Surface energies in nonconvex discrete systems

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1 Introduction

Nonconvex interactions in lattice systems lead to a number of interesting phenomena that can be translated into a variety of energies within their limit continuum description as the lattice size tends to zero. These effects may be due to different superposed causes. When only nearest-neighbour interactions are taken into account, a scaling effect for nonconvex energy densities with non-faster-than-linear growth at infinity (such as Lennard-Jones potentials or the 'weak membrane' energies considered by Blake and Zisserman in Image Processing) show the appearance of a competing surface term besides a convex bulk integral. In this way one can derive the Mumford Shah functional of Computer Vision as the limit of finite-difference schemes [18], explain Griffith's theory of Fracture as a phase transition with one 'well' at infinity [29], or give a microscopical interpretation of softening phenomena [10]. In the one-dimensional case a complete description can be given highlighting in addition oscillations and micro-cracking (see [14] and also Del Piero and Truskinowsky [21] for a Mechanical insight).

For energies with 'superlinear' growth (these growth conditions are expressed in terms of the scaled difference quotients) Alicandro and Cicalese [2] have shown that, upon some natural decay conditions on the energy densities ϕ_ε, the Γ-limit as $\varepsilon \to 0$ of an arbitrary system of interactions

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

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

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

The simplest case is when only nearest-neighbour interactions are present, in which case the function φ is computed via a convexification process [2]. When not only nearest-neighbour interactions are taken into account, in contrast, the description of the limit problem turns out more complex involving in general some 'homogenization' process (see [15], [2]). It is worth noting that the necessity of such a complex description arises also for simple linear spring models where the nonlinearity is of a more 'geometrical' origin (see [22]). Even in the simple one-dimensional case of next-to-nearest-neighbour interaction the limit bulk energy density is described by a formula of 'convolution type' that highlights a non-trivial balance between first and second neighbours (see [26], [8]). Additional phenomena arise in the case when the range of interaction does not vanish with the lattice size, in which case a complex non-local interaction can take place (see [9]).

In this paper we provide a higher-order description of one-dimensional next-to-nearest-neighbour systems of the form

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

using the terminology of developments by Γ-convergence (introduced in Anzellotti and Baldo [4]) and equivalence of variational theories (in the spirit of Braides and Truskinovsky [17]). In this one-dimensional case the integrand φ is given as the convex envelope of an effective energy ψ described by an explicit convolution-type formula describing oscillations at the lattice level

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

that allows an easier description of the phenomena. Besides the possibility of oscillatory solutions on the microscopic scale, we show some additional features: first, the appearance of a boundary-layer contribution on the boundary due to the asymmetry of the boundary interactions. This type of boundary contribution has been studied by Charlotte and Truskinovsky [19] in terms of local minima for quadratic interactions and here is described in energetical terms in the general case. The formula for the boundary contribution is quite general, and can be also formulated for higher-dimensional problems, where additional difficult technical issues arise (see *e.g.* the recent work by Theil [28]).

A second feature is the appearance of a phase-transition surface energy, that is due to the non convexity of the zero-order energy density ψ that forces the appearance of phase transitions and the appearance of internal boundary layers due to the presence of next-to-nearest neighbour interactions. By showing an equivalent family of continuum energies we highlight that second neighbours play the same role as the higher-order gradients in the gradient theory of phase transitions. It is worth noting that, under some assumptions on the geometry of displacements, by combining this result with the description of Lennard-Jones systems by Pagano and Paroni [26] we obtain a variational asymptotic theory with first and second gradients that qualitatively differs from that obtained as a pointwise limit (see *e.g.* Blanc, Le Bris and Lions [6]).

A third issue is that 'macroscopic' transitions must be coupled to 'microscopic' ones; *i.e.*, even if the limit deformation is an affine function $u(t)=zt$ the corresponding microscopic deformations may be forced to have oscillations corresponding to a minimizing pair (z_1,z_2) with $z_1=(u^{i+1}-u^i)/\varepsilon$ for i odd mixed with oscillations corresponding to the same pair, but with $z_1=(u^{i+1}-u^i)/\varepsilon$ for i even, thus introducing an 'anti-phase' boundary that may not be detected by the macroscopic averaged field u. This justifies a necessarily more complex description of the limit in terms of a vector variable $\mathbf{u}=(u_1,u_2)$ that separately describes 'even' and 'odd' oscillations. If we integrate out microscopic patters the limit theory takes a non-local form where the internal surface terms are influenced by the boundary and also between themselves. Note that anti-phase boundaries necessarily arise under some boundary conditions. Similar phenomena arise in the study of spin systems (see [1] for their description using Γ-convergence). It must be remarked that the use of the new vector variable **u** brings more information than the description by Young measures (see Paroni [27]), by which the interaction of micro-oscillations with phase transitions cannot be detected.

Finally, an additional fourth feature appears in the description of Lennard-Jones type microscopic interactions, where the higher-order Γ-limit gives a fracture term. The microscopic pattern influence the value of the fracture energy through the appearance of boundary layers on the two sides of the fracture (an alternative description of this phenomena justified by a renormalization-group approach, under a different scaling of the energy, is provided by Braides, Lew and Ortiz [16]). The computation can be compared with that with a fixed interface by Blanc and Le Bris [5]. Note that these fracture boundary layer may compete with those forced by boundary conditions; as a consequence, for example, for Lennard-Jones interactions subject to forced displacement at the boundary we obtain that fracture at the boundary is energetically favoured, in contrast with the nearest-neighbour case when fracture may appear anywhere in the sample.

2 Setting of the problem

We will consider one-dimensional next-to-nearest neighbour interactions on (a portion of) a lattice $\lambda_n\mathbb{Z}$ of the form $E_n(u) : \mathcal{A}_n(0,L) \to [0,+\infty)$ given by

$$E_n(u) = \sum_{i=0}^{n-1} \lambda_n \psi_1\Big(\frac{u^{i+1}-u^i}{\lambda_n}\Big) + \sum_{i=0}^{n-2} \lambda_n \psi_2\Big(\frac{u^{i+2}-u^i}{2\lambda_n}\Big),$$

where ψ_1, ψ_2 are Borel functions bounded from below (this condition can be relaxed). Here and in the following of the paper $\lambda_n = \frac{L}{n}$, $\mathcal{A}_n(0,L)$ is the set of all functions $u : \lambda_n\mathbb{Z} \cap [0,L] \to \mathbb{R}$ and we often use the notation $u^i = u(i\lambda_n)$. We will also make the identification of such functions with their piecewise-affine interpolations and thus simply write

$$\mathcal{A}_n(0,L) = \{u : \mathbb{R} \to \mathbb{R} :\ u \in C(\mathbb{R}),\ u(t) \text{ is affine for } t \in (i, i{+}1)\lambda_n,\ i \in \{0,\dots,n{-}1\}\}.$$

We will also consider problems with fixed boundary data. To this end, given $l \in \mathbb{R}$ we define $E_n^l(u) : \mathcal{A}_n(0,L) \to [0,+\infty]$ as

$$E_n^l(u) = \begin{cases} E_n(u) & \text{if } u(0) = 0,\ u(L) = l \\ +\infty & \text{otherwise.} \end{cases} \tag{2.1}$$

We also define the *effective* (*zero-order*) *energy density* of the system ψ_0 by

$$\psi_0(\alpha) = \psi_2(\alpha) + \frac{1}{2}\inf\{\psi_1(z_1) + \psi_1(z_2)\ :\ z_1 + z_2 = 2\alpha\} \tag{2.2}$$

obtained by 'minimizing out' the nearest-neighbour interactions (see [15], [26], [8]).

For any $\alpha \in \mathbb{R}$, we define the set of (microscopic) *minimal states* of the effective energy density $\mathbf{M}^\alpha$ as the set of all the pairs optimizing the minimum problem for $\psi_0(\alpha)$; *i.e.*

$$\mathbf{M}^\alpha := \{(z_1, z_2) \in \mathbb{R}^2 : z_1 + z_2 = 2\alpha,\ \psi_0(\alpha) = \psi_2(\alpha) + \frac{1}{2}\left(\psi_1(z_1) + \psi_1(z_2)\right)\}.$$

The case $\#\mathbf{M}^\alpha = 1$, so that $\mathbf{M}^\alpha = \{(\alpha, \alpha)\}$ and $\psi_0^{**}(\alpha) = \psi_1(\alpha) + \psi_2(\alpha)$, is usually referred to as the *strict Cauchy-Born hypothesis*, while the case $\#\mathbf{M}^\alpha = 2$ as *the local Cauchy-Born hypothesis*. In this case $\mathbf{M}^\alpha = \{(z_1^\alpha, z_2^\alpha), (z_2^\alpha, z_1^\alpha)\}$ with $z_2^\alpha \neq z_1^\alpha$.

For $l \in \mathbb{R}$, if $\psi_0^{**}(\frac{l}{L}) < \psi_0(\frac{l}{L})$, then ψ_0^{**} coincides with an affine function on a neighborhood of $(\frac{l}{L})$. We denote by r such affine function and let $N(l)$ be the number of α_i such that $\psi_0(\alpha_i) = \psi_0^{**}(\alpha_i) = r(\alpha_i)$. In the following we will make the assumption that $\#N(l) < +\infty$. We also define the set $\mathbf{M}_l$ as follows:

$$\mathbf{M}_l = \begin{cases} \emptyset & \text{if} \quad \psi_0^{**}(\frac{l}{L}) = +\infty \\ \mathbf{M}^{\frac{l}{L}} & \text{if} \quad \psi_0^{**}(\frac{l}{L}) = \psi_0(\frac{l}{L}) \\ \bigcup\limits_{i=1}^{N(l)} \mathbf{M}^{\alpha_i} & \text{if} \quad \psi_0^{**}(\frac{l}{L}) < \psi_0(\frac{l}{L}). \end{cases}$$

Let $\mathbf{z}^\alpha = (z_1^\alpha, z_2^\alpha) \in \mathbf{M}^\alpha$; we define the *minimal energy configurations* $u_{\mathbf{Z}^\alpha} : \mathbb{Z} \to \mathbb{R}$ and $\overline{u}_{\mathbf{Z}^\alpha} : \mathbb{Z} \to \mathbb{R}$ by

$$u_{\mathbf{Z}^\alpha}(i) = \left[\frac{i}{2}\right] z_2^\alpha + \left(i - \left[\frac{i}{2}\right]\right) z_1^\alpha, \quad \overline{u}_{\mathbf{Z}^\alpha}(i) = u_{\mathbf{Z}^\alpha}(i+1) - z_1^\alpha$$

and $u_{\mathbf{Z}^\alpha, n} : \lambda_n\mathbb{Z} \to \mathbb{R}$, $\overline{u}_{\mathbf{Z}^\alpha, n} : \lambda_n\mathbb{Z} \to \mathbb{R}$ by

$$u_{\mathbf{Z}^\alpha, n}(x_i^n) = u_{\mathbf{Z}^\alpha}(i)\lambda_n, \quad \overline{u}_{\mathbf{Z}^\alpha, n}(x_i^n) = \overline{u}_{\mathbf{Z}^\alpha}(i)\lambda_n. \tag{2.3}$$

Note that the gradient of (the piecewise affine interpolation corresponding to) $u_{\mathbf{Z}^\alpha}$ takes the values z_1^α, z_2^α on intervals $(i, i+1)$ with i even/odd respectively while the converse holds for $\overline{u}_{\mathbf{Z}^\alpha}$ and that the piecewise affine interpolations of both $u_{\mathbf{Z}^\alpha, n}$ and $\overline{u}_{\mathbf{Z}^\alpha, n}$ converge uniformly to αt.

2.1 Even and odd interpolation

In order to describe the fine behaviour of discrete minimizers we will separately consider even and odd indices. In order to separately track the limits of the corresponding interpolations, given $u : \mathcal{A}_n(0, L) \to \mathbb{R}$ we define the *even interpolator function* $u_1 : \mathcal{A}_n(0, L) \to \mathbb{R}$ and the *odd interpolator function* $u_2 : \mathcal{A}_n(0, L) \to \mathbb{R}$ as follows:

$$u_1^0 = 0, \quad u_1^{i+1} - u_1^i = \begin{cases} u^{i+1} - u^i & \text{i is even} \\ u^i - u^{i-1} & \text{i is odd} \end{cases}$$

$$\text{if n is even,} \quad u_2^0 = 0 \quad u_2^{i+1} - u_2^i = \begin{cases} u^{i+1} - u^i & \text{i is odd} \\ u^{i+2} - u^{i+1} & \text{i is even} \end{cases}$$

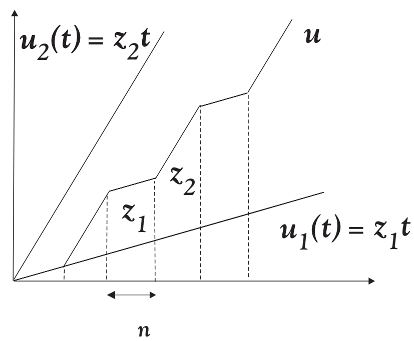

Figure 1: Interpolator functions for minimal energy configuration.

$$\text{if n is odd,} \qquad u_2^0 = 0 \quad u_2^{i+1} - u_2^i = \begin{cases} u^{i+1} - u^i & \text{i is odd} \\ u^{i+2} - u^{i+1} & \text{i is even, } i < n-1 \\ u^i - u^{i-1} & i = n-1. \end{cases}$$

We will say that a sequence of functions u_n belonging to $\mathcal{A}_n(0, L)$ converges to $\mathbf{u} = (u_1, u_2)$ in L^p $(1 \leq p \leq \infty)$ if $\mathbf{u}_n = (u_{n,1}, u_{n,2})$ converges to $\mathbf{u} = (u_1, u_2)$ in L^p. Note that this convergence implies that (but is not equivalent to) $u_n \to \frac{1}{2}(u_1 + u_2)$ in the usual sense in L^p. Moreover, for any functional space $\mathcal{B}$, we will write $\mathbf{u} \in \mathcal{B}$ meaning that $u_1, u_2 \in \mathcal{B}$.

With this notation the *minimal energy configurations* $u_{\mathbf{Z}^\alpha}$ and $\overline{u}_{\mathbf{Z}^\alpha}$ can be respectively identified with

$$\mathbf{u}_{\mathbf{Z}^\alpha}(i) = (z_1^\alpha i, z_2^\alpha i), \quad \overline{\mathbf{u}}_{\mathbf{Z}^\alpha}(i) = (z_2^\alpha i, z_1^\alpha i)$$

(see Fig. 1).

2.2 Crease and boundary-layer energies

We will show that (proper scalings of) the energies E_n give rise to phase-transition energies with interfacial energy and boundary terms. The quantification of these energies will be done by optimizing boundary and transition layers on the lattice level on the whole lattice (or only its positive part in the case of boundary layers) with minimal configurations as conditions at infinity. To this end we introduce the energy densities below. Note that the energies do not depend only on $\mathbf{z}$, but we have to take into account also a possible 'shift' since it may occur that it is energetically convenient not to match the minimal configuration exactly but its translation by a constant (which gives the same bulk contribution). Note that such a fixed translation is lost in the passage to the continuum.

Let $\mathbf{z} = (z_1, z_2) \in \mathbb{R}^2$, $\phi,\ l \in \mathbb{R}$. The *right-hand side boundary layer energy* of

$\mathbf{z}$ with shift ϕ is

$$B_+(\mathbf{z},\phi) = \inf_{N\in\mathbb{N}} \min\Big\{\tfrac{1}{2}\psi_1(u^1-u^0) + \sum_{i\geq 0}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^i\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big) : u:\mathbb{N}\to\mathbb{R}, u(0)=0, u^i = u^i_{\mathbf{z}} - \phi \text{ if } i\geq N\Big\}.$$

The *left-hand side boundary layer energy* of $\mathbf{z}$ with shift ϕ is

$$B_-(\mathbf{z},\phi) = \inf_{N\in\mathbb{N}} \min\Big\{\tfrac{1}{2}\psi_1(u^{-1}-u^0) + \sum_{i\leq 0}\Big(\psi_2\Big(\tfrac{u^{i}-u^{i-2}}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i}-u^{i-1}\Big)+\psi_1\Big(u^{i-1}-u^{i-2}\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big) : u:-\mathbb{N}\to\mathbb{R}, u(0)=0, u^i = u^i_{\mathbf{z}} + \phi \text{ if } i\leq -N\Big\}.$$

Let $\mathbf{z}' = (z_1', z_2') \in \mathbb{R}^2$. The (crease) *transition energy* between $\mathbf{z}$ and $\mathbf{z}'$ with shift ϕ is

$$\begin{aligned}C(\mathbf{z},\mathbf{z}',\phi) = \inf_{N\in\mathbb{N}} \min\Big\{&\tfrac{1}{2}\psi_1(u^0-u^{-1}) + \sum_{i\leq -1}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^i\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big)\\ &+ \tfrac{1}{2}\psi_1(u^1-u^0) + \sum_{i\geq 0}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^i\Big)\Big) - \psi_0\Big(\tfrac{z_1'+z_2'}{2}\Big)\Big) :\\ &u:\mathbb{Z}\to\mathbb{R},\quad u^i = u^i_{\mathbf{z}}+\phi_1 \text{ if } i\leq -N\\ &u^i = u^i_{\mathbf{z}'}+\phi_2 \text{ if } i\geq N,\quad \phi=\phi_1-\phi_2\Big\}.\end{aligned}$$

Remark 2.1 Note that $B_+(\mathbf{z},\phi) = B_-(\overline{\mathbf{z}},-\phi)$. In the case of affine minimal-energy configurations, which is to say when $\#\mathbf{M}^z = \#\mathbf{M}^{z'} = 1$, we often have a simpler description of the limit. We introduce a slightly different notation for this case. If $\mathbf{z}=(z,z)$ and $\mathbf{z}'=(z',z')$ we set

$$B_\pm(z,\phi) = B_\pm(\mathbf{z},\phi) \quad \text{and} \quad C(z,z',\phi) = C(\mathbf{z},\mathbf{z}',\phi).$$

Remark 2.2 If ψ_1,ψ_2 are such that $\psi_0\in C^1(\mathbb{R})$, then it can be easily shown that, for all $\mathbf{z},\mathbf{z}'\in\mathbb{R}^2$, B_+, B_- and C are shift independent, thus it is possible to rewrite the previous energies as follows

$$B_+(\mathbf{z}) = \inf_{N\in\mathbb{N}} \min\Big\{\tfrac{1}{2}\psi_1(u^1-u^0) + \sum_{i\geq 0}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^i\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big) : u:\mathbb{N}\to\mathbb{R}, u(0)=0,\ (u_1^{i+1}-u_1^i)=z_1,\ (u_2^{i+1}-u_2^i)=z_2 \text{ if } i\geq N\Big\}$$

$$B_-(\mathbf{z}) = \inf_{N\in\mathbb{N}} \min\Big\{ \tfrac{1}{2}\psi_1(u^{-1}-u^0) + \sum_{i\le 0}\Big(\psi_2\Big(\tfrac{u^i-u^{i-2}}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^i-u^{i-1}\Big)+\psi_1\Big(u^{i-1}-u^{i-2}\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big) : u:-\mathbb{N}\to\mathbb{R}, u(0)=0,\ (u_1^{i+1}-u_1^i)=z_1,\ (u_2^{i+1}-u_2^i)=z_2 \text{ if } i\le -N\Big\}$$

$$C(\mathbf{z},\mathbf{z}') = \inf_{N\in\mathbb{N}} \min\Big\{ \tfrac{1}{2}\psi_1(u^0-u^{-1}) + \sum_{i\le -1}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^{i}\Big)\Big) - \psi_0\Big(\tfrac{z_1+z_2}{2}\Big)\Big) + \tfrac{1}{2}\psi_1(u^1-u^0) + \sum_{i\ge 0}\Big(\psi_2\Big(\tfrac{u^{i+2}-u^i}{2}\Big) + \tfrac{1}{2}\Big(\psi_1\Big(u^{i+2}-u^{i+1}\Big)+\psi_1\Big(u^{i+1}-u^{i}\Big)\Big) - \psi_0\Big(\tfrac{z_1'+z_2'}{2}\Big)\Big) : u:\mathbb{Z}\to\mathbb{R}, (u_1^{i+1}-u_1^i)=z_1,\ (u_2^{i+1}-u_2^i)=z_2 \text{ if } i\le -N, (u_1^{i+1}-u_1^i)=z_1',\ (u_2^{i+1}-u_2^i)=z_2' \text{ if } i\ge N\Big\}.$$

Remark 2.3 By the previous two remarks we observe that, in the case $\#\mathbf{M}^z = 1$, if ψ_1, ψ_2 are such that $\psi_0 \in C^1(\mathbb{R})$, then $B_+(z) = B_-(z)$. Moreover, by the formula defining $B_\pm$ one easily gets that, set $\mathbf{z} = (z, z)$, if z is a minimum point for ψ_1, then $B_\pm(z) = \frac{1}{2}\min\psi_1$.

