Discrete-to-Continuum Variational Methods for Lattice Systems

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Abstract. I review some recent results regarding the description of the behaviour of energy-driven discrete systems, and more precisely lattice systems, through the construction of approximate continuous problems. On one hand methods of weak convergence, homogenization, integral representation and gradient flow dynamics already used for continuum problems have been adapted to the discrete setting, on the other hand the new discrete dimension has brought new phenomena, novel problems and interesting results. I will limit my description to systems with interfacial energies, but focus on methods that can be adapted to a multi-scale analysis.

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1. Introduction

The presence of discrete systems is ubiquitous in the applications of Mathematics to Science and Technology, ranging from problems parameterized by the pixels of a screen in Computer Vision, to nodes on a network for Flow Dynamics, to the location of atoms in simulations of Continuum Mechanics problems, to that of larger ensembles in coarse-grained theories in Statistical Physics, etc. In many cases, the variables are directly parameterized on a *lattice*, or a portion of it (as in Image Processing or in the design of conducting networks), while in other cases this may be a simplifying assumption on the geometry or on the admissible states of the system. A paradigmatic example of the latter situation is the analysis of Lennard-Jones systems close to a ground state, for which a *crystallization* result holds; i.e., that minimal states can be parameterized on a regular lattice. Even this expected property of ground states is a very subtle issue and has been proved only in dimension two and for a class of interatomic potentials (see [61]).

We will consider only *variational* lattice systems; i.e., we will assume that their behaviour is governed by an energy functional depending on the values of a

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parameter u defined on the elements (nodes) of the lattice. We will mainly focus on a particular type of interactions, when the parameter u can take *only two values*, which we take being ± 1 (*spin variable*), the energy can be written as the sum of the interactions between pair of values of the parameter (*pair interactions*), and we will be interested in problems where the limit behaviour can be approximated by a continuous *surface energy*.

It must be noted that the methods we will use are to some extent independent of the simplification that we are making. In many problems, surface energies appear only at some energy scale, or in competition with bulk terms (*free-discontinuity problems*). This is the case for example of models in Computer Vision (e.g., Blake and Zisserman's [15], whose continuous counterpart is the Mumford and Shah variational model [56]) or Lennard-Jones systems from which one can deduce continuous variational models in Fracture Mechanics [35]. Nevertheless, blow-up and localization techniques often allow to decouple surface and bulk contribution, and assume that the parameters are locally constant on both sides of interfaces, so that the results we are going to illustrate can be thought as describing a part of a technically more complex energy depending on a continuous parameter.

The main points of the presentation will be the following:

• a variety of techniques constructed for continuum energies such as *homogenization*, Γ-*convergence*, *multi-scale analysis*, *variational motions*, *Geometric Measure Theory*, are naturally suited for this discrete setting, and provide a natural environment to define a continuum approximation;

• conversely, the discrete dimension provides a much more natural environment where to state and solve some problems which in the continuum case can be stated only with complex topological and geometrical constructions;

• in some cases the choice of the parameters for the continuum description are the main difficulty. This choice gives different effects and provides new problems with respect to the continuum setting.

2. A variational setting for spin systems

We will fix a periodic lattice $\mathcal{L}$ in $\mathbb{R}^d$. For reasons of simplicity we will mainly think of $\mathbb{Z}^d$ or of the triangular lattice $\mathcal{T}$ in $\mathbb{R}^2$, but we may consider as well non-Bravais lattices such as the hexagonal lattice in $\mathbb{R}^2$, fcc or hcp lattices in $\mathbb{R}^3$, etc.

The energy setting. We will consider functions $u : \mathcal{L} \to \{1, -1\}$, whose value at $i \in \mathcal{L}$ is denoted by u_i, and pair-interaction energies defined on such functions. It will be sometimes convenient to write the energies in such a way that they are zero on the two constant states ± 1. Upon additive and multiplicative constants the general form of these functionals is

$$E(u) = \frac{1}{8} \sum_{ij} c_{ij}(u_i - u_j)^2. \tag{1}$$

The normalization constant $1/8$ is due to the fact that the pair (i, j) is accounted for twice and that $u_i - u_j \in \{-2, 0, 2\}$. It is more customary, especially in Statistical

Physics, to write such energies as

$$E(u) = -\sum_{ij} c_{ij} u_i u_j, \tag{2}$$

which is an equivalent form if only a finite number of indices are taken into account (finite domain). If $c_{ij} \geq 0$ (*ferromagnetic interactions*) form (1) allows to directly consider an infinite domain and avoids $+\infty - \infty$ indeterminations. If interactions are not positive, it will be otherwise necessary to rewrite the energy in a different fashion with a suitable renormalization.

Convergence of discrete functions. We may use several notions of convergence of discrete functions. In most cases, given a family (u^ε) with $u^\varepsilon : \mathcal{L} \to \{\pm 1\}$ we consider functions $\widetilde{u}^\varepsilon$ which are piecewise-constant interpolations of the function with value u_i^ε on the node $\varepsilon i \in \varepsilon\mathcal{L}$. This correspond to scaling the lattice of a factor ε. The resulting functions belong to $L^1_{\mathrm{loc}}(\mathbb{R}^d)$. We can therefore consider the convergence $\widetilde{u}^\varepsilon \to u$ in this topology. In this way we have defined a *convergence $u^\varepsilon \to u$ of discrete functions to a continuum limit*. Other notions of convergence of $\widetilde{u}^\varepsilon$ to u will be used, and the corresponding convergences of u^ε to u.

