Models of Discrete Thin Films

Andrea Braides (Roma *Tor Vergata*)

Workshop: New Challenges for the Calculus of Variations Stemming From Problems in the Materials Sciences and Image Processing

In Honour of the 60th Birthday of Irene Fonseca

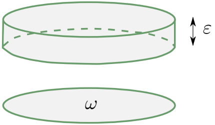
CRM, Montreal, May 17 2016

My first encounter with Irene (possibly) in the early '90s

In the 1990s we lived parallel mathematical lives, working on similar problems but never really interacting, then, finally, collaboration started in 1998 at the Max-Planck Institute in Leipzig!

Elastic Thin Films

Irene explained to me the problem of dimension-reduction.
For those who may not know, it consists in looking at objects with one (or more) dimension smaller than others. In picture, for example in 3D



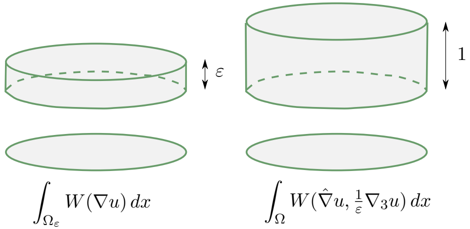
the "small domain" is $\Omega_\varepsilon = \omega \times (0, \varepsilon)$ ($\omega \subset \mathbb{R}^2$) with thickness ε.

For (homogeneous) elastic thin films we have (scaled) energies

$$F_\varepsilon(u) = \frac{1}{\varepsilon^\alpha} \int_{\Omega_\varepsilon} W(\nabla u)\, dx \qquad u : \Omega_\varepsilon \to \mathbb{R}^3$$

with W an energy function with p-growth ($p > 1$)
In the case is $\alpha = 1$ we expect a membrane theory on ω
(varying α, a hierarchy of theories; cf. Friesecke, James, Müller)

Scaling to a common domain $\Omega = \omega \times (0,1)$ we get a family of energies with a degenerate dependence on $\nabla_3 u$.



This allows to conclude that the domain of the limit is some

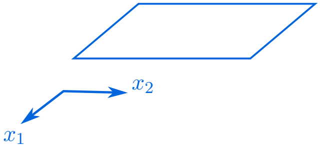
$$W^{1,p}(\omega : \mathbb{R}^3) \sim \{u \in W^{1,p}(\omega : \mathbb{R}^3) : \nabla_3 u = 0\},$$

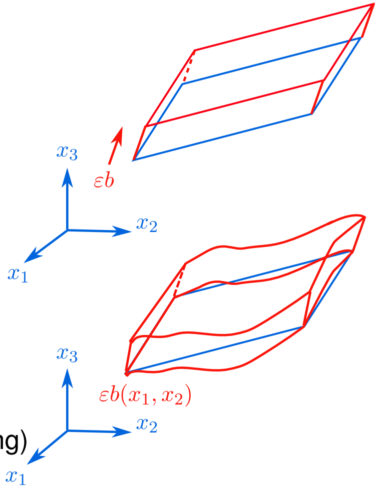
defines a convergence $u_\varepsilon \to u$, and provides a lower bound with

$$\overline{W}(A) = \min\{W(A,b) : b \in \mathbb{R}^3\} \qquad A \in \mathbb{M}^{3\times 2}$$

Le Dret and Raoult (J.Math.Pures Appl.1995) showed that this bound is not sharp since $\overline{W}$ may not be quasiconvex, and the recovery sequence might develop microstructure.

($\overline{W}$ quasiconvex $\Rightarrow b$ constant)





($\overline{W}$ not quasiconvex $\Rightarrow b$ oscillating)

The Le Dret-Raoult relaxation formula: the Γ-limit is given by

$$\int_\omega Q_{3\times 2}\overline{W}(\nabla u)\, dx_1 dx_2$$

where $Q_{3\times 2}$ denotes the 3×2-quasiconvexification (optimization on oscillations).

