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Multi-scale Problems for Lattice Systems

Multi-scale Problems in Sustainable Resource Management
The Royal Netherlands Academy of Arts and Sciences

September 9, 2010

Discrete system: with discrete variables $u = \{u_i\}$ indexed on a lattice (e.g., $\Omega \cap \mathbf{Z}^d$)

Discrete energy: (e.g., pair interactions)

$$E(u) = \sum_{ij} f_{ij}(u_i, u_j)$$

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Effective continuous theory: obtained by Γ-limit as $\varepsilon \to 0$.

B. Γ-convergence for Beginners, OUP 2002
B. Handbook of Γ-convergence (Handbook of Diff. Eqns, Elsevier, 2006)

Fine multi-scale effects occur even for the simplest discrete systems.
Starting example:

Cubic lattice: variables parameterized on $\Omega \cap \mathbf{Z}^d$

Binary systems: variable taking only **two values**; wlog $u_i \in \{-1, 1\}$ (spins).

Nearest-neighbour interactions: the energies depend only on (u_i, u_j) with $|i - j| = 1$.

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Only two possible energies (up to affine change of variables):

$$E(u) = E_{\rm ferr}(u) = -\sum_{\rm NN} u_i u_j \qquad \text{(ferromagnetic energy)}$$

(with two trivial minimizers $u_i \equiv 1$ and $u_i \equiv -1$)

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Note: the change of variables $v_i = (-1)^i u_i$ is such that $E_{\rm anti}(v) = E_{\rm ferro}(u)$, so actually we have only one energy

BINARY SYSTEMS: Continuous limits of ferromagnetic energies

Bulk scaling: (mixtures of ground states)

$$E_\varepsilon(u) = -\sum \varepsilon^d u_i u_j \longrightarrow \int_\Omega \psi(u)\,dx, \quad \text{with} \quad \psi(u) = \begin{cases} -1 & \text{if } -1 \le u \le 1 \\ +\infty & \text{otherwise} \end{cases}$$

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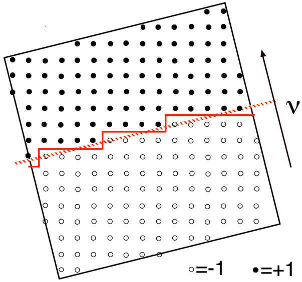
Surface scaling: (crystalline perimeter) $u \in BV(\Omega; \{\pm 1\})$

$$E_\varepsilon(u) = \sum \varepsilon^{d-1}(1 - u_i u_j) \longrightarrow 2\int_{\Omega \cap \partial\{u=1\}} \|\nu\|\, d\mathcal{H}^{d-1}, \quad \text{with} \quad \|\nu\| = \sum_k |\nu_k|$$



Equivalent Cahn-Hilliard Theory: the analysis above shows that

$$-\sum \varepsilon^d u_i u_j \sim \int_\Omega \psi_{\mathrm{eff}}(u)\,dx + \varepsilon^2 \int_\Omega \|\nabla u\|^2\,dx$$

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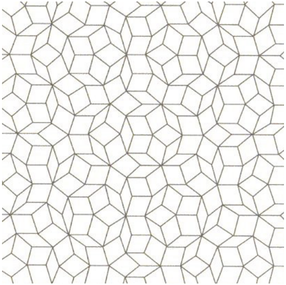
Equivalent Ginzburg-Landau Theory/screw dislocations: a similar expansion holds for the $2D$ **vector case**: $d = 2$ and $u_i \in S^1 \subset \mathbb{R}^2$ and

$$-\sum \varepsilon^d \langle u_i, u_j\rangle \sim \int_\Omega \psi_{\rm eff}(u)\,dx + \varepsilon^2 \int_\Omega |\nabla u|^2\,dx$$

($\psi_{\rm eff}$ a suitable two-well energy with minima in S^1), but the relevant scaling is $\varepsilon^2|\log\varepsilon|$, in which case we have **vortices** (**Alicandro-Cicalese, ARMA 2009**). This formulation is 'dual' to screw-dislocation energies (**Alicandro-Cicalese-Ponsiglione, Indiana UMJ 2010**)

With the due changes the process can be repeated on more general periodic lattices (e.g. triangular, exagonal, FCC, BCC, etc.); even though we do not have in general a duality between ferro- and anti-ferromagnetic energies (**frustration**).

