Variational methods for lattice systems

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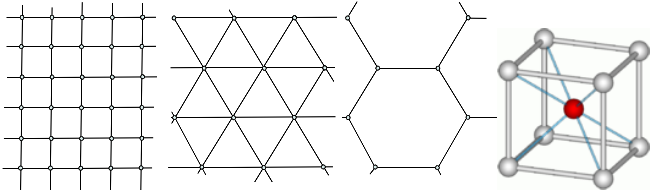
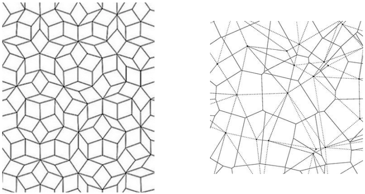
Geometry. We will consider a parameter $u : i \mapsto u_i$ defined on a (part of a) lattice $\mathcal{L}$, which can be a periodic lattice



or an aperiodic lattice, or a random lattice, etc.



Methods (but not results) will be independent of the lattice

Energy. The behaviour of the parameter is governed by an *internal energy*, that usually is written

$$E(u) = \sum_{i \neq j} \phi_{ij}(u_i, u_j)$$

(*pair interactions*). Again the methods are valid for more general energies.

Motivations: from Continuum Mechanics, Statistical Physics, Computer Vision, etc.

We will focus mainly on some simple energies, in order to highlight the methods and some of the related issues.

General references: Alicandro, Braides, Cicalese. *The Importance of Being Discrete* (provisional title, book in preparation)
A. Braides. Lecture Notes of the Würzburg Winter School 2012 on Calculus of Variations in Physics and Materials Science (available at my web page).

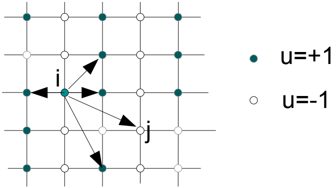
Parameter: $u : \Omega \cap \mathbb{Z}^d \to \{-1, 1\}$

Energy:

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

or, up to additive/multiplicative constants

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



Variational Analysis.

Ferromagnetic interactions. If $c_{ij} \geq 0$ then $u \equiv 1$ or $u \equiv -1$ are *ground states*.

Also in this case, non-trivial minimum problems may be obtained by adding some conditions; e.g.
Volume-constrained problems

$$\min\{E(u) : \#\{i : u_i = 1\} = N\}$$

Problems with an external field

$$\min\Big\{E(u) + \sum_i H_i u_i\Big\}$$

We are interested in the **behaviour of such problems when the number** i **of indices involved diverges**.

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 $\varepsilon \to 0$.

Scaled variable: $u : \varepsilon\mathcal{L} \to \mathbb{R}^m$

Scaled energies:

$$E_\varepsilon(u) = \sum_{i,j} \phi^\varepsilon_{ij}(u_i, u_j)$$

(usually, up to constants, $\phi^\varepsilon_{ij}(u_i, u_j) = \varepsilon^\alpha \phi^\varepsilon_{ij}(\varepsilon^\beta u_i, \varepsilon^\beta u_j)$).

This is a **multi-scale problem**: the behaviour of the same ϕ_{ij} can be analysed through different scalings.

Functional setting. Identify $u : \varepsilon\mathcal{L} \to \mathbb{R}^m$ 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.

Weak convergence methods.
Define a **discrete-to-continuum convergence**

$$u^\varepsilon : \varepsilon\mathcal{L} \to \mathbb{R}^m \qquad \longrightarrow \qquad u : \mathbb{R}^d \to \mathbb{R}^m$$

as the *convergence of the interpolations* (or sum of deltas). Usually, weak L^1-convergence (convergence of averages), 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.

Define 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".

Integral representation theory. The description of F depends on the scaling and the parameter. Abstract results allow to recognise an integral form of F; e.g.

$$F(u) = \int f(x,u)\,dx \qquad f \text{ convex}$$

$$F(u) = \int f(x,u,\nabla u)\,dx \qquad f \text{ quasiconvex}$$

$$F(u) = \int_S g(\psi)\,d\mathcal{H}^{d-1} \text{ if } \quad u = \psi\mathcal{H}^{d-1} \llcorner S \text{ (surface energy)} \qquad g \text{ BV-elliptic}$$

$$F(u) = \sum_i \Psi(c_i) \text{ if } \qquad u = \textstyle\sum_i c_i\delta_{x_i} \text{ (point energy)} \qquad \Psi \text{ subadditive,}$$

etc.

