Boundary layer energies in discrete systems: an approach via Γ-convergence

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 variational description of boundary layer phenomena arising in studying the 'discrete to continuum' limit of pair-interaction lattice systems.

By boundary layer phenomena we mean the non vanishing contribution of proper scaling of the energy of the system which affects the geometry of the ground states near the boundary of the sample. These effects have been studied from different perspectives; ours is the variational one, by which we intend to highlight the coupling of this phenomena with the asymptotic behaviour of discrete systems when the lattice spacing vanishes.

We will proceed by recalling some general facts about discrete systems and making several example of boundary layer effect borrowed from different models.

For energies with 'superlinear' growth (these growth conditions are expressed in terms of the scaled difference quotients) it has been shown in [3] that, upon some natural decay conditions on the energy densities ϕ_ε, the Γ-limit as $\varepsilon \to 0$ of an arbitrary system of interactions

$$\sum_{i,j \in \varepsilon \mathbb{Z}^N \cap \Omega} \varepsilon^N \phi_\varepsilon \Big(\frac{i-j}{\varepsilon}, \frac{u_j - u_i}{\varepsilon} \Big)$$

(Ω a bounded open subset of $\mathbb{R}^N$) always exists (upon passing to subsequences) and is expressed as an integral functional

$$\int_\Omega \varphi(Du) \; dx.$$

The simplest case is when only nearest-neighbour interactions are present, in which case the function φ is computed via a convexification process [3]. When not only nearest-neighbour interactions are taken into account, in contrast, the description of the limit problem turns out more complex involving in general some 'homogenization' process (see [5], [3]). Even in the simple one-dimensional case of next-to-nearest-neighbour interaction the limit bulk energy density is described by a formula of 'convolution type' that highlights a non-trivial balance between first and second neighbours.

As a first example of boundary layer phenomena, we discuss a higher-order description of one-dimensional next-to-nearest-neighbour systems of the form

$$\sum_{i,i+1 \in \varepsilon \mathbb{Z} \cap \Omega} \varepsilon \psi_1 \Big(\frac{u^{i+1} - u^i}{\varepsilon} \Big) + \sum_{i,i+2 \in \varepsilon \mathbb{Z} \cap \Omega} \varepsilon \psi_2 \Big(\frac{u^{i+2} - u^i}{2\varepsilon} \Big)$$

using the terminology of developments by Γ-convergence (introduced in Anzellotti and Baldo [4]). In this case the integrand φ is given as the convex envelope of an effective

energy ψ described by an explicit convolution-type formula describing oscillations at the lattice level

$$\psi(z) = \psi_2(z) + \frac{1}{2}\min\{\psi_1(z_1) + \psi_1(z_2) : z_1 + z_2 = 2z\},$$

that allows an easier description of the phenomena. Besides the possibility of oscillatory solutions on the microscopic scale, we show the appearance of a boundary-layer contribution on the boundary due to the asymmetry of the boundary interactions. The quantification of these energies will be done by optimizing boundary layers on the lattice level on the whole lattice with minimal configurations as conditions at infinity.

When ψ_1 and ψ_2 are Lennard-Jones type potentials, the higher-order Γ-limit gives a fracture term. Here the microscopic pattern influence the value of the fracture energy through the appearance of boundary layers on the two sides of the fracture (an alternative description of this phenomena justified by a renormalization-group approach, under a different scaling of the energy, is provided by Braides, Lew and Ortiz [6]). Note that these fracture boundary layer may compete with those forced by boundary conditions; as a consequence, for example, for Lennard-Jones interactions we obtain that fracture at the boundary is energetically favoured, in contrast with the nearest-neighbour case when fracture may appear anywhere in the sample.

Similar issues will be presented also for a 2-D next to nearest neighbours model for binary discrete systems of ferromagnetic-antiferromagnetic type studied in [2].

Eventually, we will discuss pair-interaction 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 where 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 that, this time, is of the same order as the bulk energy (see [2]).

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