Techniques must be refined to take care of **a-periodic lattices** (e.g. Penrose tilings or quasicrystals)



(B-Solci M^{3}AS 2010)

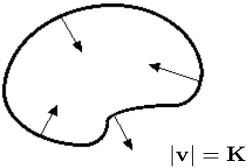
Continuous "flows" of the perimeter

Motion is obtained by introducing a discrete time-step τ, define a time-discrete motion by successive minimizations for fixed τ, and pass to the limit as $\tau \to 0$

Perimeter-driven motion of sets

$\Downarrow$

motion by mean curvature
(Almgren-Taylor-Wang SIAM J.Control.Optim. 1983)



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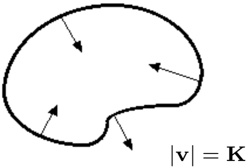
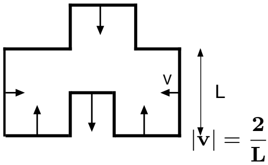


Crystalline perimeter-driven motion of sets

$\Downarrow$

motion by crystalline mean curvature
(**Almgren-Taylor J.Diff.Geom. 1995** in 2D)



Pinning/depinning transition: **(B-Gelli-Novaga ARMA 2009)** We follow the Almgren-Taylor-Wang scheme letting $\varepsilon, \tau \to 0$ at the same time.

- For $\tau << \varepsilon$ the motion $E(t)$ is trivial (**pinning**):

$$E(t) = E_0$$

for all (sufficiently regular) bounded initial sets E_0;

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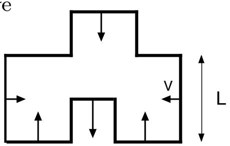
• At the **critical scale** $\tau = \alpha\varepsilon$ we have **'quantized' cristalline motion**

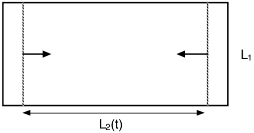


$$|\mathbf{v}| = \frac{\mathbf{1}}{\alpha}\left\lfloor \frac{\mathbf{2}\alpha}{\mathbf{L}} \right\rfloor$$

Discreteness effects at the critical scale

(i) (**critical pinning side length**) If all $L > 2\alpha$ then the motion is trivial: $E(t) = E_0$;

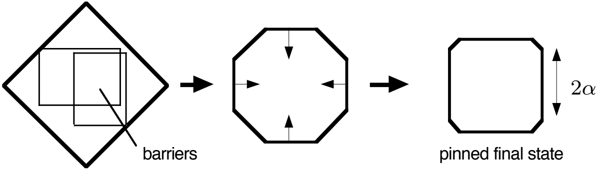
(ii) (**partial pinning and non strict inclusion principle**; e.g for rectangles) If $L_1 < 2\alpha$ and $L_2 > 2\alpha$ only one side is (initially) pinned



(iii) (**quantized velocity**)
$2\alpha/L(t) \notin \mathbb{N} \Rightarrow$ velocity integer multiple of $1/\alpha$;

(iv) (**non-uniqueness**)
$2\alpha/L(t) \in \mathbb{N} \;\Rightarrow\;$ velocity not uniquely determined $\;\Rightarrow\;$ non-uniqueness

(v) (**non-convex pinned sets**)
(vi) (**pinning after initial motion**)



Coming back to the **static framework**, within binary systems ($u \in \{\pm 1\}$) we may have more complex interactions:

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

Conditions of the type
- (**uniform minimal states**) $\sigma_{ij} \geq 0$
- (**coerciveness conditions**) $\sigma_{ij} \geq c > 0$ for $|i - j| = 1$
- (**decay conditions**) $\sum_j \sigma_{ij} \leq C < +\infty$ for all i

guarantee that (up to subsequences)

$$\sum_{ij} \varepsilon^{d-1} \sigma_{ij}(1 - u_i u_j) \longrightarrow \int_{\Omega \cap \partial\{u=1\}} \varphi(x, \nu)\, d\mathcal{H}^{d-1}$$

i.e., the limit is still a (possibly inhomogeneous) interfacial energy.