3 Γ-convergence for superlinear growth densities

3.1 Zero-order Γ-limit

In this section we give a description of the (zero-order) Γ-limit of the sequence E_n showing that the result by Braides, Gelli and Sigalotti [15] can be extended to Dirichlet and periodic boundary conditions. We have to take some extra care in that we do not assume that our potentials are everywhere finite. For the sake of simplicity, and without losing in generality, we will suppose $\psi_1,\ \psi_2$ to be non negative.

Theorem 3.1 (Zero order Γ-limit - Dirichlet boundary data) *Let $\psi_1, \psi_2 : \mathbb{R} \to [0, +\infty]$ be Borel functions such that the following hypotheses hold:*

[A1] $\operatorname{dom}\psi_1 = \operatorname{dom}\psi_2$ *is an interval of* $\mathbb{R}$*,*
[A2] ψ_1 *and* ψ_2 *are lower semicontinuous on their domain,*
[A3] $\lim_{|z|\to+\infty} \frac{\psi_1(z)}{|z|} = +\infty$.

Then the Γ-limit of E_n^l with respect to the L^1-topology is given by

$$E^l(u) = \begin{cases} \displaystyle\int_0^L \psi_0^{**}(u'(t))dt & u \in W^{1,1}(0,L),\ u(0)=0,\ u(L)=l \\ +\infty & \textit{otherwise} \end{cases}$$

on $L^1(0, L)$.

Remark 3.2 It is possible to weaken hypothesis [A1] supposing that dom $\psi_1 = \bigcup_i A_i$ where A_i is an interval of the real line. In this case some extra condition is needed. For example, one can suppose that, if $z \in$ dom ψ_0 and $z_1,\ z_2$ are optimal for z in the sense of (2.2), then $z_1,\ z_2 \in A_i$ and that dom ψ_2 contains the convex hull of dom ψ_1.

Proof of Theorem 3.1. In the following we suppose that $L = 1$. Let $u_n \to u$ in $L^1(0,1)$ and be such that $\sup_n E^l_n(u_n) < +\infty$, then, up to subsequences $u_n \rightharpoonup u$ weakly in $W^{1,1}(0,1)$ and $u(0) = 0$, $u(1) = l$. Moreover

$$\liminf_n E^l_n(u_n) \geq \int_{(0,1)} \psi_0^{**}(u'(t))\, dt.$$

To prove the Γ-lim sup inequality we consider two cases:

$$(a)\ l \text{ is an internal point of dom } \psi_0, \qquad (b)\ l \in \partial\text{dom } \psi_0.$$

In case (a) we use a density argument. Let u be such that $E^l(u) < +\infty$. Then $u'(t) \in \text{dom}\psi_0$ for a.e. $t \in (0,1)$. Without loss of generality we may suppose that $\text{dom}\psi_0 = [0,+\infty)$ or $\text{dom}\psi_0 = (0,+\infty)$. If $u' \geq c > 0$ the density argument is easy as it is possible to construct a sequence of piecewise affine functions (u_n) such that $u'_n \geq \frac{c}{2} > 0$, $u_n \to u$ in $W^{1,1}(0,1)$ and $\lim_n \int_0^1 \psi_0^{**}(u'_n) = \int_0^1 \psi_0^{**}(u')$. If otherwise $\inf u' = 0$, then $|\{t :\ u'(t) > l\}| \neq 0$ and $\eta > 0$ exists such that $|\{t :\ l + \eta < u'(t) < \frac{1}{\eta}\}| > 0$. Let $u_T \in W^{1,\infty}(0,1)$ be such that $u_T(0) = 0$ and $u'_T = u' \vee T$, and let

$$v_T(t) = u_T(t) + c_T \int_0^t \chi_{\{t:\ u' \in (l+\eta, \frac{1}{\eta})\}} \text{ where } c_T = \frac{l - u_T(1)}{|\{t :\ l + \eta < u' < \frac{1}{\eta}\}|}.$$

Observe that $\lim_{T\to 0^+} c_T = 0$. We have that $v_T \in W^{1,\infty}(0,1)$, $v_T(0) = 0$, $v_T(1) = l$ and that, for $T \to 0^+$, $v_T \to u$ in $W^{1,1}(0,1)$. By lower semicontinuity we have

$$\liminf_{T\to a} \int_{(0,1)} \psi_0^{**}(v'_T(t))\, dt \geq \int_{(0,1)} \psi_0^{**}(u'(t))\, dt.$$

Moreover

$$\begin{aligned}\int_{(0,1)} \psi_0^{**}(v'_T)\, dt = & \int_{\{t:\ u' \leq T\}} \psi_0^{**}(T)\, dt + \int_{\{t:\ T < u' \leq l+\eta\}} \psi_0^{**}(u')\, dt \\ & + \int_{\{t:\ l+\eta \leq u' \leq \frac{1}{\eta}\}} \psi_0^{**}(u' + c_T)\, dt + \int_{\{t:\ u' > \frac{1}{\eta}\}} \psi_0^{**}(u')\, dt. \end{aligned} \tag{3.1}$$

Observe that, thanks to the uniform continuity of ψ_0^{**} on compact sets, we have

$$\lim_{T\to 0^+} \int_{\{t:\ l+\eta \leq u' \leq \frac{1}{\eta}\}} \psi_0^{**}(u' + c_T)\, dt = \int_{\{t:\ l+\eta \leq u' \leq \frac{1}{\eta}\}} \psi_0^{**}(u')\, dt. \tag{3.2}$$

To pass to the limit in the equality (3.1) we need to consider the following two cases:

$$\text{(i)} \lim_{T\to 0^+} \psi_0^{**}(T) = +\infty, \quad \text{(ii)} \lim_{T\to 0^+} \psi_0^{**}(T) < +\infty.$$

In case (i), for T small enough we have that $\psi_0^{**}(T) \leq \psi_0^{**}(u'(t))$ for a.e. t such that $u'(t) \leq T$, hence

$$\int_{\{t:\ u' \leq T\}} \psi_0^{**}(T)\, dt \leq \int_{\{t:\ u' \leq T\}} \psi_0^{**}(u')\, dt.$$

In case (ii) we have that ψ_0^{**} is uniformly continuous in $[0, \frac{1}{\eta}]$. Hence, passing to the limit as $T \to 0^+$ in (3.1), thanks to (3.2) we finally have that

$$\limsup_{T\to 0^+} \int_{(0,1)} \psi_0^{**}(v_T'(t))\, dt \leq \int_{(0,1)} \psi_0^{**}(u'(t))\, dt. \tag{3.3}$$

Thanks to (3.3) and a density argument it suffices to prove the Γ- lim sup inequality for $u(t)$ piecewise affine. For the sake of simplicity we prove it for $u(t) = zt$ with z such that $\psi_0^{**}(z) = \psi_0(z)$ as the general case can be easily obtained by a convexity argument. Thanks to hypothesis [A2] there exist $\mathbf{z} = (z_1, z_2) \in \mathbf{M}^l$. Setting $u_n = u_{\mathbf{Z},n}$ as in (2.3), then $u_n \to u$ in $L^1(0,1)$ and $\lim_n E_n(u_n) = \int_{(0,1)} \psi_0(u')\, dt$. Defining

$$v_n(t) = \begin{cases} u_n(t) & \text{if } t \in [0, 1-\lambda_n] \\ u_n(1-\lambda_n) + \dfrac{(l - u_n(1-\lambda_n)}{\lambda_n}(t - 1 + \lambda_n) & \text{if } t \in [1-\lambda_n, 1] \end{cases}$$

then $v_n(0) = 0$, $v_n(1) = z$ and it holds

$$E_n(u_n) - E_n(v_n) \leq \lambda_n |\psi_2(z) - \psi_2(\frac{z + z_2}{2})| + \lambda_n |\psi_1(z_1) - \psi_1(z)|.$$

Thanks to hypotheses [A1] we have that

$$\lim_n (E_n(u_n) - E_n(v_n)) = 0,$$

thus proving that v_n is the recovery sequence for our problem.

In case (b), observing that $\psi_0^{**}(l) = \psi_0(l)$ and that $u(t) = lt$, the proof is easily obtained as the boundary condition is automatically satisfied for $u_n = u_{\mathbf{Z},n}$ when $z_1 = z_2 = l$. □

Remark 3.3 Observe that in the previous proof the construction of v_n is simplified in the case of *even* lattices.

We now state the analog result in the periodic case. Set

$$\mathcal{A}_n(\mathbb{R}) := \{u : \mathbb{R} \to \mathbb{R} :\ u \in C(\mathbb{R}),\ u(t) \text{ is affine for } t \in (i, i+1)\lambda_n \ \text{ for all } \ i \in \mathbb{Z}\},$$

let $E_n^{\#,l}(u) : \mathcal{A}_n(\mathbb{R}) \to [0, +\infty]$ be defined as

$$E_n^{\#,l}(u) = \begin{cases} \displaystyle\sum_{i=0}^{n-1} \lambda_n \psi_1\Big(\frac{u^{i+1} - u^i}{\lambda_n}\Big) + \sum_{i=0}^{n-1} \lambda_n \psi_2\Big(\frac{u^{i+2} - u^i}{2\lambda_n}\Big) & \text{if } u \in \mathcal{A}_n^{\#,l}(0, L) \\ +\infty & \text{otherwise,} \end{cases}$$

where $\mathcal{A}_n^{\#,l}(0, L) := \{u \in \mathcal{A}_n(\mathbb{R}) \ : u((i + n)\lambda_n) = u(i\lambda_n) + l\}$ (*i.e.*, $u(t)$ are $L-$periodic perturbation of the affine function $\frac{l}{L}t$).

Theorem 3.4 (Zero order Γ-limit - Periodic boundary data) *In the hypotheses of Theorem* 3.1 *the* Γ*-limit of* $E_n^{\#,l}$ *with respect to the* $L^1_{\rm loc}$*-topology is given by*

$$E^{\#,l}(u) = \begin{cases} \displaystyle\int_0^L \psi_0^{**}(u'(t))\, dt & \text{if } u \in W^{1,1}_{\#,l}(0, L) \\ +\infty & \text{otherwise} \end{cases}$$

on $L^1_{\rm loc}(\mathbb{R})$*, where* $W^{1,1}_{\#,l}(0, L) := \{u \in W^{1,1}_{\rm loc}(\mathbb{R}) : \ u(t) - lt$ is L periodic$\}$.

Proof. Supposing that $L = 1$, let $u_n \to u$ in $L^1_{\rm loc}(\mathbb{R})$ such that $\sup_n E_n^{\#,l}(u_n) < +\infty$. Then, up to subsequences, $u_n \rightharpoonup u$ weakly in $W^{1,1}_{\rm loc}(\mathbb{R})$ and a.e. in every compact set of $\mathbb{R}$. Thus

$$u(x + 1) - u(x) = \lim_n (u_n(x + 1) - u_n(x)) = \lim_n (u_n([x] + 1) - u_n([x])) = l$$

and then $u \in W^{1,1}_{\#,l}(0, 1)$. The thesis is easily obtained by arguing as in the proof of Theorem 3.1. □

3.2 First-order Γ-limit

In this section we compute the first-order Γ-limit of E_n under periodic or Dirichlet type boundary conditions, and show the appearance of phase transitions and boundary terms in the limit energy. Interfacial energies will appear in the case when ψ_0 is a non-convex function. Our model case is when ψ_0 is a double-well potential with two minimum points (in particular there is only one 'interval of non-convexity'), and each minimum point z possesses only one (in the trivial case (z, z)) or two (*i.e.*, (z_1, z_2) and (z_2, z_1) with $z_1 \neq z_2$) minimal-energy configuration. We nevertheless treat a more general case, for which some hypotheses (that are always satisfied except for 'degenerate' cases) must be made clear as follows:

[H1](*discreteness of the energy states*)

$$\#(\{x \in \mathbb{R} : \psi_0(x) = \psi_0^{**}(x)\} \cap \{x \in \mathbb{R} : \psi_0 \text{ is affine}\}) < +\infty.$$

This condition is necessary in order to deal with a finite number of accessible energy states;

[H2] (*finiteness of minimal energy configurations*) for every $\alpha \in \mathbb{R}$ such that $\psi_0(\alpha) = \psi_0^{**}(\alpha)$

$$\#\mathbf{M}^\alpha < +\infty;$$

[H3] (*compatibility of minimal energy configurations*) for every α, $\beta \in \mathbb{R}$ with $\alpha \neq \beta$, such that $\psi_0(\alpha) = \psi_0^{**}(\alpha)$ and $\psi_0(\beta) = \psi_0^{**}(\beta)$ and for every $\mathbf{z}^\alpha = (z_1^\alpha, z_2^\alpha) \in \mathbf{M}^\alpha$ and $\mathbf{z}^\beta = (z_1^\beta, z_2^\beta) \in \mathbf{M}^\beta$ it holds

$$z_i^\alpha \neq z_j^\beta \quad i, j \in \{1, 2\}.$$

This condition is necessary in order to have a non-zero surface energy for the transition from α to β;

[H4] (*continuity and growth conditions*) $\psi_1,\ \psi_2\ : \mathbb{R} \to [0, +\infty]$ are Lipschitz functions such that

$$\psi_1(z) \geq mz + q$$

for some $m, q \in \mathbb{R}$ with $m \neq 0$ (note that m is not required to be positive) and that l is such that

$$\lim_{|z| \to +\infty} \psi_0(z) - pz = +\infty \qquad \text{for all } p \in \partial\psi_0^{**}(l);$$

[H5] (*non-degeneracy for the boundary datum*) l is such that

$$\lim_{|z| \to +\infty} \psi_1(z) - pz = +\infty \qquad \text{for all } p \in \partial\psi_0^{**}(l);$$

[H6] (*finiteness of the intervals of non-convexity*) l is such that $N(l) < +\infty$ ($N(l)$ defined as in (2.3)).

The following compactness result states that functions u_n such that $E_n^l(u_n) = \min E^l + O(\lambda_n)$ locally have microscopic oscillations close to minimal-energy configurations belonging to $\mathbf{M}_l$, except for a finite number of interactions that concentrate on a finite set S in the limit.

Proposition 3.5 (Compactness - Dirichlet boundary data) *Suppose that hypotheses* [H1]–[H6] *hold. If $\{u_n\}$ is a sequence of functions such that*

$$\sup_n E_n^{1,l}(u_n) = \sup_n \frac{E_n^l(u_n) - \min E^l}{\lambda_n} < +\infty \tag{3.4}$$

then there exists a set $S \subset (0, L)$ with $\#S < +\infty$ such that, up to subsequences, u_n converges to $\boldsymbol{u} = (u_1, u_2)$ in $W^{1,\infty}_{\mathrm{loc}}((0, L) \setminus S)$ where u_1, u_2 are piecewise-affine functions and $u_1(L) + u_2(L) = 2l$. Moreover $\boldsymbol{u}'(t) \in \boldsymbol{M}_l$ for a.e. $t \in (0, L)$ and $S(\boldsymbol{u}') = S(u_1') \cup S(u_2') \subseteq S$.

Proof. For simplicity of notation we can suppose that $L = 1$ and that n is even, the proof being analogous in the general case.

Set

$$\tilde\psi_1(z) = \psi_1(z) - \frac{m}{2} z,$$

(m as in [$H4$]) we have that

$$\tilde{\psi}_1(z) \geq c(|z|-1) \tag{3.5}$$

for some $c > 0$. Thus we have

$$\begin{aligned} +\infty > E_n(u_n) &\geq \sum_{i=0}^{n-1} \lambda_n \psi_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big) \\ &= \sum_{i=0}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big) + \frac{m}{2}\sum_{i=0}^{n-1}(u_n^{i+1}-u_n^i) \\ &= \sum_{i=0}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big) + \frac{m}{2} l. \end{aligned}$$

Then, by the definition of even and odd interpolations, we have

$$\begin{aligned} +\infty &> 2\sum_{i=0,\ even}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big) + 2\sum_{i=0,\ odd}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big) \\ &= \sum_{i=0}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_{1,n}^{i+1}-u_{1,n}^i}{\lambda_n}\Big) + \sum_{i=0}^{n-1} \lambda_n \tilde{\psi}_1\Big(\frac{u_{2,n}^{i+1}-u_{2,n}^i}{\lambda_n}\Big) \\ &= \int_0^1 \tilde{\psi}_1(u_{1,n}'(t))\,dt + \int_0^1 \tilde{\psi}_1(u_{2,n}'(t))\,dt. \end{aligned}$$

Thanks to (3.5) we get, for $h \in \{1,2\}$

$$\int_0^1 |u_{h,n}'(t)|\,dt < +\infty. \tag{3.6}$$

Let $\{J_j\},\ \{K_j\}$ be two families of intervals of the real line where ψ_0^{**} is, respectively, a straight line or a strictly convex function, satisfying

$$\begin{aligned} \partial\psi_0^{**}(x) \neq \partial\psi_0^{**}(y) \quad &\text{for all } x \in J_j,\ y \in J_{j+1} \\ K_j,\ K_{j+1} &\text{ are not contiguous,} \end{aligned}$$

where we have denoted by $\partial\psi_0^{**}(x)$ the sub-differential of ψ_0^{**} in x. Note that, by the growth conditions on ψ_0, J_j is a bounded interval. Suppose that $l \in J_j$ for some j and that $p(l) \in \partial\psi_0^{**}(l)$. We define $r_j(x) = p(l)(x-l) + \psi_0^{**}(l)$, the straight line such that $\psi_0^{**}(x) = r_j(x)$ for all $x \in J_j$. Since $\min E^l = \psi_0^{**}(l)$, by (3.4) we get

$$\begin{aligned} C \geq E_n^{1,l}(u_n) &= \sum_{i=0}^{n-2}\Big(\psi_2\Big(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big)\Big) - \psi_0^{**}(l)\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{n}-u_n^{n-1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^1-u_n^0}{\lambda_n}\Big)\Big) - \psi_0^{**}(l) \end{aligned}$$

$$= \sum_{i=0}^{n-2} \mathcal{E}_n^i(u_n) + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^1 - u_n^0}{\lambda_n}\Big) - r_j\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big) - r_j\Big(\frac{u_n^1 - u_n^0}{\lambda_n}\Big)\Big),$$

where we have set

$$\mathcal{E}_n^i(u_n) = \psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big)\Big) - r_j\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big).$$

Thanks to the continuity of $\psi_1(z)$ and $r_j(z)$ and to hypothesis [H5], we have that $\psi_1(z) - r_j(z)$ has a finite minimum since $\lim_{|z|\to+\infty}(\psi_1(z) - r_j(z)) = +\infty$. It follows that

$$\sum_{i=0}^{n-2} \mathcal{E}_n^i(u_n) \le C. \tag{3.7}$$

We infer that, for every $\eta > 0$, if we define $I_n(\eta) := \{i \in \{0, 1, \ldots, n-2\} : \mathcal{E}_n^i(u_n) > \eta\}$, then

$$\sup_n \# I_n(\eta) \le C(\eta) < +\infty.$$

Let $i \notin I_n(\eta)$; then by (3.7)

$$0 \le \psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big)\Big) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) \le \eta$$
$$0 \le \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) - r_j\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) \le \eta\ .$$

Let $\varepsilon = \varepsilon(\eta)$ be defined so that if

$$0 \le \psi_0(z) - r_j(z) \le \eta,$$
$$0 \le \psi_2(z) + \frac{1}{2}\Big(\psi_1(z_1) + \psi_1(z_2)\Big) - \psi_0(z) \le \eta \quad \text{with } z_1 + z_2 = 2z,$$

then

$$\mathrm{dist}\,((z_1, z_2), \mathbf{M}_l) \le \varepsilon(\eta).$$

Chosen $\eta > 0$ such that

$$2\varepsilon(\eta) < \min\{|\mathbf{z}' - \mathbf{z}''|,\ \mathbf{z}', \mathbf{z}'' \in \mathbf{M}_l\},$$

we deduce that, if $i-1,\ i \notin I_n(\eta)$ then there exists $\mathbf{z} \in \mathbf{M}_l$ such that

$$\Big|\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}, \frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) - \mathbf{z}\Big| \le \varepsilon$$

and

$$\Big|\Big(\frac{u_n^i - u_n^{i-1}}{\lambda_n}, \frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - \overline{\mathbf{z}}\Big| \le \varepsilon.$$

