From Discrete Systems to Continuum Problems

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Preface

These are the lecture notes of the six-lecture course that I gave in Würzburg at the Winter School "Calculus of Variations in Physics and Materials Science" beautifully organized by Anja Schlömerkemper and Giuliano Lazzaroni from January 8 to 13, 2012, to whom go my thanks, as well as to John Ball and Stefan Müller who gave the other courses with stimulating interactions between the courses, and to the very receptive audience. The content of Lecture 1 is subdivided into Chapter 1 and Chapter 2, while the other lectures are contained in the corresponding chapters.

The subject of the course are discrete systems, more precisely lattice systems, and their continuous description by variational methods. This is an extremely broad subject. I will focus on a series of examples with the aim of

• show how we can adapt 'macro' techniques such as homogenization, relaxation, multi-scale analysis, etc. to compute continuum limits;

• exhibit a variety of interesting limits starting from a limited set of very simple lattice interactions;

• highlight new 'micro' effects that add up to the usual 'macro' energies.

Disclaimer

Part of the written material comes from a previous PhD course at the University of Rome in collaboration with Roberto Alicandro and Marco Cicalese, and the final chapter from a Summer School at the University of Utah. Hence, there might be some slight incoherences from chapter to chapter. One of those may come from summation conventions, so that e.g. a sum on nearest neighbours may be understood sometimes as counting once or sometimes twice a connection (when parameterized as pairs (i, j) by its nodes), another one comes from the convenience at times to use as a parameter a subset of $\mathbb{Z}^d$ (especially if $d = 1$) and at other times a subset of $\varepsilon\mathbb{Z}^d$. Moreover, the reader should consider that constants may have been dropped without advice. All this will be corrected in a (near- or distant-) future version. I have thought anyhow to present this "preliminary" version for the sake of immediacy soon after the end of the school.

Chapter 1

Γ-convergence and discrete problems

Γ-convergence has been developed to analyze the behavior of variational problems, such as homogenization and phase changes, where there appear small parameters that make the treatment of the problem complex or numerically expensive. The idea then is to substitute to these problems a new 'effective' problem, where these parameters do not appear, or appear in a simplified manner. It is surprising that discrete systems, in which problems are defined, for example, on lattices characterized by a vanishing lattice size, with apparent analytical and numerical applications, have come rather late to the attention of the experts of this branch of the Calculus of Variations. In these notes we will examine some issues arising from the passage from discrete systems to continuous energies with a special attention to those features that are characteristic of the microscopic variable.

Our energies will be defined on spaces of functions whose domain is a portion of a lattice. We can take as a model the cubic lattice $\mathbb{Z}^d$, but we can also think of different lattices (eg a triangular lattice in in $\mathbb{R}^2$) and not necessarily of Bravais lattices (for example, the hexagonal lattice in $\mathbb{R}^2$). In this context, our variables are functions

$$u : l\mathbb{Z}^d \cap \Omega \to \mathbb{R}^m, \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$ is a reference open set, and l is the characteristic lattice size. For brevity of notations we put

$$\Omega_l = l\mathbb{Z}^d \cap \Omega, \qquad u_i = u(i) \text{ for } i \in \Omega_l \tag{1.2}$$

The nature of the energies defined on these functions may be of different origins, and lead to a number of problems of variational character.

Many of the problems we are interested in can be reduced to minimum problems

$$\min\{E_l(u) + \text{boundary conditions, constraints, etc.} : u : \Omega_l \to \mathbb{R}^m\},$$

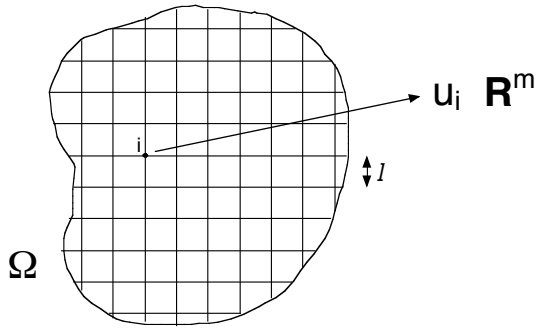


Figure 1.1: representation of the discrete environment

and their analysis for $l \ll 1$. Our aim will be to carry on this analysis with the language and methods of Γ-convergence

Example 1.0.1 (i) (*binary systems/lattice gas*) Let $u : \mathbb{Z}^d \to \{-1, 1\}$ and consider the energy (the so-called *ferromagnetic energy*)

$$-\sum_{|i-j|=1} u_i u_j \,,$$

where the sum is extended to neighbouring nodes in a set Ω only. The value u_i can be interpreted as the spin of a particle sitting at i, or a parameter indicating whether at the site i is present or not a gas particle. The energy is minimized when all u_i are equal. If we fix the average spin or the total number of gas particles then the minimizer is not trivial.

In problems of Statistical Mechanics it is the number of particles that tends to $+\infty$. We equivalently scale the lattice and consider functions parameterized on $l\mathbb{Z}^d \cap \Omega$. In this case $l \approx N^{-1/d}$ where N is the number of the particles of the sample, so that $l \ll 1$ is equivalent to $N \gg 1$. We will see that, up to an additive term of order l^{-d} (not depending on u) the energy of minimizers scales as l^{1-d}. The relevant energies will then be of the form

$$E_l(u) = -\sum_{|i-j|=l} l^{d-1} u_i u_j \,.$$

(ii) (*conducting or elastic networks*) we consider a portion of a cubic network contained in an open set Ω. The scalar variable u is parameterized on the network nodes $l\mathbb{Z}^d \cap \Omega$ and may be thought either to represents the value of an electric potential or the displacement of the node in the reference configuration. For linear interactions the overall energy of the system can be written as

$$\sum_{|i-j|=l} c_{ij} \left| \frac{u_i - u_j}{l} \right|^2 ,$$

where c_{ij} can be interpreted as a material constant of the piece of the network connecting the nodes i and j. The correct scaling gives the energies

$$E_l(u) = \sum_{|i-j|=l} l^d c_{ij} \Big| \frac{u_i - u_j}{l} \Big|^2 .$$

(iii) (*pairwise interatomic potentials*) If $\{u_i\}_{i=0,\dots,N}$ are points in $\mathbb{R}^d$ and ϕ is a potential describing the interaction between pair of atoms sitting at those points, the total energy of this system is given by

$$\sum_{i,j} \phi(u_i, u_j),$$

where now the sum is extended to all pairs. This can be approximated as a problem defined on a lattice under the hypothesis of *crystallization* (ie, that ground states sit at a regular lattice $\mathbb{L}$; up to dilations, if $d = 1$ this lattice can be often proved to be $\mathbb{Z}$, while if $d = 2$ it is the triangular lattice $\mathbb{T}$). In this case u_i can be interpreted as the displacement from a reference position. As for spins then we may introduce a reference set Ω and consider functions parameterized on $l\mathbb{L} \cap \Omega$. Under decay hypotheses on ϕ as the distance of atoms diverges it can be shown that the energy of ground states decays as N, the number of atoms; ie, as l^{-d}, so that now the correct scaled energies are

$$E_l(u) = \sum_{i,j} l^d \phi(u_i, u_j),$$

An additional simplification is that only interactions up to a certain range be taken into account; again the simplest case is that the sum be extended only to nearest neighbours in the reference lattice.

1.1 Definition and properties

The idea of Γ-convergence is to approximate minimum problems

$$\min\{F_\varepsilon(x) : x \in X\}, \tag{1.3}$$

by a problem

$$\min\{F(x) : x \in X\}, \tag{1.4}$$

independent of the small parameter ε (the lattice size l in the previous section). This is done via a notion of convergence of the energies given in 'local terms' (ie, through the characterization of the behavior of the energies of convergent sequences of points x_ε) and is 'compatible with continuous perturbations'. Here and later we will call a *sequence* a family parametrized by either $\varepsilon > 0$, (x_ε), or by $j \in \mathbb{N}$; eg, (x_j).

Definition 1.1.1 (Γ-convergence) *Let X be a metric space and let $F_\varepsilon, F : X \to [-\infty, +\infty]$ be functionals on X. We say that (F_ε)* Γ-converges *to F, or that F is the* Γ-limit *of (F_ε), as $\varepsilon \to 0^+$ (with respect to the metric X), and we will write*

$$F = \Gamma\text{-}\lim_{\varepsilon \to 0^+} F_\varepsilon \tag{1.5}$$

if for all $x \in X$ the two following conditions hold

(i) (liminf inequality) *for all $x_\varepsilon \to x$ we have $F(x) \leq \liminf_{\varepsilon \to 0^+} F_\varepsilon(x_\varepsilon)$*

(ii) (limsup inequality) *there exist $x_\varepsilon \to x$ such that $F(x) \geq \limsup_{\varepsilon \to 0^+} F_\varepsilon(x_\varepsilon)$.*

Taking (i) *into account condition* (ii) *can be rephrased as the existence of a* recovery sequence*, ie $x_\varepsilon \to x$ such that $F(x) = \lim_{\varepsilon \to 0^+} F_\varepsilon(x_\varepsilon)$.*

The first condition requires that F provide an estimate from below of the limit (of the minima) of the energies F_ε, while the second ensures that this limit is reached. The definition is designed so that the following theorem applies.

Theorem 1.1.2 (Fundamental theorem of Γ-convergence) *If a compact $K \subset X$ exists such that $\inf F_\varepsilon = \inf_K F_\varepsilon$, then there exists $\min F$ and we have*

$$\min F = \lim_{\varepsilon \to 0^+} \inf F_\varepsilon.$$

Moreover, if x_ε is a precompact sequence such that $F_\varepsilon(x_\varepsilon) = \inf F_\varepsilon + o(1)$ with a subsequence converging to $\overline{x} \in X$, then $F(\overline{x}) = \min F$.

Proof. It suffices to prove the second assertion. We can then consider a sequence (x_{ε_j}) such that at the same time we have $\lim_j F_{\varepsilon_j}(x_{\varepsilon_j}) = \liminf_{\varepsilon \to 0^+} \inf F_\varepsilon$ and $x_{\varepsilon_j} \to \overline{x}$. We then have $F(\overline{x}) \leq \liminf_{\varepsilon \to 0^+} F_\varepsilon(x_\varepsilon) \leq \lim_j F_{\varepsilon_j}(x_{\varepsilon_j}) = \liminf_{\varepsilon \to 0^+} \inf F_\varepsilon$ thanks to (i). From (ii) instead for all $x \in X$there exists a sequence $(\overline{x}_\varepsilon)$ such that $F(x) \geq \limsup_{\varepsilon \to 0^+} F_\varepsilon(x_\varepsilon) \geq \limsup_{\varepsilon \to 0^+} \inf F_\varepsilon$, which concludes the proof by taking the infimum in x and comparing with the previous inequality. □

Remark 1.1.3 (comments on the definition) (a) (*lower semicontinuity*) from (i) the convergence of a constant sequence $F_\varepsilon = F_0$ is possible only if F_0 is *lower semicontinuous* (lsc for short), ie if for each $x_j \to x$

$$F_0(x) \leq \liminf_j F_0(x_j); \tag{1.6}$$

(b) (*relaxation*) if $F_\varepsilon = F_0$ the Γ-limit exists and is equal to the *lower-semicontinuous envelope* of F_0, ie the functional $\overline{F}$ given by

$$\overline{F}(x) = \sup\{G(x) : G \text{ is lower semicontinuous and } G \leq F\}; \tag{1.7}$$

(c) (*choice of the topology*) In order to apply the Fundamental Theorem it is convenient to choose weak (metrizable) topologies, so as to have more converging sequences. This makes it easy to construct recovery sequences, but it makes it more difficult to satisfy the liminf inequality.

1.2 Computation of Γ-limits

In this section we make some observations that are useful in the actual computation of a Γ-limit.

Proposition 1.2.1 (compactness of Γ-convergence) *If X is a separable metric space then from every sequence (F_j) with $F_j : X \to [-\infty, +\infty]$ we can extract a Γ-converging subsequence.*

Proposition 1.2.2 (stability under subsequences) *A sequence (F_ε) Γ-converges to F if and only if from every subsequence (F_{ε_j}) we can extract a subsequence converging to F.*

These results are useful when first we extract converging subsequences by compactness, and then we characterize the Γ-limit showing it does not depend on the subsequence.

Proposition 1.2.3 (stability under continuous perturbations) *If (F_ε) Γ-converges to F and G is continuous, then $(F_\varepsilon + G)$ Γ-converges to $F + G$.*

The use of this proposition is twofold. On one hand it can be applied to the study of sequences (H_ε) whose elements can be written as $H_\varepsilon = F_\varepsilon + G$ with G continuous and (F_ε) with a known Γ-limit. On the other hand, by writing $F_\varepsilon = (F_\varepsilon - G) + G$, one can sometime choose G such that the computation of the Γ-limit of $(F_\varepsilon - G)$ is more handy or meaningful, and then add G to the result.

1.2.1 Upper and lower bounds

The computation of a Γ-limit can be reduced to two separate estimates in the same way as the computation of an ordinary limit can be seen as the equality of an upper and a lower limit.

Definition 1.2.4 (Γ-lim inf / Γ-lim sup) *If $F_\varepsilon : X \to [-\infty, +\infty]$ we define the* Γ-lower limit *and the* Γ-upper limit *of (F_ε) as*

$$\Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon(x) := \inf\Big\{\liminf_{\varepsilon\to 0^+} F_\varepsilon(x_\varepsilon) : x \to x\Big\} \tag{1.8}$$

$$\Gamma\text{-}\limsup_{\varepsilon\to 0^+} F_\varepsilon(x) := \inf\Big\{\limsup_{\varepsilon\to 0^+} F_\varepsilon(x_\varepsilon) : x \to x\Big\}, \tag{1.9}$$

respectively.

Note the asymmetry of the definition. Note moreover that the quantities (1.8) and (1.9) always exist.

The two inequalities characterizing the Γ-limit can be rewritten as a lower and upper estimate for the Γ-lim inf and the Γ-lim sup

$$F(x) \leq \Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon(x), \qquad \Gamma\text{-}\limsup_{\varepsilon\to 0^+} F_\varepsilon(x) \leq F(x), \tag{1.10}$$

which can be treated separately. To that end, two useful observations are contained in the following proposition.

Proposition 1.2.5 (lower semicontinuity and Γ-limits)
(i) *The functionals F' and F'' defined by*

$$F'(x) := \Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon(x), \qquad F''(x) := \Gamma\text{-}\limsup_{\varepsilon\to 0^+} F_\varepsilon(x) \tag{1.11}$$

are lower semicontinuous on X;
(ii) *If $\overline{F}_\varepsilon$ denotes the lower-semicontinuous envelope of F_ε, ie*

$$\overline{F}_\varepsilon(x) = \sup\{G(x) : G \leq F_\varepsilon,\ G \text{ lower semicontinuous}\}, \tag{1.12}$$

then we also have

$$F'(x) = \Gamma\text{-}\liminf_{\varepsilon\to 0^+} \overline{F}_\varepsilon(x), \qquad F''(x) = \Gamma\text{-}\limsup_{\varepsilon\to 0^+} \overline{F}_\varepsilon(x). \tag{1.13}$$

The first observation allows us to limit our choice of candidate Γ-limits to lower-semicontinuous functionals. The second one allows to sometime simplify the form of F_ε.

Example 1.2.6 If $X = L^p(\Omega)$ endowed with the weak topology on bounded sets (which is metrizable) then in the class of integral functionals

$$F(u) = \int_\Omega f(u)\,dx$$

we have that F is lower semicontinuous if and only if f is *convex* and lower semicontinuous (this condition is implied by convexity if f takes only finite values). Furthermore the lower-semicontinuous envelope of F is exactly

$$\overline{F}(u) = \int_\Omega f^{**}(u)\,dx,$$

where f^{**} is the convex and lower-semicontinuous envelope of f, and a recovery sequence can be constructed composed of piecewise-affine functions.

Remark 1.2.7 (lower bound - supremum of measures) The way one often proves a lower bound is by optimizing a family of inequalities; ie by finding a family of lsc functionals G_λ (for discrete-to-continuous processes those will be functionals on the continuum; eg those in the previous remark, so that they will satisfy simplifying convexity conditions) such that

$$F'(x) = \Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon(x) \geq G_\lambda(x). \tag{1.14}$$

This condition is verified in particular if the inequality $F_\varepsilon \geq G_\lambda$ holds on the domain of F_ε. From (1.14) we then deduce that

$$\Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon \geq \sup_\lambda G_\lambda \tag{1.15}$$

(we recall that the supremum of a family of lsc functionals is lower semicontinuous).

This inequality can be further sharpened whenever we have a 'localized' version of $\Gamma\text{-}\liminf_{\varepsilon\to 0^+} F_\varepsilon$, (for integral functional 'localizing' on a set A means simply to integrate only on A, and the corresponding Γ-limits are computed by only requiring convergence on A itself) by using the following lemma (with A the Γ-liminf localized on A).

Lemma 1.2.8 (supremum of measures) *Let μ be a function defined on the open bounded subsets of $\mathbb{R}^d$ such that $\mu(A\cup B) \geq \mu(A) + \mu(B)$ if $\overline{A}\cap\overline{B} = \emptyset$, let σ be a Borel measure and (f_λ) a countable family of Borel functions. If $\mu(A) \geq \int_A f_\lambda d\sigma$ for all λ and A bounded open set, then $\mu(A) \geq \int_A \sup_\lambda f_\lambda d\sigma$.*

Remark 1.2.9 (upper bound by relaxation) The upper bound depends on a construction or *Ansatz* on recovery sequences. By the lsc properties of the Γ-limsup in general it is not necessary to construct such sequences for all $x \in X$, but we may proceed as follows:

- we choose a subset $D \subset X$ and for all $x \in D$ we construct $\overline{x}_\varepsilon \to x$ so that

$$F''(x) = \limsup_{\varepsilon\to 0^+} F_\varepsilon(u_\varepsilon) \leq G(x) \text{ for all } x \in D \tag{1.16}$$

for some functional G.

- from this inequality we deduce that

$$F''(x) \leq \overline{G_D}(x) \text{ for all } x \in X, \tag{1.17}$$

where

$$G_D(x) = \begin{cases} G(x) & \text{if } x \in D \\ +\infty & \text{otherwise,} \end{cases}$$

and $\overline{G_D}$ it its lower-semicontinuous envelope.

A trivial upper bound is obtained choosing $x_\varepsilon = x$ where possible (for lattice energies taking x_ε the discretization of x).

Remark 1.2.10 (upper bound by density) In the particular case when in the previous remark $\overline{G_D} = G$, ie when D is dense in X, G is lsc and for all $x \in X$ there exists $(x_j) \subset D$, $x_j \to x$ such that $G(x_j) \to G(x)$, we deduce that

$$F''(x) \leq G(x) \text{ for all } x \in X. \tag{1.18}$$

Hence, we obtain an upper bound thanks to a construction on a dense set D and the computation of a lsc envelope. Particular choices of D will be regular or piecewise simple functions or sets, which are dense in a stronger topology for which G is continuous.

1.2.2 Equivalence by Γ-convergence

Γ-convergence defines an equivalence relation as in the following definition, which will allow us to state that discrete energies are 'equivalent' to energies on the continuum.

Definition 1.2.11 (equivalence by Γ-convergence) *Two families (F_ε) and (G_ε) are* equivalent by Γ-convergence *if from all sequences (ε_j) we may extract a subsequence (still denoted by (ε_j)) and there exists a sequence of real numbers (m_j) such that there exits the*Γ*-limits*

$$\Gamma\text{-}\lim_j (F_{\varepsilon_j} - m_j), \qquad \Gamma\text{-}\lim_j (G_{\varepsilon_j} - m_j),$$

they are equal and they are not trivial*; ie, they do not take the value $-\infty$ and are not identically $+\infty$.*

Remark 1.2.12 (i) even though the limits are defined in the same space, the domains of F_ε and G_ε will in general be different;

(ii) the translation by m_j allows us to define the equivalence also for families whose Γ-limits are trivial or identically $\pm\infty$. In this case, for example, two diverging sequences with different 'speeds' are not equivalent (eg, the constant functions $F_\varepsilon(u) = \varepsilon^{-2}$ and $G_\varepsilon(u) = \varepsilon^{-1}$).

(iii) if the Γ-limit H of $(F_\varepsilon - m_\varepsilon)$ exists, in particular (F_ε) is equivalent to $(H + m_\varepsilon)$;

(iv) if X is separable then a family (F_ε) with $\inf F_\varepsilon \in \mathbb{R}$ is equivalent to itself. This is ensured by Proposition 1.2.1 applied to $(F_\varepsilon - \inf F_\varepsilon)$.

1.3 Discrete-to-continuous convergence of lattice functions

1.3.1 Interpolations

Lattice energies are defined on sets depending on the lattice parameters. In order to apply the methods of Γ-convergence we have to identify such sets with subspaces of a common

metric space. To that end the simplest identification is with subspaces of $L^1(\Omega;\mathbb{R}^m)$: a function $u : \Omega \cap \varepsilon\mathbb{Z}^d \to \mathbb{R}^m$ is identified with its *piecewise-constant interpolation* on the lattice $\varepsilon\mathbb{Z}^d$ given by

$$u(x) = \begin{cases} u_i & \text{if } x \in Q_i^\varepsilon,\ i \in \Omega \cap \varepsilon\mathbb{Z}^d, \\ 0 & \text{otherwise,} \end{cases} \qquad Q_i^\varepsilon = i + \left(-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)^d. \tag{1.19}$$

Note that in this way $u \in L^\infty(\mathbb{R}^d;\mathbb{R}^m)$.

Note also that the 0-extension for the indices not contained in Ω is convenient to have the interpolated function defined on the whole Ω.

Depending on the energies considered we will then choose $X = L^p(\Omega;\mathbb{R}^m)$ for some $p \geq 1$ equipped with one of the convergences:

• strong convergence (in L^1)

• weak convergence on bounded sets of L^p for some $p > 1$, or weak* if $p = \infty$ (which are metrizable).

Remark 1.3.1 (convergence of averages) We recall that for bounded sequences in L^p the weak convergence $u_\varepsilon \rightharpoonup u$ is equivalent to the convergence on integrals on open sets; i.e., to

$$\lim_{\varepsilon\to 0} \int_A u_\varepsilon \, dx = \int_A u \, dx$$

for all A regular open set. For lattice functions we can interpret this equality as the requirement that u represent the asymptotic statistical properties of the discrete variables u_ε; ie, that

$$\lim_{\varepsilon\to 0} \sum_{i \in A \cap \varepsilon\mathbb{Z}^d} \varepsilon^d u_\varepsilon(i) = \int_A u \, dx$$

for all A with a boundary of null Lebesgue measure. In fact this sum and the integral above differ by an infinitesimal quantity as $\varepsilon \to 0$.

The Γ-convergence of a sequence of lattice energies E_ε each defined on the spaces

$$X_\varepsilon := \{u : \Omega \cap \varepsilon\mathbb{Z}^d \to \mathbb{R}^m\}$$

is then identified with the convergence of the energies F_ε defined on $L^p(\Omega;\mathbb{R}^m)$ by

$$F_\varepsilon(u) = \begin{cases} E_\varepsilon(u) & \text{if } u \in X_\varepsilon \\ +\infty & \text{otherwise,} \end{cases} \tag{1.20}$$

with the identification of X_ε with a subspace of $L^p(\Omega;\mathbb{R}^m)$ as illustrated above.

Alternatively to L^p weak or strong convergences, we may also consider the topology of convergence in measure, or the convergence in $L^p_{\text{loc}}(\Omega;\mathbb{R}^m)$ (the latter is useful if we do not want to take into account the precise definition on interpolated functions close to the boundary of Ω).

Remark 1.3.2 (different interpolations) It is sometime useful to consider other interpolations of lattice functions such as piecewise-affine interpolations over a triangulation of the space. It is usually easy to check that the convergence to functions on the continuum can be equivalently stated in terms of these functions; for example, remarking that piecewise-affine interpolations can be written as convex combination of piecewise-constant functions converging to the same limit. In dimension one the piecewise-affine interpolation $\widetilde{u}_\varepsilon$ on $\varepsilon\mathbb{Z}$ can be written in term of a piecewise-constant interpolation as

$$\widetilde{u}_\varepsilon(t) = u_\varepsilon(t)\Big(1 - \Big(\frac{t}{\varepsilon} - \Big\lfloor \frac{t}{\varepsilon} \Big\rfloor\Big)\Big) + u_\varepsilon(t+\varepsilon)\Big(\frac{t}{\varepsilon} - \Big\lfloor \frac{t}{\varepsilon} \Big\rfloor\Big).$$

If $u_\varepsilon \to u$ then also $\widetilde{u}_\varepsilon \to u$.

1.3.2 Compactness conditions

Even though it may be interesting to compute Γ-limits in stronger topologies, usually it is meaningful to study them with respect to topologies weak enough so that compactness conditions hold and we may apply the Fundamental Theorem of Γ-convergence.

• *Weak-compactness conditions.* Those can be obtained directly from estimates on $\|u_\varepsilon\|_{L^p}$; for example, whenever the energies E_ε satisfy $E_\varepsilon(u) \geq C(\|u\|^p_{L^p} - 1)$ with $p > 1$, or whenever they are finite only on bounded sets of L^∞ (this is the case of spin energies).

• *Strong-compactness conditions.* These may be obtained from compactness criteria *à la* Fréchet-Kolmogorov.

A criterion that allows to reduce the analysis to one-dimensional sections is the following.

Theorem 1.3.3 (Sectional compactness criterion) *Let (u_ε) be a bounded sequence in $L^p(\Omega)$ for some $p > 1$and such that for all $\delta > 0$ and $k = 1, \dots, d$ there exists a sequence (v_ε) such that*

- (i) $\|v_\varepsilon - u_\varepsilon\|_{L^1(\Omega)} \leq \delta$
- (ii) *foe almost all $y \in \mathbb{R}^{d-1}$ the sequence of one-dimensional functions (v^y_ε) defined as $v^y_\varepsilon : \Omega^y \to \mathbb{R}$ setting*

$$\Omega^y = \{t \in \mathbb{R} : (y_1, \dots, y_k, t, y_{k+1}, \dots, y_d) \in \Omega\} \tag{1.21}$$
$$v^y_\varepsilon(t) = v_\varepsilon(y_1, \dots, y_k, t, y_{k+1}, \dots, y_d) \tag{1.22}$$

is precompact in $L^1(\Omega^y)$ whenever $\Omega^y \neq \emptyset$,

then the sequence (u_ε) is precompact in $L^1(\Omega)$.

Remark 1.3.4 (1D compactness) The criterion stated above will be applied to sequences of functions $u_\varepsilon \in X_\varepsilon$, often reducing the study directly to the analysis of their one-dimensional sections u_ε^y (ie, with $v_\varepsilon = u_\varepsilon$). We easily obtain the precompactness of one-dimensional sequences (u_ε) for which the following energies are equibounded (we suppose that Ω is a bounded interval):

(1) (*spins*) we write the energies as $E_\varepsilon(u) = \sum_i (u_i - u_{i-\varepsilon})^2$ with the constraint $|u| = 1$. We immediately deduce that the functions u_ε are piecewise constant with a finite number of discontinuity points. The compactness of the functions is equivalent to the compactness of the sequences of discontinuity points (Bolzano-Weierstrass Theorem).

(2) (*finite-differences*) $E_\varepsilon(u) = \sum_i \varepsilon \left| \frac{u_i - u_{i-\varepsilon}}{\varepsilon} \right|^p$ with $p \geq 1$. In this case we identify discrete functions with their piecewise-affine interpolations, and use the compact embedding of $W^{1,1}$ in L^1 in dimension 1;

(3) (*free-discontinuity energies*) $E_\varepsilon(u) = \sum_i \varepsilon \left(\left(\frac{u_i - u_{i-\varepsilon}}{\varepsilon} \right)^2 \wedge \frac{1}{\varepsilon} \right)$ (the Blake-Zisserman energy). In this case we use a piecewise-affine interpolation of u between $i - \varepsilon$ and i if $\left(\frac{u_i - u_{i-\varepsilon}}{\varepsilon} \right)^2 \leq \frac{1}{\varepsilon}$, and with the constant value u_i otherwise. Compactness follows by combining the arguments in the cases (1) and (2).