The integrand φ is determined by a family of discrete (non-local) minimal-surface problems. In the $2D$ case and if only nearest-neighbours are considered ($\sigma_{ij} = 0$ if $|i - j| > 1$) equivalently it is given by an **asymptotic distance** on the lattice $\mathbb{Z}^2$ (where the distance between the nodes i and j is σ_{ij}) (**B-Piatnitsky 2010**)

Non-coercive spin systems (only $\sigma_{ij} \geq 0$). We may consider ω a realization of an **i.i.d. random variable** in $\mathbb{Z}^2$, and the corresponding energy

$$E^\omega(u) = -\sum_{i,j} \sigma^\omega_{ij} u_i u_j \qquad \text{with} \qquad \sigma^\omega_{ij} = \begin{cases} 1 & \text{with propability } p \\ 0 & \text{with propability } 1-p \end{cases}$$

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Percolation Theorem (B-Piatnitsky 2010)

In the surface scaling, the Γ-limit F_p of E^ω_ε is a.s.

(1) $F_p(u) = 0$ on all $u \in L^1(\Omega; [-1,1])$ for $p \leq 1/2$

(2) $F_p(u) = \displaystyle\int_{\Omega \cap \partial\{u=1\}} \varphi_p(\nu)\, d\mathcal{H}^1$ for $p > 1/2$

The limit is deterministic and $\varphi_p(\nu)$ is given by a *first-passage percolation* formula for $p > 1/2$.

Deterministic toy problem: discrete 'perforated domain'; the case $p > 1/2$ corresponds to well-separated 'holes'; i.e., where $\sigma_{ij} = 0$.

Interactions with changing sign

Ferromagnetic/antiferromagnetic interactions: an **open problem** is when

$$E^\omega(u) = -\sum_{i,j} \sigma^\omega_{ij} u_i u_j \qquad \text{with} \qquad \sigma^\omega_{ij} = \begin{cases} 1 & \text{with propability } p \\ -1 & \text{with propability } 1-p \end{cases}$$

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Deterministic 'toy' problem (for the case $p \sim 0$): discrete 'perforated domain' with well-separated 'holes' where $\sigma_{ij} = -1$ (**B-Piatnitsky 2010**). In this case

- need **stronger separation conditions** between the perforations
- the Γ-limit may be still described by an interfacial energy $\displaystyle\int_{\Omega\cap\partial\{u=1\}} \varphi(\nu)\, d\mathcal{H}^1$

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($\Longrightarrow$ probabilistic approach beyond percolation theory)

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Note: when $0 < p < 1$ it is not even clear what should be the **correct parameter** in the limit

When not only nearest neighbours are taken into account we do not have a correspondence between ferromagnetic and anti-ferromagnetic energies.

1) **Anti-ferromagnetic spin systems in 2D** **(B-Alicandro-Cicalese NHM 2006)**

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

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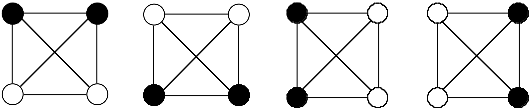
(NNN = next-to-nearest neighbours)
For suitable positive c_1 and c_2 the ground states are 2-periodic



(representation in the unit cell)

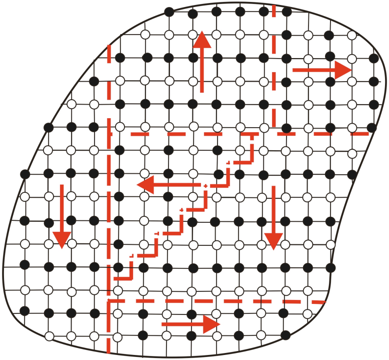
The correct order parameter is the **orientation** $v \in \{\pm e_1, \pm e_2\}$ of the ground state.

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

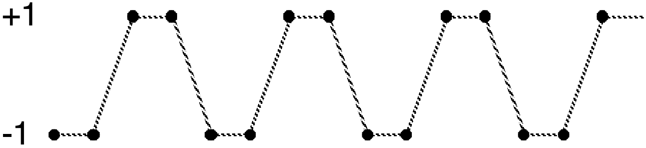
Microscopic picture of a limit state with finite energy



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

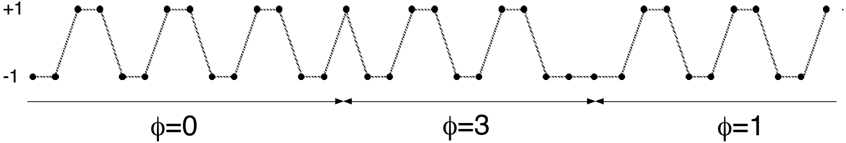
$$E(u) = -c_1 \sum_{\mathrm{NN}} u_i u_j + c_2 \sum_{\mathrm{NNN}} u_k u_l \qquad u_i \in \{\pm 1\}$$