Homogenization: computation of the energy densities of F through formulas that involve the microscopic formulation (fundamental for numerical analysis, optimal design, etc.)

Example : spin systems - II

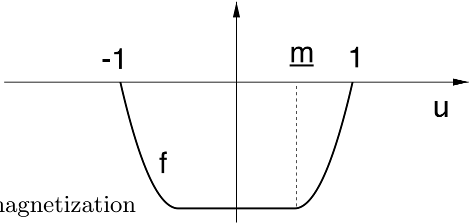
Bulk scaling. Convergence = weak L^1-convergence
Limit $u(x)$ (*magnetization*) = average value of u_ε "around x".
Scaling

$$E_\varepsilon(u) = \sum_{ij} \varepsilon^d c_{ij}(u_i - u_j)^2 \qquad i \in \varepsilon\mathbb{Z}^2$$

The limit of the form

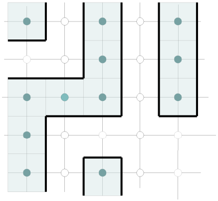
$$F(u) = \int f(x, u(x))\,dx \qquad u : \mathbb{R}^d \to [-1, 1]$$

If, e.g., $c_{ij} = c_{j-i}$, $f = f(z)$ is given by an optimal location problem for u_i on large cubes $[0, T]^d$ subject to the condition $\sum_i u_i = zT^d$. $f : [-1, 1] \to \mathbb{R}$ is convex:



$\underline{m}$ = effective magnetization

Surface scaling.
For **nearest-neighbour ferromagnetic interactions** ($c_{ij} = 0$ for $|i-j| > 1$, $c_{ij} = 1$ if $|i-j| = 1$)) E can be viewed as a **surface energy**



Scaled energies

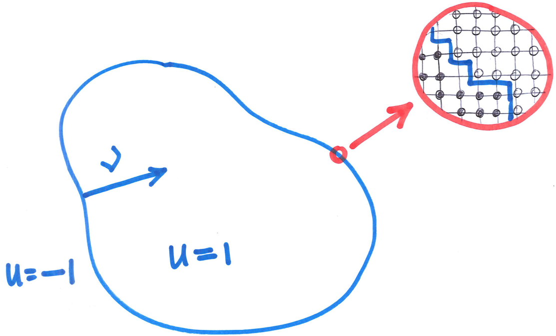
$$E_\varepsilon(u) = \sum_{i,j} \varepsilon^{d-1} (u_i - u_j)^2$$

Convergence = strong L^1-convergence/weak BV-convergence

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 $\partial\{u=1\}$

General Ferromagnetic Homogenization Result

B.-Piatnitski JFA 2012

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: $\sum_{k'\in\mathbb{Z}^d} C_{kk'} < +\infty$ (e.g. $C_{kk'} = 0$ for $|k-k'| > M$ or $C_{kk'} \sim |k-k'|^{-\gamma}$ with $\gamma > d$)

Then 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 least-area homogenization formula. Periodicity can be substituted by a random dependence ($\Rightarrow$ a.s. result).

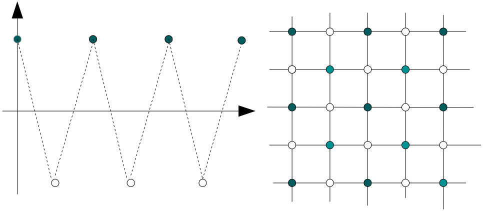
Note. If we relax the periodicity and decay assumptions we may obtain non-local energies; e.g.,

$$F(u) = \int_{\Omega\cap\partial\{u=1\}} \varphi_{\text{hom}}(\nu)\,d\mathcal{H}^{d-1} + \iint_{\Omega\times\Omega} k(x,y)|u(x)-u(y)|\,dx\,dy$$

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

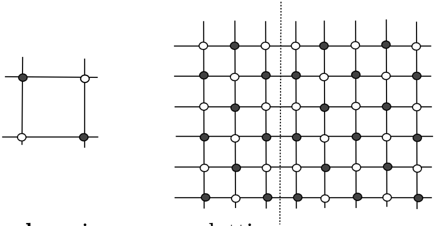
$$E(u) = \sum_{NN} (u_i + u_j)^2$$

Ground states: alternating states.