Surface scaling and compactness. We will consider families of energies

$$E_\varepsilon(u) = \frac{1}{8} \sum_{ij} \varepsilon^{d-1} c_{ij}^\varepsilon (u_i - u_j)^2, \tag{3}$$

where in principle the sum runs over all pairs in $\mathbb{Z}^d \times \mathbb{Z}^d$ (with $i \neq j$). The scaling ε^{d-1} corresponds to considering $E_\varepsilon(u^\varepsilon)$ as surface energies if interpreted in the scaled parameter $\widetilde{u}^\varepsilon$. Indeed, in the simplest situation of *nearest-neighbour interactions* in the cubic lattice $\mathcal{L} = \mathbb{Z}^d$, with $c_{ij}^\varepsilon = 1$ if $|i - j| = 1$ and $c_{ij}^\varepsilon = 0$ otherwise, we have

$$E_\varepsilon(u^\varepsilon) = \mathcal{H}^{d-1}(\partial\{\widetilde{u}^\varepsilon = 1\}); \tag{4}$$

i.e., the energy coincides with the $d-1$-dimensional Hausdorff measure of the interface $\partial\{\widetilde{u}^\varepsilon = 1\}$, or, equivalently the perimeter of the set $\{\widetilde{u}^\varepsilon = 1\}$. From the theory of sets of finite perimeter, we deduce then that families with equibounded $E_\varepsilon(u^\varepsilon)$ are precompact with respect to the convergence $u^\varepsilon \to u$ (see e.g. [19]).

Static picture: Γ-limit. Functionals E_ε can be set in the framework of surface energies on sets of finite perimeter [11], and their behaviour is described by Γ-limits of the form

$$F(u) = \int_{\partial\{u=1\}} \varphi(x, \nu)\, d\mathcal{H}^{d-1}, \tag{5}$$

where ∂A denotes the *reduced boundary* of the set A, and ν its *measure-theoretical normal*.

In the homogeneous case $\varphi(x, \nu) = \varphi(\nu)$ this Γ-convergence will guarantee in particular the convergence (up to translations) of minimizers $\overline{u}^\varepsilon$ with the (limit) volume constraint $\#(\{\overline{u}^\varepsilon = 1\}) = M_\varepsilon$ and $M_\varepsilon\, \varepsilon^d \to 1$ to the function $\overline{u} = 2\chi_{\overline{A}} - 1$, where $\overline{A}$ is the *Wulff shape* of φ; i.e., $\overline{A}$ minimizes

$$A \mapsto \int_{\partial A} \varphi(\nu)\, d\mathcal{H}^{d-1}$$

among the sets of finite perimeter with unit volume, $|A| = 1$. Indeed the knowledge of the Wulff shape itself is sufficient to describe φ and hence the Γ-limit. In the simplest case (4) we have

$$\varphi(\nu) = \|\nu\|_1 := |\nu_1| + \cdots |\nu_d| \tag{6}$$

and $\overline{A}$ is a unit coordinate cube.

Dynamic picture: minimizing movement along a sequence of functionals. The knowledge of the Γ-limit does not give information sufficient to describe gradient-flow type dynamics, which may depend on the interaction between the *space scale* ε and the relevant *time scale* τ, and is defined by an implicit-time discretization scheme along E_ε (see [23] and Section 5 below).

Note that for sufficiently slow time scales the behaviour of the systems is approximated by the gradient-flow dynamics related to the Γ-limit, which can therefore be used as a comparison motion. In case (6) and $d = 2$ the related dynamics is the *crystalline motion* of the sets $A_t := \{x : u(t, x) = 1\}$. In the case of an initial datum a square, the sets are all squares, with side length L satisfying the ODE

$$L' = -\frac{2}{L} \tag{7}$$

until extinction time [9].

3. Positive interactions

As remarked above, the simplest case for energies (1) is when all interactions are non-negative; in which case the only ground states are the uniform states. In that framework it is not restrictive, for the sake of notational simplicity, to limit the analysis to the cubic lattice $\mathcal{L} = \mathbb{Z}^d$. In the case of nearest-neighbour interactions; i.e., if $c_{ij} = 0$ if $|i - j| \neq 1$ energies E_ε can be directly rewritten as surface integrals. The discrete setting allows also to consider *long-range interactions*; i.e., interactions between non-neighbouring points.

3.1. Integral-representation results. A general question is whether an approximation by a surface energy can be used. The answer is positive if the decay of the interaction is sufficiently fast, as in the following theorem (where the hypotheses are simplified for the sake of simplicity of presentation).

Theorem 3.1 (compactness). *Let c^ε_{ij} be non-negative numbers satisfying*
(i) (coerciveness) $c^\varepsilon_{ij} \geq c_1 > 0$ *if* $|i - j| = 1$*;*
(ii) (decay) $|c^\varepsilon_{ij}| \leq c_2|i - j|^{-r}$ *with* $r > d + 1$*,*
and let E_ε be defined by (3)*. Then, up to subsequences, E_ε Γ-converge to a surface energy of the form* (5) *for some Carathéodory integrand whose positively homogeneous extension of degree one in the second variable is convex. The domain of F is $BV_{\rm loc}(\mathbb{R}^d; \{\pm 1\})$.*

Remark 3.2. (a) Conditions (i) and (ii) are simplified for expository reasons and can be easily improved;

(b) **(non-local limits)** if (ii) is relaxed to a growth condition only guaranteeing that F be finite on $BV_{\rm loc}(\mathbb{R}^d;\{\pm 1\})$, we may lose *locality*; e.g., F may be of the form

$$F(u)=\int_{\partial\{u=1\}}\varphi(x,\nu)d\mathcal{H}^{d-1}+\int_{\mathbb{R}^d\times\mathbb{R}^d}k(x,y)(u(x)-u(y))^2\,dx\,dy; \qquad (8)$$

(c) **(boundary terms)** in a finite domain Ω we can consider energies obtained by restricting the interactions in the definition of E_ε to i,j belonging to $\frac{1}{\varepsilon}\Omega$. If Ω is a sufficiently smooth bounded set, then the corresponding limit takes the same form, but is restricted to functions in $BV(\Omega;\{\pm 1\})$ and takes into account only the part of $\partial\{u=1\}$ contained in Ω, up to a constant term concentrated on $\partial\Omega$. Note that this term may be relevant to problems where Ω is a *design parameter*.