...but Irene (and Gilles, working with her on the subject) was not happy with this formula since it relies on a very particular geometry and works for homogeneous energies

Our contribution to the theory

AB, I.Fonseca, G.Francfort.
3D-2D Asymptotic Analysis for Inhomogeneous Thin Films.
Indiana Univ. Math. J. 2000

(. . . my *most-cited paper!*, according to MathSciNet. . .)

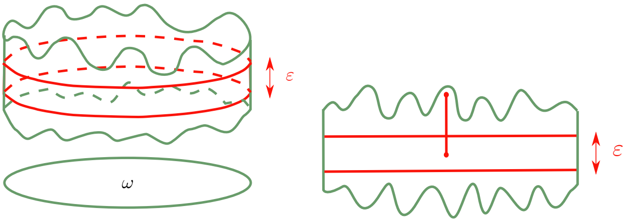
We developed a general method for dimension-reduction, valid for inhomogeneous thin films with possibly varying thickness (with boundary of graph type).

The two (simple but effective) **main ideas** are

• that for the definition of a limit parameter it is sufficient to have a uniform minimal thickness

• the application of the localization method of Γ-convergence on cylindrical sets

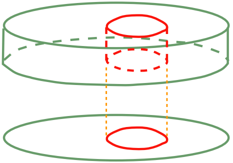
Sufficiency of a uniform minimal thickness



(we first define a limit u on the “normal” thin film, and then deduce that the limit is the correct parameter by using a Poincaré inequality in the vertical direction)

Note. The fact of having a thin film of “graph type” is somewhat necessary to apply this Poincaré argument (cf. Bhattacharya-B. *R.Soc.Lond.Proc. A* 2002)

The localization method of Γ-convergence



(we use cylindrical sets and the fact that the limit u depends only on (x_1, x_2))

This method allows to treat energies on Ω_ε with oscillating profile and W_ε inhomogeneous, concluding the existence (up to subsequences) of a Γ-limit

$$F(u) = \int_\omega \widehat{W}(x_1, x_2, \nabla u) dx_1 \, dx_2$$

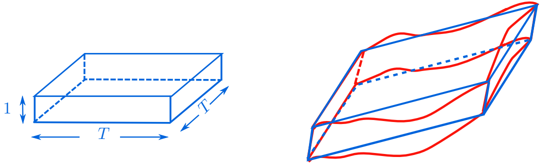
(and, of course, it extends to k-dimensional thin objects in $\mathbb{R}^n$)

A homogenization formula

(e.g., when $W_\varepsilon(x,\xi) = W(x/\varepsilon,\xi)$ and the profile is flat)

$$\widehat{W}(A) = \lim_{T\to+\infty} \frac{1}{T^2} \inf\Big\{ \int_{(0,T)^2\times(0,1)} W(y,\nabla w)dy : \\ w = A(x_1,x_2) \text{ on } (\partial(0,T)^2)\times(0,1) \Big\}$$

This relies on a simple scaling argument by $T = 1/\varepsilon$

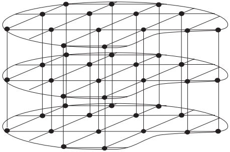


(Note: when $W_\varepsilon = W(\xi)$, this provides an alternative formula for $Q_{3\times2}\overline{W}$)

Discrete Thin Films

The study of thin objects is important in nano-environments, where ε is at the atomic scale.

It seems interesting to study energies directly defined on discrete thin objects; e.g., portions of $\lambda\mathbb{Z}^3$ contained in a “bulky” thin film, as atomistic interaction systems.



In this case the thickness parameter is the number N of “layers”, and $\varepsilon = (N-1)\lambda$.