1.3.3 Sets of finite perimeter

Functions taking two values (ie, spins) can be identified with characteristic functions and then with sets. The notion of sets of finite perimeter is particularly useful when dealing with energies that can be interpreted as surface energies on sets and thus provide easy compactness properties.

Let $\Omega \subset \mathbb{R}^d$ be an open set, $\mathcal{B}(\Omega)$ denote the family of Borel subsets of Ω. We denote by $\mathcal{H}^{d-1}$ the $d-1$-dimensional Hausdorff measure.

A good notion of perimeter from the standpoint of the Calculus of Variations will satisfy the following properties

$$\mathcal{P}(G) = \mathcal{H}^{d-1}(\partial G \cap \Omega) \text{ if } G \text{ is a polyhedral set;} \tag{1.23}$$

$$\mathcal{P}(G) \leq \liminf_{n \to +\infty} \mathcal{P}(G_n) \tag{1.24}$$

if G_n converges to G in measure; ie, $|G_n \triangle G| \to 0$. One way to define such a perimeter is by relaxation; ie, by setting

$$\mathcal{P}(G) = \inf\{\liminf_{n \to +\infty} \mathcal{H}^{d-1}(\partial G_n \cap \Omega) : \ G_n \to G \text{ in measure, } G_n \text{ polyhedral}\}.$$

In other words $G \subset \Omega$ has *finite perimeter* (in Ω) if and only if there exists a sequence of polyhedral sets G_n converging to G in measure and such that $\mathcal{H}^{d-1}(G_n \cap \Omega)$ is bounded.

The following theorem summarizes the main structure properties of sets of finite perimeter.

Theorem 1.3.5 *If G has finite perimeter then there exists a set $\partial^* G \subseteq \partial G$, called the* reduced boundary *of G, such that*

$$\mathcal{P}(G) = \mathcal{H}^{d-1}(\partial^* G);$$

$\partial^* G$ is rectifiable; that is, $\partial^* G \subset \bigcup_{h\in\mathbb{N}} \Gamma_h \cup N$ for a sequence (Γ_h) of compact subsets of C^1-hypersurfaces and with $\mathcal{H}^{d-1}(N) = 0$. Moreover there exists a function $\nu_G : \partial^* G \to S^{d-1}$, the inner normal *to G, such that*

$$\lim_{\rho\to 0^+} \frac{|B_\rho^+(x, \nu_G(x)) \setminus G|}{\rho^d} = 0 \quad \forall x \in \partial^* G,$$

where $B_\rho^+(x,\nu) := \{y \in \mathbb{R}^d : \|y - x\| < \rho,\ \langle y - x, \nu\rangle > 0\}$.

The following compactness and lower-semicontinuity theorems will be very useful.

Theorem 1.3.6 (compactness) *Let $(G_n) \subset \mathcal{B}(\Omega)$ be a sequence of sets of finite perimeter such that $\sup_{n\in\mathbb{N}} \mathcal{P}(G_n) < +\infty$. Then there exists a subsequence (G_{n_k}) converging in measure to a set G of finite perimeter. Moreover,*

$$\mathcal{P}(G) \le \liminf_{n\to+\infty} \mathcal{P}(G_n).$$

Theorem 1.3.7 (lower semicontinuity) *Let Ω have Lipschitz boundary. If φ is a norm, the functional*

$$F(G) = \int_{\Omega\cap\partial^* G} \varphi(\nu_G)\, d\mathcal{H}^{d-1}$$

is lower-semicontinuous with respect to the convergence in measure. Moreover, for all G there exists a sequence (G_n) of polyhedral sets converging to G such that

$$\lim_n F(G_n) = F(G).$$

1.4 Development by Γ-convergence

The Fundamental Theorem of Γ-convergence can be iteratively applied to get a better description of the behaviour of minimum problems for energies F_ε whenever the first Γ-limit $F^{(0)}$ possesses a non-trivial set of minimizers. The iterative process goes as follows:

• we conjecture a second *scale* (that is, an infinitesimal function ofε), say ε^α (but it is not necessarily a polynomial scale). This means that we find a converging sequence (x_ε^α) such that $F_\varepsilon(x_\varepsilon^\alpha) = \min F^{(0)} + O(\varepsilon^\alpha)$;

• we consider the scaled functional

$$F_\varepsilon^{(\alpha)}(x) = \frac{F_\varepsilon(x) - \inf F}{\varepsilon^\alpha}. \tag{1.25}$$

Note that $F_\varepsilon^{(\alpha)}$ has the same minimizers as F_ε. Set

$$m_\varepsilon := \inf F_\varepsilon, \qquad m^{(0)} := \inf F^{(0)}, \qquad m_\varepsilon^{(\alpha)} := \inf F_\varepsilon^{(\alpha)} \tag{1.26}$$

so that

$$m_\varepsilon^{(\alpha)} = \frac{m_\varepsilon - m^{(0)}}{\varepsilon^\alpha}; \tag{1.27}$$

• we compute the Γ-limit (Γ-*limit of* (F_ε) *at scale* ε^α)

$$F^{(\alpha)}(x) = \Gamma\text{-}\lim_{\varepsilon\to 0} F_\varepsilon^{(\alpha)}(x); \tag{1.28}$$

• if this limit is not trivial then we have the following result, immediately obtained from the Fundamental Theorem of Γ-convergence.

Theorem 1.4.1 (development of minimum problems) *Under the coerciveness hypotheses of the Fundamental Theorem of* Γ*-convergence there exits the minima* $\min F^{(0)}$ *and* $m^{(\alpha)} := \min F^{(\alpha)}$*, and* $m_\varepsilon^{(\alpha)} \to m^{(\alpha)}$*, so that*

$$m_\varepsilon = m^{(0)} + \varepsilon^\alpha m^{(\alpha)} + o(\varepsilon^\alpha). \tag{1.29}$$

Moreover, if (x_ε) *is a* ε^α*-minimizing sequence of* (F_ε)*, ie, such that* $F_\varepsilon(x_\varepsilon) = \inf F_\varepsilon + o(\varepsilon^\alpha)$*, and* x *is one of its limit points, then* x *is a minimizer both for* $F^{(0)}$ *and* $F^{(\alpha)}$*.*

Remark 1.4.2 (i) From the definition of $F^{(\alpha)}$ its domain is contained in the set of minimizers of $F^{(0)}$; ie, $F^{(\alpha)}(x) = +\infty$ if $F^{(0)}(x) \neq \min F^{(0)}$;

(ii) in the hypotheses of the theorem there can still exits an intermediate scale, say still a polynomial ε^β with $\varepsilon^\alpha << \varepsilon^\beta << 1$, such that

$$F^{(\beta)}(x) = \Gamma\text{-}\lim_{\varepsilon\to 0} \frac{F_\varepsilon(x) - \inf F}{\varepsilon^\beta} \tag{1.30}$$

exist and is not trivial, but in that case we must have $\min F^{(\beta)} = 0$, otherwise development (1.29) would be violated;

(iii) if for all intermediate scale $\varepsilon^\alpha << s_\varepsilon << 1$ we have

$$\Gamma\text{-}\lim_{\varepsilon\to 0} \frac{F_\varepsilon(x) - \inf F}{s_\varepsilon} = \begin{cases} 0 & \text{if } F^{(0)}(x) = \min F^{(0)} \\ +\infty & \text{otherwise} \end{cases} \tag{1.31}$$

then we say that the development is *complete at scale* ε^α;

(iv) if the domain of $F^{(\alpha)}$ is dense in the set of minimizers of $F^{(0)}$then the development is complete at scale ε^α;

(v) the process can be iterated, introducing a second scale, say $\varepsilon^\gamma << \varepsilon^\alpha$ and applying the process to $F_\varepsilon^{(\alpha)}$, and so on.

The definition of development by Γ-convergence given above allows us to extend the equivalence relation by Γ-convergence.

Definition 1.4.3 (Equivalence by Γ-convergence at scale ε^α) *We say that two families (F_ε) and (G_ε) are* equivalent by Γ-convergence at scale ε^α *if from every sequence (ε_j) we can extract a subsequence (still denoted by (ε_j)) and there exists a sequence (m_j) of real numbers such that there exist the Γ-limits*

$$\Gamma\text{-}\lim_j \frac{F_{\varepsilon_j} - m_j}{\varepsilon_j^\alpha}, \qquad \Gamma\text{-}\lim_j \frac{G_{\varepsilon_j} - m_j}{\varepsilon_j^\alpha},$$

they coincide and are not trivial.

In particular, in the hypotheses of the theorem above and taking $m_j = m_{\varepsilon_j}$, we have that F_ε is equivalent to $m_\varepsilon + \varepsilon^\alpha F^{(\alpha)}$ at scale ε^α.

1.5 Bibliographical notes

An elementary introduction to Γ-convergence, mostly in dimension one can be found in
[1] A. Braides, Γ-*convergence for Beginners*, Oxford University Press, Oxford, 2002.

More examples and techniques in dimension higher than one are contained in
[2] A. Braides, A handbook of Γ-convergence. In *Handbook of Differential Equations. Stationary Partial Differential Equations, Volume* 3 (M. Chipot and P. Quittner, eds.), Elsevier, 2006.

A general introduction to integral functionals and to homogenization by Γ-convergence is
[3] A. Braides and A. Defranceschi,*Homogenization of Multiple Integrals.* Oxford University Press, Oxford, 1998.

The standard reference to the general properties of Γ-convergence, also in non-metrizable spaces, its metric properties, etc., is
[4] G. Dal Maso, *An Introduction to* Γ-*convergence*, Birkhäuser, Boston, 1993.

Definitions and examples about description by Γ-convergence at multiple scales and various notions of equivalence are found in
[5] A. Braides and L. Truskinovsky. Asymptotic expansions by Gamma-convergence. *Cont. Mech. Therm.* **20** (2008), 21–62

Chapter 2

Some simple 1D examples

2.1 Point energies. 'Mesoscopic' oscillations

We consider lattice energies defined as

$$E_\varepsilon(u) = \sum_{i \in \Omega_\varepsilon} \varepsilon^d \, W(u_i), \qquad u : \Omega_\varepsilon \to \mathbb{R}, \tag{2.1}$$

where Ω is a regular bounded open set. and $W : \mathbb{R} \to (-\infty, +\infty]$ is bounded below and with polynomial growth at infinity. Without loss of generality we shall suppose that

$$W \geq 0, \qquad W(u) \geq c(|u|^p - 1) \tag{2.2}$$

for some $p > 1$. The energies E_ε are (identified with) equi-coercive functionals in $L^p(\Omega)$ with respect to the weak topology. We may take as prototypical W non-convex energies such as

$W(u) = \min\{(u-1)^2, (u+1)^2\}$ or $W(u) = (u^2-1)^2$ (*double-well potentials*)

$W(u) = \begin{cases} 0 & \text{if } u = 1 \text{ or } u = -1 \\ +\infty & \text{otherwise.} \end{cases}$

We fix $\lambda > 0$; for ε sufficiently small we have

$$\bigcup \{Q_i^\varepsilon : i \in \Omega_\varepsilon, \ \operatorname{dist}(i, \partial\Omega) > \lambda/2\} \supset \Omega(\lambda) := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) > \lambda\}$$

so that

$$E_\varepsilon(u) \geq \int_{\Omega(\lambda)} W(u) \, dx$$

for all $u \in X_\varepsilon$. If we recall the lower-semicontinuity theorems for integral energies in L^p-spaces, equivalent to lower semicontinuity (in $\mathbb{R}$) and convexity of the integrand, we can take as G_λ

$$G_\lambda(u) = \int_{\Omega(\lambda)} W^{**}(u) \, dx.$$

For all our examples we have

$$W^{**}(u) = \begin{cases} W(u) & \text{if } |u| \geq 1 \\ 0 & \text{if } |u| < 1. \end{cases}$$

We trivially have $E_\varepsilon(u) \geq G_\lambda(u)$, so that, taking the limit as $e \to 0$, we have

$$\Gamma\text{-}\limsup_{\varepsilon \to 0^+} E_\varepsilon(u) \leq G_\lambda(u).$$

Taking the sup in λ (ie, letting $\lambda \to 0$) by Beppo Levi's Theorem we deduce

$$E_\varepsilon(u) \geq \sup_\lambda \int_{\Omega(\lambda)} W^{**}(u)\,dx = \int_\Omega W^{**}(u)\,dx := G(u)$$

In this case the introduction of the parameter λ has been useful to avoid estimating the contribution of points close to the boundary. Here we have used the hypothesis that W be bounded below.

As the upper bound is concerned, in this case we may fix as D the space of piecewise-constant functions on a family of sufficiently regular sets (eg, constant on cubes of $\mathbb{R}^d$). In that case we take $u_\varepsilon(i) = u(i)$, obtaining

$$\Gamma\text{-}\limsup_{\varepsilon \to 0^+} E_\varepsilon(u) \leq G(u)$$

for $u \in D$. By using a relaxation argument we conclude the upper bound with G, and conclude the proof.

In the terminology of equivalence by Γ-convergence, the family of discrete energies E_ε is equivalent (as $\varepsilon \to 0$) to the continuous energy $\int_\Omega W^{**}(u)\,dx$.

Remark 2.1.1 (microscopic relaxation and mesoscopic oscillations) The argument by relaxation above makes the proof very fast, but hides the details of recovery sequences, which may be relevant to a more refined analysis of the behaviour of minimum problems.

To construct a recovery sequence, we preliminarily relax functional E_ε. In this case, since Ω_ε is a finite set of parameters, the lower semicontinuity of E_ε is equivalent to the lower semicontinuity of W. The lower-semicontinuous envelope of E_ε is then

$$\overline{E}_\varepsilon(u) = \sum_{i \in \Omega_\varepsilon} \varepsilon^d\, \overline{W}(u),$$

where $\overline{W}$ is the lower-semicontinuous envelope (in $\mathbb{R}$) of W. We may then suppose that W itself be lower-semicontinuous. From the growth condition and the lower semicontinuity of W we have

$$W^{**}(u) = \min\{t\,W(v) + (1-t)W(w) : u, v \in \mathbb{R};\ 0 \leq t \leq 1,\ tv + (1-t)w = u\}. \quad (2.3)$$

Consider for simplicity the one-dimensional case, with $\Omega = (0,1)$ and a constant target function u. The relaxation argument on the continuum can be realized by choosing as functions $u_j \rightharpoonup u$ those constructed by taking a periodic function $\overline{u}$ of period 1 with

$$\overline{u}(s) = \begin{cases} v & \text{if } 0 < s \leq t \\ w & \text{if } t < s \leq 1, \end{cases}$$

where v and w are given by (2.3) and $u_j(s) = \overline{u}(T_j s)$, where $T_j \to +\infty$. In order to repeat this argument with u_ε a discretization of $\overline{u}(T_\varepsilon s)$ we have to require $T_\varepsilon << 1/\varepsilon$ so that the oscillation period T_ε^{-1} of $\overline{u}(T_\varepsilon s)$ does not interfere with the discrete scale ε. Hence, such type of 'regular' oscillations generated by the non-convexity of W must take place at a scale much larger than ε, even if infinitesimal (a *mesoscopic* scale).

Remark 2.1.2 In one dimension, we can consider equivalently functionals

$$E_\varepsilon(z) = \sum_{i, i-\varepsilon \in \Omega_\varepsilon} \varepsilon\, W\Big(\frac{z_i - z_{i-\varepsilon}}{\varepsilon}\Big), \qquad z : \Omega_\varepsilon \to \mathbb{R}. \tag{2.4}$$

The Γ-limit can be computed with respect to the strong L^1-convergence of z_ε, and is given by the same energy function as above:

$$F(z) = \int_\Omega W^{**}(z')\, dx$$

with domain contained in $W^{1,p}(\Omega)$. The proof is as above with $u_i = \frac{z_i - z i-\varepsilon}{\varepsilon}$. The only thing to note is that by Remark 1.3.4 the functionals are equi-coercive in $L^1(\Omega)$.

2.2 Homogenization. 'Multi-phase' limits

We consider a simple variant to the previous problem, where the integrand depends periodically on the site i (we can think that we have a number K^d of different 'species' of variables). We then have

$$E_\varepsilon(u) = \sum_{i \in \Omega_\varepsilon} \varepsilon^d W_{i/\varepsilon}(u_i)$$

where $k \mapsto W_k$ is periodic of period K in every coordinate direction (ie, $W_k = W_{k+Ke_j}$ for all$j = 1, \dots, d$). In this case we can consider the sub-lattices

$$\Omega^j_{K\varepsilon} = \varepsilon j + \varepsilon K \mathbb{Z}^d \text{ for all} j \in \{1, \dots, K\}^d.$$

By the previous example we can study the convergence of

$$E^j_\varepsilon(u) = \sum_{i \in \Omega^j_{K\varepsilon}} (K\varepsilon)^d W_j(u_i),$$

whose limit is

$$F^j(u) = \int_\Omega W_j^{**}(u)\,dx.$$

If $u_\varepsilon : \Omega_\varepsilon \to \mathbb{R}$, we set $u_\varepsilon^j(i) = u_\varepsilon(i)$, identified now with an element of the space $X_{K\varepsilon}$ of the functions constant on the cubes $Q_i^{K\varepsilon}$. If u_ε is a sequence with equibounded energy, $E_\varepsilon(u_\varepsilon) \le c < +\infty$, then every sequence (u_ε^j) is bounded in L^p and then we can extract from it a converging sequence to some u^j for all j. if moreover $u_\varepsilon \rightharpoonup u$ then we have

$$u = \frac{1}{K^d} \sum_{j\in\{1,\dots,K\}^d} u^j.$$

In addition, we have

$$E_\varepsilon(u_\varepsilon) = \sum_{j\in\{1,\dots,K\}^d} \frac{1}{K^d} E_\varepsilon^j(u_\varepsilon^j),$$

so that we deduce the liminf inequality

$$\liminf_{\varepsilon\to 0^+} E_\varepsilon(u_\varepsilon) \ge \sum_{j\in\{1,\dots,K\}^d} \frac{1}{K^d} F^j(u^j) \ge \int_\Omega W_{\rm hom}(u)\,dx, \tag{2.5}$$

where $W_{\rm hom}$ is given by the *homogenization formula*

$$W_{\rm hom}(z) = \min\Big\{ \sum_{j\in\{1,\dots,K\}^d} \frac{1}{K^d} W_j^{**}(z_j) :\ z = \frac{1}{K^d} \sum_{j\in\{1,\dots,K\}^d} z_j \Big\}. \tag{2.6}$$

The upper bound for $u = z$ constant can be obtained by considering optimal z_j in the homogenization formula. Given those, we may consider the oscillating u_ε^j constructed in the previous example and optimal for $F^j(z_j)$. the optimal sequences for $u = z$ are then given by $u_\varepsilon(i) = u_\varepsilon^j(i)$ if $i \in \Omega_{K\varepsilon}^j$. Hence, the functional

$$F_{\rm hom}(u) = \int_\Omega W_{\rm hom}(u)\,dx$$

represents theΓ-limit of E_ε.

Remark 2.2.1 (the homogenization formula) Formula (2.6) corresponds to those in the homogenization theory for scalar integral functionals. It must be noted that the continuous formula can be set as a minimum problem on a periodicity cell, while in this formula we use a convexification involving a mesoscopic scale (and hence a possibly infinite number of cells). Note moreover that on the continuum a relaxation argument allows to consider convex energy densities.

Remark 2.2.2 ("Coarse graining") A proof alternative to the introduction of the variables u^j consists in directly considering the mesoscopic scale, by introducing an average on many periodicity cells (*coarse graining*). To this end, we take $M \in \mathbb{N}$ and estimate the energy $E_\varepsilon(u)$ by the energy $E_\varepsilon^M(v)$ defined on functions $v \in X_{MK\varepsilon}$ by

$$E_\varepsilon^M(v) = \sum_{i \in \Omega_{MK\varepsilon}} (MK\varepsilon)^d \, W^M(v_i),$$

v is given by the average of u; ie,

$$v_i = \frac{1}{(MK)^d} \sum_{k \in \varepsilon\mathbb{Z}^d \cap Q_i^{MK\varepsilon}} u_k.$$

and W^M is given by

$$W^M(z) = \min\Big\{ \sum_{j \in \{1,\dots,MK\}^d} \frac{1}{(MK)^d} W_j(z_j) : \; z = \frac{1}{(MK)^d} \sum_{j \in \{1,\dots,MK\}^d} z_j \Big\}. \tag{2.7}$$

Letting $M \to +\infty$ we have a lower bound with $\inf_M W^M$ (*asymptotic homogenization formula*), which, in this case, coincides with $W_{\rm hom}$ defined above. This *coarse graining* argument is more general than the one used above, and is usually applied to vector problems (ie, when u is a vector) where the 'periodicity cell' description of the limit integrand fails.

Remark 2.2.3 (multi-phase limits) The argument in (2.5) shows that we may equivalently compute the Γ-limit with respect to the convergence $u_\varepsilon \to \mathbf{u} := (u^j)_{j \in \{1,\dots,K\}^d}$ defined by $u_\varepsilon^j \rightharpoonup u^j$ for all j. In this case the Γ-limit is defined on the space of vector-valued functions $L^p(\Omega; \mathbb{R}^{K^d})$, and is given by

$$F(\mathbf{u}) = \sum_{j \in \{1,\dots,K\}^d} \frac{1}{K^d} F^j(u^j).$$

In this way we separately describe the energy relative to each 'species' j. Note that the convergence of (u_ε) thus defined is still compact.

2.3 Nearest-neighbours energies. Microscopic oscillations

In the previous examples we have used arguments where the continuum techniques of relaxation, convexification and homogenization have been adapted to the discrete setting. We now examine an example where a new type of argument must be envisaged to treat the discrete variable.

We consider the case $d = 1$ and Ω a bounded interval. In this case we use a different parameterization of discrete functions. If $N = \#(\varepsilon\mathbb{Z} \cap \Omega)$, then we may reparameterize our energies taking as domain of our functions the set $\{\frac{j}{N} : j = 1, \dots, N\}$ and, with an abuse of notation, we set

$$\varepsilon = \frac{1}{N}, \qquad u_j = u(j\varepsilon).$$

In terms of the functionals we consider this amounts to divide by εN $(= |\Omega| + o(1)$ as $\varepsilon \to 0^+)$ and to reparameterize on $(0, 1)$ the continuum energies.

The energies we are now considering can be written as

$$E_\varepsilon(u) = \sum_{j=1}^{N} \varepsilon W_1(u_j) + \sum_{j=1}^{N-1} \varepsilon W_2(u_j + u_{j+1}).$$

Hence, they sum to a point energy another energy taking into account interactions of *nearest neighbours*. On W_1 and W_2 we make for simplicity the same hypotheses (2.2) of the previous example. By a relaxation argument we can suppose that they are lower semicontinuous.

We briefly examine the estimates that we obtain by repeating the arguments used above, Note that if $u_\varepsilon \rightharpoonup u$ then also for the functions $\overline{u}_\varepsilon$ defined by $(\overline{u}_\varepsilon)_j = ((u_\varepsilon)_j + (u_\varepsilon)_{j+1})/2$ we have $\overline{u}_\varepsilon \rightharpoonup u$. We then obtain the lower bound

$$\begin{aligned} \liminf_{\varepsilon\to 0^+} E_\varepsilon(u_\varepsilon) &\geq \liminf_{\varepsilon\to 0^+} \sum_{j=1}^{N} \varepsilon W_1((u_\varepsilon)_j) + \liminf_{\varepsilon\to 0^+} \sum_{j=1}^{N-1} \varepsilon W_2(2(\overline{u}_\varepsilon)_j) \\ &\geq \int_{(0,1)} W_1^{**}(u)\, dx + \int_{(0,1)} W_2^{**}(2u)\, dt. \end{aligned} \tag{2.8}$$

Conversely, testing the upper bound with $u_\varepsilon(\varepsilon j) = u(\varepsilon j)$ (eg, if u is piecewise constant) we obtain

$$\lim_{\varepsilon\to 0^+} E_\varepsilon(u_\varepsilon) = \int_{(0,1)} (W_1(u) + W_2(2u))\, dt,$$

and then, by relaxation,

$$\Gamma\text{-}\limsup_{\varepsilon\to 0^+} E_\varepsilon(u) \leq \int_{(0,1)} (W_1(u) + W_2(2u))^{**}\, dt. \tag{2.9}$$

The functionals in these bounds are in general different, and then do not allow to conclude the Γ-convergence.

In order to compute the Γ-limit we use a different optimization argument for the nearest-neighbour interactions. In order to formalize it, we write

$$E_\varepsilon(u) = \sum_{j=1}^{N} \varepsilon \frac{1}{2} W_1(u_j) + \sum_{j=0}^{N-1} \varepsilon \frac{1}{2} W_1(u_{j+1}) + \sum_{j=1}^{N-1} \varepsilon W_2(u_j + u_{j+1})$$

$$
\begin{aligned}
&= \sum_{j=1}^{N-1} \varepsilon\Big(\frac{1}{2}W_1(u_j) + \frac{1}{2}W_1(u_{j+1}) + W_2(u_j + u_{j+1})\Big) + \frac{1}{2}\varepsilon W_1(u_N) + \frac{1}{2}\varepsilon W_1(u_1) \\
&\geq \sum_{j=1}^{N-1} \varepsilon W_{\text{eff}}\Big(\frac{u_j + u_{j+1}}{2}\Big), \qquad (2.10)
\end{aligned}
$$

where

$$
W_{\text{eff}}(z) = \min\Big\{\frac{1}{2}W_1(z_1) + \frac{1}{2}W_1(z_2) : \frac{z_1 + z_2}{2} = z\Big\} + W_2(z). \qquad (2.11)
$$

In this way we obtain the lower bound

$$
\Gamma\text{-}\liminf_{\varepsilon\to 0^+} E_\varepsilon(u) \geq \int_{(0,1)} W_{\text{eff}}^{**}(u)\, dt.
$$

In order to check the upper bound we cannot use the discretization of the limit function. If $u = z$ is a constant then we choose u_ε defined by

$$
u_\varepsilon(\varepsilon j) = \begin{cases} z_1 & \text{if } j \text{ is even} \\ z_2 & \text{if } j\text{is odd,} \end{cases}
$$

where z_1 and z_2 minimize the problem in (2.11). The same construction can be repeated if u is piecewise constant, obtaining

$$
\lim_{\varepsilon\to 0^+} E_\varepsilon(u_\varepsilon) = \int_{(0,1)} W_{\text{eff}}(u)\, dt,
$$

and then, by relaxation, the desired upper bound. In conclusion, the Γ-limit is

$$
\Gamma\text{-}\liminf_{\varepsilon\to 0^+} E_\varepsilon(u) = \int_{(0,1)} W_{\text{eff}}^{**}(u)\, dt \qquad (2.12)
$$

and recovery sequences exhibit *microscopic oscillations* on the period 2ε (described by the formula that optimizes the interaction between nearest neighbours, which is a kind of homogenization formula) and mesoscopic oscillations highlighted by the second convexification procedure.

