Homogenization of spin systems

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(Scalar) spin systems: a prototypical lattice energy

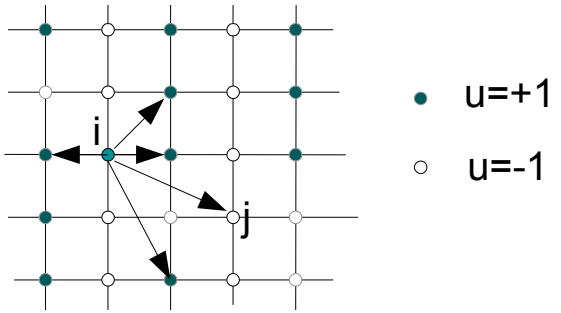
Geometrical setting: a lattice $\mathcal{L}$; e.g. $\mathbb{Z}^d$ ($d = 2$ in this talk) or a trianguar lattice in 2D, etc.

Parameter: $u : \Omega \cap \mathcal{L} \to \{-1, 1\}$ with the notation $u_i = u(i)$
Energy: (pair-interaction energy)

$$E(u) = -\sum_{i,j} c_{ij} u_i u_j \qquad \textbf{Ising model/Lattice gas}$$

or, up to additive/multiplicative constants

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



$c_{ij} > 0$ **"attractive" (ferromagnetic) interactions**
$c_{ij} < 0$ **"repulsive" (antiferromagnetic) interactions**

Discrete-to-continuous analysis–I

Given energies (in general with ε-depending coefficients)

$$F_\varepsilon(u) = \sum_{i,j} c_{ij}^\varepsilon (u_i - u_j)^2 \qquad u : \mathcal{L} \to \{\pm 1\}$$

with $\mathcal{L} \subset \mathbb{R}^d$, we proceed following a general procedure

Introduction of a small scale parameter $\varepsilon > 0$. The overall behaviour of the system for a large number of interacting particles will be rephrased as a **continuum limit** of the interactions on the lattice $\varepsilon\mathcal{L}$ as $\varepsilon \to 0$.

Scale variables: $u : \varepsilon\mathcal{L} \to \{\pm 1\}$

Scale energies:

$$E_\varepsilon(u) = \sum_{i,j} \varepsilon^{d-1} c^\varepsilon_{i/\varepsilon\, j/\varepsilon} (u_i - u_j)^2$$

(**surface scaling** – other scalings are possible $\Rightarrow$ multi-scale problem)

Discrete-to-continuous analysis–II

Choice of the macroscopic parameter: Identify $u : \varepsilon\mathcal{L} \to \{\pm 1\}$ with a continuum quantity; e.g. with its *piecewise-constant interpolation* (or to a sum of scaled Dirac deltas on the nodes of the lattice).
In this way all u are defined on the same space.

Use of weak convergence methods.
Define a discrete-to-continuum convergence

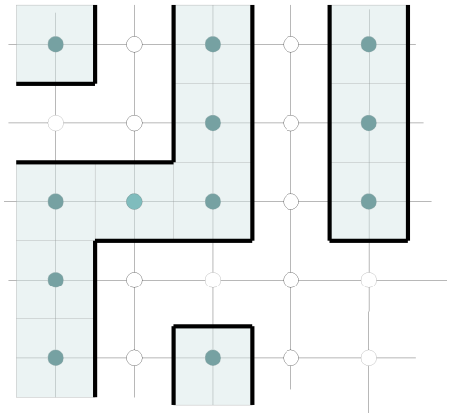
$$u^\varepsilon : \varepsilon\mathcal{L} \to \mathbb{R} \qquad \longrightarrow \qquad u : \mathbb{R}^d \to \mathbb{R} \text{ (in some cases } \mathbb{R}^m)$$

as the *convergence of the interpolations*. In general, may use weak L^1-convergence, weak* convergence of measures, etc., so that we have to be ready to find in the limit u to be also a Dirac delta, a surface distribution, etc.
We will see less immediate definitions of convergence.

Definition of a continuum energy F which describes the "behaviour" of the energies E_ε as $\varepsilon \to 0$.
Γ-convergence. In a variational setting, F is given by the **Γ-limit** of E_ε (with respect to the convergence $u_\varepsilon \to u$), which guarantees the "convergence of minimum problems".

Choice of the surface scaling/ferromagnetic interactions

For **ferromagnetic interactions** ($c_{ij} \geq 0$) E can be viewed as a **surface energy**. In the case of **nearest-neighbour (NN) interactions** ($c_{ij} = 0$ for $|i-j| > 1$; e.g., $c_{ij} = 1$ if $|i-j| = 1$) the picture is



Scaled energies ($\frac{1}{8}$ normalization constant)

