Variational coarse graining of lattice systems

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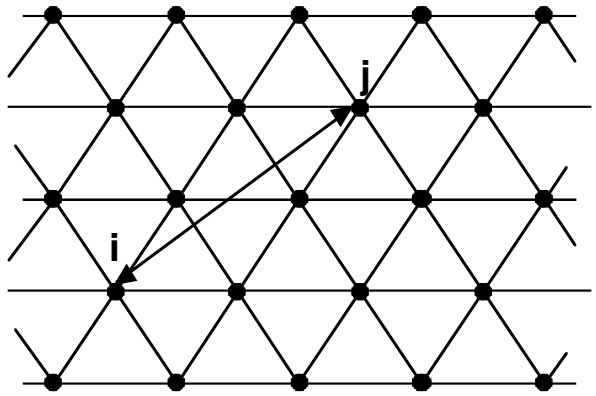
Analysis of complex lattice systems

Starting point:
lattice systems (interactions parameterized on an underlying lattice $\mathcal{L}$)
pair interactions depending on a parameter $u = u_i$ through potentials $f_{ij} = f_{ij}(u_i - u_j)$ (but may be generalized to any n-point interactions)

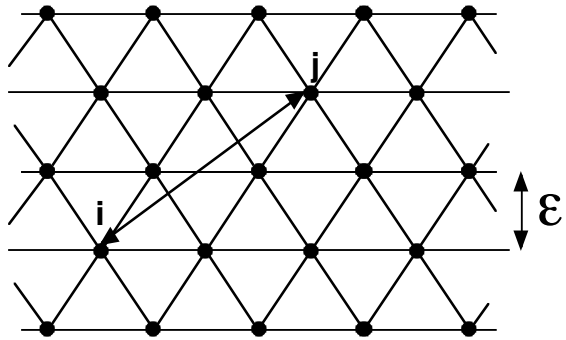


Energies: $E(u) = \sum_{i,j \in \Omega \cap \mathcal{L}} f_{ij}(u_i - u_j)$ (Ω=reference set)

GOAL: description of overall properties of equilibria of E when the number of points contained in Ω is very large.

From discrete systems to continuous variational problems

- **Introduction of a small scaling parameter** ε
- **Scale the lattice** (keeping the reference set Ω fixed)



- **Scale the energy densities** (from f_{ij} to some f_{ij}^{ε}) so that the overall energy retains the relevant features of E

SCALED ENERGIES: $E_\varepsilon(u) = \sum_{i, i \in \Omega \cap \varepsilon\mathcal{L}} f_{ij}^{\varepsilon}(u_i - u_j)$

GOAL: find a **continuous energy** F that describes the main properties of E_ε (as $\varepsilon \to 0$)

Definition of the limit energy

Minimal requirements:

• (**convergence**) fixed ϕ, minimum problems of the type

$$\min\{E_\varepsilon(u) : u = \phi \text{ on } \partial\Omega\}$$

(boundary conditions must be understood properly and can be replaced by other types of conditions) are *approximated* by

$$\min\{F(u) : u = \phi \text{ on } \partial\Omega\}$$

• (“**locality**”) the form of F is independent of Ω (and ϕ)

NOTE: “approximation” means that minimizers $\overline{u}_\varepsilon$ for E_ε are “close” to minimizers $\overline{u}$ of F. To this end an identification of u_ε with piecewise-constant functions is understood, so that a convergence $u_\varepsilon \to u$ is defined.

Gamma-convergence

The two requirements above imply that F is the **Γ-limit** of E_ε. In analytical terms

(1) (*ansatz-free lower bound*) $F(u) \leq \liminf_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon)$ if $u_\varepsilon \to u$

(2) (*existence of recovery sequences*) for all u there exists $u_\varepsilon \to u$ such that $F(u) = \lim_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon)$

This convergence has been introduced by **De Giorgi** in the 1970s and has been extensively applied to integral energies.

Its application to discrete energies is particularly interesting since the definition of the limit parameter u and the scaling of E to obtain E_ε are interlinked with the computation of the Γ-limit.

Example: bulk limit energy

Q.(**elasticity scaling**) Under what scaling law the limit is a bulk energies, i.e., of the form

$$F(u) = F(u, \Omega) = \int_\Omega W(\nabla u)\, dx \quad ?$$

The locality property suggests to look at **scaling properties** of samples with respect to their dimensions

We expect for fixed u

$$F(u, \Omega) \approx |\Omega|$$

e.g. (taking $\Omega = (0, \delta)^d$ – a small sample in macroscopic units) $F(u, (0, \delta)^d) \approx \delta^d$

A variational coarse-graining principle for W:

If $\varepsilon << \delta << 1$ we can transfer back the scaling property of F to E_ε using the convergence of minima : if $\xi = \nabla \overline{u}(x_0)$ (eg $x_0 = 0$)

$$W(\xi) \approx \min\Big\{ \int_{(0,\delta)^d} W(\nabla u)\, dx : u = \xi x \text{ on } \partial(0,\delta)^d \Big\}$$

(note that at that scale $\nabla u \approx \xi$, so that $\phi \approx \xi x$)

$$\approx \min\Big\{ \sum_{i,j \in (0,\delta)^d \cap \varepsilon\mathcal{L}} f_{ij}^{\varepsilon}(u_i - u_j) : u = \xi x \text{ on } \partial(0,\delta)^d \Big\}$$

