Dimension reduction for discrete systems

Marco Cicalese

Dipartimento di Matematica e Applicazioni 'R. Caccioppoli' - Università 'Federico II' via Cintia, 80126 Napoli cicalese@unina.it

Object of this talk is the description of the overall behaviour of variational pairinteraction lattice systems defined on 'thin' domains of \mathbb{Z}^N ; *i.e.* on domains consisting on a finite number M of mutually interacting copies of a portion of a N-1-dimensional discrete lattice.

On one hand we draw a parallel with the analog theories for 'continuous' thin films showing that general compactness and homogenization results can be proven by adapting the techniques commonly used for problems on Sobolev spaces; on the other hand we show that new phenomena arise due to the different nature of the microscopic interactions, and in particular that for long-range interactions a surface energy on the free surfaces of the film due to boundary layer effects renders the effective behaviour depend in a non-trivial way on the number M of layers.

In a more precise notation, we consider energies depending on functions parameterized on a portion of the lattice \mathbb{Z}^N consisting of a 'cylindrical' set

$$\mathcal{Z}(\omega, M) = (\omega \cap \mathbb{Z}^{N-1}) \times \{1, \dots M\}$$

of the form

$$\sum_{\alpha,\beta\in\mathcal{Z}(\omega,M)}\varphi_{\alpha,\beta}(u_{\alpha}-u_{\beta}), \qquad u:\mathcal{Z}(\omega,M)\to\mathbb{R}^{d}$$

when the size of ω is large. Upon introducing a small positive parameter ε and scaling ω to a fixed size, obtaining the discrete thin domain

 $\mathcal{Z}_{\varepsilon}(\omega, M) = (\omega \cap \varepsilon \mathbb{Z}^{N-1}) \times \{\varepsilon, 2\varepsilon, \dots M\varepsilon\},\$

this problem can be reformulated as the description of the Γ -limit of energies of the form

$$F_{\varepsilon}(u) = \sum_{\alpha,\beta\in\mathcal{Z}_{\varepsilon}(\omega,M)} \varepsilon^{N-1} f_{\alpha,\beta}^{\varepsilon} \left(\frac{u_{\alpha} - u_{\beta}}{\varepsilon}\right), \qquad u: \mathcal{Z}_{\varepsilon}(\omega,M) \to \mathbb{R}^{d}$$

(at this point a more general dependence of the energy densities on ε is introduced for the sake of generality).

The energies above may be viewed as the discrete analog of thin-film energies of the form

$$\mathcal{F}_{\varepsilon}(u) = \frac{1}{\varepsilon} \int_{\omega \times (0, M\varepsilon)} W_{\varepsilon}(x, Du(x)) \, dx \qquad u \in W^{1, p}(\omega \times (0, M\varepsilon); \mathbb{R}^d).$$

For such functionals a number of results in the framework of variational convergence have been obtained since the pioneering work of Le Dret and Raoult [6]; in particular if

M. Cicalese

 W_{ε} uniformly satisfy some *p*-growth conditions, a general compactness result by Braides, Fonseca and Francfort [4] shows that, upon subsequences, we can always suitably define a Γ -limit energy in the lower-dimensional set ω of the form

$$\mathcal{F}(u) = \int_{\omega} W(\hat{x}, Du(\hat{x})) \, d\hat{x}, \qquad u \in W^{1, p}(\omega; \mathbb{R}^d)$$

(here, $\hat{x} = (x_1, \ldots, x_{n-1})$). Particular cases are when $W_{\varepsilon} = W_0(Du)$ is independent of ε and x, in which the limit W is simply given [6] by

$$W(A) = M \, Q \overline{W}_0(A), \qquad \overline{W}_0(A) = \inf_z W_0(A \mid z),$$

where Q stands for the operation of quasiconvexification (note the trivial dependence on M), and when $W_{\varepsilon}(x, A) = W(x/\varepsilon, A)$, in which suitable homogenization formulas hold [4].