Example 2.3.1 A simple example is obtained by taking

$$
W_1(z) = \begin{cases} 0 & \text{if } z = 1 \text{ or } z = -1 \\ +\infty & \text{otherwise} \end{cases} \qquad W_2(z) = \frac{1}{4}z^2.
$$

Then we have

$$
\min\Big\{\frac{1}{2}W_1(z_1) + \frac{1}{2}W_1(z_2) : \frac{z_1 + z_2}{2} = z\Big\} = \begin{cases} 0 & \text{if } z \in \{-1, 0, 1\} \\ +\infty & \text{otherwise} \end{cases}
$$

and

$$W_{\rm eff}(z) = \begin{cases} z^2 & \text{if } z \in \{-1, 0, 1\} \\ +\infty & \text{otherwise} \end{cases} \qquad W^{**}_{\rm eff}(z) = \begin{cases} |z| & \text{if } |z| \le 1 \\ +\infty & \text{otherwise.} \end{cases}$$

The functions obtained in (2.8) and (2.9) are instead

$$W_1^{**}(z) + W_2^{**}(2z) = \begin{cases} z^2 & \text{if } |z| \le 1 \\ +\infty & \text{otherwise} \end{cases}$$

$$(W_1(z) + W_2(2z))^{**} = \begin{cases} 1 & \text{if } |z| \le 1 \\ +\infty & \text{otherwise.} \end{cases}$$

A comparison with the integrand of the Γ-limit is drawn in Figure 2.1.

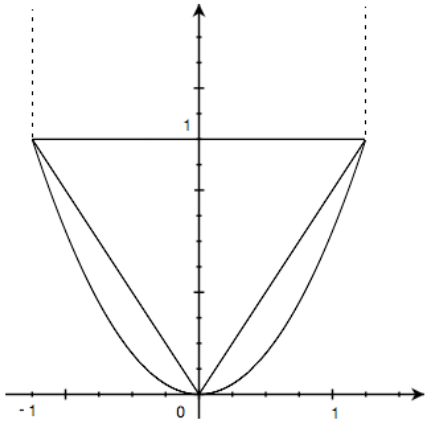


Figure 2.1: the energy function of the Γ-limit in Example 2.3.1 and its comparison with the trivial estimates

Remark 2.3.2 As in Remark 2.1.2 we can equivalently consider functionals

$$E_\varepsilon(z) = \sum_i \varepsilon\, W_1\Big(\frac{z_i - z_{i-1}}{\varepsilon}\Big) + \sum_i \varepsilon\, W_2\Big(\frac{z_{i+1} - z_{i-1}}{\varepsilon}\Big), \tag{2.13}$$

and obtain that the Γ-limit with respect to the strong L^1-convergence, is given by the same energy function as above:

$$F(z) = \int_\Omega W^{**}_{\rm eff}(z')\, dx$$

with domain contained in $W^{1,p}(\Omega)$.

Remark 2.3.3 (open problem) We may consider longer range of interactions; eg, next-to-nearest neighbour interactions, with energy of the form

$$E_\varepsilon(u) = \sum_{j=1}^{N} \varepsilon W_1(u_j) + \sum_{j=1}^{N-1} \varepsilon W_2(u_j + u_{j+1}) + \sum_{j=2}^{N-1} \varepsilon W_3(u_{j-1} + u_j + u_{j+1}).$$

Note that the Γ-limit can always be proven to exist and its energy function is described by an asymptotic homogenization formula W_{asy} obtained by coarse graining.

Question. Is there an analog of formula W_{eff}; ie, a minimization formula over period functions with a fixed finite period (not necessarily 3) such that the Γ-limit can be expressed in the same way (2.12) as above?

Conjecture. The answer to the previous question is negative; ie, there exist W_1, W_2, W_3 such that for all periods the relative formula W_{eff} is strictly larger than W_{asy} at some point.

2.4 One-dimensional spins

We consider one-dimensional energies defined on functions $u : \varepsilon\mathbb{Z} \to \{-1, +1\}$ (*spins*), with nearest-neighbour interaction

$$E_\varepsilon(u) = \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon f(u_i, u_j)$$

(we adopt the notation $u_i = u(\varepsilon i)$).

We now show that we may consider f of a simplified form: first of all, since

$$E_\varepsilon(u) = \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon\Big(\frac{f(u_i, u_j) + f(u_j, u_i)}{2}\Big)$$

we may suppose that f be symmetric: $f(u, v) = f(v, u)$. Hence, up to reparameterization of the points in Ω_ε we may suppose to have the energy

$$E_\varepsilon(u) = \sum_{i=1}^{N} \varepsilon f(u_i, u_{i-1}),$$

with $N = 1/\varepsilon$.

We may rewrite

$$E_\varepsilon(u) = \sum_{i=1}^{N} \varepsilon(f(u_i, u_{i-1}) + g(u_i, u_{i-1})) - \sum_{i=1}^{N} \varepsilon g(u_i, u_{i-1}), \tag{2.14}$$

where $g(u,u) := f(-u,-u)$ and $g(1,-1) = g(-1,1) := \frac{1}{2}(f(1,1) + f(-1,-1))$. By adding such g the integrand in the first sum has the same value in $(-1,-1)$ and $(1,1)$. Note that

$$g(u,v) = \frac{1}{2}g(u,u) + \frac{1}{2}g(v,v), \tag{2.15}$$

and hence we have

$$\sum_{i=1}^{N} \varepsilon g(u_i, u_{i-1}) = \sum_{i=1}^{N-1} \varepsilon\, g(u_i,u_i) + \frac{1}{2}\varepsilon\, g(u_0,u_0) + \frac{1}{2}\varepsilon\, g(u_N,u_N).$$

Since the last two terms can be neglected, the second sum in (2.14) can be rewritten as $\sum_{i=1}^{N-1} \varepsilon W_0(u_i)$, where W_0 is the affine function such that $W_0(\pm 1) = g(\pm 1, \pm 1)$. Note that this sum corresponds to $G(u) = \int_{(0,1)} W_0(u)\, dt$, which is a continuous functional with respect to the weak L^1-convergence, and hence commuted with the Γ-limit. We may limit to considering only the first sum in (2.14). This is an example in which the addition of a continuous perturbation allows us to simplify the form of the functionals we consider.

Summing up, it is not restrictive to suppose that f be symmetric and $f(1,1) = f(-1,-1)$. Hence, excluding the trivial case f constant, there are the two cases: $f(1,1) < f(1,-1)$ and $f(1,1) > f(1,-1)$. Up to translations we may suppose that the two values taken by f be 0 and 1. We may rewrite the two cases as

$$f(u,v) = \frac{1}{4}(u-v)^2, \qquad f(u,v) = \frac{1}{4}(u+v)^2.$$

Note again that, up to multiplicative and additive constants, the two cases correspond, respectively, to

$$f(u,v) = -uv, \qquad f(u,v) = uv.$$

We only treat the first case since the second one can be reduced to the first by the change of variables $w_i = (-1)^i u_i$. We finally consider

$$E_\varepsilon(u) = \frac{1}{4}\sum_{i=1}^{N} \varepsilon (u_i - u_{i-1})^2 \qquad u_i \in \{-1,1\}. \tag{2.16}$$

We may compare E_ε with an energy of the type $\widetilde{E}_\varepsilon(v) = \sum_i \varepsilon W(v_i)$ by setting

$$v_i = \frac{u_i + u_{i-1}}{2}, \qquad W(v) = \begin{cases} 0 & \text{if } v = -1 \text{ or } v = 1 \\ 1 & \text{if } v = 0 \\ +\infty & \text{otherwise.} \end{cases} \tag{2.17}$$

Note that if $u_\varepsilon \rightharpoonup u$ then also $v_\varepsilon \rightharpoonup u$, so that

$$\liminf_{\varepsilon\to 0^+} E_\varepsilon(u_\varepsilon) \geq \liminf_{\varepsilon\to 0^+} \widetilde{E}_\varepsilon(v_\varepsilon) \geq \int_{(0,1)} W^{**}(u)\, dt.$$

The Γ-limsup inequality for E_ε cannot be directly deduced from that for $\widetilde{E}_\varepsilon$ since not all recovery sequences for v_ε are derived from u_ε by (2.17). In order to highlight the error due to the lack of this last correspondence, note that in order to weakly approximate a constant with functions oscillating we have again to introduce a mesoscopic scale $\varepsilon \ll \eta_\varepsilon \ll 1$, and take u_ε oscillating on this scale between 1 and -1. We need only to specify this construction when the limit function is a constant $0 < z < 1$. In that case we define the function $u_z : \mathbb{R} \to \{-1, 1\}$ periodic of period 1 and such that

$$u_z(s) = \begin{cases} 1 & \text{if } 0 < s \leq \frac{z+1}{2} \\ -1 & \text{if } \frac{z+1}{2} < s \leq 1 \end{cases} \qquad \text{and} \qquad u_\varepsilon(i) = u_z\Big(\frac{\varepsilon i}{\eta_\varepsilon}\Big).$$

Since $u_z(t/\eta_\varepsilon) \rightharpoonup z$, also $u_\varepsilon \rightharpoonup z$ and it may be easily checked that it gives the desired value. Hence, we have

$$\Gamma\text{-}\lim_{\varepsilon \to 0^+} E_\varepsilon(u) = \begin{cases} 0 & \text{if } |u| \leq 1 \text{ almost everywhere} \\ +\infty & \text{otherwise.} \end{cases}$$

We may now analyze the Γ-limit at the scale ε. This scale is suggested from the fact that ε is the error that we make when we have a transition from a minimal state identically 1 or -1. In this case we simply have

$$E^{(1)}_\varepsilon(u) = \frac{1}{4} \sum_{i=1}^{N} (u_i - u_{i-1})^2 \qquad u_i \in \{-1, 1\}. \tag{2.18}$$

Hence, if $E^{(1)}_\varepsilon(u_\varepsilon) \leq c < +\infty$ then the piecewise-constant extension of u_ε has a set of discontinuity points $S(u_\varepsilon)$ of cardinality at most c. If

$$\liminf_{\varepsilon \to 0^+} \#S(u_\varepsilon) = M$$

we may then suppose that, up to subsequences, such discontinuity points (t^j_ε) satisfy $0 < t^1_\varepsilon < t^2_\varepsilon < \cdots < t^M_\varepsilon < 1$ and converge to points t^j with $0 \leq t^1 \leq \cdots \leq t^M \leq 1$. Hence, u_ε converges (strongly) to a piecewise-constant function ui,whose set of discontinuity points $S(u)$ is contained in $\{t^j : j = 1, \ldots, M\}$. We then have

$$\liminf_{\varepsilon \to 0^+} E^{(1)}_\varepsilon(u_\varepsilon) = \liminf_{\varepsilon \to 0^+} \#(S(u_\varepsilon)) \geq \#(S(u)).$$

The converse inequality is obtained by taking $u_\varepsilon(\varepsilon i) = u(\varepsilon i)$. Hence, the Γ-limit at scale ε is

$$F^{(1)}(u) = \begin{cases} \#(S(u)) & \text{if } u \text{ is piecewise constant and } u \in \{1, -1\} \text{ a.e.} \\ +\infty & \text{otherwise.} \end{cases}$$

We may hence conclude that E_ε is equivalent to $F_\varepsilon = \varepsilon F^{(1)}$ at scale ε. In this case we may also choose other functionals on the continuum equivalent to E_ε; eg the functionals from the gradient theory of phase transitions

$$F_\varepsilon(u) = \int_0^1 (W_0(u) + \varepsilon^2 |u'|^2)\, dt, \qquad u \in H^1(0,1),$$

with W_0 a double-well potential with minimum in -1 and 1 and such that

$$2\int_{-1}^{1} \sqrt{W(s)}\, ds = 1.$$

Note that the functions on which $F^{(1)}$ is finite are dense for the weak topology in the set of the minimizers of $F^{(0)}$ and hence the development at scale ε is complete.

Remark 2.4.1 (anti-phase interfaces) Note that the parameter w defined by $w_i = (-1)^i u_i$ changes an antiferromagnetic energy (in u) into a ferromagnetic energy (in w). A phase A phase boundary for w corresponds to an *antiphase boundary* of u; ie a passage from a state $(-1)^i$ to $(-1)^{i+1}$.

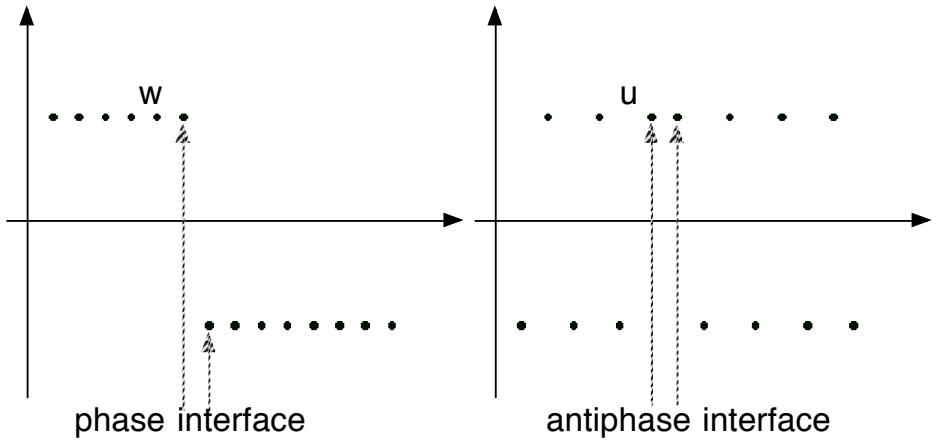


Figure 2.2: phase boundary and corresponding antiphase boundary

Exercise 2.4.2 (homogenization) Let

$$E_\varepsilon(u) = -\sum_i c_i \varepsilon u_i u_{i-1} \text{ with } |u_i| = 1$$

where $i \mapsto c_i$ is positive and M-periodic. Compute the Γ-limit at scale 1 and ε. In particular, prove that the Γ-limit at scale ε is given by

$$F(u) = \Big(\min_i c_i\Big)\, \#S(u).$$

Exercise 2.4.3 (asymmetric case) Let

$$E_\varepsilon(u) = \sum_i \varphi(u_i, u_{i-1}) \text{ with } |u_i| = 1$$

where φ is a non-negative function with $\varphi(u, v) = 0$ only when $u = v$, but not necessarily symmetric. Compute the Γ-limit F of E_ε, showing that if $\varphi(1, -1) \neq \varphi(-1, 1)$ then we have a unique minimizer to the problem

$$\min\Big\{F(u) : \int_0^1 u\, dt = C\Big\},$$

contrary to the symmetric case where we have two minimizers for $|C| < 1$.

Exercise 2.4.4 (long-range interactions) Compute the Γ-limit of

$$E_\varepsilon(u) = \frac{1}{2}\sum_i \sum_{k=1}^K c_k(1 - u_i u_{i-k}) \text{ with } |u_i| = 1$$

(with periodic conditions).

Note first that if we write for $k = 1, \dots, K$, $j = 1, \dots, K$

$$E_\varepsilon^{k,j}(u) = \frac{1}{2}\sum_i c_k(1 - u_{ik+l} u_{(i-1)k+l})$$

each such $E_\varepsilon^{k,j}$ is a n.n. ferromagnetic energy on a lattice of size length εk. Deduce the equality

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon(u) = \sum_{k=1}^K \sum_{j=1}^k E_\varepsilon^{k,j}(u) = \sum_{k=1}^K k c_k\ \#(S(u)).$$

2.5 Boundary layers

As we have remarked earlier, the interaction between nearest neighbours may add to an integral energy an additional phase transition effect. In Section 2.4 the transition is 'sharp', by the nature of the energies; we now examine an example, of general nature, where this transition involves 'boundary layers' at the lattice level. To this end we consider a non-convex point energy perturbed by a nearest-neighbour interaction.

Example 2.5.1 (spins with elastic potential - analysis at scale 1) We consider a spin system where the constraint $u_i \in \{-1, 1\}$ is substituted by a double-well potential; we take

$$W(u) = (|u| - 1)^2,$$

and the energy ($\varepsilon = 1/N$ and $K \in \mathbb{R}$)

$$\begin{aligned} E_\varepsilon(u) &= \sum_{i=1}^{N} \varepsilon(W(u_i) + Ku_iu_{i-1}) \\ &= \sum_{i=1}^{N} \varepsilon\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i + u_{i-1}}{2}\Big)^2\Big) \\ &\quad -\frac{1}{2}\varepsilon W(u_0) + \frac{1}{2}\varepsilon W(u_N). \end{aligned} \tag{2.19}$$

We first analyze the behaviour of E_ε at scale 1.

1. If $K \geq 1$ then we cannot apply the analysis of Section 2.4 to the potential $W(u) - Ku^2$. In this case the Γ-limit is identically $-\infty$. To check that, it suffices to exhibit for all u and for all $M > 0$ a sequence $u_\varepsilon \rightharpoonup u$ such that $E_\varepsilon(u_\varepsilon) \leq -M$. We show that for $u = z$ constant. In this case fix $t > |z|$ and take

$$u_\varepsilon(\varepsilon i) = z + (-1)^i t.$$

We then have

$$E_\varepsilon(u_\varepsilon) \leq (t-1)^2 + z^2 + K(z^2 - t^2) + \varepsilon(t + |z|)^2.$$

Since the second term tends to $-\infty$ per $t \to +\infty$ we have the desired estimate.

2. Conversely, if $K \leq -1$ the nearest-neighbours term gets unbounded and again the Γ-limit is identically $-\infty$. In this case if u is continuous it suffices to take $u_\varepsilon(\varepsilon i) = u(\varepsilon i)$, obtaining

$$\lim_{\varepsilon \to 0^+} E_\varepsilon(u_\varepsilon) = \int_{(0,1)} \Big((|u| - 1)^2 + Ku^2\Big)\, dt.$$

Since the convex envelope of the integrand on the right-hand side is $-\infty$ the desired estimate follows by relaxation.

3. If $-1 < K < 1$ we can apply the analysis of Section 2.4, obtaining the 'effective' integrand

$$W_{\rm eff}(u) = \frac{K}{K-1} + 2Ku^2 + (1-K)\min\Big\{\Big(|u| - \frac{1}{1-K}\Big)^2, u^2\Big\}.$$

Such a function may take three different shapes as in Figure 2.3.

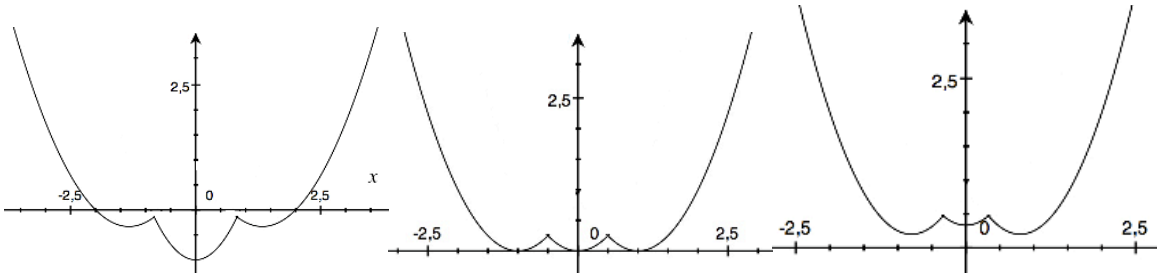


Figure 2.3: 'effective integrands' for elastic spins ($0 < K < 1$, $K = 0$ and $-1 < K < 0$)

Example 2.5.2 (analysis at scale ε: boundary layers) We may now examine the next scale, that, as in the case of spins, is ε. We examine the three non-trivial cases of the previous example.

1: $-1 < K < 0$. In this case the minimizers of the limit energy are all the functions u with $\|u\|_\infty \le \frac{1}{1+K}$, and their common value of the energy is $\frac{K}{K+1}$

We examine the energy

$$\begin{aligned} E_\varepsilon^{(1)}(u) &= \sum_{i=1}^{N}\Big(W(u_i) + Ku_iu_{i-1} - \frac{K}{K+1}\Big) \\ &= \sum_{i=1}^{N}\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2 - \frac{K}{K+1}\Big) \\ &\quad -\frac{1}{2}W(u_0) + \frac{1}{2}W(u_N). \end{aligned} \tag{2.20}$$

From $E_\varepsilon^{(1)}(u) \le M$ we first deduce that we may estimate the number of indices i where $(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2$ is not close to its minimum $\frac{K}{K+1}$. Since that minimum is obtained only for $u_i = u_{i-1} \in \{-1/(1+K), 1/(1+K)\}$, more precisely, we have:

• with fixed $\eta > 0$ the number of indices i such that we do not have at the same time $|u_i - \frac{1}{1+K}| \le \eta$ and $|u_{i-1} - \frac{1}{1+K}| \le \eta$, or at the same time $|u_i + \frac{1}{1+K}| \le \eta$ and $|u_{i-1} + \frac{1}{1+K}| \le \eta$ is bounded by a constant $C(\eta, M)$ independent of ε.

We may hence consider such indices and regroup then in sets of consecutive indices (we omit the dependence on ε): $\{i_k^j : j \in \{0,\dots,J+1\},\ k \in \{0,\dots,M_j\}$. We may suppose that $i_0^0 = 0$ and $i_{M_{J+1}}^{J+1} = N$ and moreover that if $|u_i - 1/(1+K)| \le \eta$ for $i = i_0^j - 1$, then for $i = i_{J_j}^j + 1|$ we have $|u_i + 1/(1+K)| \le \eta$ (ie, in each such group of indices, except the extreme ones, the function has a phase transition approximately between $1/(1+K)$ and $-1/(1+K)$).

We may hence give a lower bound of our energy taking into account only the contribution from those sets of indices, by $2B_\eta + D_\eta J$, where

$$\begin{aligned} B_\eta &= \inf\Big\{\sum_{i=1}^{M}\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2 - \frac{K}{K+1}\Big) \\ &\quad -\frac{1}{2}W(u_0) : |u_{M-1} - 1/(K+1)| \le \eta, |u_M - 1/(K+1)| \le \eta,\ M \in \mathbb{N}\Big\} \end{aligned}$$

and

$$\begin{aligned} D_\eta &= \inf\Big\{\sum_{i=-M}^{M}\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2 - \frac{K}{K+1}\Big) : \\ &\quad |u_{\pm M-1} \pm 1/(K+1)| \le \eta, |u_{\pm M} \pm 1/(K+1)| \le \eta,\ M \in \mathbb{N}\Big\}. \end{aligned}$$

As $\eta \to 0$ these two quantities tend, respectively, to

$$\begin{aligned} B &= \inf\Big\{\sum_{i=-M}^{M}\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2 - \frac{K}{K+1}\Big) \\ &\quad -\frac{1}{2}W(u_0) : u_{M-1} = \frac{1}{(K+1)},\ u_M = \frac{1}{(K+1)},\ M \in \mathbb{N}\Big\} \end{aligned}$$

and

$$\begin{aligned} D &= \inf\Big\{\sum_{i=1}^{M}\Big(\frac{1}{2}(W(u_i) - Ku_i^2) + \frac{1}{2}(W(u_{i-1}) - Ku_{i-1}^2) + 2K\Big(\frac{u_i+u_{i-1}}{2}\Big)^2 - \frac{K}{K+1}\Big) : \\ &\quad u_{\pm M-1} = \pm\frac{1}{(K+1)},\ u_{\pm M} = \pm\frac{1}{(K+1)},\ M \in \mathbb{N}\Big\}. \end{aligned}$$

The constant B represent the energy of an *external boundary layer*, with a condition at infinity given by the constant minimal state $\frac{1}{(K+1)}$. The constant D represents the energy of an *internal boundary layer*, with conditions at $\pm\infty$ the two minimal states $\pm\frac{1}{(K+1)}$, respectively.

By applying this argument to a sequence u_ε with bounded energy we obtain that

• up to subsequences it converges to a piecewise-constant function u with $u \in \{\pm 1/(K+1)\}$;

• having denoted by $S(u)$ the set of discontinuity points of u we have

$$\liminf_{\varepsilon \to 0^+} E_\varepsilon(u_\varepsilon) \geq 2B + D\#(S(u)).$$

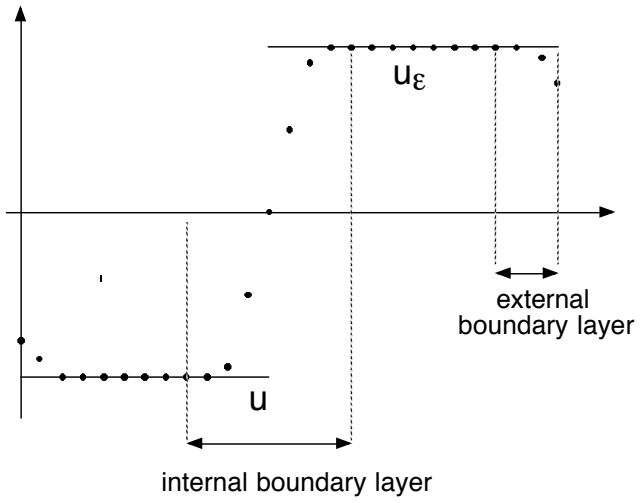


Figure 2.4: boundary layers

From the definition of B and D it is immediate also to construct a recovery sequence for a piecewise-constant function u with $u \in \{1/(K+1), -1/(K+1)\}$, by joining constant interpolations with (almost) minimal transitions for the problems defining the two constants (see Figure 2.4).

For the sake of completeness we also include the analysis of the other two cases.

2: $0 < K < 1$. Consider for simplicity periodic boundary conditions: $u_0 = u_N$ and N even. In this case the Γ-limit of the scaled functionals is simply

$$F^{(1)}(u) = \begin{cases} 0 & \text{if } u = 0 \\ +\infty & \text{otherwise.} \end{cases}$$

Recovery sequences for $u = 0$ are given by $u_\varepsilon(\varepsilon i) = \frac{1}{1-K}(-1)^i$ and $u_\varepsilon(\varepsilon i) = -\frac{1}{1-K}(-1)^i$.

Note that if instead N is odd, the Γ-limit must take into account the presence of anti-phase interfaces due to the incompatibility of recovery sequences at the periodicity condition. In this case we have to introduce a new parameter as in the case of antiferromagnetic spins.

3: K=0. In this case the effect of the nearest neighbours disappears and the analysis at scale ε^α for all $\alpha > 0$ is particularly simple. The Γ-limit of

$$E_\varepsilon^{(\alpha)}(u) = \sum_{i=1}^{N} \varepsilon^{1-\alpha}\, W(u_i)$$

is

$$F^{(\alpha)}(u) = \begin{cases} 0 & \text{if } \|u\|_\infty \leq 1 \\ +\infty & \text{otherwise.} \end{cases}$$

Since the Γ-limit must be $+\infty$ except than on minimizers of the Γ-limit at scale 1 it suffices to check that $F^{(\alpha)}(u) = 0$ if $\|u\|_\infty \leq 1$. This is an immediate consequence of $W(1) = W(-1) = 0$.

2.6 Limits depending on a *pattern variable*

We now show how we may have limits where the relevant parameter in the final energy must be carefully chosen so as to distinguish different ground states. A very simple case is that of anti-ferromagnetic spin systems where ground states are two two-periodic states oscillating between 1 and -1. In that case we have again two parameters and a change of variable allows to go back to the analysis of ferromagnetic spin systems. We now see how we can modify that example to obtain more complex ground states.

We consider the one-dimensional spin energies defined on $u : \varepsilon\mathbb{Z} \cap [0,1] \to \mathbb{R}$ with nearest and next-to-nearest interactions of the form

$$E_\varepsilon(u) = \sum_{i=0}^{N} \varepsilon(\alpha u_i u_{i-1} + u_{i-1}u_{i+1})$$

(with the notation $u_i = u(\varepsilon i)$), where we suppose that $N = 1/\varepsilon$ be integer. In order to avoid boundary effects we consider periodic boundary conditions

$$u_N = u_0; \qquad u_{N+1} = u_1; etc.,$$

so that we may write

$$E_\varepsilon(u) = \sum_{i=0}^{N} \varepsilon\Big(\frac{1}{2}\alpha(u_i u_{i-1} + u_{i+1}u_i) + u_{i-1}u_{i+1}\Big)$$

Ground states of E_ε can be looked for among the functions (if they exist) that for all i minimize the corresponding term in the sum. Depending on α we obtain the three cases:

(1) $\alpha < 2$. In this case the nearest-neighbour ferromagnetic term dominates and the minimizers are the constants ± 1;

(2) $\alpha > 2$. In this case the oscillations between nearest neighbours dominate, and we have the two minimizers $\pm(-1)^i$, of period 2;

(3) $|\alpha| < 2$. In this case the interactions between second neighbours dominates; hence, we have four minimizers, corresponding to the four possible combinations of the 'antiferromagnetic' oscillating minimizers for second neighbours. The ground states are 4-periodic functions of the form

$$(u^k)_i = v_{i+k},$$

$(k = 0, 1, 2, 3)$, where $v = u^0$ is given by

$$v_j = \begin{cases} 1 & \text{if } j = 1, 2 \\ 1 & \text{if } j = 3, 4. \end{cases}$$

(see Figure 2.5).

