# 2. Finite-difference systems

# 1 Introduction

In the past years a number of researches have been devoted to the study of discrete systems with a large number of interactions viewed as a variational limit of energies indexed by the number of nodes of the system. In this framework the setting in which we have a fairly complete set of results is that of *central interactions* for *lattice systems*; i.e., systems where the reference positions of the interacting points lie on a prescribed lattice, whose parameters change as the number of points increases, and each point of the lattice interacts separately with each other point. In more precise terms, we consider an open set  $\Omega \subset \mathbb{R}^n$  and take as reference lattice  $Z_{\varepsilon} = \Omega \cap \varepsilon \mathbb{Z}^n$ . The general form of a pair-potential energy is then

$$E_{\varepsilon}(u) = \sum_{i,j \in Z_{\varepsilon}} f_{ij}^{\varepsilon}(u(i), u(j)), \qquad (1.1)$$

where  $u: Z_{\varepsilon} \to \mathbb{R}^m$ . The analysis of energies of the form (1.1) has been performed under various hypotheses on  $f_{ij}$ . The first simplifying assumption is that F is invariant under translations (in the target space); that is,

$$f_{ij}^{\varepsilon}(u,v) = g_{ij}^{\varepsilon}(u-v).$$
(1.2)

Furthermore, an important class is that of homogeneous interactions (*i.e.*, invariant under translations in the reference space); this condition translates into

$$f_{ij}^{\varepsilon}(u,v) = g_{(i-j)/\varepsilon}^{\varepsilon}(u,v).$$
(1.3)

If both conditions are satisfied, we may rewrite the energies  $E_{\varepsilon}$  above as

$$E_{\varepsilon}(u) = \sum_{k \in \mathbb{Z}^n} \sum_{i,j \in \mathbb{Z}_{\varepsilon}, i-j=\varepsilon k} \varepsilon^n \psi_k^{\varepsilon} \left( \frac{u(i) - u(j)}{\varepsilon} \right), \tag{1.4}$$

where  $\psi_k^{\varepsilon}(\xi) = \varepsilon^{-n} g_k^{\varepsilon}(\varepsilon\xi)$ . In this new form the interactions appear through the (discrete) difference quotients of the function u. Upon identifying each function u with its piecewise-constant interpolation (extending the definition of u arbitrarily outside  $\Omega$ ), we can consider  $E_{\varepsilon}$  as defined on (a subset of)  $L^1(\Omega; \mathbb{R}^m)$ , and hence consider the  $\Gamma$ -limit with respect to the  $L^1_{\text{loc}}$ -topology. Under some coerciveness conditions the computation of the  $\Gamma$ -limit will give a continuous approximate description of the behaviour of minimum problems involving the energies  $E_{\varepsilon}$  for  $\varepsilon$  small (see further for definitions, and [11] for a quick introduction to the subject). The scaling in (1.4) is heuristically motivated by interpreting  $\frac{u(i)-u(j)}{\varepsilon}$  as the (scaled) gradient of the piecewise-affine interpolation  $u_{\varepsilon}$  of u, and  $\varepsilon^n$  as an integral factor. In the case of only nearest-neighbor interactions in one space dimension for example, we may rewrite

$$E_{\varepsilon}(u) = \sum_{i \in Z_{\varepsilon}} \varepsilon \psi^{\varepsilon} \Big( \frac{u(i+\varepsilon) - u(i)}{\varepsilon} \Big) \approx \int_{\Omega} \psi^{\varepsilon}(u') \, dt.$$

### 1.1 Some convergence results. Continuum energies on Sobolev spaces

Now we address the following question:

• given a sequence of energies  $E_{\varepsilon}$ , do we have some limit energy (up to subsequences)? is this limit a 'local' integral energy?

Growth conditions on the energy densities  $\psi_k^{\varepsilon}$  imply correspondingly boundedness conditions on gradient norms of piecewise-affine interpolations of functions with equi-bounded energy. The simplest type of growth condition that we encounter is on *nearest neighbours*; *i.e.*, for |k| = 1. If p > 1 exists such that

$$c_1 |z|^p - c_2 \le \psi_k^{\varepsilon}(z) \le c_2 (1 + |z|^p) \tag{1.5}$$

 $(c_1, c_2 > 0 \text{ for } |k| = 1)$ , and if  $\psi_k^{\varepsilon} \ge 0$  for all k then the energies are *equi-coercive*: if  $(u_{\varepsilon})$  is a bounded sequence in  $L^1(\Omega; \mathbb{R}^m)$  and  $\sup_{\varepsilon} E_{\varepsilon}(u_{\varepsilon}) < +\infty$ , then from every sequence  $(u_{\varepsilon_j})$  we can extract a subsequence converging to a function  $u \in W^{1,p}(\Omega; \mathbb{R}^m)$ . In this section we will consider energies satisfying this assumption. Hence, their  $\Gamma$ -limits are defined in the Sobolev space  $W^{1,p}(\Omega; \mathbb{R}^m)$ .