Connection with continuum theories

Energies defined on "bulky sets"; e.g., on $u : \Omega \cap \lambda\mathbb{Z}^3 \to \mathbb{R}^3$ of the form

$$F_\lambda(u) = \sum_{ij} \lambda^3 \, W_{ij}^\lambda\Big(\frac{u_i - u_j}{\lambda}\Big),$$

with

- W of p-growth
- decay conditions when $|i-j| \to +\infty$
- coerciveness on nearest neighbours

Then we have a compactness theorem with respect to the convergence of the piecewise-constant interpolations $u_\lambda \to u$, obtaining in the limit continuum energies

$$\int_\Omega W(x, \nabla u)\, dx \qquad u : \Omega \to \mathbb{R}^3$$

(Alicandro, Cicalese. *SIAM J. Math Anal* 2004)

Elastic Discrete Thin Films

As a consequence of the "bulky" result if we let first N (the number of layers) diverge, keeping $\varepsilon = \lambda N$ fixed, and then $\varepsilon \to 0$, we obtain the usual continuum thin-film theory.

What about N fixed?

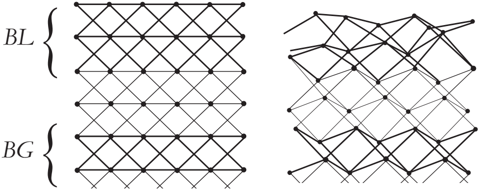
In Alicandro-B-Cicalese (*Calc. Var.* 2008) we considered thin films with W^{λ}_{ij} exactly as above defined in $(\omega \times [0, \lambda N]) \cap \mathbb{Z}^3$, and proved

• the compactness method of BFF can be adapted with the additional difficulty that discrete energies are non-local by nature. Controlled decay conditions allow to prove the locality of the limit, and the representation

$$\int_{\omega} W(x, \nabla u)\, dx_1\, dx_2$$

If W_{ij}^{λ} are translation-invariant (i.e., homogeneous; corresponding to the Le Dret-Raoult case) then

• the limit energy density depends on N (contrary to the continuum case). This is due to a boundary-layer effect giving a surface energy of the same order as the bulk energy

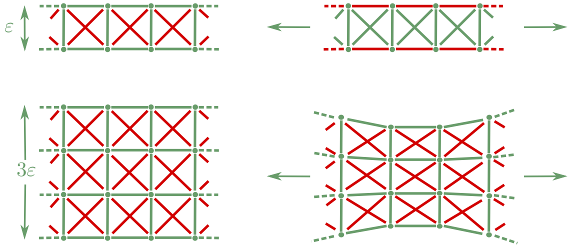


(BL = boundary layer, BG = bulk geometry)

• commutability (under some symmetry conditions); i.e., by letting $N \to +\infty$ we obtain the continuum thin-film limit

(**Open question**: does this hold without symmetry conditions?)

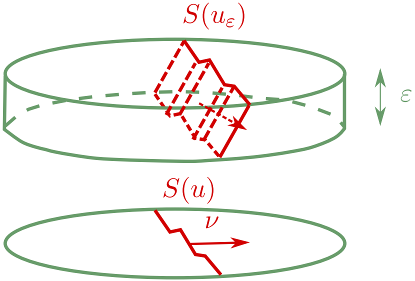
Note: in terms used by Friesecke and Theil, we might have more Cauchy-Born states as N increases



Brittle Thin Films

Back to the continuum setting ...

... Irene and I considered thin films with possibility of fracture (*Appl. Math. Optim.* 2001) in an SBV setting. The passage to the limit is also interesting for interfacial energies only



showing the possibility of oscillations of cracks.

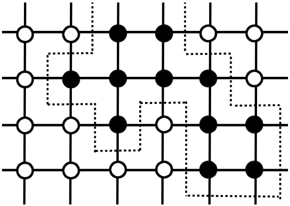
Discrete Interfacial Energies: Spin Systems

Simplest model of discrete interfaces: cubic lattice $\lambda\mathbb{Z}^n$,
$u_i \in \{-1, +1\}$ spin variable ($i \in \mathbb{Z}^n$),

Model energies: (**ferromagnetic interactions**)

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

with the sum running over (i, j) nearest neighbours in $\lambda\mathbb{Z}^n$
(note the scaling by λ^{n-1}(surface scaling))
A spin function $u : \lambda\mathbb{Z}^n \to \{\pm 1\}$ is identified with its
piecewise-constant interpolation $\sim$ set $\{u = 1\}$