Homogenization formulas. In the *periodic case*; i.e., if $c^\varepsilon_{ij}=C_{ij}$ and there exists $T\in\mathbb{N}$ such that $C_{ij}=C_{i+kT\ j+kT}$ for all $i,j,k\in\mathbb{Z}^d$ then $\varphi(x,\nu)=\varphi(\nu)$ and it is described by an asymptotic formula involving the computation of minimum problems with Dirichlet boundary conditions on a family of invading cubes [38]. The same result holds under *almost-periodicity assumptions*.

The use of homogenization formulas often allows to provide bounds on φ, and in some cases its actual computation. This is valid in particular when $T=1$, so that $C_{ij}=C'_{i-j}$. For example, in the two-dimensional case with $C'_k=1$ for $|k|\le\sqrt{2}$ and $C'_k=0$ otherwise (*next-to-nearest neighbour interactions*) φ is described by its Wulff shape, which is an octagon.

We now give some examples in which the analysis of the effect of the discrete dimension in the homogenization formulas allows to highlight differences and new applications with respect to the analogous continuum problems.

3.2. Optimal design of networks.

Lattice energies may be used to describe metric properties of networks. For the sake of simplicity we illustrate only a two-dimensional framework. In this case nearest-neighbour interaction energies on $\mathbb{Z}^2$ can be interpreted as a length functional on curves defined in the nodes of the translated lattice $(1/2,1/2)+\mathbb{Z}^2$, with piecewise-constant weights $a^\varepsilon_{(i+j)/2}=c^\varepsilon_{ij}$. The continuum counterpart of such energies are *Riemannian metrics* of the form

$$F_\varepsilon(\gamma)=\int_0^1 a^\varepsilon(\gamma(t))|\gamma'(t)|^2\,dt, \qquad (9)$$

whose limits are given by *Finsler metrics* with the integrands $\varphi=\varphi(x,\nu)$ computed at $x=\gamma$ and $\nu=\gamma'$ [29, 24]. *Optimal-design problems* for such energies amount to finding the general form of such φ when a^ε are subject to some *design constraint*. The simplest such constraint is requiring that $a^\varepsilon\in\{\alpha,\beta\}$ where α and β are two positive constants (*mixture of two conductors*). In the continuum case such a description for φ is an open problem, with only bounds available [46]. The discrete

case, where we require that $c^\varepsilon_{ij} \in \{\alpha, \beta\}$, allows a simple solution of this type of problems as follows.

A general observation (the "Dal Maso-Kohn localization principle" [22])) states that in order to describe general $\varphi(x, \cdot)$ it suffices to consider the case of periodic coefficients $C_{ij} \in \{\alpha, \beta\}$ with prescribed proportion of α and β connections (*microgeometries*). Often, the "extreme microgeometries" are then obtained by taking connections in parallel or in series. While this cannot be done in all directions at once in the continuum, such geometries are easily constructed in the discrete setting. As a result, reading the limit in terms of Finsler metrics, we obtain all functional of the form

$$F(\gamma) = \int_0^1 \varphi(\gamma(t), \gamma'(t))\, dt, \tag{10}$$

where $\varphi(x, \cdot)$ is any convex function satisfying

$$\alpha(|\nu_1| + |\nu_2|) \le \varphi(x, \nu) \le c_1|\nu_1| + c_2|\nu_2|,$$

where the coefficients c_1 and c_2 satisfy

$$c_1 \le \beta, \quad c_2 \le \beta, \qquad c_1 + c_2 = 2(\theta\beta + (1-\theta)\alpha)$$

and θ is the limit local proportion of β connections at x.

3.3. Discrete thin objects. Theories of thin objects starting from three-dimensional bodies through a dimension-reduction procedure have been a very successful way to obtain rigorous simplified theories for membranes, shells, rods, etc. [54, 31, 49]. For elastic membranes, the three-dimensional energies have the form

$$F_\varepsilon(u) = \frac{1}{\varepsilon} \int_{D\times(0,\varepsilon)} W(\nabla u)\; dx_1\, dx_2\, dx_3\,, \tag{11}$$

and the resulting energies as $\varepsilon \to 0$ can be written on two-dimensional functions as

$$F(u) = \int_D \overline{W}(\nabla_\alpha u)\; dx_1\, dx_2, \tag{12}$$

where $\overline{W}$ is defined through a minimization and quasiconvexification procedure, and ∇_α denotes the gradient in dimension two. An analog description can be given for interfacial problems [30].

Similar energies can be considered in a discrete setting, simply restricting the summation in the definition of energies E_ε in (3) to a stripe

$$S^T_n = \{x \in \mathbb{R}^{d+1} : |\langle x, n\rangle| \le T\}, \tag{13}$$

where $T > 0$ and $n \in S^d$. Note that the corresponding notion of convergence of function $u^\varepsilon \to u$ gives a limit function u defined on $\{x \in \mathbb{R}^{d+1} : |\langle x, n\rangle| = 0\}$, which we identify with $\mathbb{R}^d$. A compactness theorem, analogous to Theorem 3.1, guarantees, under the corresponding decay assumptions, that we have a limit functional of the form (5) defined in $\mathbb{R}^d$. Nevertheless, with respect to the continuum case, we have some notable differences.

1. Surface effects. Even in the simpler case of periodic C_{ij} and coordinate thin films; e.g., when $n = e_{d+1}$ is a coordinate vector, we have a non-trivial dependence of the resulting φ on T. This is due to the non-local character of discrete interactions, giving a boundary term which is predominant for small values of T.

2. Quasicrystals. When n is not rational (i.e., it is not a multiple of a vector in $\mathbb{Z}^{d+1}$) then the part of the lattice included in S_n^T cannot be considered as the superposition of copies of $\mathbb{Z}^d$. Nevertheless, almost-periodic techniques allow to cover also these cases, which are connected to the modeling of quasicrystals [28].