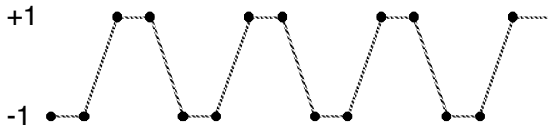


Figure 2.5: a 4-periodic minimizer

In the case $\alpha = -2$ we have six ground states (both those for $\alpha < -2$ and those for $|\alpha| < 2$), and analogously in the case $\alpha = 2$.

2.6.1 Analysis at scale ε

The interesting case is (3). Note that in order to have absolute minimizers compatible with ground states we would have to suppose that N be a multiple of 4 In any case, we may scale our functional noting that for ground states we have

$$\frac{1}{2}\alpha(v_i v_{i-1} + v_{i+1} v_i) + v_{i-1} v_{i+1} = -1$$

and consider the scales energies

$$E_\varepsilon^{(1)}(u) := \frac{1}{\varepsilon}(E_\varepsilon(u) - \min E_\varepsilon) = \sum_{i=0}^{N} \Big(\frac{1}{2}\alpha(u_i u_{i-1} + u_{i+1} u_i) + u_{i-1} u_{i+1} + 1 \Big)$$

(in the case N is not a multiple of 4 the translation does not correspond to the value of the minimum of E_ε).

To understand the behaviour of this energy consider the particular case $\alpha = 0$ and N even. In such a case the interactions between odd and even indices are decoupled,

and correspond to two antiferromagnetic disjoint systems. To each of such energy we can associate a macroscopic variable, v_1 (odd) and v_2 (even) with values ± 1 corresponding to the alternating microscopic states. The overall continuous variable is then the vector variable $v = (v_1, v_2)$ and the limit energy is

$$F(v) = \#(S(v_1)) + \#(S(v_2)),$$

which can also be written in a more general form as

$$\sum_{t \in S(v)} \psi(|v_1^+ - v_1^-| + |v_2^+ - v_2^-|),$$

with $\psi(t) = t/2$. In the general case when the odd and even lattices are not decoupled, then it is more convenient to introduce a *pattern variable*.

Compactness. Note that if $\sup_\varepsilon E_\varepsilon^{(1)}(u_\varepsilon) < +\infty$ then, up to subsequences, there exist $K \in \mathbb{N}$ and a finite number of indices $I_1^\varepsilon, \dots, i_K^\varepsilon$ such that $\varepsilon i_j^\varepsilon \to x_j \in [0,1]$ and, having set $x_0 = 0$ and $x_{K+1} = 1$, if $x_j \neq x_{j-1}$ then there exists $\phi_j \in \{0,1,2,3\}$ such that

$$u_\varepsilon(\varepsilon i) = v_i + \phi_j \text{ definitively locally in } (x_{j-1}, x_j) \tag{2.21}$$

Definition of the order parameter. Let $\phi : [0,1] \to \{0,1,2,3\}$ be a piecewise-constant function. We say that $u_\varepsilon \to \phi$ if there exists a finite set of points $0 = x_0 < x_1 < \dots < x_M = 1$ such that $\phi = \phi_j$ on (x_{j-1}, x_j) and (2.21) holds.

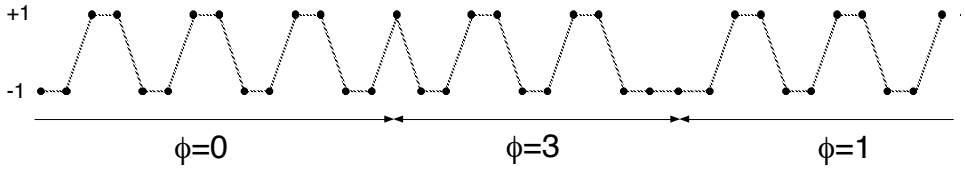


Figure 2.6: a function u and its corresponding *phase parameter* ϕ

Computation of the Γ-limit. We may localize the reasoning and compute the Γ-limit just for an optimal transition between two states corresponding to u^k and u^{k+l} with $l \in \{1,2,3\}$. The energy of such a transition is obtained by a minimal-transition problem

$$\begin{aligned} \psi(l) \quad = \quad & \min\Big\{ \sum_{i=-\infty}^{+\infty} \Big(\frac{1}{2}\alpha(u_i u_{i-1} + u_{i+1} u_i) + u_{i-1} u_{i+1} + 1 \Big) : \\ & u_i = (u^0)_i \text{ for } i \le -4, u_i = (u^l)_i \text{ for } i \ge -4 \Big\}. \end{aligned}$$

This value is computed over a finite set of states, and can be easily seen to be

$$\psi(l) = \begin{cases} \min\{6 - 3\alpha, 2 + \alpha\} & \text{if } l = 1 \\ 2 - 2|\alpha| & \text{if } l = 2 \\ \min\{6 + 3\alpha, 2 - \alpha\} & \text{if } l = 3. \end{cases}$$

The Γ-limit has the form

$$F(\phi) = \sum_{t \in S(\phi) \cap [0,1)} \psi(|\phi(t^+) - \phi(t^-)|),$$

where ϕ is extended periodically outside $(0, 1)$.

2.6.2 Three-point interactions

We may consider (directly in the surface scaling) interaction between three (or more) neighbouring points; i.e., of the form

$$E_\varepsilon(u) = \sum_i f(u_{i-1}, u_i, u_{i+1})$$

It is interesting to note that next-to-nearest neighbours interactions can be seen as a particular case of three-point interactions where

$$f(u_{i-1}, u_i, u_{i+1}) = \frac{1}{2}\Big(f_1(u_i, u_{i+1}) + f_1(u_{i-1}, u_i)\Big) + f_2(u_{i-1}, u_{i+1}).$$

The pattern energy above can be recovered when f is minimized by triplets of the form $(\pm 1, \pm 1, \mp 1)$ and $(\pm 1, \mp 1, \mp 1)$.

2.7 Ternary systems: multiscale limits

We now highlight a further phenomenon due to the presence of more than two competing 'species' of phases. We consider $u : \varepsilon\mathbb{Z} \cap [0, 1] \to \{-1, 0, 1\}$, and $\varphi : \{-1, 0, 1\}^2 \to \mathbb{R}$ satisfying the following properties:

(i) (symmetry) $\varphi(u, v) = \varphi(v, u) = \varphi(-u, -v)$

(ii) (uniform ground states) $\operatorname{argmin} \varphi = \{(1, 1), (-1, -1)\}$ and, wlog, $\min \varphi = 0$;

(iii) (optimal phase transition) $\varphi(-1, 1) > 2\,\varphi(0, 1) > 0$.

The energies we consider are

$$E_\varepsilon(u) = \sum_i \varphi(u_i, u_{i-1}).$$

As usual we suppose that $N = 1/\varepsilon$ is integer and we assume periodic boundary conditions so as to avoid boundary effects. Condition (ii) ensures that ground states are only the constant functions identically equal to 1 and -1. Condition (iii) implies that if we have a transition between 1 and -1 it is energetically favourable to insert a 0 phase

If $\{u_\varepsilon\}$ is a sequence with $\sup E_\varepsilon(u_\varepsilon) = C < +\infty$ then we deduce that $\varphi((u_\varepsilon)_i(u_\varepsilon)_{i-1}) = 0$ except for a finite set of i. Up to subsequences, we may suppose that this set may be written as

$$I_\varepsilon := \{i_1^\varepsilon, \dots, i_M^\varepsilon\}$$

for some M. We also define $i_0^\varepsilon = 0$ and $i_{M+1}^\varepsilon = N$. Note that condition (i) gives

- $(u_\varepsilon)_i = (u_\varepsilon)_{i_k^\varepsilon} \in \{-1, 1\}$ for $i = i_k^\varepsilon, \dots, i_{k+1}^\varepsilon - 1$ for all $k = 0, \dots M$;
- if $J_\varepsilon := \{\varepsilon i : (u_\varepsilon)_i = 0\}$ then $\#J_\varepsilon \leq M$.

Note then the 'multiscale behaviour' of the parameters:

(i) the 0-phase is not detected by L^1-convergence; moreover, the piecewise-constant extensions of u_ε converge to a function $u \in BV((0,1); \{\pm 1\})$;

(ii) the 0-phase is concentrated on a finite number of points, which converge, up to subsequences, to points in the set $J := \{x_1, \dots, x_M\}$. Note that some of these points may coincide.

It is convenient to consider the measures

$$\mu_\varepsilon = \sum_{i \in J_\varepsilon} \delta_{\varepsilon i} \, .$$

Up to subsequences these measures converge weakly* to a measure

$$\sum_{x \in J} k(x) \delta_x,$$

with $k(x) \in \mathbb{N}$ representing the number of sequences in J_ε converging to x.

We may alternatively compute the Γ-limit with respect to L^1-convergence (thus integrating out the effect of the 0-phase in the limit), or with respect the convergence in $L^1 \times \mathcal{M}$. The energies are coercive with respect to both convergences. The second Γ-limit gives more information, and is compatible with more constraints (eg, if we fix the total mass of μ_ε or, equivalently the number of points in J_ε).

Theorem 2.7.1 (multiphase limits) *The Γ-limit is finite on pairs function/measures (u, μ) as above, and is of the form*

$$F(u, \mu) = C_0 \#(S(u) \setminus J) + \sum_{x \in J} (C_1 + C_2(k(x) - 1)) \, ,$$

where

$$\begin{aligned} C_0 &= \varphi(1, -1), \\ C_1 &= 2\,\varphi(0, 1), \\ C_2 &= \min\{\varphi(0, 0), 2\,\varphi(0, 1)\} \, . \end{aligned}$$

Proof. If $x \in S(u) \setminus J$ then there exist no sequences of points of $\varepsilon J_\varepsilon$ converging to x; hence we have at least one index i with $\varepsilon i \to x$ and $\varphi((u_\varepsilon)_i, (u_\varepsilon)_{i-1}) = \varphi(1, -1)$

If $x \in J$ then there exist at least two indices i such that $\varphi((u_\varepsilon)_i(u_\varepsilon)_{i-1}) = \varphi(0, \pm 1)$; The other interactions of i where $(u_\varepsilon)_i = 0$ or $(u_\varepsilon)_{i-1} = 0$ satisfy

$$\varphi((u_\varepsilon)_i, (u_\varepsilon)_{i-1}) \geq \min\{\varphi(0,1), \varphi(0,0)\}$$

so that (taking into account that $(0,0)$ pairs are counted twice) for any such x we have a contribution of at least $C_1 + C_2(k(x) - 1)$.

The recovery sequences are constructed by optimizing the process above, and are pictured in Figures 2.7 and 2.8. □

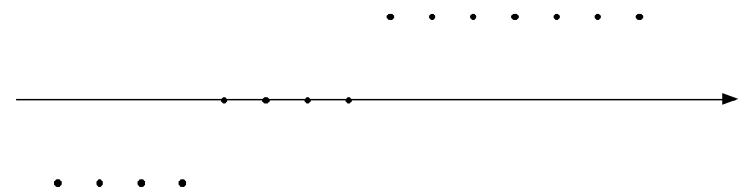


Figure 2.7: recovery sequence in the case $\varphi(0,0) < 2\,\varphi(0,1)$ for $k(x) = 4$

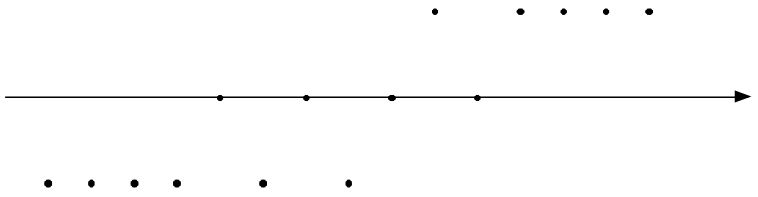


Figure 2.8: recovery sequence in the case $\varphi(0,0) > 2\,\varphi(0,1)$ for $k(x) = 4$

Note that we may rewrite F as

$$F(u,\mu) = \sum_{x \in S(u)} \psi(k(x)) + \sum_{x \in J \setminus S(u)} \left(C_1 + C_2(k(x) - 1)\right),$$

where ψ given by

$$\psi(k) = \begin{cases} C_0 & \text{if } k = 0 \\ C_1 - C_2 + C_2 k & \text{if } k \geq 1 \end{cases}$$

highlights the effect of the 0-variable on the interface.

Corollary 2.7.2 *The Γ-limit with respect to the L^1-convergence is given by*

$$F(u) = C_1 \#(S(u)).$$

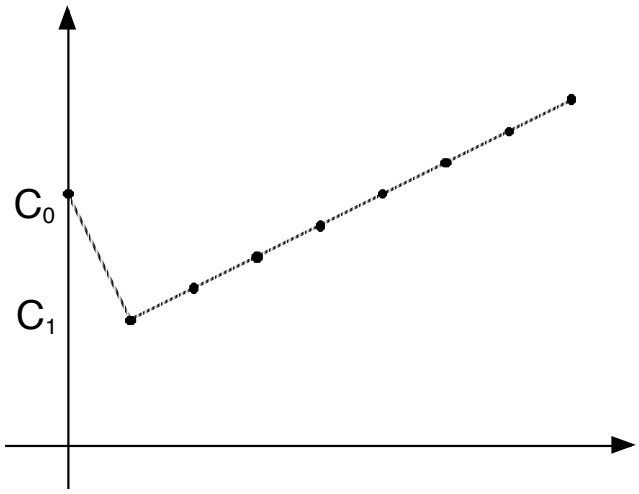


Figure 2.9: dependence of the interfacial energy on the 0-variable density

Proof. The Γ-limit is obtained from the theorem above by choosing $J = S(u)$ and $k(x) = 1$; ie $\mu = \sum_{x \in S(u)} \delta_x$. □

Exercise 2.7.3 Let $K > 0$ be a fixed natural number and let $E_\varepsilon(u)$ be defined as above with the constraint that $\#\{i : u_i = 0\} = K$. Prove that the Γ-limit with respect to the L^1-convergence is given by

$$F(u) = \begin{cases} C_1 + C_2(K-1) & \text{if } u \text{ is constant} \\ (C_1 - C_2)\#\, S(u) + C_2\, K & \text{otherwise.} \end{cases}$$

2.8 Bibliographical notes

One-dimensional examples can also be found in
[1] A. Braides and M.S. Gelli. From discrete systems to continuous variational problems: an introduction. In *Topics on concentration phenomena and problems with multiple scales* (A. Braides and V. Chiadò Piat, eds.), *Lect. Notes Unione Mat. Ital.* **2** Springer, Berlin, 2006, 3–77.

Boundary layers are described in
[2] A. Braides and M.Cicalese. Surface energies in nonconvex discrete systems. *M3AS* **17** (2007) 985-1037

Ternary systems (in any dimension) are studied in
[3] R. Alicandro, M. Cicalese, and L. Sigalotti. Phase transition in the presence of surfactants: from discrete to continuum. Preprint cvgmt.sns.it

Chapter 3

Spin Systems

In this section we consider energies defined on functions $u : \Omega_\varepsilon := \varepsilon\mathbb{Z}^d \cap \Omega \to \{-1, +1\}$.

3.1 Nearest-neighbour interactions

We first consider energies taking into account only nearest-neighbour interactions; i.e., of the form

$$E_\varepsilon(u) = \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon^d f(u_i, u_j)$$

(we adopt the notation $u_i = u(\varepsilon i)$).

Following the arguments in Section 2.4, which are valid in any dimension, it is not a restriction to limit our analysis to two f:

i) $f(u, v) = \frac{1}{4}(u - v)^2$ (ferromagnetic energies). In this case the minimization of E_ε favours uniform states $u \equiv 1$ or $u \equiv -1$;

ii)$f(u, v) = \frac{1}{4}(u - v)^2$ (antiferromagnetic energies). In this case the minimization of E_ε favours configurations with nearest neighbours of changing sign.

We will mainly concentrate on the first of the two cases, as the second one can be reduced to the first (for the cubic lattice) by the change of variables $w_i = (-1)^i u_i$, where $(-1)^i = (-1)^{i_1+i_2+\ldots+i_d}$.

Hence, we consider the family of energies

$$E_\varepsilon(u) = \frac{1}{4} \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon^d (u_i - u_j)^2 \qquad u_i \in \{-1, 1\}. \tag{3.1}$$

As in the one-dimensional case, we may relate to E_ε a point-energy functional as follows. We introduce the 'dual lattice' of $\mathbb{Z}^d$

$$\mathcal{Z} = \Big\{ \frac{i+j}{2} : i, j \in \mathbb{Z}^d, |i-j| = 1 \Big\},$$

and correspondingly

$$\Omega'_\varepsilon = \varepsilon\mathcal{Z} \cap \Omega$$

and to every $u : \Omega_\varepsilon \to \{-1, +1\}$ we associate a new function $v : \Omega'_\varepsilon \to \{-1, 0, +1\}$ defined by

$$v_k = \frac{u_i + u_j}{2}, \text{ where } k \in \mathcal{Z} \text{ and are such that } k = \frac{i+j}{2},\ i, j \in \mathbb{Z}^d,\ |i-j| = 1. \tag{3.2}$$

Note that v is such that

$$v_k = \begin{cases} -1 & \text{if } u_i = u_j = -1 \\ 0 & \text{if } u_i = -u_j \\ 1 & \text{if } u_i = u_j = 1. \end{cases}$$

We then obtain

$$E_\varepsilon(u) = \sum_{\varepsilon k \in \Omega'_\varepsilon} \varepsilon^d W(v_k) =: \widetilde{E}_\varepsilon(v),$$

where

$$W(v) = \begin{cases} 0 & \text{if } v = -1 \text{ or } v = 1 \\ 1 & \text{if } v = 0 \\ +\infty & \text{otherwise.} \end{cases} \tag{3.3}$$

Note that if $u_\varepsilon \rightharpoonup u$ then also $v_\varepsilon \rightharpoonup u$ (here v_ε is identified with its piecewise-constant interpolations on the cells of the dual lattice, so that

$$\liminf_{\varepsilon \to 0^+} E_\varepsilon(u_\varepsilon) \geq \liminf_{\varepsilon \to 0^+} \widetilde{E}_\varepsilon(v_\varepsilon) \geq d \int_\Omega W^{**}(u)\, dt,$$

where in the last inequality we have taken into account that the measure of the reference unit cell in the dual lattice $\mathcal{Z}$ is $\frac{1}{d}$

As in one dimension the Γ-limsup inequality for E_ε cannot be directly deduced from that for $\widetilde{E}_\varepsilon$. In the case when the limit function is of the form $u = 2\chi_C - 1$ with C sufficiently regular, eg C a finite union of cubes of $\mathbb{R}^d$, then a recovery sequence is given by $u_\varepsilon(\varepsilon i) = u(\varepsilon i)$. Indeed, for these functions the energy concentrates on the interface $\partial C \cap \Omega$; ie, all the strictly positive contributions derive from nearest-neighbour interactions with $\varepsilon i, \varepsilon j$ on opposite sides of ∂C (for which we have $v_\varepsilon(\varepsilon k) = 0$ for $k = \frac{i+j}{2}$) and

$$\lim_{\varepsilon \to 0} E_\varepsilon(u_\varepsilon) = \lim_{\varepsilon \to 0} \varepsilon(d-1\text{-dimensional measure of } \partial C \cap \Omega) = 0. \tag{3.4}$$

Hence, we have

$$\Gamma\text{-}\lim_{\varepsilon \to 0^+} E_\varepsilon(u) = \begin{cases} 0 & \text{if } |u| \leq 1 \text{ a.e.} \\ +\infty & \text{otherwise.} \end{cases}$$

3.1.1 Phase and anti-phase transitions

As in the one-dimensional case, the construction of recovery sequences at scale 1 suggest to analyze the limit at scale ε. We then scale the energy as

$$E_\varepsilon^{(1)}(u) = \frac{E_\varepsilon(u)}{\varepsilon} = \frac{1}{4} \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon^{d-1}(u_i - u_j)^2 \qquad u_i \in \{-1, 1\}. \tag{3.5}$$

From now on we suppose that Ω has a Lipschitz boundary. Let u_ε be such that $\sup_\varepsilon E_\varepsilon^{(1)}(u_\varepsilon) < +\infty$ and set $G_\varepsilon := \{u_\varepsilon = 1\}$. Note that the interaction energy between two nearest neighbours is 0 if $\varepsilon i,\ \varepsilon j \in G_\varepsilon$ and is ε^{d-1} otherwise; that is, exactly the $d-1$-dimensional measure of the common boundary of the two cells $\varepsilon(i + [-\frac{1}{2}, \frac{1}{2})^d)$ and $\varepsilon(j + [-\frac{1}{2}, \frac{1}{2})^d)$. Hence, having set

$$I_\varepsilon := \left\{ i \in \mathbb{Z}^d : \varepsilon\Big(i + [-\frac{1}{2}, \frac{1}{2})^d\Big) \subset \Omega \right\}, \qquad \tilde{\Omega}_\varepsilon := \bigcup_{i \in I_\varepsilon} \varepsilon\Big(i + [-\frac{1}{2}, \frac{1}{2})^d\Big),$$

we have

$$E_\varepsilon^{(1)}(u_\varepsilon) \geq \mathcal{H}^{d-1}(\partial G_\varepsilon \cap \tilde{\Omega}_\varepsilon). \tag{3.6}$$

Moreover, since Ω has Lipschitz boundary,

$$\mathcal{H}^{d-1}(\partial G_\varepsilon \setminus \tilde{\Omega}_\varepsilon) \leq c\mathcal{H}^{d-1}(\partial\Omega). \tag{3.7}$$

Hence, by Theorem 1.3.6, from (3.6) and (3.7) we deduce that, up to subsequences, G_ε converges in measure to a set of finite perimeter $G \subset \Omega$; ie, u_ε converges strongly in L^1 to $u = -1 + 2\chi_G$. We now analyze the Γ-limit of $E_\varepsilon^{(1)}$ with respect to the L^1-convergence.

We may optimize estimate (3.6) by observing that ν_{G_ε} may only take the values $\pm e_k,\ k = 1, \dots, d$, and then, for all $\Omega' \subset\subset \Omega$, we have

$$E_\varepsilon^{(1)}(u_\varepsilon) \geq \int_{\partial G_\varepsilon \cap \Omega'} \varphi(\nu_{G_\varepsilon})\, d\mathcal{H}^{d-1}, \tag{3.8}$$

for every norm φ such that $\varphi(e_k) \leq 1$ for all $k = 1, \dots, d$. The largest such norm is

$$\|\nu\|_1 := \sum_{k=1}^d |\nu_k|, \quad \nu = (\nu_1, \dots, \nu_d).$$

Hence, thanks to (3.8) and Theorem 1.3.7, we have

$$\liminf_{\varepsilon \to 0} E_\varepsilon^{(1)}(u_\varepsilon) \geq \sup_{\Omega' \subset\subset \Omega} \int_{\partial^* G \cap \Omega'} \|\nu_G\|_1\, d\mathcal{H}^{d-1} = \int_{\partial^* G} \|\nu_G\|_1\, d\mathcal{H}^{d-1}. \tag{3.9}$$

As for the Γ-lim sup inequality, it is sufficient to construct a recovery sequence for a polyhedral set G. For such a set we may easily check that the sequence $u_\varepsilon(\varepsilon i) := -1 + 2\chi_G(\varepsilon i)$ is such that

$$\lim_{\varepsilon\to 0} E_\varepsilon^{(1)}(u_\varepsilon) = \int_{\partial G} \|\nu_G\|_1 \, d\mathcal{H}^{d-1}.$$

Hence, we have

$$E^{(1)}(G) := \Gamma\text{-}\lim_{\varepsilon\to 0^+} E_\varepsilon^{(1)}(G) = \begin{cases} \displaystyle\int_{\partial^* G} \|\nu_G\|_1 \, d\mathcal{H}^{d-1} & \text{if } Per(G) < +\infty \\ +\infty & \text{otherwise.} \end{cases} \tag{3.10}$$

Remark 3.1.1 (minimal interface problems) We consider the minimum problems

$$m_\varepsilon := \min\left\{ E_\varepsilon^{(1)}(u) : \ \#\{i : \ u_i = 1\} = p_\varepsilon \#\, \Omega_\varepsilon \right\},$$

where p_ε is chosen such that $m_\varepsilon \not\equiv +\infty$ (eg, we may take p_ε such that $p_\varepsilon \#\Omega_\varepsilon \in \mathbb{N}$) and $p_\varepsilon \to p \in [0,1]$. Then thanks to the previous Γ-convergence result, we have that minimizers of m_ε converge to functions minimizing

$$m := \min\left\{ \int_{\partial^* G} \|\nu_G\|_1 \, d\mathcal{H}^{d-1} : \ |G| = p\,|\Omega| \right\}.$$

To check this it suffices to check that for $|G| = p\,|\Omega|$ we may construct a recovery sequence u_ε for G in such a way that $\#\{i : \ u_\varepsilon(\varepsilon i) = 1\} = p_\varepsilon \#\, \Omega_\varepsilon$. It is sufficient to show this for G a polyhedral set. In this case, consider the recovery sequence $\tilde{u}_\varepsilon(\varepsilon i) = -1 + 2\chi_G(\varepsilon i)$ (which may not satisfy $\#\{i : \ \tilde{u}_\varepsilon(\varepsilon i) = 1\} = p_\varepsilon \#\, \Omega_\varepsilon$)strongly converging in L^1 to $-1+2\chi_G$. Having set $\tilde{c}_\varepsilon := \#\{i : \ \tilde{u}_\varepsilon(\varepsilon i) = 1\}$, $\varepsilon^d \tilde{c}_\varepsilon$ converges to $p|\Omega|$. Hence, if we set $c_\varepsilon := p_\varepsilon \#\Omega_\varepsilon$, we have $\varepsilon^d(c_\varepsilon - \tilde{c}_\varepsilon) \to 0$. We may suppose, eg, that $c_\varepsilon > \tilde{c}_\varepsilon$ and set $l_\varepsilon := (c_\varepsilon - \tilde{c}_\varepsilon)^{\frac{1}{d}}$, $\bar{l}_\varepsilon := [l_\varepsilon]$, where we denote by $[t]$ the integer part of $t \in \mathbb{R}$. Note that $\varepsilon l_\varepsilon \to 0$ and $0 < l_\varepsilon^d - \bar{l}_\varepsilon^d \le d l_\varepsilon^{d-1}$. We choose i_ε such that $Q_\varepsilon := \varepsilon i_\varepsilon + [0, \bar{l}_\varepsilon \varepsilon)^d \subset \Omega \setminus G$ and let $J_\varepsilon \subset (\Omega \setminus (G \cup Q_\varepsilon)) \cap \varepsilon\mathbb{Z}$ be such that $\# J_\varepsilon = l_\varepsilon^d - \bar{l}_\varepsilon^d$. We then set

$$u_\varepsilon(\varepsilon i) = \begin{cases} 1 & \text{if } \varepsilon i \in Q_\varepsilon \cup J_\varepsilon \\ \tilde{u}_\varepsilon(\varepsilon i) & \text{otherwise.} \end{cases}$$

By construction then, u_ε satisfies the constraint $\#\{i : u_\varepsilon(\varepsilon i) = 1\} = c_\varepsilon$ and moreover

$$E_\varepsilon(u_\varepsilon) \le E_\varepsilon(\tilde{u}_\varepsilon) + C\varepsilon^{d-1}(\#(\partial Q_\varepsilon \cap \varepsilon\mathbb{Z}^d) + \# J_\varepsilon) \le E_\varepsilon(\tilde{u}_\varepsilon) + C(\varepsilon l_\varepsilon)^{d-1},$$

from which the conclusion.