Hence, there exists a finite number of indices $0 = i_1 < i_2 < \ldots < i_{N_n} = n$ such that for all $k = 1, 2, \ldots, N_n$ there exists $\mathbf{z}_k^n = (z_{1,k}^n, z_{2,k}^n) \in \mathbf{M}_l$ such that for all $i \in \{i_{k-1}+1, i_{k-1}+2, \ldots, i_k - 1\}$ we have

$$\Big|\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}, \frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) - \mathbf{z}_k^n\Big| \leq \varepsilon.$$

Then, by the definitions of even and odd interpolations it can be easily seen that

$$\begin{aligned} \Big|\frac{u_{1,n}^{i+1} - u_{1,n}^i}{\lambda_n} - z_{1,k}^n\Big| &\leq \varepsilon \quad i \in \{i_{k-1}+2, i_{k-1}+3, \ldots, i_k - 1\}, \\ \Big|\frac{u_{2,n}^{i+1} - u_{2,n}^i}{\lambda_n} - z_{2,k}^n\Big| &\leq \varepsilon \quad i \in \{i_{k-1}+1, i_{k-1}+2, \ldots, i_k - 2\}. \end{aligned} \tag{3.8}$$

Let $\{j_1, j_2, \ldots, j_{M_n}\}$ be the maximal subset of $0 = i_1 < i_2 < \ldots < i_{N_n} = n$ defined by the requirement that if $\mathbf{z}_{j_k}^n \in \mathbf{M}^\beta$ then $\mathbf{z}_{j_k+1}^n \in \mathbf{M}^\gamma$ with $\beta \neq \gamma$ and $\mathbf{M}^\beta, \mathbf{M}^\gamma \subset \mathbf{M}_l$. Thanks to (3.4) there exists $C(\eta) > 0$ such that $E_n^1(u_n) \geq C(\eta) M_n$. Thus, up to further subsequences, we can suppose that $M_n = M$, $\mathbf{z}_{j_k}^n = \mathbf{z}_k = (z_{1,k}, z_{2,k})$ and that $x_{j_k}^n \to x_k$. Fix δ, set $S = \bigcup_k x_k$ and $S_\delta = \bigcup_k (x_k - \delta, x_k + \delta)$. Then, by (3.8) we get

$$\sup_{t \in (0,1) \setminus S_\delta} |u_{s,n}'(t) - z_{s,k}| \leq \varepsilon \quad s \in \{1, 2\}.$$

The previous estimates, together with (3.6) ensure that $\mathbf{u}_n$ is an equicontinuous and equibounded sequence in $(0,1) \setminus S_\delta$. Thus, thanks to the arbitrariness of δ, up to passing to a further subsequence (not relabelled), $\mathbf{u}_n$ converges in $W^{1,\infty}_{\rm loc}((0,1) \setminus S)$ to a function $\mathbf{u}$ such that $\mathbf{u}'(t) \in \mathbf{M}_l$ a.e. $t \in (0,1)$. Moreover $S(\mathbf{u}') \subseteq S$.

To prove that u_1 and u_2 are piecewise affine functions, we need to prove that they are continuous. Suppose by contradiction that $S(u_1) \neq \emptyset$. Then, for n large enough,

$$\text{for all } M \in \mathbb{N} \ \text{ there exits } i: \ \Big|\frac{u_{1,n}^{i+1} - u_{1,n}^i}{\lambda_n}\Big| > M. \tag{3.9}$$

Then, by (3.4), we have that, for some j

$$\begin{aligned} C \quad \geq \quad & \sum_{i=0,\ even}^{n-2} \Bigg(\psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2} - u_n^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big)\Big) \\ & - r_j\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Bigg). \end{aligned}$$

Then, for i even, by the definition of even and odd interpolations, we get

$$C \geq \frac{1}{2}\Big(\psi_1\Big(\frac{u_{2,n}^{i+2} - u_{2,n}^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_{1,n}^{i+1} - u_{1,n}^i}{\lambda_n}\Big)\Big) - r_j\Big(\frac{u_{2,n}^{i+2} - u_{2,n}^{i+1} + u_{1,n}^{i+1} - u_{1,n}^i}{2\lambda_n}\Big).$$

Since $r_j(z) = pz + q$ with $p \in \partial\psi_0^{**}(l)$, the previous estimate gives

$$C \geq \frac{1}{2}\Big(\psi_1\Big(\frac{u_{2,n}^{i+2} - u_{2,n}^{i+1}}{\lambda_n}\Big) - p\Big(\frac{u_{2,n}^{i+2} - u_{2,n}^{i+1}}{\lambda_n}\Big) + \psi_1\Big(\frac{u_{1,n}^{i+1} - u_{1,n}^i}{\lambda_n}\Big) - p\Big(\frac{u_{1,n}^{i+1} - u_{1,n}^i}{\lambda_n}\Big)\Big).$$

By the previous inequality, we get the contradiction thanks to (3.9) and to hypothesis [H5].

The same argument can be exploited also in the case $l \in K_j$ for some j. □

Remark 3.6 (Boundary terms blow-up) Observe that, if hypothesis [H5] is dropped, it is possible to produce an example of ψ_1 and ψ_2 and a sequence (u_n) equibounded in energy such that

$$\lim_n \frac{1}{2}\Big(\psi_1\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big)+\psi_1\Big(\frac{u_n^1 - u_n^0}{\lambda_n}\Big)-r_j\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big)-r_j\Big(\frac{u_n^1 - u_n^0}{\lambda_n}\Big)\Big) = -\infty \tag{3.10}$$

preventing us from deducing inequality (3.7). In fact if

$$\psi_1(z) = |z| - 1, \qquad \psi_2(z) = \begin{cases} -2z-6 & z \in (-\infty, -1], \\ 5z+1 & z \in (-1, 0], \\ -z+1 & z \in (0, 1], \\ 4z-4 & z \in (1, +\infty), \end{cases}$$

we have that

$$\psi_0^{**}(z) = \begin{cases} -3z-7 & z \in (-\infty, -1], \\ 2z-2 & z \in (-1, +\infty). \end{cases}$$

For $l = 1$ we have that $\partial\psi_0^{**}(l) = \{2\}$ and that

$$\lim_{z\to\infty} \psi_1(z) - 2z = -\infty,$$

thus not fulfilling hypothesis [H5]. The sequence

$$u_n^0 = 0, \qquad u_n^{i+1} - u_n^i = \begin{cases} \sqrt{\lambda_n} & i = 0, \\ \lambda_n & i = 1, 2, \dots, n-2, \\ 2\lambda_n - \sqrt{\lambda_n} & i = n-1, \end{cases}$$

satisfies (3.10) and is such that $E_n^{1,l}(u_n) = 0$.

The first Γ-limit is given in terms of the variables $\mathbf{u}$ (giving microscopic oscillations) and s (the shift). It describes transitions between different phases through the term C and with the boundary through the terms $B_\pm$. The final form of the limit is obtained by optimizing in the shift term, taking care of the compatibility restrictions due to the boundary conditions. Note the difference in the limit boundary conditions in the even and odd cases.

Theorem 3.7 (First order Γ-limit - Dirichlet boundary data) *Suppose that hypotheses* [H1]–[H6] *hold and let* $E_n^{1,l} : \mathcal{A}_n(0, L) \to [0, +\infty]$ *be defined by*

$$E_n^{1,l}(u) = \frac{E_n^l(u) - \min E^l}{\lambda_n}.$$

We then have:

(Case n even) $E_n^{1,l}$ Γ*-converges with respect to the* L^∞*-topology to*

$$E^{1,l}_{even}(\boldsymbol{u}) = \inf\Big\{E^{1,l}_{even}(\boldsymbol{u}, s): \ s: S(\boldsymbol{u}') \cup \{0, L\} \to \mathbb{R}, \sum_{t \in S(\boldsymbol{u}') \cup \{0,L\}} s(t) = l\Big\}$$

where

$$E^{1,l}_{even}(\boldsymbol{u}, s) = \begin{cases} \sum\limits_{t \in S(\boldsymbol{u}')} C(\boldsymbol{u}'(t-), \boldsymbol{u}'(t+), s(t)) + B_+(\boldsymbol{u}'(0), s(0)) + B_-(\boldsymbol{u}'(L), s(L)), \\ \qquad\qquad \text{if } \boldsymbol{u}' \in PC(0, L),\ \boldsymbol{u}' \in \boldsymbol{M}_l,\ u_1(L) + u_2(L) = 2l \\ +\infty \qquad\qquad \text{otherwise} \end{cases}$$

on $W^{1,\infty}(0, L)$.

(Case n odd) $E_n^{1,l}$ Γ*-converges with respect to the* L^∞*-topology to*

$$E^{1,l}_{odd}(\boldsymbol{u}) = \inf\Big\{E^{1,l}_{odd}(\boldsymbol{u}, s): \ s: S(\boldsymbol{u}') \cup \{0, L\} \to \mathbb{R}, \sum_{t \in S(\boldsymbol{u}') \cup \{0,L\}} s(t) = l\Big\}$$

where

$$E^{1,l}_{odd}(\boldsymbol{u}, s) = \begin{cases} \sum\limits_{t \in S\boldsymbol{u}'} C(\boldsymbol{u}'(t-), \boldsymbol{u}'(t+), s(t)) + B_+(\boldsymbol{u}'(0), s(0)) + B_-(\overline{\boldsymbol{u}'(L)}, s(L)) \\ \qquad\qquad \text{if } \boldsymbol{u}' \in PC(0, L),\ \boldsymbol{u}' \in \boldsymbol{M}_l,\ u_1(L) + u_2(L) = 2l \\ +\infty \qquad\qquad \text{otherwise} \end{cases}$$

on $W^{1,\infty}(0, L)$.

PROOF. The general case being dealt with similarly, in the following we will suppose that n is even, $L = 1$ and, using the notation of the previous proof, that $l \in J_j$ for some j.

Γ-liminf inequality. Let $u_n \to \mathbf{u}$ in $L^\infty(0, 1)$ be such that $E_n^{1,l}(u_n) < +\infty$. Then, thanks to Proposition 3.5 there exist $M \in \mathbb{N}$, $\alpha_1, \alpha_2, \ldots, \alpha_M \in \mathbf{M}_l$ and $0 = x_0 < x_1 < \ldots < x_M = 1$ such that

$$u_n'(t) \to \mathbf{z}^{\alpha_j} \quad t \in (x_{j-1}, x_j) \quad j \in \{1, 2, \ldots, M\}. \tag{3.11}$$

For $i \in \{0, 1, \ldots, M\}$, let $\{k_n^i\}_n$ be a sequence of indices such that $k_n^0 = 0$ and

$$\lim_n \Big(k_n^i - \sum_{j=1}^{i} \frac{x_j - x_{j-1}}{\lambda_n}\Big) = 0, \tag{3.12}$$

and let $\{h_n^i\}_n$ be a sequence of indices such that

$$\lim_n \lambda_n h_n^i = \frac{x_i - x_{i-1}}{2}.$$

Since ψ_0^{**} is affine in J_j, we have that

$$n\psi_0^{**}(l) \quad = \quad n\psi_0^{**}\Big(\sum_{j=1}^{M} \alpha_j(x_j - x_{j-1})\Big) = \sum_{j=1}^{M} n(x_j - x_{j-1})\psi_0^{**}(\alpha_j)$$

$$
\begin{aligned}
&= \sum_{j=1}^{M} \sum_{i=k_n^{j-1}}^{k_n^j-1} n \frac{(x_j - x_{j-1})}{(k_n^j - k_n^{j-1})} \psi_0(\alpha_j) \\
&= \sum_{j=1}^{M-1} \sum_{i=k_n^{j-1}}^{k_n^j-1} \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \sum_{i=k_n^{M-1}}^{n-2} \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \psi_0(\alpha_M) + R_n,
\end{aligned}
$$

with

$$
\begin{aligned}
R_n &= \sum_{j=1}^{M-1} \sum_{i=k_n^{j-1}}^{k_n^j-1} \Big(\Big(n \frac{(x_j - x_{j-1})}{(k_n^j - k_n^{j-1})}\Big) \psi_0(\alpha_j) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Big) \\
&\quad + \sum_{i=k_n^{M-1}}^{n-2} \Big(n \frac{(x_M - x_{M-1})}{(k_n^M - k_n^{M-1})}\Big) \Big(\psi_0(\alpha_M) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Big) \\
&\quad + \Big(n \frac{(x_M - x_{M-1})}{(k_n^M - k_n^{M-1})} - 1\Big) \psi_0(\alpha_M).
\end{aligned}
$$

Thanks to Proposition 3.5, (3.12) and to the continuity of ψ_0 we have that $R_n \to 0$. To get the Γ-liminf inequality it is useful to rewrite the energy as follows:

$$
\begin{aligned}
E_n^1(u_n) = &\sum_{i=0}^{n-2} \psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \sum_{i=0}^{n-1} \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) \\
&- \sum_{j=1}^{M-1} \sum_{i=k_n^{j-1}}^{k_n^j-1} \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) - \sum_{i=k_n^{M-1}}^{n-2} \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) - \psi_0(\alpha_M) - R_n \\
= &\; E_n^1(u_n, h_n^1) + \sum_{j=1}^{M-1} E_n^1(u_n, h_n^j, h_n^{j+1}) + E_n^1(u_n, h_n^M) - R_n \qquad (3.13)
\end{aligned}
$$

where we have set

$$
\begin{aligned}
E_n^1(u_n, h_n^1) &= \sum_{i=0}^{h_n^1-1} \Big(\psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Big), \\
E_n^1(u_n, h_n^j, h_n^{j+1}) &= \sum_{i=h_n^j}^{h_n^{j+1}-1} \Big(\psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Big), \\
E_n^1(u_n, h_n^M) &= \sum_{i=h_n^M}^{n-2} \Big(\psi_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + \psi_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - \psi_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big)\Big) \\
&\quad + \psi_1\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big) - \psi_0(\alpha_M).
\end{aligned}
$$

As the general case can be obtained by slightly modifying the definition of $\tilde{\mathbf{u}}_n$, in the sequel we will suppose that $h_n^j, k_n^j, h_n^j - k_n^j, h_n^{j+1} - k_n^j$ are even. Defining

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \dfrac{\mathbf{u}_n^i}{\lambda_n} & \text{if } i \in \{0, 1, \dots, h_n^1\} \\ \mathbf{u}_{\mathbf{Z}^{\alpha_1}}(i) - \mathbf{u}_{\mathbf{Z}^{\alpha_1}}(h_n^1) + \dfrac{\mathbf{u}_n^{h_n^1}}{\lambda_n} & \text{if } i \geq h_n^1, \end{cases}$$

by the continuity of ψ_1 and ψ_2, we can find a suitable continuous function $\omega(\varepsilon) : \mathbb{R} \to \mathbb{R}$, $\omega(0) = 0$ such that, as $\tilde{\mathbf{u}}_n^i$ is a test function for the minimum problem defining $B_+(\mathbf{u}'(0), \phi(0))$, for any $\varepsilon > 0$, we have, for n large enough,

$$\begin{aligned} E_n^1(u_n, h_n^1) &= \frac{1}{2}\psi_1(\tilde{u}_n^1 - \tilde{u}_n^0) + \sum_{i \geq 0} \Big(\psi_2\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\tilde{u}_n^{i+2} - \tilde{u}_n^{i+1}\Big) + \psi_1\Big(\tilde{u}_n^{i+1} - \tilde{u}_n^i\Big)\Big) - \psi_0\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big)\Big) + \omega(\varepsilon) \\ &\geq B_+(\mathbf{u}'(0), \phi(0)) + \omega(\varepsilon), \end{aligned} \tag{3.14}$$

where

$$\phi(0) = u_{\mathbf{Z}^{\alpha_1}}(h_n^1) - \frac{u_n^{h_n^1}}{\lambda_n}.$$

Exploiting the same argument, for $j \in \{1, 2, \dots, M-1\}$, we can define

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \mathbf{u}_{\mathbf{Z}^{\alpha_j}}(i) - \mathbf{u}_{\mathbf{Z}^{\alpha_j}}(h_n^j - k_n^j) + \dfrac{\mathbf{u}_n^{h_n^j}}{\lambda_n} & \text{if } i \leq h_n^j - k_n^j, \\ \dfrac{\mathbf{u}_n^{i+k_n^j}}{\lambda_n} & \text{if } h_n^j - k_n^j \leq i \leq h_n^{j+1} - k_n^j, \\ \mathbf{u}_{\mathbf{Z}^{\alpha_{j+1}}}(i) - \mathbf{u}_{\mathbf{Z}^{\alpha_{j+1}}}(h_n^{j+1} - k_n^j) + \dfrac{\mathbf{u}_n^{h_n^{j+1}}}{\lambda_n} & \text{if } i \geq h_n^{j+1} - k_n^j\ , \end{cases}$$

and we have that

$$\begin{aligned} E_n^1(u_n, h_n^j, h_n^{j+1}) &= \frac{1}{2}\psi_1(\tilde{u}_n^0 - \tilde{u}_n^{-1}) + \sum_{i \leq -1} \Big(\psi_2\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\tilde{u}_n^{i+2} - \tilde{u}_n^{i+1} + \psi_1\Big(\tilde{u}_n^{i+1} - \tilde{u}_n^i\Big)\Big) - \psi_0\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big)\Big) \\ &\quad + \frac{1}{2}\psi_1(\tilde{u}_n^1 - \tilde{u}_n^0) + \sum_{i \geq 0} \Big(\psi_2\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\tilde{u}_n^{i+2} - \tilde{u}_n^{i+1}\Big) + \psi_1\Big(\tilde{u}_n^{i+1} - \tilde{u}_n^i\Big)\Big) - \psi_0\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big)\Big) \\ &\quad + \omega(\varepsilon) \\ &\geq C(\mathbf{u}'(x_j-), \mathbf{u}'(x_j+), \phi(x_j)) + \omega(\varepsilon), \end{aligned} \tag{3.15}$$

with

$$\phi(x_j) = \frac{u_n^{h_n^j}}{\lambda_n} - u_{\mathbf{Z}^{\alpha_j}}(h_n^j - k_n^j) + u_{\mathbf{Z}^{\alpha_{j+1}}}(h_n^{j+1} - k_n^j) - \frac{u_n^{h_n^{j+1}}}{\lambda_n}.$$

Finally, with

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \mathbf{u}_{\mathbf{Z}^{\alpha_M}}(i) - \mathbf{u}_{\mathbf{Z}^{\alpha_M}}(h_n^M - n) + \dfrac{\mathbf{u}_n^{h_n^M}}{\lambda_n} & \text{if } i \le h_n^M - n, \\ \dfrac{\mathbf{u}_n^{i+n}}{\lambda_n} - \dfrac{l}{\lambda_n} & h_n^M - n \le i \le 0, \end{cases}$$

we obtain

$$\begin{aligned} E_n^1(u_n, h_n^M) &= \frac{1}{2}\psi_1(\tilde{u}_n^0 - \tilde{u}_n^{-1}) + \sum_{i\le 0}\Big(\psi_2\Big(\frac{\tilde{u}_n^i - \tilde{u}_n^{i-2}}{2}\Big) \\ &\quad + \frac{1}{2}\Big(\psi_1\Big(\tilde{u}_n^i - \tilde{u}_n^{i-1}\Big) + \Big(\tilde{u}_n^{i-1} - \tilde{u}_n^{i-2}\Big)\Big) - \psi_0\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big)\Big) + \omega(\varepsilon) \\ &\ge B_-(\mathbf{u}'(1), \phi(1)) + \omega(\varepsilon), \end{aligned} \tag{3.16}$$

where

$$\phi(1) = \frac{u_n^{h_n^M}}{\lambda_n} - u_{\mathbf{Z}^{\alpha_M}}(h_n^M - n).$$