3. Aperiodic lattices. Penrose tilings. Some aperiodic lattices can be constructed through a "cut-and-project" procedure from a higher-dimensional lattice on a lower-dimensional subspace. This is the case of Penrose tilings on the plane, for example, which can be constructed as a projection of a subset of $\mathbb{Z}^5$ on a suitable "irrational" two-dimensional subspace. To such a construction the techniques used for "quasicrystals" can be adapted, obtaining an effective interfacial energy [41].

Question. *Is the Wulff shape of such an interfacial energy a pentagon? How do these pentagons differ (depending on the corresponding Penrose tiling)?*

4. Objective structures. Nanotubes. The definition of homogenized interfacial energies can be extended from periodicity assumptions to *objective structures* [52]. As a particular case we can treat models of "brittle nanotubes", for which the effective interfacial energy can depend on the *chirality* of the model. It is interesting to note that, even though described by the same general formulas, the value of the fracture toughness depends very much on the type of underlying lattice considered.

3.4. Random models. Percolation.

In a fashion connected to problems in Statistical Physics one can maintain a fixed lattice, and consider a random choice of coefficients. For simplicity we suppose that only nearest-neighbour interactions are taken into account and that $c_{ij}^{\varepsilon} \in \{\alpha, \beta\}$, in which case we can interpret this as a model of a uniform network with randomly placed defects or inclusions. In a two-dimensional framework (to which we limit our description), by the identification of boundaries with curves the limit can be interpreted as describing the overall metric properties of a random network. The precise statement requires the introduction of an i.i.d. random variable, which gives, for each of its realizations ω, a random choice of the coefficients $C_{ij}^{\omega} \in \{\alpha, \beta\}$ with

$$\begin{cases} C_{ij}^{\omega} = \beta & \text{with probability } p \\ C_{ij}^{\omega} = \alpha & \text{with probability } 1 - p, \end{cases}$$

and in (3) we simply consider $c_{ij}^{\varepsilon} = C_{ij}^{\omega}$. In this way we obtain a family of functionals E_{ε}^{ω} indexed by the realizations of our random variable. The analysis of the Γ-limit for each fixed ω corresponds to fixing a distribution of connections through the realization ω of the random medium, and computing its overall properties, which in general may depend on ω; the question is if *almost surely* they do not (*deterministic limit*) and how can the limit be described in terms of known probabilistic quantities. In the case of $0 < \alpha \leq \beta < +\infty$ for each fixed ω the functionals

are in the class taken into account by Theorem 3.1. Hence, a strictly positive and finite limit $\varphi = \varphi^\omega$ is always defined. Indeed, such a $\varphi^\omega = \varphi_p^{\alpha,\beta}$ is shown to almost surely depend only on the probability p and on the two values α and β, and can be described by the corresponding *first-passage percolation* formula [38, 18].

In the extreme cases, when $\alpha = 0$ or $\beta = +\infty$ (in this second case we use the convention that $+\infty \cdot 0 = 0$, so that $\beta(u_i - u_j)^2$ is finite, and equal to 0, if and only if $u_i = u_j$), the description of the limit is related to the properties of the *infinite clusters* of *bonds* (i.e., infinite connected components of elements of the dual lattice corresponding to pairs (i, j) with C_{ij}^ω taking the value α if $p < 1/2$, or, respectively, β if $p > 1/2$).

Theorem 3.3 (dilute-spin percolation theorem [37]). *Let $\alpha = 0$. Then we have*

(i) (trivial surface tension) *if $p \le 1/2$ then the corresponding Γ-limit is almost surely 0 for all u;*

(ii) (non-trivial deterministic surface tension) *if $p > 1/2$ then there exists a homogeneous strictly positive surface tension $\varphi = \varphi_p^{0,\beta}$ such that (5) holds.*

The function $\varphi_p^{0,\beta}$ is given by the dilute first-passage percolation *formula* [64, 44].

For $p < 1/2$ the existence of an infinite cluster yields that the limit of minimal-length problems in the homogenization formula are always trivial. In the case $p > 1/2$ the discrete environment can be interpreted as a randomly perforated medium, for which the main issue is the estimate of the effect of 'large' holes (whose probability is very small), which is negligible thanks to the i.i.d. hypothesis.

Theorem 3.4 (rigid-spin percolation theorem [59]). *Let $\beta = +\infty$. Then we have*

(i) (non-trivial deterministic surface tension) *if $p \le 1/2$ then there exists a homogeneous strictly positive surface tension $\varphi = \varphi_p^{\alpha,\infty}$ such that (5) holds;*

(ii) (degenerate surface tension) *if $p > 1/2$ then the corresponding Γ-limit is almost surely equal to the functional identically $+\infty$ for all u, except for the trivial cases $u = 1$ and $u = -1$.*

The function $\varphi_p^{\alpha,\infty}$ is given by the chemical distance *on the strong cluster* [51]. *Furthermore, we have the continuity result $\varphi_p^{\alpha,\beta} \to \varphi_p^{\alpha,\infty}$ as $\beta \to +\infty$.*

The key point in this result is a variational characterization of the chemical distance (the asymptotic distance in the infinite cluster). It is interesting to note that the continuity result is not trivial, and relies on a lemma provided by H. Kesten [36], which we may state informally as follows.

Lemma 3.5. *Fixed $L < 1$, let γ be a long path in the infinite cluster with length less than L times the corresponding chemical distance between its endpoints. Then it must contain a fixed proportion $P = P(L)$ of connections in the complement of the infinite cluster.*

It is interesting and promising to note the mutual exchange of results and problems between variational results and the corresponding percolation techniques.

3.5. Some interesting generalizations. The hypotheses of the compactness Theorem 3.1 can be extended in several interesting directions.

1. Random lattices. The compactness Theorem 3.1 can be extended to random perturbations of a given lattice. Other cases than can be covered using similar techniques are Poisson processes. It would be very interesting to prove percolation results in this context.