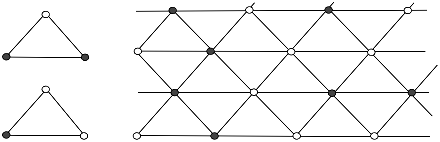


Note: in $\mathbb{Z}^d$ we can reduce to ferromagnetic interactions introducing the variable $v_i = (-1)^i u_i$ (only for NN systems).

Dependence on the lattice: the reduction to ferromagnetic interactions is not always possible, and the description is lattice-dependent.



Anti-phase boundary in a square lattice



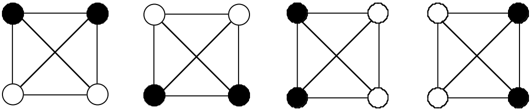
No anti-phase boundaries in a triangular lattice

In general magnetization is not a meaningful order parameter.

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)

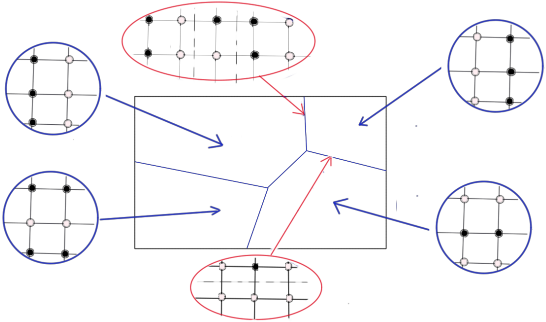
The correct order parameter is the **orientation** $v \in \{\pm e_1, \pm e_2\}$ of the ground state.

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

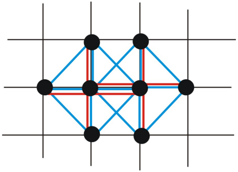
Macroscopic picture of a limit state with finite energy



We may consider a $2D$ spin model accounting for NN (nearest neighbors), NNN (next-to-nearest neighbors) and NNNN (next-to-next-to...) interactions

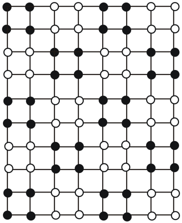
$u : \varepsilon\mathbb{Z}^2 \to \{\pm 1\}$

$$E_\varepsilon(u) = \sum_{NN} \varepsilon u_i u_j + c_1 \sum_{NNN} \varepsilon u_i u_j + c_2 \sum_{NNNN} \varepsilon u_i u_j$$



It is possible to regroup the interactions to study the ground states

For suitable c_1 and c_2, for ε small enough we obtain 4-periodic minimizers as:



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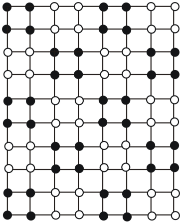

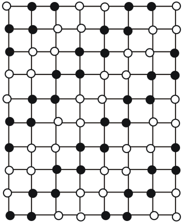

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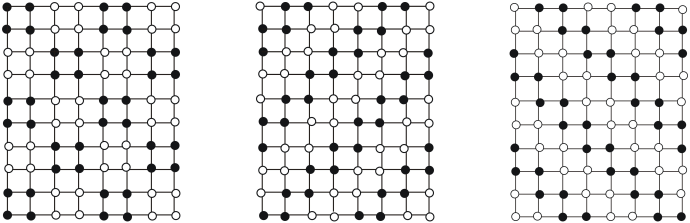

