Variational problems for antiferromagnetic systems

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Lattice Spin Systems

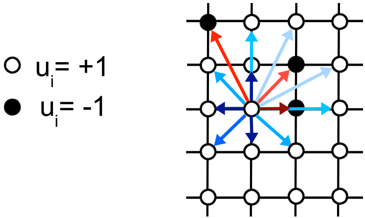
- **Underlying reference lattice** $\mathcal{L}$

In this talk $\mathcal{L} = \mathbb{Z}^2$ (*square lattice*) or $\mathcal{L} = \mathbb{T}$ (*triangular lattice*)

- (**Spin variable**) Parameter $u = \{u_i\}$ defined on the nodes i of the lattice $\mathcal{L}$ with $u_i \in \{+1, -1\}$
- **Energy**

$$E(u) = \sum_{i,j \in \mathcal{L}} \sigma_{ij}(u_i - u_j)^2$$

Pictorial representation:



We may have **two types of interactions**

ferromagnetic

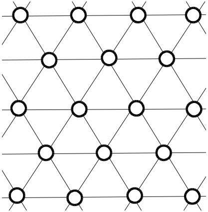
$\sigma_{ij} > 0$

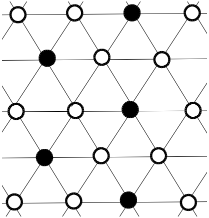
uniform ground states

antiferromagnetic

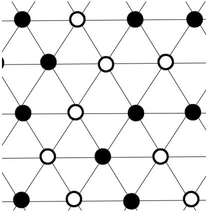
$\sigma_{ij} < 0$

microstructure





ordered



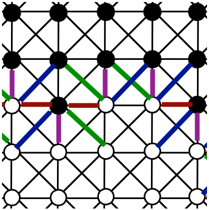
disordered

Ground states = minimizers w.r.t. local perturbations
(or, if possible, minimizing a “cell energy” for all cells)

We briefly examine **ferromagnetic interactions**

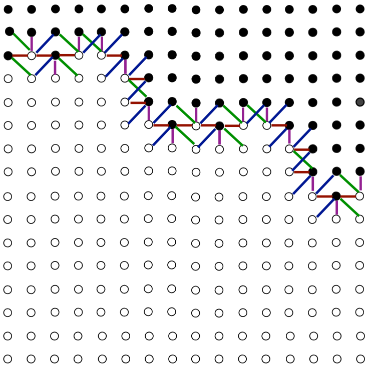
$$E(u) = \sum_{ij} \sigma_{ij}(u_i - u_j)^2$$

with $\sigma_{ij} \geq 0$



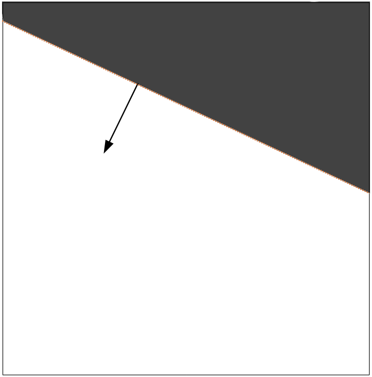
Here we depict a next-to-nearest neighbour system.
The coloured segments highlight the 'active' interactions $(u_i \neq u_j)$, the different colours possible anisotropy and the dependence of σ_{ij} on ij

Large-scale behaviour - heuristics



As we ‘zoom out’, the energy tends to concentrate on an interface.