2. Double-porosity models. Such models in the continuum case are used in applications, e.g., to the study of the flow in a naturally fractured reservoir [13, 26]. In a discrete setting the complex topological assumptions necessary to their modeling are simplified, and reduce to a degenerate coerciveness condition, where (i) in Theorem 3.1 is weakened to $c_{ij}^{\varepsilon} \geq \varepsilon$ for a part of the interactions. If we suppose that the part in which (i) remains valid in the strong form determines a finite family of N infinite periodic connected sets, each of which can be treated as a separate perforated set, then the limit depends on a N-dimensional variable $u \in BV_{\rm loc}(\mathbb{R}^d; \{\pm 1\})^N$, and takes the form

$$F(u) = \sum_{j=1}^{N} \int_{\partial\{u_j=1\}} \varphi_j(\nu_j) d\mathcal{H}^{d-1} + \int_{\mathbb{R}^d} \psi(u_1, \dots, u_N)\, dx,$$

where ψ is an interaction term. Note that we may add lower-order terms, which influence the form of ψ in a non-trivial way.

3. Energies depending on a finite number of parameters. Surfactants. The compactness theorem can be extended to functions taking finitely many values. Even in the simplest case of $u \in \{-1, 0, 1\}$ and supposing that we still have the trivial ground states ± 1, the effect of the extra variable can be described in detail by a different type of energy. As an example, in the *Blume-Emery-Griffith* model the 0-phase, suitably scaled, converges to a positive measure μ, and the limit can be written as

$$F(u, \mu) = \int_{\partial\{u=1\}} \phi\Big(\frac{d\mu}{d\mathcal{H}^{d-1}}, \nu\Big) d\mathcal{H}^{d-1} + c\|\mu\|(\mathbb{R}^d \setminus \partial\{u = 1\})$$

(see [7]). This functional describes the energetic effect of the 0-phase, which is different when we have "deposition" on the interface between the 1-phase and the -1-phase, or "dilution" on the interior of the phases. If we do not have constraints on μ, we may define $\varphi(\nu) = \min_{z \geq 0} \phi(z, \nu)$ and integrate out the measure variable, reobtaining a representation as in Theorem 3.1. Note that this optimization may not be possible if for example the total mass of μ is prescribed.

4. Interactions with negative or changing sign

When in (1) or (2) the interactions c_{ij}^{ε} may take a negative sign then formally the functional is not bounded below and then, in the case of the infinite domain, it must be suitably scaled, taking care to avoid $+\infty - \infty$ indeterminations [1]. Even

after scaling in such a way that it becomes bounded from below, as in (3), the representation of the Γ-limit, and its computation, may be different than the one described in Theorem 3.1. As a simple example one can consider the triangular lattice and only the *anti-ferromagnetic* nearest-neighbour interactions; i.e., such that $c^\varepsilon_{ij} = -1$ when $|i-j| = 1$. In this geometry it is not possible that all pair interactions take the minimal value (*frustration*), so that minimal states are all those u not taking the same value at all vertices of each triangle. Note that in this case we may take the *magnetization* as the parameter for the Γ-limit, which is then trivially constant for all u with values in $[-1/3, 1/3]$ (the value $1/3$ corresponding to spins taking two values $+1$ and one -1 on each triangle, and analogously for $-1/3$), and no interfacial energy is present.

In the case of the cubic lattice $\mathbb{Z}^d$ the anti-ferromagnetic nearest-neighbour energies can be reduced, up to scaling, to ferromagnetic ones via a *change of parameter*, setting $v_i = (-1)^i u_i$ (where $(-1)^i = \Pi_k (-1)^{i_k}$). The phase boundaries for v are called *anti-phase boundaries* of u. Note that in this case the corresponding magnetization for u is always 0, both when $v = 1$ and $v = -1$. This shows that not always the magnetization is a good order parameter. The simple definition of v as above is not meaningful in general. For example, if we have nearest and next-to-nearest neighbour interactions in the square lattice with all antiferromagnetic interactions, such a change of variable gives an energy with still antiferromagnetic interactions, so that it cannot be rephrased as a ferromagnetic energy in terms of v. This shows that in general the determination of a limit order parameter is a non-trivial, and in general essential, part of the question.

4.1. Limits parameterized on ground states. The line followed in Theorem 3.1 can be repeated in this more general context if we can describe the *ground states* for the energy E. Actually, some care must be taken in the definition of ground states themselves. To that end, in the context of the cubic lattice, we assume to being able to rewrite our energies (upon additive constants) as

$$E_\varepsilon(u) = \sum_i \varepsilon^{d-1} \Psi(\{u_{i+j}\}_{j \in \mathbb{Z}^d}),$$

and denote the energy localized to a set I by $E(u, I) = \sum_{i \in I} \Psi(\{u_{i+j}\}_{j \in \mathbb{Z}^d})$. Then the analog of Theorem 3.1 reads as follows.

Theorem 4.1. *Suppose that we have*

(i) (existence of periodic ground states) *there exist* $N, K \in \mathbb{N}$ *and* $\{v^1, \dots, v^K\}$ *N-periodic functions such that, setting* $Q_N = \{1, \dots, N\}^d$ *we have* $E(v^j, Q_N) = 0$, *and* $E(u, Q_N) \geq C > 0$ *if* $u \neq v^j$ *in* Q_N *for all* j;

(ii) (incompatibility of ground states) *if* $u = \begin{cases} v^l & \text{in } Q_N \\ v^m & \text{in } k + Q_N \end{cases}$ *with* $k \in \mathbb{Z}^d$ *such that* $Q_N \cap (k + Q_N) \neq \emptyset$, *then* $E(u, Q_N \cup (k + Q_N)) > 0$;

(iii) (decay of the energy) *if* $u = u'$ *in* $R\,Q_N$ *then* $|E(u', Q_N) - E(u, Q_N)| \leq C_R$ *and* $\sum_R C_R R^{d-1} < \infty$.