**Remark 1.1 (conditions for the limit to be finite on**  $W^{1,p}$ ) The energies  $E_{\varepsilon}$  can also be seen as an integration with respect to measures concentrated on Dirac deltas at the points of  $Z_{\varepsilon} \times Z_{\varepsilon}$ . If each  $\psi_k^{\varepsilon}$  satisfies a growth condition

$$\psi_k^{\varepsilon}(z) \le c_k^{\varepsilon}(1+|z|^p),$$

then we have

$$E_{\varepsilon}(u) \leq \int_{\Omega \times \Omega} (1 + |u(x) - u(y)|^p) d\mu_{\varepsilon}(x, y) ,$$

where

$$\mu_{\varepsilon} = \sum_{k \in \mathbb{Z}^n}^{\infty} \sum_{i-j=\varepsilon k, \ i,j \in Z_{\varepsilon}} c_k^{\varepsilon} \frac{1}{\varepsilon^p} \delta_{(i,j)}.$$

A natural condition for the finiteness of the limit of  $E_{\varepsilon}$  is the equi-boundedness of these measures (as  $\varepsilon \to 0$ ), regardless to the set  $\Omega$ ; namely, (taking into account that the number of interaction at range  $\varepsilon k$  is proportional to  $(\operatorname{diam} \Omega/\varepsilon) - |k|$ )

$$\limsup_{\varepsilon \to 0} \sum_{|k| \le K/\varepsilon} \frac{(K - \varepsilon |k|)^{n-1}}{\varepsilon^{p+n}} c_k^{\varepsilon} < +\infty$$

for each fixed K > 0 (for fixed  $\Omega$  this condition is applied with  $K = \operatorname{diam} \Omega$ ). However, under such assumption, example can be shown exhibiting a non-local  $\Gamma$ -limit, of the form

$$F(u) = \int_{\Omega} f(\nabla u(x)) \, dx + \int_{\Omega \times \Omega} \psi(u(x) - u(y)) d\mu(x, y)$$

where  $\mu$  is the weak\*-limit of the measures  $\mu_{\varepsilon}$  outside the 'diagonal' of  $\mathbb{R}^n \times \mathbb{R}^n$ . (see [10] for more detailed examples).

Under some decay conditions, such long-range behaviour may be ruled out: the following compactness result proved by Alicandro and Cicalese [1] shows that a wide class of discrete systems possesses a 'local' continuous limit. We state it in a general 'space-dependent' case.

**Theorem 1.2 (compactness)** Let p > 1 and let  $\psi_k^{\varepsilon}$  satisfy:

(i) (coerciveness on nearest neighbours) there exits  $c_1 > 0$  such that for all  $(x, z) \in \Omega \times \mathbb{R}^m$ and  $i \in \{1, ..., n\}$ 

$$c_1|z|^p - c_2 \le \psi_{e_i}^{\varepsilon}(x, z) \tag{1.6}$$

(ii) (decay of long-range interactions) for all  $(x, z) \in \Omega \times \mathbb{R}^m$ , and  $k \in \mathbb{Z}^n$ 

$$\psi_k^\varepsilon(x,z) \le c_k^\varepsilon (1+|z|^p),\tag{1.7}$$

where  $c_k^{\varepsilon}$  satisfy

(H1): 
$$\limsup_{\varepsilon \to 0^+} \sum_{k \in \mathbb{Z}^n} c_k^{\varepsilon} < +\infty;$$
  
(H2): for all  $\delta > 0$   $M_{\delta} > 0$  exists such that 
$$\limsup_{\varepsilon \to 0^+} \sum_{|k| > M_{\delta}} c_k^{\varepsilon} < \delta.$$

Let  $E_{\varepsilon}$  be defined by

$$E_{\varepsilon}(u) = \sum_{k \in \mathbb{Z}^n} \sum_{i \in R_{\varepsilon}^k} \varepsilon^n \psi_k^{\varepsilon} \left( i, \frac{u(i + \varepsilon k) - u(i)}{\varepsilon |k|} \right),$$

where  $R_{\varepsilon}^k := \{i \in Z_{\varepsilon} : i + \varepsilon k \in Z_{\varepsilon}\}$ . Then for every sequence  $(\varepsilon_j)$  of positive real numbers converging to 0, there exists a subsequence  $(\varepsilon_{j_k})$  and a Carathéodory function  $f : \Omega \times \mathbb{R}^{d \times N}$  satisfying

$$c(\|M\|^p - 1) \le f(x, M) \le C(\|M\|^p + 1),$$

with 0 < c < C, such that  $(E_{\varepsilon_{j_k}}(\cdot))$   $\Gamma$ -converges with respect to the  $L^p(\Omega)$ -topology to the functional  $F: L^p(\Omega) \to [0, +\infty]$  defined as

$$F(u) = \begin{cases} \int_{\Omega} f(x, \nabla u) \, dx & \text{if } u \in W^{1, p}(\Omega; \mathbb{R}^m) \\ +\infty & \text{otherwise.} \end{cases}$$
(1.8)

Moreover, for any  $u \in W^{1,p}(\Omega)$  and  $A \in \mathcal{A}(\Omega)$ ,

$$\Gamma - \lim_{k} F_{\varepsilon_{j_k}}(u, A) = \int_A f(x, \nabla u) \, dx$$

**Remark 1.3 (multi-phase limits)** The condition of coerciveness on nearest-neighbors is the easiest one that ensure that the limit is described by just one variable. The trivial counterexample to this in one dimension is when only second neighbors are taken into account; *e.g.*,

$$E_{\varepsilon}(u) = \sum_{i} \varepsilon \Big| \frac{u(i+2\varepsilon) - u(i)}{\varepsilon} \Big|^{2}.$$