(write $\delta = T\varepsilon$ and change variables $u = \varepsilon v$)

$$\approx \min\Big\{ \frac{1}{T^d} \sum_{i,j \in (0,T)^d \cap \mathcal{L}} \frac{1}{\varepsilon^d} f_{ij}^{\varepsilon}\big(\varepsilon(v_i - v_j)\big) : v = \xi x \text{ on } \partial(0,T)^d \Big\}$$

Scaling of the energy densities: suggested scaling to reduce from f_{ij}^{ε} to f_{ij}

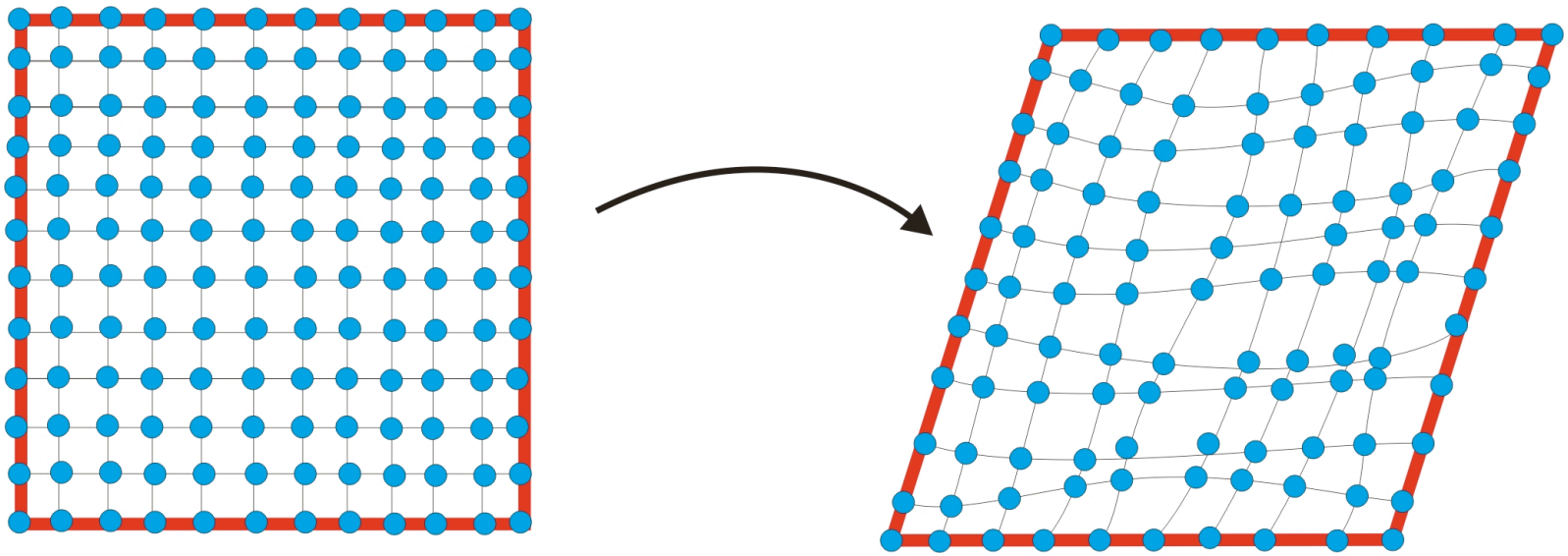
$$f_{ij}^{\varepsilon}(u_i - u_j) = \varepsilon^d \, f_{ij}\left(\frac{u_i - u_j}{\varepsilon}\right) \qquad \text{(if } \Omega \subset \mathbb{R}^d\text{)}$$

In this way the **coarse-graining principle for W** is

$$W(\xi) = \lim_{T\to+\infty} \min\Big\{ \frac{1}{T^d} \sum_{i,j\in(0,T)^d\cap\mathcal{L}} f_{ij}\big(v_i - v_j\big) : v = \xi x \text{ on } \partial(0,T)^d \Big\}$$

(existence of the limit $\Rightarrow$ “ansatz-free coarse graining”)

This is a **homogenization formula**: optimization over oscillations at all micro-scales T with fixed "overall strain" ξ



Application: derivation of elasticity theories from interactions f_{ij} with polynomial growth conditions (Alicandro-Cicalese '04)

Issues of convergence

No restriction on oscillations at microscopic scale
$\Rightarrow$ any competing function v with $v = \xi x$ on the boundary in the formula for W

- Wide range of applicability to convergence of minimum problems (no restriction on ξ)
- Growth restrictions on the function f
- Hard computations

Q. Can we restrict to "regular patterns" for test functions? (**Cauchy-Born rule**)

In general **no** (e.g. Friesecke-Theil '02 example – periodic ground states for NNN interactions on a square lattice. For analysis of the CB rule see E-Ming '07)

Restricted theories

Assumptions on the convergence of minimizers u_ε
$\Rightarrow$ different sets of test functions v in minimum problems
$\Rightarrow$ different forms of W
$\Rightarrow$ different range of applicability

Strong convergence $\Rightarrow$ only competing function $v = \xi x$
(**(strict) Cauchy-Born rule**) (see e.g. Blanc-Le Bris-Lions '02).
• No restriction on the function f
• Easier computations
• Smaller range of applicability to convergence of minimum problems

A COMPROMISE: **Small oscillations at microscopic scale**
$\Rightarrow$ Lipschitz bound on competing function $v = \xi x \Rightarrow$ **(weak) Cauchy-Born rule** (see e.g. Friesecke-James '00, Schmidt '08)

A different scaling: interfacial limit energy

In this case $F(u, \Omega)$ scales as a surface area.