On the other hand, a general compactness theory for discrete systems with energy densities of polynomial growth defined on 'thick' domains by Alicandro and Cicalese [2] is also available. In particular, that theory can be applied in the case above when M = 1and the energies F_{ε} are simply interpreted as defined on $\omega \cap \varepsilon \mathbb{Z}^{N-1}$. In this case again an energy of the same form as \mathcal{F} above can be proven to be the Γ -limit in a suitable sense of such F_{ε} (discrete functions must be identified with piecewise-constant interpolations). Appropriate homogenization formulas apply as well if the discrete interactions possess some periodicity.

In the general case M > 1 we note that the energies F_{ε} can also be seen as defined on M copies of $\omega \cap \varepsilon \mathbb{Z}^{N-1}$ interacting through pair-interactions corresponding to $\beta - \alpha$ with a non-zero component in the N-th variable. We first show that functions on which the limit energy is finite, that are thus defined on M copies of ω , are actually equal on each of these copies, so that the limit energy can be defined on the only set ω . To prove a general compactness and representation theorem for the limit we adapt both the localization techniques on cylindrical domains used by Braides, Fonseca and Francfort [4] to prove a compactness result for energies on continuous thin films, and those used by Alicandro and Cicalese [2] for thick discrete systems, where the main difficulty is taking care of long-range interactions. More precise homogenization formulas are given in the case when the energy densities are periodic; *i.e.* $f_{\alpha,\beta}^{\varepsilon} = f_{\alpha/\varepsilon,\beta/\varepsilon}$ and there exists an integer k such that $f_{i,j} = f_{i',j'}$ if $i - i' = j - j' \in k\mathbb{Z}^{N-1}$. As in [4] these formulas are defined through minimum problems on rectangles with boundary conditions on the lateral boundaries only. In the discrete case it must be noted that these formulas are necessary also in the 'trivial' case when $f_{i,j} = f_{j-i}$; *i.e.* the energy densities depend only on the distance of α and β in the unscaled reference lattice \mathbb{Z}^N , as already observed for 'thick' domains, except when only nearest-neighbour interactions are taken into account. In the case of thin domains an additional scale effect must be taken into account, since long-range interactions (next-to nearest interactions and further) produce different effects close to the upper and lower free boundaries than in the interior. These effects can be viewed as generating a surface energy through a boundary layer (see [3, 5]) that for thin films is of the same order as the bulk energy.

Eventually the Cauchy-Born rule, stating that microscopic arrays corresponding to affine boundary conditions are regularly spaced on a lattice with the same overall affine deformation will be discussed. It will be shown that the domain of affine boundary condition where the Cauchy-Born rule fails decreases with the number M of layers.

The results presented here are mostly contained in a paper in collaboration with R. Alicandro and A. Braides [1].

REFERENCES

- 1. R. Alicandro, A. Braides and M. Cicalese, Continuum limits of discrete thin films with superlinear growth densities, Preprint 2005, (download @ http://cvgmt.sns.it/).
- 2. R. Alicandro and M. Cicalese, Representation result for continuum limits of discrete energies with superlinear growth, *SIAM J. Math Anal.*, vol. 36, 2004, 1–37.
- 3. A. Braides and M. Cicalese, Surface energies in nonconvex discrete systems, Preprint, 2004 (download @ http://cvgmt.sns.it/).
- 4. A. Braides, I. Fonseca and G. Francfort, 3D-2D asymptotic analysis for inhomogeneous thin films. *Indiana Univ. Math. J.*, vol. 49, 2000, 1367–1404.
- 5. A. Braides, A.J. Lew and M. Ortiz, Effective cohesive behavior of layers of interatomic planes, *Arch. Ration. Mech. Anal.*, in press.
- 6. H. Le Dret and A. Raoult, The nonlinear membrane model as variational limit of nonlinear three-dimensional elasticity, *J.Math. Pures Appl.*, vol. 74, 1995, 549–578.