In this case the lattices of even and odd interactions are completely decoupled, and the correct limit is described by two variables

$$F(u_1, u_2) = \frac{1}{2} \int_{\Omega} (|u_1'|^2 + |u_2'|^2) dt,$$

where, for example, u is the limit of interpolations in the 'even' lattice and v the limit of interpolations in the 'odd' one. We may even have a more complex situation, as in the example

$$E_{\varepsilon}(u) = \sum_{i} \varepsilon \left( \left| \frac{u(i+2\varepsilon) - u(i)}{\varepsilon} \right|^2 + |u(i+\varepsilon) - u(i)|^2 \right),$$

where  $c_1 = \varepsilon$ , and the limit is

$$F(u_1, u_2) = \frac{1}{2} \int_{\Omega} (|u_1'|^2 + |u_2'|^2) dt + \int_{\Omega} |u_1 - u_2|^2 dt,$$

with a coupling between  $u_1$  and  $u_2$ . This type of limits arise in some kinds of homogenization problems in the continuum, where some complex geometries are usually involved. It must be remarked that their appearance seems much more 'natural' in a discrete setting.

Coerciveness conditions on nearest neighbors may be obtained indirectly; for examples in dimension one by difference by requiring an analogous growth condition both on second and third neighbors.

Remark 1.4 (homogenization) In the case of energies defined by a scaling process; i.e., when

$$\psi_k^{\varepsilon}(x,z) = \psi_k \left(\frac{z}{\varepsilon}\right),\tag{1.9}$$

then the limit energy density  $\varphi(M) = f(x, M)$  is independent of x and of the subsequence, and is characterized by the *asymptotic homogenization formula* 

$$\varphi(M) = \lim_{T \to +\infty} \frac{1}{T^N} \min \left\{ \mathcal{F}_T(u), \ u|_{\partial Q_T} = Mi \right\}, \tag{1.10}$$

where  $Q_T = (0, T)^N$ ,

$$\mathcal{F}_T(u) = \sum_{k \in \mathbb{Z}^n} \sum_{i \in R_1^k(Q_T)} \psi_k\left(\frac{u(i+k) - u(i)}{|k|}\right)$$

and  $u|_{\partial Q_T} = Mi$  means that "near the boundary" of  $Q_T$  the function u is the discrete interpolation of the affine function Mx (see [1] for further details). In the one-dimensional case this formula was first derived in [18] (see also (3.4) below), and it is the discrete analog of the nonlinear asymptotic formula for the homogenization of nonlinear energies of the form  $G_{\varepsilon}(u) = \int_{\Omega} g(x/\varepsilon, Du) dx$ , that reads

$$\varphi(M) = \lim_{T \to +\infty} \frac{1}{T^N} \inf \{ \mathcal{G}_T(u) : u = Mx \text{ on } \partial Q_T \},\$$

where now

$$\mathcal{G}_T(u) = \int_{Q_T} g(y, Du) \, dy$$

(see [14] for exact statements and hypotheses on g). Note however that the two formulas differ in two important aspects: the first is that (1.10) transforms functions depending on difference quotients (hence, vectors or scalars) into functions depending on gradients (hence, matrices or vectors, respectively); the second one is that the boundary conditions in (1.10) must be carefully specified, since we have to choose whether considering or not interactions that may 'cross the boundary' of  $Q_T$ . Remark 1.5 (special cases) It is worth examining formula (1.10) in some special cases. First, if all  $\psi_k$  are convex then, apart from a possible lower-order boundary contribution, the solution in (1.10) is simply  $u_i = Mi$ . In this case the  $\Gamma$ -limit coincides with the pointwise limit. Note that convexity in a sense always 'trivializes' discrete systems, in the sense that their continuous counterpart, obtained by simply substituting difference quotients with directional derivatives is already lower semicontinuous, and hence provides automatically an optimal lower bound. However, in some cases constraints are worse expressed in the continuous translation rather than in the original lattice notation, so that a direct treatment of the discrete system is easier. A striking and simple example is the computation of bounds for composite linear conducting networks as shown by Braides and Francfort [15].

Next, if only *nearest-neighbour interactions* are present then it reduces to

$$\varphi(M) = \sum_{i=1}^{n} \psi_i^{**}(Me_i),$$

where  $\psi_i = \psi_{e_i}$  and  $f^{**}$  denotes the lower semicontinuous and convex envelope of f. Note that convexity is not a necessary condition for lower semicontinuity at the discrete level: this convexification operation should be interpreted as an effect due to oscillations at a 'mesoscopic scale' (i.e., much larger than the 'microscopic scale'  $\varepsilon$  but still vanishing as  $\varepsilon \to 0$ ). If not only nearest neighbours are taken into account then the mesoscopic oscillations must be coupled with microscopic ones (see [18, 32] and the next section).

Finally, note that also in the non-convex case (the relaxation of) the pointwise limit always gives an upper bound for the  $\Gamma$ -limit and is not always trivial (see e.g. the paper by Blanc, Le Bris and Lions [8]).

#### 1.2 Microscopic oscillations: the Cauchy-Born rule

One issue of interest in the study of discrete-to-continuous problems is whether to a 'macroscopic' gradient there corresponds at the 'microscopic' scale a 'regular' arrangements of lattice displacement. For energies deriving from a scaling process as in (1.9) this can be translated into the asymptotic study of minimizers for the problems defining  $\varphi(M)$ ; in particular whether  $u_i = Mi$  is a minimizer (in which case we say that the (strict) Cauchy-Born rule holds at M), or if minimizers tend to a periodic perturbation of Mi; i.e. ground states are periodic (in which case we say that the weak Cauchy-Born rule holds at M). Note that the strict Cauchy-Born rule can be translated into the equality

$$\varphi(M) = \sum_{k \in \mathbb{Z}^N} \psi_k \Big( \frac{Mk}{|k|} \Big), \tag{1.11}$$

and that it always holds if all  $\psi_k$  are convex, as remarked above.