Scaling:

$$f_{ij}^{\varepsilon}(u_i - u_j) = \varepsilon^{d-1} f_{ij}\left(\frac{u_i - u_j}{\varepsilon}\right)$$

Particular case: Phase-transition limits. F is defined on functions $u : \Omega \to \{\pm 1\}$ (a parametrization of two preferred phases) and

$$F(u) = \int_{\Omega \cap S(u)} \varphi(\nu)\, d\mathcal{H}^{d-1} \quad \text{where} \quad S(u) = \partial\{u = 1\}$$

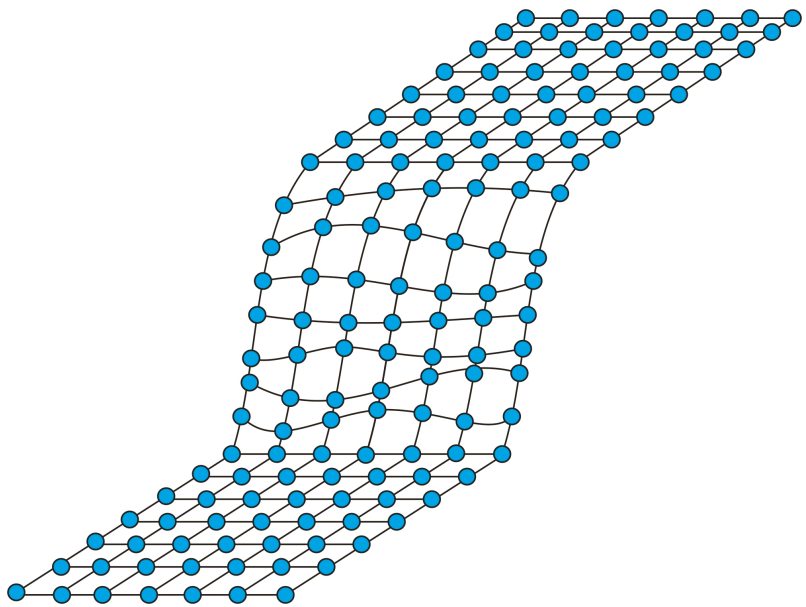
(phase boundary) ν = normal to $S(u)$

A variational coarse-graining principle for φ:

in 1D φ = surface tension constant, given by

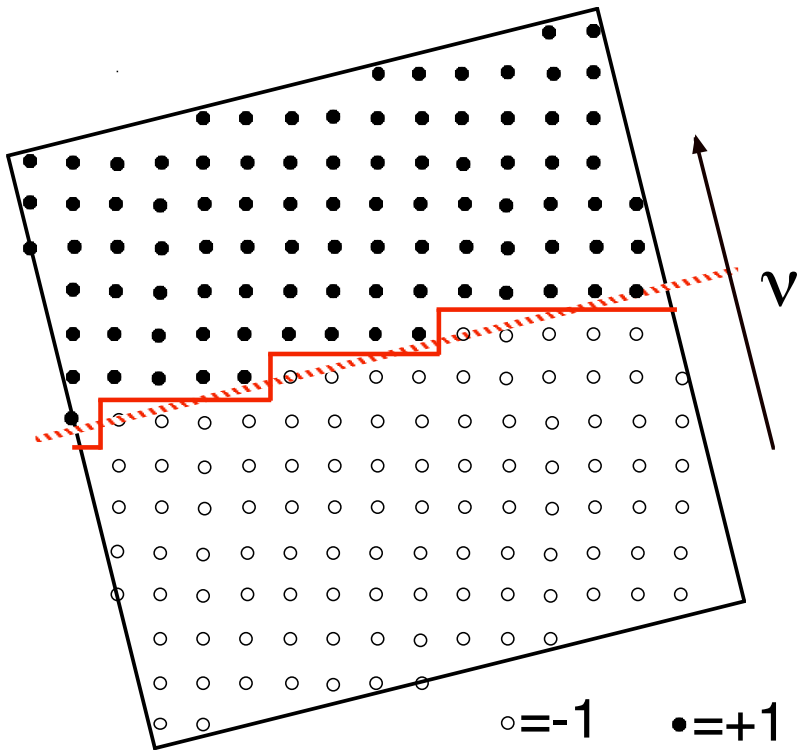
$$\varphi = \min\Big\{ \sum_{i,j\in\mathbf{Z}} f_{ij}(v_i - v_j) : v(-\infty) = -1,\ v(+\infty) = 1 \Big\}$$

(**optimal-profile problem**)
In dimension d the minimum problem is among transitions v from -1 to 1 oriented with ν on cubes of side-lenght $T \to +\infty$



Range of applications:

- *high-order analysis* of non-convex discrete systems: here ± 1 represent a parametrization of two "wells" of the energy computer using the bulk variational principle
- "spin systems" ($u_i \in \{\pm 1\}$): $\psi(\nu)$ **optimal-interface problem**



(connections with Statistical Mechanics, Percolation)

Multiscale analysis

The examples above are an **over-simplified view**.

