

Chapter 2

Continuum Limits of Discrete Models via Γ -Convergence

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In memory of my beloved mother Maria Rosaria Indino.

Abstract These lecture notes are a step-by-step guide to Γ -convergence and its applications to the upscaling of discrete systems. In many cases of interest—atoms, defects in metals, crowds—one has to face the challenging problem of deriving a macroscopic model to describe the *collective* behaviour of the interacting particles. Γ -convergence is a mathematically rigorous approach to the upscaling, and has been successfully applied to several problems in material science. The focus of this contribution is on one-dimensional chains of particles, and the starting point is the interaction energy of the system. The nature of the interaction depends on the application and we will consider the case of convex and non convex potentials and both short and long-range interactions.

Keywords Γ -Convergence · Discrete-to-continuum upscaling · Lennard-Jones · Dislocations

2.1 Introduction

Systems of interacting particles are ubiquitous: crowds of people, birds flocking, fish swarming, atoms, dislocations in metals, vortices in superconductors are examples of discrete collections of particles—different in nature and in scale—which aggregate and have an interesting collective behaviour (Fig. 2.1).

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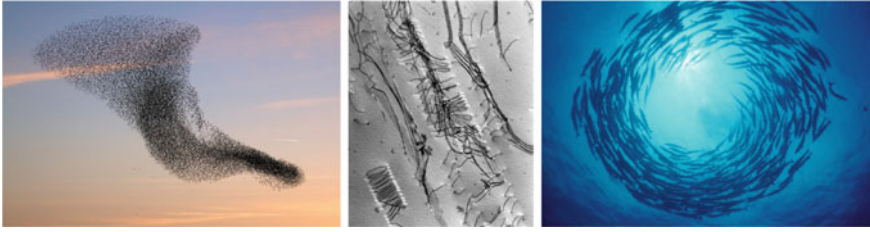


Fig. 2.1 Examples of interacting discrete systems: birds flocking, dislocations and fish swarming

Dislocations, in particular, are defects at the microscopic scale which collectively, at the macroscopic scale, determine how metals deform permanently. To understand this collective behaviour one has to bridge the scales between a microscopic, individual-based description of the system, and a macroscopic, group-led one. In other words, one has to perform a discrete-to-continuum *upscaling*, also referred to as *coarse-graining*, or *averaging* in different disciplines.

Upscaling is a *selection* mechanism in the zoo of available macroscopic theories, often derived phenomenologically and poorly justified. Since the interaction forces between particles at the discrete level are generally well (or better) understood, deriving a macroscopic model from discrete interactions is the best way to ensure that the macroscopic models are physically sound. Over the years, and in different communities, several approaches have been used, e.g. formal expansions, matched asymptotics [12, 17, 19], and statistical mechanics approaches similar to the derivation of the BBGKY hierarchy explained in Chap. 1 [15, 16]. So, what *method* should be used for the upscaling?

A mathematically rigorous way to bridge the scales is via Γ -convergence, a convergence concept for the energies of the system. The Γ -convergence approach has many advantages. In particular, it ensures that minimisers of the discrete problem are *close* to minimisers of the limit problem; hence the limit model is a good approximation of the original one, as far as minimisers are concerned. This property makes this approach very well-suited for tackling problems in materials science. Fracture mechanics [6, 9, 10, 18, 23], spin systems [1, 2], magnetomechanics [24] and dislocations [14, 22, 25] are some of the many examples where this approach has been successful. Moreover, although Γ -convergence is a convergence of energies and equilibrium configurations—hence of *static* problems—it can be combined with gradient flow or rate-independent techniques, as described above, in order to treat dynamics (see e.g. [5, 20, 21]).

In these lecture notes we are going to focus on the static case, and explain the basic concepts and difficulties of the rigorous upscaling by Γ -convergence for a one-dimensional chain of interacting particles, and for both short-range and long-range interactions.

In the systems we are going to consider the particles are ordered and interact via a pairwise interaction potential. This means that we are assuming that there is an underlying *reference lattice* that enforces the ordering of the particles, and in

particular implies that a particle has always the same neighbours. Although this assumption has some limitations, it is reasonable for the systems we study. The nature of the potential depends on the applications. For inter-atomic interactions it is typically the Lennard-Jones potential, which blows up when the atoms collide and decays rapidly by increasing the inter-atomic distance. For Coulomb interactions, the potential can model attraction or repulsion, depending on the sign of the charges. Moreover, it can be convex (like in a linear spring model, where it is quadratic) or non-convex (like the Lennard-Jones potential).

The aim of the lecture notes is to walk through the difficulties inherent to the study of discrete problems by facing one difficulty per time. We will mainly limit ourselves to nearest-neighbour interactions. In this simplified setting we will first consider superlinear energies, for which the energy functional is naturally defined on a reflexive space, and we will analyse both the case of convex and non-convex potentials. Then we will move away from the superlinearity assumption and focus on the Lennard-Jones interaction potential. The final part of the lecture notes will be devoted to the case of more interactions (next-to-nearest neighbours and more) and to the case of dislocation interactions.

2.2 Preliminaries

In this section we collect a number of preliminaries that will be needed in the rest of the lecture notes. More precisely, we are going to define Γ -convergence, and the more technical concepts of coerciveness and relaxation.

2.2.1 Γ -Convergence

This first subsection is devoted to the definition and some properties of Γ -convergence. For a more comprehensive introduction to this topic the interested reader can have a look at the excellent book by Dal Maso [13].

Definition 2.2.1 Let (X, d) be a metric space, let $E_n : X \rightarrow \mathbb{R}$ be a sequence of functionals for $n \in \mathbb{N}$, and let $E : X \rightarrow \mathbb{R}$. We say that E_n Γ -converges to E as $n \rightarrow +\infty$ if the following conditions are satisfied:

- (i) For all $x \in X$ and for every $(x_n) \subset X$, $x_n \rightarrow x$:

$$\liminf_{n \rightarrow +\infty} E_n(x_n) \geq E(x);$$

- (ii) For all $x \in X$ there exists a *recovery* sequence $(\bar{x}_n) \subset X$, $\bar{x}_n \rightarrow x$:

$$\limsup_{n \rightarrow +\infty} E_n(\bar{x}_n) \leq E(x).$$

Remark 2.2.1 Condition (i) is usually referred to as *liminf inequality* or lower bound; (ii) is referred to as *limsup inequality* or upper bound. If we think of E_n as the energy associated to a discrete system of n particles and of E as the continuum limit model, then (i) means that for a given macroscopic configuration x , the discrete energy corresponding to *any* configuration x_n close to x is larger than the limit energy computed at x . Property (ii), on the other hand, ensures that the lower bound is *sharp*, namely that it can be attained on a special discrete configuration $\bar{x}_n$.

Remark 2.2.2 Notice that the Γ -limit will depend on the convergence used in the space X . In particular, if we endow X with the distances d and d' and assume that d is stronger than d' (i.e., that convergence in d implies convergence in d') then the $\Gamma(d)$ -limit will be larger than the $\Gamma(d')$ -limit.

Γ -convergence enjoys very nice properties concerning the behaviour of minimisers and minimum values which other, more natural definitions of convergence (e.g. the pointwise convergence) do not enjoy.

Theorem 2.2.1 Let $E_n, E : X \rightarrow \mathbb{R}$, and assume the following:

- (a) $E_n \xrightarrow{\Gamma} E$ as $n \rightarrow +\infty$;
- (b) x_n is a minimiser of E_n for every $n \in \mathbb{N}$;
- (c) $x_n \rightarrow x$.

Then x is a minimiser of E .

Proof We claim that $E(x) \leq E(y)$ for every $y \in X$.

Let $y \in X$; by assumption (a) there exists a recovery sequence $\bar{y}_n \rightarrow y$ satisfying property (ii) in Definition 2.2.1. Therefore

$$E(y) \geq \limsup_{n \rightarrow +\infty} E_n(\bar{y}_n) \stackrel{(b)}{\geq} \limsup_{n \rightarrow +\infty} E_n(x_n) \geq \liminf_{n \rightarrow +\infty} E_n(x_n) \geq E(x),$$

where the last inequality follows from (c) and from property (i) in Definition 2.2.1.

Example 2.2.1 Consider the sequence $f_n : \mathbb{R} \rightarrow \mathbb{R}$ defined as

$$f_n(x) = \begin{cases} -nx & 0 \leq x \leq \frac{1}{n} \\ -2 + nx & \frac{1}{n} \leq x \leq \frac{2}{n} \\ 0 & x \notin [0, \frac{2}{n}]. \end{cases}$$

Clearly the minimum value of f_n is $\min f_n = -1$, reached at the point $\frac{1}{n}$.

Note that the pointwise limit of the sequence f_n (as $n \rightarrow +\infty$) is the function $f_p \equiv 0$ for every $x \in \mathbb{R}$. In particular for the pointwise limit f_p the conclusion of Theorem 2.2.1 does not hold true, since $\min f_p = 0 \neq -1$. Hence, the pointwise limit is not the right object if we are interested in the behaviour of minimisers and minimum values.

It is easy to check that the Γ -limit of f_n as $n \rightarrow +\infty$ is the function f_∞ defined as

$$f_\infty(x) = \begin{cases} -1 & x = 0 \\ 0 & x \neq 0, \end{cases}$$

which instead has the same minimum value of f_n .

In conclusion, Γ -convergence is the natural convergence concept if one is interested in the asymptotic behaviour of minimisers. Note however that Theorem 2.2.1 states that if we want to infer, from Γ -convergence, that minimisers of the energies E_n converge to a minimiser of the limit energy E , we need to prove property (c). More precisely, we need to prove that minimisers of E_n converge to some limit configurations. Next section focuses on this point.

2.2.2 Coerciveness

The concept of coerciveness for an energy is intimately related to its minimisation. More precisely, it is related to the concept of minimising sequences, i.e., sequences along which the functional reaches its minimum value. If such a sequence has a limit, then the limit is the natural candidate for being the minimum point of the limit energy. The fact that such a sequence of energy minimisers converges depends on the bounds that the energy provides; and this is the essence of coerciveness.

Given the relation between Γ -convergence and convergence of minimisers, it is clear that coerciveness is also related to Γ -convergence. More precisely, the choice of the convergence in the space X in Definition 2.2.1 is determined by the coerciveness of the functionals E_n .

The definition of *coerciveness* will be given for functionals defined in general topological spaces (which are not necessarily metric spaces). The reason for that is that we are going to work often with energy bounds ensuring only weak convergence of the sequences.

Definition 2.2.2 Let X be a topological space and let $E : X \rightarrow \mathbb{R}$. The functional E is said to be (sequentially) coercive if for every t there exists a (sequentially) compact set K_t such that

$$S_t := \{x \in X : E(x) \leq t\} \subset K_t.$$

Recall that a set K is said to be *sequentially compact* if every sequence in K has a converging subsequence to a point in K .

Remark 2.2.3 Since the definition of the coerciveness in Definition 2.2.2 is very abstract, there is a characterisation of coerciveness that is used in practice when X is a reflexive Banach space:

F is coercive in the weak topology of X if and only if $F(x)$ tends to infinity as $\|x\| \rightarrow +\infty$.

This gives a simple criterion for the weak coerciveness. In fact, if the functional satisfies the lower bound $F(x) \geq C\|x\|$, with a constant $C > 0$, then it is weakly coercive. This means that if we can prove some *a priori* bounds for the energy with respect to some norm, then we directly have compactness, in a weak or in a strong sense, as we will see.

The concrete meaning of the definition and of the remark above will be made clear in the following, more familiar examples.

Example 2.2.2 Recall that $L^p(0, 1)$ and $W^{1,p}(0, 1)$, for $p > 1$, are reflexive Banach spaces; recall also that a bounded sequence in a reflexive space has a weakly convergent subsequence (see, e.g. [11]).

Let us consider the following examples, where $p > 1$.

- (a) The functional $F : L^p(0, 1) \rightarrow \mathbb{R}$ defined as

$$F(u) = \int_0^1 |u|^p ds$$

is weakly sequentially coercive.

- (b) The functional $F : W^p(0, 1) \rightarrow \mathbb{R}$ defined as

$$F(u) = \int_0^1 |u'|^p ds + \int_0^1 |u|^p ds$$

is weakly sequentially coercive in $W^{1,p}$ and strongly sequentially coercive in L^p .

2.2.2.1 Weak Compactness in L^1

This section is very technical and might be skipped on a first reading. The results stated here, however, will be heavily used in the applications studied in Sect. 2.3 and therefore are needed to make these lecture notes self-contained.