We conclude that, in order to minimize $E_\varepsilon^{(1)}$ the spins 1 and -1 arrange in a fashion so as to minimize the 'interface' between the two regions $\{u_\varepsilon = -1\}$ and $\{u_\varepsilon = 1\}$. In other words, the two 'phases' 1 and -1 do not mix, and they generate a 'sharp' interface minimizing an anisotropic 'crystalline' perimeter.

Exercise 3.1.2 Consider anisotropic microscopic interactions; i.e., energies of the form

$$E_\varepsilon(u) = \frac{1}{4} \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} c_{i-j} \varepsilon^d (u_i - u_j)^2 \qquad u_i \in \{-1, 1\}. \tag{3.11}$$

with $c_k = c_{-k}$. Prove that in the surface scaling we obtain the energy

$$F^{(1)}(G) = \int_{\partial^* G \cap \Omega} \sum_{k=1}^{d} c_k |\nu_k| \, d\mathcal{H}^{d-1} \, . \tag{3.12}$$

The antiferromagnetic case: antiphase boundaries

As in the one-dimensional case with the change of variables $w_i = (-1)^i u_i$, an antiferromagnetic energy (in u) turns into a ferromagnetic energy (in w). Moreover, to a phase interface for w there corresponds an *antiphase boundary* for u; i.e. the passage from a state $(-1)^i$ to $(-1)^{i+1}$. Note that the two ground states are 'indistinguishable' as the average spin is concerned, being zero in both cases.

3.1.2 The triangular lattice. Frustration

The analysis of nearest-neighbour interactions for ferromagnetic systems can be carried on following exactly the same line for other lattices, such as the triangular lattice. The change of parameter that carries an antiferromagnetic variable into a ferromagnetic variable, thus reducing the study to a single energy is possible on lattices where all cycles have even order (eg, the hexagonal lattice in two dimension), but does not hold for example for the triangular lattice (where we have cycles of order 3). In this case the behaviour of antiferromagnetic systems is completely different in the surface scaling regime.

We consider in two dimensions the triangular lattice $\mathbb{T}$ generated by the vectors $v_1 = (1, 0)$ and $v_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$; ie, $\mathbb{T} = \mathbb{Z}v_1 \oplus \mathbb{Z}v_2$. This lattice entails a partition of $\mathbb{R}^2$ into equilateral triangles, where every node i of the lattice has six nearest neighbours: $i \pm v_1$, $i \pm v_2$ and $i \pm (\frac{-1}{2}, \frac{\sqrt{3}}{2})$. We consider nearest-neighbour energies defined on functions $u : \varepsilon\mathbb{T} \cap \Omega \to \{\pm 1\}$. We may identify such functions with their piecewise-constant extensions to parallelograms centered in the nodes εi and edges parallel to v_1 and v_2 which take on these sets their value in the center εi.

For ferromagnetic energies the analysis is similar to the one for the square lattice. The Γ-limit at order 1 is still of the form (3.10) with a norm φ with hexagonal symmetry in the place of $\|\cdot\|_1$. We consider in detail the antiferromagnetic case; ie, energies

$$E_\varepsilon(u) = \frac{1}{4} \sum_{\varepsilon i, \varepsilon j \in \Omega_\varepsilon, |i-j|=1} \varepsilon^2 (u_i + u_j)^2.$$

It is again useful to rewrite the energy in terms of a new variable. More precisely, to every discrete function u we associate an auxiliary variable v defined as follows: for every triple $(i,j,k) \in \mathbb{T}^3$ of nodes which are the vertices of a triangle of minimal area in the lattice, we set

$$v(\varepsilon i, \varepsilon j, \varepsilon k) = \frac{1}{3}(u_i + u_j + u_k).$$

Note that if $u_\varepsilon \rightharpoonup u$, then also $v_\varepsilon \rightharpoonup u$ (here, v_ε is identified with its piecewise-constant interpolation taking the value $v_\varepsilon(\varepsilon i, \varepsilon j, \varepsilon k)$ on the triangle with vertices $\varepsilon i, \varepsilon j, \varepsilon k$). We also have

$$v(\varepsilon i, \varepsilon j, \varepsilon k) = \begin{cases} \pm 1 & \text{if } u_i = u_j = u_k = \pm 1 \\ \frac{1}{3} & \text{if } u_i = u_j = 1 \text{ and } u_k = -1 \\ -\frac{1}{3} & \text{if } u_i = u_j = -1 \text{ e } u_k = 1. \end{cases}$$

We then set

$$W(v) = \begin{cases} \frac{3}{2} & \text{if } v = \pm 1 \\ \frac{1}{2} & \text{if } v = \pm \frac{1}{3} \\ +\infty & \text{otherwise.} \end{cases}$$

so that

$$W(v(\varepsilon i, \varepsilon j, \varepsilon k)) = \frac{1}{2} \sum_{i,j,k} \varepsilon^2 \frac{1}{4}((u_i + u_j)^2 + (u_j + u_k)^2 + (u_k + u_i)^2)$$

(the factor $\frac{1}{2}$ is due to the fact that every pair of such points belong to two different triangles). We may then write

$$E_\varepsilon(u) = \sum_{(i,j,k)} \varepsilon^2 W(v(\varepsilon i, \varepsilon j, \varepsilon k)) + o(1) =: \tilde{E}_\varepsilon(v) + o(1), \tag{3.13}$$

where the sum is computed on all triples which are vertices of triangles contained in Ω. The term $o(1)$ is an error due to the contribution of triangles which intersect the boundary of Ω.

We may then repeat the arguments as in the computation of the Γ-limit of ferromagnetic energies on the square lattice, to show that the Γ-limit of E_ε coincides with that of $\tilde{E}_\varepsilon$ and is given by

$$\Gamma\text{-}\lim_{\varepsilon \to o} E_\varepsilon(u) = \begin{cases} \dfrac{4}{\sqrt{3}} \displaystyle\int_\Omega W^{**}(u)\, dx & \text{if } |u| \le 1 \text{ a.e.} \\ +\infty & \text{otherwise.} \end{cases}$$

We may explicit the limit energy density W^{**}:

$$W^{**}(u) = \begin{cases} \frac{1}{2} & \text{if } |u| \le \frac{1}{3} \\ \frac{3}{2}|u| & \text{if } \frac{1}{3} \le |u| \le 1. \end{cases}$$

Note that such energy density takes its minimum in the whole interval $[-\frac{1}{3}, \frac{1}{3}]$; ie, minimizing sequences can be constructed by mixing in arbitrary proportion (periodic) minimal configurations corresponding to $v = -\frac{1}{3}$ and $v = \frac{1}{3}$. It is interesting to note that in this case the geometry of the lattice allows phase transitions without interfacial penalization at any scale. In fact, we may construct sequences of lattice functions converging to piecewise-constant functions with values $\frac{1}{3}$ and $-\frac{1}{3}$ with interfaces in the lattice directions, and minimizing the energy at every single microscopic triangle, as pictured in Figure 3.1 (dark dots corresponding to $+1$, empty dots to -1). By a density argument, we may approximate all functions u with $|u| \leq \frac{1}{3}$. This shows that in this case we may have arbitrarily complex patterns of ground states (*frustration*)

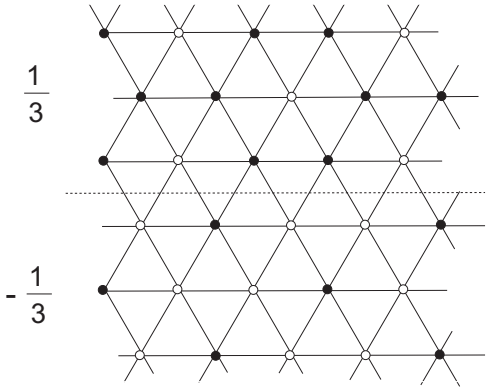


Figure 3.1: microscopic pattern of a transition with zero-energy interface (dotted line)

The absence of an interfacial energy can be described by studying the Γ-limit of the scaled energy

$$E_\varepsilon^{(1)}(v) = \sum_{(i,j,k)} \varepsilon \left(W(v(\varepsilon i, \varepsilon j, \varepsilon k)) - \frac{1}{2} \right).$$

If we take $\Omega = [0,1]v_1 \oplus [0,1]v_2$, $\varepsilon = \frac{1}{n}$, $n \in \mathbb{N}$, and v, eg, satisfying periodicity conditions, then by using the previous construction we may show that the Γ-limit of $E_{\frac{1}{n}}^{(1)}$ is 0 on all the functions v with $|v| \leq \frac{1}{3}$. Note that, taking Ω arbitrary, boundary interactions may give a non-negligible contribution to the limit.

3.1.3 The XY model: vortices

We briefly outline an important variant to the scalar spin model, where instead the variable u is vectorial. We only treat the two-dimensional case $d = 2$; i.e., $u : \varepsilon\mathbb{Z}^2 \cap \Omega \to \mathbb{R}^2$ and

satisfies $|u| = 1$ (ie, $u \in S^1$). The energy (after normalization) is

$$E_\varepsilon(u) = \sum_{ij} \varepsilon^2 (1 - \langle u_i, u_j \rangle)\,. \tag{3.14}$$

In this case the vectors u_i tend to be aligned at neighbouring points.

Note that E_ε can also be written as

$$E_\varepsilon(u) = \frac{1}{2}\varepsilon^2 \sum_{ij} \varepsilon^2 \Big| \frac{u_i - u_j}{\varepsilon} \Big|^2 = \frac{1}{2}\varepsilon^2 \int_\Omega |\nabla u|^2 \, dx\,, \tag{3.15}$$

where u is now identified with a piecewise-affine interpolation on a triangulation of $\varepsilon\mathbb{Z}^2$. This shows that the Γ-limit is 0 on $H^1(\Omega, S^1)$ at all scales ε^α with $\alpha < 2$; in particular it is 0 at the surface scale ε.

We note that the energy can also be viewed as a penalization of the distance to S^1; in particular (after regrouping terms) we can write

$$E_\varepsilon(u) \geq C \int_\Omega (|u|^2 - 1)^2 \, dx \tag{3.16}$$

(note that, while $u_i \in S^1$, its piecewise-affine extension does not satisfy the constraint $|u| = 1$).

Discrete Ginzburg-Landau energies

We may scale the energy above by $\varepsilon^2 |\log \varepsilon|$, and define

$$E^v_\varepsilon(u) = \frac{1}{\varepsilon^2 |\log \varepsilon|} \sum_{ij} \varepsilon^2 (1 - \langle u_i, u_j \rangle)\,. \tag{3.17}$$

Taking into account (3.15) and (3.16), for all fixed $1 > \delta > 0$ we may estimate

$$E^v_\varepsilon(u) \geq \frac{\delta}{2|\log \varepsilon|} \int_\Omega |\nabla u|^2 \, dx + \frac{(1-\delta)}{\varepsilon^2 |\log \varepsilon|} \int_\Omega (|u|^2 - 1)^2 \, dx. \tag{3.18}$$

The latter is a *Ginzburg-Landau* energy. Its Γ-limit is finite on functions u such that there exist $x_1 \dots x_N \in \Omega$ and $u \in H^1_{\rm loc}(\Omega \setminus \{x_1 \dots x_N\}, S^1)$. For each such x_j we may define the *degree* $d_j \in \mathbb{Z}$ of u at x_j. Then, we have

$$\Gamma\text{-}\lim_{\varepsilon \to 0} \Big(\frac{\delta}{2|\log \varepsilon|} \int_\Omega |\nabla u|^2 \, dx + \frac{(1-\delta)}{\varepsilon^2 |\log \varepsilon|} \int_\Omega (|u|^2 - 1)^2 \, dx \Big) = \delta \pi \sum_{j=1}^N |d_j|\,. \tag{3.19}$$

By letting $\delta \to 1$ we obtain an optimal lower bound.

From the density results on Ginzburg-Landau vortices it is sufficient to check the upper bound only at functions with degree -1 or $+1$; e.g., for $u = x/|x|$. For this the computation reduces to a Riemann sum giving π as a limit. We finally obtain that

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon^v(u) = \pi \sum_{j=1}^{N} |d_j|$$

is a *vortex energy* (v for vortex).

Liquid crystal-type singularities

A further variation of the scalar energy (after normalization) is

$$E_\varepsilon(u) = \sum_{ij} \varepsilon^2 \Big(1 - (\langle u_i, u_j\rangle)^2\Big), \tag{3.20}$$

with $u \in S^1$. In this case the vectors u_i tend to have the same direction at neighbouring points, but may also have opposite versus. The same reasoning as above applies, but the limit parameter is a function with vortices of degree in $\frac{1}{2}\mathbb{Z}$.

3.2 Next-to-nearest neighbours

We proceed with a brief study of the subsequent case (in order of complexity), when each point in a square lattice 'interacts' with its nearest and second-nearest neighbours. Again, the pattern that may appear depend on the 'sign' of the interactions that may favour or disfavour oscillating configurations, but also on the balance between first and second-neighbour interactions. We treat the two-dimensional setting only, in the case that we consider the most interesting.

We fix an open bounded set Ω in $\mathbb{R}^2$ with regular boundary. Our energy will be of the form

$$E_\varepsilon(u) = \frac{1}{4}c_1 \sum_{n.n.} \varepsilon^2 u_i u_j + \frac{1}{4}c_2 \sum_{n.n.n.} \varepsilon^2 u_i u_j,$$

where n.n. (nearest neighbours) entails that the sum is taken over all $i, j \in \mathbb{Z}^2$ such that $\varepsilon i, \varepsilon j \in \Omega$ and $|i-j| = 1$, while n.n.n. (next-to-nearest neighbours) are such that $|i-j| = \sqrt{2}$ (corresponding to the diagonals of the squares of the lattice).

3.2.1 Ferromagnetic interactions: superposition

Consider next-to-nearest neighbour ferromagnetic interactions; i.e. with $c_1, c_2 < 0$. We immediately obtain a lower bound by considering separately n.n. and n.n.n. interactions. In fact,

$$E_\varepsilon(u) \geq E_\varepsilon^1(u) + E_\varepsilon^{2,e}(u) + E_\varepsilon^{2,o}(u),$$

where

$$E^1_\varepsilon(u) = \frac{1}{4}c_1 \sum_{n.n.} \varepsilon^2 u_i u_j, \qquad E^{2,e/o}_\varepsilon(u) = \frac{1}{4}c_2 \sum_{even/odd\ n.n.n.} \varepsilon^2 u_i u_j,$$

and by even/odd indices we mean those $i \in \varepsilon\mathbb{Z}^2$ for which $\sum_k i_k/\varepsilon$ is even/odd. In this way we have regrouped the interactions as interactions on three separate square lattices (see Fig. 3.2):

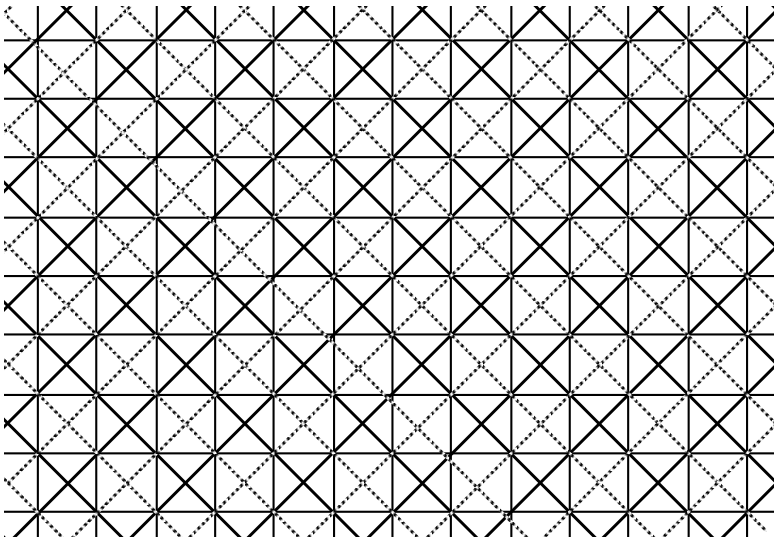


Figure 3.2: nnn interactions as the superposition of three nn systems

$$\varepsilon\mathbb{Z}^2, \qquad \sqrt{2}\varepsilon J\mathbb{Z}^2, \qquad \text{and } \sqrt{2}\varepsilon\Big(\Big(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}}\Big) + J\mathbb{Z}^2\Big).$$

where J is the rotation by $\pi/4$. By the results for nearest neighbours we have

$$\begin{aligned}
\Gamma\text{-}\lim_{\varepsilon\to 0} E^1_\varepsilon(u) &= c_1 \int_{S(u)} \|\nu(u)\|_1 d\mathcal{H}^1 \\
\Gamma\text{-}\lim_{\varepsilon\to 0} E^{2,e}_\varepsilon(u) &= \frac{c_2}{\sqrt{2}} \int_{S(u)} \|J\nu(u)\|_1 d\mathcal{H}^1 = c_2 \int_{S(u)} \|\nu(u)\|_\infty d\mathcal{H}^1 \\
\Gamma\text{-}\lim_{\varepsilon\to 0} E^{2,o}_\varepsilon(u) &= \frac{c_2}{\sqrt{2}} \int_{S(u)} \|J\nu(u)\|_1 d\mathcal{H}^1 = c_2 \int_{S(u)} \|\nu(u)\|_\infty d\mathcal{H}^1 d\mathcal{H}^1
\end{aligned}$$

Since we have

$$\liminf_\varepsilon E_\varepsilon(u_\varepsilon) \geq \liminf_\varepsilon E^1_\varepsilon(u_\varepsilon) + \liminf_\varepsilon E^{2,e}_\varepsilon(u_\varepsilon) + \liminf_\varepsilon E^{2,o}_\varepsilon(u_\varepsilon),$$

we immediately obtain

$$\Gamma\text{-}\liminf_{\varepsilon\to 0} E_\varepsilon(u) \geq \int_{S(u)} \varphi(\nu(u)) d\mathcal{H}^1,$$

where

$$\varphi(\nu) = c_1\|\nu\|_1 + 2c_2\|\nu\|_\infty\,.$$

On the other hand we have remarked that for nearest-neighbour interactions recovery sequences are simply given by the discretization of the target function; hence, they are the same for the three Γ-limits and indeed

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon(u) = \int_{S(u)} \varphi(\nu(u))d\mathcal{H}^1\,.$$

The shape of $\{\varphi(\nu) = 1\}$ is described in Fig. 3.3.

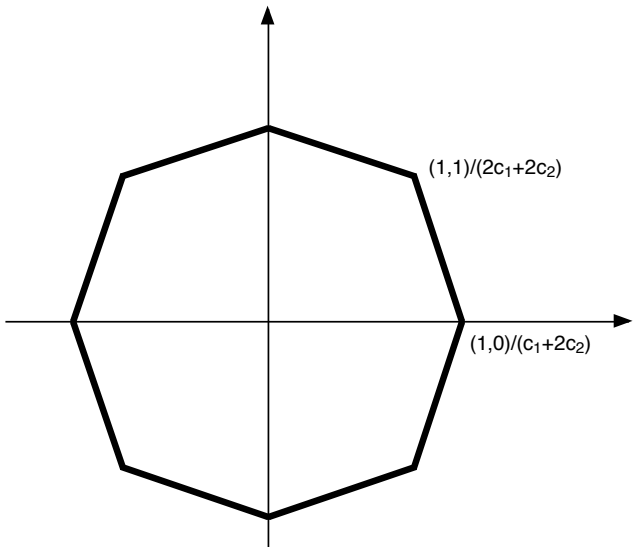


Figure 3.3: energy density level set for nnn ferromagnetic interactions

Exercise 3.2.1 Let φ be a symmetric norm in $\mathbb{R}^2$; ie, $\varphi(\nu) = \varphi(-\nu)$. Then prove that φ can be obtained as the energy function of a system of long-range interactions

$$E_\varepsilon(u) = \frac{1}{4}\sum_{k\in\mathbb{Z}^2\setminus\{0\}}\sum_{|i-j|=\varepsilon k} \varepsilon^2 c_k u_i u_j.$$

(Treat first the case of φ crystalline (ie, $\{\varphi = 1\}$ a polygon) with vertices corresponding to directions $k \in \mathbb{Z}^2 \setminus \{0\}$ with $|k| \le M$ for a fixed M).

Deduce that minimizer for the minimum problem with constraint $\varepsilon^2\#\{i : u_i = 1\} = C_\varepsilon$ with $C_\varepsilon \to C$ converge to an octagon.

3.2.2 Anti-ferromagnetic interactions: partitions and patterns

In this case it is convenient to rewrite the energy taking into account the local interactions in a fashion similar to that used for the hexagonal lattice. Indeed we may rewrite

$$E_\varepsilon(u) = \frac{1}{4}\sum_{i,j,k,l} \varepsilon^2\Big(\frac{1}{2}c_1(u_iu_j + u_ju_k + u_ku_l + u_lu_i) + c_2(u_iu_k + u_ju_l)\Big) + o(1)$$

where the sum is taken over all i, j, k, l vertices of a lattice square, ordered in such a way that $|i-j| = |j-k| = |k-l| = |l-i| = 1$ and $|i-k| = |j-l| = \sqrt{2}$. The factor $\frac{1}{2}$ comes from the fact that each pair of nearest neighbours belongs to two such lattice squares, and again the error $o(1)$ is due to the squares close to the boundary. Note that each cube is considered four times.

Note that indeed the sum above can be rewritten as parameterized on the centres of the cubes; *i.e.* on the points $m = \frac{1}{4}(i+j+k+l)$. We would like to introduce equivalent energies of a simpler form

$$F_\varepsilon(v) = \sum_m \varepsilon^2 f(v_m),$$

and

$$v_m = \frac{1}{4}(u_i + u_j + u_k + u_l).$$

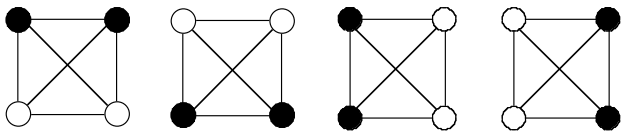


Figure 3.4: possible patterns of interactions on a cube

The possible values of v are

$$\begin{aligned}
u_i = u_j = u_k = u_l = 1 &\implies v_m = 1\\
u_i = u_j = u_k = u_l = -1 &\implies v_m = -1\\
u_i = u_j = u_k = 1,\ u_l = -1 &\implies v_m = \frac{1}{2}\\
u_i = u_j = u_k = -1,\ u_l = 1 &\implies v_m = -\frac{1}{2}\\
u_i = u_j = -1,\ u_k = u_l = 1 &\implies v_m = 0\\
u_i = u_k = -1,\ u_j = u_l = 1 &\implies v_m = 0.
\end{aligned}$$

The list comprises all different cases (upon cyclical permutation of the indices), which are pictured in Figure 3.4.

How to define f? There is no ambiguity for $v = \pm 1$ and $v = \pm\frac{1}{2}$. In these cases

$$f(v_m) = \frac{1}{2}c_1(u_iu_j + u_ju_k + u_ku_l + u_lu_i) + c_2(u_iu_k + u_ju_l)$$

so that

$$f(v) = \begin{cases} 2c_1 + 2c_2 & \text{if } |v| = 1 \\ 0 & \text{if } |v| = \frac{1}{2}. \end{cases}$$

For $v = 0$ the definition must take into account the two values $-2c_2$, corresponding to the case $u_i = u_j = -1$ $u_k = u_l = 1$, and $-2c_1 + 2c_2$, corresponding to the case $u_i = u_k = -1$ $u_j = u_l = 1$. As we are interested in minimum energy configurations, the 'natural' definition for f is then

$$f(0) = \min\{-2c_2,\ -2c_1 + 2c_2\}.$$

This is a very simple case of a *homogenization formula* that gives the overall value of an averaged quantity in terms of a minimum problem among functions (in this case just two possible states) satisfying some average conditions (in this case, that their average be zero).

We have two cases, whether

$$-2c_2 \geq -2c_1 + 2c_2 \qquad (i.e.,\ 2c_2 \leq c_1)$$

or not. In the first case, when $f(0) = -2c_1 + 2c_2$, the minimum configuration is the same alternating state as that we encountered in the 'plus case' for nearest neighbours.

The case $f(0) = -2c_2$ is more interesting since the minimizers have less symmetries. We will consider this case only. We make the assumptions

$$0 < c_1 < 2c_2, \qquad c_1 + 2c_2 > 0$$

(in particular, $f(0) = -2c_2 < 0$). In this case, the convex envelope of f is given by

$$\psi(v) = \begin{cases} 4c_2\Big(|v| - \frac{1}{2}\Big) & \text{if } |v| \leq \frac{1}{2} \\ 4(c_1 + c_2)\Big(|v| - \frac{1}{2}\Big) & \text{if } \frac{1}{2} \leq |v| \leq 1, \end{cases}$$

and the Γ-limit can be again described by $\int_\Omega \psi(u)\,dx$ with the constraint that $|u| \leq 1$. The proof of this fact is the same as for nearest neighbours; the only care is in using the minimal configuration in the computation of $f(0)$ (that now corresponds to a layering of ones and minus ones).

The limit minimal state is now 0, as in the 'plus case' for nearest neighbours, where anti-phase boundaries appeared in the description of the second Γ-limit. In that computation, a

simple change of sign in the variables allowed to use the computation for the 'minus case'. Here, this is not possible since the minimal configuration have more symmetries.

Note that the locally minimal configurations u in $\mathbb{Z}^2$ (for $\varepsilon = 1$) are periodic with period two. Hence, it is natural to parameterize them after a translation in $2\mathbb{Z}^2$ to a reference cube. The four configurations we have after this translation may then be parameterized by four parameters, that is suggestive to take $\pm e_1$ and $\pm e_2$. We have the correspondence

$$\begin{aligned}
&u(0,0) = u(0,1) = -1,\ u(1,0) = u(1,1) = 1 \quad \text{corresponds to} \quad e_1\\
&u(0,0) = u(1,0) = -1,\ u(0,1) = u(1,1) = 1 \quad \text{corresponds to} \quad e_2\\
&u(0,0) = u(0,1) = 1,\ u(1,0) = u(1,1) = -1 \quad \text{corresponds to} \quad -e_1\\
&u(0,0) = u(1,0) = 1,\ u(0,1) = u(1,1) = -1 \quad \text{corresponds to} \quad -e_2.
\end{aligned}$$

If we may neglect the effects of the boundary of Ω (for example, if Ω is a cube and we have periodic conditions for u), then we may describe the Γ-limit of the scaled functional

$$E_\varepsilon^{(1)}(u) = \frac{1}{4}c_1 \sum_{n.n.} \varepsilon u_i u_j + \frac{1}{4}c_2 \sum_{n.n.n.} \varepsilon(u_i u_j + 1)$$

in terms of a new four-dimensional parameter: for each u_ε we may define $w : 2\mathbb{Z}^2 \to \mathbb{R}^4$

$$w(\varepsilon i) = (u_i, u(\varepsilon(i + (1,0))), u(\varepsilon(i + (1,1)), u(\varepsilon(i + (0,1))).$$

If we follow a sequence (u_ε) with $\sup_\varepsilon E_\varepsilon^{(1)}(u_\varepsilon) < +\infty$ then we deduce that $u_\varepsilon \to 0$ and $w_\varepsilon \to w$, where w takes a.e. only the values $(-1,1,1,-1)$, $(-1,-1,1,1)$, $(1,-1,-1,1)$ and $(1,1,-1,-1)$, corresponding to $e_1, e_2, -e_1, -e_2$ above. In this case the surface energy depends also on the two states on both sides of the interface, and can be written as

$$F(w) = \int_{S(w)} \varphi(w^+, w^-, \nu_w) d\mathcal{H}^1,$$

where $w^\pm$ are the traces of w on both sides of the jump set $S(w)$.