Large-scale behaviour - heuristics



The 'discrete interface' can be approximately described as a continuous one, smooth enough as to have a normal ν well defined

We expect to have a *continuum surface tension* which *approximately describes the behaviour of E.*

Discrete-to-continuum analysis by scaling

Objective: description of the behaviour of **large systems** driven by E with a **continuum theory** characterized by some **continuum energy** $E_{\rm cont}$

- Introduction of a **scale parameter** $\varepsilon \to 0$
- Definition of a **scaled energy** $E_\varepsilon(u^\varepsilon) = \sum_{ij} \sigma^\varepsilon_{ij}(u^\varepsilon_i - u^\varepsilon_j)^2$ with u^ε identified with functions defined on $\varepsilon\mathcal{L}$
- Definition of a **continuous limit parameter** u (and of a discrete-to-continuum convergence $u^\varepsilon \to u$)
- Definition of an **effective continuous energy** $E_{\rm cont}$.

The requirement for such energy is that: "**solutions to problems related to E_ε are close to solutions related to $E_{\rm cont}$**"

In our case the **surface scaling** $\sigma^\varepsilon_{ij} = \sigma_{ij}\,\varepsilon^{n-1}$ is the relevant one and the **convergence** is L^1 convergence of the interpolates of u^ε_i on $\varepsilon\mathbb{Z}^n$

Static analysis: Γ-convergence

Basic question: *existence of a limit surface energy?*

Theorem (Compactness and continuum description)
(Caffarelli-de la Llave 2005, B-Piatnitsky 2013, Alicandro-Gelli 2014)

Suppose $E_\varepsilon(u) = \sum_{ij} \varepsilon^{n-1}\sigma^\varepsilon_{ij}(u_i - u_j)^2$ with $\sigma^\varepsilon_{ij} \geq 0$ satisfying:

(i) (decay) $|\sigma^\varepsilon_{ij}| \leq C|i-j|^{-r}$ with $r > n+1$;
(ii) (coerciveness of NN interactions) $\sigma^\varepsilon_{ij} \geq \sigma_0 > 0$ if $|i-j| = 1$
(iii) (negligible long-range tail) $\lim_{T\to+\infty} \sum_{|i-j|>T} \sigma^\varepsilon_{ij} = 0$

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Then (up to subsequences) there exists g with $g > 0$ on S^{n-1} and $g(x,\cdot)$ convex and positively 1-homogeneous such that $E_\varepsilon \to E_{\rm cont}$ where

$$E_{\rm cont}(u) = \int_{\partial\{u=1\}} g(x,\nu)\, d\mathcal{H}^{n-1}$$

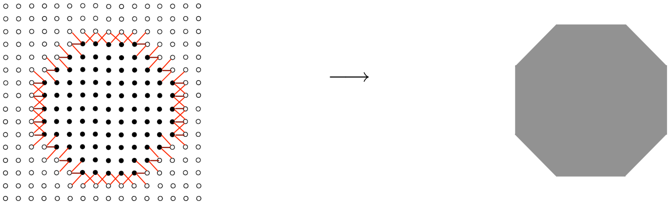
is defined on $BV_{\rm loc}(\mathbb{R}^n; \{\pm 1\})$ and ν is the normal to $\partial\{u=1\}$

The Wulff problem (a good way to picture convergence)

If $g = g(\nu)$ (homogeneous limit) then we deduce the convergence of *problems with* **volume constraint** ($C_\varepsilon \to C$)

$$\min\{E_\varepsilon(u) : \varepsilon^n \#\{i : u_i = 1\} = C_\varepsilon\}$$
$$\to \quad \min\Big\{\int_{\partial\{u=1\}} g(\nu) d\mathcal{H}^{n-1} : |\{u=1\}| = C\Big\} \quad \textbf{(Wulff problem)}$$

A minimizer of the latter (normalized e.g. to unit energy) is called a **Wulff shape**.



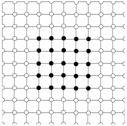
(for NNN interactions the Wulff shape is an octagon)

Conversely, the knowledge of the Wulff shape determines g and characterizes the Γ-convergence of E_ε.

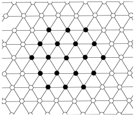
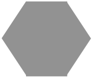
Some Wulff shapes

It is instructive then to look at the Wulff shape related to some easy discrete systems (and how it reflects the lattice structure)...