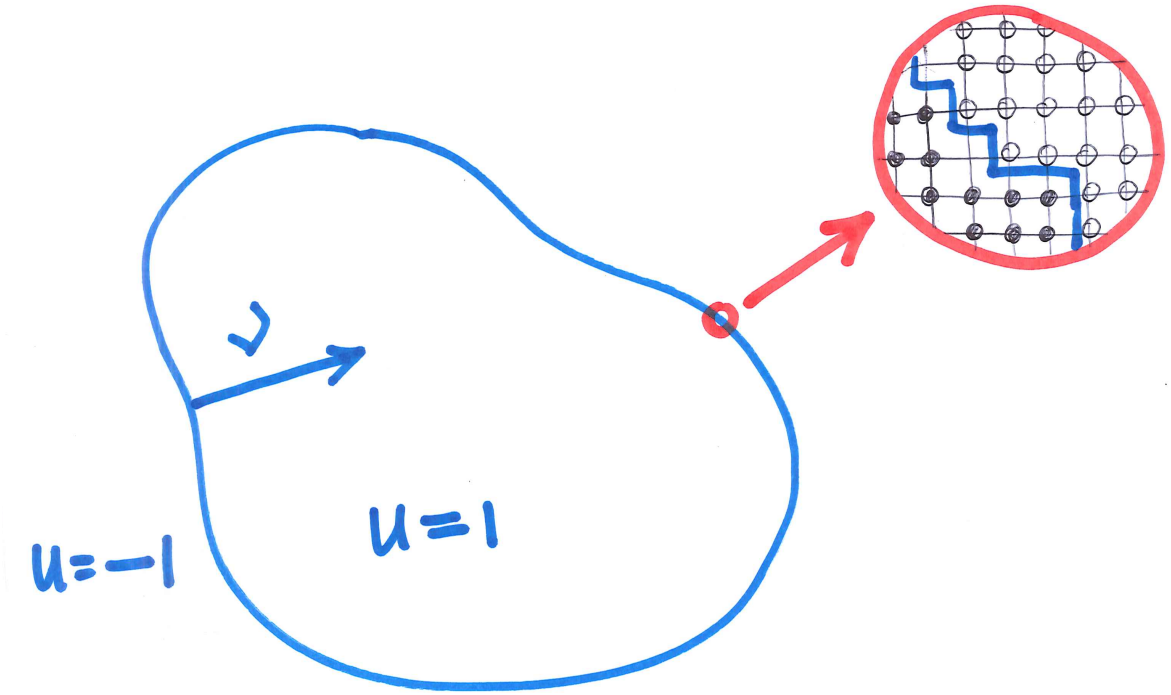
$$E_\varepsilon(u) = \frac{1}{8} \sum_{i,j} \varepsilon^{d-1} (u_i - u_j)^2$$

Convergence = strong L^1-convergence/weak BV-convergence
(for which we have **compactness**: the limit is a BV-functions with values in $\{\pm 1\}$ $\sim$ set of finite perimeter)

Limit **surface energy**:

$$F(u) = \int_{\partial\{u=1\}} \|\nu\|_1 d\mathcal{H}^{d-1}$$

$\|\nu\|_1 = |\nu_1| + \cdots + |\nu_d|$



ν = normal to the interface $\partial\{u = 1\}$

The Wulff-shape problem

Note: for general energies, if the Γ-limit is a (homogeneous) perimeter

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

then the minimum problems

$$\min\Big\{ E_\varepsilon(u) : \varepsilon^d \#\{i : u_i = 1\} = 1 + o(1) \Big\}$$

converge to a minimum perimeter problem

$$\min\Big\{ \int_A \varphi(\nu) d\mathcal{H}^{d-1} : |A| = 1 \Big\}$$

(identifying u with $A = \{u = 1\}$).
Equivalently, we may consider the maximal area problem

$$\max\Big\{ |A| : \int_A \varphi(\nu) d\mathcal{H}^{d-1} = 1 \Big\}$$

A minimizer of the latter (which differs from a minimizer for the perimeter by a dilation) is called the **Wulff shape** of φ (and indeed describes φ and hence F)

Note: for NN homogeneous ferromagnetic systems in $\mathbb{Z}^d$ the **Wulff shape** is a **cube**.

General Ferromagnetic Homogenization Results

B.-Piatnitski JFA 2012 (see also Caffarelli-De la Llave JSP 2006)

Let $E_\varepsilon(u) = \sum_{i,j} \varepsilon^{d-1} c^\varepsilon_{ij} (u_i - u_j)^2$. Under the assumptions

- **Ferromagnetic interactions**: $c^\varepsilon_{ij} \geq 0$
- **Periodicity**: $c^\varepsilon_{ij} = C_{\frac{i}{\varepsilon}\frac{j}{\varepsilon}}$ and $C_{(k+K)(l+K)} = C_{kl}$ for $K \in T\mathbb{Z}^d$
- **Decay**: $\sum_{k' \in \mathbb{Z}^d} k' C_{kk'} < +\infty$

(e.g. short-range interactions $C_{kk'} = 0$ for $|k - k'| > M$)

E_ε Γ-converge to an interfacial energy

$$F(u) = \int_{\Omega \cap \partial\{u=1\}} \varphi_{\text{hom}}(\nu) d\mathcal{H}^{d-1} \qquad u : \Omega \to \{-1, 1\}$$

where φ_{hom} is given by a discrete (non-local) least-area homogenization formula.

Note. In dimension 2 and with only NN interactions $\varphi_{\text{hom}}(\nu)$ can also be seen as a least length homogenization formula in direction $\nu^\perp$.

Some homogenization problems

Starting from the general framework outlined above, we will describe

1. Optimal design of mixtures of ferromagnetic interactions (a "G-closure" problem)

2. Interfacial energies for frustrated systems (with antiferromagnetic interactions)

3. An asymptotic result for dilute antiferromagnetic interactions.

1- A G-closure problem (bounds on ferromagnetic mixtures)

(part of the PhD thesis of L.Kreutz (GSSI))

A prototypical case: mixtures of two ferromagnetic interactions

We consider an arbitrary family of energies in dimension 2

$$F_\varepsilon(u) = \frac{1}{8}\sum_{NN} \varepsilon\, c_{ij}^\varepsilon (u_i - u_j)^2$$

(NN = only nearest-neighbour interactions) where
$c_{ij}^\varepsilon \in \{\alpha, \beta\}$, with $0 < \alpha < \beta$.