Here we are going to consider the problem of compactness in L^1 and in $W^{1,1}$, which is mathematically more subtle since the unit ball in these spaces is not weakly compact (as the spaces are not reflexive). The next two theorems offer a good way to check the coerciveness of a functional in L^1 by means of some useful (and typically easier to check) characterizations.

We will state the theorems in the general setting of functionals defined in $L^1(\Omega)$, for $\Omega \subset \mathbb{R}^N$ and $N \geq 1$.

Theorem 2.2.2 (Dunford-Pettis) Let $\mathcal{F} \subset L^1(\Omega)$, with Ω bounded. The following statements are equivalent:

- (1) $\mathcal{F}$ is relatively compact in the weak topology of L^1 (i.e., every sequence has a weakly convergent subsequence);
- (2) the family $\mathcal{F}$ is uniformly integrable, i.e., for every $\varepsilon > 0$ there exists $c > 0$ such that:

$$\int_{|f|>c} |f| ds < \varepsilon \quad \text{for every } f \in \mathcal{F}.$$

Remark 2.2.4 There are a number of characterisations of the *uniform integrability* that might be easier to check in practice. One of them is that the family $\mathcal{F}$ is bounded and uniformly (in $\mathcal{F}$) absolutely continuous.

We recall that we say that the *absolute continuity* of the integrand holds uniformly in $\mathcal{F}$ if for every $\varepsilon > 0$ there exists $\delta > 0$ such that for every measurable set A with $|A| < \delta$:

$$\int_A |f| ds < \varepsilon \quad \text{for every } f \in \mathcal{F}.$$

In the formula above, $|A|$ denotes the (Lebesgue) measure of the set A .

Another useful criterion is the following:

Theorem 2.2.3 *Let $\mathcal{F} \subset L^1(\Omega)$, with Ω bounded. Assume that there exists $\psi : \mathbb{R} \rightarrow [0, +\infty)$ continuous such that*

$$\lim_{|z| \rightarrow +\infty} \frac{\psi(z)}{|z|} = +\infty,$$

and with the property that there exists $M > 0$ such that

$$\int_{\Omega} \psi(|f|) ds < M \quad \text{for every } f \in \mathcal{F}.$$

Then the family $\mathcal{F}$ is uniformly integrable.

Proof By the superlinearity assumption on ψ it follows that for every a there exists a radius R such that, for every $|z| > R$:

$$\frac{\psi(z)}{|z|} > a.$$

So, if $f \in \mathcal{F}$ and if $s \in \{\xi \in \Omega : |f(\xi)| > R\}$, then

$$\frac{\psi(f(s))}{|f(s)|} > a.$$

In particular, since ψ is nonnegative:

$$\int_{\Omega} \psi(|f(\xi)|) d\xi \geq \int_{|f|>R} \psi(|f(s)|) ds \geq a \int_{|f|>R} |f(s)| ds.$$

Now, let $\varepsilon > 0$ be fixed and let a be such that $\frac{M}{a} < \varepsilon$. Then, by assumption and by the previous inequalities:

$$M \geq \int_{\Omega} \psi(|f(\xi)|) d\xi \geq a \int_{|f|>R} |f(s)| ds.$$

Hence

$$\frac{M}{a} \geq \int_{|f|>R} |f(s)| ds,$$

implying the claim.

Remark 2.2.5 The converse implication follows if ψ is convex.

Corollary 2.2.1 *Under the assumptions of Theorem 2.2.3 it follows that the family $\mathcal{F}$ is in fact relatively compact with respect to the weak convergence in L^1 .*

2.2.3 Lower Semicontinuity and Relaxation

Lower semicontinuity is, together with coerciveness, the key assumption ensuring the existence of minimisers.

Also in this section we will assume that X is a general topological space.

Definition 2.2.3 A functional $F : X \rightarrow \mathbb{R}$ is said to be lower semicontinuous if for every t the sublevels

$$S_t := \{x \in X : F(x) \leq t\}$$

are closed.

The following sequential definition is more used in practice (and coincides with Definition 2.2.3 for metric spaces).

Definition 2.2.4 A functional $F : X \rightarrow \mathbb{R}$ is said to be sequentially lower semicontinuous if for every $x \in X$ and for every sequence (x_j) converging to x as $j \rightarrow +\infty$:

$$F(x) \leq \liminf_{j \rightarrow +\infty} F(x_j).$$

Example 2.2.3 Consider the following cases:

- The functional in Example 2.2.2 (a) is strongly continuous and weakly lower semicontinuous in L^p ;
- The functional in Example 2.2.2 (b) is strongly continuous and weakly lower semicontinuous in $W^{1,p}$.

Note that the integrand in both cases is a convex function. This is not a coincidence: As we will see, for integral functionals, lower semicontinuity is strictly related to the convexity of the integrand.

The connection between lower semicontinuity and coerciveness on the one hand, and existence of minimisers on the other hand is made clear by the following theorem.

Theorem 2.2.4 *Let $F : X \rightarrow \mathbb{R}$ be a coercive and lower semicontinuous functional. Then there exists a minimiser of F .*

Proof Let (x_j) be a minimising sequence for F , namely $\lim_{j \rightarrow \infty} F(x_j) = \inf_X F$. By coerciveness we deduce that x_j converges to some $x \in X$. The fact that x is a minimiser of F follows by lower semicontinuity, since

$$\inf_X F = \lim_{j \rightarrow \infty} F(x_j) \geq F(x).$$

Remark 2.2.6 (Lower semicontinuity and Γ -convergence) The Γ -limit defined by properties (i) and (ii) of Definition 2.2.1 is lower semicontinuous.

Remark 2.2.7 Given a sequence of functionals $F_n : X \rightarrow \mathbb{R}$ it is possible to define the following functionals:

$$\begin{aligned} F'(x) &:= \inf \{ \liminf_{n \rightarrow +\infty} F_n(y_n) : y_n \rightarrow x \} \\ F''(x) &:= \inf \{ \limsup_{n \rightarrow +\infty} F_n(y_n) : y_n \rightarrow x \}. \end{aligned}$$

The functionals F' and F'' are lower semicontinuous and the sequence F_n Γ -converges if and only if $F' = F''$ (and the common value is the Γ -limit of F_n).

If a functional F is not lower semicontinuous one can construct a lower semicontinuous functional related to F , as in Definition 2.2.5.

Definition 2.2.5 Given a functional $F : X \rightarrow \mathbb{R}$, its *lower semicontinuous envelope* (or *relaxed functional*) is defined as

$$\text{sc}^- F(x) := \sup \{ G(x) \mid G : X \rightarrow \mathbb{R}, G \text{ lower semicontinuous}, G \leq F \}.$$

Remark 2.2.8 Given a functional $F : X \rightarrow \mathbb{R}$, we can define the sequence $F_n := F$ for every $n \in \mathbb{N}$. Then the Γ -limit of the sequence F_n coincides with the relaxation

of F . The functional $\text{sc}^- F$ is therefore characterized by the same properties of the Γ -limit.

From the point of view of Γ -convergence, the ‘right’ space would be the space of lower semicontinuous functionals.

It is possible to prove that F and $\text{sc}^- F$ have the same ‘ground states’ in some sense. Therefore, from the point of view of the minimisation, the energies F and $\text{sc}^- F$ are the same.

2.2.3.1 Lower Semicontinuity in L^1

As for the coerciveness, also for the lower semicontinuity in the case of non-reflexive spaces requires some care and will be dealt with separately.

The proof of the next theorem is quite technical and can be skipped by a reader who is not familiar with convergence of measures. The lower semicontinuity result will be heavily used in the applications in the next sections.

Theorem 2.2.5 *Let $\psi : \mathbb{R} \rightarrow \mathbb{R}$ be a convex function such that $\psi(z) = +\infty$ for $z < 0$, $\lim_{z \rightarrow 0^+} \psi(z) = +\infty$ and $\lim_{z \rightarrow +\infty} \psi(z) = \beta$, for some $\beta \in \mathbb{R}$.*

For $u \in W^{1,1}(0, 1)$ satisfying the Dirichlet boundary conditions $u(0) = 0$ and $u(1) = \ell > 0$ we define the functional

$$u \mapsto F(u) = \int_0^1 \psi(u'(s)) ds;$$

the functional F is lower semicontinuous with respect to the strong convergence in L^1 .

Proof Let $(u_j) \subset W^{1,1}(0, 1)$ and let $u \in W^{1,1}(0, 1)$ be such that $u_j(0) = 0 = u(0)$, $u_j(1) = \ell = u(1)$ and $u_j \rightarrow u$ strongly in $L^1(0, 1)$. We claim that

$$\liminf_{j \rightarrow +\infty} F(u_j) \geq F(u).$$

We assume further that $F(u_j) \leq c$ (otherwise the claim is trivial).

From the assumptions on F it follows that u_j are increasing; moreover, they are bounded uniformly by ℓ by the monotonicity. For the derivative we have the following uniform bound (where we use that functions in $W^{1,1}(0, 1)$ are absolutely continuous, see e.g. [11]):

$$\int_0^1 |u'_j(s)| ds = \int_0^1 u'_j(s) ds = u_j(1) - u_j(0) = \ell.$$

Therefore the sequence (u_j) is bounded in $W^{1,1}$ and consequently the sequence $(u_j)'$ regarded as a sequence of measures converges weakly* to u' . By [3, Proposition 5.1–Theorem 5.2] we have that the functional F on absolutely continuous measures (with respect to the Lebesgue measure) is lower semicontinuous with respect to the weak convergence of measures, which implies the thesis. (To apply the theorem just observe that $\psi_\infty = 0$, where ψ_∞ denotes the *recession* function of the convex function ψ .)

2.3 Discrete Systems: Short-Range Interactions

As a first step we establish the setup of one-dimensional discrete models. This general setup will be used also in Sect. 2.4.

2.3.1 One-Dimensional Discrete Setting

Consider $n + 1$ points, for $n \in \mathbb{N}$, representing $n + 1$ particles in a one-dimensional chain. Set $\lambda_n := \frac{1}{n}$. We define a reference lattice, which, roughly speaking, provides an ordering of the particles. In the reference lattice the $n + 1$ particles occupy $n + 1$ uniformly spaced points in the interval $[0, 1]$ (with no loss of generality). More precisely, the positions of the particles in the reference lattice are $\lambda_n i = \frac{i}{n}$, for $i \in \{0, \dots, n\}$. We denote with I_n the reference lattice, i.e.,

$$I_n := [0, 1] \cap \lambda_n \mathbb{Z}.$$

The real, *current* positions of the particles will be described by means of a function defined on I_n , denoted by $u : I_n \rightarrow \mathbb{R}$. In practice, u is nothing but a collection of $n + 1$ ordered values, which are the evaluations of u on I_n . In Sects. 2.3.2.2 and 2.3.3 the values $\{u_i : i = 0, \dots, n\}$ represent the *displacement* that each of the particles undergoes. Therefore, the current position of the i -th particle is $\lambda_n i + u_i$. In Sect. 2.3.4 the function u is instead a *deformation*, hence the values $\{u_i\}$ are the positions of the particles in the current, deformed configuration.

The function u (displacement or deformation) can be equivalently regarded as a continuous piecewise affine function (affine interpolation of the $n + 1$ values). In formulas, given $\{u_i : i = 0, \dots, n\}$, we define $\tilde{u} : [0, 1] \rightarrow \mathbb{R}$ as

$$\tilde{u}(s) := u_i + \frac{u_{i+1} - u_i}{\lambda_n} (s - \lambda_n i), \quad s \in (\lambda_n i, \lambda_n (i + 1)).$$

Notice that

$$\tilde{u}'(s) := \frac{u_{i+1} - u_i}{\lambda_n}, \quad s \in (\lambda_n i, \lambda_n (i + 1)).$$



Fig. 2.2 Sketch of nearest neighbour interactions in the reference configuration

We denote with $\mathcal{A}_n(0, 1)$ the set of discrete values of u or, equivalently, the set of piecewise affine functions $\tilde{u}$ defined as above. Notice that $\mathcal{A}_n(0, 1) \subset W^{1,1}(0, 1)$ and $\mathcal{A}_n(0, 1) \subset W^{1,\infty}(0, 1)$.