Since we have

$$\sum_{t\in S(\mathbf{u}')\cup\{0,1\}} \phi(t) = l, \tag{3.17}$$

we obtain that, thanks to (3.13), (3.14), (3.15) and (3.16),

$$\begin{aligned} E_n^{1,l}(u_n) &\ge B_+(\mathbf{u}'(0), \phi(0)) \\ &\quad + \sum_{t\in S(\mathbf{u}')} C(\mathbf{u}'(t-), \mathbf{u}'(t+), \phi(t)) + B_-(\mathbf{u}'(1), \phi(1)) + c\omega(\varepsilon) - R_n \\ &\ge \inf\Big\{E_{even}^{1,l}(u,s) : \ s : S(\mathbf{u}')\cup\{0,1\} \to \mathbb{R}, \sum_{t\in S(\mathbf{u}')\cup\{0,1\}} s(t) = l\Big\} + c\,\omega(\varepsilon) - R_n. \end{aligned}$$

Thus, by the arbitrariness of ε, we get

$$\liminf_n E_n^{1,l}(u_n) \ge \inf\Big\{E_{even}^{1,l}(u,s) : \ s : S(\mathbf{u}')\cup\{0,1\} \to \mathbb{R}, \sum_{t\in S(\mathbf{u}')\cup\{0,1\}} s(t) = l\Big\}. \tag{3.18}$$

Γ-limsup inequality. Let $\mathbf{u}$ be such that $E_{even}^{1,l}(\mathbf{u}) < +\infty$. Then there exist $M \in \mathbb{N}$, $\alpha_1, \alpha_2, \ldots, \alpha_M \in \mathbf{M}_l$ and $0 = x_0 < x_1 < \ldots < x_M = 1$ such that $\#S(\mathbf{u}') = M - 1$ and

$$\mathbf{u}'(t) = \mathbf{z}^{\alpha_j} \quad t \in (x_{j-1}, x_j) \quad j \in \{1, 2, \ldots, M\}. \tag{3.19}$$

Thanks to the boundary conditions on $\mathbf{u}$, we have that $\sum_{i=1}^{M-1}(x_{i+1} - x_i) = 1$. For $\varepsilon > 0$ let $\varphi : S(\mathbf{u}')\cup\{0,1\} \to \mathbb{R}$ be such that

$$\sum_{t\in S(\mathbf{u}')\cup\{0,1\}} \varphi(t) = l,$$

$$\sum_{t\in S(\mathbf{u}')} C(\mathbf{u}'(t-),\mathbf{u}'(t+),\varphi(t)) + B_+(\mathbf{u}'(0),\varphi(0)) + B_-(\mathbf{u}'(1),\varphi(1))$$
$$\leq E^{1,l}_{even}(\mathbf{u}) + \varepsilon. \tag{3.20}$$

Fix $\eta > 0$. For $j \in \{1, 2, \dots, M-1\}$ let $\mathbf{v}_1 = (v_{1,1}, v_{1,2})$, $\mathbf{v}_{j,j+1} = (v_{j,j+1,1}, v_{j,j+1,2})$ and $\mathbf{v}_M = (v_{M,1}, v_{M,2})$ be such that

$$v_1^0 = 0, \qquad v_1^i = u^i_{\mathbf{Z}^{\alpha_1}} - \varphi(0) \quad \text{for } i \geq N,$$
$$v^i_{j,j+1} = \begin{cases} u^i_{\mathbf{Z}^{\alpha_j}} + \phi_1^{j,j+1} & \text{for } i \leq -N, \\ u^i_{\mathbf{Z}^{\alpha_{j+1}}} + \phi_2^{j,j+1} & \text{for } i \geq N, \end{cases}$$
$$v_M^0 = 0, \qquad v_M^i = u^i_{\mathbf{Z}^{\alpha_M}} - \varphi(1) \quad \text{for } i \leq -N,$$

where

$$\phi_1^{j,j+1} = -\sum_{k=0}^{j} \varphi(x_k), \qquad \phi_2^{j,j+1} = -\sum_{k=0}^{j+1} \varphi(x_k)$$

and

$$\frac{1}{2}\psi_1(v_1^1 - v_1^0) + \sum_{i\geq 0}\Big(\psi_2\Big(\frac{v_1^{i+2} - v_1^i}{2}\Big)$$
$$+\frac{1}{2}\Big(\psi_1\Big(v_1^{i+2} - v_1^{i+1}\Big) + \psi_1\Big(v_1^{i+1} - v_1^i\Big)\Big) - \psi_0(\alpha_1)\Big)$$
$$\leq B_+(\mathbf{u}'(0),\varphi(0)) + \eta,$$

$$\frac{1}{2}\psi_1(v^0_{j,j+1} - v^{-1}_{j,j+1}) + \sum_{i\leq -1}\Big(\psi_2\Big(\frac{v^{i+2}_{j,j+1} - v^i_{j,j+1}}{2}\Big)$$
$$+\frac{1}{2}\Big(\psi_1\Big(v^{i+2}_{j,j+1} - v^{i+1}_{j,j+1}\Big) + \psi_1\Big(v^{i+1}_{j,j+1} - v^i_{j,j+1}\Big)\Big) - \psi_0\Big(\frac{z_1^{\alpha_j} + z_2^{\alpha_j}}{2}\Big)\Big)$$
$$+\frac{1}{2}\psi_1(v^1_{j,j+1} - v^0_{j,j+1}) + \sum_{i\geq 0}\Big(\psi_2\Big(\frac{v^{i+2}_{j,j+1} - v^i_{j,j+1}}{2}\Big)$$
$$+\frac{1}{2}\Big(\psi_1\Big(v^{i+1}_{j,j+1} - v^i_{j,j+1}\Big) + \psi_1\Big(v^{i+1}_{j,j+1} - v^i_{j,j+1}\Big)\Big) - \psi_0\Big(\frac{z_1^{\alpha_{j+1}} + z_2^{\alpha_{j+1}}}{2}\Big)\Big)$$
$$\leq C(\mathbf{u}'(x_j-),\mathbf{u}'(x_j+),\varphi(x_j)) + \eta,$$

$$\frac{1}{2}\psi_1(v_M^1 - v_M^0) + \sum_{i\leq 0}\Big(\psi_2\Big(\frac{v_M^i - v_M^{i-2}}{2}\Big)$$
$$+\frac{1}{2}\Big(\psi_1\Big(v_M^i - v_M^{i-1}\Big) + \psi_1\Big(v_M^{i-1} - v_M^{i-2}\Big)\Big) - \psi_0(\alpha_M)\Big)$$
$$\leq B_-(\mathbf{u}'(1),\varphi(1)) + \eta.$$

Consider the sequence of functions $(\mathbf{u}_n)$ defined as follows

$$\mathbf{u}_n^i = \begin{cases} \lambda_n \mathbf{v}_1^i & \text{if } 0 \le i \le [x_1 n] - N, \\ \lambda_n \mathbf{v}_{j,j+1}^{i-[x_j n]} + \lambda_n D_j & \text{if } [x_j n] - N \le i \le [x_{j+1} n] - N \\ & j \in \{1, 2, \ldots, M-1\}, \\ \lambda_n \mathbf{v}_M^{i-n} + \lambda_n D_M & \text{if } n - N \le i \le n-1, \\ 0 & \text{if } i = n, \end{cases}$$

where

$$\begin{aligned} D_1 &= -u_{\mathbf{Z}^{\alpha_1}}(-N) + u_{\mathbf{Z}^{\alpha_1}}([x_1 n] - N), \\ D_j &= -\sum_{k=1}^{j-1} u_{\mathbf{Z}^{\alpha_k}}(-N) + \sum_{k=1}^{j} u_{\mathbf{Z}^{\alpha_k}}([x_k n] - \sum_{h=1}^{j-1} [x_h n] - N) \quad j \in \{2, 3, \ldots, M\}. \end{aligned}$$

Then $\mathbf{u}_n \to \mathbf{u}$ in L^∞ and

$$\begin{aligned} E(u_n) \le\ & B_+(\mathbf{u}'(0), \varphi(0)) + \sum_{j=1}^{M-1} C(\mathbf{u}'(x_j-), \mathbf{u}'(x_j+), \varphi(x_j)) + B_-(\mathbf{u}'(1), \varphi(1)) \\ & + \tilde{R}_n + c\eta, \end{aligned} \tag{3.21}$$

where

$$\begin{aligned} \tilde{R}_n =\ & \psi_2\Big(\frac{v_M^0 - v_M^{-2}}{2}\Big) + \frac{1}{2}\Big(\psi_1(v_M^0 - v_M^{-1}) + \psi_1(v_M^{-1} - v_M^{-2})\Big) \\ & -\psi_0\Big(\frac{v_M^0 - v_M^{-2}}{2}\Big) - \psi_2\Big(\frac{u_n^n - u_n^{n-2}}{2\lambda_n}\Big) - \frac{1}{2}\Big(\psi_1(\frac{u_n^n - u_n^{n-1}}{\lambda_n}) \\ & +\psi_1(\frac{u_n^{n-1} - u_n^{n-2}}{\lambda_n})\Big) + \psi_0\Big(\frac{u_n^n - u_n^{n-2}}{2\lambda_n}\Big) \end{aligned}$$

and, by the continuity of ψ_1, ψ_2 and ψ_0, $\tilde{R}_n \to 0$. Thanks to (3.20) and (3.21) we have that

$$\limsup_n E_n(u_n) \le E^{1,l}_{even}(\mathbf{u}) + c\eta + \varepsilon.$$

We obtain the thesis thanks to the arbitrariness of η and ε. □

Remark 3.8 In the case that ψ_1, ψ_2 are such that $\psi_0 \in C^1(\mathbb{R})$ then, thanks to Remark 2.2, the first order Γ-limit has no shift minimization formula:

(Case n even)

$$E^{1,l}_{even}(\mathbf{u}) = \begin{cases} \sum_{t \in S(\mathbf{u}')} C(\mathbf{u}'(t-), \mathbf{u}'(t+)) + B_+(\mathbf{u}'(0)) + B_-(\mathbf{u}'(L)), \\ \qquad \text{if } \mathbf{u}' \in PC(0,L),\ \mathbf{u}' \in \mathbf{M}_l,\ u_1(L) + u_2(L) = 2l, \\ +\infty \qquad \text{otherwise}, \end{cases}$$

(Case n odd)

$$E^{1,l}_{odd}(\mathbf{u}) = \begin{cases} \sum_{t \in S\mathbf{u}'} C(\mathbf{u}'(t-), \mathbf{u}'(t+)) + B_+(\mathbf{u}'(0)) + B_-(\overline{\mathbf{u}'(L)}), \\ \qquad \text{if } \mathbf{u}' \in PC(0,L),\ \mathbf{u}' \in \mathbf{M}_l,\ u_1(L) + u_2(L) = 2l, \\ +\infty \qquad \text{otherwise}. \end{cases}$$

Remark 3.9 In the case that

$$\#\mathbf{M}^{\alpha} = 1 \qquad \text{for all } \alpha \in \mathbb{R} \text{ such that } \psi_0(\alpha) = \psi_0^{**}(\alpha),$$

then, by Remark 2.1, the first order Γ-limit does not depend on the parity of the lattice, or, in formula,

$$E^{1,l}(u) = \inf \Big\{ E^{1,l}(u,s): \; s: S(u') \cup \{0,L\} \to \mathbb{R}, \sum_{t \in S(u') \cup \{0,L\}} s(t) = l \Big\}$$

where

$$E^{1,l}(u,s) = \begin{cases} \sum_{t \in S(u')} C(u'(t-), u'(t+), s(t)) + B_+(u'(0), s(0)) + B_-(u'(L), s(L)), \\ \qquad\qquad \text{if } u' \in PC(0,L),\ (u',u') \in \mathbf{M}_l,\ u(0)=0,\ u(L)=l, \\ +\infty \qquad\quad \text{otherwise.} \end{cases}$$

The Γ-limit in the periodic case is similar to that with Dirichlet boundary conditions, except for the absence of boundary terms. Note that in the case of odd interactions non-uniform minimal-energy configurations are not admissible test functions, and hence phase transitions may be forced by the periodicity constraints.

Theorem 3.10 (First-order Γ-limit - Periodic boundary data) *Suppose that hypotheses* [H1]–[H4] *and* [H6] *hold and let* $E^{\#,l}_{1,n} : \mathcal{A}^{\#,l}_n(0,L) \to [0,+\infty]$ *be defined by*

$$E^{\#,l}_{1,n}(u) = \frac{E^{\#,l}_n(u) - \min E^{\#,l}}{\lambda_n}. \tag{3.22}$$

We then have:

(Case n even) $E^{\#,l}_{1,n}$ *Γ-converges with respect to the* $L^\infty_{\rm loc}$*-topology to*

$$E^{\#,l}_1(\boldsymbol{u}) = \begin{cases} \sum_{t \in S(\boldsymbol{u}') \cap [0,L)} C(\boldsymbol{u}'(t-), \boldsymbol{u}'(t+)), & \text{if } \boldsymbol{u}' \in PC_{\rm loc}(\mathbb{R}),\ \boldsymbol{u}' \in \boldsymbol{M}_l, \\ & u(t) - lt \text{ is } L\text{-periodic}, \\ +\infty & \text{otherwise} \end{cases}$$

on $W^{1,\infty}_{\rm loc}(\mathbb{R})$ *and* $u_1'(0+) = u_1'(L+)$ *and* $u_2'(0+) = u_2'(L+)$.

(Case n odd) *The same results hold but* $u_1'(0+) = u_2'(L+)$ *and* $u_2'(0+) = u_1'(L+)$.

Proof. Since the Γ-liminf and the Γ-limsup inequalities are easily deducible from the proof of Theorem 3.7, we will only prove the compactness result.

In the following, without loss of generality, we suppose $L=1$, n even and $l \in J_j$ for some j. Moreover, with the same notation of the previous proposition, we define r_j to be the straight line such that $\psi_0^{**}(x) = r_j(x)$ for all $x \in J_j$. Let $u_n \to \mathbf{u}$ in $L^\infty_{\rm loc}(\mathbb{R})$ be such that $\sup_n E^{\#,l}_{1,n}(u_n) < +\infty$. By the definition of $E^{\#,l}_{n,1}$, we have that u_n is such that $\sup_n E^{\#,l}_n(u_n) < +\infty$, and then, as in Theorem 3.4,

$$\frac{u_1(t) + u_2(t)}{2} - lt = u(t) - lt \text{ is 1-periodic.}$$

Thanks to the periodicity assumption, we have that

$$\frac{u_n^{n+1}-u_n^n}{\lambda_n}=\frac{u_n^1-u_n^0}{\lambda_n}$$

and then

$$\begin{aligned}
+\infty > E_{n,1}^{\#,l}(u_n) &= \sum_{i=0}^{n-1}\Big(\psi_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big)+\psi_2\Big(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\Big)-\psi_0^{**}(l)\Big)\\
&= \sum_{i=0}^{n-1}\Big(\psi_2\Big(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\Big)\\
&\quad +\frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\Big)+\psi_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big)\Big)-\psi_0^{**}(l)\Big)\\
&= \sum_{i=0}^{n-1}\mathcal{E}_n^i(u_n) \qquad (3.23)
\end{aligned}$$

where

$$\mathcal{E}_n^i(u_n)=\psi_2\Big(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\Big)+\frac{1}{2}\Big(\psi_1\Big(\frac{u_n^{i+2}-u_n^{i+1}}{\lambda_n}\Big)+\psi_1\Big(\frac{u_n^{i+1}-u_n^i}{\lambda_n}\Big)\Big)-r_j\Big(\frac{u_n^{i+2}-u_n^i}{2\lambda_n}\Big).$$

Thanks to (3.23) we can deduce, as in the proof of Proposition 3.5, that there exists $S\subset(0,1]$ with $\#(S)<+\infty$ such that, up to subsequences, $u_n\to\mathbf{u}$ in $W^{1,\infty}_{\rm loc}(\mathbb{R}\setminus(S+k))$, $k\in\mathbb{Z}$ and that $\mathbf{u}'\in\mathbf{M}_l$. By the definition of even and odd interpolations, thanks to the periodicity hypothesis, we have

$$\begin{aligned}
\frac{u_{1,n}^1-u_{1,n}^0}{\lambda_n}&=\frac{u_n^1-u_n^0}{\lambda_n}=\frac{u_n^{n+1}-u_n^n}{\lambda_n}=\frac{u_{1,n}^{n+1}-u_{1,n}^n}{\lambda_n},\\
\frac{u_{2,n}^1-u_{2,n}^0}{\lambda_n}&=\frac{u_n^2-u_n^1}{\lambda_n}=\frac{u_n^{n+2}-u_n^{n+1}}{\lambda_n}=\frac{u_{2,n}^{n+1}-u_{2,n}^n}{\lambda_n}.
\end{aligned}$$

Passing to the limit in the previous expressions we get that $u_1'(0+)=u_1'(1+)$ and $u_2'(0+)=u_2'(1+)$. □

Remark 3.11 We observe that, in contrast with Theorem 3.7, here, the absence of boundary layer terms in the limit, allowed us to skip hypothesis [H5] to obtain inequality (3.23).

Remark 3.12 Note that in the case n is odd, if $\mathbf{u}'\equiv(z_1,z_2)$ in $(0,L)$ with $z_1\neq z_2$, then $kL\in S(\mathbf{u}')$ for all $k\in\mathbb{Z}$.

4 Γ-convergence for Lennard-Jones type densities

In this section we deal with the zero- and first-order Γ-limit, under periodic and Dirichlet boundary conditions, of energies H_n of the form

$$H_n(u)=\sum_{i=0}^{n-1}\lambda_n J_1\Big(\frac{u^{i+1}-u^i}{\lambda_n}\Big)+\sum_{i=0}^{n-2}\lambda_n J_2\Big(\frac{u^{i+2}-u^i}{2\lambda_n}\Big),$$

where J_1 and J_2 are Lennard-Jones type potentials. Our model case being the standard $(6,12)$ Lennard-Jones potential, we will treat more general energy densities. With the same notation of the previous section we define $H_n^{\#,l}(u) : \mathcal{A}_n(\mathbb{R}) \to [0,+\infty]$ as

$$H_n^{\#,l}(u) = \begin{cases} H_n(u) & \text{if } u \in \mathcal{A}_n^{\#,l}(0,L) \\ +\infty & \text{otherwise} \end{cases}$$

and $H_n^l(u) : \mathcal{A}_n(0,L) \to [0,+\infty]$ as

$$H_n^l(u) = \begin{cases} H_n(u) & \text{if } u(0)=0,\ u(L)=l \\ +\infty & \text{otherwise.} \end{cases} \tag{4.1}$$

We also set

$$\begin{aligned} J_0(z) &= J_2(z) + \frac{1}{2}\inf\{J_1(z_1)+J_1(z_2) :\ z_1+z_2=2z\}, \\ BV^{\#,l}(0,L) &= \{u \in BV_{\text{loc}}(\mathbb{R}) :\ u(t)-lt \text{ is } L \text{ periodic}\}, \\ BV^l(0,L) &= \{u \in BV(0,L) :\ u(0+)=0,\ u(L-)=l\}, \end{aligned}$$

and use the analogous notation for SBV spaces.

Adapting the proof of Theorem 3.2 in [12] it is possible to prove the following two theorems which are the analogue of Theorem 3.4 and Theorem 3.1.

Theorem 4.1 (Zero order Γ-limit - Periodic boundary data) *Let $\psi_j : \mathbb{R} \to (-\infty,+\infty]$ be Borel functions bounded below. Suppose that there exists a convex function $\Psi : \mathbb{R} \to [0,+\infty]$ such that*

$$\lim_{z\to-\infty} \frac{\Psi(z)}{|z|} = +\infty$$

and there exist constants $c_1,\ c_2 > 0$ such that

$$c_1(\Psi(z)-1) \le J_j(z) \le c_2 \max\{\Psi(z),|z|\} \quad \text{for all } z \in \mathbb{R}, \quad j=1,2,$$

then the Γ-limit of $H_n^{\#,l}$ with respect to the L^1_{loc}-topology is given by

$$H^{\#,l}(u) = \begin{cases} \displaystyle\int_0^L J_0^{**}(u'(t))\,dt & \text{if } u \in BV^{\#,l}(0,L),\ D^s u > 0 \\ +\infty & \text{otherwise} \end{cases}$$

on $L^1_{\text{loc}}(\mathbb{R})$, where $D^s u$ denotes the singular part of the measure Du with respect to the Lebesgue measure.