Integral representation. (Alicandro-Gelli SIMA 2016): up to subsequences F_ε Γ-converge to some F of the form

$$F(u) = \int_{\Omega \cap \partial\{u=1\}} \varphi(x,\nu) d\mathcal{H}^1 \qquad u : \Omega \to \{-1, 1\}$$

Note. In dimension 2 such energies are "dual" to energies on curves

$$F(u) = \int_a^b \varphi^\perp(\gamma, \gamma') dt \qquad \gamma : (a,b) \to \Omega$$

where $\varphi^\perp(x, z^\perp) = \varphi(x, z)$

Two-phase G-closure problem: characterize all possible φ

(analogous problem for conduction networks: B-Francfort RS London Proc.2004)

Local percentage of α-bonds: up to subsequences, $\{c_{ij}^\varepsilon\}$ determine a function $\theta : \Omega \to [0,1]$, defined e.g. as the density of the weak* limit of

$$\frac{1}{2} \sum_{(i,j):c_{ij}^\varepsilon = \alpha} \varepsilon^2 \delta_{\frac{i+j}{2}}$$

Problem: find all possible φ that can be obtained by $\{c_{ij}^\varepsilon\}$ with a given local percentage of α-bonds $\theta = \theta(x)$.

Continuum analogue for metrics: find all possible φ such that the Finsler length energy $\int \varphi(\gamma, \gamma')dt$ can be obtained as limit of anisotropic Euclidean length energies $\int a^\varepsilon(\gamma)|\gamma'|dt$ with $a^\varepsilon(x) \in \{\alpha, \beta\}$ given θ the weak limit of $\chi_{\{a^\varepsilon = \alpha\}}$ (non-sharp bounds by Davini-Ponsiglione JAM 2007)

A localization principle

• Given $\theta_0 \in (0,1)$ we define the set $\mathcal{H}(\theta_0)$ of all $\psi = \psi(\nu)$ that can be obtained by homogenization of periodic systems $\{C_{ij}\}$ with percentage of α given by θ_0 (with arbitrary period N).
• The definition of $\mathcal{H}(\theta_0)$ makes sense if $\theta_0 \in \mathbb{Q} \cap (0,1)$. By approximation we define $\mathcal{H}(\theta_0)$ for all $\theta_0 \in [0,1]$

Lemma ("Dal Maso & Kohn"-type) The reachable φ are exactly those such that $\varphi(x,\cdot) \in \mathcal{H}(\theta(x))$ for almost all $x \in \Omega$.

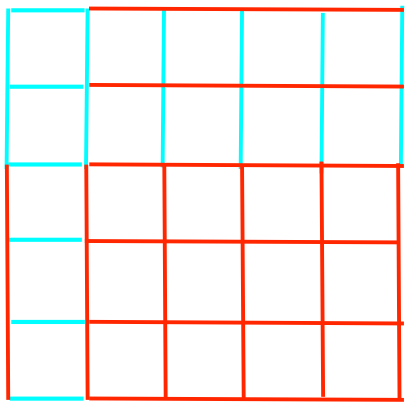
Technical points:
• in order to reduce to a periodic setting the energies are extended to BV by $\displaystyle\int_\Omega \varphi\Big(x, \frac{Du}{|Du|}\Big)|Du|$ (and the discrete analog). These are convex, and can be localized by blow-up and characterized by cell problems (B-Chiadò Piat JCA 1995, Chambolle-Thouroude NHM 2009);
• in order to construct c^ε_{ij} one uses the identification with $\displaystyle\int_a^b \varphi^\perp(\gamma,\gamma')dt$ and constructions for Riemannian metrics (B-Buttazzo-Fragalà Asy.An. 2002, Davini Diff.Int.Eqns 2005)

Description of the set $\mathcal{H}(\theta)$. Optimal bounds.

The problem is then to describe $\mathcal{H}(\theta)$ showing "optimal bounds" for the Wulff shape.

Trivial bounds: $\alpha\|\nu\|_1 \leq \psi(\nu) \leq \beta\|\nu\|_1$.

Sharpness of the trival lower bound: by layering "in series" in both directions we have a path with minimal length using only α-bonds



This can be done using a percentage of α-bonds of order $1/N$

This bound can be interpreted as a geometrical constraint on the Wulff shape of ψ, which be contained in the square Wulff shape of $\alpha\|\nu\|_1$.

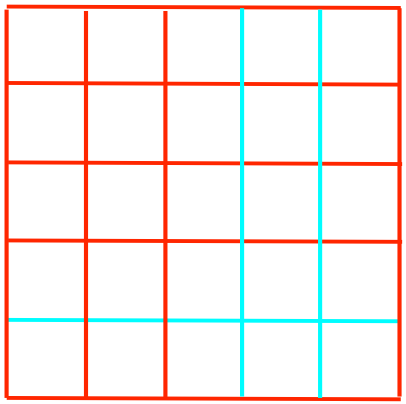
Bounds-II

An "upper bound" by averaging: if ψ is the homogenized energy density of C_{ij} we have

$$\psi(\nu) \leq C^h|\nu_1| + C^v|\nu_2|.$$

where $C^h =$ average of horizontal C_{ij}, $C^v =$ average of vertical C_{ij} (i.e., $C^h = \theta^h\alpha + (1-\theta^h)\beta$ with θ^h percentage of horizontal α-bonds, ...)