Remark 2.3.1 It is possible to provide an alternative description of the current positions of the $n + 1$ particles $\{u_i : i = 0, \dots, n\}$ in terms of *empirical measure*. The empirical measure associated to the current configuration is μ_n defined as

$$\mu_n := \frac{1}{n} \sum_{i=0}^n \delta_{u_i}.$$

2.3.2 Nearest-Neighbour Interactions

In this section we focus on *nearest-neighbour* interactions, as sketched in Fig. 2.2 for the reference lattice.

The interaction energy for particles interacting with their nearest neighbours via an interaction potential φ is a functional $E_n : \mathcal{A}_n(0, 1) \rightarrow \mathbb{R}$ defined as

$$E_n(\{u_i\}) := \lambda_n \sum_{i=0}^{n-1} \varphi \left(\frac{u_{i+1} - u_i}{\lambda_n} \right).$$

The pairwise interaction described by the functional E_n depends only on the ratio between the difference of the displacements of two consecutive particles (or the deformed distance between consecutive particles) and their distance in the reference lattice. In what follows we will consider different expressions for the potential φ , corresponding to different types of interaction.

As we noticed, $\mathcal{A}_n(0, 1) \subset W^{1,1}(0, 1)$. Nevertheless, as we will see, the most natural setting for this type of functionals is $L^1(0, 1)$. Therefore we will use the extension of the functional to $L^1(0, 1)$, (still denoted by E_n) defined as

$$E_n(\{u_i\}) := \begin{cases} \lambda_n \sum_{i=0}^{n-1} \varphi \left(\frac{u_{i+1} - u_i}{\lambda_n} \right) & u \in \mathcal{A}_n(0, 1), \\ +\infty & u \in L^1(0, 1) \setminus \mathcal{A}_n(0, 1). \end{cases} \quad (2.3.1)$$

Remark 2.3.2 The extension in (2.3.1) has a great advantage. In fact, while the original functionals E_n are defined on the domains $\mathcal{A}_n$ that depend on n , the extended functionals E_n are defined on a common domain $L^1(0, 1)$ independent of n .

2.3.2.1 Rewriting the Energy as an Integral

Using the identification of the discrete function $\{u_i\}$ with its piecewise affine interpolation $\tilde{u}$ we can rewrite the sum in E_n as an integral. In fact

$$\varphi\left(\frac{u_{i+1} - u_i}{\lambda_n}\right) = \frac{1}{\lambda_n} \int_{\lambda_n i}^{\lambda_n(i+1)} \varphi(\tilde{u}'(s)) ds,$$

and therefore

$$\lambda_n \sum_{i=0}^{n-1} \varphi\left(\frac{u_{i+1} - u_i}{\lambda_n}\right) = \int_0^1 \varphi(\tilde{u}'(s)) ds. \quad (2.3.2)$$

2.3.2.2 Convex and Superlinear Interaction

In this section we consider discrete energies E_n with a convex and superlinear interaction potential φ . The model case is $\varphi(z) = z^2$, corresponding to spring-type interactions. Notice that such a convex interaction favours configurations where the relative displacement is zero. In particular, in the case of clamped boundary conditions $u_0 = u_n = 0$, the minimum energy configuration is the reference configuration, i.e., $u_i = 0$ for every i .

We want to study the Γ -convergence of the energies E_n in the ‘many particles’ limit $n \rightarrow +\infty$. The goal is to obtain a continuum, upscaled energy.

Finding the Γ -limit is a procedure that consists of two main steps, as we already pointed out. The first step is to determine the *natural* convergence in the domain of the functional (the space X in Definition 2.2.1). The second step is to prove the lower and upper bounds (i) and (ii) in Definition 2.2.1.

We start by focusing on the second step and we skip the first step for now. In Theorem 2.3.1 we state and prove Γ -convergence with respect to the strong convergence in $W^{1,1}(0, 1)$. In what follows we will see that this is not the natural convergence to be used, and we will determine the natural convergence by studying the coerciveness of the functionals E_n in (2.3.1).

Theorem 2.3.1 *Let E_n be defined as in (2.3.1) and assume that φ is continuous, convex and nonnegative. The Γ -limit of E_n with respect to the strong convergence in $W^{1,1}$ is the functional E defined for $u \in W^{1,1}(0, 1)$ as*

$$E(u) = \int_0^1 \varphi(u'(s)) ds.$$

Proof (Liminf inequality) Let $u \in W^{1,1}(0, 1)$ and $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ such that $\{u_i^n\} \rightarrow u$ in $W^{1,1}$. (Notice that the convergence is meant in terms of the convergence of the

piecewise affine interpolations $\tilde{u}^n$.) We claim that

$$\liminf_{n \rightarrow +\infty} E_n(\{u_i^n\}) \geq E(u).$$

Using the identification (2.3.2), this is equivalent to proving that

$$\liminf_{n \rightarrow +\infty} \int_0^1 \varphi((\tilde{u}^n)'(s)) ds \geq \int_0^1 \varphi(u'(s)) ds.$$

First of all, we reduce to a subsequence $\tilde{u}^j := \tilde{u}^{n_j}$ of $\tilde{u}^n$ such that

$$\liminf_{n \rightarrow +\infty} \int_0^1 \varphi((\tilde{u}^n)'(s)) ds = \lim_{j \rightarrow +\infty} \int_0^1 \varphi((\tilde{u}^j)'(s)) ds.$$

Clearly, the subsequence $\tilde{u}^j$ converges to u in $W^{1,1}$ as $j \rightarrow +\infty$, hence in particular $(\tilde{u}^j)'$ converges to u' in L^1 . Consequently, there exists a further subsequence $\tilde{u}^{j_k}$ such that $(\tilde{u}^{j_k})'$ converges to u' a.e. on $(0, 1)$ as $k \rightarrow +\infty$. Being φ continuous, this implies that

$$\lim_{k \rightarrow +\infty} \varphi((\tilde{u}^{j_k})') = \varphi(u') \quad \text{a.e.}$$

It follows that

$$\int_0^1 \lim_{k \rightarrow +\infty} \varphi((\tilde{u}^{j_k})'(s)) ds = \int_0^1 \varphi(u'(s)) ds. \quad (2.3.3)$$

By Fatou's Lemma (φ measurable and nonnegative) it follows that

$$\int_0^1 \lim_{k \rightarrow +\infty} \varphi((\tilde{u}^{j_k})'(s)) ds \leq \liminf_{k \rightarrow +\infty} \int_0^1 \varphi((\tilde{u}^{j_k})'(s)) ds;$$

by (2.3.3) this implies that

$$\int_0^1 \varphi(u'(s)) ds \leq \liminf_{k \rightarrow +\infty} \int_0^1 \varphi((\tilde{u}^{j_k})'(s)) ds,$$

and hence the claim. Notice that in the proof of the lower bound we did not make use of the assumption that φ is convex.

Limsup inequality. Let $u \in W^{1,1}(0, 1)$; we define the recovery sequence as the evaluations of u on I_n (well defined since u is continuous), i.e.,

$$u_i^n := u(\lambda_n i).$$

Also, since u is absolutely continuous (being in $W^{1,1}(0, 1)$), the Fundamental Theorem of Calculus can be applied to u and gives

$$\frac{u_{i+1}^n - u_i^n}{\lambda_n} = \frac{1}{\lambda_n} \int_{\lambda_n i}^{\lambda_n(i+1)} u'(s) ds.$$

Then, for the functionals E_n we have

$$\begin{aligned} E_n(\{u_i^n\}) &= \lambda_n \sum_{i=0}^n \varphi\left(\frac{u_{i+1}^n - u_i^n}{\lambda_n}\right) = \lambda_n \sum_{i=0}^n \varphi\left(\frac{1}{\lambda_n} \int_{\lambda_n i}^{\lambda_n(i+1)} u'(s) ds\right) \\ &\stackrel{(*)}{\leq} \lambda_n \sum_{i=0}^n \frac{1}{\lambda_n} \int_{\lambda_n i}^{\lambda_n(i+1)} \varphi(u'(s)) ds = \int_0^1 \varphi(u'(s)) ds, \end{aligned}$$

where the $(*)$ inequality follows by Jensen's inequality.

Remark 2.3.3 Notice that by the convexity assumption the functionals E_n also Γ -converge to E with respect to the weak convergence in $W^{1,1}$.

The recovery sequence is clearly the same, since a strongly convergent sequence converges weakly to the same limit. The only difference in the proof is in the liminf-inequality, where one has to prove the lower semicontinuity of the functionals with respect to the weak convergence in $W^{1,1}$. Thanks to the convexity of φ , this stronger lower-semicontinuity property follows directly from Theorem 2.3.2:

Theorem 2.3.2 *Let X be a Banach space, let $F : X \rightarrow \mathbb{R}$ be convex. Then F is strongly lower semicontinuous if and only if it is weakly lower semicontinuous.*

Now we focus on the step we skipped so far, namely on the identification of the *natural* convergence for the energies E_n . This will be the result of a coerciveness result for the functionals E_n . In Theorem 2.3.3 we consider the general case of a nonnegative and continuous energy density φ with superlinear growth, and analyse the coerciveness of the corresponding integral functional.

Theorem 2.3.3 *Let E_n be defined as in (2.3.1) and assume that φ is continuous and nonnegative and satisfies*

$$\lim_{|z| \rightarrow +\infty} \frac{\varphi(z)}{|z|} = +\infty.$$

Let $(u^n) \subset W^{1,1}(0, 1)$ be such that $\|u^n\|_{L^1(0,1)} \leq c$ and such that

$$E_n(u^n) := \int_0^1 \varphi((u^n)'(s)) ds \leq c.$$

Then there exists $u \in W^{1,1}(0, 1)$ such that $u^n \rightharpoonup u$ weakly in $W^{1,1}$.

Proof The assumptions on φ imply that the sequence (u^n) is bounded in $W^{1,1}$; hence, by the compact embedding of $W^{1,1}(0, 1)$ into $L^1(0, 1)$, there exists a subsequence of u^n (not re-labelled) and $u \in L^1(0, 1)$ such that

$$u^n \rightarrow u \quad \text{strongly in } L^1(0, 1).$$

The superlinearity of φ also implies that the sequence $(u^n)'$ is uniformly integrable, by Theorem 2.2.3. This means, by Theorem 2.2.2, that there exists $g \in L^1(0, 1)$ such that

$$(u^n)' \rightharpoonup g \quad \text{weakly in } L^1(0, 1).$$

Hence $u \in W^{1,1}(0, 1)$ and $u' = g$, as we obtain by passing to the limit $n \rightarrow +\infty$ in the following equality, valid for test functions $\phi \in C_c^1(0, 1)$:

$$\int_0^1 u^n(s) \phi'(s) ds = - \int_0^1 (u^n)'(s) \phi(s) ds.$$

Remark 2.3.4 Notice that in the proof of the coerciveness no convexity is assumed. The main role of the convexity is to guarantee the lower semicontinuity of the integral functional with respect to weak convergence (see Theorem 2.3.2).

Remark 2.3.5 The conclusion of Theorem 2.3.3 follows also if the a-priori L^1 -bound for the sequence u^n is replaced by some Dirichlet boundary conditions (which imply the L^1 -bound by the Poincaré Inequality).

Theorem 2.3.3 suggests that the natural convergence for the discrete functionals E_n in (2.3.1) is the weak convergence in $W^{1,1}$ (instead of the strong convergence used in Theorem 2.3.1). Nevertheless, since it is always desirable to deal with a metric space, we prefer to consider the Γ -convergence with respect to the strong convergence in L^1 (which is implied by the weak convergence in $W^{1,1}$, thanks to the compactness embedding of $W^{1,1}(0, 1)$ in $L^1(0, 1)$).

Therefore, the most natural Γ -convergence result is the following:

Theorem 2.3.4 *Let E_n be defined as in (2.3.1) and assume that φ is continuous, convex, nonnegative and superlinear at infinity, i.e.,*

$$\lim_{|z| \rightarrow +\infty} \frac{\varphi(z)}{|z|} = +\infty.$$

Then the Γ -limit of E_n with respect to the strong convergence in L^1 is the functional E defined for $u \in L^1(0, 1)$ as

$$E(u) = \begin{cases} \int_0^1 \varphi(u'(s)) ds & u \in W^{1,1}(0, 1), \\ +\infty & u \in L^1(0, 1) \setminus W^{1,1}(0, 1). \end{cases} \quad (2.3.4)$$

Proof (Compactness of sequences with bounded energy) Let $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ be such that $E_n(\{u_i^n\}) \leq c$ and assume, additionally, that $\|\tilde{u}^n\|_{L^1} \leq c$, where $\tilde{u}^n$ denotes the piecewise affine interpolation of $\{u_i^n\}$.¹ By Theorem 2.3.3 it follows that there exists $u \in W^{1,1}(0, 1)$ such that

$$\tilde{u}^n \rightharpoonup u \text{ weakly in } W^{1,1}.$$

This shows that the natural convergence is the weak convergence in $W^{1,1}$, and hence that the domain of the Γ -limit is $W^{1,1}(0, 1)$.