Theorem 4.2 (Zero order Γ-limit - Dirichlet boundary data) *Let $\psi_j : \mathbb{R} \to (-\infty,+\infty]$ be Borel functions bounded below satisfying the same conditions as in the previous theorem; then the Γ-limit of H_n^l with respect to the L^1_{loc}-topology is given by*

$$H^l(u) = \begin{cases} \displaystyle\int_0^L J_0^{**}(u'(t))\,dt & \text{if } u \in BV^l(0,L),\ D_s u > 0 \\ +\infty & \text{otherwise} \end{cases}$$

on $L^1(0,L)$.

In the same spirit of Section 3.2, we now deal with the problem of computing the first order $\Gamma-$limit of H_n in order to describe boundary layer phenomena in the continuum limit. The following set of hypotheses makes clear what kind of Lennard-Jones type potentials we will consider in this case:

$[H1]_{LJ}$(*discreteness of the energy states*)

$$\#(\{x \in \mathbb{R} : J_0(x) = J_0^{**}(x)\} \cap \{x \in \mathbb{R} : J_0 \text{ is affine}\}) < +\infty,$$

$[H2]_{LJ}$ (*finiteness of minimal energy configurations*) for every $\alpha \in \mathbb{R}$ such that $J_0(\alpha) = J_0^{**}(\alpha)$

$$\#\mathbf{M}^\alpha < +\infty,$$

$[H3]_{LJ}$ (*compatibility of minimal energy configurations*) for every $\alpha,\ \beta \in \mathbb{R}$ with $\alpha \neq \beta$, such that $J_0(\alpha) = J_0^{**}(\alpha)$ and $J_0(\beta) = J_0^{**}(\beta)$ and for every $\mathbf{z}^\alpha = (z_1^\alpha, z_2^\alpha) \in \mathbf{M}^\alpha$ and $\mathbf{z}^\beta = (z_1^\beta, z_2^\beta) \in \mathbf{M}^\beta$ it holds

$$z_i^\alpha \neq z_j^\beta \quad i, j \in \{1, 2\},$$

$[H4]_{LJ}$ (*continuity and growth conditions*) $J_1,\ J_2\ : \mathbb{R} \to (-\infty, +\infty]$ are sufficiently smooth functions bounded below such that $J_0 \in C^1(\mathbb{R})$ and there exists a convex function $\Psi : \mathbb{R} \to [0, +\infty]$ and constants $c_1,\ c_2 > 0$ such that

$$\lim_{z \to -\infty} \frac{\Psi(z)}{|z|} = +\infty,$$

and

$$c_1(\Psi(z) - 1) \leq J_j(z) \leq c_2 \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}, \quad j = 1, 2;$$

$[H5]_{LJ}$ (*structure of* $J_1,\ J_2$ *and* J_0) the following limits exist:

$$\lim_{z \to +\infty} J_1(z) = J_1(+\infty), \quad \lim_{z \to +\infty} J_2(z) = J_2(+\infty) \quad \lim_{z \to +\infty} J_0(z) = J_0(+\infty),$$

$J_0(z) = \min J_0$ if and only if $z = \gamma$, and $J_0(+\infty) > J_0(\gamma)$;

$[H6]_{LJ}$ (*finiteness of the intervals of non-convexity*) l is such that $N(l) < +\infty$ ($N(l)$ defined as in (2.3)).

The following compactness result will be used in proving Theorem 4.4. It describes functions with $H_n^{\#,l}(u_n) = \min H^{\#,l} + O(\lambda_n)$, stating that below the threshold γ they behave as in the Sobolev case and develop no discontinuity. Above the threshold they may develop a finite number of discontinuities, behaving otherwise as in the Sobolev case with periodic condition corresponding to γ.

Proposition 4.3 (Compactness - Periodic boundary data) *Suppose that hypotheses* $[H1]_{LJ}$–$[H6]_{LJ}$ *hold. If* $\{u_n\}$ *is a sequence of functions such that*

$$\sup_n H_{1,n}^{\#,l}(u_n) = \sup_n \frac{H_n^{\#,l}(u_n) - \min H^{\#,l}}{\lambda_n} < +\infty \tag{4.2}$$

and there exists $t \in [0, L)$ *such that* $\sup_n |u_n(t)| < +\infty$*, then, up to subsequences,* $u_n \to \boldsymbol{u}$ *strongly in* $L^1_{\text{loc}}(\mathbb{R})$ *where* $\boldsymbol{u} \in SBV^{\#,l}(0, L)$ *is such that*

(i) $\#(S(\boldsymbol{u}) \cap [0, L)) < +\infty$. *In particular*

(a) *if* $l \leq \gamma$ *then* $S(\boldsymbol{u}) = \emptyset$,

(b) *if* $l > \gamma$ *then* $0 < \#(S(\boldsymbol{u}) \cap [0, L)) < +\infty$,

(ii) $[\boldsymbol{u}_s(t)] > 0 \quad s = 1, 2 \quad$ *for all* $t \in S(\boldsymbol{u})$,

(iii) $\#(S(\boldsymbol{u}') \cap [0, L)) < +\infty$,

(iv) $\boldsymbol{u}'(t) \in \boldsymbol{M}_l$ *a.e.* $t \in (0, L)$. *In particular*

(a) *if* $l \leq \gamma$ *then* $\boldsymbol{u}'(t) \in \boldsymbol{M}^{\frac{l}{L}}$,

(b) *if* $l > \gamma$ *then* $\boldsymbol{u}'(t) \in \boldsymbol{M}^{\gamma}$.

PROOF. To fix the ideas let us suppose that $u_n(0) = 0$ and that $L = 1$. Let us observe that (4.2) implies that

$$\sup_n H_n^{\#,l}(u_n) \leq C < +\infty. \tag{4.3}$$

With the notation so far used, let us set $\mathbf{u}_n = (u_{n,1}, u_{n,2})$. Since if $u_{n,1} = u_{n,2}$ it is possible to prove that $u_n \to u$ strongly in $L^1_{loc}(\mathbb{R})$ and that $u \in SBV^{\#,l}(0, L)$ repeating the same proof of Theorem 3.7 in [13] first and then using Theorem 3.1 in [13], we only sketch this part of the proof. For all $n \in \mathbb{N}$, let $T_n \in \mathbb{R}$ be such that $\lim_n T_n = +\infty$, $\lim_n \lambda_n T_n = 0$ and set $I_n := \{i \in \{0, 1, \ldots, n-1\} : \ |u_n^{i+1} - u_n^i| > \lambda_n T_n\}$. Let w_n be defined as

$$w_n(t) = \begin{cases} 0 & \text{if } t = 0 \\ u_n(t) & \text{if } t \in (i, i+1)\lambda_n,\ i \notin I_n \\ u_n(i\lambda_n) & \text{if } t \in (i, i+1)\lambda_n,\ i \in I_n \end{cases}$$

and let $v_n(t)$ be an extension of $w_n(t)$ given by the following formula $v_n(t + k) = w_n(t) + kl$ for all $k \in \mathbb{Z}$. By (4.3), thanks to the growth hypotheses, by arguing as in [13] (Theorem 3.7), we have that $\|v_n\|_{BV_{loc}(\mathbb{R})} \leq C$. Then, up to subsequences not relabelled, $v_n \to u$ strongly in $L^1_{loc}(\mathbb{R})$. The same holds true for u_n since, by construction, for all compact sets $K \subset \mathbb{R}$, $\lim_n \int_K |u_n(t) - v_n(t)|\, dt = 0$. Set

$$\mathcal{H}_n^1(u_n) = \sum_{i=0}^{n-2} \Big(J_0\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) - J_0(\gamma)\Big), \tag{4.4}$$

by (4.2) we have that $\sup_n \mathcal{H}_n^1(u_n) \leq C < +\infty$. Let us set $\mathbf{v}_n^i = \mathbf{u}_n^i - i\lambda_n \mathbf{z}^\gamma$ and $\tilde{J}_0(z) = J_0(z + \gamma) - J_0(\gamma)$. We have that the sequence of functionals $\mathcal{H}_n^1$ satisfies all the hypotheses of Theorem 3.1 in [13] which implies in particular that $u \in SBV^{\#,l}(0, L)$. In the general case, when $u_{n,1}(t) \neq u_{n,2}(t)$ for some $t \in [0, 1)$, the previous argument need to be modified in order to prove the convergence of even and odd interpolator functions independently. In this case, observing that $H_n^{\#,l}(u_n) = \frac{1}{2} \sum_{s=1}^{2} \mathcal{E}_{n,s}^{\#,l}(u_{n,s})$, where

$$\mathcal{E}_{n,s}^{\#,l}(u_{n,s}) = \sum_{i=0}^{n-1} \lambda_n J_1\Big(\frac{u_{n,s}^{i+1} - u_{n,s}^i}{\lambda_n}\Big) + \sum_{i=0}^{n-2} \lambda_n J_2\Big(\frac{u_{n,s}^{i+2} - u_{n,s}^i}{2\lambda_n}\Big),$$

we get

$$\sup_n \mathcal{E}^{\#,l}_{n,s}(u_{n,s}) \leq C < +\infty. \tag{4.5}$$

Thus the convergence to $\mathbf{u} \in SBV^{\#,l}(0,L)$ can be now easily proved using the argument we have exploited before independently for $s = 1, 2$. By (4.5) and Theorem 4.1 we also get *(ii)*. The proof of (iii) and (iv) can be obtained arguing as in the proof of Theorem 3.7. Let us prove (ii) in case (a). If $l < \gamma$ then, thanks to the hypothesis $[H5]_{LJ}$ on J_0, we have that for all $p \in \partial J_0^{**}(l)$ $\lim_{|z|\to+\infty} J_0(z) - pz = +\infty$ and the claim follows again arguing as in the proof of Theorem 3.10. If $l = \gamma$, by the boundary conditions and (iv), $u(t) = \frac{u_1(t)+u_2(t)}{2} = \gamma t$ *a.e.* $t \in (0,1)$, thus $S(u) \cap [0,1) = \emptyset$. This, together with (i), for $s = 1, 2$, implies that $S(u_s) \cap [0,1) = \emptyset$ and then the claim follows by the definition of $S(\mathbf{u})$.

Let us prove (ii) in the case (b). Arguing as in the proof of Theorem 3.7, set

$$\mathcal{H}^1_n(u_{s,n}) = \sum_{i=0}^{n-2} \Big(J_0\Big(\frac{u^{i+2}_{s,n} - u^i_{s,n}}{2\lambda_n}\Big) - J_0(\gamma)\Big), \tag{4.6}$$

by (4.2) we have that $\sup_n \mathcal{H}^1_n(u_{s,n}) \leq C < +\infty$. Let us set $\mathbf{v}^i_n = \mathbf{u}^i_n - i\lambda_n \mathbf{z}^\gamma$ and $\tilde{J}_0(z-\gamma) = J_0(z) - J_0(\gamma)$. Observing that $\mathbf{M}_l = \mathbf{M}^\gamma$, $\mathbf{v}_n \to \mathbf{u} - t\mathbf{z}^\gamma$ strongly in $L^1_{\mathrm{loc}}(\mathbf{R})$. Thus, by Theorem 3.1 in [14], for $s = 1, 2$ we have

$$\begin{aligned} C \geq \liminf_n \mathcal{H}^1_n(u_{s,n}) &= \liminf_n \sum_{i=0}^{n-2} \tilde{J}_0\Big(\frac{v^{i+2}_{s,n} - v^i_{s,n}}{2\lambda_n}\Big) \\ &\geq \int_{(0,1)} F(u'_s(t))\,dt + \sum_{t \in S(u_s)\cap(0,1)} G([u_s](t), \end{aligned} \tag{4.7}$$

where

$$F(z) = \begin{cases} 0 & \text{if } z = \gamma \\ +\infty & \text{otherwise} \end{cases}$$

and

$$G(w) = \begin{cases} J_0(+\infty) - J_0(\gamma) & \text{if } w > 0 \\ 0 & \text{if } w = 0 \\ +\infty & \text{if } w < 0. \end{cases}$$

By (4.7) and hypothesis $[H5]_{LJ}$ we finally get that

$$\#S(\mathbf{u}) = \# \bigcup_{s=1}^{2} S(u_s) \leq C < +\infty.$$

The Γ-limit described below takes into account both phase transitions and discontinuities. Note that the energy of a discontinuity takes into account boundary layers on both sides of the jump. For simplicity of notation we define

$$SBV^{\#,l}_c(0,L) = \{\mathbf{u} \in SBV^{\#,l}(0,L) : \text{ (i)-(iv) of Proposition 4.3 hold}\}. \tag{4.8}$$

Theorem 4.4 (First order Γ-limit - Periodic boundary data) *Suppose that hypotheses $[H1]_{LJ} - [H6]_{LJ}$ hold and let $H^{\#,l}_{1,n} : \mathcal{A}^{\#,l}_n(0,L) \to [0,+\infty]$ be defined by*

$$H^{\#,l}_{1,n}(u) = \frac{H^{\#,l}_n(u) - \min H^{\#,l}}{\lambda_n}. \tag{4.9}$$

We then have:

(Case n even)

(i) *if* $l \le \gamma$

$H^{\#,l}_{1,n}$ *Γ-converges with respect to the L^∞_{loc}-topology to*

$$H^{\#,l}_1(\boldsymbol{u}) = \begin{cases} \sum\limits_{t\in S(\boldsymbol{u}')\cap[0,L)} C(\boldsymbol{u}'(t-),\boldsymbol{u}'(t+)), & \text{if } \boldsymbol{u} \in SBV^{\#,l}_c(0,L), \\ +\infty & \text{otherwise} \end{cases}$$

on $W^{1,\infty}_{\mathrm{loc}}(\mathbf{R})$, where $SBV^{\#,l}_c(0,L)$ is defined in (4.8), and $u_1'(0+) = u_1'(L+)$ and $u_2'(0+) = u_2'(L+)$.

(ii) *if* $l > \gamma$

$H^{\#,l}_{1,n}$ *Γ-converges with respect to the L^1_{loc}-topology to*

$$H^{\#,l}_1(\boldsymbol{u}) = \begin{cases} \sum\limits_{t\in S(\boldsymbol{u}')\setminus S(\boldsymbol{u})\cap[0,L)} C(\boldsymbol{u}'(t-),\boldsymbol{u}'(t+)) + \sum\limits_{t\in S(\boldsymbol{u})\cap[0,L)} B_J(\boldsymbol{u}'(t-),\boldsymbol{u}'(t+)), \\ \qquad\qquad \text{if } \boldsymbol{u} \in SBV^{\#,l}_c(0,L), \\ +\infty \qquad\qquad \text{otherwise} \end{cases}$$

on $L^1_{\mathrm{loc}}(\mathbf{R})$ where

$$B_J(\boldsymbol{z},\boldsymbol{z}') = B_+(\boldsymbol{z}) + B_-(\boldsymbol{z}') - 2J_0(\gamma) + 2J_2(+\infty) + J_1(+\infty)$$

and $u_1'(0+) = u_1'(L+)$ and $u_2'(0+) = u_2'(L+)$.

(Case n odd) *The same results hold but $u_1'(0+) = u_2'(L+)$ and $u_2'(0+) = u_1'(L+)$.*

Proof. Since the proof is similar to that of Theorem 3.10, we only highlight the main differences in the case $l > \gamma$ proving the Γ-liminf inequality for the second term in the energy.

In the following we will suppose that $L = 1$ and n is even. Let $u_n \to \mathbf{u}$ in $L^1_{\mathrm{loc}}(\mathbf{R})$ be such that $\sup_n H^{\#,l}_{1,n}(u_n) < +\infty$. Then, thanks to Proposition 4.3 and to the translation invariance of the energies, without loss of generality, we can further suppose that

$$\mathbf{u}(0) = 0, \quad \mathbf{u}(1) = l, \qquad S(\mathbf{u}) \cap [0,1) = S(\mathbf{u}') \cap [0,1) = \{\bar{t}\}.$$

Let $\mathbf{z}^\gamma_1,\ \mathbf{z}^\gamma_2 \in \mathbf{M}^\gamma$ be such that

$$\mathbf{u}'(\bar{t}-) = \mathbf{z}^\gamma_1, \quad \mathbf{u}'(\bar{t}+) = \mathbf{z}^\gamma_2$$

and let $\{h_n\}_n$ be a sequence of indices such that,

$$\lambda_n h_n \leq \bar{t} \quad \text{and} \quad \lim_n \lambda_n h_n = \bar{t}. \tag{4.10}$$

It is convenient to rewrite the energy as follows

$$\begin{aligned} H_{1,n}^{\#,l}(u_n) &= \mathcal{H}_n(u_n, h_n-) + \mathcal{H}_n(u_n, h_n+) + J_2\Big(\frac{u_n^{h_n+1} - u_n^{h_n-1}}{2\lambda_n}\Big) \\ &+ J_2\Big(\frac{u_n^{h_n+2} - u_n^{h_n}}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\Big) - 2J_0(\gamma), \end{aligned} \tag{4.11}$$

where

$$\begin{aligned} \mathcal{H}_n(u_n, h_n-) &= \sum_{i=0}^{h_n-2} \Big(J_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - J_0(\gamma)\Big) \\ &\quad + J_1\Big(\frac{u_n^{h_n} - u_n^{h_n-1}}{\lambda_n}\Big) \end{aligned}$$

and

$$\begin{aligned} \mathcal{H}_n(u_n, h_n+) &= \sum_{i=h_n+1}^{n-2} \Big(J_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - J_0(\gamma)\Big) \\ &\quad + J_1\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big) - J_0(\gamma). \end{aligned}$$

Defining

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \dfrac{\mathbf{u}_n^{i+h_n+1}}{\lambda_n} & \text{if } 0 \leq i \leq n - h_n - 1 \\ \dfrac{\mathbf{u}_n^n}{\lambda_n} + u_{\mathbf{z}_2^\gamma}(i) - u_{\mathbf{z}_2^\gamma}(n - h_n - 1) & \text{if } i \geq n - h_n - 1, \end{cases}$$

by the continuity of J_1 and J_2, we can find a suitable continuous function $\omega(\varepsilon) : \mathbf{R} \to \mathbf{R}$, $\omega(0) = 0$ such that,for all $\varepsilon > 0$, as $\tilde{\mathbf{u}}_n^i$ is a test function for the minimum problem defining $B_+(\mathbf{z}_2^\gamma)$, for n large enough we have

$$\begin{aligned} \mathcal{H}_n(u_n, h_n+) &= \frac{1}{2} J_1(\tilde{u}_n^1 - \tilde{u}_n^0) + \sum_{i\geq 0} \Big(J_2\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big) \\ &\quad + \frac{1}{2}\Big(J_1\Big(\tilde{u}_n^{i+2} - \tilde{u}_n^{i+1}\Big) + J_1\Big(\tilde{u}_n^{i+1} - \tilde{u}_n^i\Big)\Big) - J_0(\gamma)\Big) + \omega(\varepsilon) \\ &\geq B_+(\mathbf{z}_2^\gamma) + \omega(\varepsilon). \end{aligned} \tag{4.12}$$

Analogously, defining

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \dfrac{\mathbf{u}_n^0}{\lambda_n} + u_{\mathbf{z}_1^\gamma}(i) - u_{\mathbf{z}_1^\gamma}(-h_n) & \text{if } i \leq -h_n, \\ \dfrac{\mathbf{u}_n^{i+h_n}}{\lambda_n} & \text{if } -h_n \leq i \leq 0, \end{cases}$$

we have,

$$\begin{aligned}\mathcal{H}_n(u_n, h_n-) &= \frac{1}{2}J_1(\tilde{u}_n^0 - \tilde{u}_n^{-1}) + \sum_{i\le 0}\Big(J_2\Big(\frac{\tilde{u}_n^i - \tilde{u}_n^{i-2}}{2}\Big) \\ &\quad + \frac{1}{2}\Big(J_1\Big(\tilde{u}_n^i - \tilde{u}_n^{i-1}\Big) + \Big(\tilde{u}_n^{i-1} - \tilde{u}_n^{i-2}\Big)\Big) - J_0(\gamma)\Big) + \omega(\varepsilon) \\ &\ge B_-(\mathbf{z}_1^\gamma) + \omega(\varepsilon). \end{aligned} \tag{4.13}$$

Thanks to inequalities (4.12), (4.13) and formula (4.11), we get

$$\begin{aligned} H_{1,n}^{\#,l}(u_n) &\ge J_2\Big(\frac{u_n^{h_n+1} - u_n^{h_n-1}}{2\lambda_n}\Big) + J_2\Big(\frac{u_n^{h_n+2} - u_n^{h_n}}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{h_n+1} - u_n^{h_n}}{\lambda_n}\Big) \\ &\quad -2J_0(\gamma) + B_-(\mathbf{z}_1^\gamma) + B_+(\mathbf{z}_2^\gamma) + c\,\omega(\varepsilon). \end{aligned}$$

By (4.10), the definition of $\bar{t}$ and hypothesis $[H5]_{LJ}$, we have

$$\begin{aligned} \liminf_n H_{1,n}^{\#,l}(u_n) &\ge 2J_2(+\infty) + J_1(+\infty) - 2J_0(\gamma) + B_-(\mathbf{z}_1^\gamma) + B_+(\mathbf{z}_2^\gamma) + c\omega(\varepsilon) \\ &= B_J(\mathbf{u}'(\bar{t}-), \mathbf{u}'(\bar{t}+)) + c\,\omega(\varepsilon). \end{aligned}$$

The claim follows by the arbitrariness of ε.