Sharpness of the upper bound given C^h and C^v (which determine the percentage of vertical and horizontal α-bonds): obtained by layering "in parallel"



Note that $\frac{1}{2}(C^h + C^v) = \theta\alpha + (1-\theta)\beta$

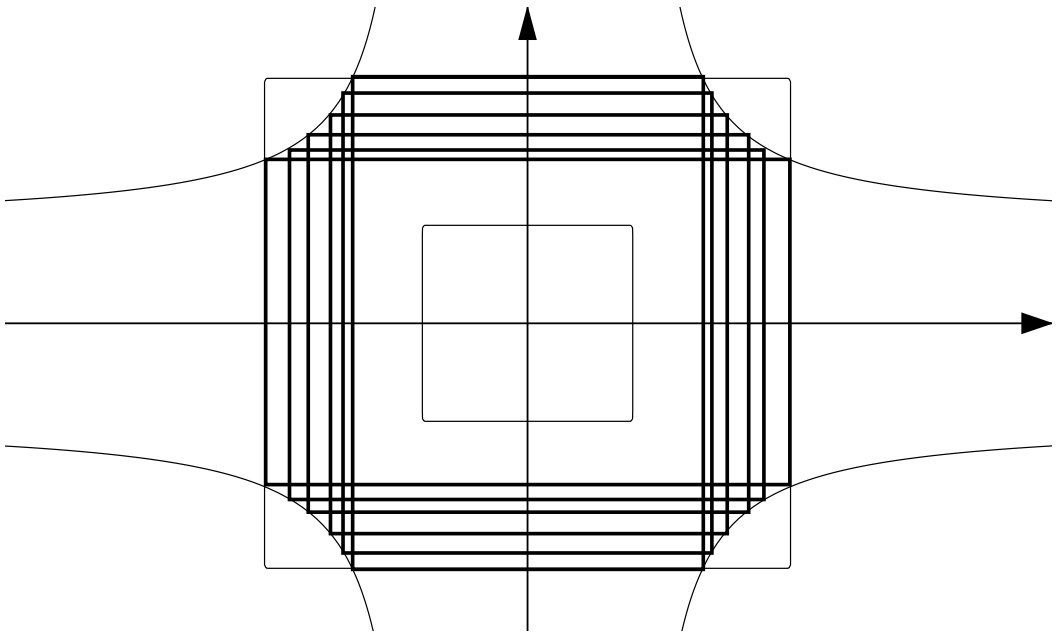
Bounds-III

The optimal upper bound is :

$$\psi(\nu) \leq (C^h|\nu_1| + C^v|\nu_2|) \vee \beta\|\nu\|_1$$

for some $\alpha \leq C^h, C^v \leq \beta$ with $C^h + C^v = 2(\theta\alpha + (1-\theta)\beta)$.

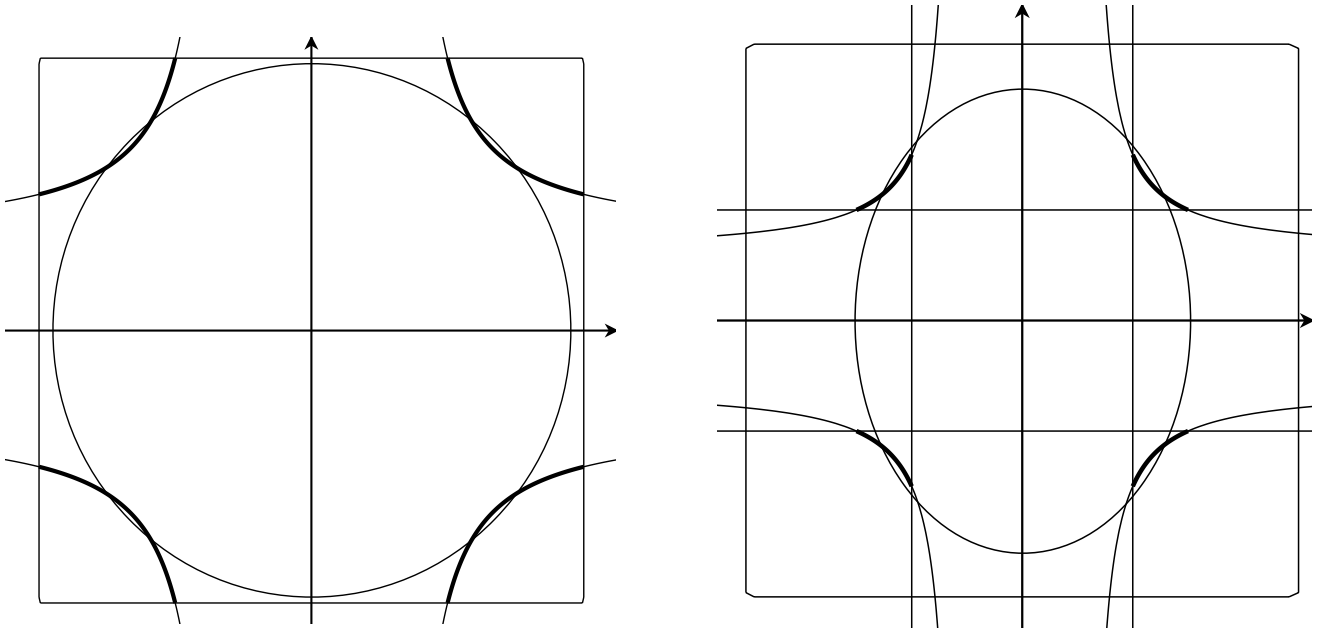
This can be interpreted as a geometrical constraint on the Wulff shape of ψ: it should contain one of the Wulff shapes of $C^h|\nu_1| + C^v|\nu_2|$ (rectangles in figure)



Representation of the bounds on the Wulff shape

Possible Wulff shape should be symmetric with respect to the origin and cross the four **curves in bold**, of equation

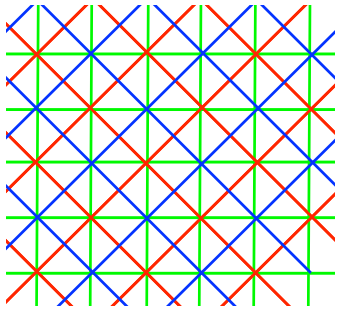
$$\frac{1}{|x_1|} + \frac{1}{|x_2|} = 16(\theta\alpha + (1-\theta)\beta)$$