Liminf inequality. Let $u \in W^{1,1}(0, 1)$ and $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ such that $\tilde{u}^n \rightarrow u$ in L^1 . We claim that

$$\liminf_{n \rightarrow +\infty} E_n(\tilde{u}^n) \geq E(u).$$

We can assume that $E_n(\tilde{u}^n) \leq c$, otherwise the claim is trivial. By the previous step the energy bound implies that $\tilde{u}^n \rightharpoonup u$ weakly in $W^{1,1}$. Then the claim follows by the lower semicontinuity of the integral functional

$$v \mapsto \int_0^1 \varphi(v'(s)) ds$$

with respect to the weak convergence in $W^{1,1}$, which in its turn follows by the convexity of φ .

Limsup inequality. The recovery sequence is the same as in Theorem 2.3.1.

¹This bound can be guaranteed by some additional term in the discrete energy, or by Dirichlet boundary conditions for the admissible displacements, e.g. $u_0^n = 0 = u_n^n$ for every n .

2.3.3 Non-convex and Superlinear Interaction

In this section we drop the convexity assumption for the interaction potential φ . The Γ -limit will involve a convexification process at a small scale, which is smaller than the macroscopic one, but larger than the microscopic scale λ_n of the lattice.

Definition 2.3.1 (*Convex envelope*) For a function φ the lower semicontinuous and convex envelope of φ , denoted by φ^{**} , is the largest convex and lower semicontinuous function below φ . If φ is lower semicontinuous then the definition of φ^{**} simplifies to:

$$\varphi^{**}(z) = \min \{t\varphi(z_1) + (1-t)\varphi(z_2) : t \in [0, 1], z = tz_1 + (1-t)z_2\}. \quad (2.3.5)$$

Remark 2.3.6 (*Geometric interpretation of the convex envelope*) Consider a continuous function φ . If φ is convex, then for every z

$$\varphi^{**}(z) = \varphi(z),$$

since the optimal choice in (2.3.5) is $z_1 = z_2 = z$.

If instead φ is not convex, then the equality $\varphi^{**} = \varphi$ is not anymore true for every z . Consider for instance the case of the double-well potential $\varphi(z) = (z^2 - 1)^2$. Then

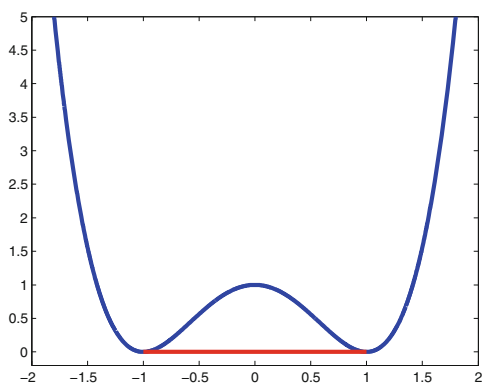
$$\varphi^{**}(z) = \begin{cases} \varphi(z) & z \leq -1, z \geq 1, \\ 0 & -1 \leq z \leq 1. \end{cases}$$

This follows easily by noticing that for every $-1 \leq z \leq 1$ the optimal choice in (2.3.5) is $z_1 = -1$ and $z_2 = 1$. See Fig. 2.3.

Next theorem is a Γ -convergence result for E_n , without the convexity assumption on φ .

Theorem 2.3.5 *Let E_n be defined as in (2.3.1) and assume that φ is continuous, nonnegative and superlinear at infinity i.e.,*

Fig. 2.3 Plot of the function φ (in blue). The convexification of φ differs from φ only in $(0, 1)$ and its plot in $(0, 1)$ is shown in red (color online)



$$\lim_{|z| \rightarrow +\infty} \frac{\varphi(z)}{|z|} = +\infty.$$

Then the Γ -limit of E_n with respect to the strong convergence in L^1 is the functional E defined for $u \in L^1(0, 1)$ as

$$E(u) = \begin{cases} \int_0^1 \varphi^{**}(u'(s)) ds & u \in W^{1,1}(0, 1), \\ +\infty & u \in L^1(0, 1) \setminus W^{1,1}(0, 1), \end{cases}$$

where φ^{**} denotes the convex and lower semicontinuous envelope of φ .

Proof (Compactness of sequences with bounded energy) Since the proof of the coerciveness of E_n in Theorem 2.3.4 did not make use of the convexity of φ , the result in this case is the same, i.e., the natural convergence is the weak convergence in $W^{1,1}$, and hence the domain of the Γ -limit is $W^{1,1}(0, 1)$.

Liminf inequality. Let $u \in W^{1,1}(0, 1)$ and $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ be such that $\tilde{u}^n \rightarrow u$ in L^1 . Since $\varphi^{**} \leq \varphi$, we have the bound

$$E_n(\{u_i^n\}) \geq \int_0^1 \varphi^{**}((\tilde{u}^n)'(s)) ds. \quad (2.3.6)$$

The lower bound for the energies E_n follows by the lower semicontinuity (with respect to the weak convergence in $W^{1,1}$) of the functional in the right-hand side of (2.3.6).

Limsup inequality. For the construction of the recovery sequence we will use a density argument. We first recall that piecewise affine functions are dense in $W^{1,1}(0, 1)$ with respect to the strong convergence in $W^{1,1}$. Moreover, the Γ -limit functional E is continuous with respect to the strong convergence in $W^{1,1}$. The continuity of E follows by the general result:

Let X be a normed space and let $F : X \rightarrow \mathbb{R}$ be a bounded convex function on $B = \{x \in X : \|x\| \leq 1\}$. Then F is continuous at $x = 0$.

The continuity of E and the density of piecewise affine functions in $W^{1,1}(0, 1)$ allow us to restrict our attention to the case of piecewise affine functions u . Moreover, the case of piecewise affine functions can be obtained from the simpler case of linear functions by superposition. In conclusion, it is sufficient to consider only the case of linear functions, i.e., $u(s) = zs$.

Let then $u(s) = zs$, and let t, z_1, z_2 be given by (2.3.5) so that

$$\varphi^{**}(z) = t\varphi(z_1) + (1-t)\varphi(z_2).$$

The idea is to construct for every n a *zig-zag function* with slopes z_1 and z_2 , oscillating at a small scale δ_n , with $\delta_n \rightarrow 0$ as $n \rightarrow +\infty$ (which we need in order to have a recovery sequence), but with $\delta_n \gg \lambda_n$.

Let therefore $\ell_n \in \mathbb{N}$ be such that $\ell_n \rightarrow +\infty$ and $\lambda_n \ell_n \rightarrow 0$ as $n \rightarrow +\infty$ and define $\delta_n := \lambda_n \ell_n$. Let $K_n \in \{0, \dots, \ell_n\}$ be so that $\frac{K_n}{\ell_n} \rightarrow t$, and define the recovery sequence $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ as $\tilde{u}^n(s) := zs + \tilde{v}^n(s)$, where $\{v_i^n\} \subset \mathcal{A}_n(0, 1)$ are $\lambda_n \ell_n$ -periodic, with derivative (almost everywhere) given by

$$(\tilde{v}^n)'(s) = \begin{cases} z_1 - z & 0 \leq s < \lambda_n K_n, \\ z_2 - z & \lambda_n K_n \leq s < \lambda_n \ell_n. \end{cases}$$

Notice that, by definition,

$$(\tilde{u}^n)'(s) = \begin{cases} z_1 & 0 \leq s < \lambda_n K_n, \\ z_2 & \lambda_n K_n \leq s < \lambda_n \ell_n. \end{cases}$$

Moreover, $\|\tilde{v}^n\|_{L^\infty(0,1)} = \lambda_n K_n |z_1 - z| \leq \lambda_n \ell_n |z_1 - z| \rightarrow 0$ as $n \rightarrow +\infty$, and therefore $\tilde{u}^n \rightarrow u$ uniformly. (Notice that $\tilde{u}^n$ converges to u also strongly in $W^{1,1}$, so it is admissible for any convergence we might want to consider.)

It remains to check the convergence of the energies E_n along the sequence $\tilde{u}^n$. We have

$$\begin{aligned} E_n(\{u_i^n\}) &= \int_0^1 \varphi((\tilde{u}^n)'(s)) ds \\ &= \lambda_n K_n \left(\frac{1}{\lambda_n \ell_n} \right) \varphi(z_1) + \lambda_n (\ell_n - K_n) \left(\frac{1}{\lambda_n \ell_n} \right) \varphi(z_2). \end{aligned}$$

Moreover, by the definition of ℓ_n and K_n it follows that

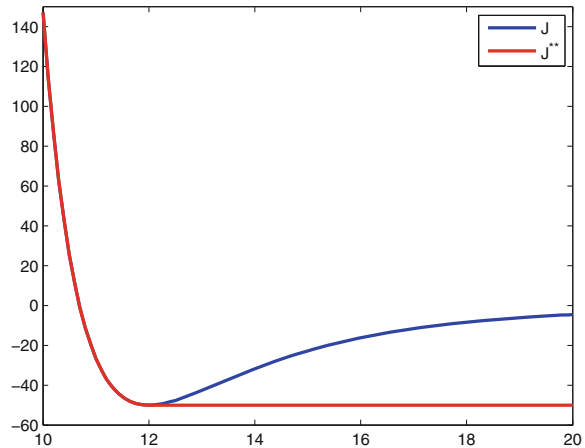
$$\lim_{n \rightarrow +\infty} E_n(\{u_i^n\}) = t\varphi(z_1) + (1-t)\varphi(z_2) = \varphi^{**}(z) = \int_0^1 \varphi^{**}(u'(s)) ds,$$

which proves that $\{u_i^n\}$ is a recovery sequence for E_n .

2.3.4 Lennard-Jones Interactions

In the previous section we showed that dropping the convexity assumption for the potential φ , but keeping the superlinearity at infinity, had the sole effect of giving rise to a convexification of the limit energy (necessary to have lower semicontinuity, which the Γ -limit has to satisfy).

Fig. 2.4 Lennard-Jones potential defined as in (2.3.7) with $\alpha = 50$ and $z_0 = 12$



A different situation arises when the growth condition is weakened—or dropped. In this case the compactness becomes more subtle and limit deformations might develop discontinuities (notice that so far the limit deformations were in $W^{1,1}(0, 1)$, therefore continuous). This is clearly the right type of interaction to be considered for problems in fracture mechanics. A fracture, indeed, corresponds to a discontinuity of the deformation, and hence it is natural to consider weaker growth conditions for the energy to allow jumps to occur with a finite cost, in terms of elastic energy.

The typical energy potential used in this case is the *Lennard-Jones interaction* potential (see Fig. 2.4)

$$J(z) = \alpha \left(\frac{z_0}{z^{12}} \right) - 2\alpha \left(\frac{z_0}{z^6} \right), \quad z > 0, \quad (2.3.7)$$

where z_0 is the minimum point (location of the well) and $-\alpha$ is the minimum value (depth of the well). Note that J can be negative (unlike in the previous cases) and moreover

$$\lim_{z \rightarrow +\infty} \frac{J(z)}{z} = 0.$$

More in general, we will consider Lennard-Jones-type energies. The assumptions we require for $J : \mathbb{R} \rightarrow \mathbb{R}$ are listed below.

(LJ-1) *Non-interpenetration condition:*

$$J(z) = +\infty \quad \text{for every } z < 0;$$

(LJ-2) *Strong repulsion:*

$$\lim_{z \rightarrow 0^+} J(z) = +\infty;$$

(LJ-3) *Regularity and behaviour at infinity.* The potential J is smooth in $(0, \infty)$; moreover the strength of the interaction decays at infinity, i.e.,

$$\lim_{z \rightarrow +\infty} J(z) = 0.$$

(LJ-4) *Structure of the potential.* There exists a unique minimiser $\gamma > 0$ and there exists $\delta > 0$ such that J is strictly convex in $(0, \gamma + \delta)$ and strictly concave in $(\gamma + \delta, +\infty)$. In particular, by assumption (LJ-3) we have that $J(\gamma) < 0$.