Then we have

(a) (compactness) *If $E_\varepsilon(u_\varepsilon) \le C < +\infty$. Then there exist $A_{1,\varepsilon}, \dots, A_{K,\varepsilon} \subseteq \mathbb{Z}^N$ (identified with the union of the cubes centered on their points) such that $u_\varepsilon = v^j$ on $A_{j,\varepsilon}$, we have $\chi_{A_{j,\varepsilon}} \to \chi_{A_j}$ in the sense of convergence from discrete to continuum (Section 2), and $A_1, \dots, A_K$ is a partition of $\mathbb{R}^d$. We denote this convergence as*

$$u_\varepsilon \to u := \sum_{j=1}^{K} j\chi_{A_j};$$

(a) (Γ-convergence) *the Γ-limit can be written as*

$$F(u) = \int_{S(u)} \psi(u^+, u^-, \nu)\ d\mathcal{H}^{d-1}$$

where $S(u) := \bigcup_{i,j} \partial\{u = i\} \cap \partial\{u = j\}$ and $u^\pm$ denote the traces of u on both sides of $S(u)$, for a suitable BV-elliptic *function ψ.*

This result generalizes the previous compactness theorem provided that we enlarge our class of limit energies to *functionals defined on partitions of sets of finite perimeter* [11], and that we take the ground states themselves as *order parameters*. Conditions (ii) and (iii) have the same role as the hypotheses of Theorem 3.1.

In the case of nearest-neighbour antiferromagnetic energies on a cubic lattice, we have $K = N = 2$, with two 2-periodic ground states, corresponding to v^1 given by $v^1_i = (-1)^i$ and $v^2 = -v^1$.

4.2. Patterns. The parameterization of ground states can describe different *types of patterns* at the microscopic level. We list a few examples, where we do not explicit the translation that gives zero energy to ground states.

(1) for $d = 1$ and $E(u) = \sum_i (\alpha u_i u_{i-1} + u_{i-1}u_{i+1})$ with $|\alpha| < 2$ (strong anti-ferromagnetic next-to-nearest neighbour interactions in 1D) we have four 4-periodic ground states, differing by a translation, so that the order parameter can be interpreted as a *shift*;

(2) for $d = 2$ and $E(u) = c_1 \sum_{|i-j|=1} u_i u_j + c_2 \sum_{|k-l|=\sqrt{2}} u_k u_l$ in the square lattice, with $c_2 > 0$ and $2c_2 > c_1$ (strong anti-ferromagnetic next-to-nearest neighbour interactions in 2D) we have four 2-periodic ground states $v^1, \dots, v^4$ given by $v^1_i = (-1)^{i_1}$, $v^2_i = (-1)^{i_2}$, $v^3 = -v^1$, and $v^4 = -v^2$. In this case we have *striped* ground states. The two ground states v^1 and v^2 can be interpreted as the directions e_1 and e_2 while v^3 and v^4 as the opposite directions $-e_1$ and $-e_2$. The interface between v^1 and v^3, e.g., can be considered an *anti-phase boundary*. Note that the Wulff shape of $\psi(e_k, e_l, \cdot)$ can be either a square or an irregular hexagon [1];

(3) for $d = 2$ and $E(u) = c_1 \sum_{|i-j|=1} u_i u_j + c_2 \sum_{|k-l|=\sqrt{3}} u_k u_l$ in the triangular lattice, with $c_1 > 0$ and $c_2 < 0$ (anti-ferromagnetic nearest neighbour interactions and ferromagnetic next-to-nearest neighbour interactions) then we have six ground states, which are $\sqrt{3}$ periodic in the direction $(1/2, \sqrt{3}/2)$.

Remark 4.2 (boundary terms). Contrary to the ferromagnetic case, in general the additional boundary term appearing in problems on a bounded domain Ω is

not a constant, and depends on the trace of the ground state at the boundary; i.e., the Γ-limit takes the form

$$F(u) = \int_{S(u)\cap\Omega} \psi(u^+, u^-, \nu)\ d\mathcal{H}^{d-1} + \int_{\partial\Omega} \phi(u, n) d\mathcal{H}^{d-1},$$

where n is the normal to $\partial\Omega$. As a consequence, minimizers can depend on the interplay between the geometry of the domain and the microstructure of ground states.

Remark 4.3 (ferromagnetic parameters). In some cases it is possible to infer, as in the case of dilute spin systems, that the relevant parameters can still be interpreted as the two ferromagnetic phases. This is the case of periodic antiferromagnetic inclusions, provided that the distance between the inclusion is sufficiently large with respect to their size. In this case the parameter indexing the ground states represents the *majority phase* in the ferromagnetic matrix. It is interesting to note that even in the two-dimensional setting the minimum problems giving the interfacial energy cannot be directly interpreted as minimal-length problems, as their computation may involve the value on large antiferromagnetic inclusions.

Remark 4.4 (change in parameters - open problems). Simple examples show that we may have a change in the limit parameter in dependence of the volume fraction between ferromagnetic and antiferromagnetic interactions. Optimal-design and random problems are widely open. For example, it is not proved whether *there exists a small but positive probability p such that a random i.i.d. distribution of antiferromagnetic interactions in a matrix of ferromagnetic interactions is still described by only two (ferromagnetic) states.*

4.3. Change of patterns in thin films. As we have observed in the ferromagnetic case, a boundary contribution can influence the limit description of discrete thin films. In that case, the influence was described by a varying value of the interfacial energy. In the case of the presence of antiferromagnetic interactions, taking into account that boundary conditions and the geometry influence the form of the ground states, we may have a more striking influence in dependence of the thickness of the thin film.