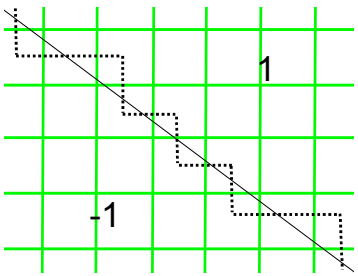
Left: case $\theta > 1/2$
Right: case $\theta \leq 1/2$ (here we must also take into account that $C^h, C^v \leq \beta$)

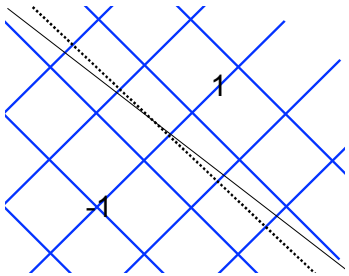
Longer-range interactions

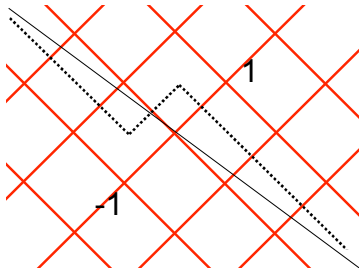
For longer-range interactions the bounds are obtained by a **superposition argument**: e.g., a system of NNN interactions



can be considered as three superposed lattices, where to estimate interfacial energies separately.







A multi-scale argument for the construction of the optimal geometries is needed in this case.

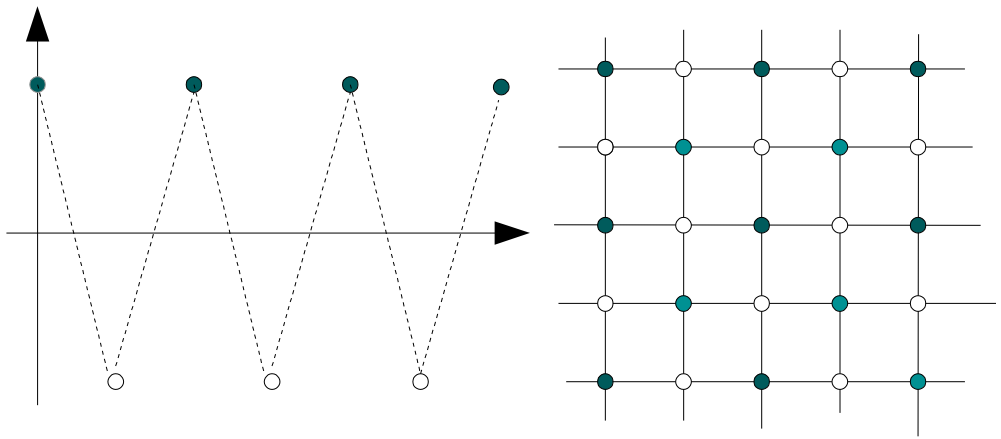
2- Homogenization of frustrated systems

When also antiferromagnetic interactions are considered then minimizers can be **frustrated**: i.e. not all interactions are separately minimized.

Simplest case: nearest-neighbour energies $E(u) = \sum_{NN} u_i u_j$, or, up to additive/multiplicative constants

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

Ground states: alternating states.



Note: in $\mathbb{Z}^d$ we can reduce to ferromagnetic interactions introducing the variable $v_i = (-1)^i u_i$ (only for NN systems).

An example with non-trivial macroscopic parameter

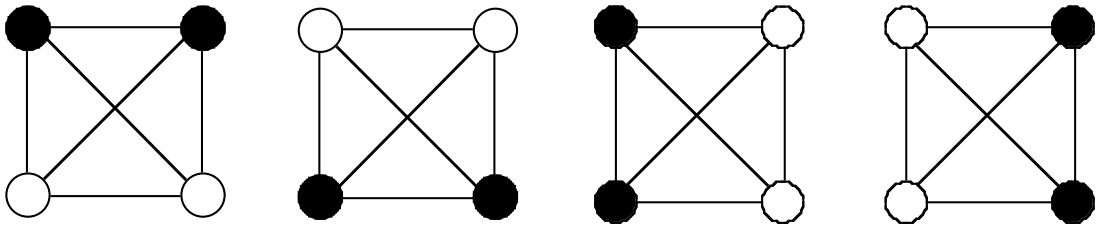
Alicandro-B.-Cicalese NHM 2006

In general ± 1 are not meaningful order parameters.

An example: anti-ferromagnetic spin systems in 2D

$$E(u) = c_1 \sum_{NN} u_i u_j + c_2 \sum_{NNN} u_k u_l \qquad u_i \in \{\pm 1\}$$

For suitable positive c_1 and c_2 the ground states are 2-periodic



(representation in the unit cell)