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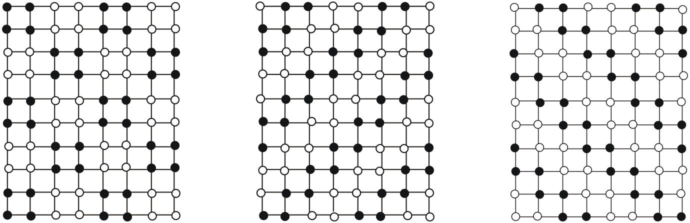
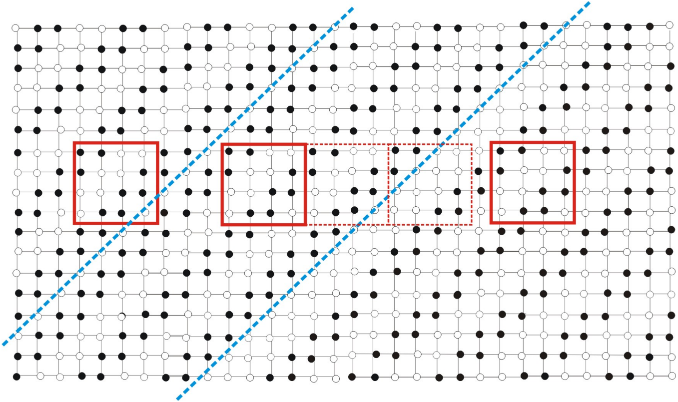
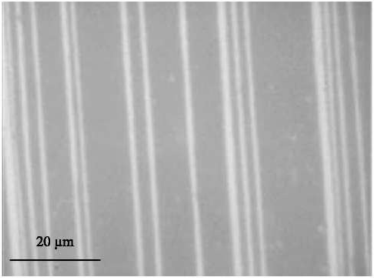


(counting translations, they are 16)

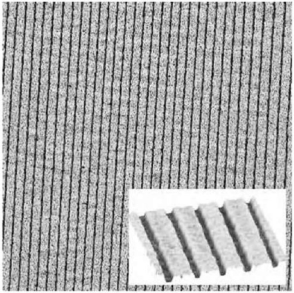


The Γ-limit can be expressed in terms of a **phase variable**.
The limit functional is the energy of the shift transitions in spatially-modulated phases.

Formation of stripe patterns during Langmuir-Blodgett condensation



fast process



slow process

General Phase-Shift energies

$X \subset \mathbb{R}$ finite space of configurations
For $u : \varepsilon\mathbb{Z}^d \to X$ let $E_\varepsilon(u) = \sum_i \varepsilon^{n-1}\Psi(\{u_{i+j}\}_{j\in\mathbb{Z}^d})$ be such that

H1 (presence of periodic minimizers)
$\exists N, K \in \mathbb{N}$ 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)

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

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H3 (locality of the energy)
$u = u'$ in $Q_{RN} \Rightarrow |E_\varepsilon(u', Q_N) - E_\varepsilon(u, Q_N)| \leq C_R$ and
$\sum_R C_R R^{d-1} < \infty$

The following results states that, under reasonable assumptions, a spin system can be interpreted as a phase-shif energy

Compactness:
Let u_ε be such that $E_\varepsilon(u_\varepsilon) \leq C < +\infty$. Then, under $H1, H2$ and $H3$, $\exists A_{1,\varepsilon}, \ldots, A_{K,\varepsilon} \subseteq \mathbb{Z}^N$ (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 $A_1, \ldots, A_N$ is a partition of $\mathbb{R}^d$.

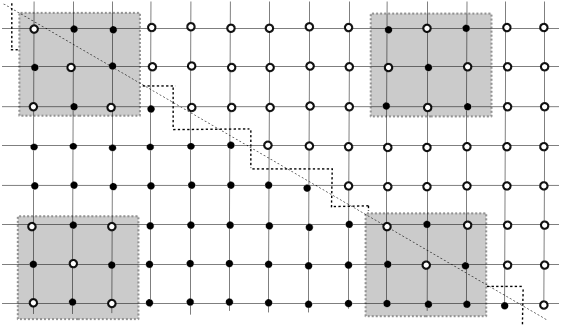
Γ-convergence:

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

Ferromagnetic vs antiferromagnetic interactions

B-Piatnitski, J.Stat.Phys. 2012

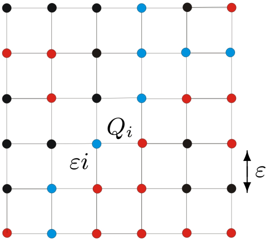
In general, when ferromagnetic and anti-ferromagnetic interaction are present (**spin glass**) the behaviour at the surface scaling and the macroscopic order parameter may not be clear. For small volume fractions of the antiferromagnetic phase we still have a continuum interfacial energy and an order parameter $u : \mathbb{R}^d \to \{-1, 1\}$ (representing the *majority phase*).



grey area = anti-ferromagnetic interactions

As the volume fraction of the antiferromagnetic phase grows the order parameter has to change. In this case the hypotheses of the phase-shift characterization are not valid.