The discrete energy is defined for functions $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ as

$$E_n(\{u_i^n\}) = \lambda_n \sum_{i=0}^n J\left(\frac{u_{i+1}^n - u_i^n}{\lambda_n}\right). \quad (2.3.8)$$

We will see that unlike in Sects. 2.3.2.2 and 2.3.3, where the superlinearity of the potential ensured the weak compactness in $W^{1,1}$ of sequences with bounded energy, in this case one can only get a bound in $W^{1,1}$, which is not enough for weak compactness (since $W^{1,1}$ is not reflexive). Moreover, the $W^{1,1}$ bound for sequences with bounded energy does not follow from growth conditions of the potential J , but only on the non-interpenetration condition (LJ-1). That assumption, in particular, forces admissible deformations to be increasing. And sequences of increasing functions enjoy nice compactness properties, as we are going to show.

Note that in Sects. 2.3.2.2 and 2.3.3, since u plays the role of a displacement and not of a deformation, the difference quotient in the argument of φ had no sign restriction. Also, for the convex potential $\varphi(z) = z^2$ the minimum energy configuration (under appropriate Dirichlet boundary conditions) is the reference configuration. In the case of Lennard-Jones interactions the energy is minimised by the $\lambda_n \gamma$ -equispaced configuration (under appropriate boundary conditions).

To simplify what follows, we restrict the space of admissible sequences $\{u_i^n\}$ to the following subset of $\mathcal{A}_n(0, 1)$:

$$\mathcal{A}_n^{bc}(0, 1) := \{u_i \in \mathcal{A}_n(0, 1) : u_0 = 0, u_n = \ell\}. \quad (2.3.9)$$

Theorem 2.3.6 *Let E_n be defined as in (2.3.8), and let $(u^n) \subset \mathcal{A}_n^{bc}(0, 1)$ be such that $E_n(u^n) \leq c$. Then the sequence (u^n) is bounded in $W^{1,1}$.*

Proof Notice that, since the sequence $\{u_i^n\}$ has bounded energy and by assumption (LJ-1) $J(z) = +\infty$ for $z < 0$, the difference quotients $(u_{i+1}^n - u_i^n)/\lambda_n$ have to be nonnegative. Moreover, since $\mathcal{A}_n(0, 1) \subset W^{1,1}(0, 1)$, the sequence $(\tilde{u}^n)$ (namely the affine interpolation of $\{u_i^n\}$) is continuous. Therefore for every n the function $\tilde{u}^n$ is continuous and increasing.

The monotonicity and the common boundary conditions $\tilde{u}^n(0) = 0$ and $\tilde{u}^n(1) = \ell$ give the uniform bound $\|\tilde{u}^n\|_{L^\infty(0,1)} \leq \ell$.

For the first derivatives notice that, by the Fundamental Theorem of Calculus, which can be applied since functions in $W^{1,1}(0, 1)$ are absolutely continuous,

$$\int_0^1 (\tilde{u}^n)'(s) ds = \tilde{u}^n(1) - \tilde{u}^n(0) = \ell.$$

Moreover, by the monotonicity of $\tilde{u}^n$, $(\tilde{u}^n)' \geq 0$ (a.e.); hence

$$\int_0^1 |(\tilde{u}^n)'(s)| ds = \int_0^1 (\tilde{u}^n)'(s) ds = \tilde{u}^n(1) - \tilde{u}^n(0) = \ell. \quad (2.3.10)$$

The bound (2.3.10), together with the uniform bound on $(\tilde{u}^n)$ guarantees the desired $W^{1,1}$ -bound for the sequence $(\tilde{u}^n)$.

Corollary 2.3.1 *Under the same assumptions of Theorem 2.3.6 we can conclude that, in particular, $u^n \rightarrow u$ strongly in L^1 , and that the limit function u is increasing (being limit almost everywhere of increasing functions).*

Moreover, the derivatives $(u^n)'$, regarded as measures, converge *weakly** to a limit measure μ with bounded variation. Clearly, $\mu = u'$ in distributional sense.

We remark once more that the limit deformation u can have discontinuities, since it is only an L^1 -function. We restrict our attention to a subclass of the limit deformations, namely on functions that are *piecewise* $W^{1,1}(0, 1)$. We follow Braides' notation (see e.g. [8]) and we denote such a space by $P\text{-}W^{1,1}(0, 1)$. More precisely:

Definition 2.3.2 For every $p > 1$ we define

$$P\text{-}W^{1,p}(0, 1) := W^{1,p}(0, 1) + PC(0, 1), \quad (2.3.11)$$

where $PC(0, 1)$ denotes the space of piecewise constant functions.

Notice that, since the only functions that are both in $W^{1,p}(0, 1)$ and $PC(0, 1)$ are the constants, the decomposition in (2.3.11) is unique modulo a constant.

In practice, a given $u \in P\text{-}W^{1,p}(0, 1)$ is the sum of a function $v \in W^{1,p}(0, 1)$ (in particular continuous) and a piecewise constant function $w \in PC(0, 1)$. This implies in particular that

$$u' = v' \text{ (a.e.)}, \quad S(u) = S(w), \quad u^\pm(x) = v(x) + w^\pm(x) \quad \forall x \in S(u).$$

In the formula above, $S(u)$ denotes the discontinuity set of u , and $u^\pm$ denote the right and left limits of u at a discontinuity point x .

Now we can identify the restriction of the Γ -limit of E_n to the space $P\text{-}W^{1,1}(0, 1)$.

Theorem 2.3.7 *Let E_n be defined as in (2.3.8), and consider its restriction to the space $\mathcal{A}_n^{bc}(0, 1)$. Then the Γ -limit of E_n with respect to the strong convergence in L^1 is the functional E defined for $u \in P\text{-}W^{1,1}(0, 1)$ as*

$$E(u) = \begin{cases} \int_0^1 J^{**}(u'(s))ds & u(0) = 0, u(1) = \ell, u \text{ increasing}, \\ 0 & \\ +\infty & \text{otherwise.} \end{cases}$$

Proof (Liminf inequality) Let $u \in P\text{-}W^{1,1}(0, 1)$ be an increasing function satisfying the boundary conditions, and let $(\tilde{u}^n) \subset \mathcal{A}_n^{bc}(0, 1)$ be such that $\tilde{u}^n \rightarrow u$ strongly in L^1 and $E_n(\tilde{u}^n) \leq c$. Since $u \in P\text{-}W^{1,1}(0, 1)$, there exist $N + 1$ points $0 = y_0 < y_1 < \dots < y_N = 1$ such that

$$(0, 1) \setminus S(u) = \bigcup_{k=1}^N (y_{k-1}, y_k), \quad u|_{(y_{k-1}, y_k)} \in W^{1,1}(y_{k-1}, y_k).$$

Moreover, by Theorem 2.2.5 the functional

$$u \in W^{1,1}(y_{k-1}, y_k) \mapsto \int_{y_{k-1}}^{y_k} J^{**}(u'(s))ds$$

is lower semicontinuous with respect to the strong convergence in L^1 . This means that, for every $k = 1, \dots, N$:

$$\liminf_{n \rightarrow \infty} \int_{y_{k-1}}^{y_k} J^{**}((\tilde{u}^n)'(s))ds \geq \int_{y_{k-1}}^{y_k} J^{**}(u'(s))ds.$$

Adding up the previous inequality for every k leads to

$$\begin{aligned} E(u) &= \sum_{k=1}^N \int_{y_{k-1}}^{y_k} J^{**}(u'(s))ds \leq \sum_{k=1}^N \liminf_{n \rightarrow \infty} \int_{y_{k-1}}^{y_k} J^{**}((\tilde{u}^n)'(s))ds \\ &\leq \liminf_{n \rightarrow \infty} \sum_{k=1}^N \int_{y_{k-1}}^{y_k} J^{**}((\tilde{u}^n)'(s))ds \leq \liminf_{n \rightarrow \infty} \int_0^1 J^{**}((\tilde{u}^n)'(s))ds. \end{aligned}$$

In the previous estimate we have used that, for sequences $\{a_n\}$ and $\{b_n\}$,

$$\liminf_{n \rightarrow \infty} (a_n + b_n) \geq \liminf_{n \rightarrow \infty} a_n + \liminf_{n \rightarrow \infty} b_n.$$

Finally, the claim follows from the bound $J^{**} \leq J$.

Limsup inequality. Let $u \in P\text{-}W^{1,1}(0, 1)$ be an increasing function satisfying the Dirichlet boundary conditions. Let $0 = y_0 < y_1 < \dots < y_N = 1$ be $N + 1$ points such that

$$(0, 1) \setminus S(u) = \bigcup_{k=1}^N (y_{k-1}, y_k), \quad u_k := u|_{(y_{k-1}, y_k)} \in W^{1,1}(y_{k-1}, y_k).$$

Let us fix $k \in \{1, \dots, N\}$; we are going to construct a recovery sequence $\tilde{u}_k^n$ in the interval (y_{k-1}, y_k) . The recovery sequence $\tilde{u}^n$ in $[0, 1]$ will be simply defined as $\tilde{u}^n|_{(y_{k-1}, y_k)} := \tilde{u}_k^n$.

Since $u_k \in W^{1,1}(y_{k-1}, y_k)$, we can use density arguments to reduce to the case of a linear function with slope z_k , i.e., $u_k = z_k s$. If we take $\tilde{u}_k^n$ to be simply the affine interpolation of the values of u_k on the lattice $I_n \cap (y_{k-1}, y_k)$, then we will miss the convexification of J , as the limit will be $J(z_k)$ instead of $J^{**}(z_k)$.

Therefore we have to take a zig-zag sequence that approximates u_k in the strong convergence in $W^{1,1}(y_{k-1}, y_k)$ and with oscillations at scale $\delta_n \gg \lambda_n$ so that

$$\lim_{n \rightarrow \infty} \int_{y_{k-1}}^{y_k} J((\tilde{u}_k^n)'(s)) ds = \int_{y_{k-1}}^{y_k} J^{**}(u'(s)) ds.$$

The details of the construction are as in Theorem 2.3.5.

2.4 Discrete Systems: Long-Range Interactions

In the previous section we considered the case of particles interacting only with their nearest neighbours. Clearly in reality particles interact with all their neighbours, not only with the closest ones, and truncating the energy to the first neighbours can potentially lead to a wrong limit energy. Hence it should be avoided, even in the case of a rapidly decaying interaction potential, like the Lennard Jones potential for instance.

In this section we consider long-range interactions, starting with the case of *next-to-nearest neighbour* interactions illustrated in Fig. 2.5.

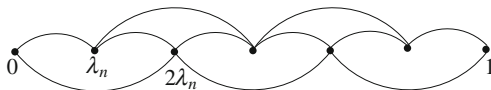


Fig. 2.5 Sketch of next-to-nearest neighbour interactions in the reference configuration

2.4.1 Next-to-Nearest-Neighbour Interactions

For given $\varphi^1, \varphi^2 : \mathbb{R} \rightarrow [0, \infty)$ we define

$$E_n(\{u_i\}) := \lambda_n \sum_{i=0}^{n-1} \varphi^1 \left(\frac{u_{i+1} - u_i}{\lambda_n} \right) + \lambda_n \sum_{i=0}^{n-2} \varphi^2 \left(\frac{u_{i+2} - u_i}{2\lambda_n} \right). \quad (2.4.1)$$

Like in the previous sections, we identify $\{u_i\}$ with its piecewise interpolation $\tilde{u}$. Also, as in (2.3.2), we rewrite the discrete energy (2.4.1) in integral form; for the nearest-neighbour interaction term we have

$$\lambda_n \sum_{i=0}^{n-1} \varphi^1 \left(\frac{u_{i+1} - u_i}{\lambda_n} \right) = \int_0^1 \varphi^1(\tilde{u}'(s)) ds.$$

For the next-to-nearest neighbour interaction term we first notice that, for $i = 0, \dots, n-2$,

$$\begin{aligned} \frac{u_{i+2} - u_i}{2\lambda_n} &= \frac{1}{2} \frac{u_{i+2} - u_{i+1}}{\lambda_n} + \frac{1}{2} \frac{u_{i+1} - u_i}{\lambda_n} \\ &= \frac{1}{2} \tilde{u}'(s + \lambda_n) + \frac{1}{2} \tilde{u}'(s), \quad s \in (\lambda_n i, \lambda_n(i+1)). \end{aligned} \quad (2.4.2)$$

Therefore, the second term in the energy (2.4.1) can be rewritten as

$$\lambda_n \sum_{i=0}^{n-2} \varphi^2 \left(\frac{u_{i+2} - u_i}{2\lambda_n} \right) = \int_0^{1-\lambda_n} \varphi^2 \left(\frac{\tilde{u}'(s + \lambda_n) + \tilde{u}'(s)}{2} \right) ds.$$

In conclusion, the discrete energy E_n can be rewritten as

$$E_n(u) = \int_0^1 \varphi^1(\tilde{u}'(s)) ds + \int_0^{1-\lambda_n} \varphi^2 \left(\frac{\tilde{u}'(s + \lambda_n) + \tilde{u}'(s)}{2} \right) ds. \quad (2.4.3)$$

The following Theorems 2.4.1 and 2.4.2 have been proved by Braides and collaborators (see e.g. [8]) and establish the Γ -convergence of E_n for convex and non convex interaction potentials.