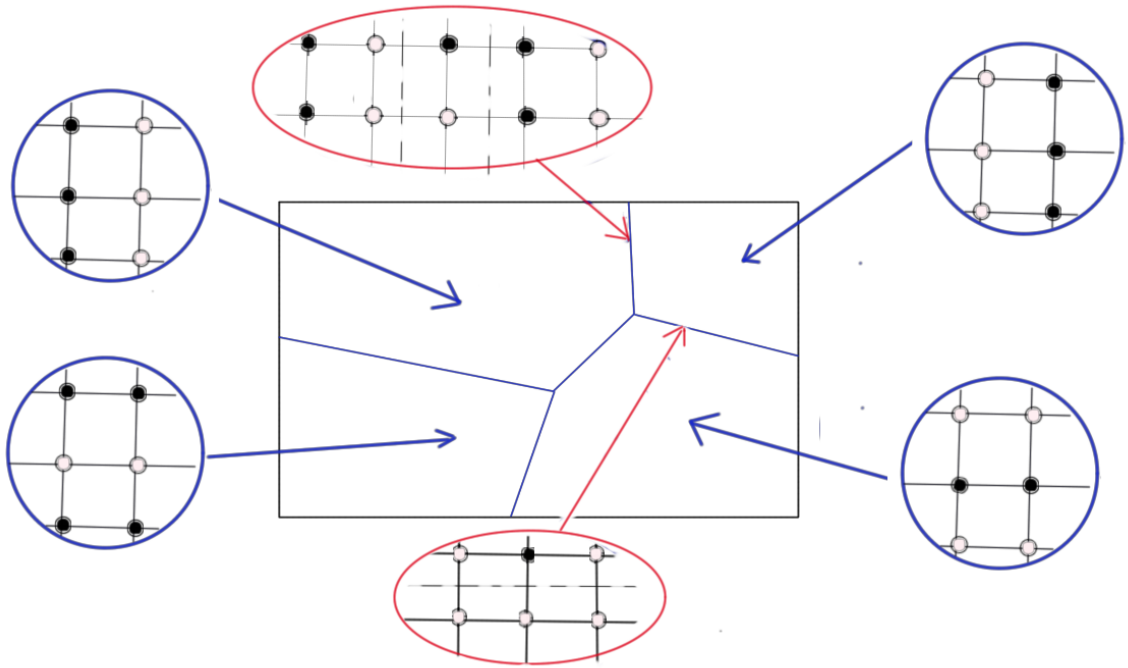
The correct order parameter is the **orientation** $v \in \{\pm e_1, \pm e_2\}$ of the ground state.

Γ-limit of scaled E_ε:

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

$S(v)$ = discontinuity lines; ν = normal to $S(v)$
ψ given by an optimal-profile problem

Macroscopic picture of a limit state with finite energy



Energies with periodic ground states

$X \subset \mathbb{R}$ finite space of configurations
For $u : \varepsilon\mathbb{Z}^d \to X$ let

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

(Ψ_i is obtained by regrouping and normalizing interactions: in the example above Ψ_i takes into account interactions in a single square labeled by i)
be such that $i \mapsto \Psi_i$ is periodic and

H1 (presence of periodic minimizers) let $Q_N = \{1, \dots, N\}^d$
there exist $N, K \in \mathbb{N}$ and $\{v_1, \dots, v_K\}$ Q_N-periodic functions such that
$u \neq v_j$ in $Q_N \Rightarrow E_\varepsilon(u, Q_N) \geq C > 0$
$u = v_j$ in $Q_N \Rightarrow E_\varepsilon(u, Q_N) = 0$

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H2 (incompatibility of minimizers) let Q'_N be a N-cube with $Q_N \cap Q'_N \neq \emptyset$ and $l \neq m$. Then

$$u = \begin{cases} v_l & \text{in } Q_N \\ v_m & \text{in } Q'_N \end{cases} \quad \Longrightarrow \quad E_\varepsilon(u, Q_N \cup Q'_N) > 0,$$

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H3 (decay conditions) there exist C_R with $\sum_R C_R R^{d-1} < \infty$ such that
$u = u'$ in $Q_{RN} \Rightarrow |E_\varepsilon(u', Q_N) - E_\varepsilon(u, Q_N)| \leq C_R$

A compactness result with ground states (patterns) as parameters

B-Cicalese 2015, to appear

The following results states that, under assumptions H1–H3, a spin system can be interpreted as a multi-component surface energy

Compactness:

Let u_ε be such that $E_\varepsilon(u_\varepsilon) \leq C < +\infty$. Then, under $H1, H2$ and $H3$, there exist sets $A_{1,\varepsilon}, \dots, A_{K,\varepsilon} \subseteq \mathbb{Z}^N$ (identified with the union of the ε-cubes centered on their points) such that $u_\varepsilon = v_j$ on $A_{j,\varepsilon}$, $A_{j,\varepsilon} \to A_j$ in $L^1_{loc}(\mathbb{R}^d)$ and $A_1, \dots, A_N$ is a partition of $\mathbb{R}^d$.

Γ-convergence:

$$\Gamma\text{-}\lim_\varepsilon E_\varepsilon(u) = \sum_{i,j} \int_{\partial A_j \cap \partial A_j} \psi(i,j,\nu)\, d\mathcal{H}^{n-1}$$

Mixtures of ferro+antiferro spin energies

The previous theorem may be appied to periodic mixtures where Ψ_i regroupes (and normalizes) interactions

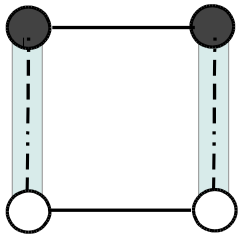
$$C_{ij} \in \{+1, -1\}.$$

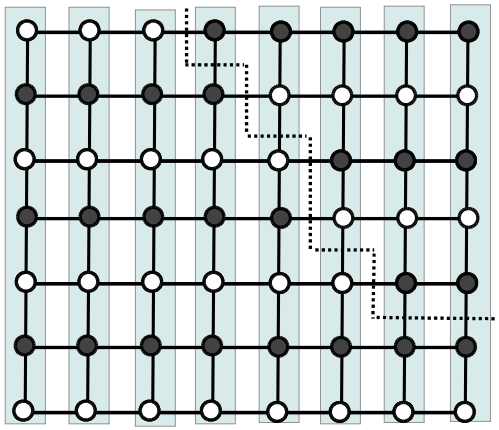
Question: what conditions to require on $\{C_{ij}\}$ in order that Ψ_i satisfy H1–H3?
Question: can we bescribe the limit energies in some classes of coefficients?
This is not trivial even when we only have nearest-neighbour interactions.

How to state a G-closure problem?