We now examine the effect of more than two phases.



Three phases: $-1, 0, 1$

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

$$u : \mathbb{Z}^2 \cap \Omega \mapsto \{-1, 0, 1\}, \ k \in \mathbb{R}$$

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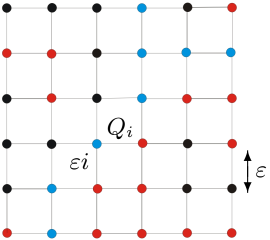

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New effects for $\frac{1}{3} < k < 1$: in this case

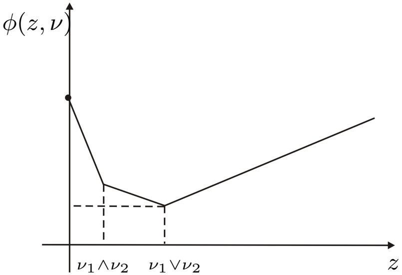
- minimal phases are $u \equiv 1$ and $u \equiv -1$
- the presence of the phase 0 is energetically-favourable on the interfaces

The description of the limit depends on the positive parameter k.

Surfactant energies

The continuum limit of the BEG model involves: a parameter $u : \mathbb{R}^2 \to \{-1, 1\}$ and a measure μ representing the limit concentration of the 0-phase. In these variables the continuum description is as follows.

$$F = F(u,\mu) = \int_{\partial\{u=1\}} \phi\Big(\frac{d\mu}{d\mathcal{H}^1\lfloor_{\partial\{u=1\}}}, \nu\Big) d\mathcal{H}^1 + 2(1-k)|\mu|(\mathbb{R}^2 \setminus \partial\{u=1\}),$$



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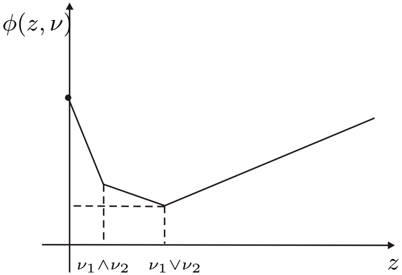

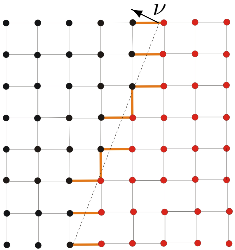

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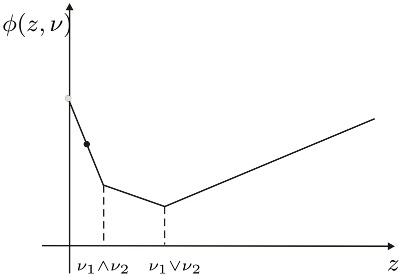

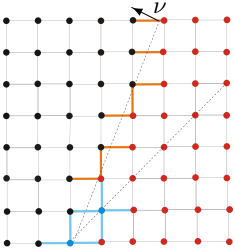

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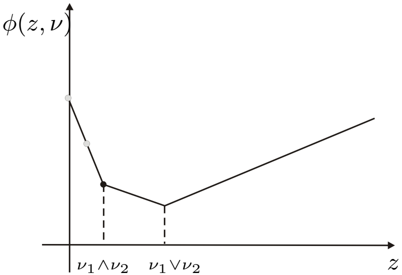

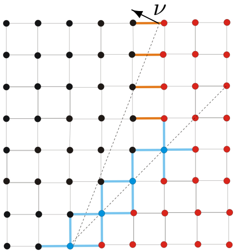

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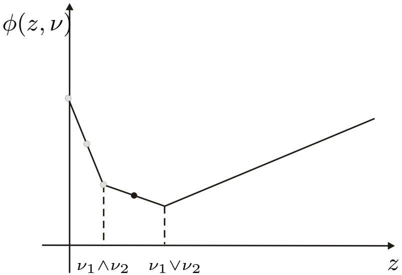

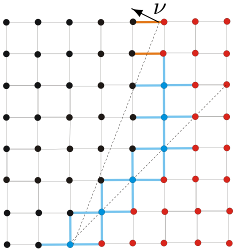

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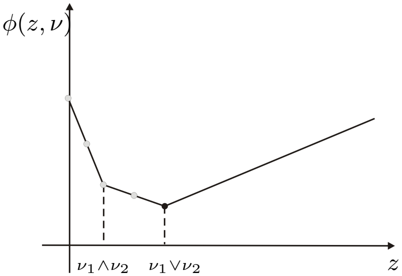

