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)
Parameter: \( u : \Omega \cap \mathbb{Z}^d \rightarrow \{ -1, 1 \} \)

Energy:

\[
E(u) = - \sum_{i,j} c_{ij} u_i u_j \quad \text{Ising model/Lattice gas}
\]

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**

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

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:

\[
E_\varepsilon(u) = \sum_{i,j} \phi_{ij}^\varepsilon(u_i, u_j)
\]

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

This is a multi-scale problem: the behaviour of the same \( \phi_{ij} \) can be analysed through different scalings.
Functional setting. Identify $u : \varepsilon L \to \mathbb{R}^m$ e.g. with its \textit{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 \textit{discrete-to-continuum convergence}

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

as the \textit{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 \textbf{continuum energy} $F$ which describes the “behaviour” of the energies $E_\varepsilon$ as $\varepsilon \to 0$. 
\textbf{\textit{\Gamma}}-convergence. In a variational setting, $F$ is given by the \textbf{\textit{\Gamma}}-limit of $E_\varepsilon$ (with respect to the convergence $u_\varepsilon \to u$), which guarantees the “convergence of minimum problems”.

\textbf{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.

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

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

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

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

etc.

\textbf{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 $u_\varepsilon$ “around $x$”.

Scaling

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

The limit of the form

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

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 $\sum_i u_i = z T^d$. $f : [-1, 1] \to \mathbb{R}$ is convex:

$\bar{m} = \text{effective magnetization}$
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:

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

\[ ||\nu||_1 = |\nu_1| + \cdots + |\nu_d| \]

\( \nu = \) normal to the interface \( \partial\{u = 1\} \)
**General Ferromagnetic Homogenization Result**
B.-Piatnitski JFA 2012

**Ferromagnetic interactions:** $c_{i,j}^\varepsilon \geq 0$

**Periodicity:** $c_{i,j}^\varepsilon = C_{i,j}^\varepsilon$ 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 $E_\varepsilon$ $\Gamma$-converge to an interfacial energy

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

where $\varphi_{\text{hom}}$ 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.,

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

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**

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

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.
$\Gamma$-limit of scaled $E_\varepsilon$:

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

$S(v) = \text{discontinuity lines}$; $\nu = \text{normal to } S(v)$

$\psi$ 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

\[ u : \varepsilon \mathbb{Z}^2 \rightarrow \{ \pm 1 \} \]

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

It is possible to regroup the interactions to study the ground states
For suitable $c_1$ and $c_2$, for $\varepsilon$ small enough we obtain $4$-periodic minimizers as:
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![Diagram of 4-periodic minimizers]

(counting translations, they are 16)
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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
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)
\[ \exists N, K \in \mathbb{N} \text{ and } \{v_1, \ldots, v_K\} \text{ } Q_N\text{-periodic functions such that} \]
\[ u \neq v_j \text{ in } Q_N \Rightarrow E_\varepsilon(u, Q_N) \geq C > 0 \]
\[ u = v_j \text{ in } Q_N \Rightarrow E_\varepsilon(u, Q_N) = 0 \]
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**H2** (incompatibility of minimizers)

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

3. **H3** (locality of the energy)
   \[
   u = u' \text{ in } Q_{RN} \Rightarrow |E_\varepsilon(u', Q_N) - E_\varepsilon(u, Q_N)| \leq C_R \text{ and}
   \]
   \[
   \sum_R C_R R^{d-1} < \infty
   \]
The following results states that, under reasonable assumptions, a spin system can be interpreted as a phase-shif energy

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

**Γ-convergence:**

$$\Gamma\lim_{\varepsilon} E_\varepsilon(u) = \sum_{i,j} \int_{\partial A_j \cap \partial A_j} \psi(i,j,\nu) \, d\mathcal{H}^{n-1}$$
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: $-1, 0, 1$

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

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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 $u : \mathbb{R}^2 \rightarrow \{-1, 1\}$ and a measure $\mu$ representing the limit concentration of the 0-phase. In these variables the continuum description is as follows.

$$F = F(u, \mu) = \int_{\partial\{u=1\}} \phi\left( \frac{d\mu}{d\mathcal{H}^1|_{\partial\{u=1\}}}, \nu \right) d\mathcal{H}^1 + 2(1 - k)|\mu|(\mathbb{R}^2 \setminus \partial\{u = 1\}),$$
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![Diagram](image)
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Vector spin systems: the XY model
Alicandro-Cicalese ARMA 2009

Nearest-neighbour model

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

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

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

degree 1

degree $-1$

The limit energy is defined on "vortices"

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

for which

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

\[ E_\varepsilon(u) = \sum_{ij} \|u_i - u_j\|^2 = \sum_{ij} \varepsilon^2 \left\| \frac{u_i - u_j}{\varepsilon} \right\|^2 \]

Interpreting \( \frac{u_i - u_j}{\varepsilon} \sim \nabla u \) gives

\[ F(u) = \int |\nabla u|^2 \, dx \quad \text{for } |u| = 1 \]

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

\[ F_\varepsilon(u) = \int \left( |\nabla u|^2 + \frac{1}{\varepsilon} (|u|^2 - 1)^2 \right) \, dx \]

(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 displacement 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!