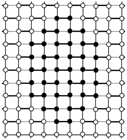
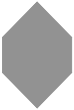
Square NN (**nearest-neighbour**) interactions $\longrightarrow$ square

 $\longrightarrow$ 

Triangular NN interactions $\longrightarrow$ hexagon

 $\longrightarrow$ 

Inhomogeneous square NN interactions $\longrightarrow$ (irregular) polygon

 $\longrightarrow$ 

For finite-range interactions we have crystalline surface tensions

An application: Discrete Optimal Design Problems

Optimal design problems = construction of structures with "**extreme properties**" subject to design constraints

Analytical tools = **homogenization** formulas (nonlinear, nonperiodic, non-convex) (cf. the books by Allaire and Milton)

Discrete structures $\Rightarrow$ **more flexible design constraints** with respect to the continuum case

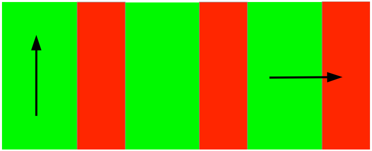
Example: composites of two ferromagnetic materials
This translates in the computation of all possible limits of

$$E_\varepsilon(u) = \sum_{ij} \varepsilon^{n-1} \sigma_{ij} (u_i - u_j)^2$$

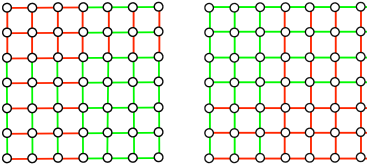
with periodic $\sigma_{ij} \in \{\alpha, \beta\}$ with given proportions.

Optimal discrete geometries

In the continuum often extremal properties are obtained by "laminates", which "extremize" different properties in different directions

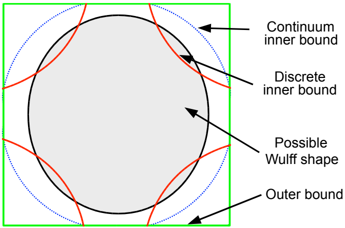


In a discrete setting we can extremize *the same* property in different directions by discrete lamination



Description of the “G-closure” in terms of Wulff shapes

We can describe all possible surface tensions φ in terms of the *proportion* θ of β-connections. E.g., for $\theta \leq 1/2$ these are all convex symmetric shapes internal to the cube of side-length $\frac{1}{4\alpha}$ and intersecting the curve $\frac{1}{|x_1|} + \frac{1}{|x_2|} = 16(\theta\beta + (1-\theta)\alpha)$



With respect to the analogous continuum case (homogenization of metrics)

- *exact* bounds
- *much larger* set of reachable φ

(in the continuum case Wulff shapes must intersect the blue lines in the discrete case Wulff shapes must intersect the red lines)

(B. arXiv 2014)

‘Evolutionary’ framework

Variational evolution: an *implicit Euler scheme* (Almgren-Taylor-Wang 1993, De Giorgi 1995, Ambrosio-Gigli-Savaré 2005) can be adapted to study evolution of discrete systems: fix initial data u_0, time-step τ and space scale ε, define the *space/time-discrete evolution* of E_ε *at time-scale* τ as

- $u_0^{\tau,\varepsilon} = u_0$
- $u_{i+1}^{\tau,\varepsilon}$ **a minimizer** of

$$E_\varepsilon(u) + \frac{1}{\tau} D(u, u_i^{\tau,\varepsilon})$$

(D = “dissipation” measuring the “L^2-distance of interfaces”)
Up to subsequences, we define a **space/time-continuum limit**

$$u(t) = \lim_{\varepsilon \to 0} u_{\lfloor t/\tau \rfloor}^{\tau,\varepsilon}$$

as $\tau, \varepsilon \to 0$ (**Minimizing movement** of E_ε at scale τ from u_0)