Remark 4.5 (variation of the parameters by boundary effects). We can take the two-dimensional antiferromagnetic/ferromagnetic Example (3) in Section 4.2, on a thin film with normal perpendicular to a direction of the lattice vectors. If we have a "very thin film" of a single layer, then we simply have a one-dimensional antiferromagnetic lattice, with 2 parameters. As we increase the number of layers, the number of parameters varies depending on the ratio c_1/c_2 and for a sufficiently large film it reaches the number of the parameter of the bulk case (i.e., 6).

Remark 4.6 (coerciveness by boundary effects). As we have remarked above, the antiferromagnetic triangular lattice is degenerate, with zero surface tension in the limit. In the case of thin films this is not the case. Not only, as above we have the one-dimensional antiferromagnetic lattice, with 2 parameters when we

have a single layer, but we have a non degenerate interfacial energy for all number of layers, with the number of parameters that diverges as 2^N. Other interesting effects that can be highlighted on this simple example are the dependence on the thin film direction, and the asymmetry of the interfacial energy density.

5. Gradient-flow type dynamics

For energy-driven systems a notion of gradient-flow dynamics can be given through a time-discrete approximation scheme. For a sequence of parameterized energies F_ε defined on a Hilbert space X the *minimizing movement* $x(t)$ *along the sequence* F_ε with time scale $\tau = \tau(\varepsilon)$ from an initial datum x^0 (or from a family of initial data $x^0_\varepsilon \to x^0$) is defined as the limit of the (time-discrete) trajectories x^ε defined as follows: we set $x^\varepsilon_0 = x^0$ and define recursively x^ε_{k+1} as a solution of the minimum problem

$$\min\Big\{F_\varepsilon(x) + \frac{1}{2\tau}\|x - x^\varepsilon_k\|^2\Big\}, \tag{14}$$

and then $x^\varepsilon(t) = x^\varepsilon_{\lfloor x/\tau \rfloor}$ [12, 23]. This scheme can be adapted to discrete systems and energies of the type E_ε following a variant due to Almgren, Taylor and Wang [10] (which indeed precedes the formalization of minimizing movements). Note that the minimizing movement x depends on the time scale $\tau(\varepsilon)$. In particular we have the following extreme cases, under proper coerciveness assumptions, which are satisfied by our E_ε.

Theorem 5.1 (extreme minimizing movements). *Let F_ε be a sequence of functionals defined on discrete spaces. Let $x^0_\varepsilon \to x^0$ with $F_\varepsilon(x^0_\varepsilon) \le C < +\infty$ and let F_ε be equicoercive, non-negative and Γ-converge to F. Then*

(i) (pinning scale) *there exists a (sufficiently fast) scale τ_p such that if $\tau \le \tau_p$ then $x(t) = x^0$ for all t;*

(ii) (commutation scale) *there exists a (sufficiently slow) scale τ_c such that if $\tau \ge \tau_c$ then $x(t)$ coincides with the* minimizing movement *for F from x^0 (defined by taking $F_\varepsilon = F$).*

The existence of a pinning scale is a consequence of the discreteness of the space, and is independent of the Γ-convergence of F_ε. Loosely speaking, in the notation of (14) there exists a function f such that we have $\|x^0_\varepsilon - x\|^2 \ge f(\varepsilon)$ for all $x \ne x^0_\varepsilon$, so that the minimum in (14) is x^0_ε for all k if $\tau < f(\varepsilon)/2C =: \tau_p$.

The interesting regimes are those excluded by Theorem 5.1, which interpolate between the extreme scales. The relevant problems can be summarized as

(i) determine the *critical regime(s)* $\tau = \tau(\varepsilon)$ such that we neither have pinning nor commutation;

(ii) compute the corresponding continuum *effective minimizing movement*, and describe the additional features that make it differ from the "trivial" one of the commutative case.

These novel type of dynamic homogenization problems constitutes a very interesting and wide class of gradient-flow type dynamics. We only give a few examples in the case of discrete energies converging to a crystalline perimeter.

5.1. Homogenized dynamics for positive interactions. For many ferromagnetic (nearest-neighbour) interactions the Γ-limit F is given by the crystalline perimeter. In two dimensions, Almgren and Taylor have shown that the minimizing movement (*flat flow*) for this functional is given by motion by *crystalline curvature* [9]. This motion can be easily described for coordinate rectangles, in which case each side moves inwards with velocity given by its curvature κ, which in the crystalline case is defined by $\kappa = 2/L$, L being the length of the side. The same description holds for coordinate polyrectangles provided we define $\kappa = -2/L$ (i.e., the motion is outwards) if the set is concave at the side, and $\kappa = 0$ if the set is neither concave or convex at the side.

Remark 5.2 (partial pinning/quantization of the velocity [34]). If E_ε are ferromagnetic nearest-neighbour interactions with $c_{ij} = 1$ if $|i - j| = 1$, then we have

(i) the *critical regime* is $\varepsilon \sim \tau$;

(ii) if $\tau/\varepsilon \to \gamma$ then the *effective minimizing movement* is described by the law

$$v = \frac{1}{\gamma}\big\lfloor \gamma\kappa \big\rfloor,$$

with the convention on the crystalline curvature κ as above.

The integer part is explained by the fact that the "discrete sides" must move by a finite quantity (proportional) to ε. Note that, as a consequence, we have *partial pinning*; i.e., pinning of sides only when they are larger than 2γ, and that, contrary to the motion by crystalline curvature, we may have initial data which may be pinned after an initial motion.

Remark 5.3 (homogenization of the velocity [39]). As remarked in the case of the optimal design of ferromagnetic materials, we may have the same crystalline perimeter even when we have periodic inclusions with $c_{ij} = \beta > 1$ in a matrix of unit nearest-neighbour interactions. These inclusions do not influence the Γ-limit, but they do influence the resulting minimizing movement, the reason being that the "discrete sides" avoid the inclusions for energetic reasons. We still have an effective minimizing movement, with sides moving with a velocity

$$v = \frac{1}{\gamma} f_{\rm hom}\big(\gamma\kappa\big),$$

with γ as in the previous remark. The *homogenized velocity function* can be described through a homogenization formula, and takes into account the geometry and distribution of the strong inclusions.