Some general issues:

• **more scales** are present at the same time $\Rightarrow$ **iteration of Γ-convergence** to obtain a **development** or **expansion**

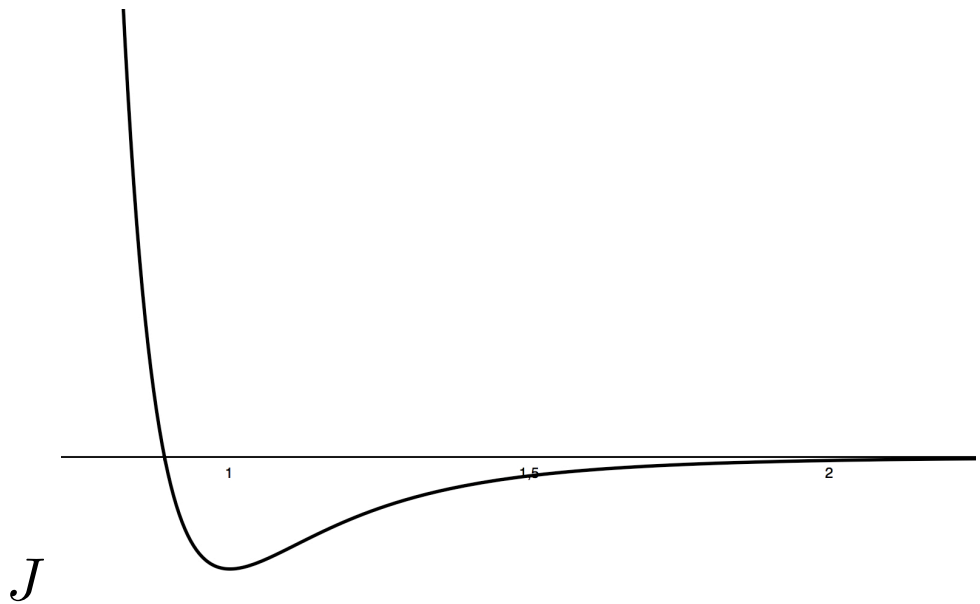
• a single **macroscopic scaling** may result from **superposition of microscopic effects** $\Rightarrow$ **separation of scales** must be described

• the **relevant macroscopic order parameter** is part of the unknown $\Rightarrow$ derivation of the order parameter by looking at **ground states**

Example of expansions: fracture from Lennard Jones interactions

Equilibrium configurations linked to the energy

$$\sum_{i \neq j} J(|u_i - u_j|) \qquad J \text{ Lennard-Jones potential}$$

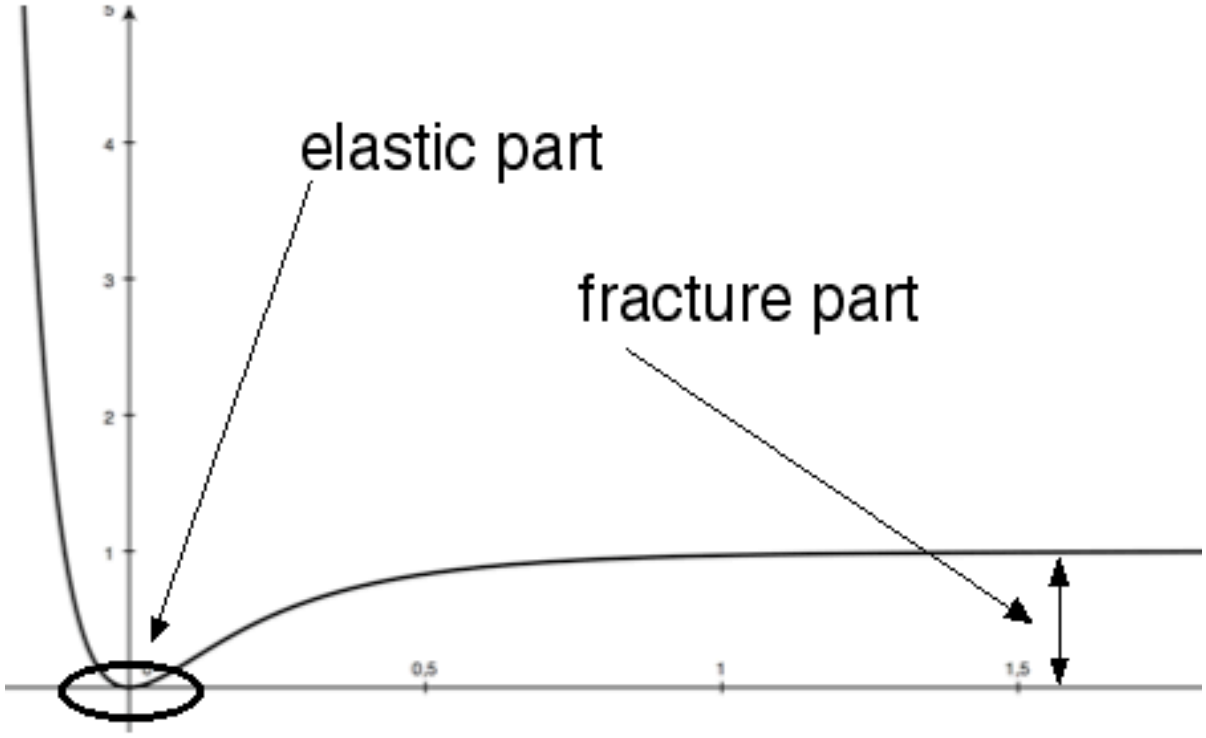


u_i = position of the i-th atom; (number of atoms $\to +\infty$)