Theorem 2.4.1 *Let E_n be defined as in (2.4.1) (and (2.4.3)) and assume that φ^1 and φ^2 are continuous, convex and nonnegative. Assume, moreover, that φ^1 is superlinear at infinity. Then the Γ -limit of E_n with respect to the strong convergence in L^1 is the functional E defined for $u \in L^1(0, 1)$ as*

$$E(u) = \begin{cases} \int_0^1 \varphi(u'(s))ds & u \in W^{1,1}(0, 1) \\ 0 & \\ +\infty & u \in L^1(0, 1) \setminus W^{1,1}(0, 1), \end{cases}$$

where $\varphi(t) = \varphi^1(t) + \varphi^2(t)$.

Proof (Compactness of sequences with bounded energy) Since the potential φ^2 is nonnegative, if a sequence $\{u_i^n\}$ has bounded energy E_n , then in particular the nearest-neighbour interaction term of the energy is bounded along the sequence. Therefore the convergence of the sequence follows directly from Theorem 2.3.4, under the additional assumption that the L^1 -norm of the sequence is bounded. (Remember that this additional bound is guaranteed by Dirichlet boundary conditions for the sequence.) Recall that the sequence converges also weakly in $W^{1,1}$.

Liminf inequality. Let $u \in W^{1,1}(0, 1)$ and let $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ be such that $\tilde{u}^n \rightarrow u$ strongly in L^1 and $E_n(\tilde{u}^n) \leq c$. From the compactness result we have that $\tilde{u}^n \rightharpoonup u$ weakly in $W^{1,1}$. Since the first term of the energy E_n is of the same type as the energy considered in Theorem 2.3.4, it follows directly that

$$\liminf_{n \rightarrow \infty} \lambda_n \sum_{i=0}^{n-1} \varphi^1 \left(\frac{u_{i+1}^n - u_i^n}{\lambda_n} \right) \geq \int_0^1 \varphi^1(u'(s))ds.$$

For the second term we observe that $\bar{u}^n(s) := \frac{\tilde{u}^n(s) + \tilde{u}^n(s + \lambda_n)}{2}$ also converges weakly in $W^{1,1}$ to u . Therefore, for $\eta > 0$, by (2.4.3) and by the definition of $\bar{u}^n$ we have

$$\begin{aligned} \liminf_{n \rightarrow \infty} \lambda_n \sum_{i=0}^{n-2} \varphi^2 \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) &\geq \liminf_{n \rightarrow \infty} \int_0^{1-\eta} \varphi^2((\bar{u}^n)'(s))ds \\ &\geq \int_0^{1-\eta} \varphi^2(u'(s))ds. \end{aligned}$$

The last inequality is a consequence of the lower semicontinuity of the functional

$$v \rightarrow \int_0^{1-\eta} \varphi^2(v'(s))ds$$

with respect to the weak convergence in $W^{1,1}$. Then the liminf inequality follows by the arbitrariness of η .

Limsup inequality. Let $u \in W^{1,1}(0, 1)$. We define $u_i^n := u(\lambda_n i)$ for every $i = 0, \dots, n$; by the Fundamental Theorem of Calculus and by Jensen's inequality

$$\begin{aligned}
E_n(u^n) &= \lambda_n \sum_{i=0}^{n-1} \varphi^1 \left(\int_{\lambda_n i}^{\lambda_n(i+1)} u'(s) ds \right) + \lambda_n \sum_{i=0}^{n-2} \varphi^2 \left(\int_{\lambda_n i}^{\lambda_n(i+2)} u'(s) ds \right) \\
&\leq \sum_{i=0}^{n-1} \int_{\lambda_n i}^{\lambda_n(i+1)} \varphi^1(u'(s)) ds + \frac{1}{2} \sum_{i=0}^{n-2} \int_{\lambda_n i}^{\lambda_n(i+2)} \varphi^2(u'(s)) ds \\
&\leq \int_0^1 \varphi^1(u'(s)) ds + \int_0^1 \varphi^2(u'(s)) ds.
\end{aligned}$$

We conclude this section by proving the analogue of Theorem 2.4.1 for non convex potentials.

Theorem 2.4.2 *Let E_n be defined as in (2.4.1) (and (2.4.3)) and assume that φ^1 and φ^2 are continuous and nonnegative. Assume, moreover, that φ^1 is superlinear at infinity. Then the Γ -limit of E_n with respect to the strong convergence in L^1 is the functional E defined for $u \in L^1(0, 1)$ as*

$$E(u) = \begin{cases} \int_0^1 \varphi(u'(s)) ds & u \in W^{1,1}(0, 1) \\ +\infty & u \in L^1(0, 1) \setminus W^{1,1}(0, 1), \end{cases}$$

where $\varphi(z) = (\varphi^1 \# \varphi^2)^{**}(z)$, and $\varphi^1 \# \varphi^2$ denotes the inf-convolution of the two potentials, defined as

$$(\varphi^1 \# \varphi^2)(z) = \varphi^2(z) + \frac{1}{2} \inf \{ \varphi^1(z_1) + \varphi^1(z_2) : z_1 + z_2 = 2z \}.$$

Remark 2.4.1 Notice that if φ^1 is convex, then $(\varphi^1 \# \varphi^2)(z) = \varphi^1(z) + \varphi^2(z)$.

Proof (Compactness of sequences with bounded energy) As in Theorem 2.4.1 the convergence follows directly from Theorem 2.3.4, since φ^2 is nonnegative.

Liminf inequality. Let $u \in W^{1,1}(0, 1)$ and let $\tilde{u}^n \rightarrow u$ strongly in L^1 , with $E_n(\tilde{u}^n) \leq c$. From the compactness result we have that $\tilde{u}^n \rightharpoonup u$ weakly in $W^{1,1}$.

In this case it is very convenient to rewrite the energy in an alternative way. We can look at the lattice I_n as obtained by the superposition of two lattices with double spacing $2\lambda_n$, with a relative λ_n -shift. For convenience we can write

$$I_n = I_n^{\text{odd}} \cup I_n^{\text{even}}, \quad I_n^{\text{odd}} \cap I_n^{\text{even}} = \emptyset,$$

where $I_n^{\text{odd}} = \{\lambda i : i \text{ odd}\}$, and $I_n^{\text{even}} = \{\lambda i : i \text{ even}\}$.

Therefore, splitting the sums in E_n into even and odd lattice,

$$\begin{aligned}
 E_n(\tilde{u}^n) &= \sum_{\substack{i=0 \\ \text{odd}}}^{n-2} \lambda_n \left\{ \varphi^2 \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) + \frac{1}{2} \varphi^1 \left(\frac{u_{i+1}^n - u_i^n}{\lambda_n} \right) + \frac{1}{2} \varphi^1 \left(\frac{u_{i+2}^n - u_{i+1}^n}{\lambda_n} \right) \right\} \\
 &+ \sum_{\substack{i=0 \\ \text{even}}}^{n-2} \lambda_n \left\{ \varphi^2 \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) + \frac{1}{2} \varphi^1 \left(\frac{u_{i+1}^n - u_i^n}{\lambda_n} \right) + \frac{1}{2} \varphi^1 \left(\frac{u_{i+2}^n - u_{i+1}^n}{\lambda_n} \right) \right\} \\
 &+ \frac{1}{2} \lambda_n \varphi^1 \left(\frac{u_n^n - u_{n-1}^n}{\lambda_n} \right) + \frac{1}{2} \lambda_n \varphi^1 \left(\frac{u_1^n - u_0^n}{\lambda_n} \right).
 \end{aligned}$$

Using the definition of the inf-convolution and the fact that $\varphi^1 \geq 0$ we have

$$\begin{aligned}
 E_n(\tilde{u}^n) &\geq \sum_{\substack{i=0 \\ \text{odd}}}^{n-2} \lambda_n (\varphi^1 \# \varphi^2) \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) + \sum_{\substack{i=0 \\ \text{even}}}^{n-2} \lambda_n (\varphi^1 \# \varphi^2) \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) \\
 &\geq \sum_{\substack{i=0 \\ \text{odd}}}^{n-2} \lambda_n (\varphi^1 \# \varphi^2)^{**} \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right) + \sum_{\substack{i=0 \\ \text{even}}}^{n-2} \lambda_n (\varphi^1 \# \varphi^2)^{**} \left(\frac{u_{i+2}^n - u_i^n}{2\lambda_n} \right).
 \end{aligned}$$

Therefore it only remains to write the sums as integrals, as usual. To this aim, we define *odd and even interpolants* on the lattices I_n^{odd} and I_n^{even} , say $\tilde{u}_{\text{odd}}^n$ and $\tilde{u}_{\text{even}}^n$. In formula,

$$(u_{\text{odd}}^n)'(s) = \frac{u_{i+2}^n - u_i^n}{2\lambda_n}, \quad s \in (\lambda_n i, \lambda_n(i+2)), \quad i \text{ odd},$$

and analogously for u_{even}^n . The previous estimate implies that, for every $\eta > 0$,

$$E_n(\tilde{u}^n) \geq \frac{1}{2} \int_{\eta}^{1-\eta} (\varphi^1 \# \varphi^2)^{**}((\tilde{u}_{\text{odd}}^n)'(s)) ds + \frac{1}{2} \int_{\eta}^{1-\eta} (\varphi^1 \# \varphi^2)^{**}((\tilde{u}_{\text{even}}^n)'(s)) ds.$$

Notice that also such interpolants converge weakly in $W^{1,1}$ to u . The claim then follows by lower semicontinuity, since the integrands are convex.

Limsup inequality. As usual, via density arguments we can restrict to the case of a linear function $u(s) = zs$. Moreover, to focus on the inf-convolution rather than on the convexification we assume that $(\varphi^1 \# \varphi^2)^{**}(z) = (\varphi^1 \# \varphi^2)(z)$.

Let now $\eta > 0$, and z_1 and z_2 be such that $z_1 + z_2 = 2z$ and

$$\varphi^2(z_2) + \frac{1}{2} \varphi^1(z_1) + \frac{1}{2} \varphi^1(z_2) < (\varphi^1 \# \varphi^2)^{**}(z) + \eta. \quad (2.4.4)$$

The idea for the recovery sequence in this case is that it should have constant slope z on the larger $2\lambda_n$ -lattices I_n^{odd} and I_n^{even} , and slope alternatively z_1 and z_2 on the smaller λ_n -lattice I_n . In this way the energy term coming from the next-to-nearest neighbour interactions will be $\varphi^2(z)$, while half of the nearest neighbour interactions, say, the even ones, will contribute $\varphi^1(z_1)$, and the odd ones $\varphi^1(z_2)$. More in detail, the recovery sequence is

$$u_i^n = \begin{cases} \lambda_n i z & i \text{ odd}, \\ \lambda_n (i-1) z + \lambda_n z_1 & i \text{ even}. \end{cases}$$

It is easy to check that $u_{i+2}^n - u_i^n = 2\lambda_n z$ for both i odd and even. Instead

$$u_{i+1}^n - u_i^n = \begin{cases} \lambda_n z_2, & i \text{ odd}, \\ \lambda_n z_1, & i \text{ even}. \end{cases}$$

Therefore,

$$E_n(\{u_i^n\}) = \varphi^2(z) + \lambda_n \sum_{\substack{i=0 \\ \text{odd}}}^{n-1} \varphi^1(z_2) + \lambda_n \sum_{\substack{i=0 \\ \text{even}}}^{n-1} \varphi^1(z_1),$$

which implies the claim by (2.4.4).