We do not describe the form of φ, but only give a picture of the 'optimal transitions' in Figure 3.5 where the microscopical transitions are shown between the states (from left to right) e_2, e_1, $-e_1$ and $-e_2$. The grey squares are those where the value of the interactions between the corners is not minimal. It must be noted that the transition between e_2 and $-e_2$ is less energetically favourable since it must use a 'diffuse' interface, while the transition between $-e_2$ and $-e_1$ with an interface at an angle of $\pi/4$ is more advantageous than that at $\pi/2$. Even though this does not immediately suggest the form of φ, it shows that it must be more complex than the surface energy in the nearest-neighbour case.

Exercise 3.2.2 (Three-point interactions) Consider the energy function f in Section 2.6.2, and the two-dimensional version of the energy therein; ie,

$$\sum_i \Big(f(u_{i+\varepsilon e_1}, u_i, u_{i-\varepsilon e_1}) + f(u_{i+\varepsilon e_2}, u_i, u_{i-\varepsilon e_2}) \Big).$$

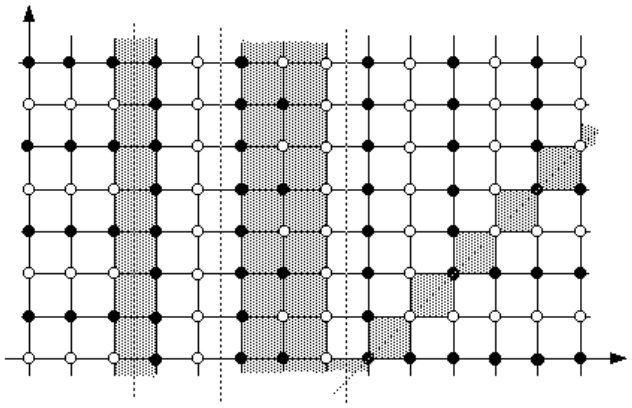


Figure 3.5: microscopical transitions between four different phases

Describe the 16 ground states for this energy.

3.3 Bibliographical Notes

Most of this section is derived from
[1] R. Alicandro, A. Braides and M. Cicalese. Phase and anti-phase boundaries in binary discrete systems: a variational viewpoint. *Netw. Heterog. Media* **1** (2006), 85–107

The study of the XY model is contained in
[2] R. Alicandro and M. Cicalese. Variational Analysis of the Asymptotics of the XY Model. *Arch. Rational Mech. Anal.* **192** (2009), 501–536

A concise introduction to sets of finite perimeter can be found in
[3] A. Braides. *Approximation of Free-Discontinuity Problems.* Lecture Notes in Math. **1694**, Springer Verlag, Berlin, 1998.

Chapter 4

Homogenization of spin systems

4.1 Ferromagnetic homogenization

We consider inhomogeneous interactions. The corresponding energies are then of the form

$$E_\varepsilon(u) = -\sum_{ij} c_{ij}^\varepsilon u_i u_j,$$

with the sum ranging on nearest neighbours. If $c_{ij} \geq 0$ then the constant functions $u = \pm 1$ are absolute minimizers. We can then consider the scaled energies

$$E_\varepsilon(u) = \sum_{ij} \varepsilon^{d-1} c_{ij}^\varepsilon (1 - u_i u_j),$$

and study their asymptotic behaviour.

Note that if

$$+\infty > C_2 \geq \sup_{ij} c_{ij}^\varepsilon \geq \inf_{ij} c_{ij}^\varepsilon \geq C_1 > 0$$

then the functionals are coercive, and we immediately obtain the lower estimate

$$\begin{aligned} C_2 \int_{S(u)} \|\nu\|_1 d\mathcal{H}^{d-1} &\geq \Gamma\text{-}\limsup_{\varepsilon\to 0} E_\varepsilon(u) \\ &\geq \Gamma\text{-}\liminf_{\varepsilon\to 0} E_\varepsilon(u) \geq C_1 \int_{S(u)} \|\nu\|_1 d\mathcal{H}^{d-1} \end{aligned}$$

Note that the same problem makes sense also when long-range interactions are taken into account. In this case a condition for the lower estimate to hold is that

$$\inf_{|i-j|=1} c_{ij}^\varepsilon \geq C_1 > 0,$$

while the upper estimate holds (taking trivial interpolations as recovery sequences) if we have

$$\sup_i \sum_{k=1}^{\infty} \sum_{|j-i|\geq k} c_{ij}^{\varepsilon} \leq C_2 < +\infty.$$

We are interested in cases when we expect the limit to be translationally invariant. This is reasonable in the following cases.

Periodic setting

In this case we have a N-periodic function c_{ij} on $\mathbb{Z}^d \times \mathbb{Z}^d$; ie such that

$$c_{i+N,j} = c_{i,j+N} = c_{ij}$$

and define the coefficient c_{ij}^{ε} on $\varepsilon\mathbb{Z}^d \times \varepsilon\mathbb{Z}^d$ by

$$c_{i,j}^{\varepsilon} = c_{i/\varepsilon, j/\varepsilon}\,.$$

Random setting

In this case the function $c_{ij} = c_{ij}^{\omega}$ on $\mathbb{Z}^d \times \mathbb{Z}^d$ depends on the realization of a random variable, and again we set the coefficient c_{ij}^{ε} on $\varepsilon\mathbb{Z}^d \times \varepsilon\mathbb{Z}^d$ by

$$c_{i,j}^{\varepsilon} = c_{i/\varepsilon, j/\varepsilon}^{\omega}\,.$$

4.1.1 The surface homogenization formula

We consider the two-dimensional case $d = 2$. The idea of an asymptotic formula translates the *ansatz* that in the limit we will have a homogeneous energy of the form $F(G) = \int_{\partial^* G} \varphi(\nu) d\mathcal{H}^1$. If this is the case, then we may use the knowledge that φ must be convex for lower semicontinuity reasons. This means that

$$\varphi(\nu) = \min\Big\{ \int_{\partial^* G \cap Q^\nu} \varphi(\nu) d\mathcal{H}^1 : \chi_G = \chi_{\Pi_\nu} \text{ on } \partial Q^\nu \Big\}. \tag{4.1}$$

Here:

- $Q_\nu = Q_\nu(0)$ is a unit square centered in 0 with a side orthogonal to ν
- Π_ν is the half plane $\{\langle x, \nu\rangle \geq 0\}$,

formula (4.1) states that the plane Π_ν is minimal among variations contained in Q_ν. With the notation

$$F(G, A) = \int_{A \cap \partial^* G} \varphi(\nu) d\mathcal{H}^1, \tag{4.2}$$

we then have

$$\varphi(\nu) = \min\Big\{F(G,A) : \chi_G = \chi_{\Pi_\nu} \text{ on } \partial Q^\nu\Big\}, \tag{4.3}$$

and, introducing the same notation for discrete problems and using the Fundamental Theorem of Γ-convergence

$$\varphi(\nu) = \lim_{\varepsilon\to 0} \min\Big\{E_\varepsilon(u,A) : u = \chi_{\Pi_\nu} \text{ on } \partial Q^\nu\Big\}. \tag{4.4}$$

By scaling ε to 1 (here below T plays the role of $1/\varepsilon$) we finally obtain the *asymptotic homogenization formula*

$$\varphi(\nu) = \lim_{T\to+\infty} \frac{1}{T} \min\Big\{\sum_{i \text{ or } j\in\mathbb{Z}^2\cap TQ^\nu} : u = \chi_{\Pi_\nu} \text{ outside } \partial TQ^\nu\Big\}. \tag{4.5}$$

Note that we have had to modify a little our boundary conditions since in general ∂TQ_ν does not intersect $\mathbb{Z}^2$.

4.1.2 Periodic Homogenization

In this case we can show that the limit in (4.5) holds.

Lemma 4.1.1 *The limit* (4.5) *exists for all* $\nu \in S^1$.

Proof. The proof is by *subadditivity*. Let

$$g(T) = \min\Big\{\sum_{i \text{ or } j\in\mathbb{Z}^2\cap TQ^\nu} : u = \chi_{\Pi_\nu} \text{ outside } \partial TQ^\nu\Big\}.$$

Let $S > T$; then by covering (most part of) $SQ_\nu \cap \partial\Pi_\nu$ with copies of TQ_ν we may construct a test function for $g(S)$ from the minimizer of $g(T)$ obtaining

$$g(S) \le \frac{S}{T} g(T) + o(S)$$

as $S \to +\infty$ and $T \to +\infty$. The existence of the limit is then proven after dividing by S and taking first the limsup for $S \to +\infty$ and then the liminf for $T \to +\infty$. □

Theorem 4.1.2 (periodic homogenization theorem) *In the periodic setting above we have*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon(G) = \int_{\partial^* G} \varphi(\nu) d\mathcal{H}^1 =: F_{\hom}(G) \tag{4.6}$$

where φ *is given by* (4.5).

Proof. We outline the proof, which follows standard arguments of homogenization theory. The lower bound is obtained by *blow-up*: if $u_\varepsilon \to G$ we can define the measures

$$\mu_\varepsilon = \sum_{ij} c_{ij}^\varepsilon \varepsilon \frac{1}{2}(u_i^\varepsilon - u_j^\varepsilon)^2 \delta_{(i+j)/\varepsilon},$$

so that $E_\varepsilon(u_\varepsilon) = \mu_\varepsilon(\mathbb{R}^2)$, and their weak* limit μ. In order to prove that $\liminf_\varepsilon E_\varepsilon(u_\varepsilon) \geq F_{\rm hom}(G)$ it suffices to prove that

$$\frac{d\mu}{d\mathcal{H}^1{}_{|G}}(x) \geq \varphi(\nu(x))$$

at $\mathcal{H}^1$ a.a. points of G. Using the derivation formula

$$\frac{d\mu}{d\mathcal{H}^1{}_{|G}} = \lim_{\rho\to 0} \frac{\mu(Q_{\rho\nu}(x))}{\rho}$$

and the fact that

$$\lim_{\rho\to 0} \mu_\varepsilon(Q_{\rho\nu}(x)) = \mu(Q_{\rho\nu}(x))$$

except for a countable number of ρ, upon introducing $T = \rho/\varepsilon$, we finally obtain that

$$\frac{d\mu}{d\mathcal{H}^1{}_{|G}}(x) = \lim_{T\to+\infty} \frac{1}{T} E_1(u_T, TQ_\nu(x)),$$

where u_T are obtained by scaling u_ε. At this point it suffices to note that

- upon a slight modification that does not change the limit of u_T and the limit energy we may suppose that $u_T = \chi_{x+\Pi_\nu}$ close to $\partial TQ_\nu(x)$
- we may translate x to 0 by the periodicity of c_{ij}.

In this way $E_1(u_T, TQ_\nu(x)) \geq g(T)$ with $\nu = \nu(x)$ in the notation of the lemma above, and we have the lower bound.

The upper bound close to a linear interface of normal ν is obtained by covering it by copies of translations of εTQ_ν for $T >> 1$ and using the minimal u_T for g_T. For a polygon the construction is repeated locally. The general case is recovered by density. □

Exercise 4.1.3 Let $0 < \alpha < \beta < +\infty$ and let c_{ij} be the N-periodic function given by

$$c_{ij} = \begin{cases} \alpha & \text{if } i_1 i_2 = 0 \\ \beta & \text{otherwise} \end{cases}$$

on $\{0, \dots, N-1\}^2$. Prove that the homogenized energy density is $\alpha\|\nu\|_1$ as in the case when c_{ij} is identically α.

Remark 4.1.4 (open problem) A typical problem in Optimal Design (usually for integral functionals) is that of the *G-closure*, which in its simplest form can be translated into examining all possible energies that can be obtained by 'homogenizing' mixtures of two types of homogeneous energies. In our case we can think of mixing 'bonds' of type α and β as in the previous exercise, but with fixed proportion, say of α bonds.

Problem 1: Given a proportion $\theta \in [0,1]$ compute the set of the limits φ of all possible φ_h that can be obtained starting from periodic geometries of α and β of arbitrary period and proportions θ_h of α bonds (and correspondingly $1-\theta_h$ of β bonds) with $\theta_h \to \theta$.

Problem 2: A simpler problem is that of giving (sharp) bounds for the φ described in Problem 1. Note that the exercise above shows that for all $\theta \in [0,1]$ we have a sharp bound $\alpha\|\nu\|_1 \leq \varphi(\nu)$, independent of θ.

4.1.3 A simplified view to percolation theory

We want to compute a Γ-limit as in the previous section, of an energy where we randomly mix coefficients. To this end we have to introduce some notions of percolation theory for what is called the 'bond percolation model' (*i.e.*, when the random choice is thought to be performed on the connections. A different model, that can be treated similarly, is the *site percolation model*. In our intuition it would correspond to choosing weak and strong nodes – and to define a weak connection as a connection between two nodes of which at least one is a weak node).

We do not want to introduce the formal definition of a random variable, but just to look at the relevant elements of percolation theory that will allow us to describe our models. From now on we will restrict to the two-dimensional case $N = 2$. We start by introducing the dual lattice

$$\mathcal{Z} = \Big\{ \frac{i+j}{2} : i,j \in \mathbb{Z}^2,\ |i-j| = 1 \Big\}.$$

Let

$$0 < \alpha < \beta < +\infty$$

A choice of connections between nodes of $\mathbb{Z}^2$ is a function $\omega : \mathcal{Z} \to \{\alpha, \beta\}$. We identify each point $\gamma \in \mathcal{Z}$ with the segment $[i,j]$ such that $i,j \in \mathbb{Z}^2$ and $2\gamma = i + j$.

We now want to express the fact that

$$\omega(\gamma) = \begin{cases} \alpha & \text{with probability } 1-p \\ \beta & \text{with probability } p. \end{cases}$$

This can be done rigorously by introducing some 'independent identically distributed' random variables. This is not however the scope of our presentation. It suffices to describe the 'almost-sure' properties of such ω.

Let $i, j \in \mathbb{Z}^2$. A *path* L between i and j is a family $\{i_l : \ l = 0, \dots, N\}$ in $\mathbb{Z}^2$ with $|i_l - i_{l-1}| = 1$, $i_0 = i$ and $i_N = j$. The *length of a path* is given by

$$|L|_\omega = \sum_{l=0}^{N} \omega\Big(\frac{i_l + i_{l-1}}{2}\Big),$$

and corresponding to endowing the lattice $\mathcal{Z}$ (thought as the union of the segments) with an inhomogeneous Riemannian distance. The *distance* between i and j is

$$d^\omega(i, j) = \min\{|L|_\omega : L \text{ path between } i \text{ and } j\}.$$

The following result can be derived from *first-passage percolation* results.

Lemma 4.1.5 (first-passage percolation formula) *The limit*

$$\varphi^p(\nu) = \lim_{K\to+\infty} \liminf_{T\to+\infty} \inf\Big\{\frac{1}{|T|} d^\omega(i, i') : i - i' = T\nu + o(T); |i| + |i'| \le KT\Big\} \tag{4.7}$$

is finite and independent of ω for all ν, except for a set of ω with zero probability.

From this lemma in particular we infer the existence of the limit defining the function φ in (4.5) taking $\nu^\perp$ in place of ν in (4.7) and i and i' points close to $\Pi_\nu \cap \partial T Q_\nu$, and that $\varphi = \varphi^p$. In addition, we also have that

$$\varphi(\nu) = \lim_{T\to+\infty} \frac{1}{T} \min\Big\{ \sum_{i \text{ or } j\in\mathbb{Z}^2\cap TQ^\nu} : u = \chi_{x_T+\Pi_\nu} \text{ outside } \partial(x_T + TQ^\nu)\Big\}. \tag{4.8}$$

for any choice of points $\{x_T\}$ with $\sup_T |x_T| = O(T)$. This allows to carry on the proof of the lower bound of the following theorem in the same way as for Theorem 4.1.2. Similarly, we can also construct a recovery sequence.

Theorem 4.1.6 (Random homogenization theorem) *In the random setting above we almost surely have*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon(G) = \int_{\partial^* G} \varphi^p(\nu) d\mathcal{H}^1 =: F_{\text{hom}}(G) \tag{4.9}$$

where φ is given by (4.7).

4.2 Variational Percolation

In this section we consider two extreme cases when the final Γ-limit, which depends on p exhibits a "percolation" phenomenon; ie, below (or above) some threshold is degenerate, while above (or below) it is described by a usual surface energy.

4.2.1 Percolation Clusters

In the notation of Section 4.1.3, we may deal with the two extreme cases $\alpha = 0$ or $\beta = +\infty$. To this end we will have to introduce the notion of *percolation cluster*. As a matter of notation, the case α will corresponds to a *strong connection*, and β to a *weak connection*.

Given ω, we say that two points $\gamma, \gamma' \in \mathcal{Z}$ such that $\omega(\gamma) = \omega(\gamma')$ are *connected* if there exists a path in $\mathcal{Z}$ such that each element of this path γ'' is such that $\omega(\gamma'') = \omega(\gamma)$. Such a path is called a *weak channel* if $\omega(\gamma) = \alpha$ and a *strong channel* if $\omega(\gamma) = \beta$. In this way, we subdivide $\mathcal{Z}$ into 'connected subsets' where either $\omega(\gamma) = \alpha$ or β.

If $p < 1/2$ then it is 'more probable' to have some γ with $\omega(\gamma) = \alpha$; not only, it is not likely to have a large number of connected points with $\omega(\gamma) = \beta$. This is expressed by the fact that there is one (necessarily unique) infinite connected component of $\{\omega = \alpha\}$. We call this set the *infinite weak cluster* (or simply weak cluster). Of course, the situation is symmetrical for $p > 1/2$, in which case we have an *infinite strong cluster*.

The weak cluster (and the strong cluster for $p > 1/2$) are 'well distributed'. This can be expressed in the following way (*channel property*): there exist constants $c(p) > 0$ and $c_1(p) > 0$ such that a.s. for any δ, $0 < \delta \leq 1$ there is a large enough number $N_0 = N_0(\omega, \delta)$ such that for all $N > N_0$ and any square of size length δN contains at least $c(p)\delta N$ disjoint weak channels which connect opposite sides of the square. Moreover, the length of each such a channel does not exceed $c_1(p)\delta N$.

The dilute case: $\alpha = 0$

In this case we normalize $\beta = 1$. Note that a path of weak connections has length 0.

The function φ^p can be defined as in Section 4.1.3. In this case we have φ^p identically equal to 0 if $p \leq 1/2$, while we have

$$\min\{\varphi^p(\nu) : \nu \in S^1\} > 0$$

if $p > 1/2$.

In this case the main difficulty is defining the convergence with respect to which to compute the Γ-limit. In fact, given u with $E_\varepsilon(u) < +\infty$, we can construct $\widetilde{u}$ by setting $\tilde{u}_i = -u_i$ at every i in the "interior" of the weak cluster; ie, such that $\omega((i+j)/2) = 0$ whenever $|i - j| = 1$. Clearly, we still have $E_\varepsilon(u) = E_\varepsilon(\widetilde{u})$ since the changes are not detected by the energy. This shows that we cannot expect a strong convergence of the piecewise-constant interpolations. In the case $p > 1/2$ we may nevertheless change the parameter by choosing the limit u as the "majority" phase defined on the strong cluster. The convergence we consider is the following: let $\mathcal{S}$ be the set of nodes corresponding to bonds in the strong cluster; we say that $u_\varepsilon \to u$ if we have that

$$\lim_{\varepsilon \to 0} \sum_{i \in \varepsilon\mathcal{S}} \varepsilon^2 |(u_\varepsilon)_i - u_i| = 0\,.$$

Lemma 4.2.1 (compactness) *Almost surely, from every sequence with $E_\varepsilon(u_\varepsilon) \leq C < +\infty$ we can extract a subsequence, and a function $u \in BV(\Omega; \{\pm 1\})$ such that $u_\varepsilon \to u$.*

Proof. The complement of the weak cluster is composed of finite-size "open" (ie, coinciding with their interior in the sense above) connected sets of nodes (*islands*). It can be shown that a.s. large islands are negligible. Given u_ε as above, we can define $\widetilde{u}_\varepsilon$ as equal to u_ε on $\varepsilon\mathcal{S}$, and on each island equal to the "majority phase" on the boundary (the boundary is defined as the set in the strong cluster with distance 1 to the island). Note that

$$E_\varepsilon(\widetilde{u}_\varepsilon) \leq E_\varepsilon(u_\varepsilon).$$

Then $\widetilde{u}_\varepsilon$ can be shown to have equibounded ferromagnetic energy, and hence be strongly precompact in L^1. This means that

$$0 = \lim_{\varepsilon\to 0} \sum_i \varepsilon^2 |(\widetilde{u}_\varepsilon)_i - u_i| = \lim_{\varepsilon\to 0} \sum_{i\in\varepsilon\mathcal{S}} \varepsilon^2 |(\widetilde{u}_\varepsilon)_i - u_i| = \lim_{\varepsilon\to 0} \sum_{i\in\varepsilon\mathcal{S}} \varepsilon^2 |(u_\varepsilon)_i - u_i|\,,$$

as desired. □

Theorem 4.2.2 (dilute percolation theorem) *Almost surely in ω, the Γ-limit of E_ε is deterministic. Moreover, we have*

(i) *if $p \leq 1/2$ the Γ-limit is identically 0 on the whole $L^1(\Omega)$;*

(ii) *if $p > 1/2$ the Γ-limit F depends on p through φ^p, and we have*

$$F(u) = \int_{S(u)} \varphi^p(\nu(u)) d\mathcal{H}^1$$

on its domain.

Proof. (i) By the channel property we immediately see that $F(u) = 0$ if $\{u = 1\}$ is the characteristic function of a polyhedron. The result follows then by density.

(ii) If $\widetilde{u}$ is constructed as in the previous lemma, we can use the previous result with $\alpha > 0$ and $\beta = 1$ and obtain that

$$\liminf_\varepsilon E_\varepsilon(u_\varepsilon) \geq \liminf_\varepsilon E_\varepsilon(\widetilde{u}_\varepsilon) \geq \int_{S(u)} \varphi^p_\alpha(\nu) d\mathcal{H}^1 - C\alpha \geq \int_{S(u)} \varphi^p(\nu) d\mathcal{H}^1 - C\alpha,$$

so that the liminf inequality follows by letting $\alpha \to 0$.

The construction of a recovery sequence follows as for the case $\alpha > 0$. □

The rigid case: $\beta = +\infty$

In this case we normalize $\alpha = 1$. The energy we consider is defined by

$$E_\varepsilon(u) = \varepsilon^{d-1}\#\{u_i \neq u_j,\ |i-j| = 1\},$$

if $\omega((i+j)/2) = 1$ for all i, j in the set above, and $E_\varepsilon(u) = +\infty$ otherwise (ie, the interface must all lie in the weak cluster).

Note that a path has finite length if all its connections are weak, and in this case $|L|_\omega = |L|$ is simply the number of connections in the path.

If $p < 1/2$ and two points γ and γ' belong to the weak cluster then there is at least one path L in the cluster joining γ and γ'. The *chemical distance* of γ and γ' is defined as

$$d^\omega(\gamma, \gamma') = \min |L|,$$

where the minimum is taken over all such paths L.

This distance is not isotropic (it suffices to think about the trivial case $p = 0$) and depends on ω. Nevertheless, its limit behavior as the points γ and γ' are scaled properly is well defined and independent of ω: we define

$$\varphi^p(\nu) = \lim_{K\to+\infty} \liminf_{T\to+\infty} \inf\Big\{ \frac{1}{|T|} d^\omega(\gamma, \gamma') : \gamma - \gamma' = T\nu,\ |\gamma| + |\gamma'| \leq KT \Big\}.$$

This limit is finite and independent of ω for all ν, except for a set of ω with zero probability. Note that for $p = 1$ we have $\varphi^p(\nu) = \|\nu\|_1$.

The number $\varphi^p(\nu)$ describes the average distance on the weak cluster in the direction ν (and by symmetry also in the orthogonal direction). Its value cannot be decreased by using 'small portions' of strong connections: if $\delta > 0$ then there exists $T > 0$ and $c = c(\delta) \in (0, 1)$ such that if L is a path joining γ and $\gamma' = \gamma + T\nu$ and $|L| < (\varphi^p(\nu) - \delta)T$, then there are at least $c(\delta)T$ strong connections in the path L.

Theorem 4.2.3 (rigid percolation theorem) *Almost surely in ω, the Γ-limit of E_ε is deterministic. Moreover, we have*

(i) *if $p > 1/2$ the Γ-limit is identically $+\infty$ on the whole $L^1(\Omega)$ except for u constant identically ± 1;*

(ii) *if $p < 1/2$ the Γ-limit F depends on p through φ^p, and we have*

$$F(u) = \int_{S(u)} \varphi^p(\nu(u)) d\mathcal{H}^1$$

on its domain.

Proof. (i) If u is not constant then there exists at least a point in $S(u)$. By the channel property there must be at least one pair i, j of nearest neighbours in the strong cluster such that $(u_\varepsilon)_i \neq (u_\varepsilon)_j$ so that $E_\varepsilon(u_\varepsilon) = +\infty$. □

4.3 Bibliographical Notes

The material in this section is contained in two recent papers.
[1] A. Braides and A. Piatnitski. Homogenization of surface and length energies for spin systems. Preprint, 2010.
[2] A. Braides and A. Piatnitski. Variational problems with percolation: dilute spin systems at zero temperature Preprint 2011.

The case of rigid spins is contained in a forthcoming paper of G. Scilla.

Another application of 'rigid' percolation in the context of free-discontinuity problems is found in
[3] A. Braides and A. Piatnitski. Overall properties of a discrete membrane with randomly distributed defects. *Arch. Ration. Mech. Anal.*, **189** (2008), 301–323

Chapter 5

Motion of discrete interfaces

In this section we will see how it is possible to describe a motion of a lattice system driven by a ferromagnetic spin-type energy. How we have already observed, the continuum Γ-limit of such energies is a functional of 'crystalline-perimeter' type. To such an energy we can associate a motion by curvature. In the following sections we will briefly describe a variational approach to such a motion.

5.1 Motion by curvature

In this section we provide a simplified view of motion by curvature in the continuum. For simplicity of exposition we consider the two-dimensional case. The motion by curvature of a set $E_0 \subset \mathbb{R}^2$ is continuous function E defined on an interval $[0,T]$ with values subsets of $\mathbb{R}^2$ such that

- $E(0) = E_0$;
- for $t \in [0,T)$ the boundary $\partial E(t)$ at a point x moves with velocity proportional to the curvature κ in the point x (which is meant to point towards the center of curvature).