Derivation of bulk and surface energies

Two regimes:

(after translation of J in 0)

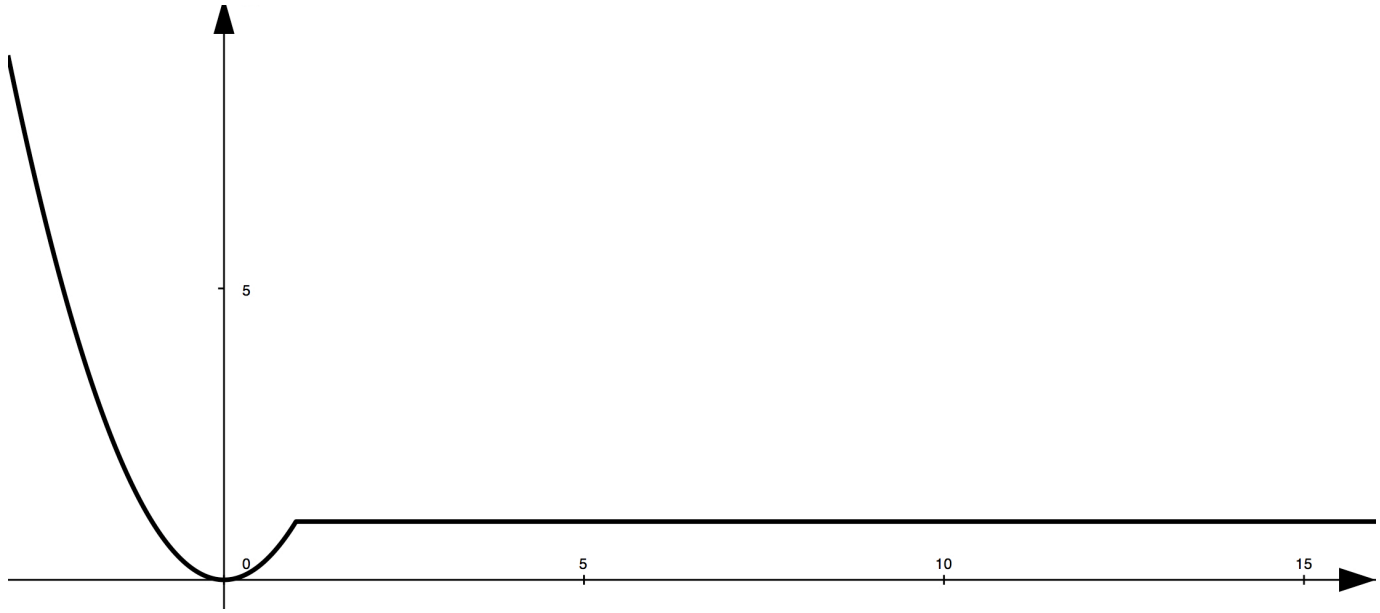


Note: surface and bulk scalings are different

A comparison energy: Blake-Zisserman model in Computer Vision

$$\Psi_\varepsilon(z) = \begin{cases} \min\left\{z^2, \frac{1}{\varepsilon}\right\} & \text{if } z > 0 \\ z^2 & \text{if } z \leq 0 \end{cases}$$

1D analysis (atomic chain)