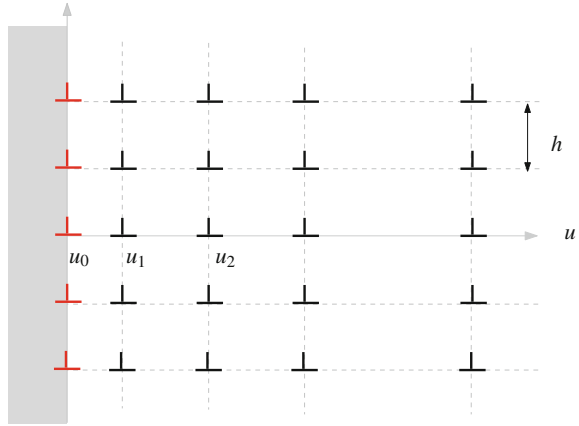
2.4.2 Long-Range Interactions: The Case of Dislocations

In this section we consider long-range interactions. The particles in this case are *dislocations*, i.e., defects in the arrangement of the atoms in a crystal lattice of a metal, steel for instance. Dislocations are of great importance for their role as main carriers of the permanent or plastic deformation in metals. The main mechanism of plastic deformation is the relative slip of planes of atoms, and the presence and the motion of large numbers of dislocations make the slip energetically possible. Typically, the number of dislocations in a portion of metal is very large, and therefore a discrete model that keeps track of each dislocation is not useful in practice. Hence the need for *upscaled* models, in terms of a continuum, averaged quantity: The dislocation density.

Similarly as in the cases considered before, the starting point of our analysis is a one-dimensional discrete energy describing the pairwise interaction among dislocations. In this case, however, we will consider all interactions, not only nearest and next-to-nearest neighbour interactions. Actually, the interactions we consider are not among *single* dislocations, but among vertical *walls* of dislocations as in Fig. 2.6.

Each wall is h -periodic, where $h > 0$ is the spacing between consecutive dislocations within the wall. Therefore the discrete function $\{u_i\} \subset \mathcal{A}_n(0, 1)$ represents the n deformed positions of the dislocations walls with respect to the reference lattice I_n .

Fig. 2.6 The dislocation configuration. Infinite, vertical walls of equispaced dislocations are free to move in the horizontal direction. A wall of fixed dislocations is pinned at $u_0 = 0$ and acts as a repellent



The discrete dislocation energy is defined as

$$\mathcal{E}_n(\{u_i\}) := 2K \sum_{i=0}^n \sum_{\substack{j=0 \\ j \neq i}}^n V\left(\frac{u_i - u_j}{h}\right) + \sigma \sum_{i=0}^n u_i, \quad (2.4.5)$$

where $K > 0$ is a mechanical constant, $\sigma > 0$ is an applied load, and the interaction energy V is shown in Fig. 2.7 and is defined as

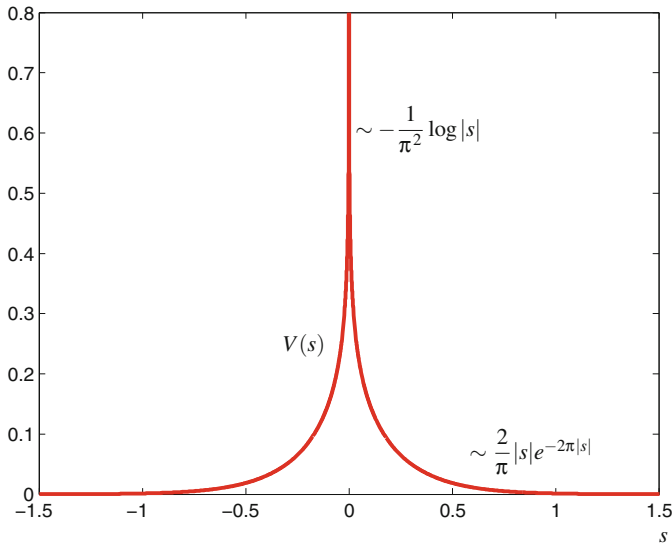


Fig. 2.7 The interaction energy V

$$V(s) := \frac{1}{\pi} s \coth \pi s - \frac{1}{\pi^2} \log(2 \sinh \pi s) = \frac{2}{\pi} \frac{|s|}{(e^{2\pi|s|} - 1)} - \frac{1}{\pi^2} \log(1 - e^{-2\pi|s|}).$$

Therefore the first term in the discrete energy $\mathcal{E}_n$ is fully repulsive: each pair of walls repels each other, with a potential that diverges logarithmically as the walls approach each other. The second term of the energy, accounting for the applied load, drives the walls to the left. Moreover, we impose a Dirichlet boundary condition for the left most wall, $u_0 = 0$, which models pinning.

In the special case where the vertical distance h between consecutive dislocations within a wall and the *average* distance between consecutive dislocations in the horizontal direction is of the same order, non-dimensionalising the energy leads to

$$E_n(\{u_i\}) := 2\lambda_n \sum_{i=0}^n \sum_{\substack{j=0 \\ j \neq i}}^n V\left(\frac{u_i - u_j}{\lambda_n}\right) + \lambda_n \sum_{i=0}^n u_i,$$

which looks more similar to the discrete energies considered so far. The fact that V is even, moreover, allows us to rewrite the energy in the more convenient form

$$E_n(\{u_i\}) := \lambda_n \sum_{k=1}^n \sum_{i=0}^{n-k} V\left(\frac{u_{i+k} - u_i}{\lambda_n}\right) + \lambda_n \sum_{i=0}^n u_i. \quad (2.4.6)$$

Notice that the energy V is convex, but is not superlinear; in particular it decays exponentially to zero (recall that the Lennard-Jones potential had a polynomial decay).

As in the Lennard-Jones case the lack of the superlinear growth entails that the limit deformations can have discontinuities. In what follows, however, we will only identify the Γ -limit on a subspace of the limit deformations, i.e., on continuous functions in $W^{1,1}(0, 1)$. In this way we will only focus on the effect of long-range interactions. For the general case we refer to [14, 22] (see also [25] for the case of a bounded domain $[0, L]$ for the positions of the walls).

Theorem 2.4.3 *The functionals E_n in (2.4.6) Γ -converge with respect to the weak convergence in $W^{1,1}$ to the functional E defined for increasing functions $u \in W^{1,1}(0, 1)$ as*

$$E(u) = \int_0^1 V_{\text{eff}}(u'(s)) ds + \int_0^1 u(s) ds,$$

where $V_{\text{eff}}(t) := \sum_{k=1}^{\infty} V(kt)$ for every $t \in \mathbb{R}$.

Proof (Liminf inequality) Let $u \in W^{1,1}(0, 1)$ be an increasing function, and let $\{u_i^n\} \subset \mathcal{A}_n(0, 1)$ be a sequence with bounded energy E_n and such that the interpolants $\tilde{u}^n \rightharpoonup u$ weakly in $W^{1,1}$.

We first rewrite the functional E_n in a more convenient way. For every $k \in \mathbb{N}$ we define the function $V^k(t) := V(kt)$. Hence we have

$$E_n(\{u_i^n\}) = \lambda_n \sum_{k=1}^n \sum_{j=0}^{n-k} V^k \left(\frac{u_{i+k}^n - u_i^n}{k\lambda_n} \right) + \lambda_n \sum_{i=0}^n u_i^n. \quad (2.4.7)$$

The expression in the argument of V^k resembles a gradient, and we make the gradient term appear explicitly using the affine interpolant $\tilde{u}^n$ of the $\{u_i^n\}$. For fixed $k \in \{0, \dots, n-1\}$ and $\ell \in \{0, \dots, n-1\}$ and for $i \leq \ell \leq k+i-1$, we have

$$\frac{u_{i+k}^n - u_i^n}{k\lambda_n} = \frac{1}{k} \sum_{m=i-\ell}^{i-\ell+k-1} \frac{u_{\ell+m+1}^n - u_{\ell+m}^n}{\lambda_n} = \frac{1}{k} \sum_{m=i-\ell}^{i-\ell+k-1} (\tilde{u}^n)'(s + \lambda_n m)$$

for every $s \in (\frac{\ell}{n}, \frac{\ell+1}{n})$. Then

$$\begin{aligned} \lambda_n V^k \left(\frac{u_{i+k}^n - u_i^n}{k\lambda_n} \right) &= \frac{1}{k} \sum_{\ell=i}^{i+k-1} \int_{\frac{\ell}{n}}^{\frac{\ell+1}{n}} V^k \left(\frac{1}{k} \sum_{m=i-\ell}^{i-\ell+k-1} (\tilde{u}^n)'(s + \lambda_n m) \right) ds \\ &\stackrel{(j=\ell-i)}{=} \frac{1}{k} \sum_{j=0}^{k-1} \int_{\frac{j+i}{n}}^{\frac{j+i+1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds. \end{aligned}$$

Therefore, we can rewrite the first term in (2.4.7) in terms of the functions $\tilde{u}^n$, as

$$\begin{aligned} \sum_{i=0}^{n-k} \lambda_n V^k \left(\frac{u_{i+k}^n - u_i^n}{k\lambda_n} \right) &= \frac{1}{k} \sum_{i=0}^{n-k} \sum_{j=0}^{k-1} \int_{\frac{j+i}{n}}^{\frac{j+i+1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds \\ &= \frac{1}{k} \sum_{j=0}^{k-1} \int_{\frac{j}{n}}^{\frac{n-k+j+1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds \\ &= \frac{1}{k} \sum_{j=0}^{k-1} \int_{\frac{j}{n}}^{1-\frac{k-j-1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds. \end{aligned}$$

We claim that for every fixed integer N the following lower bound is satisfied:

$$\liminf_{n \rightarrow +\infty} E_n(\{u_i^n\}) \geq \int_0^1 V_{\text{eff}}^N(u'(s)) ds + \int_0^1 u(s) ds, \quad (2.4.8)$$

where the energy density V_{eff}^N is defined as $V_{\text{eff}}^N(t) := \sum_{k=1}^N V(kt)$ for every $t \in \mathbb{R}$. This claim implies the lower bound by the arbitrariness of N .

We focus on the first term of the discrete energy E_n ; since by assumption $\tilde{u}^n \rightharpoonup u$ in $W^{1,1}$, in particular $\tilde{u}^n \rightarrow u$ strongly in L^1 , therefore the convergence of the second term of the energy follows directly. (Notice that the second term in the discrete energy is a Riemann sum for the integral of $\tilde{u}^n$.)

Let N be fixed (independent of n). Then, for $n \geq N$,

$$\begin{aligned} \lambda_n \sum_{k=1}^n \sum_{i=0}^{n-k} V^k \left(\frac{u_{i+k}^n - u_i^n}{k\lambda_n} \right) \\ \geq \sum_{k=1}^N \frac{1}{k} \sum_{j=0}^{k-1} \int_{\frac{j}{n}}^{1-\frac{k-j-1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds. \end{aligned}$$

We note that, since j and k run through a finite set independent of n , for every $\eta > 0$ there exists an integer $\nu(\eta)$ such that, if $n \geq \nu(\eta)$, then

$$\begin{aligned} \int_{\frac{j}{n}}^{1-\frac{k-j-1}{n}} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds \\ \geq \int_{\eta}^{1-\eta} V^k \left(\frac{1}{k} \sum_{m=-j}^{k-1-j} (\tilde{u}^n)'(s + \lambda_n m) \right) ds \end{aligned}$$

for every j and for every k . Moreover, for every k and j , also the convex combination

$$\tilde{u}_{k,j}^n(s) := \frac{1}{k} \sum_{m=-j}^{k-1-j} \tilde{u}^n(s + \lambda_n m)$$

converges to u weakly in $W^{1,1}(\eta, 1-\eta)$. Therefore, for every k and j

$$\liminf_{n \rightarrow \infty} \int_{\eta}^{1-\eta} V^k((\tilde{u}_{k,j}^n)'(s)) ds \geq \int_{\eta}^{1-\eta} V^k(u'(s)) ds, \quad (2.4.9)$$

since the integral functional in (2.4.9) is lower semicontinuous with respect to the weak convergence in $W^{1,1}$, by the convexity of V^k . In conclusion,

$$\begin{aligned}
\liminf_{n \rightarrow \infty} E_n(\{u_i^n\}) &\geq \sum_{k=1}^N \frac{1}{k} \sum_{j=0}^{k-1} \int_{\eta}^{1-\eta} V^k(u'(s)) ds + \int_0^1 u(s) ds \\
&= \sum_{k=1}^N \int_{\eta}^{1-\eta} V^k(u'(s)) ds + \int_0^1 u(s) ds \\
&= \int_{\eta}^{1-\eta} V_{\text{eff}}^N(u'(s)) ds + \int_0^1 u(s) ds,
\end{aligned}$$

and the claim (2.4.8) follows by the arbitrariness of N and η .