Slightly modifying the construction made in the proof of Γ-limsup inequality in Theorem 3.7, it can be proven that this bound is optimal. □

We find useful to set

$$\tilde{\mathbf{u}}(t) = \begin{cases} \mathbf{u}(0+) & \text{if } t = 0 \\ \mathbf{u}(t) & \text{if } t \in (0, L) \\ \mathbf{u}(L-) & \text{if } t = L. \end{cases} \tag{4.14}$$

The proof of the following result can be straightly derived by that of Proposition 4.3.

Proposition 4.5 (Compactness - Dirichlet boundary data) *Suppose that hypotheses $[H1]_{LJ}$–$[H6]_{LJ}$ hold. If $\{u_n\}$ is a sequence of functions such that*

$$\sup_n H_{1,n}^l(u_n) = \sup_n \frac{H_n^l(u_n) - \min H^l}{\lambda_n} < +\infty, \tag{4.15}$$

then, up to subsequences, $u_n \to \boldsymbol{u}$ strongly in $L^1_{\rm loc}(0, L)$ where $\boldsymbol{u} \in SBV^l(0, L)$ is such that

(i) $\#S(\tilde{\boldsymbol{u}}) < +\infty$ *($\tilde{\boldsymbol{u}}$ defined in (4.14)). In particular*

  (a) *if $l \le \gamma$ then $S(\tilde{\boldsymbol{u}}) = \emptyset$,*

  (b) *if $l > \gamma$ then $0 < \#(S(\tilde{\boldsymbol{u}})) < +\infty$,*

(ii) $[\tilde{\boldsymbol{u}}_s(t)] > 0 \quad s = 1, 2 \quad$ *for all $t \in S(\boldsymbol{u})$,*

(iii) $\#(S(\boldsymbol{u}')) < +\infty$,

(iv) $\boldsymbol{u}'(t) \in \boldsymbol{M}_l$ *a.e.* $t \in (0, L)$. *In particular*

   (a) *if* $l \leq \gamma$ *then* $\boldsymbol{u}'(t) \in \boldsymbol{M}^{\frac{l}{L}}$,

   (b) *if* $l > \gamma$ *then* $\boldsymbol{u}'(t) \in \boldsymbol{M}^{\gamma}$.

The Γ-limit for Dirichlet boundary conditions takes the form below, where boundary-layer effects at the boundary are taken into account. For simplicity of notation we define

$$SBV_c^l(0,L) = \{u \in SBV^l(0,L) : \text{ conditions (i)-(iv) of Proposition 4.5 hold}\}. \tag{4.16}$$

Theorem 4.6 (First order Γ-limit - Dirichlet boundary data) *Suppose that hypotheses* $[H1]_{LJ}$*–*$[H6]_{LJ}$ *hold and let* $H^l_{1,n} : \mathcal{A}_n(0,L) \to [0,+\infty]$ *be defined by*

$$H^l_{1,n}(u) = \frac{H^l_n(u) - \min H^l}{\lambda_n}. \tag{4.17}$$

We then have:

(i) *if* $l \leq \gamma$
   $H^l_{1,n}$ Γ*-converges with respect to the* L^∞*-topology to*

$$H^l_1(\boldsymbol{u}) = \begin{cases} \sum\limits_{t \in S(\boldsymbol{u}')} C(\boldsymbol{u}'(t-), \boldsymbol{u}'(t+)), & \textit{if } \boldsymbol{u} \in SBV_c^l(0,L), \\ +\infty & \textit{otherwise} \end{cases}$$

   on $W^{1,\infty}(0,L)$, *with* $SBV_c^l(0,L)$ *defined in* (4.16).

(ii) *if* $l > \gamma$ *and* $\#\boldsymbol{M}^\gamma = 1$
   $H^l_{1,n}$ Γ*-converges with respect to the* $L^1_{\rm loc}$*-topology to*

$$H^l_1(u) = \begin{cases} C(\gamma,\gamma)\#(S(u') \setminus S(u)) + B_{IJ}\#S(u) + B_{BJ}\#S(\tilde{u}) + 2B(\gamma) \\ \qquad\qquad\qquad \textit{if } u \in SBV_c^l(0,L) \\ +\infty \qquad\qquad\quad \textit{otherwise} \end{cases}$$

   on $L^1_{\rm loc}(\mathbf{R})$, *where*

$$B_{BJ} = J_1(+\infty) + J_2(+\infty) - J_0(\gamma)$$

   is the boundary layer energy for a jump at the boundary of the domain, and

$$B_{IJ} = 2B(\gamma) - 2J_0(\gamma) + 2J_2(+\infty) + J_1(+\infty)$$

   is the boundary layer energy for a jump at an internal point of the domain.

Remark 4.7 Note that, compared to the periodic case, we have further restricted our analysis to the case $\#\mathbf{M}^\gamma = 1$ when $l > \gamma$. In the general case a dependence on the parity of the lattice would appear in the limit as in Theorem 3.7.

Proof of Theorem 4.6. Since the proof is similar to that of Theorem 3.10, we only highlight the main differences in the case $l > \gamma$ proving the Γ-liminf inequality for the last term in the energy. In what follows we will suppose $L = 1$ and n even. Let $u_n \to \mathbf{u}$ in $L^1_{\rm loc}(0, L)$ be such that $\sup_n H^l_{1,n}(u_n) < +\infty$. Moreover, for simplicity, suppose that

$$S(\mathbf{u}) = \{0\}. \tag{4.18}$$

By the compactness result of Proposition 4.5, we have that $\mathbf{u}'(t) = \mathbf{z}^\gamma \in \mathbf{M}^\gamma$ for a.e. $t \in (0, L)$. Let $\{h_n\}_n$ be a sequence of indices such that $\lim_n \lambda_n h_n = \frac{1}{2}$. It is convenient to rewrite the energy as follows:

$$\begin{aligned} H^l_{1,n}(u_n) &= \mathcal{H}_n(u_n, 0+) + \mathcal{H}_n(u_n, 1-) + J_1\Big(\frac{u_n^1 - u_n^0}{\lambda_n}\Big) \\ &\quad + J_2\Big(\frac{u_n^2 - u_n^0}{2\lambda_n}\Big) - J_0(\gamma), \end{aligned} \tag{4.19}$$

where

$$\mathcal{H}_n(u_n, 0+) = \sum_{i=1}^{h_n} \Big(J_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - J_0(\gamma)\Big),$$

$$\begin{aligned} \mathcal{H}_n(u_n, 1-) &= \sum_{i=h_n+1}^{n-2} \Big(J_2\Big(\frac{u_n^{i+2} - u_n^i}{2\lambda_n}\Big) + J_1\Big(\frac{u_n^{i+1} - u_n^i}{\lambda_n}\Big) - J_0(\gamma)\Big) \\ &\quad + J_1\Big(\frac{u_n^n - u_n^{n-1}}{\lambda_n}\Big) - J_0(\gamma). \end{aligned}$$

Defining

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \dfrac{\mathbf{u}_n^{i+1}}{\lambda_n} & \text{if } 0 \le i \le h_n - 1 \\ \dfrac{\mathbf{u}_n^{h_n}}{\lambda_n} + u_{\mathbf{z}^\gamma}(i) - u_{\mathbf{z}^\gamma}(h_n) & \text{if } i \ge h_n - 1, \end{cases}$$

by the continuity of J_1 and J_2, we can find a suitable continuous function $\omega(\varepsilon) : \mathbf{R} \to \mathbf{R}$, $\omega(0) = 0$ such that,for all $\varepsilon > 0$, as $\tilde{\mathbf{u}}_n^i$ is a test function for the minimum problem defining $B(\gamma)$, for n large enough we have

$$\begin{aligned} \mathcal{H}_n(u_n, 0+) &= \frac{1}{2} J_1(\tilde{u}_n^1 - \tilde{u}_n^0) + \sum_{i \ge 0} \Big(J_2\Big(\frac{\tilde{u}_n^{i+2} - \tilde{u}_n^i}{2}\Big) \\ &\quad + \frac{1}{2}\Big(J_1\Big(\tilde{u}_n^{i+2} - \tilde{u}_n^{i+1}\Big) + J_1\Big(\tilde{u}_n^{i+1} - \tilde{u}_n^i\Big)\Big) - J_0(\gamma)\Big) + \omega(\varepsilon) \\ &\ge B_+(\mathbf{z}^\gamma) + \omega(\varepsilon). \end{aligned} \tag{4.20}$$

Analogously, defining

$$\tilde{\mathbf{u}}_n^i = \begin{cases} \dfrac{\mathbf{u}_n^{h_n}}{\lambda_n} + u_{\mathbf{z}^\gamma}(i) - u_{\mathbf{z}^\gamma}(h_n - n) & \text{if } i \le h_n - n, \\ \dfrac{\mathbf{u}_n^{i+n}}{\lambda_n} - \dfrac{l}{n} & \text{if } h_n - n \le i \le 0, \end{cases}$$

we have,

$$\begin{aligned}\mathcal{H}_n(u_n,1-) &= \frac{1}{2}J_1(\tilde u_n^0-\tilde u_n^{-1})+\sum_{i\le 0}\Big(J_2\Big(\frac{\tilde u_n^i-\tilde u_n^{i-2}}{2}\Big)\\ &\quad+\frac{1}{2}\Big(J_1\Big(\tilde u_n^i-\tilde u_n^{i-1}\Big)+\Big(\tilde u_n^{i-1}-\tilde u_n^{i-2}\Big)\Big)-J_0(\gamma)\Big)+\omega(\varepsilon)\\ &\ge B(\gamma)+\omega(\varepsilon). \end{aligned}\tag{4.21}$$

By (4.18) and hypothesis $[H5]_{LJ}$, we have

$$\begin{aligned}\liminf_n H^l_{1,n}(u_n) &\ge J_1(+\infty)+J_2(+\infty)-J_0(\gamma)+2B(\gamma)+c\omega(\varepsilon)\\ &= B_{BJ}+2B(\gamma)+c\omega(\varepsilon).\end{aligned}$$

The Γ-liminf inequality follows by the arbitrariness of ε. □

In the following two examples we consider the case of standard *Lennard-Jones* and *Morse* potentials pointing out some interesting features about phase transition energies in these cases.

Example 4.8 Let us consider the Lennard-Jones case:

$$J_1(z)=\begin{cases}+\infty & \text{if } z\le 0\\ \dfrac{k_1}{z^{12}}-\dfrac{k_2}{z^6} & \text{if } z>0,\end{cases}\qquad J_2(z)=J_1(2z)$$

for some $k_1,k_2>0$. Set $z_{\min}=(2k_1/k_2)^{\frac{1}{6}}$ the minimum point of J_1 and γ the minimum point of J_0, it can be proven that

$$J_0^{**}(z)=\begin{cases}J_0(z) & \text{if } 0<z\le\gamma:=\Big(\frac{1+2^{-12}}{1+2^{-6}}\Big)^{\frac{1}{6}}z_{\min}\\ J_0(\gamma) & \text{otherwise.}\end{cases}$$

Hence no mesoscopic phase transition energies come into play because $N(l)=1$ being

$$\mathbf{M}_l=\begin{cases}\emptyset & \text{if } l/L\le 0\\ \mathbf{M}^{\frac{l}{L}} & \text{if } 0<l/L<\gamma\\ \mathbf{M}^\gamma & \text{otherwise.}\end{cases}$$

It is also possible to show that neither microscopic phase transition energies appear as $\#\mathbf{M}_l\le 1$.

Example 4.9 Let us consider the Morse case:

$$J_1(z)=k_1\Big(1-e^{-k_2(z-z_{\min})}\Big)^2,\quad J_2(z)=J(2z)$$

for some $k_1,k_2>0$. Set γ the minimum point of J_0, it can be proven that

$$J_0^{**}(z)=\begin{cases}J_0(z) & \text{if } z\le\gamma<z_{\min}\\ J_0(\gamma) & \text{otherwise.}\end{cases}$$

This again gives that no mesoscopic phase transition energy appear in the first order Γ-limit as $N(l) = 1$ being

$$\mathbf{M}_l = \begin{cases} \mathbf{M}^{\frac{l}{L}} & \text{if } l/L < \gamma \\ \mathbf{M}^{\gamma} & \text{otherwise.} \end{cases}$$

We now give an example of Lennard-Jones type potentials leading to mesoscopic phase transition terms in the limit.

Example 4.10 Let

$$\begin{aligned} J_1(z) &= (z - z_m)^2 \wedge t\chi_{(z_m,+\infty)}(z) \\ J_2(z) &= J_1(z/k) \end{aligned}$$

for some $t < z_m^2$ and $k > \frac{z_m + \sqrt{t/2}}{z_m - \sqrt{t/2}}$. Then (see Fig. 2)

$$J_0(z) = \begin{cases} (z - z_m)^2 + (\frac{1}{k}z - z_m)^2 & \text{if } z \le z_m + \sqrt{t/2} \\ (\frac{1}{k}z - z_m)^2 + \frac{1}{2}\,t & \text{if } z_m + \sqrt{t/2} < z \le k(z_m + \sqrt{t}) \\ \frac{3}{2}t & \text{if } z > k(z_m + \sqrt{t}) \end{cases}$$

and

$$J_0^{**}(z) = \begin{cases} J_0(z) & \text{if } z \le z_m + \sqrt{\frac{t}{2(1+k^2)}} \\ a(z - z_m - \sqrt{\frac{t(1+k^2)}{2}}) + b & \text{if } z_m + \sqrt{\frac{t}{2(1+k^2)}} < z \le z_m + \sqrt{\frac{t(1+k^2)}{2}} \\ J_0(z) & \text{if } z_m + \sqrt{\frac{t(1+k^2)}{2}} < z \le kz_m \\ \frac{t}{2} & \text{if } z > kz_m, \end{cases}$$

where

$$a = \frac{2}{k^2}\Big(z_m(1-k) + \sqrt{\frac{t(1+k^2)}{2}}\Big), \quad b = \frac{1}{k^2}\Big(z_m(1-k) + \sqrt{\frac{t(1+k^2)}{2}}\Big)^2 + \frac{t}{2}.$$

In this case we have that

$$\mathbf{M}_l = \begin{cases} \mathbf{M}^{\frac{l}{L}} & \text{if } l/L \le \alpha \\ \mathbf{M}^{\alpha} \cup \mathbf{M}^{\beta} & \text{if } \alpha < l/L \le \beta \\ \mathbf{M}^{\frac{l}{L}} & \text{if } \beta < l/L \le \gamma \\ \mathbf{M}^{\gamma} & \text{otherwise} \end{cases}$$

where

$$\alpha = z_m + \sqrt{\frac{t}{2(1+k^2)}}, \quad \beta = z_m + \sqrt{\frac{t(1+k^2)}{2}}, \quad \gamma = kz_m.$$

A mesoscopic phase transition energy will occur in the limit being $N(l) = 2$ for $\alpha \le \frac{l}{L} \le \beta$.

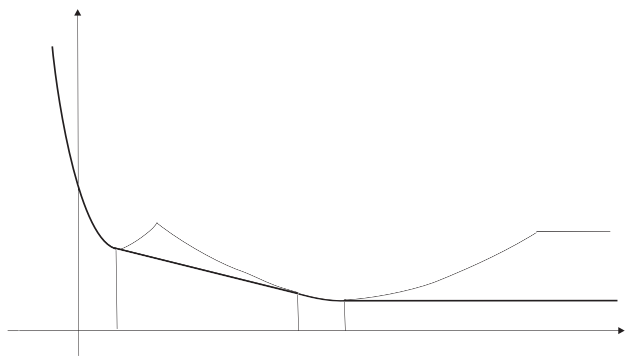

Figure 2: J_0 and J_0^{**} (bold line) in Example 4.10

5 Minimum Problems

In this section we describe the structure of the minima for the first order discrete energies we studied in Section 3 and 4 in some special cases. In particular we will focus on the periodic case for superlinear growth densities and on the Dirichlet case for Lennard-Jones densities.

5.1 Superlinear-growth densities

The next theorem deals with the convergence of minimizer for first-order discrete energies of the form (3.22) in two special cases. For the sake of simplicity and without losing in generality we can set $L = 1$.

Theorem 5.1 *Suppose that hypotheses* [H1]–[H4] *and* [H6] *hold and suppose that* ψ_0 *is such that*

$$\boldsymbol{M}_l = \boldsymbol{M}^\alpha \cup \boldsymbol{M}^\beta \ \textit{if} \ \ l \in (\alpha, \beta).$$

Then the minimizers $(\boldsymbol{u}_n)$ *of* $\min\{E^{\#,l}_{1,n}(u)\}$, *for* n *even and* $l \in (\alpha, \beta)$, *converge, up to subsequences, to one of the functions:*

(i) *if* $\boldsymbol{M}^\alpha = \{(\alpha, \alpha)\}$, $\boldsymbol{M}^\beta = \{(\beta, \beta)\}$, *then* $\boldsymbol{u} = (u, u)$,

$$u(t) = \alpha\chi_I(t) + \beta\chi_{(0,1)\setminus I}(t)$$

where $I \subset (0, 1)$ *is an interval such that* $|I|\alpha + (1 - |I|)\beta = l$. *Moreover* $E^{\#,l}_1(u) = 2C(\alpha, \beta)$.

(ii) *if* $\boldsymbol{M}^\alpha = \{(\alpha, \alpha)\}$, $\boldsymbol{M}^\beta = \{(\beta_1, \beta_2), (\beta_2, \beta_1)\}$, *then* $\boldsymbol{u} = (u_1, u_2)$,

$$u_1(t) = \alpha\chi_I(t) + \beta_1\chi_{(0,1)\setminus I}(t)$$

$$u_2(t) = \alpha\chi_I(t) + \beta_2\chi_{(0,1)\setminus I}(t)$$

where $I \subset (0,1)$ is an interval such that $|I|\alpha + (1-|I|)\beta = l$. Moreover $E_1^{\#,l}(u) = 2C((\alpha,\alpha),(\beta_1,\beta_2))$.

Proof. The claim follows thanks to Theorem 3.10 applying the minima convergence result in Γ-convergence problem (see [8] and [20]) and observing that we have

$$E_1^{\#,l}(u) \geq 2C((\alpha,\alpha),(\beta,\beta)),$$

$$E_1^{\#,l}(u) \geq C((\alpha,\alpha),\mathbf{z}^\beta) + C((\alpha,\alpha),\mathbf{z}_1^\beta) \quad \text{for all } \mathbf{z}^\beta,\ \mathbf{z}_1^\beta \in \mathbf{M}^\beta.$$

in case (i) and (ii), respectively. □

5.2 A graphic reduction method

In what follows we describe a graphic reduction method which can be useful to treat cases more complicated than those seen in the previous theorem. Let $l \in (\alpha,\beta)$. We introduce some terminology: the plane (z_1,z_2) is said to be the *micro-phase plane (m-p plane)*. A point $\mathbf{w} = (w_1,w_2)$ in the m-p plane is said to be a *micro-configuration (m-c)* if $\mathbf{w} \in \mathbf{M}_l$. An arrow in the m-p plane connecting two m-cs, starting from a m-c $(\overline{z}_1,\overline{z}_2)$ and pointing to a m-c $(\tilde{z}_1,\tilde{z}_2)$ is said to be a *phase-transition (p-t)* and is indicated by $(\overline{z}_1,\overline{z}_2) \to (\tilde{z}_1,\tilde{z}_2)$.