Remark 5.4 (bulk effects). We can consider periodic inclusions as in the previous example but with $c^\varepsilon_{ij} = \varepsilon$ (*double-porosity scaling*). The effect of these inclusions is negligible in the Γ-limit, which can be treated as a perforated domain giving, upon properly scaling the energy, still the same crystalline perimeter F. Nevertheless, in this case the effective minimizing movement has an additional term taking into account that the weak inclusions may be regarded as a bulk effect. We may have in the limit a velocity of the form

$$v = \frac{1}{\gamma}\big\lfloor \gamma c\kappa + c(\gamma) \big\rfloor.$$

Note that in this case the limit for very slow time scales is not the motion of the crystalline perimeter. The failure of Theorem 5.1(ii) is due to the non equi-coerciveness of E_ε in the double-porosity case. A similar type of effect is encountered in the study of convection in mushy layers [63].

5.2. Homogenized dynamics for non-positive interactions. We only highlight some phenomena in the case of antiferromagnetic interactions

Remark 5.5 (mobility and motion by creation of defects). In the case of multiple ground states the limit behaviour is connected to the motion of networks rather than sets. Even in the simplifying case when only two phases are present in the continuum description we may have

(i) (*mobility*) the velocity law may depend on the orientation of the boundary normal and on the two phases;

(ii) (*motion by the creation of defects*) the interface may move by using an intermediate phase which is non optimal for static problems. This may also happen at corner points.

Remark 5.6 (motion by maximization). The discrete setting allows to define another kind of motion, e.g., by taking in the minimizing-movement scheme an antiferromagnetic interaction. In this way we formally define a motion following a *maximization criterion* of the ferromagnetic energy or a backward motion for the perimeter functional. In particular we may take as initial datum a single point (*nucleation*) from which we have an expanding family of sets at constant velocity, whose shape depends (on the energy and) on the distance [40].

6. Conclusion: surface scaling as part of a multi-scale analysis

For general discrete systems, the surface-energy description analyzed above must be placed in a proper multi-scale framework, together with effects related to other types of scaling. Note that, even when only energetic contributions are taken into account in a static picture described by a Γ-limit process, the same type of functionals can be considered with different scaling depending on the energy level. For the same quadratic energies we may have, e.g.,

(a) (*bulk scaling*) $\sum_{ij} \varepsilon^d c_{ij}|u_i - u_j|^2$ giving integral energies $\int f(x, u(x))\,dx$;

(b) (*surface scaling*) $\sum_{ij} \varepsilon^{d-1} c_{ij}|u_i - u_j|^2$ giving surface energies as described in this presentation above;

(c) (*vortex scaling*) $\sum_{ij} \varepsilon^{d-2}|\log\varepsilon|^{-1} c_{ij}|u_i - u_j|^2$ giving *vortex energies* defined on point singularities;

(d) (*gradient scaling*) $\sum_{ij} \varepsilon^{d-2} c_{ij}|u_i - u_j|^2$ giving integral energies depending on gradients $\int f(x, \nabla u(x))\,dx$, etc.

Such effects, and others, may be present at the same time. For some of them, methods corresponding to those described for surface energies have been developed and used. Some issues that have a direct link with the results described above are

• *vortex and dislocation models* from *vector spin systems* (the so-called XY *model*; i.e., with $u_i \in \mathbb{R}^2$ and $|u_i| = 1$) [4]. Even though the interactions are formally the same as the ferromagnetic one, here the relevant scaling gives a behaviour equivalent to *Ginzburg-Landau energies* both for the static and the dynamic case, and has applications in the theory of dislocations [6, 8];

• *liquid-crystal type models*. Here a very interesting issue is the choice of the parameter, which can be for example the *magnetization* or the *Q-tensor*, giving different limit theories even at the first bulk scaling [28];

• *microscopic order/disorder*. For computational and modelling reasons it is very important to know whether macroscopic energies correspond to a regular arrangements of discrete values (*Cauchy-Born rule*) or not, and how this 'regularity' properties depend on parameters (e.g. thickness of thin films) [50, 33, 47, 2, 58];

• *interaction between surface and bulk contribution for free-discontinuity problems*. Both in Computer Vision and Fracture Mechanics, among other applications, we encounter competing bulk and surface energies, which can be derived from atomistic Lennard-Jones interactions [35] or optimized among lattice energies (see e.g. [45]);

• *quasicontinuum methods*. Computational problems involving free-discontinuity problems for which details of interfacial interactions are important require a coupling between continuum discretization procedures and atomistic fine-mesh analysis (see e.g. [60, 16, 57]);

• *derivation of nonlinear and linear theories in Continuum Mechanics*. The interpretation of discrete energies as describing the deformation of a lattice ground state lead to the derivation of elastic energies. We may have nonlinear elastic energies even from very simple lattice interactions [3, 17], while linear elastic energies can be rigorously derived [42] using powerful rigidity estimates [48];

• *optimal-design problems*. As highlighted for surface energies, optimal design problems can be treated also for conducting or elastic networks [32] in the spirit of optimal design of composites [55]. Little has been done in this direction, which seems natural for applications;

• *surface relaxation and crystal shapes*. Surface energies may arise as a result of asymmetric interactions at internal or external boundaries as a higher-order effect [27, 62]. When other bulk interactions are close to a ground state an important effect of the surface energy is the determination of optimal shapes of crystals [14].

Among the general directions of research that have been taken, some that may be singled out are the elaboration of new notions in the direction to allow to bridge the scales (in the variational setting e.g. 'equivalence by Γ-convergence' [43]), the extension of variational techniques to non-zero temperature [53], and the removal of the assumption of an underlying lattice [14, 61]. Many more new questions have been raised, with a wide range of applications, but still, even in the simplest variational setting, many remain open.

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