A simple example in order to understand how the validity and failure of the Cauchy-Born rule can be understood in terms of the form of  $\varphi$  is given by the one-dimensional case with next-to-nearest neighbours; i.e. when only  $\psi_1$  and  $\psi_2$  are non zero. In this case  $\varphi = \psi^{**}$ , where

$$\psi(z) = \psi_2(2z) + \frac{1}{2} \min \Big\{ \psi_1(z_1) + \psi_1(z_2) : z_1 + z_2 = 2z \Big\}.$$
(1.12)

The second term, obtained by minimization, is due to oscillations at the microscopic level: nearest neighbours rearrange so as to minimize their interaction coupled with that between second neighbours (see [11] for a simple treatment of these one-dimensional problems). In this case we can read the microscopic behaviour as follows (for the sake of simplicity we suppose that the minimum problem in (1.12) has a unique solution, upon changing  $z_1$  into  $z_2$ ):

(i) first case:  $\psi$  is convex at z (i.e.,  $\psi(z) = \varphi(z)$ ). We have the two cases

(a)  $\psi(z) = \psi_1(z) + \psi_2(z)$ ; in this case  $z = z_1 = z_2$  minimizes the formula giving  $\varphi$  and (1.11) holds; hence, the strict Cauchy-Born rules applies;

(b)  $\psi(z) < \psi_1(z) + \psi_2(z)$ ; in this case we have a 2-periodic ground state with 'slopes'  $z_1$  and  $z_2$ , and the weak Cauchy-Born rules applies;

(ii) second case:  $\psi$  is not convex at z (i.e.,  $\psi(z) > \varphi(z)$ ). In this case the Cauchy-Born rule is violated, but a finer analysis (see below) shows that minimizers are fine mixtures of states satisfying the conditions above; hence the condition holds 'locally'.

For energies in higher-dimensions this analysis is more complex. A similar argument as in the one-dimensional case is used in [28] to show the non-validity of the Cauchy-Born rule even for some types of very simple lattice interactions in dimension two, with nonlinearities of geometrical origin.

Finally, it must be noted that formula (1.10) does not simplify even in the simplest case of three levels of interactions in dimension one (as suggested by the physical literature as in [30]), thus showing that this effect, typical of nonlinear homogenization, is really due to the lattice interactions and not restricted to vector-valued functions as in the case of homogenization on the continuum.

#### Higher-order developments: phase transitions

In the case of failure of the Cauchy-Born rule, non-uniform states may be preferred as minimizers, and surface energies must be taken into account in their description. A first attempt to rigorously describe this phenomena can be found in Braides and Cicalese [12], again in the simplest nontrivial case of next-to-nearest neighbour interactions of the form independent of  $\varepsilon$ . In that case, using the notion of equivalence by  $\Gamma$ -convergence (see [19]) we may infer that (under some technical assumptions) the discrete systems are equivalent to the perturbation of a non-convex energy on the continuum, of the form

$$\int_{\Omega} \psi(u') \, dt + \varepsilon^2 C \int_{\Omega} |u''|^2 \, dt,$$

thus recovering a well-known formulation of the gradient theory of phase transitions. This result shows that a surface term (generated by the second gradient) penalizes high oscillations between states locally satisfying some Cauchy-Born rule.

#### **1.3** Continuous energies on functions of bounded variation

In this paper we extend the homogenization formula as above for systems whose continuous counterpart is naturally defined on some set of functions of bounded variation (see below for definitions). In particular we will consider energies defined on the Ambrosio-De Giorgi SBV spaces (see [6, 25, 4, 9]). In the one-dimensional case we can picture a function  $u \in SBV(a, b)$  as a piecewise-Sobolev functions. If denoting by S(u) its set of discontinuity points, then (local, homogeneous and translation-invariant) energies on SBV(a, b) are of the form

$$\mathcal{E}(u) = \int_{a}^{b} f(u'(x)) \, dx + \sum_{t \in S(u)} g([u](t)), \tag{1.13}$$

where  $u^{\pm}(t)$  are the right and left-hand side limits of u at t.

The pioneering example for this case is due to Chambolle [20], who treated the limit of some finite-difference schemes in Computer Vision (see [7]), producing as the continuum counterpart the one-dimensional version of the Mumford-Shah functional ([31]). That is however a 'limit' case when the potential is a truncated quadratic function and the decoupling process between bulk and surface parts is obtained by considering the effect of the quadratic and constant parts separately. A different approach is started in a subsequent paper by Braides, Dal Maso and Garroni [13], who consider potentials of convex-concave type and express the limit in terms of different scalings of the two parts (the same type of interactions are analyzed by Truskinovsky [35]).

The general case of nearest-neighbour interactions has been treated by Braides and Gelli in [17], where the following result is proved (for missing definitions see the sections below).