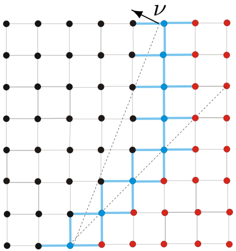

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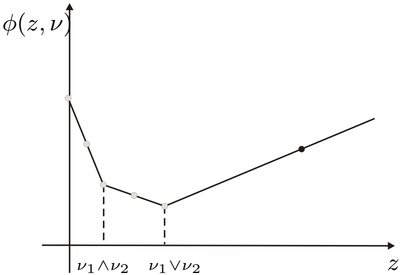

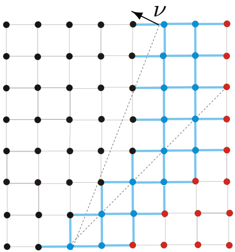

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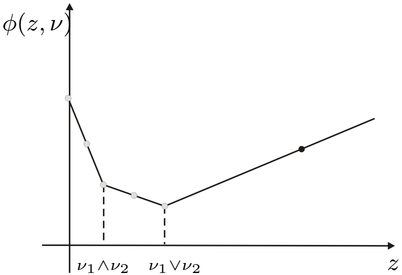
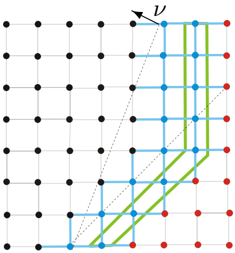




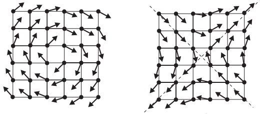
Nearest-neighbour model

$$E(u) = \sum_{ij} \|u_i - u_j\|^2 \sim -\sum_{ij} \langle u_i, u_j \rangle \qquad u : \mathbb{Z}^2 \to \mathbb{R}^2,\ |u_i| = 1$$

New energy scales: **vortex scaling**

$$E_\varepsilon(u) = \frac{1}{|\log \varepsilon|} \sum_{ij} \|u_i - u_j\|^2$$

As $\varepsilon \to 0$ the energy concentrates on vortex singularities



degree 1 degree -1

The limit energy is defined on "vortices"

$$u = \sum_i c_i \delta_{x_i} \qquad c_i \in \mathbb{Z}$$

for which

$$F(u) = \pi \sum_i |c_i|\,.$$

gradient scaling

$$E_\varepsilon(u) = \sum_{ij} \|u_i - u_j\|^2 = \sum_{ij} \varepsilon^2 \Big\| \frac{u_i - u_j}{\varepsilon} \Big\|^2$$

Interpreting $\frac{u_i - u_j}{\varepsilon} \sim \nabla u$ gives $\qquad F(u) = \int |\nabla u|^2 \, dx \qquad$ for $|u| = 1$

Note: (1) The XY model presents a complete analogy with the **Ginzburg-Landau** theory with energy

$$F_\varepsilon(u) = \int \Big(|\nabla u|^2 + \frac{1}{\varepsilon}(|u|^2 - 1)^2 \Big) dx$$

(theory of *superconductivity*)
(2) discrete vortices can be interpreted as *screw dislocations*;
(3) for models with head-to-tail symmetry the same argument gives a *nematic liquid crystal theory*

Conclusions

Even for simple lattice spin system a complex continuum theory has been obtained with a multi-scale (bulk, surface, gradient, vortex,...) nature involving vector parameters, surface energies, measures, etc.

The analysis has moved beyond what we have seen, including
• the analysis of gradient-flow type motions for spin systems obtaining geometric flows with pinning and homogenized velocity formulas;
• the treatment of *displacemet fields* $u_i \in \mathbb{R}^m$, with issues such as *crystallization*: description of the ground states as a regular lattice; *derivation of elasticity theories* both nonlinear and linear; *derivation of fracture theories*,
etc.

Many questions remain unanswered. In particular
• *remove the assumption of a reference lattice*
• *treat the case of non-zero temperature*
etc.

Thanks for the attention!