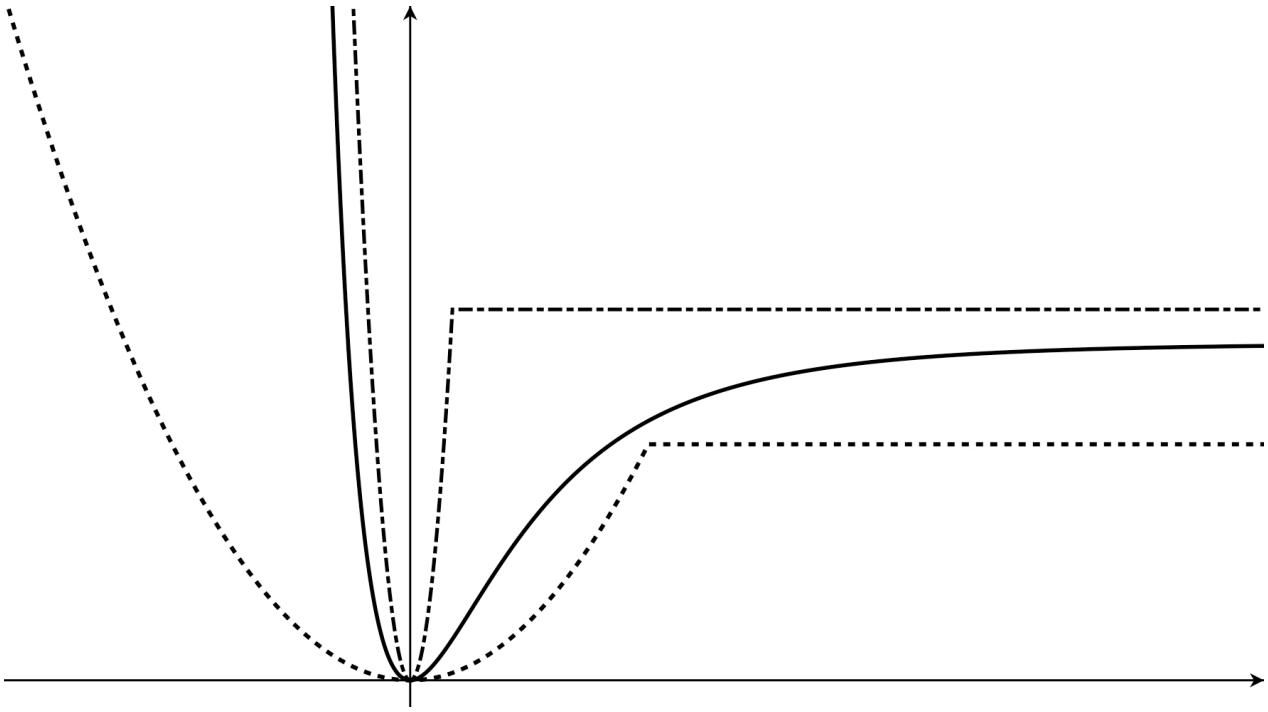


Γ-limit: $\int |u'|^2\, dt + \#(S(u))$ $\qquad u^+ > u^-$ on $S(u)$

(*Griffith brittle fracture energy with unilateral constraint* - Chambolle 1993)

‘Universal form’ of the Blake-Zisserman energy

Analysis by comparison with (scaled) Blake-Zisserman energies:



$$\min\Big\{\alpha' z^2, \beta'\Big\} \leq J(z) \leq \min\Big\{\alpha'' z^2, \beta''\Big\} \qquad (z > 0)$$

NOTE: $\sup \alpha' = \inf \alpha'' = \frac{1}{2} J''(0) =: \alpha$ (Taylor expansion at 0)

$\sup \beta' = \inf \beta'' = J(+\infty) =: \beta$ (depth of the well)

Scaling argument to recover Griffith fracture (B-Lew-Ortiz '06):

$$\min\Big\{\alpha' z^2, \frac{\beta'}{\varepsilon}\Big\} \le \frac{1}{\varepsilon}\, J(\sqrt{\varepsilon} z) \le \min\Big\{\alpha'' z^2, \frac{\beta''}{\varepsilon}\Big\}$$

Change of variables ('linearization' around 0) $u = \sqrt{\varepsilon}\, v$

$$\begin{aligned}
E_\varepsilon(u) &= \sum_i \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) = \varepsilon \sum_i \varepsilon \cdot \frac{1}{\varepsilon} J\Big(\sqrt{\varepsilon}\frac{v_i - v_{i-1}}{\varepsilon}\Big) \\
&\approx \varepsilon\Big(\alpha \int |v'|^2\, dt + \beta \#(S(v))\Big) \\
&= \varepsilon\Big(\alpha \int \Big|\frac{u'}{\sqrt{\varepsilon}}\Big|^2\, dt + \beta \#(S(u))\Big) \\
&= \alpha \int |u'|^2\, dt + \varepsilon\beta \#(S(u)) \qquad \text{(with } u^+ > u^-\text{)}
\end{aligned}$$

Differences from the bulk/surface scalings

New scaling argument

In this case a 'linearization' argument is combined with the scaling

$$f^{\varepsilon}(z) = f(\sqrt{\varepsilon} z)$$

Different form of the limit

The limit energy retains the small parameter ε (Γ-expansion, B-Truskinovsky '08)

$$F(u) = \alpha \int |u'|^2 \, dt + \varepsilon \, \beta \#(S(u)) \qquad \text{(with } u^+ > u^- \text{)}$$

(*Griffith fracture energy with an internal parameter*)

Separation of scales

The macroscopic behavior can result from the superposition of micro/meso-scopic effects.

Example (NNN interactions for non-convex energies)

(B Gelli '02) Bulk scaling for a $1D$ energy

$$E_\varepsilon(u) = \sum_i \varepsilon f_1\left(\frac{u_{i+1}-u_i}{\varepsilon}\right) + \sum_i \varepsilon f_2\left(\frac{u_{i+1}-u_{i-1}}{\varepsilon}\right)$$