Connections with the static analysis

If E_ε Γ-converge to $E_{\rm cont}$ and D is a continuous perturbation then

$$E_\varepsilon(\cdot)+\frac{1}{\tau}D(\cdot,\overline{u}^\varepsilon)$$

Γ-converge to

$$E_{\rm cont}(\cdot)+\frac{1}{\tau}D(\cdot,\overline{u})$$

if $\overline{u}^\varepsilon\to\overline{u}$, from which we deduce that *if $\varepsilon\to 0$ fast enough with respect to τ* then $u(t)$ *is the minimizing movement of the Γ-limit* $E_{\rm cont}$ from u_0

Hence, the Γ-limit gives also a description of the evolution but only for "slow time". In general, the limit $u(t)$ *does depend on the mutual behaviour of ε and τ* (B Lecture Notes Math 2013)

An Example: Flat Flow

Example. If we take NN ferromagnetic interactions in $\mathbb{Z}^2$ then the Γ-limit is the crystalline perimeter with a square Wulff shape. Its evolution (flat flow) is **motion by crystalline curvature** (Almgren-Taylor 1995)

$$v = \kappa, \qquad \kappa = \text{ crystalline curvature}$$

where e.g. each side of a rectangle moves inwards with velocity

$$v = \frac{2}{L} \qquad \text{i.e., } \kappa = \frac{2}{L} \text{ (crystalline curvature of the side)}$$

($L =$ length of the side).

This evolution is also as the minimizing movement for E_ε at scale τ if $\varepsilon << \tau$.

Pinning and Evolutionary Homogenization of Flat Flow

The time/space-discrete (τ/ε) evolution generally gives

- completely pinned motion for *fast time*; i.e., $\tau \to 0$ fast enough
- convergence to the evolution of the static Γ-limit for *slow time*; i.e., $\varepsilon \to 0$ fast enough

Hence we have **existence of one or more *critical time scales* with non-trivial evolution**. In particular at such scales we obtain the evolution of a *"corrected"* Γ-limit (ε and τ-dependent)

Example (B-Gelli-Novaga 2010) For NN ferromagnetic interactions in $\mathbb{Z}^2$ the *critical scale* is $\varepsilon/\tau \to \gamma$ for which the motion is

$$v = \frac{1}{\gamma}\lfloor \gamma\kappa \rfloor \qquad (\lfloor t \rfloor \text{ is the integer part of } t)$$

- large sets (of size depending on γ) are **pinned**; in particular
  - as $\gamma \to 0$ all initial sets are pinned
  - as $\gamma \to +\infty$ we recover motion by crystalline curvature

Differently from the continuum case
• velocity is "quantized" (due to rows of microscopic energy barriers)
• (*partial pinning*) we may have non-trivial motions of compact sets existing for all time (and not always finite-time existence)

Example (B-Scilla 2013) The geometry of discrete interactions may give evolutionary effects that are **not detected by the Γ-limit**. For NN ferromagnetic interactions in $\mathbb{Z}^2$ with "defects" the limit motion may be of the form

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

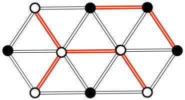
where $f_{\rm hom}$ is a *homogenized velocity* obtained implicitly by showing the existence of "asymptotically periodic" orbits of an auxiliary problem
Note. Even for simple distributions of defects the computation of $f_{\rm hom}$ raises non-trivial combinatorial issues

Lattice Microstructure

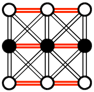
For (mixtures of ferromagnetic and) **antiferromagnetic interactions** ground states may be **frustrated**; i.e., not all interactions are minimized $\Longrightarrow$ **lattice microstructure**

Examples (all antiferromagnetic interactions)
We may have ground states with frustrated interactions (in red)

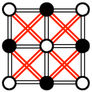
NN Triangular lattice
('disordered' ground states)



NNN square lattice
(periodic ground states)

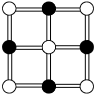


or



(depending on σ_{ij})