Continuous limit: we have

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

We will identify a function $u \in \{\pm 1\}$ with the set $A = \{u = 1\}$
$\Rightarrow$ the limit is a crystalline perimeter

We can consider more general energies

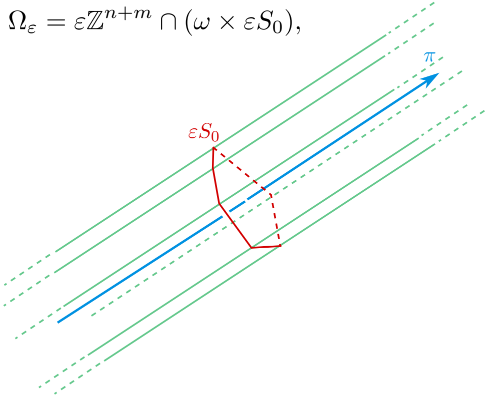
$$E_\lambda(u) = \sum_{(i,j)} \lambda^{n-1} c_{ij}(u_i - u_j)^2$$

($i \in \lambda\mathbb{Z}^n$) with $c_{ij} \geq 0$

Quasicrystalline geometries

For such simple systems we can concentrate on more complex geometries in $\mathbb{R}^{n+m}$; for example, thin objects of the form

$$\Omega_\varepsilon = \varepsilon\mathbb{Z}^{n+m} \cap (\omega \times \varepsilon S_0),$$

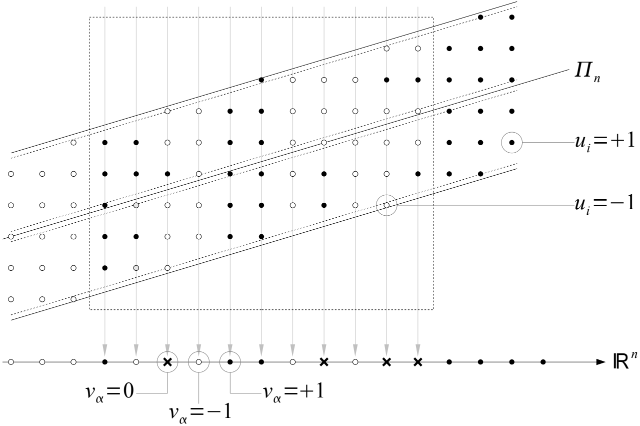


(from now on we may consider the case $\lambda = \varepsilon$, since we do not consider the number of layers N) where $\omega \subset \pi$, $\pi = \Pi_n$ is an n-dimensional linear subspace of $\mathbb{R}^{n+m}$ and S_0 is a subset of the orthogonal complement to π (connected and containing 0 for simplicity)

Note: if $m = 1$ then necessarily S_0 is a segment. Even in that case, the geometry of $\mathbb{Z}^{n+m} \cap (\pi \times S_0)$ has interesting features if the normal to π is not an "integer" direction and its projection on π is often referred to as a quasicrystal. If π is a coordinate hyperplane then we have the "usual" layered thin film.

A refinement of the "projection method" in BFF

We can directly project on a suitable n-dimensional space, up to introducing a "negligible" third phase $u_i = 0$



Surface Energies on Quasicrystals

Proceeding as in BFF (+BF), we obtain the existence of a limit (up to subsequences) that can be written as

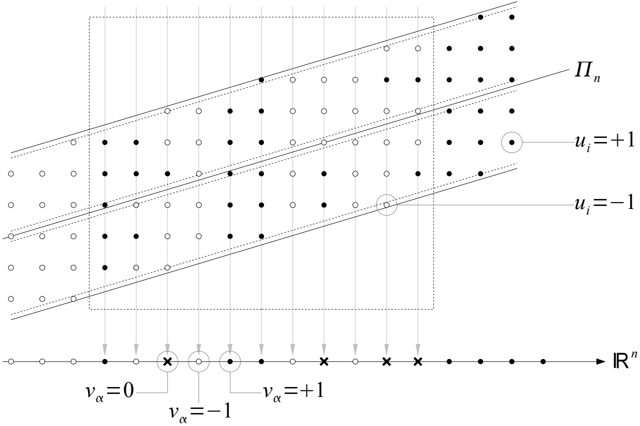
$$\int_\omega \varphi(x,\nu)\,d\mathcal{H}^{n-1}.$$