The precise definition of such a motion and its study is a complex problem which is not in the scope of these notes. For our purposes, in order to have an idea of how a set evolves by curvature it will suffice to examine the case when$E_0 = B_{R_0}$ is a disk of (center 0 and) radius R_0. In this case the curvature is constant at every point of ∂E_0 and hence $E(t)$ is a disk $B_{R(t)}$ for all t. The radius $R(t)$ satisfies the ODE

$$\begin{cases} \dot{R} = -C\dfrac{1}{R} \\ \\ R(0) = R_0, \end{cases} \tag{5.1}$$

whose solution is

$$R(t) = \sqrt{R_0 - 2Ct}, \qquad T = \frac{R_0}{2C}. \tag{5.2}$$

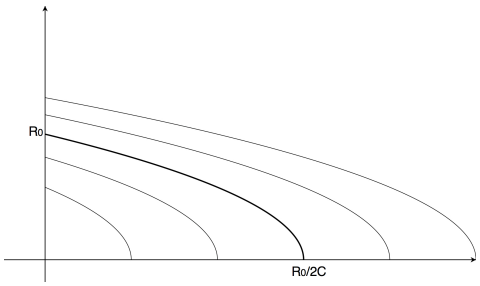


Figure 5.1: Motion by curvature of disks in terms of their radius

Since it is possible to prove an *inclusion principle* for motion by curvature (ie, that if $E(t)$ and $E'(t)$ are two motions of E_0 and E_0' with $E_0 \subset E_0'$ then the motion by curvature maintains the inclusion at all times: $E(t) \subset E'(t)$) we deduce that for all bounded E_0 the motion by curvature will be defined up to a maximal time T, where either we have *extinction* of the motion (as in the case of a disk) or we do not have enough regularity of the boundary of $E(T)$ as to guarantee that the motion be rigorously defined.

5.2 A variational approach to motion by curvature

We now briefly illustrate an approach due to Almgren, Taylor and Wang to define the motion by curvature by means of discrete-time motions obtained by iterative minimization. The scheme is as follows.

• fix a *time scale* τ and define a family (E_i^τ) recursively by setting:

$E_0^\tau = E_0$,
E_i^τ is a minimizing set of

$$\min\Big\{\mathrm{Per}\,(E) + \frac{1}{\tau} D(E, E_{i-1}^\tau)\Big\}, \tag{5.3}$$

where Per denotes the (euclidean) perimeter of E, and D is a suitable distance between sets (the choice of this distance is crucial as remarked below);

• define the motion

$$E\tau(t) = E_{[t/\tau]}^\tau; \tag{5.4}$$

• prove that (up to subsequences in τ) these exists the limit

$$E(t) = \lim_{\tau \to 0^+} E^\tau(t),$$

not empty for $t \in [0, T)$ and this is a motion by curvature of E_0.

Remark 5.2.1 (i) In this procedure the sets E_i^τ a priori are only sets of finite perimeter.

(ii) We may try a heuristic explanation of this approach: the Euler-Lagrange equations for the functional $\mathrm{Per}(E)$ (suitably interpreted) give an integral of the curvature on the boundary of E. If

$$D(E, E') = |E \triangle E'|, \tag{5.5}$$

then this can be interpreted as an L^2-distance

$$D(E, E') = \int |\chi_E - \chi_{E'}|^2 \, dx, \tag{5.6}$$

from which we get, in the Euler-Lagrange equations of (5.3), the integral of the difference quotient

$$\frac{\chi_{E_i^\tau} - \chi_{E_{i-1}^\tau}}{\tau},$$

corresponding to a discretization of the time derivative of $E(t)$.

(iii) Unfortunately, the choice of D as in (5.6) is not possible. To see this, consider the initial datum $E_0 = B_{R_0}$. In this case we expect that the motions E_i^τ be composed of disks with centre 0. With fixed τ, if $B_{R_1} \subset E_0$ is a minimizing disk for the first minimum problem, every other disk $B_{R_1}(x)$ of the same radius still contained in E_0 is clearly still a minimizing set. Hence, we may easily choose such disks in a way that the resulting motion concentrates at the extinction time at an arbitrary point of the closure of the initial disk.

The choice of Almgren, Taylor and Wang for the distance D is

$$D(E, E') = \int_{E \triangle E'} \mathrm{dist}\,(x, \partial E') \, dx. \tag{5.7}$$

We will se how this choice in (5.3) favours sets E 'uniformly distant' to the boundary of E_i^τ.

In the following example we will now briefly examine the model case of E_0 a disk, with a proof that we may easily adapt to the crystalline perimeter, and then in many points to the discrete case.

Example 5.2.2 Let $E_0 = B_R$; it will suffice to examine the minimum problem (5.3) with $i = 1$. We start with some preliminary observations:

1) the sets E in (5.3) may be chosen with every connected component contained in B_R. Indeed otherwise taking $E \cap B_R$ would decrease both perimeter and symmetric difference with B_R;

2) the sets E in (5.3) can be chosen with convex connected components, by the same reason;

3) if E' is a connected component of E not containing the center, we may consider the set obtained by substituting E' with

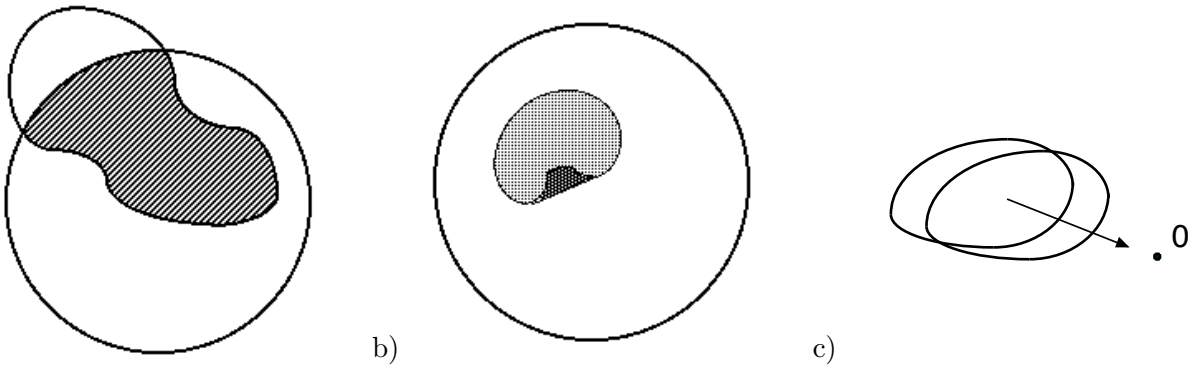
$$E'(s) = E' - sx_{E'}, \qquad \text{where } x_{E'} := \int_{E'} x\,dx$$

is the baricenter of E' and $s > 0$ is sufficiently small. Note that the derivative of our energy along this path for $s = 0$ is

$$-\int_{E'} \frac{1}{|x|}\langle x, x_{E'}\rangle\,dx < 0.$$

Hence, we may conclude that the minimum E_1^τ has a unique connected component (which is convex) containing 0.

Figure 5.2 pictures points 1)–3) above.



a) b) c)

Figure 5.2: simplification of the sets E in (5.3) by: a) intersection; b) convexification; c) translation towards 0

4) We now check that the minimal set is a disk of center 0. Let $A = |E_1^\tau|$, and consider our minimum problem with such an area constraint. By the isoperimetric inequality the perimeter term is minimized on disks; it then suffices to show that the term $D(E, E_0)$ has a disk of center 0. To this end we use polar coordinates and denote $f(\theta) = \sup\{\rho : \rho e^{i\theta} \in E\}$, so that

$$A = \int_0^{2\pi}\int_0^{f(\theta)} \rho\,d\rho d\theta = \frac{1}{2}\int_0^{2\pi} |f(\theta)|^2 d\theta$$

(Figure 5.3). By introducing the function $u(\theta) = \pi|f(\theta)|^2$ our volume constraint becomes simply

$$A = \frac{1}{2\pi}\int_0^{2\pi} u(\theta)d\theta.$$

By this condition, we may write

$$D(E, E_0) \;=\; \int_0^{2\pi}\int_{f(\theta)}^{R} (R - \rho)\,d\rho\,d\theta$$

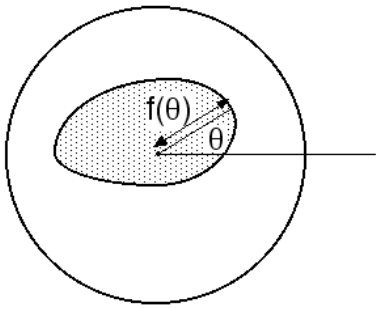


Figure 5.3: introduction of the variable f

$$\begin{aligned} &= \frac{1}{3}\pi R^2 - RA + \frac{1}{3}\int_0^{2\pi} |f(\theta)|^3 d\theta \\ &= \frac{1}{3}\pi R^2 - RA + \frac{1}{3\pi^{3/2}}\int_0^{2\pi} |u(\theta)|^{3/2} d\theta. \end{aligned}$$

By the strict convexity of $s \mapsto s^{3/2}$, applying Jensen's inequality we obtain that the minimum is obtained only on the constant function $u = A$; ie, the minimal set is a disk centered in 0.

5) We may now compute the radius r of the minimal disk, which is the minimum point of

$$\min\Big\{2\pi r + \frac{2\pi}{\tau}\int_r^R (R-\rho)\rho d\rho\Big\},$$

and hence satisfies $2\pi - \frac{2\pi}{\tau}(R-r)r = 0$.

The computations above may be repeated iteratively for all radii r_{i-1}^τ in the place of R and r_i^τ in the place of r,obtaining

$$\frac{r_i^\tau - r_{i-1}^\tau}{\tau} = -\frac{1}{r_i^\tau},$$

which is exactly the discretization of the equation $\dot{R} = -1/R$ characterizing motion by curvature of disks.

5.3 Crystalline motion

The functional given by the Γ-limit of ferromagnetic energies does not non correspond to the euclidean perimeter, but to a crystalline anisotropic perimeter. The scheme proposed

by Almgren, Taylor and Wang has been applied by Almgren and Taylor in dimension two with

$$\mathrm{Per}\,(E) = \int_{\partial^* E} \|\nu\|_1 d\mathcal{H}^1, \qquad D(E,E') = \int_{E\triangle E'} \mathrm{dist}_\infty(x,\partial E')\,dx.$$

For this choice the resulting motion (called *crystalline motion*) is more complex to describe in general by the of the non-local definition of 'crystalline curvature'. We may instead examine the relevant case when the initial set E_0 is a rectangle (this is the analog of the disk for the euclidean perimeter). We may follow the line of the previous chapter.

Example 5.3.1 (crystalline motion of a rectangle) Let E_0 be a rectangle centered in 0 with edges L_0^1 and L_0^2; ie, $E_0 = [-L_0^1/2, L_0^1/2] \times [-L_0^2/2, L_0^2/2]$. With fixed $\tau > 0$ we now characterize the set E_1 minimizing

$$\int_{\partial^* E} \|\nu\|_1 d\mathcal{H}^1 + \frac{1}{\tau}\int_{E\triangle E_0} \mathrm{dist}_\infty(x,\partial E_0)\,dx\,. \tag{5.8}$$

by adapting the argument of the previous section.

1) Note that $E_1 \subset E_0$. Otherwise, $E_1 \cap E_0$ both decreases the perimeter and the symmetric difference with E_0;

2) Note that every connected component of E_1 is a rectangle. Otherwise, we substitute to this connected component the minimal rectangle containing it, possibly repeating this operation if two of these rectangles intersect. The set thus obtained has a perimeter not greater than the previous one, but symmetric difference with E_0 strictly decreasing;

3) By translating each connected component of E_1 not containing 0 towards the origin the second integral in (5.8) strictly decreases (same computation as point 3 in Example 5.2.2). This shows that there is a unique connected component and that this component contains the origin.

We may hence take sets E in (5.8) only of the form $(-x_1, x_2) \times (-y_1, y_2) \subset E_0$. Up to an uniformly small error as $\tau \to 0$ the minimum problem becomes hence the minimization of

$$\begin{aligned} f(x_1,x_2,y_1,y_2) \;&=\; 2(x_2+x_1) + 2(y_2+y_1) + \frac{1}{\tau}\left(\frac{1}{2}\Big(\frac{L_0^1}{2} - x_1\Big)^2 L_0^2 + \frac{1}{2}\Big(\frac{L_0^1}{2} - x_2\Big)^2 L_0^2\right. \\ &\left. + \frac{1}{2}\Big(\frac{L_0^2}{2} - y_1\Big)^2 L_0^1 + \frac{1}{2}\Big(\frac{L_0^2}{2} - y_2\Big)^2 L_0^1\right). \end{aligned} \tag{5.9}$$

From the stationarity condition for f we obtain

$$\begin{aligned} 2 - \frac{1}{\tau}\Big(\frac{L_0^1}{2} - x_1\Big)L_0^2 \;&=\; 2 - \frac{1}{\tau}\Big(\frac{L_0^1}{2} - x_2\Big)L_0^2 = 0 \\ 2 - \frac{1}{\tau}\Big(\frac{L_0^2}{2} - y_1\Big)L_0^1 \;&=\; 2 - \frac{1}{\tau}\Big(\frac{L_0^2}{2} - y_2\Big)L_0^1 = 0. \end{aligned} \tag{5.10}$$

We deduce that E_1 is a rectangle of the form $E_0 = [-L_1^1/2, L_1^1/2] \times [-L_1^2/2, L_1^2/2]$, where $L_1^1 = x_1 + x_2$ and $L_1^2 = y_1 + y_2$ satisfy

$$\frac{L_1^1 - L_0^1}{\tau} = -\frac{4}{L_0^2} \qquad \frac{L_1^2 - L_0^2}{\tau} = -\frac{4}{L_0^1}. \tag{5.11}$$

The computation can be repeated iteratively, obtaining two sequences $(L_i^{\tau,1})$ and$(L_i^{\tau,2})$ that satisfy

$$\frac{L_i^{\tau,1} - L_{i-1}^{\tau,1}}{\tau} = -\frac{4}{L_i^{\tau,2}} \qquad \frac{L_i^{\tau,2} - L_{i-1}^{\tau,2}}{\tau} = -\frac{4}{L_i^{\tau,1}}, \tag{5.12}$$

up to a uniformly small error as $\tau \to 0$, and $L_0^{\tau,1} = L_0^1$, $L_0^{\tau,2} = L_0^2$. By letting $\tau \to 0$ we hence deduce the following characterization of the crystalline motion of E_0.

Proposition 5.3.2 (crystalline evolution of rectangles) *The evolution by crystalline curvature of a rectangle E_0 of edges L_0^1, L_0^2 obtained as limit of time-discrete evolutions is given by a family $E(t)$ of rectangles with the same center and of edges $L_1(t), L_2(t)$ satisfying the system of ODE*

$$\begin{cases} \dot{L}_1 = -\dfrac{4}{L_2}, \qquad \dot{L}_2 = -\dfrac{4}{L_1} \\ L_1(0) = L_0^1, \qquad L_2(0) = L_0^2\,. \end{cases} \tag{5.13}$$

Remark 5.3.3 *1) The rectangles are all similar. Indeed we have*

$$\frac{d}{dt}\Big(\frac{L_2}{L_1}\Big) = \frac{L_1\dot{L}_2 - L_2\dot{L}_1}{(L_1)^2} = 0;$$

2) the area $A(t) = L_1L_2$ of the rectangles decreases linearly:

$$\frac{d}{dt}A(t) = L_1\dot{L}_2 + L_2\dot{L}_1 = -8,$$

from which we deduce that $A(t) = L_0^1L_0^2 - 8t$, and that the extinction time of the motion is

$$T = \sqrt{\frac{L_0^1L_0^2}{8}}.$$

5.4 Motion (and 'pinning') of discrete interfaces

We may now examine the motion of discrete sets, with in mind the crystalline motion of the previous section. In this case we have to understand the role of the 'discrete spatial scale' ε and its interaction with the 'discrete time scale' τ which appear in the time-discrete minimization scheme.

In the case of spin systems with nearest-neighbour interactions in the place of the crystalline perimeter we have its discrete version. If $E \subset \varepsilon\mathbb{Z}^2$ is identified with the set where $u_i = 1$ the ferromagnetic energy considered above can be written as

$$P_\varepsilon(E) := \varepsilon \#\{(i,j) : \varepsilon i \in E, \varepsilon j \in \varepsilon\mathbb{Z}^2 \setminus E\}.$$

The distance between subsets of $\varepsilon\mathbb{Z}^2$ analogous to D can be written as

$$D_\varepsilon(E,E') = \varepsilon^2 \sum_{i \in E\setminus E'} \mathrm{dist}_\infty(i,E') + \varepsilon^2 \sum_{i \in E'\setminus E} \mathrm{dist}_\infty(i, \varepsilon\mathbb{Z}^2 \setminus E').$$

We may then fix τ and ε and proceed by successive minimization starting from an initial set of indices$E_0 = E_0^{\varepsilon,\tau}$. We will describe the motion only when the initial set is a rectangle, so as to compare it with the continuum crystalline motion obtained in the previous section.

Example 5.4.1 (discrete motion of a rectangle) As in the previous examples we may describe the set E minimizing

$$P_\varepsilon(E) + \frac{1}{\tau} D_\varepsilon(E, E_0) \tag{5.14}$$

among the sets $\varepsilon\mathbb{Z}^2$. As in Example 5.3.1 note that we may limit to considering E in the class of rectangles contained in E_0:

1) if E is not contained in E_0 we may consider $E_0 \cap E$ for which we have both $P_\varepsilon(E_0 \cap E) < P_\varepsilon(E)$ and $D_\varepsilon(E_0 \cap E, E_0) < D_\varepsilon(E, E_0)$;

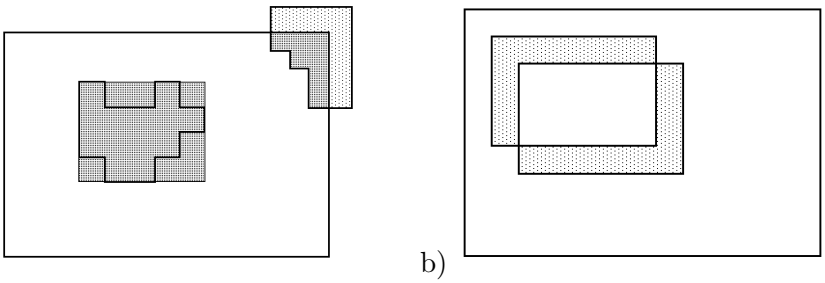
2) if (a connected component of) E is not a rectangle then we may substitute it with the least rectangle E' containing it. We have both $P_\varepsilon(E') \le P_\varepsilon(E)$ and $D_\varepsilon(E', E_0) < D_\varepsilon(E, E_0)$;

3) if a connected component does not contain the center of E_0 we may translate it towards the center. This operation maintains constant the perimeter and decreases the second term in (5.14). By repeating this operation we translate this component until it reaches another component (and then we apply point 2) or it contains 0.

From points 1)–3), pictured in Figure 5.4, we deduce that each minimizer of (5.14) is a rectangle contained in E_0.

We now characterize the side length of the minimizer. Suppose that

$$E_0 = ([-\varepsilon M_1, \varepsilon M_2] \times [-\varepsilon M_2, \varepsilon M_2]) \cap \varepsilon\mathbb{Z}^2,$$



a) b)

Figure 5.4: simplification of sets E in (5.14) by: a) intersection and 'rectangular envelope'; b) translation towards the center

where we drop the dependence on ε of $M_1 = M_1^\varepsilon$ and $M_2 = M_2^\varepsilon$. Then the minimizer of (5.14), up to negligible error as $\tau \to 0$, is a rectangle

$$E_1 = ([-\varepsilon(M_1 - n_1), \varepsilon(M_1 - n_2)] \times [-\varepsilon(M_2 - m_1), \varepsilon(M_2 - m_2)]) \cap \varepsilon\mathbb{Z}^2.$$

where n_1, n_2, m_1, m_2 minimize

$$\begin{aligned} f(n_1, n_2, m_1, m_2) &= -2\varepsilon(n_1 + n_2) - 2\varepsilon(m_1 + m_2) \\ &+ \frac{1}{\tau}\varepsilon^2 \left((2M_2 + 1)\Big(\sum_{k=1}^{n_1} \varepsilon k + \sum_{k=1}^{n_2} \varepsilon k\Big) + (2M_1 + 1)\Big(\sum_{j=1}^{m_1} \varepsilon k + \sum_{j=1}^{m_2} \varepsilon k\Big) \right). \end{aligned} \tag{5.15}$$

To understand this computation, we may refer to Figure 5.5. The rectangle E_1 is obtained by removing n_1 columns of $2M_2 + 1$ points on the 'left' side of E_0, n_2 columns of $2M_2 +$ 1points in the 'right' of E_0, m_1 rows of $2M_1 + 1$ points in the 'lower' part of E_0, m_2 rows of $2M_1 + 1$ points in the 'upper' part of E_0. The k-th column removed on the left is composed by points at a distance εk from $\varepsilon\mathbb{Z}^2 \setminus E_0$ (except those points in the smaller rectangles of size $\varepsilon^2 n_i m_j$, which are negligible when τ is small), and gives rise to the first sum. In an analogous way we can explain the terms in the other sums.

By using the formula $\sum_{k=1}^{n} k = \frac{1}{2}n(n+1)$ we obtain

$$\begin{aligned} f(n_1, n_2, m_1, m_2) &= -2\varepsilon(n_1 + n_2) - 2\varepsilon(m_1 + m_2) \\ &+ \frac{\varepsilon^3}{2\tau}\Big((2M_2 + 1)(n_1(n_1 + 1) + n_2(n_2 + 1)) \\ &+ (2M_1 + 1)(m_1(m_1 + 1) + m_2(m_2 + 1)) \Big). \end{aligned} \tag{5.16}$$

We may consider separately the dependence of f on each variable and examine the parabola $g(x) = -2x + \frac{\varepsilon^2}{2\tau}(x^2 + x)M$ whose minimum is obtained by $x = \frac{2\tau}{M\varepsilon^2} - \frac{1}{2}$. Hence, we have that n_1 is characterized by the inequalities

$$n_1 - \frac{1}{2} \le \frac{2\tau}{(2M_2 + 1)\varepsilon^2} - \frac{1}{2} \le n_1 + \frac{1}{2};$$

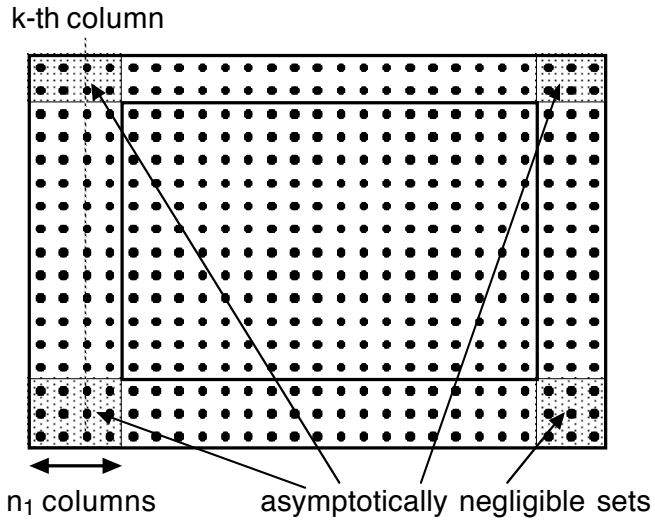


Figure 5.5: computation of the minimal set in (5.14)

ie,

$$n_1 = \begin{cases} \left[\dfrac{2\tau}{(2M_2+1)\varepsilon^2}\right] & \text{if } \left[\dfrac{2\tau}{(2M_2+1)\varepsilon^2}\right] \notin \mathbb{N} \\ \left[\dfrac{2\tau}{(2M_2+1)\varepsilon^2}\right] \text{ oppure } \left[\dfrac{2\tau}{(2M_2+1)\varepsilon^2}\right] - 1 & \text{if } \left[\dfrac{2\tau}{(2M_2+1)\varepsilon^2}\right] \in \mathbb{N}. \end{cases} \tag{5.17}$$

Analogous conditions hold for the other indices.

Three different regimes. We now describe the limit motion by choosing τ in function of ε. By assuming that the initial data converge to a 'continuum' rectangle $E_0 = [-L_1/2, L_1/2] \times [-L_2/2, L_2/2]$; ie, that

$$\varepsilon(2M_1+1) = \varepsilon(2M_1+1)^{\varepsilon} \to L_1, \qquad \varepsilon(2M_2+1) = \varepsilon(2M_2+1)^{\varepsilon} \to L_2 \tag{5.18}$$

we may define the discrete motions by successive minimization by $E^{\varepsilon}(t) = E^{\varepsilon,\tau}_{[t/\tau]}$ and consider their limit motion $E(t)$. We have the three following cases.

1: pinning. If $\tau << \varepsilon$ then the motion limit is trivial: $E(t) = E_0$ at all times. Indeed, by (5.17) we have definitively $n_1 = n_2 = m_1 = m_2 = 0$;

2: crystalline motion. If $\tau >> \varepsilon$ then by (5.17) we obtain an equation for the motion of

$L_1(t)$ as a limit of the corresponding discrete motions $(L_i^{1,\varepsilon})$. We have

$$\frac{L_i^{1,\varepsilon} - L_{i-1}^{1,\varepsilon}}{\tau} = -\frac{\varepsilon(n_1+n_2)}{\tau} \approx -2\frac{\varepsilon}{\tau}\left[\frac{2\tau}{L_i^{2,\varepsilon}\varepsilon}\right] \approx -\frac{4}{L_i^{2,\varepsilon}} \tag{5.19}$$

and then

$$\dot{L}_1 = -\frac{4}{L_2},$$

which, together with the companion equation for $\dot{L}_2$, characterizes the (continuum) crystalline motion of E_0;

2: interaction between scales. In the regime when $\tau \approx \varepsilon$ we may assume that the limit

$$\alpha := \lim_{\varepsilon\to 0}\frac{\tau}{\varepsilon}$$

exist. Then, the discrete motions are characterized by the equation

$$\frac{L_i^{1,\varepsilon} - L_{i-1}^{1,\varepsilon}}{\tau} = -\frac{\varepsilon(n_1+n_2)}{\tau} = \begin{cases} -\dfrac{2}{\alpha}\left[\dfrac{2\alpha}{L_i^{2,\varepsilon}}\right] & \text{if } \left[\dfrac{2\alpha}{L_i^{2,\varepsilon}}\right] \notin \mathbb{N} \\ -\dfrac{2}{\alpha}\left[\dfrac{2\alpha}{L_i^{2,\varepsilon}}\right] \text{ oppure } -\dfrac{2}{\alpha}\left[\dfrac{2\alpha}{L_i^{2,\varepsilon}} - 1\right] & \text{if } \left[\dfrac{2\alpha}{L_i^{2,\varepsilon}}\right] \in \mathbb{N}. \end{cases} \tag{5.20}$$

Proposition 5.4.2 *The motion is characterized by the differential inclusion*

$$\dot{L}_1 \in \begin{cases} \left\{-\frac{2}{\alpha}\left[\frac{2\alpha}{L_2}\right]\right\} & \text{if } \frac{2\alpha}{L_2} \notin \mathbb{N} \\ \left[-\frac{2}{\alpha}\left[\frac{2\alpha}{L_2}\right], -\frac{2}{\alpha}\left[\frac{2\alpha}{L_2} - 1\right]\right] & \text{otherwise,} \end{cases} \tag{5.21}$$

and by the analogous differential inclusion for $\dot{L}_2$

Proof. The proof i immediately obtained by passing to the limit in (5.20), and noting that if $\left[\frac{2\alpha}{L_2}\right] \in \mathbb{N}$ both choices n_1 and n_2 maintain the difference quotient in the desired interval. □

Remark 5.4.3 (differences with the continuum) 1) Pinning: we note a *pinning threshold*: if the edges of the initial datum satisfy

$$\min\{L_1, L_2\} > 2\alpha$$

then by (5.21) we have $\dot{L}_1 = \dot{L}_2 = 0$, and the motion is trivial;

2) 'Speed quantization': the speed of each edge is always an integer multiple of $\frac{2}{\alpha}$, and is then locally constant, except for a discrete set of points;

3) not self-similar motion: by (5.21) we obtain $\frac{d}{dt}(L_1/L_2) \neq 0$ and hence $E(t)$ is not in genera similar to E_0.