Definition 5.2 *Two p-ts $(z_1,z_2) \to (z_1',z_2')$, $(w_1,w_2) \to (w_1',w_2')$ are said to be* connected *if $(z_1,z_2) \equiv (w_1',w_2')$ or if $(z_1',z_2') \equiv (w_1,w_2)$. A set of connected p-ts is said to be a* loop *if every m-c is starting and ending point for two p-ts. A loop is said to be of* length $n \in \mathbf{N}$ *(or an n-loop) if it is built connecting n p-ts.*

Definition 5.3 *A real function F defined on the cartesian product of two m-p planes is called an* energy.

Let F be a given energy. The energy of a phase transition $(\overline{z}_1,\overline{z}_2) \to (\tilde{z}_1,\tilde{z}_2)$ is $F((\overline{z}_1,\overline{z}_2),(\tilde{z}_1,\tilde{z}_2))$. The energy of a sets of p-ts is the sum of the energies of all p-ts. Two sets of p-ts are said to be (energetically) equivalent *if they have the same energy. An n-loop is said to be* reducible *if it is equivalent to another set of p-ts containing an m-loop with $m < n$.*

We are interested in solving the minimum problem for the Γ-limit of energies of the type (3.22) in the same hypotheses of the previous theorem where, following the definitions above, $F(\mathbf{z}_1,\mathbf{z}_2) = C(\mathbf{z}_1,\mathbf{z}_2)$. Observe that, by the compactness result obtained in the previous section and the definition of transition energy $C(\cdot,\cdot)$, we know that

(R1) $\mathbf{u}' \in \mathbf{M}_l = \mathbf{M}^\alpha \cup \mathbf{M}^\beta$,

(R2) $\mathbf{u}'$ is 1-periodic,

(R3) $C(\mathbf{z}^\alpha,\mathbf{z}^\beta) = C(\overline{\mathbf{z}}^\alpha,\overline{\mathbf{z}}^\beta) = C(\overline{\mathbf{z}}^\beta,\overline{\mathbf{z}}^\alpha) = C(\mathbf{z}^\beta,\mathbf{z}^\alpha)$,

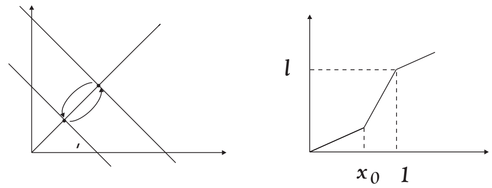

Figure 3: 2-loop and minimizing configuration in Example 5.4

(R4) $C(\cdot,\cdot) > 0$.

Thanks to $(R1)$ and the definition of $\mathbf{M}^\alpha$ and $\mathbf{M}^\beta$, we know that the m-cs we have to consider in the m-p plane, where we are going to plot our minimal configurations, are those laying on the straight lines

$$z_1 + z_2 = 2\alpha, \qquad z_1 + z_2 = 2\beta.$$

Moreover, by $(R2)$, we know that the allowed p-ts form a loop. By $(R3)$ two p-ts symmetric with respect to $z_1 = z_2$ as well as two p-ts with starting and ending points exchanged are equivalent. We will describe this graphic method with three examples. The first two are cases (i) and (ii) in Theorem (5.1).

Example 5.4 Let $\mathbf{M}^\alpha = \{(\alpha,\alpha)\}$ and $\mathbf{M}^\beta = \{(\beta,\beta)\}$. In this case only one 2-loop is possible. Thus there is only one minimizing configuration (see Fig. 3).

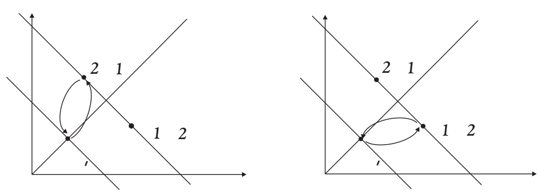

Figure 4: equivalent 2-loops (Example 5.5)

Example 5.5 Let $\mathbf{M}^\alpha = \{(\alpha,\alpha)\}$ and $\mathbf{M}^\beta = \{(\beta_1,\beta_2),(\beta_2,\beta_1)\}$. In this case two equivalent 2-loops can be built (see Fig.4). Moreover a 3-loop can be built, but it can be reduced to a 2-loop as shown in Fig. 5, thus the minimum configuration has two transitions and the associated fields $u = \frac{u_1+u_2}{2}$, u_1 and u_2 look like those in Fig. 6.

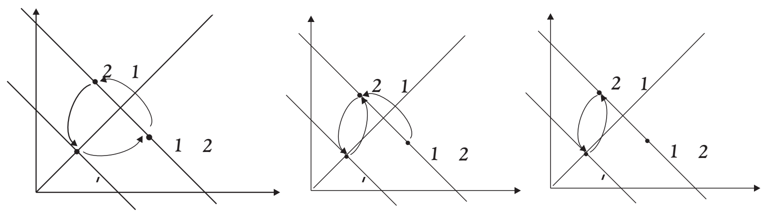

Figure 5: reduction of a 3-loop (Example 5.5)

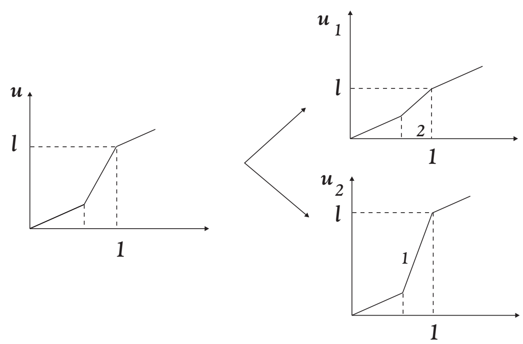

Figure 6: minimizing fields (Example 5.5)

Example 5.6 Let $\mathbf{M}^\alpha = \{(\alpha_1, \alpha_2), (\alpha_2, \alpha_1)\}$ and $\mathbf{M}^\beta = \{(\beta_1, \beta_2), (\beta_2, \beta_1)\}$. In this case two pairs of equivalent 2-loops and two of 3-loops can be built. Moreover three 4-loops can be built but each of them can be reduced to a 2-loop, thus the minimum configuration has two or three transitions. To say which loop minimizes the energy we have to compare the minimum 2-loop energy

$$m_2 \equiv \min\{2C((\alpha_1, \alpha_2), (\beta_1, \beta_2)), 2C((\alpha_1, \alpha_2), (\beta_2, \beta_1))\},$$

with the minimum 3-loop energy

$$\begin{aligned} m_3 \quad \equiv \quad & \min\{C((\alpha_1, \alpha_2), (\beta_1, \beta_2)) + C((\beta_1, \beta_2), (\beta_2, \beta_1)) + C((\beta_2, \beta_1), (\alpha_1, \alpha_2)), \\ & C((\alpha_1, \alpha_2), (\beta_1, \beta_2)) + C((\beta_1, \beta_2), (\alpha_2, \alpha_1)) + C((\alpha_2, \alpha_1), (\alpha_1, \alpha_2))\}. \end{aligned}$$

Three cases can occur. If $m_2 < m_3$ a 2-loop configuration is minimal and the corresponding minimizing fields are shown in Fig.7. If $m_2 > m_3$ a 3-loop configuration minimizes the energy and the corresponding fields are shown in Fig 8. If $m_2 = m_3$ the 2-loop and 3-loop configurations are equienergetic.

The following is an example of interaction energies ψ_1, ψ_2 leading to a ψ_0 satisfying the hypotheses of Theorem 5.1 in cases (i) and (ii).

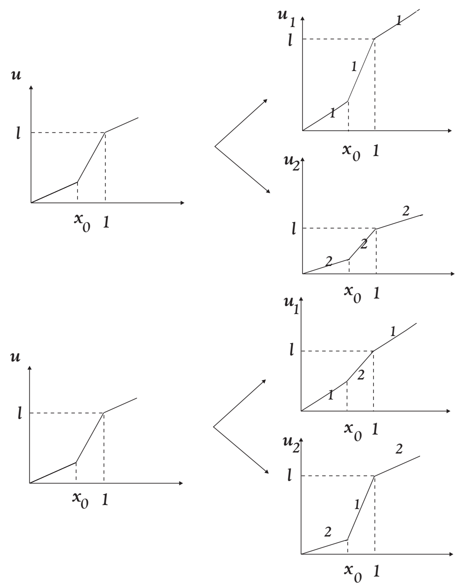

Figure 7: fields in the 2-loop configuration (Example 5.6)

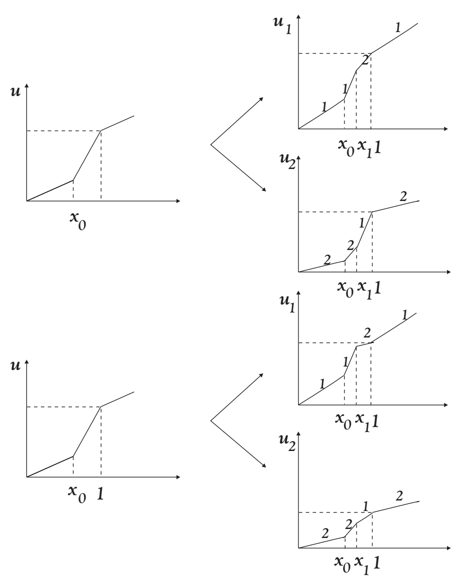

Figure 8: fields in the 3-loop configuration: $x_0 \in (0, \overline{x})$ with $\alpha\overline{x} + \beta(1 - \overline{x}) = l$, $x_1 \in (x_0, x_0 + 1 - \overline{x})$ (Example 5.6)

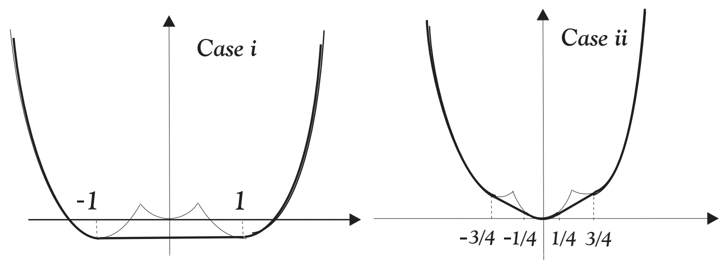

Figure 9: Example 5.7: ψ_0 and ψ_0^{**}.

Example 5.7 Consider $\psi_1 = (z+1)^2 \wedge (z-1)^2$. It is possible to compute explicitly $\phi(z) \equiv \min\{\psi_1(z_1)+\psi_1(z_2) :\ z_1+z_2 = 2z\}$ obtaining $\phi(z) = (z+1)^2 \wedge (z-1)^2 \wedge z^2$ and in particular

$$2\phi(z) = \begin{cases} \psi_1(z-1) + \psi_1(z+1) & z \in (-\frac{1}{2}, \frac{1}{2}), \\ 2\psi_1(z) & \text{otherwise} \end{cases}.$$

i) If $\psi_2 = -\frac{z^2}{2}$, computing explicitly ψ_0^{**} (see Fig. 9) one gets that, for $l \in (-1,1)$, $\mathbf{M}_l = \mathbf{M}^{-1} \cup \mathbf{M}^1$ where $\#\mathbf{M}^{-1} = \#\mathbf{M}^1 = 1$.

ii) If $\psi_2 = z^2$, computing explicitly ψ_0^{**} one gets that, for $l \in (-\frac{3}{4}, -\frac{1}{4})$, $\mathbf{M}_l = \mathbf{M}^{-\frac{3}{4}} \cup \mathbf{M}^{-\frac{1}{4}}$ and, for $l \in (\frac{1}{4}, \frac{3}{4})$, $\mathbf{M}_l = \mathbf{M}^{\frac{1}{4}} \cup \mathbf{M}^{\frac{3}{4}}$ where $\#\mathbf{M}^{-\frac{3}{4}} = \#\mathbf{M}^{\frac{3}{4}} = 1$ while $\#\mathbf{M}^{-\frac{1}{4}} = \#\mathbf{M}^{\frac{1}{4}} = 2$.

We end this section by giving an example of potentials leading to the energetic description we showed in Example 5.6.

Example 5.8 Consider $\psi_1 = (z+2)^2 \wedge z^2 \wedge (z-2)^2$ and $\psi_2 = (z+1)^2 \wedge ((z-1)^2+1)$. Again it is possible to compute $\phi(z) = (z+2)^2 \wedge (z+1)^2 \wedge (z-1)^2 \wedge (z-2)^2 \wedge z^2$. In particular

$$2\phi(z) = \begin{cases} 2\psi_1(z) & z \in (-\infty, -\frac{3}{2}) \\ \psi_1(z-1) + \psi_1(z+1) & z \in (-\frac{3}{2}, -\frac{1}{2}) \\ \psi_1(z-2) + \psi_1(z+2) & z \in (-\frac{1}{2}, \frac{1}{2}) \\ \psi_1(z-1) + \psi_1(z+1) & z \in (\frac{1}{2}, \frac{3}{2}) \\ 2\psi_1(z) & z \in (\frac{3}{2}, +\infty) \end{cases}$$

and, computing ψ_0^{**}, it can be seen that for $l \in (-\frac{7}{8}, \frac{9}{8})$ we have that $\mathbf{M}_l = \mathbf{M}^{-\frac{7}{8}} \cup \mathbf{M}^{\frac{9}{8}}$ with $\#\mathbf{M}^{-\frac{7}{8}} = \#\mathbf{M}^{\frac{9}{8}} = 2$. Observe that, to construct an example like this, it is not possible to substitute the second order asymmetric interaction we used with an even one, otherwise hypothesis [H3] would not be satisfied.

5.3 Lennard-Jones densities

Since the analysis of minimum problems for the scaled Lennard-Jones type energies of the form (4.1) when $l \leq \gamma$ does not present new features with respect to the superlinear case, we will focus on minimum problems with $l > \gamma$ when a contribution due to the crack appears in the limit. Although a more general description like the one we have provided in the previous section is possible, in order to give a simplified analysis of the phase transition phenomena for standard Lennard-Jones NNN energies, we restrict to the case $J_1(z) = J_2(2z) = J(z)$ with $\min J < J(+\infty)$ and $\#\mathbf{M}^\gamma = 1$.

For the sake of simplicity and without losing in generality we can set $L = 1$.

Theorem 5.9 (Localization of fracture) *Suppose that hypotheses $[H1]_{LJ}$–$[H6]_{LJ}$ hold and suppose that $J_1(z) = J_2(2z) = J(z)$ is such that*

$$\min J < J(+\infty), \qquad \#M^\gamma = 1. \tag{5.22}$$

Then the minimizers $(\boldsymbol{u}_n)$ of $\min\{H^l_{1,n}(u)\}$, for $l > \gamma$, converge, up to subsequences, to one of the functions:

$$u_1(t) = \gamma t, \qquad u_2(t) = \gamma t + (l - \gamma)$$

Moreover $H^l_1(u) = 3J(+\infty) - J_0(\gamma)$.

Remark 5.10 Note that the previous result asserts that, at first order in λ_n, the fracture of the ground state can be localized at the boundary of the domain.

Proof of Theorem 5.9. Thanks to Remark 2.3 we get

$$B_\pm(\gamma) = \frac{1}{2} J(\gamma).$$

Since by Theorem 4.6 we have that $\mathbf{u}'(t) = u'(t) = \gamma$ a.e. $t \in (0, L)$, we have that

$$B_{IJ} = J(\gamma) - 2J_0(\gamma) + 3J(+\infty), \qquad B_{BJ} = 2J(+\infty) - J_0(\gamma).$$

The claim follows applying the minima convergence result in Γ-convergence problems and observing that, since

$$H^l_1(u) \geq B_{IJ}(\gamma)\#S(u) + B_{BJ}\#S(\tilde{u}) + 2B(\gamma).$$

one has that $\#S(u) \leq 1$ and $\#S(\tilde{u}) \leq 1$. It remains to compare the energy $H^l_1(u)$ in the following four cases:

$$\begin{array}{ll} \text{(a) } \#S(u) = 0 \quad \#S(\tilde{u}) = 1, & \text{(b) } \#S(u) = 1 \quad \#S(\tilde{u}) = 0, \\ \text{(c) } \#S(u) = 0 \quad \#S(\tilde{u}) = 0, & \text{(d) } \#S(u) = 1 \quad \#S(\tilde{u}) = 1. \end{array}$$

By the boundary conditions, (c) must be rejected. By the positiveness of our energies (d) has an energy greater than (a) and (b). If we are in the case (a), then the only two minimizers are u_1 and u_2 while in the case (b) all the possible minimizers are functions of the type $\overline{u}(t) = \gamma t + (l - \gamma)\chi(\overline{t})$ where $\overline{t} \in (0, L)$. We have that

$$H^l_1(u_1) = H^l_1(u_2) = 3J(+\infty) - J_0(\gamma), \qquad H^l_1(\overline{u}) = 5J(+\infty) - 2J_0(\gamma),$$

and the claim follows observing that, by the definition of J_0 and thanks to hypothesis (5.22) $J_0(\gamma) \leq J(\gamma) + \min J < J(\gamma) + J(+\infty)$. □

6 Equivalence by Γ-convergence

In this section we give an interpretation of the results of Section 3 by linking them with the gradient theory of phase transitions. We show that in a sense discrete energies with next-to-nearest neighbour interactions act as singular perturbation of non-convex energies with higher-order gradients. In order to give a rigorous meaning to this statement we will use the notion of *equivalence* by Γ-convergence (see [17]).

Definition 6.1 Let $\mathcal{L}$ be a set of parameters and for $l \in \mathcal{L}$ let $F^l_\varepsilon(u)$ and $G^l_\varepsilon(u)$ be parameterized families of functionals. We say that F^l_ε and G^l_ε are *equivalent to first order* along the sequence ε_n if

(i) for all $l \in \mathcal{L}$ $\quad \Gamma\text{-}\lim_{n\to\infty} F^l_{\varepsilon_n}(u) = \Gamma\text{-}\lim_{n\to\infty} G^l_{\varepsilon_n}(u) =: F^l_0(u)$

(ii) for all $l \in \mathcal{L}$ $\quad \Gamma\text{-}\lim_{n\to\infty} \dfrac{F^l_{\varepsilon_n}(u) - \min F^l_0(u)}{\varepsilon_n} = \Gamma\text{-}\lim_{n\to\infty} \dfrac{G^l_{\varepsilon_n}(u) - \min F^l_0(u)}{\varepsilon_n}.$

With a slight abuse we use the same notation if F^l_ε and G^l_ε are defined only for $\varepsilon = \varepsilon_n$. In the following, after setting $\varepsilon_n = \lambda_n$, $F^l_{\varepsilon_n}(u) = E^{\#,l}_n(u)$, and

$$G^l_{\varepsilon_n}(u) = G^{\#,l}_n(u) = \begin{cases} \displaystyle\int_{(0,L)} \tilde\psi_0(u')\,dt + \lambda_n^2 \int_{(0,L)} |u''|^2\,dt & u \in W^{2,2}_{\rm loc}(\mathbf{R}),\\ & u - lt \text{ is } L\text{-periodic} \\ +\infty & \text{otherwise on } L^1(0,L), \end{cases}$$

we prove the following equivalence result.

Theorem 6.2 (Γ-equivalence - Periodic boundary data) *Let $\tilde\psi_0 : \mathbf{R} \to \mathbf{R}$ be a Borel function such that*

(i) $\displaystyle\lim_{|z|\to+\infty} \frac{\tilde\psi_0(z)}{|z|} = +\infty,$

(ii) $(\tilde\psi_0)^{**} = \psi_0^{**}$.

(iii) $\{z \in \mathbf{R} :\ \tilde\psi_0(z) = (\tilde\psi_0)^{**}(z)\} = \{z \in \mathbf{R} :\ \psi_0(z) = \psi_0^{**}(z)\}$

(iv) $\tilde\psi_0(z^i + z) - (\tilde\psi_0)^{**}(z^i + z) = O(z^\alpha),\ \alpha > 1$ *for all z^i such that* $\tilde\psi_0(z^i) = (\tilde\psi_0)^{**}(z^i)$

If $\{z : \psi_0^{**}$ is affine$\} = \bigcup_{i=1}^N [\alpha_i, \beta_i]$ disjoint intervals, suppose that

$$\#\boldsymbol{M}^{\alpha_j} = \#\boldsymbol{M}^{\beta_j} = 1 \text{ and} \tag{6.23}$$

$$2\int_{\alpha_j}^{\beta_j} \sqrt{\tilde\psi_0(s) - \psi_0^{**}(s)}\,ds = C(\alpha_j, \beta_j) \text{ for some } j \in \{1, 2, \dots, N(l)\}, \tag{6.24}$$

with $N(l) < +\infty$, then $F^l_{\varepsilon_n}$ and $G^l_{\varepsilon_n}$ are equivalent up to the first order for $l \in [\alpha_j, \beta_j]$.