NN square lattice
(periodic ground states)

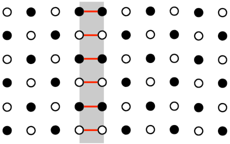


(not frustrated)

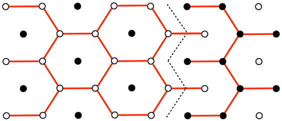
Limit analysis

Q.: can we still describe the Γ-limit? with resp. to what convergence?
Note: L^1 convergence $u^\varepsilon \to u$ in general is meaningless (e.g., for NN and NNN square lattice all ground states have 0 average)

Example (NN antif. square lattice $\Longrightarrow$ anti-phase boundaries)



(NN antif. triangular lattice $\Longrightarrow$ no interfacial energy - **"total frustration"**)



Limits parameterized on ground states

A positive convergence result

Theorem. Suppose σ_{ij} periodic, **no sign hypothesis**
Suppose that there exist $u_1, \ldots, u_N$ periodic discrete functions s.t.
(i) u_k are the "ground states" of E
(ii) "between different u_k we have an energy barrier"
(iii) "surface-type decay of the interactions" with the distance

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Then

(a) if $\sup_\varepsilon E_\varepsilon(u^\varepsilon) < +\infty$ then locally $u^\varepsilon = \sum_{k=1}^N \chi_{A_k^\varepsilon} u_k$, with (WLOG) $\varepsilon A_k^\varepsilon \to A_k$ and $\{A_k\}$ is a partition of sets of finite perimeter, and we may define the convergence $u^\varepsilon \to (A_1, \ldots, A_N)$
With an abuse of notation we may say that the limit value is u_k on A_k

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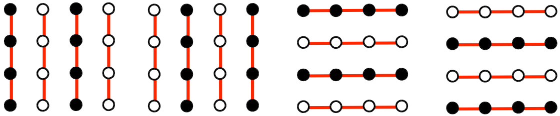
(b) E_ε Γ-converge to $E_{\rm cont}$ of the form

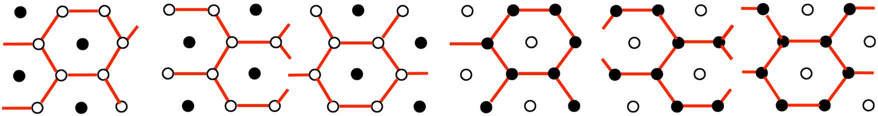
$$E_{\rm cont}(A_1, \dots, A_N) = \sum_{i \neq j} \int_{\partial A_i \cap \partial A_j} g_{ij}(\nu) d\mathcal{H}^{n-1}$$

Examples: (all σ_{ij} of period 1)

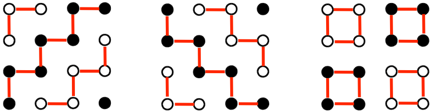
NNN antif. square lattice – 4 “striped” ground states



NN antif.+ NNN ferrom. triangular lattice – 6 “hexagonal” gr. states



NNNN squ. lattice - 16 gr. states “slanted stripes” and “checkerboard”



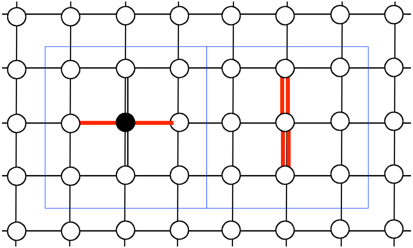
(and translations)

etc.

Classes of equivalences of ground states

Note: the theorem can be extended identifying two ground states if there is no energy barrier between them.

Example



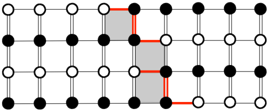
(in the picture: single line = ferrom., double line = antiferrom.)