Homogenization. For nearest-neighbour energies

$$E_\varepsilon(u) = \sum_{(i,j)\in\varepsilon\mathbb{Z}^{n+m}\cap(\omega\times\varepsilon S_0)} \varepsilon^{n-1}(u_i - u_j)^2$$

we expect the limit to be independent of subsequences and homogeneous. This should give a ferromagnetic energy density characteristic of the quasicrystal.

To prove this we may use the homogenization formula, which works if we may find a relatively dense set of translations such that the energy is (almost)-invariant under such translations.



We may use quasiperiodic arguments to find such translations. such that the corresponding geometry is repeated “almost” identical.

Note that in principle the sites that are “misplaced” by translation may give a surface contribution.

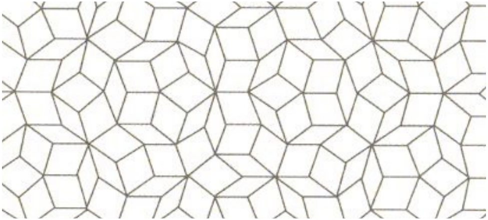
A fine additional argument must be used to describe the geometry of those misplaced” sites. To that end we have to require that S_0 be a polyhedral set
(B-Causin-Solci, *IMA J Appl Math* 2012)

(the contribution of the misplaced sites instead is negligible for “elastic” quasicrystals, for which we have no restriction on S_0).

Open question: is the hypothesis of S_0 polyhedral necessary?

Aperiodic lattices

Other aperiodic lattices can be framed in a “discrete thin film” setting. The best known is the Penrose Lattice



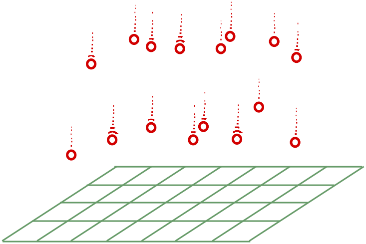
which can be seen as a 2-dimensional discrete thin film in $\mathbb{Z}^5$ with π a precise “irrational” two-dimensional plane in $\mathbb{Z}^5$ (up to some technical details; cf. B-Solci. M3AS 2011).

Open question: is the Wulff shape for the ferromagnetic energy of the Penrose lattice a pentagon?

A Model for Random Deposition

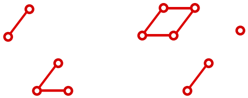
(an example of random discrete thin films - B-Cicalese-Ruf, in progress)

We may consider a spin system, with a random geometry obtained by "successive random depositions" on a neutral substrate (only forcing the sites to sit above a fixed lattice, say $\mathbb{Z}^2$).

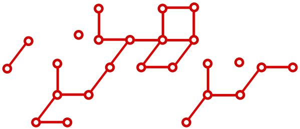


We then have “thin films” with geometry depending on the number N of iterations of the random deposition process.
We suppose

- the probability to deposit above a given site is p (according to an i.i.d. random variable)
- only nearest neighbours (in $\mathbb{Z}^3$) interact with a fixed ferromegnetic interaction.



first layer



second layer, etc.

(p small in these pictures)

We may homogenize each of these thin films obtaining almost surely

$$F_N(u) = \int_{S(u)} \varphi_N(\nu) d\mathcal{H}^1$$

We have again a dependence on N:

• if $p \leq p_c$ (critical site-percolation threshold) then we have $\varphi_N = 0$ for small N; otherwise it is positive (by comparison with the homogenized density of dilute spins in 2D; cf. B-Piatnitski *J.Stat.Phys.* 2013)

• $\lim_N \varphi_N(\nu) = p\|\nu\|_1$.