**Theorem 1.6** (Nearest-neighbour interactions) Let  $\Omega = (a, b)$  and let  $\psi_{\varepsilon} : \mathbb{R} \to [0, +\infty]$  satisfy

$$\psi_{\varepsilon}(z) \ge c_1 |z|^p - c_2 \qquad \text{for all } z < 0 \tag{1.14}$$

for some p > 1 and  $c_1 > 0$ , and let  $E_{\varepsilon}$  be given by

$$E_{\varepsilon}(u) = \sum_{i,i+\varepsilon \in Z_{\varepsilon}} \varepsilon \psi_{\varepsilon} \Big( \frac{u(i+\varepsilon) - u(i)}{\varepsilon} \Big).$$

Let  $T_{\varepsilon} \in \mathbb{R}$  be an arbitrary sequence satisfying

$$\lim_{\varepsilon \to 0^+} T_{\varepsilon} = +\infty, \qquad \lim_{\varepsilon \to 0^+} \varepsilon T_{\varepsilon} = 0, \tag{1.15}$$

and let  $F_{\varepsilon}, G_{\varepsilon} : \mathbb{R} \to [0, +\infty]$  be defined by

$$F_{\varepsilon}(z) = \begin{cases} \psi_{\varepsilon}(z) & z \leq T_{\varepsilon} \\ +\infty & z > T_{\varepsilon} \end{cases}$$
(1.16)

$$G_{\varepsilon}(z) = \begin{cases} \varepsilon \psi_{\varepsilon} \left(\frac{z}{\varepsilon}\right) & \text{if } z > \varepsilon T_{\varepsilon} \\ +\infty & \text{otherwise.} \end{cases}$$
(1.17)

Assume that there exist  $F, G : \mathbb{R} \to [0, +\infty]$  such that (note that this assumption is always satisfied, upon extracting a subsequence)

$$\Gamma - \lim_{\varepsilon \to 0^+} F_{\varepsilon}^{**} = F \ on \ \mathbb{R}, \tag{1.18}$$

$$\Gamma - \lim_{\varepsilon \to 0^+} \operatorname{sub}^- G_{\varepsilon} = G \text{ on } \mathbb{R} \setminus \{0\},$$
(1.19)

where sub<sup>-</sup>g is the lower semicontinuous and subadditive envelope of g. Then,  $(E_{\varepsilon})_{\varepsilon}$   $\Gamma$ -converges to E with respect to the convergence in  $L^1_{loc}(0,L)$  and the convergence in measure, where

$$E(u) = \begin{cases} \int_a^b \overline{F}(\dot{u}) \, dx + \sum_{S(u)} \overline{G}([u]) + \sigma Du_c^+(0, L) \\ & \text{if } u \in BV_{\text{loc}}(0, L) \ D_c u^- = 0 \ \text{and} \ [u] > 0 \ \text{on } S(u) \\ +\infty & \text{otherwise in } L^1(0, L), \end{cases}$$

where  $\overline{F}$  and  $\overline{G}$  are defined by (for notation convenience we set G(0) = 0)

$$F(z) := \inf\{F(z_1) + G^0(z_2) : z_1 + z_2 = z\},\$$

 $\overline{G}(z) := \inf\{F^{\infty}(z_1) + G(z_2) : z_1 + z_2 = z\},$ and  $\sigma := \overline{F}^{\infty}(1)$ , where  $F^{\infty}(z) = \lim_{z \to +\infty} \frac{F(z)}{z}$  and  $G^0(z) = \lim_{z \to 0^+} \frac{G(z)}{z}.$ 

The fundamental issue here is the separation of scale effect highlighted by equations (1.16)–(1.17), that allows to derive the bulk and surface energy densities of the limit from the discrete interactions. In this paper, always remaining in the one-dimensional framework, we show how in the case of long-range interactions this scale separation can be coupled with the nonlinear homogenization process described in formula (1.10) (see Theorem 3.2 further on). The general *n*-dimensional vector-valued case can be dealt with by using the localization and integral representation methods of  $\Gamma$ -convergence [2]). Particular cases when a simpler description of the limit energy densities is possible are treated in [21, 22, 16].

#### **1.4** Some results on non-central interactions

Going back to the initial paragraph of this Introduction it is worth remarking once more that all the results listed so far are concerned with "central interactions" that is, energies obtained by summing up "pairwise" interactions depending on the distance u(i) - u(j). From a general point of view it will be interesting also to study energies of type  $E_{\varepsilon}(u) = \sum_{i \in Z_{\varepsilon}} E_{\varepsilon}^{(i)}(u)$  where  $E_{\varepsilon}^{(i)}(u)$  is the energy of a single node *i* given by a potential  $\psi_i^{\varepsilon}(u) = \psi^{\varepsilon}(u(i), u(j_1), \ldots, u(j_m))$  accounting for interactions between *i* and all the nodes  $j_1, \ldots, j_m$  lying in a fixed neighbourhood of *i*, suggested by the crystalline structure underlying the model (for example a slanted or regular polyhedrum generated by fixed directions). In case  $\psi^{\varepsilon}(u(i), u(j_1), \ldots, u(j_m)) = \sum_{\ell=1,\ldots,m} \psi^{\varepsilon}(u(i), u(j_\ell))$  one goes back to the previous case but in general these interactions may have a more complex form. Actually this kind of approach has revealed to be successful (and also necessary) in order to approximate with difference schemes the functional describing the linearized elastic energy of a body with prescribed Lamè constants.

In [3] Alicandro, Focardi and Gelli have applied this approach including also the possibility of fracture and have given a variational approximation by difference schemes of the functional

$$\mu \int_{\Omega} |\mathcal{E}u|^2 dx + \frac{\lambda}{2} \int_{\Omega} |\operatorname{div}(u)|^2 dx + \int_{J_u} \Phi([u], \nu_u) d\mathcal{H}^{N-1}$$
(1.20)

defined on the space  $SBD(\Omega)$  of integrable functions u whose symmetrized distributional derivative E(u) is a bounded Radon measure with density  $\mathcal{E}u$  with respect to the Lebesgue measure and with singular part concentrated on an (N-1)-dimensional set  $J_u$  on which it is possible to define a normal  $\nu_u$  and a jump [u] (defined in a weak sense; see [6] for precise definitions).

