_2$. In fact, since

$$\int_{Q_\nu} |w_n - w| = \sum_{i_2 > \frac{\nu_1}{\nu_2} i_1} {\lambda_k}^2 |w_n^i - a| + \sum_{i_2 < \frac{\nu_1}{\nu_2} i_1} {\lambda_k}^2 |w_n^i - b| + o(1) \geq c \#(I_k^c)\lambda_k + o(1),$$

we deduce that $\#(I_k^c)\lambda_k \to 0$. Set

$$J_k = \left\{ j_2 \in \left(-\frac{\nu_1}{2\lambda_k}, \frac{\nu_1}{2\lambda_k} \right) : \exists j_1^a, j_1^b \in \left(-\frac{\nu_2}{2\lambda_k}, \frac{\nu_2}{2\lambda_k} \right) : w_k(j_1^a, j_2) = a,\ w_k(j_1^b, j_2) = b \right\}$$

$$J_k^c = \left\{ -\left[\frac{\nu_1}{2\lambda_k} \right], \left[\frac{\nu_1}{2\lambda_k} \right] + 1, \ldots, \left[\frac{\nu_1}{2\lambda_k} \right] \right\} \setminus I_k,$$

as before one can see that $\#(J_k)\lambda_k \to \nu_1$.

It suffices to prove the lemma in the following two cases:

1. $a = e_1,\ b = e_2$
2. $a = e_1,\ b = -e_1$.

Case 1. In this case $\varphi(a, b, \nu) = 2c_2(\nu_1 \vee \nu_2)$. If $i_1 \in I_k$ there must be $i_2' \in \{i_2^b, i_2^b + 1, \ldots, i_2^a\}$ such that $w_k(\lambda_k(i_1, i_2')) \in \{\pm e_4, \pm e_5, \pm e_6, \pm e_7\}$ and then the minimal energy for the transition from e_1 to e_2 in the i_1-th column is $2c_2\lambda_k$. Analogously

one can see that the minimal energy for the transition from e_1 to e_2 in the i_2-th row is $2c_2\lambda_k$ for any $i_2 \in J_k$. Then we get

$$\lim_k F_k(w_k) \geq 2c_2 \lim_k \lambda_k(\#(I_k) \vee \#(J_k)) = 2c_2(\nu_1 \vee \nu_2).$$

Case 2. In this case $\varphi(a,b,\nu) = 4c_2\nu_1 + (4c_2 - 2c_1)(\nu_2 - \nu_1)^+$.
If $i_1 \in I_k$ there must be either i_2', $\tilde{i}_2' \in \{i_2^b, i_2^b + 1, \dots, i_2^a\}$ such that $w_k(\lambda_k(i_1, i_2'))$, $w_k(\lambda_k(i_1, \tilde{i}_2')) \in \{\pm e_4, \pm e_5, \pm e_6, \pm e_7\}$ or $\hat{i}_2' \in \{i_2^b, i_2^b + 1, \dots, i_2^a\}$ such that $w_k(\lambda_k(i_1, \hat{i}_2')) \in \{\pm e_3\}$. Then the minimal energy for the transition from e_1 to $-e_1$ in the i_1-th column is $\lambda_k(4c_2 - 2c_1) = \lambda_k f(\pm e_3)$.

If $i_2 \in J_k$ there must be either i_1', $\tilde{i}_1' \in \{i_1^a, i_1^a + 1, \dots, i_1^b\}$ such that $w_k(\lambda_k(i_1', i_2))$, $w_k(\lambda_k(\tilde{i}_1', i_2)) \in \{\pm e_4, \pm e_5, \pm e_6, \pm e_7\}$ or $\hat{i}_1' \in \{i_1^a, i_1^a + 1, \dots, i_1^b\}$ such that $w_k(\lambda_k(\hat{i}_1', i_2)) \in \{\pm e_8\}$. Then the minimal energy for the transition from e_1 to e_2 in the i_2-th row is $4c_2\lambda_k$ obtained when $\tilde{i}_1' = i_1' + 1$ and $w_k(i_1, i_2) = e_1$ if $i_1 < i_1'$, $w_k(i_1, i_2) = -e_1$ if $i_1 > i_1' + 1$.