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



Γ-limit of the form

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

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

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

ψ given by an optimal-profile problem

Higher-dimensional analog

We can consider e.g. two-dimensional systems with NN, NNN, NNNN (next-to-next-...) interactions, $u_i \in \{\pm 1\}$ and

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

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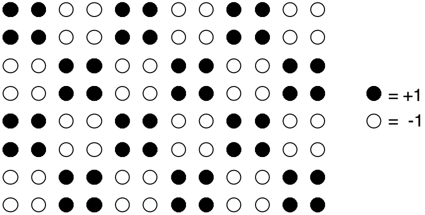
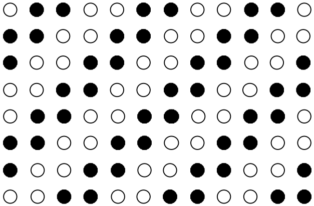
For suitable c_1 and c_2 again we have a non-trivial 4-periodic ground state



but also...



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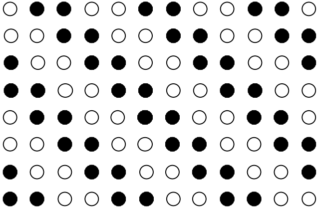
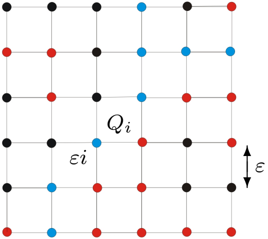


(counting translations 16 different ground states)
and a description for the surface-scaling Γ-limit combining the two previous examples

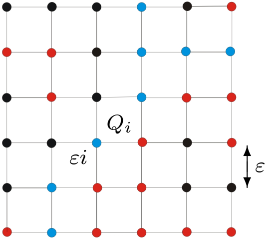


Three phases: $-1, 0, 1$

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

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

Ternary Systems: the Blume-Emery-Griffith model



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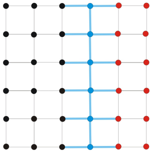
The description of the limit depends on the positive parameter k.
We focus on the case

$$\frac{1}{3} < k < 1$$

for which a **richer continuous description** is possible (the other cases are treated as in the binary case)

If $\dfrac{1}{3} < k < 1$ then

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



(Surface) scaling:

$$E_\varepsilon(u) = \sum_{\mathrm{NN}} \varepsilon(k((u_i u_j)^2 - 1) - u_i u_j + 1)$$

Blume-Emery-Griffiths Model

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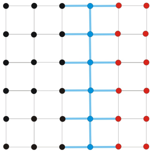

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New variables (to keep track of the 0-phase)

$$I_0(u) := \{i : u_i = 0\}; \qquad \mu(u) := \sum_{i \in I_0(u)} \varepsilon \delta_i .$$

$$E_\varepsilon(u, \mu) = \begin{cases} E_\varepsilon(u) & \text{se } \mu = \mu(u) \\ +\infty & \text{otherwise} \end{cases}$$

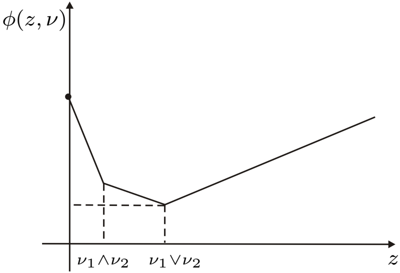
(E_ε are equi-coercive in (u, μ))

Surfactant energies as a continuous limit of the BEG model

Theorem (Alicandro-Cicalese-Sigalotti 2010)

$$E_\varepsilon(u,\mu) \xrightarrow{\Gamma} E(u,\mu) = \int_{\Omega\cap\partial\{u=1\}} \phi\Big(\frac{d\mu}{d\mathcal{H}^1\lfloor_{\partial\{u=1\}}}, \nu\Big) d\mathcal{H}^1 + 2(1-k)|\mu|(\overline{\Omega}\setminus\partial\{u=1\}),$$

$$u \in BV(\Omega;\{\pm 1\})$$



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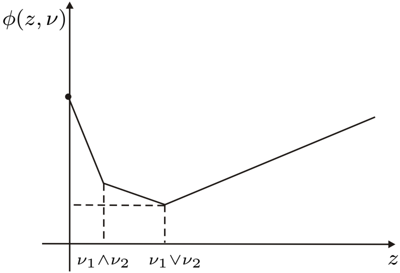