For such a functional an approximation with energies of type (1.4) leads as limit to a proper subclass of functionals in (1.20); more precisely, those with coefficients  $\mu$  and  $\lambda$  related by a fixed ratio (according to the classical computation of the Cauchy relations starting from a lattice with pairwise interactions). Here the right energies to be considered are of the form

$$E_{\varepsilon}(u) = \sum_{i \in Z_{\varepsilon}} \sum_{k \in \mathbb{Z}^N} \psi_k^{\varepsilon}(D_{\varepsilon}^k u(i) + \theta \operatorname{div}_{\varepsilon}^k u(i))$$

where  $D_{\varepsilon}^{k}u$ ,  $\operatorname{div}_{\varepsilon}^{k}u$  are proper discretizations of  $\nabla u$  and  $\operatorname{div} u$ , respectively, obtained by the interactions of i with the nodes  $j_{\ell}$  lying along each coordinate directions and having discrete distance along each coordinate equal to k ( $j_{\ell} = i \pm ke_{\ell}$ ) and  $\theta$  is a positive parameter (for more details we refer to [3]). Another type of "non-central" interactions has been studied by Focardi

and Gelli in [27] to approximate functionals of Fracture Mechanics with prescribed quasi-convex bulk density and subadditive surface density, that is functionals of the form

$$\int_{\Omega} \psi(\nabla u) \, dx + \int_{J_u} g\left(u^+ - u^-, \nu_u\right) \, d\mathcal{H}^2$$

defined for  $u \in SBV(\Omega; \mathbb{R}^3)$ , where here  $\Omega$  is an open set in  $\mathbb{R}^3$ ,  $\psi$  and g are assigned. In this last case the energy potentials considered take into account the interactions between the vertices of given simplices chosen in order to provide a regular triangulation of  $\mathbb{Z}^3$ .

For the sake of completeness it must be mentioned that according to the variational nature of the approximations all these convergence results lead to the study of convergence of minimum problems. To this regard we have to remark that in the case of the so called "long-range interactions" for functional allowing for fracture (that is, when the limit energy presents a non-zero surface part) more than one type of boundary-value problem can be formulated and an effect of boundary layer also occurs. The problem was first studied by Braides and Gelli in [16] where two type of problems where treated. The first one is to define discrete functions on the whole  $\varepsilon \mathbb{Z}^N$  and to fix the values on the nodes outside the domain  $\Omega$  equal to a fixed function  $\varphi$ ; in this case the interactions 'across the boundary of  $\Omega$ ' give rise to an additional boundary term in the limit energy of the type

$$\int_{\partial\Omega} \mathcal{G}(\gamma(u) - \varphi, \nu_{\partial\Omega}) \, d\mathcal{H}^{N-1} \tag{1.21}$$

where  $\gamma(u)$  is the inner trace of u with respect to  $\partial \Omega$  (i.e.,

$$\gamma(u)(x) = \lim_{\rho \to 0+} \oint_{B(x,\rho) \cap \Omega} u(y) \, dy)$$

The second method consists in considering the functions as fixed only on  $\partial\Omega$  that is, only a proper subset of pairwise interactions are linked with the constraint; in this case, the boundary term gives a different contribution, corresponding to a boundary-layer effect. Indeed, the additional term is still of type (1.21) but with the surface density  $\mathcal{G}'$  strictly less than  $\mathcal{G}$ , the gap magnifying with the range of interaction considered.

# 2 Lattice systems with limits defined in BV

We finally state and prove a theorem in a simple one-dimensional setting, with limit defined on functions of bounded variation. We include some preliminary definitions for the sake of completeness.

For a set A of  $\mathbb{R}$  we denote int A the interior of A. We write  $\operatorname{sgn} t$  and [t] to denote the sign of t and the integer part of t, respectively. We write  $\mathcal{L}_1(A)$  or |A| to denote the Lebesgue measure of  $A \subset \mathbb{R}$ , # for the counting measure and  $\delta_t$  for the Dirac mass at t. We use standard notation for Sobolev and Lebesgue spaces. If  $\phi$  is a measurable function then  $\int_B \phi dx$  is its mean value on the set B. If  $\mu$  is a (signed) Borel measure then  $\mu^+$  and  $\mu^-$  denote its positive and negative parts, respectively, and  $|\mu|$  its total variation; if B is a Borel set, then the measure  $\mu \sqcup B$  is defined as  $\mu \sqcup B(A) := \mu(A \cap B)$ . The letter c will denote a strictly positive constant whose value may vary from line to line.

### 2.1 Functions of bounded variation

We recall that the space BV(a, b) of functions of bounded variation on (a, b) is defined as the space of functions  $u \in L^1(a, b)$  whose distributional derivative Du is a signed Borel measure. For

each such u there exists  $f \in L^1(a, b)$ , a (at most countable) set  $S(u) \subset (a, b)$ , a sequence of real numbers  $(a_t)_{t \in S(u)}$  with  $\sum_t |a_t| < +\infty$  and a non-atomic measure  $D_c u$  singular with respect to the Lebesgue measure such that the equality of measures  $Du = f \mathcal{L}_1 + \sum_{t \in S(u)} a_t \delta_t + D_c u$  holds. It can be easily seen that for such functions the left hand-side and right hand-side approximate limits  $u^-(t), u^+(t)$  exist at every point, and that  $S(u) = \{t \in \mathbb{R} : u^-(t) \neq u^+(t)\}$  and  $a_t = u^+(t) - u^-(t) =: [u](t)$ . We will write u' = f, which is an approximate gradient of u.  $D_c u$  is called the *Cantor part* of Du. A sequence  $u_j$  converges weakly to u in BV(a, b) if  $u_j \to u$  in  $L^1(a, b)$  and  $\sup_j |Du_j|(a, b) < +\infty$ .