Limsup inequality. Let $u \in W^{1,1}(0, 1)$. The recovery sequence in this case is simply given by the evaluations of the continuous function u on the points of the lattice I_n .

Remark 2.4.2 The discrete energies E_n are coercive in $BV_{\text{loc}}(0, 1)$, and the natural convergence to be considered for the Γ -convergence is, also in this case, the strong convergence in L^1 .

2.5 Further Directions

We conclude these lecture notes by illustrating a couple of generalisations and interesting ideas.

2.5.1 Asymptotic Expansion via Γ -Convergence

Let us consider the Lennard-Jones interaction energy analysed in Theorem 2.3.7. We noticed that the limit deformations can have discontinuities, which makes the Lennard-Jones potential suitable for dealing with fracture mechanics problems. On the other hand, the Γ -limit energy obtained in Theorem 2.3.7 does not penalise in any way the occurrence of a fracture, since there is no cost associated to discontinuities of the limit deformations. Therefore in principle a deformation could have infinitely many discontinuity points. This is quite unsatisfactory from the mechanical point of view, since the opening of a crack requires energy and it is not energetically convenient for an elastic body to fracture in infinitely many points.

To understand better the limitations of the limit model, let us have a closer look at the limit energy E . For $u \in P-W^{1,1}(0, 1)$, u increasing, and $u(0) = 0$, $u(1) = \ell$,

$$E(u) = \int_0^1 J^{**}(u'(s)) ds.$$

Let $\ell < \gamma$, where γ is the unique minimum point of the interaction potential J . Then the function $\bar{u}(s) = \ell s$ is the unique minimiser of the Γ -limit. This follows from the Jensen's inequality, since for every admissible u

$$\begin{aligned} \int_0^1 J^{**}(u'(s))ds &\geq J^{**}\left(\int_0^1 u'(s)ds\right) = J^{**}(u(1) - u(0)) = J^{**}(\ell) \\ &= \int_0^1 J^{**}(\bar{u}'(s))ds. \end{aligned}$$

Hence in this case it is energetically unfavourable to create a fracture.

Assume now instead that $\ell > \gamma$. Then the continuous function $\bar{u}(s) = \ell s$ is still a minimiser, but it is not the only one. Also any increasing function u with $u' \geq \gamma$ almost everywhere is a minimiser, with the same energy.

Therefore, while in the case $\ell < \gamma$ the Γ -limit provides us with all the necessary information in order to understand the behaviour of the discrete system, in the case $\ell \geq \gamma$ the information provided by the Γ -limit is very poor, since it cannot distinguish between a continuous deformation and a deformation with infinitely many discontinuity points.

How can we improve the scenario provided by the limit energy E ? What we expect from a mechanical reasoning is that if the boundary conditions are in the convex-elastic part of J , i.e., if $\ell < \gamma$, then the best thing to do from the energetic point of view is to deform elastically, rather than creating a fracture. This is exactly what the Γ -limit predicts in the case $\ell < \gamma$. If instead the boundary condition is outside the convex-elastic part of J , i.e., if $\ell \geq \gamma$, then we expect the occurrence of a fracture. This is in contrast with the prediction provided by the energy E , for which also a continuous deformation with slope ℓ is a minimiser.

Hence, we would like to *correct* the energy for $\ell > \gamma$, and penalise continuous deformations with large slope, as well as the number of discontinuity points.

The idea is, as for the Taylor formula for functions, to look at a *higher order approximation* of the discrete energy E_n in the small parameter λ_n (see [4]). In terms of a *Taylor-expansion*, the Γ -limit can be considered as the zero-order term in λ_n . The next term to identify is the first-order one. This is done by looking at the new discrete energy:

$$E_n^{(1)}(\{u_i\}) := \frac{E_n(\{u_i\}) - \min E}{\lambda_n}.$$

Note that, for $\ell > \gamma$, $\min E = J(\gamma)$. Therefore the new energy functional is

$$E_n^{(1)}(u) := \sum_{i=0}^{n-1} \left\{ J\left(\frac{u_{i+1} - u_i}{\lambda_n}\right) - J(\gamma) \right\}. \quad (2.5.1)$$

Heuristically, the energy $E_n^{(1)}$ for large n can be finite only if almost every discrete slope equals γ . In fact in that case the terms in the sum (2.5.1), which are otherwise positive (since γ is the minimum point of J), are zero. Hence, the study of this higher order correction of the energy reduces the set of possible minimisers to the deformations with slope γ .

This result is proved in the next Theorem.

Theorem 2.5.1 *The functionals $E_n^{(1)}$ Γ -converge to the functional $E^{(1)}$ given by*

$$E_n^{(1)}(u) = \begin{cases} -J(\gamma)\#(S(u)) & u \text{ increasing, } u' = \gamma \text{ a.e.} \\ +\infty & \text{otherwise,} \end{cases}$$

on $P-W^{1,1}(0, 1)$.

Proof (Hint for the recovery sequence) Consider a function $u \in P-W^{1,1}(0, 1)$, u increasing and such that $u' = \gamma$ a.e. Assume, for simplicity, that u has only one discontinuity point, say $t \in (0, 1)$, and assume that $u^+(t) - u^-(t) = a > 0$. Define $u_i^n := u(\lambda_n i)$.

Let us choose a sequence $(t_n) \subset \mathbb{N}$, such that $t_n \rightarrow \infty$, $\lambda_n t_n \leq t$ and $\lambda_n t_n \rightarrow t$. Then, clearly,

$$\frac{u^{i+1} - u^i}{\lambda_n} = \begin{cases} \gamma & i \neq t_n, \\ \sim \frac{a}{\lambda_n} & i = t_n. \end{cases}$$

Therefore

$$E^{(1)}(u_i^n) \sim J\left(\frac{a}{\lambda_n}\right) - J(\gamma) \rightarrow -J(\gamma).$$

2.5.2 Equivalence by Γ -Convergence

Strictly related to the previous example is the concept of Γ -equivalence introduced by Braides and Truskinovsky in [10].

The key observation in [10] is that the first order Γ -expansion obtained in the previous section, namely

$$E(u) + \lambda_n E^{(1)}(u), \tag{2.5.2}$$

regarded as a function of the parameter ℓ (the elongation of the one-dimensional chain) is discontinuous at $\ell = \gamma$, where γ is the minimum point of J . The value $\ell = \gamma$ represents a threshold between the elastic regime ($\ell < \gamma$), and the regime $\ell > \gamma$ in which the chain experiences the opening of a crack.

The idea in [10] is then to construct a uniformly Γ -equivalent approximation that improves the first-order approximation (2.5.2) close to γ .

2.5.3 Empirical Measures Approach

As stated in Remark 2.3.1, it is sometimes convenient to express the discrete energy in terms of the empirical measures μ_n , rather than in terms of the piecewise affine interpolations. To illustrate this alternative formulation, let us consider again the discrete dislocation energy in (2.4.5):

$$\mathcal{E}_n(\{u_i\}) := 2K \sum_{i=0}^n \sum_{\substack{j=0 \\ j \neq i}}^n V\left(\frac{u_i - u_j}{h}\right) + \sigma \sum_{i=0}^n u_i.$$

In Sect. 2.4.2 we analysed the case where the vertical distance h between consecutive dislocations within a wall and the average distance between consecutive dislocations in the horizontal direction is of the same order. We now consider the case where h is of the same order as the *whole* pileup region. In this case, the non-dimensional discrete energy is

$$E_n(\{u_i\}) = 2 \frac{1}{n^2} \sum_{i=0}^n \sum_{\substack{j=0 \\ j \neq i}}^n V(u_i - u_j) + \frac{1}{n} \sum_{i=0}^n u_i,$$

since $\lambda_n = 1/n$. At this point the first term of the energy does not contain a gradient-like term as before, and hence the previous approach does not apply. In terms of the empirical measure $\mu_n = (\sum \delta_{u_i})/n$ instead the energy reads

$$E_n(\{u_i\}) = 2 \iint_{(0,\infty)^2 \setminus D} V(x - y) d\mu_n(x) d\mu_n(y) + \int_0^\infty x d\mu_n(x),$$

where D denotes the diagonal in $(0, \infty)^2$; from this expression is easy to guess that the Γ -limit energy is

$$E(\mu) = 2 \iint_{(0,\infty)^2} V(x - y) d\mu(x) d\mu(y) + \int_0^\infty x d\mu(x).$$

This guess can be made rigorous, and the details of the proof are in [14].

Remark 2.5.1 The measure approach has a more natural extension to higher dimensions, since no underlying lattice is required in this case.

2.5.4 Rate-Independent and Gradient Flow Evolutions

Let us focus again on the discrete dislocation energy (2.4.5). As explained above, one can couple the energy of the system with a suitable *dissipation* and consider the corresponding discrete evolution. Deriving a limit evolution is generally a very subtle issue, and relies on the results [20] (for rate-independent evolutions) and [21] (for gradient flows).

2.6 Exercises

1. Compute the Gamma-limit of the following sequences of functions:

- (a) $f_n : \mathbb{R} \rightarrow \mathbb{R}$, $f_n(x) = nxe^{-2n^2x^2}$;
- (b) $f_n = f$, where $f(x) = 1$ if $x < 1/2$ and $f(x) = 0$ if $x \geq 1/2$;
- (c) $f_n = f$, where $f(x) = 1$ if $x \leq 1/2$ and $f(x) = 0$ if $x > 1/2$.
- (d) Prove that it can be

$$\Gamma - \lim_n (f_n + g_n) \neq \Gamma - \lim_n f_n + \Gamma - \lim_n g_n.$$

- 2. Give an example of a sequence bounded in L^1 but not weakly compact.
- 3. (a) Let X be a topological space and consider $F_i : X \rightarrow \mathbb{R}$ for $i \in I$, with I countable or uncountable. Define

$$F(x) := \sup_{i \in I} F_i(x).$$

Prove that if for every i the functional F_i is sequentially lower semicontinuous, then F is sequentially lower semicontinuous.

(b) Under the same assumptions, prove or disprove that

$$G(x) := \inf_{i \in I} F_i(x)$$

is sequentially lower semicontinuous.

- 4. (a) Let X be a topological space and let $F : X \rightarrow \mathbb{R}$. If F is coercive and lower semicontinuous, then there exists a minimizer of F .

Hint. Use the following result in general topology. Let X be a topological space and let $(A_n)_n$ be closed sets, $A_n \neq \emptyset$ for every n , and decreasing, i.e.,

$$A_1 \supseteq A_2 \supseteq \cdots \supseteq A_n.$$

Assume, moreover, that there exists a compact set K such that $A_1 \subseteq K$. Then

$$\bigcap_{n=1}^{\infty} A_n \neq \emptyset.$$

(b) Let X be a topological space and let $F : X \rightarrow \mathbb{R}$. If F is sequentially coercive and sequentially lower semicontinuous, then there exists a minimizer of F .

5. (a) Does the functional

$$F(u) := \int_0^1 |u'(x)|^2 dx + \int_0^1 \frac{1}{1+u^2(x)} dx$$

have a minimum on $W^{1,2}(0, 1)$?

(b) Does the functional

$$F(u) := \int_{-1}^1 (1+x^2)|u'(x)| dx$$

have a minimum on $X := \{u \in W^{1,1}(0, 1), u(-1) = -1, u(1) = 1\}$?

(c) Does the functional

$$F(u) := \int_{-1}^1 (1+x^2)|u'(x)|^p dx, \quad p > 1,$$

have a minimum on $X := \{u \in W^{1,p}(0, 1), u(-1) = -1, u(1) = 1\}$?

(d) Does the functional

$$F(u) := \int_0^1 [(u')^2 - 1]^2 + u^4 dx$$

have a minimum on $X := \{u \in W^{1,4}(0, 1), u(0) = 0, u(1) = 0\}$?

6. Let X be a metric space and let $F : X \rightarrow \mathbb{R}$; prove that the following are equivalent:

(a) for every $x \in X$ and for every $x_n \rightarrow x$: $F(x) \leq \liminf_{n \rightarrow \infty} F(x_n)$;

(b) $S_t = \{x : F(x) \leq t\}$ is closed for every t .

7. Let $f : (0, 1) \rightarrow [0, \infty]$ be convex, C^1 and Lipschitz. Then the functional

$$F : L^1(0, 1) \rightarrow [0, \infty], \quad F(u) = \int_0^1 f(u) dt$$

is weakly lower semicontinuous in L^1 .

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