Remark 6.3 In the special case that hypotheses (i) and (iv) are satisfied by ψ_0, it is possible to restate the previous result asserting that $F^l_{\varepsilon_n}$ is equivalent up to the first order, for $l \in [\alpha_j, \beta_j]$, to the following family of functionals

$$H^l_\varepsilon(u) = \begin{cases} \displaystyle\int_{(0,L)} \psi_0(u')\,dt + k\varepsilon^2 \int_{(0,L)} |u''|^2\,dt & u \in W^{2,2}_{\mathrm{loc}}(\mathbf{R}), \\ & u - lt \text{ is } L\text{-periodic} \\ +\infty & \text{otherwise on } L^1(0,L), \end{cases}$$

where

$$k = \left(\frac{C(\alpha_j, \beta_j)}{\int_{\alpha_j}^{\beta_j} \sqrt{\psi_0(s)}\;ds} \right)^2,$$

along the sequence $\varepsilon_n = \lambda_n$.

Proof of Theorem 6.2
Zero-order equivalence. In what follows we set $L = 1$. By Theorem 3.4 we need to prove that

$$\Gamma\text{-}\lim_n G^{\#,l}_n(u) = E^{\#,l}(u) = \begin{cases} \displaystyle\int_0^1 \psi_0^{**}(u'(t))\,dt & \text{if } u \in W^{1,1}_{\#,l}(0,1) \\ +\infty & \text{otherwise on } L^1_{\mathrm{loc}}(\mathbf{R}). \end{cases}$$

First observe that, thanks to hypothesis (i) and the definition of $G^{\#,l}_n$, we have that, as in Theorem 3.4, the limit is finite only on $W^{1,1}_{\#,l}(0,1)$. Moreover, as

$$G^{\#,l}_n(u) \geq \int_0^1 \tilde{\psi}_0(u'(t))\,dt \geq \int_0^1 (\tilde{\psi}_0)^{**}(u'(t))\,dt,$$

then

$$\Gamma\text{-}\liminf_n G^{\#,l}_n(u) \geq \int_0^1 (\tilde{\psi}_0)^{**}(u'(t))\,dt.$$

By an easy density argument it suffices to obtain the $\Gamma\text{-}\limsup$ inequality for $u \in C^2(\mathbf{R})$ such that $u(t) - lt$ is 1-periodic. In this case we have, from the definition of $\Gamma\text{-}\limsup$, taking the pointwise limit of $G^{\#,l}_n(u)$ and passing to its lower semicontinuous envelope with respect to the strong L^1 convergence,

$$\Gamma\text{-}\limsup_n G^{\#,l}_n(u) \leq \int_0^1 (\tilde{\psi}_0)^{**}(u'(t))\,dt.$$

First-order equivalence. Set

$$\begin{aligned} G^{\#,l}_{1,n}(u) &:= \frac{G^{\#,l}_n(u) - \min E^{\#,l}}{\lambda_n} \\ &= \begin{cases} \displaystyle\frac{1}{\lambda_n}\int_0^1 (\tilde{\psi}_0(u') - (\tilde{\psi}_0)^{**}(l))\,dt + \lambda_n \int_0^1 |u''|^2\,dt & \text{if } u \in W^{2,2}_{\mathrm{loc}}(\mathbf{R}), \\ & u(t) - lt \text{ is 1-periodic}, \\ +\infty & \text{otherwise on } L^1_{\mathrm{loc}}(\mathbf{R}). \end{cases} \end{aligned}$$

Thanks to Theorem 3.10 and hypothesis (6.23), we need to prove that

$$\Gamma\text{-}\lim_n G^{\#,l}_{1,n}(u) = E^{\#,l}_1(u) = \begin{cases} \sum_{t\in S(\mathbf{u}')\cap(0,1]} C(u'(t-),u'(t+)), & \text{if } \mathbf{u}' \in PC_{\rm loc}(\mathbf{R}), \\ & u' \in \mathbf{M}_l,\ u(t)-lt \text{ is 1-periodic}, \\ +\infty & \text{otherwise on } W^{1,\infty}_{\rm loc}(\mathbf{R}). \end{cases}$$

Compactness. Let $u_n \to u$ in $W^{1,1}_{\rm loc}(\mathbf{R})$ be such that

$$\sup_n G^{\#,l}_{1,n}(u_n) \le c. \tag{6.25}$$

As in the proof of the zero order equivalence, we have that $u(t)-lt$ is a 1-periodic function. Without loss of generality, we may suppose that $(\tilde\psi_0)^{**}$ is a straight line in a neighborhood of l and we write $(\tilde\psi_0)^{**}(z) = r(z)$ (the case $(\tilde\psi_0)^{**}$ is strictly convex can be proved in the same way). Since

$$\int_0^1 (\tilde\psi_0)^{**}(u_n'(t))\,dt \ge (\tilde\psi_0)^{**}(l) \quad \text{and} \quad \tilde\psi_0 \ge (\tilde\psi_0)^{**},$$

we have that

$$G^{\#,l}_{1,n}(u_n) \ \ge\ \frac{1}{\lambda_n}\int_0^1 ((\tilde\psi_0)^{**}(u_n') - (\tilde\psi_0)^{**}(l))\,dt = \frac{1}{\lambda_n}\int_0^1 ((\tilde\psi_0)^{**}(u_n') - r(u_n'))\,dt$$

and

$$G^{\#,l}_{1,n}(u_n) \ \ge\ \frac{1}{\lambda_n}\int_0^1 (\tilde\psi_0(u_n') - (\tilde\psi_0)^{**}(u_n'))\,dt = \frac{1}{\lambda_n}\int_0^1 W(u_n')\,dt$$

where we have set for short $W(z) = \tilde\psi_0(z) - (\tilde\psi_0)^{**}(z)$. By (6.25) we get that , for all $\eta > 0$

$$\lim_n |\{t : (\tilde\psi_0)^{**}(u_n'(t)) - r(u_n'(t)) > \eta\} \cap \{t : W(u_n'(t)) > \eta\}| = 0.$$

Since, thanks to hypothesis (iii), we have that $\{z \in \mathbf{R} : \tilde\psi_0(z) = (\tilde\psi_0)^{**}(z) = r(z)\} = \mathbf{M}_l$, we get that, up to subsequences, $u_n' \to z$ a.e. where $z \in \mathbf{M}_l$.

Let us prove that $u' \in PC_{\rm loc}(\mathbf{R})$. By the 1-periodicity of u it suffices to consider K a compact set of $(0,1]$ and prove that $u' \in PC(K)$. Without loss of generality we can suppose that $K = [a,b]$ and that $t_1, t_2, \dots, t_M \in S(u') \cap [a,b]$. For $i = 1, 2, \dots, M$ we can find $a_i^\pm \in [a,b]$ such that

$$a < a_i^- < t_i < a_i^+ < a_{i+1}^- < b \tag{6.26}$$

and that there exist the limits

$$\lim_n u_n'(a_i^\pm) = u'(a_i^\pm) \in \mathbf{M}_l \quad \text{with} \quad u'(a_i^+) \ne u'(a_i^-). \tag{6.27}$$

It holds

$$G^{\#,l}_{1,n}(u_n) \ \ge\ \frac{1}{\lambda_n}\int_a^b W(u_n')\,dt + \lambda_n \int_a^b |u_n''|^2\,dt$$

$$\geq \sum_{i=1}^{M}\Big(\frac{1}{\lambda_n}\int_{a_i^-}^{a_i^+} W(u_n') + \lambda_n \int_{a_i^-}^{a_i^+} |u_n''|^2\Big),$$

and, by Young's inequality,

$$\begin{aligned} G_{1,n}^{\#,l}(u_n) &\geq \sum_{i=1}^{M} 2\int_{a_i^-}^{a_i^+} \sqrt{W(u_n')}|u_n''|\,dt \geq 2\sum_{i=1}^{M}\Big|\int_{a_i^-}^{a_i^+} \sqrt{W(u_n')}|u_n''|\,dt\Big| \\ &\geq 2\sum_{i=1}^{M}\Big|\int_{u_n'(a_i^-)}^{u_n'(a_i^+)} \sqrt{W(s)}\;ds\Big| = \sum_{i=1}^{M} C(u_n'(a_i^-), u_n'(a_i^+)). \end{aligned}$$

Since we have that

$$\begin{aligned} \liminf_{n\to\infty} G_{1,n}^{\#,l}(u_n) &\geq \sum_{i=1}^{M}\liminf_{n\to\infty} C(u_n'(a_i^-), u_n'(a_i^+)) \geq \sum_{i=1}^{M} C(u'(a_i^-), u'(a_i^+)) \\ &\geq M\min\{C(u'(a_i^-), u'(a_i^+)),\; i\in\{1,2,\dots,M\}\} \geq cM, \end{aligned}$$

thanks to (6.25) we get that $u'\in PC([a,b])$.

Γ-liminf inequality. Thanks to the compactness result we have just proven, we can infer that there exist $0 < t_1 < t_2 < \ldots < t_N \leq 1$ such that

$$S(u') = \{t\in\mathbf{R}:\; t+q = t_i,\; q\in\mathbf{Z},\; i = 1,2,\dots,N\}.$$

With an abuse of notation we can choose again $a_i^{\pm}$ such that (6.26) and (6.27) hold true with $a=0$, $b=1$ and $M=N$. Then, by the periodicity of u, we get

$$\begin{aligned} G_{1,n}^{\#,l}(u_n) &\geq \int_0^{a_1^-}\sqrt{W(u_n')}|u_n''|\,dt \\ &\quad+\sum_{i=1}^{N-1}\int_{a_i^-}^{a_{i+1}^-}\sqrt{W(u_n')}|u_n''|\,dt + \int_{a_N^-}^{1}\sqrt{W(u_n')}|u_n''|\,dt \\ &\geq \sum_{i=1}^{N-1}\int_{a_i^-}^{a_{i+1}^-}\sqrt{W(u_n')}|u_n''|\,dt + \int_{a_N^-}^{1+a_1^-}\sqrt{W(u_n')}|u_n''|\,dt. \end{aligned}$$

Passing to the lim inf for $n\to+\infty$ in the previous inequality we have

$$\begin{aligned} \liminf_{n} G_{1,n}^{\#,l}(u_n) &\geq \sum_{i=1}^{N-1}\liminf_{n\to+\infty}\int_{a_i^-}^{a_{i+1}^-}\sqrt{W(u_n')}|u_n''|\,dt \\ &\quad+\liminf_{n\to+\infty}\int_{a_N^-}^{1+a_1^-}\sqrt{W(u_n')}|u_n''|\,dt \\ &= \sum_{t\in S(u')\cap(0,1]} C(u'(t-), u'(t+)). \end{aligned}$$

Γ-limsup inequality. We now construct a recovery sequence (u_n) for the Γ-limsup in a periodicity cell. Fix $l\in[\alpha_j,\beta_j]$, let u be such that $E_1^{\#,l}(u) < +\infty$. Supposing, without loss of generality, that $\alpha_j = 0,\ \beta_j = 1$, since the limit energy depends only on u', our approximation construction modifies u' only in a small neighborhood of $S(u')$ and is invariant under translation, it is not restrictive to suppose that u' is the 1-periodic extension of $\chi_{(a,b)}$ where $(a,b) \subseteq [0,1]$ and that $0 < a < b \leq 1$. Following the well known construction of the recovery sequence in the Modica-Mortola problem [25] (see also [7]) it is possible to find $v_n \to u$ in $W^{1,1}(0,1)$ such that

$$\lim_{n\to+\infty} \frac{1}{\lambda_n}\int_0^1 W(v_n')\,dt + \lambda_n \int_0^1 |v_n''|^2\,dt = \sum_{t\in S(u')\cap(0,1]} C(u'(t-),u'(t+)). \tag{6.28}$$

From now on we will call (v_n) the Modica-Mortola recovery sequence for u. In the following we will modify the sequence (v_n) to obtain our recovery sequence (u_n) which has to satisfy (6.28) but also the condition

$$u_n(t) - lt \text{ is 1-periodic}$$

which can be rephrased as

$$\int_0^1 u_n'(t)\,dt = \int_0^1 u'(t)\,dt. \tag{6.29}$$

Since v_n' modifies u' only in $(a-\lambda_n, a+\lambda_n)\cup(b-\lambda_n, b+\lambda_n)$ we can define u_n' to be

$$u_n'(t) = \begin{cases} t+1-a-\lambda_n & \text{if } t\in(a+\lambda_n, a+\lambda_n+k_n) \\ -t+1+b+\lambda_n & \text{if } t\in(b-\lambda_n-k_n, b-\lambda_n) \\ 1+k_n & \text{if } t\in(a+\lambda_n+k_n, b-\lambda_n-k_n) \\ v_n'(t) & \text{otherwise} \end{cases}$$

where k_n has to be chosen such that (6.29) holds. Since

$$\int_0^1 u_n'\,dt = \int_0^1 v_n'\,dt + k_n^2 + k_n(b-a-2\lambda_n-2k_n),$$

setting

$$\alpha_n := \int_0^1 (u_n' - v_n')\,dt, \tag{6.30}$$

the equation for k_n becomes

$$k_n^2 - k_n(b-a-2\lambda_n) + \alpha_n = 0$$

and it can be chosen to be

$$k_n = \Big(\frac{b-a-2\lambda_n}{2}\Big)\Big(1-\sqrt{1-\frac{4\alpha_n}{(b-a-2\lambda_n)^2}}\Big) = O(\alpha_n).$$

By hypothesis (iv) it holds true that

$$
\begin{aligned}
G^{\#,l}_{1,n}(u_n) \;\le\; & \int_0^1 \frac{W(v_n')}{\lambda_n} + \lambda_n |v_n''|^2\,dt + \int\limits_{a+\lambda_n}^{b-\lambda_n} \frac{W(u_n')}{\lambda_n} + \lambda_n |u_n''|^2\,dt \\
\le\; & \int_0^1 \frac{W(v_n')}{\lambda_n} + \lambda_n |v_n''|^2\,dt + \int\limits_{a+\lambda_n}^{a+\lambda_n+k_n} \frac{W(t+1-a-\lambda_n)}{\lambda_n}\,dt \\
& + \int\limits_{b-\lambda_n-k_n}^{b-\lambda_n} \frac{W(-t+1+b+\lambda_n)}{\lambda_n}\,dt + 2\lambda_n k_n + \frac{(b-a-2\lambda_n-2k_n)}{\lambda_n} W(1+k_n) \\
\le\; & \int_0^1 \frac{W(v_n')}{\lambda_n} + \lambda_n |v_n''|^2\,dt + \frac{2}{\lambda_n} k_n \sup\{W(s) :\; s \in (1, 1+k_n)\} \\
& + 2\lambda_n k_n + \frac{c}{\lambda_n} O(k_n^{\alpha}).
\end{aligned}
$$

Passing to the lim sup in the previous inequality, by (6.28), observing that

$$
\alpha_n = \int_0^1 u' - v_n'\,dt \le C\lambda_n,
$$

we conclude the proof. □

Theorem 6.4 (Γ-equivalence - Dirichlet boundary data) *In the same hypotheses of Theorem* 6.2, *if* $\varepsilon_n = \lambda_n$,

$$
G^l_{\varepsilon_n}(u) = G^l_n(u) = \begin{cases} \displaystyle\int_{(0,L)} \left(\tilde{\psi}_0(u') + \lambda_n^2 |u''|^2\right) dt + \lambda_n \left(\overline{B}_+(u'(0)) + \overline{B}_-(u'(L))\right) \\ \qquad\qquad\qquad\qquad \textit{if } u \in W^{2,2}(0,L),\ u(0) = 0,\ u(L) = l, \\ +\infty \qquad\qquad\qquad\qquad\qquad\qquad \textit{otherwise on } L^1(0,L), \end{cases}
$$

where

$$
\begin{aligned}
&\overline{B}_+(z) : \mathbf{R} \to \mathbf{R} \textit{ is such that } \inf_z \{C(w,z) + \overline{B}_+(z)\} = B_+(w), \\
&\overline{B}_-(z) : \mathbf{R} \to \mathbf{R} \textit{ is such that } \inf_z \{C(w,z) + \overline{B}_-(z)\} = B_-(w),
\end{aligned} \tag{6.31}
$$

and $F^l_{\varepsilon_n}(u) = E^l_n(u)$, *then* $F^l_{\varepsilon_n}$ *and* $G^l_{\varepsilon_n}$ *are equivalent up to the first order for* $l \in [\alpha_j, \beta_j]$.

Proof. Suppose that $L = 1$. As the proof is analogous to that of the previous theorem, we only point out the main differences in the construction of the recovery sequence for the first order equivalence. As before, let $\alpha_j = 0,\ \beta_j = 1$ and let u be such that $u'(t) = \chi_{(a,b)}(t)$ with $(a,b) \subseteq (0,1)$. In the following we set

$$
G^l_{1,n}(u) \;:=\; \frac{G^l_n(u) - \min E^l}{\lambda_n}
$$

$$= \begin{cases} \displaystyle\int_0^L \Big(\frac{\tilde\psi_0(u') - (\tilde\psi_0)^{**}(u')}{\lambda_n} + \lambda_n |u''|^2 \Big)\, dt + \overline{B}_+(u'(0)) + \overline{B}_-(u'(L)) \\ \hfill \text{if } u \in W^{2,2}(0,L),\ u(0)=0,\ u(1)=l, \\ +\infty \hfill \text{otherwise on } L^1(0,1). \end{cases}$$

Fix $\varepsilon > 0$. Thanks to (6.31) there exist $\overline{z}, \tilde z$ such that

$$\begin{array}{l} C(\overline{z}, u'(0+)) + \overline{B}_+(\overline{z}) \le B_+(u'(0)) + \varepsilon \quad \text{and} \\ C(\tilde z, u'(1-)) + \overline{B}_-(\tilde z) \le B_-(u'(1-)) + \varepsilon. \end{array}$$

Fix $\eta > 0$, let $\tilde u$ be such that

$$\tilde u'(t) = \begin{cases} \overline{z} & \text{if } t \in (-\eta, 0) \\ u'(t) & \text{if } t \in (0,1) \\ \tilde z & \text{if } t \in (1, \eta), \end{cases}$$

and let $(\tilde v_n)$ be the Modica-Mortola recovery sequence for $\tilde u$. It holds that $\tilde v_n \to u$ in $W^{1,1}(0,1)$ and that

$$\begin{aligned} &\lim_n \int_0^1 \Big(\frac{\tilde\psi_0(\tilde v_n') - (\tilde\psi_0)^{**}(\tilde v_n')}{\lambda_n} + \lambda_n |\tilde v_n''|^2 \Big)\, dt \\ &= \sum_{t \in S(u') \cap (0,1)} C(u'(t-), u'(t+)) + C(\overline{z}, u'(0+)) + C(\tilde z, u'(1-)). \end{aligned} \tag{6.32}$$

As done in the proof of the previous theorem, we can modify $(\tilde v_n)$ in order to construct our recovery sequence (u_n) which fulfils the boundary conditions $u_n(0) = 0,\ u_n(1) = l$. We have that

$$G^l_{1,n}(u_n) = \int_0^1 \Big(\frac{\tilde\psi_0(\tilde v_n') - (\tilde\psi_0)^{**}(\tilde v_n')}{\lambda_n} + \lambda_n |\tilde v_n''|^2 \Big)\, dt + \overline{B}_+(\overline{z}) + \overline{B}(\tilde z).$$

Passing to the $\limsup_n$ in the previous expression, thanks to (6.32), we get that

$$\begin{aligned} \limsup_n G^l_{1,n}(u_n) &= \sum_{t \in S(u') \cap (0,1)} C(u'(t-), u'(t+)) \\ &\quad + C(\overline{z}, u'(0+)) + \overline{B}_+(\overline{z}) + C(\tilde z, u'(1-)) + \overline{B}_-(\tilde z) \\ &\le E^l_1(u) + 2\varepsilon. \end{aligned}$$

The claim follows by the arbitrariness of ε. □

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