The space SBV(a, b) of special functions of bounded variation is defined as the space of functions  $u \in BV(a, b)$  such that  $D_c u = 0$ ; i.e., whose distributional derivative Du can be written as  $Du = u' \mathcal{L}_1 + \sum_{t \in S(u)} (u^+(t) - u^-(t))\delta_t$ . This notation describes a particular case of a SBV-functions space as introduced by De Giorgi and Ambrosio [25]. We will mainly deal with functionals whose natural domain is that of piecewise- $W^{1,p}$  functions, which is a particular sub-class of SBV(a, b) corresponding to the conditions  $\dot{u} \in L^p(a, b)$  and  $\#(S(u)) < +\infty$ , but we nevertheless use the more general SBV notation for future reference and for further generalization to higher dimensions (see [5]). For an introduction to BV and SBV functions we refer to the book by Ambrosio, Fusco and Pallara [6], while approximation methods for free-discontinuity problems are discussed by Braides [9].

A class of energies on SBV(a, b) are those of the form (1.13) with  $f, g: \mathbb{R} \to [0, +\infty]$ . Lower semicontinuity conditions on  $\mathcal{E}$  are equivalent to requiring that f is lower semicontinuous and convex and g is lower semicontinuous and subadditive; i.e.,  $g(x + y) \leq g(x) + g(y)$ . The latter can be interpreted as a condition penalizing fracture fragmentation, whereas convexity penalizes oscillations. If  $\varphi$  is not lower semicontinuous and convex (respectively, subadditive) then we may consider its *lower semicontinuous and convex* (respectively, *subadditive*) *envelope*; i.e., the greatest lower semicontinuous and convex (respectively, subadditive) function not greater than  $\varphi$ , that we denote by  $\varphi^{**}$  (respectively,  $\operatorname{sub}^{-}\varphi$ ). For a discussion on the role of these conditions for the lower semicontinuity of  $\mathcal{E}$  we refer to [9] Section 2.2 or [11]. Energies in BV must satisfy further compatibility conditions between f and g.

#### 2.2 $\Gamma$ -convergence

We recall the definition of De Giorgi's  $\Gamma$ -convergence in a metric space space (X, d): given a family of functionals  $F_n : X \to [0, +\infty], n \in \mathbb{N}$ , for  $u \in X$  we define the  $\Gamma$ -lower limit and  $\Gamma$ -upper limit of  $(F_n)$  as

$$F'(u) = \Gamma(d) - \liminf_{n} F_n(u) := \inf \left\{ \liminf_{n} F_n(u_n) : \lim_{n} d(u_n, u) = 0 \right\},$$
(2.1)

and

$$F''(u) = \Gamma(d) - \limsup_{n} F_n(u) := \inf \left\{ \limsup_{n} F_n(u_n) : \lim_{n} d(u_n, u) = 0 \right\}.$$
 (2.2)

Note that the functions F' and F'' are lower semicontinuous. If these two quantities coincide then their common value is called the  $\Gamma$ -*limit* of the sequence  $(F_n)$  at u, and is denoted by  $\Gamma$ -lim<sub>n</sub>  $F_n(u)$  or  $\Gamma(d)$ -lim<sub>n</sub>  $F_n(u)$ . Equivalently,  $F(u) = \Gamma$ -lim<sub>n</sub>  $F_n(u)$  if and only if the two following conditions are satisfied:

(i) (lower semicontinuity inequality) for all sequences  $(u_n)$  converging to u in X we have  $F(u) \leq \liminf_n F_n(u_n)$ ;

(ii) (existence of a recovery sequence) there exists a sequence  $(u_n)$  converging to u in X such that  $F(u) \ge \limsup_n F_n(u_n)$ .

We will use as d the  $L^1$ -metric or a metric giving convergence in measure.

For a comprehensive study of  $\Gamma$ -convergence we refer to the books of Dal Maso [24] and Braides [11] (see also [14] Part II). The reason for the introduction of this notion is explained by the following fundamental theorem.

**Theorem 2.1** Let  $F = \Gamma - \lim_n F_n$ , and let a compact set  $K \subset X$  exist such that  $\inf_X F_n = \inf_K F_n$  for all n. Then

$$\exists \min_{Y} F = \liminf_{n} \inf_{Y} F_n.$$

Moreover, if  $(u_n)$  is a converging sequence with  $\lim_n F_n(u_n) = \lim_n \inf_X F_n$  then its limit is a minimum point for F.