The Γ-limit is of the form

$$\int W(u')\,dt$$

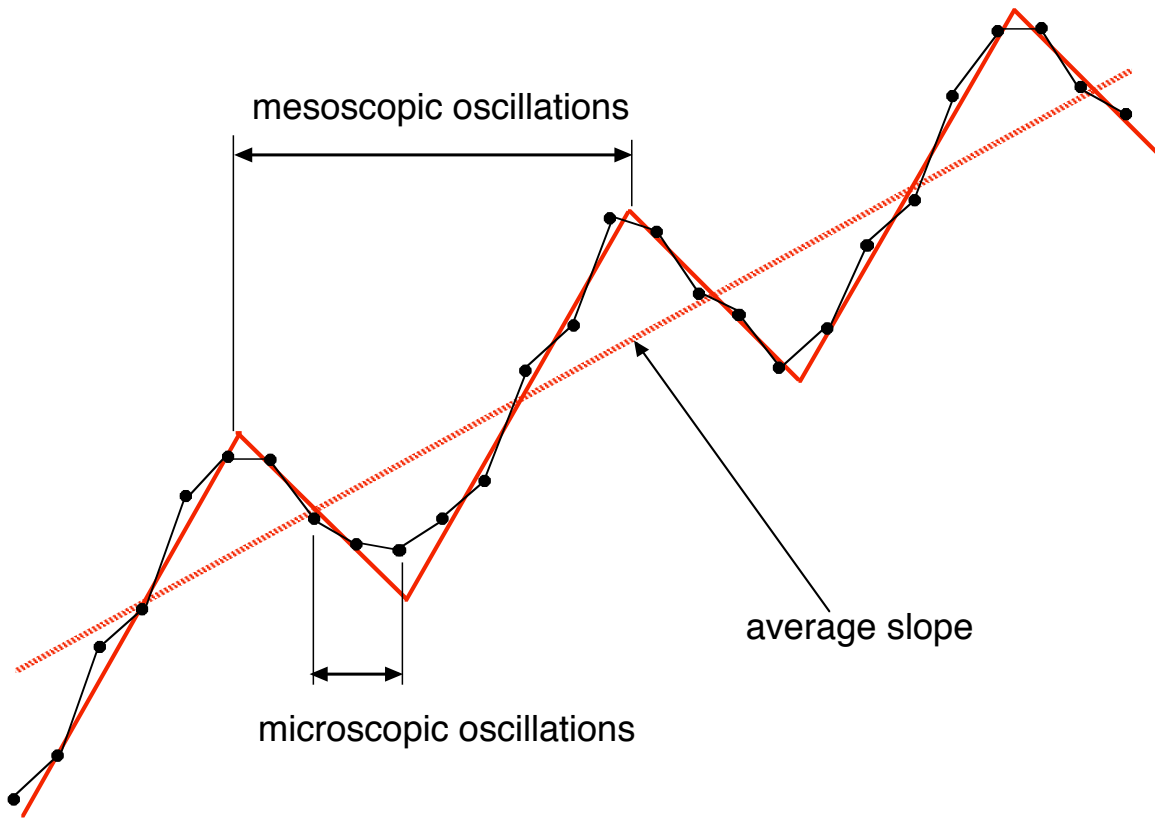
The homogenization formula for W can be simplified by separating the two effects:

- microscopic optimization
- mesoscopic relaxation

1) optimization of the effect of first-neighbors

$$f_{\text{eff}}(z) = f_2(2z) + \frac{1}{2}\min\{f_1(z_1) + f_1(z_2) : z_1 + z_2 = 2z\}$$

(note that f_{eff} may be more wiggly than f_1 and f_2)
2) optimization of mesoscopic oscillations: W=convex envelope of f_{eff}



Note: in this case the development reads as

$$\int f_{\text{eff}}(u')\,dt + C\varepsilon^2 \int |u''|^2\,dt$$

(high-order term accounting for interfacial energy)
(B-Cicalese '06)

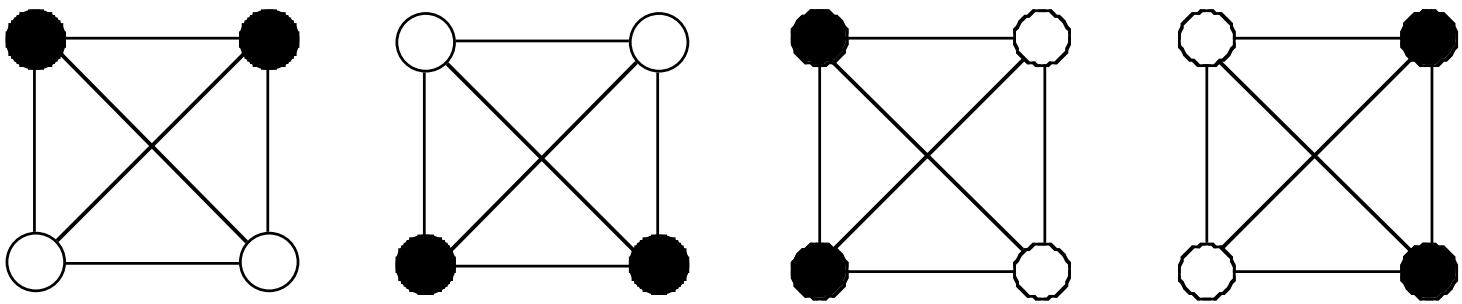
Similar multi-scale arguments:
collective behavior of dislocations
pinning effects, etc

Examples of order parameters from ground states

1) **Anti-ferromagnetic spin systems in 2D**
(B-Alicandro-Cicalese '06)

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

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



(representation in the unit cell)