In particular we get that

$$\lim_k F_k(w_k) \geq \lim_k \lambda_k(\#(J_k)) = 4c_2\nu_1.$$

If $\nu_1 \geq \nu_2$ then $\varphi(e_1, -e_1, \nu) = 4c_2\nu_1$ and we are done. If $\nu_1 \leq \nu_2$ we need a finer estimate. Set

$$m_k = \#\{i_1 \in I_k : \ \exists i_2' : w(i_1, i_2') \in \{\pm e_3\}\}.$$

Then we have that on $\#I_k - m_k$ columns the minimal transition energy is $4c_2\lambda_k$. On the other hand, by the reasoning above the same minimal transition energy is paid on $\#J_k$ columns. Then we get

$$F_k(w_k) \geq \lambda_k(4c_2((\#I_k - m_k) \vee \#J_k) + (4c_2 - 2c_1)m_k).$$

If $m_k \leq \#I_k - \#J_k$ then

$$\begin{aligned} F_k(w_k) &\geq \lambda_k(4c_2((\#I_k - m_k)) + (4c_2 - 2c_1)m_k) \\ &= \lambda_k(4c_2\#I_k - 2c_1 m_k) \geq \lambda_k(4c_2\#I_k - 2c_1(\#I_k - \#J_k)) \\ &= \lambda_k(4c_2 - 2c_1)\#I_k + 2c_1\#J_k) \\ &= \lambda_k(4c_2\#J_k + (4c_2 - 2c_1)(\#I_k - \#J_k)). \end{aligned}$$

If $m_k \geq \#I_k - \#J_k$ then

$$F_k(w_k) \geq \lambda_k(4c_2\#J_k + (4c_2 - 2c_1)(\#I_k - \#J_k)).$$

Note that in both cases we obtain the same estimate and we conclude letting k go to $+\infty$. □

Proposition 2. *We have*

$$\Gamma\text{-}\limsup_n F_n(w) \leq F(w). \tag{5.15}$$

Proof. By a density argument it suffices to show (5.15) for $w \in BV_\#(Q; \{\pm e_1, \pm e_2\})$ of the form

$$w = \sum_{l=1}^N a_l \chi_{E_l}$$

where $a_l \in \{\pm e_1, \pm e_2\}$ and (E_l) is a family of closed polyhedra whose interiors are pairwise disjoint. In particular, set $S_{l,m} := \partial E_l \cap \partial E_m$, we may write

$$S_{l,m} = \bigcup_{j=1}^{s(l,m)} S_{l,m}^j,$$

where $\{S^j_{l,m}\}$ is a family of segments.

For each $l, m \in \{1, 2, \dots, N\}$ and $j \in \{1, \dots, s(l,m)\}$ we construct a sequence $(u_n)^j_{l,m} \in C_n(Q)$ as follows. Up to a translation, we may suppose that $S^j_{l,m} \subset \Gamma^j_{l,m} := \{x \in \mathbf{R}^2 : \langle x, \nu^j_{l,m}\rangle = 0\}$ for some $\nu^j_{l,m} \in S^1$. By the continuity and the symmetry of $\varphi(a,b,\cdot)$ we may further suppose that $\nu^j_{l,m} = (\nu_1, \nu_2)$ is such that ν_1, ν_2 are nonnegative and $\frac{\nu_1}{\nu_2} \in \mathbf{Q}$. Thus there exist $h, k \in 2\mathbf{N}$ such that $\frac{\nu_1}{\nu_2} = \frac{k}{h}$.

Then $(u_n)^j_{l,m}$ is such that $(u_n)^j_{l,m}(i_1, i_2) = (u_n)^j_{l,m}(i_1 - jh, i_2 - jk)$, if $(i_1, i_2) \in \{0, 1, \dots, h\} \times \mathbf{Z} + j(h,k)$, $j \in \mathbf{Z}$, and on the set $\{0, \dots, h\} \times \mathbf{Z}$ is differently defined according to the following three different cases.

Case 1: $a_l = e_1$, $a_m = e_2$ and $\nu_1 \geq \nu_2$ (the construction being analogous in the opposite case).

$$(u_n)^j_{l,m}\Big(\frac{(i_1,i_2)}{2n}\Big) = \begin{cases} (-1)^{i_2+1} & i_1 \geq i_2 \quad i_1 \in \{0, 1 \dots, h\} \\ (-1)^{i_1+1} & i_1 < i_2 \quad i_1 \in \{0, 1 \dots, h\}. \end{cases}$$