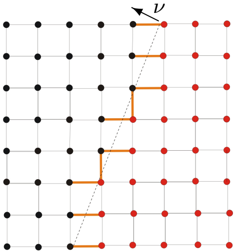

Surfactant energies as a continuous limit of the BEG model

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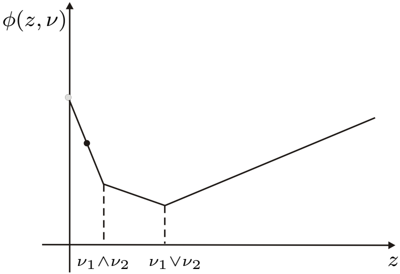

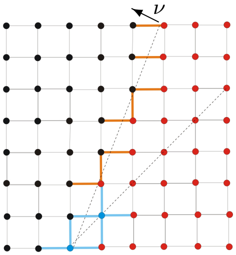

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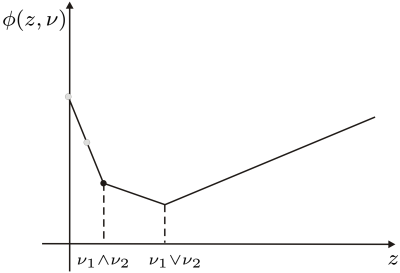

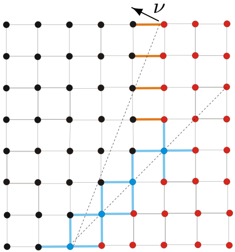

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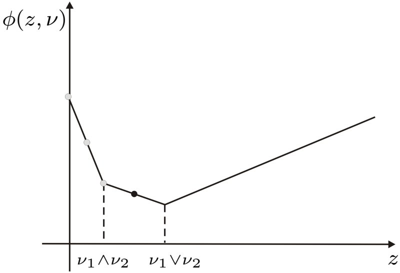

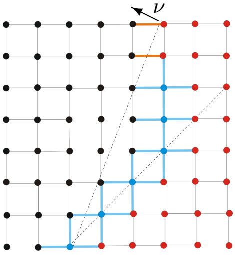

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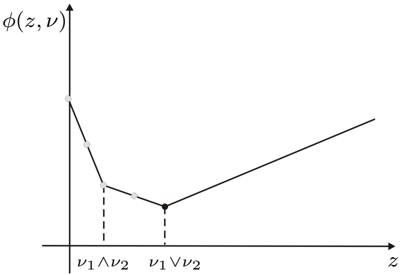

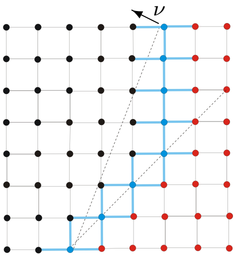

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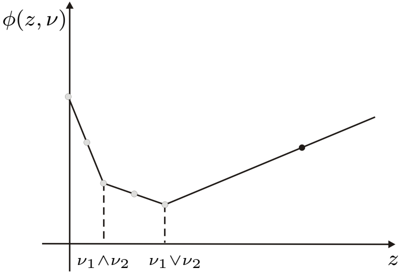

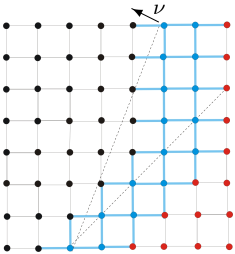

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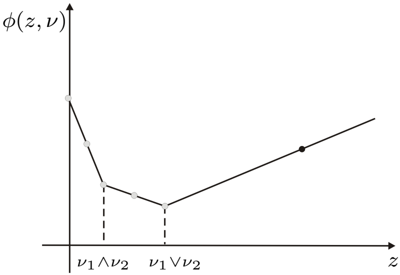

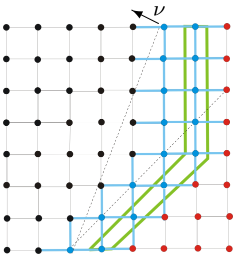

CONCLUSIONS

• As a limit of very simple discrete systems we have obtained: sharp interface energies, Cahn-Hilliard theories, multi-phase vector functionals, energies on pairs set/measure, etc. with links to homogenization, Ginzburg-Landau theory, percolation issues, Statistical Mechanics, etc.

• Such discrete-to-continuous approach allows to 'justify' continuous theories from simple atomistic or 'molecular' models

• At the same time it provides a possible simple approximation of a rich zoo of target continuous energies via lattice systems, or vice versa