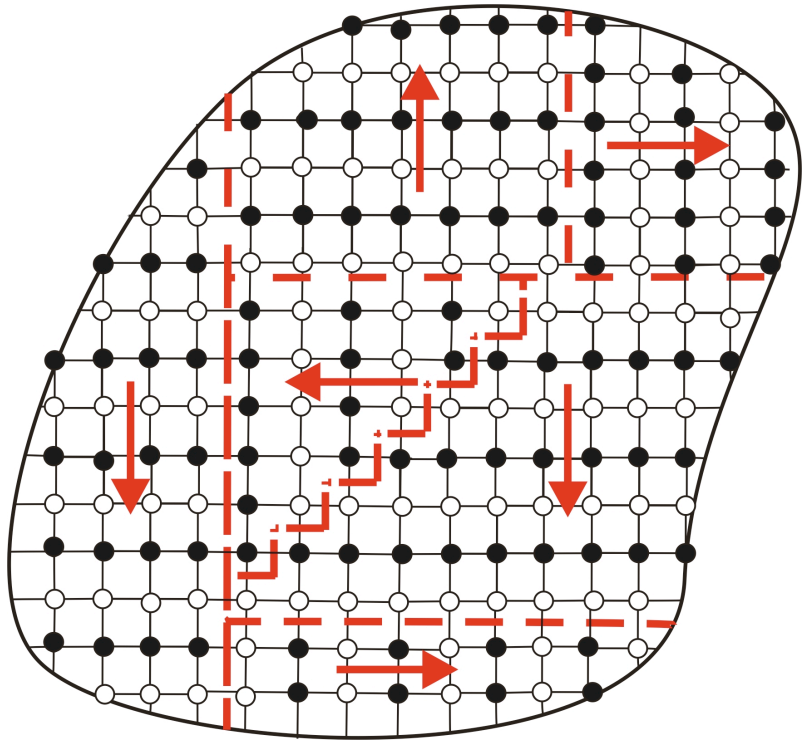
The correct order parameter is the **orientation** $v \in \{\pm e_1, \pm e_2\}$ of the ground state.

Surface-scaling limit

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

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

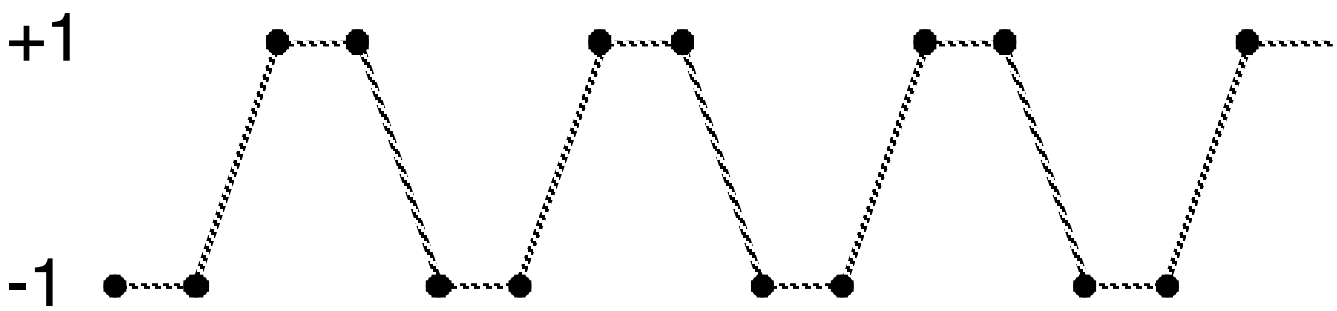
Microscopic picture of a limit state with finite energy



2) **Ferromagnetic-anti-ferromagnetic spin systems in 1D** (same form)

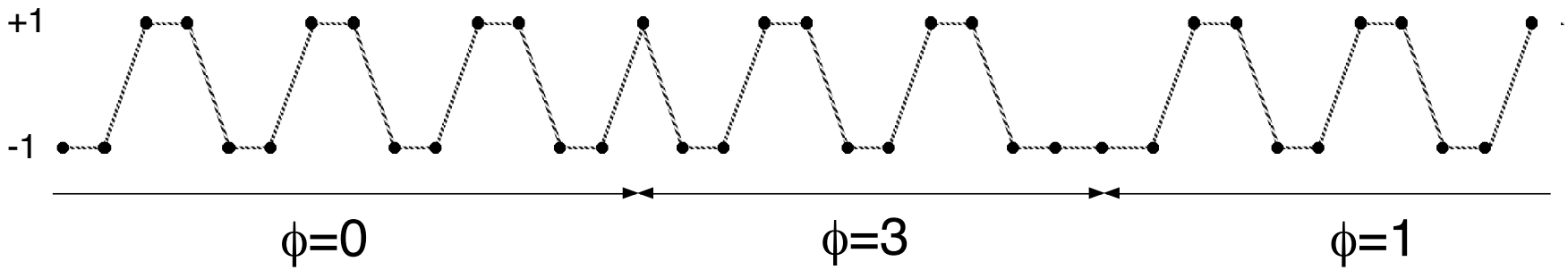
$$E(u) = -c_1 \sum_{NN} u_i u_j + c_2 \sum_{NNN} u_k u_l \qquad u_i \in \{\pm 1\}$$

For suitable positive c_1 and c_2 the ground states are 4-periodic



The correct order parameter is the **phase** $\phi \in \{0, 1, 2, 3\}$ of the ground state.

Surface-scaling limit



$$F(\phi) = \sum_{t \in S(\phi)} \psi(\phi^+(t) - \phi^-(t))$$

defined on $\phi : \Omega \to \{0, 1, 2, 3\}$

$S(\phi)$ = phase-transition set

ψ given by an optimal-profile problem

Conclusions

We have a number of variational coarse-graining principles for lattice energies based on

- scaling properties
- study of ground states
- multi-scale analysis via developments
- separation of scales arguments

These arguments are flexible and can be adapted to lattice-like environments (e.g. random lattices, layered lattices, quasicrystals), adding long-range interactions (non-local limit functionals) and taking into account also (to some extent) dynamic problems.

Do they give a complete enough picture ?
Comparison needed with experiments, numerical simulations, etc.