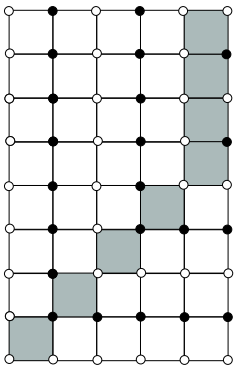

FIGURE 4: optimizing sequence in case 1

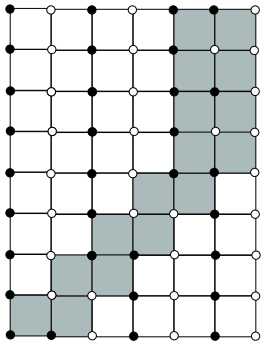

FIGURE 5: optimizing sequence in case 2

Case 2: $a_l = e_1$, $a_m = -e_1$, $\nu_1 \geq \nu_2$. Let

$$(u_n)^j_{l,m}\Big(\frac{(i_1,i_2)}{2n}\Big) = \begin{cases} (-1)^{i_1} & i_1 \geq i_2 \quad i_1 \in \{0, 1 \dots, h\} \\ (-1)^{i_1+1} & i_1 < i_2 \quad i_1 \in \{0, 1 \dots, h-1\} \\ (-1)^{i_2} & i_1 < i_2 \quad i_1 = h. \end{cases}$$

Case 3: $a_l = e_1$, $a_m = -e_1$, $\nu_1 < \nu_2$.

$$(u_n)^j_{l,m}\Big(\frac{(i_1,i_2)}{2n}\Big) = \begin{cases} (-1)^{i_1+1} & i_2 \geq 1, \quad i_1 \in \{0, 1 \dots, h-k\} \\ & i_2 > i_1 - h + k, \quad i_1 \in \{h-k+1, \dots, h\} \\ (-1)^{i_1} & i_2 \leq 0 \quad i_1 \in \{0, 1 \dots, h-k\} \\ & i_2 \leq i_1 - h + k, i_1 \in \{h-k+1, \dots, h\}. \end{cases}$$

Define, then, $(w_n)^j_{l,m}$ as

$$(w_n)^j_{l,m} = T((u_n)^j_{l,m}).$$

Note that $(w_n)^j_{l,m} = w_{a_l,a_m,\nu^j_{lm}}$, with $w_{a_l,a_m,\nu^j_{lm}}$ defined as in (5.14), except on an $\frac{1}{n}$-neighbourhood of $\Gamma^j_{l,m}$ of the type

$$(\Gamma^j_{l,m})_n := \{x \in \mathbf{R} : \ \mathrm{dist}(x, \Gamma^j_{l,m}) < C^j_{l,m}\frac{1}{n}\},$$

where the constant $C^j_{l,m}$ depend on $h \vee k$.

One can easily verify that $(w_n)^j_{l,m} \to w_{a_l,a_m,\nu^j_{lm}}$ and that the amount of the energy $F_n((w_n)^j_{l,m})$ due to the interactions in a $\frac{1}{n}$- neighbourhood of $S^j_{l,m}$ converges to $\varphi(a_l, a_m, \nu^j_{l,m})\mathcal{H}^1(S^j_{l,m})$.

Then, we may construct a recovery sequence w_n for w as follows. Set

$$S^n_w := \{x \in Q : \ \mathrm{dist}(x, S_w) \le \frac{C}{n}\},$$

with $C = \max C^j_{l,m}$. Then

$$\begin{aligned} w_n &= w && \text{on } Q \setminus S^n_w, \\ w_n &= (w_n)^j_{l,m} && \text{on } (S^j_{l,m})^n, \end{aligned}$$

where, being $a^j_{l,m}$, $b^j_{l,m}$ the endpoints of $S^j_{l,m}$, we set

$$(S^j_{l,m})^n := \{x \in Q : \ \mathrm{dist}(x, S^j_{l,m}) \le \frac{C}{n}\} \setminus B(a^j_{l,m}, \frac{C}{n}) \cup B(b^j_{l,m}, \frac{C}{n}).$$

In the set $S^n_w \setminus \bigcup (S^j_{l,m})^n$, taking care w_n to belong to $D^{\#}_n(Q)$, one can arbitrarily define w_n. Indeed, since $\#\{i \in \mathbf{Z}^2 : \frac{1}{2n} i \in S^n_w \setminus \bigcup (S^j_{l,m})^n\}$ is equibounded, the amount of the energy $F_n(w_n)$ due to the interactions in $S^n_w \setminus \bigcup (S^j_{l,m})^n$ is negligible as $n \to +\infty$.

Hence the conclusion follows by verifying that $w_n \to w$ and that

$$\lim_n F_n(w_n) = F(w).$$

□

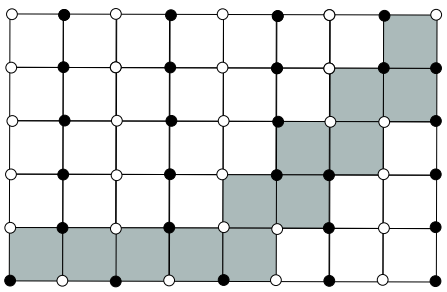

FIGURE 6: optimizing sequence in case 3

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