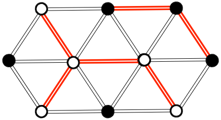
Antiferromagnetic Energies

If we have spin energies

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

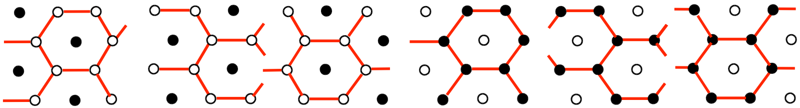
(mixing ferromagnetic and) antiferromagnetic interactions (with some $c_{ij} < 0$), then we may have *frustration*; i.e., ground states may not have the interactions minimized for all pairs (i, j). (Note that if $c_{ij} < 0$ then the interaction is minimized for $u_i \neq u_j$)

Total frustration. The simplest example is the triangular lattice with only antiferromagnetic nearest-neighbour interactions where we have 'disordered' ground states



(frustrated interactions (in red))

Periodic frustrated ground states. We also may have a finite number of periodic minimizers; e.g. in the triangular lattice with nearest-neighour antiferromagnetic and next-to-nearest-neighbour ferromagnetic interactions we have six “hexagonal” ground states



(only frustrated interactions (in red) highlighted).

Note. The ground states determine the number of parameters on which to define the Γ-limit. In this example it will be a surface energy defined on Caccioppoli partitions labelled by six parameters (B-Cicalese, ArXiv 2015).

Question: is the same type of frustration inherited by the corresponding thin films?

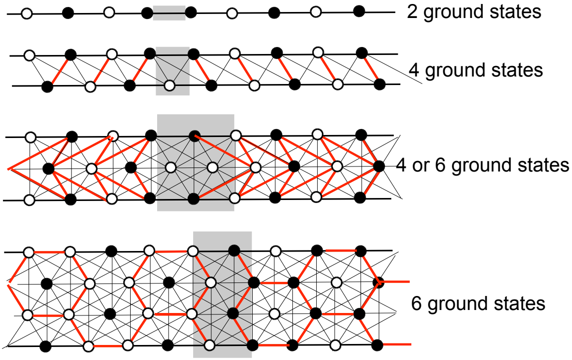
Antiferromagnetic Thin Films

For thin films the effect of internal surface energies (frustrated connections) adds up to that of boundary surface energies.

Example (dependence of $\#$ of parameters on the thickness)

The number of parameters of N-layer thin films may depend on N and ‘stabilize’ to those of the ‘bulk’ limit

E.g., for triangular NN antiferrom. + NNN ferromagnetic,

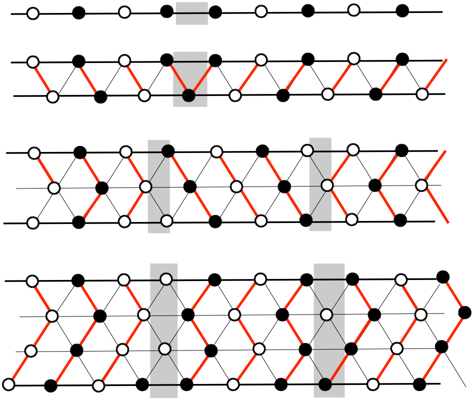


(Note: the $\#$ is not always increasing with the thickness)

Example (rigidity by boundary effects)

"Total frustration" may only occur as the number of layers $N \to +\infty$

E.g., for triangular NN antiferromagnetic, (the gray zones highlight an interface)



(in a sense the effect of the boundary is opposite to elastic thin films)

Conclusions

I have traced the approach of B-Fonseca-Francfort in recent dimension-reduction results for discrete objects.

The flexibility of the method has allowed to adapt the analysis to treat both elastic and brittle, deterministic and random thin objects.

The use of the homogenization standpoint has given the opportunity of highlighting new features as the dependence on the number of layers, or almost-periodicity issues.

We have finally seen some antiferromagnetic examples where an analysis of ground states is necessary before even starting to apply a thin-film procedure, with new questions.

There is still work to be done... maybe with Irene again...

Thank you for your attention!

. . . and. . .

Happy Birthday, Irene!