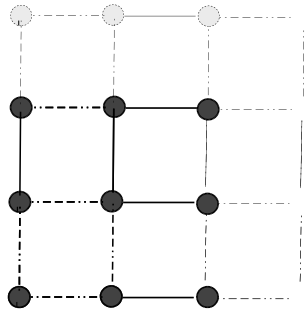
Even in the simple case of only NN interactions, and a periodic distribution of given proportions of ferro- and antiferromagnetic interactions the parameter can depend on the geometry.

Example: for half ferro and half antiferro (1-periodic arrangement) we may have a phase/antiphase description with two parameters (but no majority phase)

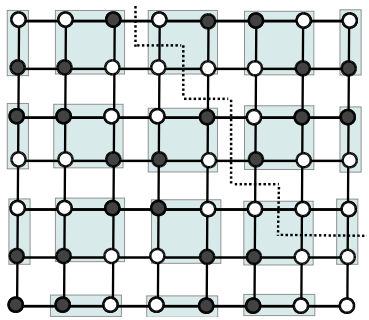




. . . the parameters may be more complex

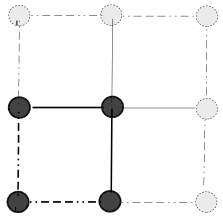


distribution of NN bonds (dotted line=antiferromagnetic bonds)



antiphase boundary

... or we may have a majority phase



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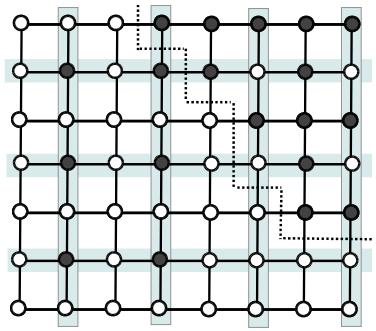
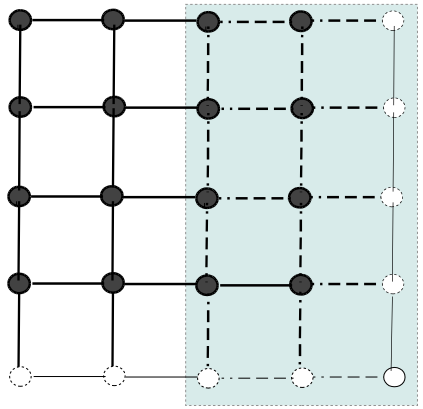
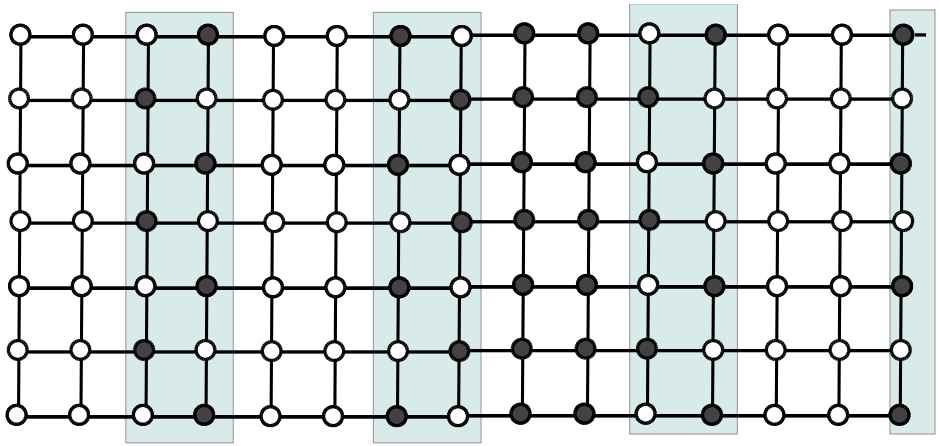


phase boundary

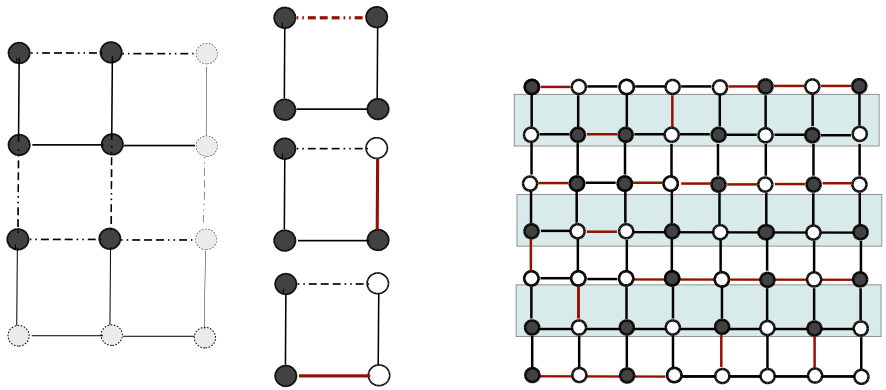
... or infinitely many ground states(4-periodic arrangement)





and a limit description not given by a perimeter energy
(must be relaxed on BV: no interfacial energy for vertical interfaces)

or **total frustration:** we may have a zero surface tension due to frustration.