Homogenization and G-closure Problems

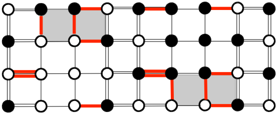
Q: compute the possible limits of mixtures of (periodic) ferromagnetic + antiferromagnetic interactions (with given proportions)

Partial answer With NN, $\sigma_{ij} = \pm 1$ and equal proportions we may obtain 2 param. and interfacial energies not greater than $|\nu_1| + |\nu_2|$

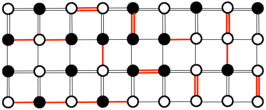
non-frustrated



frustrated/
degenerate surface energy



totally frustrated/
no surface energy



Note: question must be correctly put (equivalence by Γ-convergence B-Truskinovsky 2008).

Many (open) problems

E.g.,

Deterministic setting

Taking as the **relevant unknown** the **number of ground states**:

• if we only have NN can we have more than 2 (equivalence classes of) ground states?
• can we give a bound on the number of ground states from the periodicity and the range of interactions?
• can we estimate the "measure" of the microgeometries with N ground states (or with total frustration)?

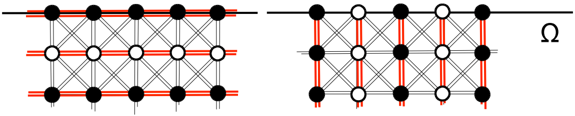
Probabilistic setting

• if we replace the percentage with the *probability* of having antiferromagnetic interactions; i.e.,
$\sigma_{ij} = \sigma^{\omega}_{ij} = -1$ (resp., 1) with probability p (resp., $1-p$)
can we keep the limit description away from $p = 0$ or 1?
• if so, how does the number of ground state changes with p?

Boundary effects for finite domains

For finite domains the energetic description is not complete.
We have a *non-trivial boundary effect*.

E.g.,



(the second configuration is energetically convenient)

$\Longrightarrow$ effective energy of the form

$$E_{\text{cont}}(A_1, \ldots, A_N) = \sum_{i \neq j} \int_{\partial A_i \cap \partial A_j \cap \Omega} g_{ij}(x, \nu) \, d\mathcal{H}^{n-1} + \sum_k \int_{\partial A_k \cap \partial \Omega} \widetilde{g}_k(x, \nu) \, d\mathcal{H}^{n-1}$$

("wetting" term)

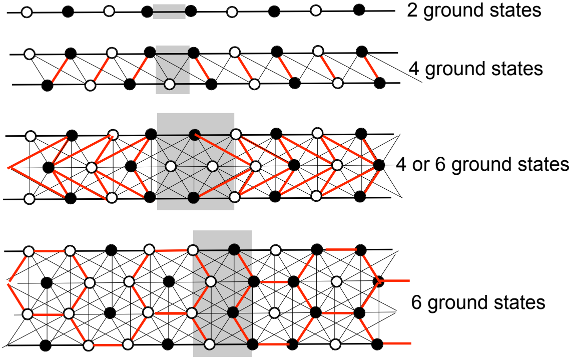
$\Longrightarrow$ Ω is an additional "design parameter"

Boundary effects for thin films - I

Boundary effects are particularly important for thin objects such as thin films.

Example (dependence of $\#$ of parameters on the thickness)
The number of parameters of N-layer thin films may depend on N and 'stabilize' to those of the 'bulk' limit

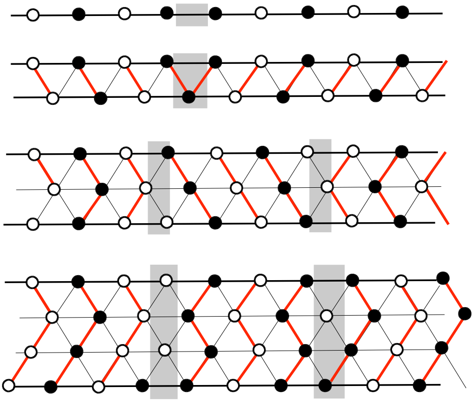
E.g., for triangular NN antiferrom. + NNN ferromagnetic,