Remark 5.4.4 (uniqueness and non-uniqueness) 1) Uniqueness: from the characterization of the motion in (5.21) we obtain that the limit motion limit is unique if $\min\{L_1, L_2\} > 2\alpha$ (ie, in the case of 'pinning') or if $\max\{L_1, L_2\} < 2\alpha$. In the second case the times when $\frac{2\alpha}{L_1} \in \mathbb{N}$ or $\frac{2\alpha}{L_2} \in \mathbb{N}$ are discrete and hence negligible;

2) Non-uniqueness: we may easily construct initial data for which we do not have uniqueness of the limit motion. For example:

(a) If $L_1 > 2\alpha$ and $\frac{2\alpha}{L_2} \in \mathbb{N}$, then we may construct motions $E(t)$ with $\dot{L}_2 = 0$ and $\dot{L}_1$ any function v with

$$v(t) \in \left[-\frac{2}{\alpha}\left[\frac{2\alpha}{L_2}\right], -\frac{2}{\alpha}\left[\frac{2\alpha}{L_2} - 1\right] \right]$$

until the value T for which $L_1(T) = 4/\alpha$;

(b) If $L_1 = L_2 = 2\alpha$, then we may construct $E(t)$ such that $E(t) = E_0$ for $t \in [0, T_1]$ and $E(t)$ a square of side length L satisfying $\dot{L} = -\frac{2}{\alpha}\left[\frac{2\alpha}{L}\right]$ and $L < 2\alpha$ for a.e. $t > T_1$ until extinction time. In Figure 5.6 we have included all the motions by crystalline curvature of squares in terms of their edge length.

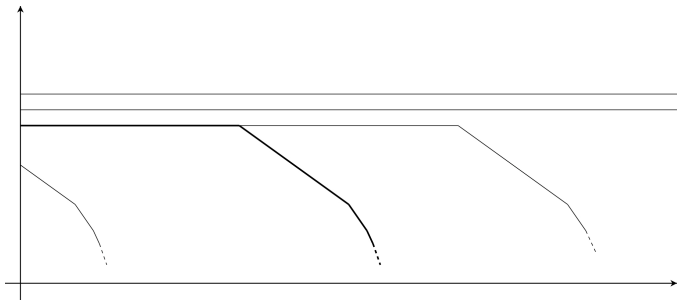


Figure 5.6: motions by crystalline curvature of squares in terms of their edge length

5.5 Bibliographical Notes

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[3] A. Braides, M.S. Gelli, and M. Novaga. Motion and pinning of discrete interfaces. *Arch. Ration. Mech. Anal.* **95** (2010), 469–498.

Chapter 6

Fracture mechanics from interatomic potentials

This section will be devoted to the study of a one-dimensional system of lattice interactions driven by some potentials that are usually involved in the description of atomic interactions. Examples of such potentials are Lennard-Jones potentials

$$J_{\mathrm{LJ}}(z) = \frac{c_1}{z^{12}} - \frac{c_2}{z^6},$$

with $c_1, c_2 > 0$ and the restriction that $z > 0$, or Morse potentials

$$J_{\mathrm{M}}(z) = -cze^{-z},$$

with $c > 0$.

The common features of these potentials $J : \mathbb{R} \to (-\infty, +\infty]$ are:

• the domain of J, $\{z : J(z) < +\infty\}$, is an interval, J admits a unique minimum point z^*, and on its domain J is (strictly) decreasing and convex for $z \leq z^*$ and (strictly) increasing for $z \geq z^*$;

• J is smooth on its domain;

• J satisfies the growth conditions at $\pm\infty$:

$$\lim_{z\to-\infty} \frac{J(z)}{|z|} = +\infty, \qquad \lim_{z\to+\infty} J(z) = 0$$

($J_{\mathrm{LJ}}(z)$ is set equal to $+\infty$ for $z \leq 0$).

6.1 Nearest-neighbors

We consider energies of the form

$$\sum_{i=1}^{n} J(v_i - v_{i-1}), \qquad v : \{0, \dots n\} \to \mathbb{R}$$

where $n \in \mathbb{N}$. For the sake of simplicity we consider a potential with the constraint that $v_i - v_{i-1} \geq 0$ (for example, Lennard-Jones potentials). This will simplify some descriptions since the function v will always be non decreasing. To remove this constraint, it is sufficient to note that the growth condition at $-\infty$ will provide strong compactness properties for the decreasing part of the function. Note that at this stage we have not performed any scaling of the energy.

6.1.1 A first scaling giving a trivial bulk energy

The first possibility is to perform the usual change of variables to interpret $v_i - v_{i-1}$ as a difference quotient, and consider energies $\varepsilon = \frac{1}{n}$,

$$E_\varepsilon(u) = \sum_{i=1}^{n} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big), \qquad u : \varepsilon\mathbb{Z} \cap [0,1] \to \mathbb{R}$$

Note that if we consider simple problems of the form

$$m_\varepsilon(L) = \min\{E_\varepsilon(u) : u(0) = 0,\ u(1) = L\},$$

then the monotonicity of test functions along with the fixed boundary conditions, provides a bound in $BV(0,1)$ of minimizers, and hence compactness in any $L^p(0,1)$ ($p < +\infty$)). We can then compute the Γ-limit of E_ε in $L^1(0,1)$ (or equivalently with respect to the weak* convergence in $BV(0,1)$). A trivial lower bound is obtained by identifying each u with its continuous piecewise-affine interpolation and correspondingly the sum with an integral: if $u_\varepsilon \to u$

$$\liminf_\varepsilon E_\varepsilon(u_\varepsilon) = \liminf_\varepsilon \int_0^1 J(u_\varepsilon')\,dt \geq \liminf_\varepsilon \int_0^1 J^{**}(u_\varepsilon')\,dt \geq \int_0^1 J^{**}(u')\,dt.$$

It must be noted that u is not AC, so that u' must be understood as the almost-everywhere defined derivative of u (that exists since u is non-decreasing). Note that u may be discontinuous (more precisely, it may have 'increasing' jumps), and that its discontinuities do not affect the value of the latter integral.

We have to check that this inequality is sharp. To this end note explicitly that

$$J^{**}(z) = \begin{cases} J(z) & \text{if } z \leq z^* \\ J(z^*) & \text{if } z \geq z^*, \end{cases}$$

and that a general $u \in BV(0,1)$ may be approximated by $u_k \in SBV(0,1)$ with a finite number of jumps and $u' \leq z^*$ in such a way that

$$\lim_k \int_0^1 J(u_k')\,dt = \int_0^1 J^{**}(u')\,dt.$$

It suffices then to consider $u \in SBV(0,1)$, with $0 < u' \leq z^*$ and with a finite number of jumps. For these functions we may just take $u_\varepsilon = u$ (more precisely, the discrete interpolation of u), and note that

$$E_\varepsilon(u_\varepsilon) = \sum_{i \in \{1,\dots,N\} \setminus I_\varepsilon^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + \sum_{i \in I_\varepsilon^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big),$$

where

$$I_\varepsilon^* = \{i : [\varepsilon(i-1), \varepsilon i) \cap S(u) \neq \emptyset\},$$

so that, for ε small enough,

$$\begin{aligned} E_\varepsilon(u_\varepsilon) &= \sum_{i \in \{1,\dots,N\} \setminus I_\varepsilon^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + \sum_{i \in I_\varepsilon^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) \\ &\leq \sum_{i \in \{1,\dots,N\} \setminus I_\varepsilon^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) \\ &= \int_0^1 J(u')\,dt + o(1), \end{aligned}$$

as desired.

We must also note that if (u_ε) is a sequence satisfying some boundary conditions; *e.g.*, $u_\varepsilon(0) = 0, u_\varepsilon(1) = L$, then the limit function for this energy may not satisfy these conditions. Anyhow, since each one of these u_ε is increasing we deduce that we have $u(0+) \geq 0$ and $u(1-) \leq L$ ($u(t\pm)$ are the traces of u at the point t). For such u the construction above still works unchanged.

As a consequence of this Γ-convergence result, we obtain that the limit of $m_\varepsilon(L)$ is given by

$$m(L) = \min\{\int_0^1 J^{**}(u')\,dt : u \text{ increasing}, \, u(0+) \geq 0, \; u(1-) \leq L\} = J^{**}(L)$$

The information we can draw from this minimum problem is that we have two types of regimes corresponding to the case:

- if $L \leq z^*$ then the unique minimizer of $m(L)$ is the linear function $u(t) = Lt$;
- if $L > z^*$ then every increasing function with $u' \geq z^*$, $u(0+) \geq 0$ and $u(1-) \leq L$ is a minimizer for $m(L)$.

If we interpret our system as a chain of atoms, then we may interpret the corresponding continuous model as having an elastic behavior in a *compressive* regime ($z \leq z^*$), while it undergoes complete failure in a *tensile* regime ($z > z^*$).

It must be noted that our result is in a sense 'trivial', as it says that E_ε can be identified with the integral

$$\int_0^1 J(u')\,dt,$$

whose relaxation is precisely $\int_0^1 J^{**}(u')\,dt$.

6.1.2 A second scaling giving Griffith fracture energy

We first perform a translation of the energy, by setting

$$\psi(z) = J(z + z^*) - J(z^*),$$

so that the minimum of ψ is $\psi(0) = 0$. We then perform a different scaling of the energies, whose underlying idea is to have the bulk and interfacial energy of the same order.

The energies we consider are now

$$E_\varepsilon(u) = \sum_{i=1}^{N} \psi\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\Big)$$

The choice of this scaling is heuristically explained as follows: if u is (the interpolation of) a smooth function, then

$$\psi\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\Big) = \psi\Big(\sqrt{\varepsilon}\frac{u_i - u_{i-1}}{\varepsilon}\Big) \approx \psi(\sqrt{\varepsilon}u'(\varepsilon i)) \approx \varepsilon\frac{1}{2}\psi''(0)(u'(\varepsilon i))^2;$$

here and after we make the assumption that

$$\alpha := \frac{1}{2}\psi''(0) > 0. \tag{6.1}$$

In this way we have

$$E_\varepsilon(u) \approx \alpha \int_0^1 |u'|^2\,dt.$$

Conversely, if we only have (increasing) jumps (*i.e.*, u is piecewise constant and non-decreasing), then if $t \in S(u) \cap [\varepsilon(i-1), \varepsilon i]$ we have

$$\psi\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\Big) \approx \psi\Big(\frac{u^+(t) - u^-(t)}{\sqrt{\varepsilon}}\Big) \approx \psi(+\infty) = -J(z^*) =: \beta,$$

and

$$E_\varepsilon(u) \approx \beta \#(S(u)).$$

Actually, what we have just shown (to have a complete proof it suffices to use a density argument by functions that are smooth except for a finite numbers of increasing jumps) is

that we have an upper bound with the functional, whose domain are SBV functions with only a finite number of increasing jumps, given by

$$F(u) = \alpha \int_0^1 |u'|^2 \, dt + \beta \#(S(u)) \qquad (u^+ > u^- \text{ on } S(u)).$$

We now show that this is also a lower bound. To do this, we compare our energy with a family of energies whose limit is easier to compute, and subsequently optimize this estimate. The family $\mathcal{F}$ of energy densities we consider are all $f \leq \psi$ of the form

$$f(z) = \begin{cases} c_1|z|^2 \wedge c_3 & \text{if } z \leq 0 \\ c_1|z|^2 \wedge c_2 & \text{if } z \geq 0, \end{cases}$$

with $c_i > 0$; *i.e.* f is a 'non-symmetrically-truncated quadratic potential'.

Note that

$$\sup\{c_1 : f \in \mathcal{F}\} = \alpha, \quad \sup\{c_2 : f \in \mathcal{F}\} = \beta, \quad \sup\{c_3 : f \in \mathcal{F}\} = +\infty. \tag{6.2}$$

Note also that

$$f\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\Big) = \begin{cases} c_3 & \text{if } \frac{u_i - u_{i-1}}{\varepsilon} \leq -\sqrt{\frac{c_3}{c_1}}\frac{1}{\sqrt{\varepsilon}} \\ \varepsilon c_1 \Big|\frac{u_i - u_{i-1}}{\varepsilon}\Big|^2 & \text{if } -\sqrt{\frac{c_3}{c_1}}\frac{1}{\sqrt{\varepsilon}} < \frac{u_i - u_{i-1}}{\varepsilon} < \sqrt{\frac{c_2}{c_1}}\frac{1}{\sqrt{\varepsilon}} \\ c_2 & \text{if } \frac{u_i - u_{i-1}}{\varepsilon} \geq \sqrt{\frac{c_2}{c_1}}\frac{1}{\sqrt{\varepsilon}}. \end{cases} \tag{6.3}$$

Let (u_ε) be a sequence converging to some u. Then we identify each u_ε with its piecewise-affine discontinuous interpolation v_ε with discontinuity set $S(v_\varepsilon) = S_\varepsilon^+ \cup S_\varepsilon^-$, where

$$S_\varepsilon^+ = \{\varepsilon i : \frac{u_\varepsilon(\varepsilon i) - u_\varepsilon(\varepsilon(i-1))}{\sqrt{\varepsilon}} \geq \sqrt{\frac{c_2}{c_1}}\}, \qquad S_\varepsilon^- = \{\varepsilon i : \frac{u_\varepsilon(\varepsilon i) - u_\varepsilon(\varepsilon(i-1))}{\sqrt{\varepsilon}} \leq -\sqrt{\frac{c_3}{c_1}}\},$$

and v_ε is constant on the corresponding intervals $(\varepsilon(i-1), \varepsilon i)$.

We then have

$$\begin{aligned} \liminf_\varepsilon E_\varepsilon(u_\varepsilon) &= \liminf_\varepsilon F_f(v_\varepsilon) \\ &=: \liminf_\varepsilon \Big(c_1 \int_0^1 |v_\varepsilon'|^2 \, dt + c_2 \#(S^+(v_\varepsilon)) + c_3 \#(S^-(v_\varepsilon)) \Big) \\ &\geq c_1 \int_0^1 |u'|^2 \, dt + c_2 \#(S^+(u)) + c_3 \#(S^-(u)), \end{aligned}$$

where

$$S^+(v) := \{t \in S(u) : u^+ > u^-\}, \qquad S^-(v) := \{t \in S(u) : u^+ < u^-\}.$$

We have used the lower semicontinuity of F_f.

We can locally optimize this estimate; *i.e.*, we may take the supremum in c_1, c_2, c_3 separately. Taking the supremum in c_3 implies that $S^-(u) = \emptyset$, while the other two 'optimizations' give the desired lower bound.

This new scaling approximates minimum boundary value problems for E_ε with

$$\begin{aligned} m(L) &= \min\{\alpha \int_0^1 |u|^2\,dt + \beta \#(\widetilde{S}(u)) : u^+ > u^-,\ u(0^+) \geq 0, u(1-) \leq L\} \\ &= \begin{cases} \min\{\alpha L^2, \beta\} & \text{if } L \geq 0 \\ \alpha L^2 & \text{if } L < 0, \end{cases} \end{aligned}$$

where we take into account that the jump of u may occur at the boundary, setting

$$\widetilde{S}(u) = S(u) \cup \{t \in \{0,1\} : \tilde{u}^-(t) < \tilde{u}^+(t)\},$$

$\tilde{u}^- = u^-$ on $(0,1]$, $\tilde{u}^+ = u^+$ on $[0,1)$, $\tilde{u}^-(0) = 0$ and $\tilde{u}^+(1) = L$.

The case $L \geq 0$ corresponds to the tensile regime in the previous scaling, and the corresponding energy may be interpreted as a *Griffith fracture energy*.

Note that for $m(L) = \beta$ we have infinitely many minimizers given by

$$u(t) = \begin{cases} 0 & \text{if } t \leq t_0 \\ L & \text{if } t > t_0; \end{cases}$$

i.e., the fracture site is not localized.

6.1.3 Equivalence by Γ-convergence

We may consider again energies of the form

$$E_\varepsilon(u) = \sum_{i=1}^n \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big), \qquad u : \varepsilon\mathbb{Z} \cap [0,1] \to \mathbb{R}$$

and interpret the second scaling as a change of variables

$$u_i = \varepsilon z^* i + \sqrt{\varepsilon} v_i,$$

so that we have

$$E_\varepsilon(u) = \sum_{i=1}^n \varepsilon J\Big(z^* + \frac{v_i - v_{i-1}}{\sqrt{\varepsilon}}\Big), \qquad v : \varepsilon\mathbb{Z} \cap [0,1] \to \mathbb{R}$$

In terms of the notation in the previous section then,

$$E_\varepsilon(u) = \varepsilon \sum_{i=1}^n \psi\Big(\frac{v_i - v_{i-1}}{\sqrt{\varepsilon}}\Big) + J(z^*). \tag{6.4}$$

The energy defined by the sum Γ-converges to

$$\alpha \int_0^1 |v'|^2 \, dt + \beta \#(S(v)).$$

Formally, carrying the argument of change of variables to the continuum, we have

$$v(t) = (u(t) - z^* t)/\sqrt{\varepsilon}$$

and the Γ-limit is rewritten as

$$\frac{1}{\varepsilon}\alpha \int_0^1 |u' - z^*|^2 \, dt + \beta \#(S(u)).$$

This suggests, plugging this argument back in (6.4), to consider the continuum energies

$$\tilde{E}_\varepsilon(u) = J(z^*) + \alpha \int_0^1 |u' - z^*|^2 \, dt + \varepsilon\beta \#(S(u)). \tag{6.5}$$

These energies are actually 'uniformly equivalent' to E_ε in the 'tensile' regime $u' \geq z^*$.

6.2 Next-to-nearest neighbors

We now consider energies taking into account first and second neighbors; *i.e.*, both terms of the form $J(u_i - u_{i-1})$ and of the form $J(u_{i+1} - u_{i-1})$.

In this case, the way boundary conditions are stated does influence the form of the limit problems. Dirichlet boundary conditions

$$u(0) = 0, \qquad u(1) = L$$

may be imposed as a pointwise condition on 0 and 1, or by requiring that u be a periodic perturbation of the linear function $u_L(t) = Lt$. In terms of minimum problems, in the first case we consider

$$\min\Big\{\sum_{i=1}^{N} J(u_i - u_{i-1}) + \sum_{i=1}^{N-1} J(u_{i+1} - u_{i-1}) : u_0 = 0, \ u_N = L\Big\}$$

(note that we have N nearest-neighbor interactions and $N-1$ next-to-nearest neighbor interactions in the interval $0, \dots, N$), while in the second one

$$\min\Big\{\sum_{i=1}^{N}\Big(J(u_i - u_{i-1}) + J(u_{i+1} - u_{i-1})\Big) : u_0 = 0, \ u_N = L, u_{N+1} = u_1 + L\Big\}$$

(equivalently, this minimum is performed among $u : \mathbb{Z} \to \mathbb{R}$ satisfying the periodicity condition $u_{i+N} = u_i + L$).

6.2.1 First scaling

In this case boundary conditions given in either way give the same limit energy. We briefly illustrate the result in a more general case, for energies of the form

$$E_\varepsilon(u) = \sum_{i=1}^{N} \varepsilon\Big(J_1\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + J_2\Big(\frac{u_{i+1} - u_{i-1}}{\varepsilon}\Big)\Big),$$

where J_1, J_2 satisfy the same conditions as the Lennard-Jones potentials.

The idea is to rewrite the energy in a more symmetric way as

$$E_\varepsilon(u) = \sum_{i=1}^{N} \varepsilon\Big(\frac{1}{2}J_1\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + \frac{1}{2}J_1\Big(\frac{u_{i+1} - u_i}{\varepsilon}\Big) + J_2\Big(\frac{u_{i+1} - u_{i-1}}{\varepsilon}\Big)\Big).$$

then to integrate out the nearest-neighbor interactions by considering

$$\tilde{J}(z) = \frac{1}{2}\min\{J(z_1) + J(z_2) : z_1 + z_2 = z\},$$

and the 'effective energy density'

$$J_{\text{eff}}(z) = J_2(2z) + \tilde{J}(2z).$$

Note that

$$\begin{aligned} & \Big(\frac{1}{2}J_1\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + \frac{1}{2}J_1\Big(\frac{u_{i+1} - u_i}{\varepsilon}\Big) + J_2\Big(\frac{u_{i+1} - u_{i-1}}{\varepsilon}\Big)\Big) \\ \geq\ & \Big(\tilde{J}\Big(\frac{u_{i+1} - u_i}{\varepsilon}\Big) + J_2\Big(\frac{u_{i+1} - u_i}{\varepsilon}\Big)\Big) = J_{\text{eff}}\Big(\frac{u_{i+1} - u_{i-1}}{2\varepsilon}\Big). \end{aligned}$$

In this way we have the inequality

$$\begin{aligned} E_\varepsilon(u) &\geq \sum_{i=1}^{N} \varepsilon J_{\text{eff}}\Big(\frac{u_{i+1} - u_{i-1}}{2\varepsilon}\Big) \\ &= \frac{1}{2}\Big(\sum_{i\ \text{even}} 2\varepsilon J_{\text{eff}}\Big(\frac{u_{i+1} - u_{i-1}}{2\varepsilon}\Big) + \sum_{i\ \text{odd}} 2\varepsilon J_{\text{eff}}\Big(\frac{u_{i+1} - u_{i-1}}{2\varepsilon}\Big)\Big), \end{aligned}$$

and hence a lower bound is given by

$$F(u) = \int_0^1 (J_{\text{eff}})^{**}(u')\, dt.$$

This is indeed the Γ-limit.

In the Lennard-Jones case

$$J_1(z) = J_2(z) = J(z)$$

the recovery sequences are simple discrete interpolations and we indeed have

$$J_{\text{eff}}(z) = J(z) + J(2z),$$

that is an energy again of Lennard-Jones type. Note that the critical state z^* giving the transition between the compressive and tensile regions is then defined as the minimizer of J_{eff}.

6.2.2 Second scaling. Periodic case

The first scaling has served in finding the minimal state z^*. Now we may scale differently the energies by setting

$$E_\varepsilon(u) = \sum_{i=1}^{N} \Big(\frac{1}{2} J\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}} + z^* \Big) + \frac{1}{2} J\Big(\frac{u_{i+1} - u_i}{\sqrt{\varepsilon}} + z^* \Big) + J\Big(\frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^* \Big) - J_{\text{eff}}(z^*) \Big).$$

A first lower bound is then obtained by the inequality

$$E_\varepsilon(u) \geq \sum_{i=1}^{N} J_{\text{eff}}\Big(\frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^* \Big)$$

The right-hand side is a superposition of two lattice energies and gives the Γ-limit

$$F_0(u) = \alpha \int_0^1 |u'|^2 \, dt + C\#(S(u)),$$

where

$$\alpha := \frac{1}{2} J''_{\text{eff}}(z^*) = \frac{1}{2} J''(z^*) + 2J''(2z^*), \qquad C := \frac{1}{2} \min J - \min J_{\text{eff}} = J_{\text{eff}}(+\infty) - \min J_{\text{eff}}.$$

This lower bound is also an upper bound if $u \in H^1(0,1)$; *i.e.*, if $S(u) = \emptyset$. Indeed, if u is smooth then a recovery sequence is simply its discrete interpolation u_ε for which

$$\begin{aligned} E_\varepsilon(u_\varepsilon) &\approx \sum_{i=1}^{N} (J(\sqrt{\varepsilon} u'(\varepsilon i) + z^*) + J(2\sqrt{\varepsilon} u'(\varepsilon i) + 2z^*) - J_{\text{eff}}(z^*)) \\ &\approx \sum_{i=1}^{N} (J_{\text{eff}}(\sqrt{\varepsilon} u'(\varepsilon i) + z^*) - J_{\text{eff}}(z^*)) \\ &\approx \sum_{i=1}^{N} \alpha\varepsilon |u'(\varepsilon i)|^2 \approx \alpha \int_0^1 |u'|^2 \, dt. \end{aligned}$$

In general the lower bound above is *not optimal* for jumps. Indeed, suppose that we have one jump (that in this periodic setting we may always suppose at 0); *i.e.*, $u_\varepsilon(0) = 0$, $u_\varepsilon(\varepsilon) \approx u(0+) = c > 0$, then

$$\begin{aligned}
&E_\varepsilon(u)\\
=\;& \Big(\frac{1}{2}J\Big(\frac{u_1}{\sqrt{\varepsilon}} + z^*\Big) + \frac{1}{2}J\Big(\frac{u_2 - u_1}{\sqrt{\varepsilon}} + z^*\Big) + J\Big(\frac{u_2 - u_0}{\sqrt{\varepsilon}} + 2z^*\Big) - J_{\text{eff}}(z^*)\Big)\\
&+ \sum_{i=2}^{N-1}\Big(\frac{1}{2}J\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}} + z^*\Big) + \frac{1}{2}J\Big(\frac{u_{i+1} - u_i}{\sqrt{\varepsilon}} + z^*\Big) + J\Big(\frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^*\Big) - J_{\text{eff}}(z^*)\Big)\\
&+ \Big(\frac{1}{2}J\Big(\frac{-u_{N-1}}{\sqrt{\varepsilon}} + z^*\Big) + \frac{1}{2}J\Big(\frac{u_1}{\sqrt{\varepsilon}} + z^*\Big) + J\Big(\frac{u_1 - u_{N-1}}{\sqrt{\varepsilon}} + 2z^*\Big) - J_{\text{eff}}(z^*)\Big)\\
\approx\;& \frac{1}{2}J\Big(\frac{u_2 - u_1}{\sqrt{\varepsilon}} + z^*\Big) - J_{\text{eff}}(z^*)\\
&+ \sum_{i=2}^{N-1}\Big(\frac{1}{2}J\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}} + z^*\Big) + \frac{1}{2}J\Big(\frac{u_{i+1} - u_i}{\sqrt{\varepsilon}} + z^*\Big) + J\Big(\frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^*\Big) - J_{\text{eff}}(z^*)\Big)\\
&+ \frac{1}{2}J\Big(\frac{u_N - u_{N-1}}{\sqrt{\varepsilon}} + z^*\Big) + J\Big(\frac{u_1 - u_{N-1}}{\sqrt{\varepsilon}} + 2z^*\Big) - J_{\text{eff}}(z^*)\\
\geq\;& 2\inf\Big\{\frac{1}{2}J(z^* + z_1) + \sum_{i=1}^{K}\Big(\frac{1}{2}J(z_i + z^*) + \frac{1}{2}J(z_{i+1} + z^*) + J(2z^* + z_i + z_{i+1})\Big)\Big\} - 2J_{\text{eff}}(z^*),
\end{aligned}$$

where K is any fixed natural number ($\leq N/2$). The optimal lower bound for a jump is then given by

$$\beta := 2B - 2\min J_{\text{eff}},$$

where

$$B := \inf_K \inf\Big\{\frac{1}{2}J(z^* + z_1) + \sum_{i=1}^{K}\Big(\frac{1}{2}J(z_i + z^*) + \frac{1}{2}J(z_{i+1} + z^*) + J(2z^* + z_i + z_{i+1})\Big)\Big\}$$

We may interpret B as a free-boundary energy: the energy to generate a discontinuity amounts to the energy $-2\min J_{\text{eff}}$ (that is positive) due to the complete detachment of the neighboring atoms plus the energy $2B$ (that is negative) due to the rearrangements of the atoms on both sides of the fracture.

Finally, the Γ-limit is again given by

$$F(u) = \alpha\int_0^1 |u'|^2\,dt + \beta\#(S(u)).$$

6.2.3 Second scaling. Boundary terms

In this case, the Γ-limit for the integral term and for interior jumps is the same, while the estimate as above performed for a jump at the boundary gives $B - \min J_{\text{eff}} = \beta/2$; hence, the resulting limit energy is

$$F(u) = \alpha \int_0^1 |u'|^2 \, dt + \beta \#(S(u)) + \frac{\beta}{2} \#(\widetilde{S}(u) \cap \{0, 1\}).$$

As a consequence we have a *localization at the boundary* of the discontinuity points.

6.3 Bibliographical Notes

The computation for nearest-neighbours can be found in
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