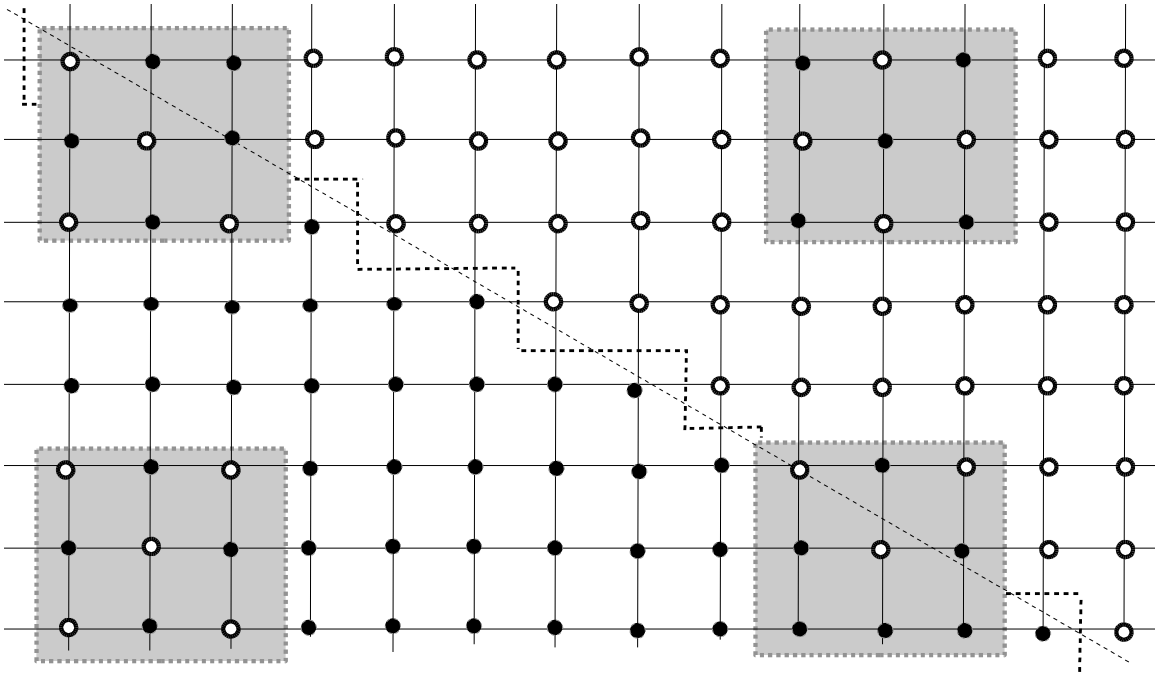


The figures picture:
– the distribution of NN bonds (dotted line=antiferromagnetic bonds)
– three minimizing patterns on a square (red lines = frustrated bonds)
– a "disordered" minimal distribution (light-blue zone = antiferromagnetic bonds)

Question: are these the only possible cases with nearest-neighbours? can we characterize the maximum number of periodic ground states from the range of the interaction?

3-Dilute antiferromagnetic inclusions

Example (B-Piatnitski, JSP 2012) If we have *small inclusions* of the antiferromagnetic bonds we may still have a continuum interfacial energy and an order parameter $u : \mathbb{R}^d \to \{-1, 1\}$ (representing the *majority phase*).



(grey area = anti-ferromagnetic interactions)
We want to show that this is the "generic" case for *small percentage* of antiferromagnetic interactions (dilute regime)

Ground states with a majority phase

(B-Causin-Piatnitski-Solci 2016)

The result. There exists a percentage $p_0 > 0$ such that for a *generic* periodic system of nearest-neighbour coefficients $C_{ij} \in \{\pm 1\}$ such that the percentage of $C_{ij} = -1$ does not exceed p_0, any minimizer of

$$\sum_{(i,j)\in\Omega} c^{\varepsilon}_{ij}(u_i - u_j)^2, \qquad \text{where} \qquad c^{\varepsilon}_{ij} = C_{i/\varepsilon\, j/\varepsilon}$$

in a bounded open set Ω satisfies: $u_i = 1$ (or $u_i = -1$) for all i in a connected set whose complement is composed of disjoint sets (i.e., of distance larger than 2ε) of size $O(\varepsilon)$.

Genericity: the genericity of $\{C_{ij}\}$ can be expressed as follows:
let $\mathcal{P}(N,p)$ be the set of all N-periodic coefficients $\{C_{ij}\}$ with a percentage of antiferromagnetic interactions not greater that p
let $\mathcal{B}(N,p)$ be the subset of $\{C_{ij}\}$ which fail to satisfy the thesis of the theorem
Then there exists $p_0 > 0$ such that $\lim_{N\to+\infty} \dfrac{\#\mathcal{B}(N,p_0)}{\#\mathcal{P}(N,p_0)} = 0.$

Outline of the proof

(combinatoric and graph-theory arguments)

• estimate the number of N-periodic arrangements $\{C_{ij}\}$ such that a path of length larger than $N/2$ exists in a periodicity square with at least half $C_{ij} = -1$. Note that the proportion of such $\{C_{ij}\}$ decreases esponentially with N.

• suppose that there exist minimizers u^ε which do not satisfy the thesis. Then for ε small there exists a "macroscopic" interface between $u^\varepsilon = 1$ and $u^\varepsilon = -1$. Such an interface must have more than half $c^\varepsilon_{ij} = -1$. We cover this interface with $O(N)$ squares.

• we use the previous observation to estimate the ratio between $\#\mathcal{B}(N, p_0)$ and $\#\mathcal{P}(N, p_0)$ with an exponentially decaying quantity.

Note: the same result holds by replacing the "proportion p_0" by a "probability p_0" and "generic" by "almost sure" (work in progress)

Conclusion

We have seen three issues in the homogenization theory for spin systems

• **Bounds for mixtures of ferromagnetic interactions**.
In this case we can exhibit exact bounds, and give a description in terms of Wulff shapes, contrary to the continuum case, still open.

• **Limits parameterized by ground states.**
We have given a general integral representation results on Caccioppoli partitions. It applies to some classes of interactions mixing ferromagnetic and antiferromagnetic interactions, but (optimal) conditions on microgeometries which ensure the applicability of the theorem are unknown.

• **Systems with ground states characterized by a majority phase.**
We have proved that "generically" systems with a low percentage of antiferromagnetic interactions have "ferromagnetic" ground states.
The extension to a Gamma-convergence result seems technically more difficult, and what happens beyond the dilute regime a matter of conjecture.

Thank you for your attention!