Boundary effects for thin films - II

Example (rigidity by boundary effects)
"Total frustration" may only occur as the number of layers $N \to +\infty$

E.g., for triangular NN antiferromagnetic,



2 ground states

4 ground states

8 ground states

16 ground states

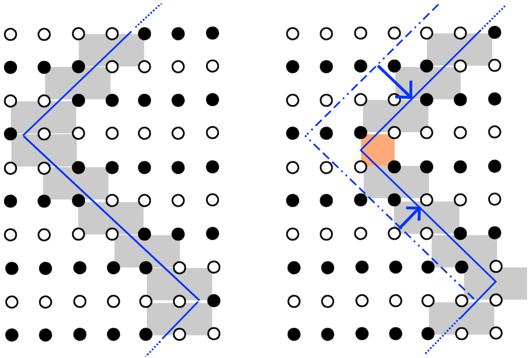
… N layers

2^N ground states

Motions by microstructures

New features in the motion of interfaces in addition to pinning and homogenization; e.g.,

(a) Motions by creation of defects (surface microstructures)



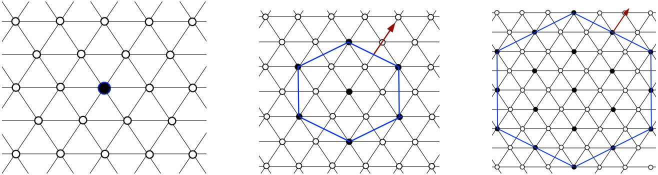
(of interfaces otherwise pinned for the Γ-limit)

(B-Cicalese-Yip, in progress)

(b) “Backwards evolution” by crystalline curvature

Approximation of crystalline perimeters by (anti-)ferromagnetic interactions may give a meaningful definition of backward motion (otherwise **ill-defined** in the continuum) by minimizing movements.

Example (nucleation in a triangular lattice driven by local maximization of the perimeter, with “hexagonal dissipation”)

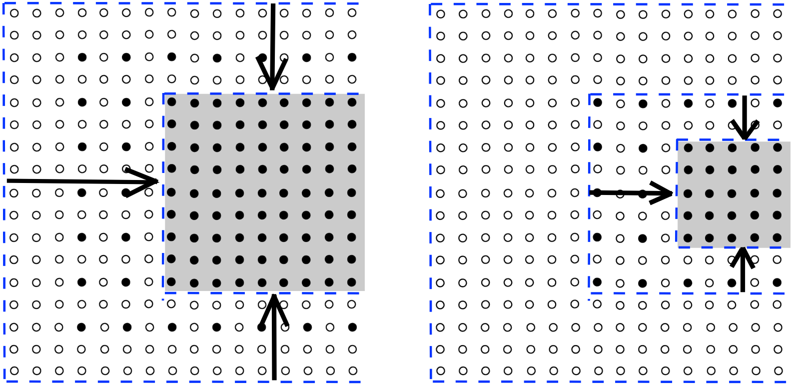


Continuum limit: hexagon expanding at constant velocity (after scaling time)

In general the motion depends on the “dissipation-distance”, and may give rise to complex patterns (linked to the problem of couting integer points inside a ball) and homogenization of the velocity (B-Scilla 2013)

(c) Motions by "mushy layers" (bulk microstructure)

(connection with Fluid Mechanics; (Grae Worster 1991))



$\Longrightarrow$ additional terms to motion by crystalline curvature

(B-Solci, in progress)

Conclusions

Microstructures and patterns are present in many continuum models, but their behaviour may be difficult to describe, such as the appearance of interfaces between patterns with an attached energy, or the relative flow.

Discrete models seem to offer the possibility of the description of the behaviour of energy-driven patterns, and anti-ferromagnetic energies seem to be a good testing ground to develop this analysis.

Thank you for your attention!