### 3 Statement of the result

With fixed L > 0, consider an open interval (0, L) of  $\mathbb{R}$  and for  $n \in \mathbb{N}$  let  $\lambda_n = L/n$ . This parameter will play the role played by  $\varepsilon$  in the Introduction. We use the notation  $x_n^i = i\lambda_n$ . We define  $\mathcal{A}_n(0, L)$  as the set of discrete functions  $u : \lambda_n \mathbb{Z} \cap [0, L] \to \mathbb{R}$ . This set will be identified as the subset of  $L^1(0, L)$  of functions constant almost everywhere on each interval  $(x_n^i - \frac{\lambda_n}{2}, x_n^i + \frac{\lambda_n}{2}), i \in \{1, \ldots, n\}.$ 

Let  $\tilde{K} \in \mathbb{N}$  be fixed and for  $n \in \mathbb{N}$  and  $j \in \{1, \ldots, K\}$  let  $\psi_n^j : \mathbb{R} \to (-\infty, +\infty]$  be given Borel functions bounded below. Define  $E_n : L^1(0, L) \to [0, +\infty]$  as

$$E_n(u) = \begin{cases} \sum_{j=1}^K \sum_{i=0}^{n-j} \lambda_n \psi_n^j \left( \frac{u(x_n^{i+j}) - u(x_n^i)}{j\lambda_n} \right) & x \in \mathcal{A}_n(0, L) \\ +\infty & \text{otherwise in } L^1(0, L). \end{cases}$$
(3.1)

We will describe the asymptotic behaviour of  $E_n$  as  $n \to +\infty$  when the energy densities are potentials of Lennard-Jones type. More precisely, we will make the following assumption:

(growth conditions: superlinearity at  $-\infty$ , mixed type at  $+\infty$ ) 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  $c_j^1$ ,  $c_j^2 > 0$  such that

$$c_j^1(\Psi(z) - 1) \le \psi_n^j(z) \le c_j^2 \max\{\Psi(z), |z|\} \quad \text{for all } z \in \mathbb{R}.$$
(3.2)

Under this hypothesis it will be possible to describe explicitly the behaviour of the energies  $E_n$  by means of their  $\Gamma$ -limit. The exact statement of the result will be given at the end of this section.

**Remark 3.1** Hypothesis (3.2) is designed to cover the case of Lennard-Jones potential (and potential of the same shape), where  $\psi_n^j = \psi$  is equal for all j and n, and

$$\psi(z) = \frac{k_1}{z^{12}} - \frac{k_2}{z^6}$$

for some  $k_1, k_2 > 0$ . In this case, we can take

$$\Psi(z) = \begin{cases} \frac{1}{z^{12}} & \text{if } z > 0\\ +\infty & \text{otherwise.} \end{cases}$$

Another case included in hypothesis (3.2) is when all functions satisfy a uniform growth condition of order p > 1; i.e.,

$$c_j(|z|^p - 1) \le \psi_n^j(z) \le C c_j(|z|^p + 1)$$

for all j and n.

Note that in the case K = 1 (nearest-neighbour interaction) the right hand-side of (3.2) can be dropped (see Theorem 1.6).

Before stating our main result, we have to introduce the counterpart of the energy densities  $F_n$  and  $G_n$  in Theorem 1.6 for the case K > 1. Following the idea already performed in [18], we consider clusters of N subsequent points (N large) and define an average discrete energy for each of those clusters, so that the energy  $E_n$  may be approximately regarded as a 'nearest neighbour interaction energy' acting between such clusters, to which the above description applies.

Actually, we fix a sequence  $(N_n)$  of natural numbers with the property

$$\lim_{n} N_n = +\infty, \qquad \lim_{n} \frac{N_n}{n} = 0, \tag{3.3}$$

and we define

$$\psi_n(z) = \min\left\{\frac{1}{N_n} \sum_{j=1}^K \sum_{i=0}^{N_n - j} \psi_n^j \left(\frac{u(i+j) - u(i)}{j}\right) : \ u : \{0, \dots, N_n\} \to \mathbb{R}, \\ u(x) = zx \text{ if } x = 0, \dots, K, N_n - K, \dots, N_n\right\}.$$
(3.4)

By using the energies  $\psi_n$  we will regard a system of  $N_n$  neighbouring points as a single interaction between the two extremal ones, up to a little error which is negligible as  $N_n \to +\infty$ . We can now state our convergence result, whose thesis is exactly the same as that of Theorem 1.6 with  $\varepsilon_n := N_n \lambda_n$ .

**Theorem 3.2** Let  $\psi_n^j$  satisfy (3.2) and let  $(E_n)$  be given by (3.1). Let  $\psi_n$  be given by (3.4) and let  $\varepsilon_n = N_n \lambda_n$ . For all  $n \in \mathbb{N}$  let  $T_n \in \mathbb{R}$  be defined as in (1.15), and let  $F_n, G_n : \mathbb{R} \to [0, +\infty]$  be defined by

$$F_n(z) = \begin{cases} \psi_n(z) & z \le T_n \\ +\infty & z > T_n \end{cases}$$
(3.5)

$$G_n(z) = \begin{cases} \varepsilon_n \psi_n \left(\frac{z}{\varepsilon_n}\right) & \text{if } z > \varepsilon_n T_n \\ +\infty & \text{otherwise.} \end{cases}$$
(3.6)

Assume that there exist  $F, G : \mathbb{R} \to [0, +\infty]$  such that

$$\Gamma - \lim_{n} F_n^{**} = F \quad on \ \mathbb{R}, \tag{3.7}$$

$$\Gamma - \limsup_{n} \operatorname{sub}^{-} G_{n} = G \ on \ \mathbb{R} \setminus \{0\}.$$
(3.8)

Note that this assumption is always satisfied, upon extracting a subsequence. Then,  $(E_n)_n \Gamma$ converges to E with respect to the convergence in  $L^1_{loc}(0,L)$  and the convergence in measure,
where

$$E(u) = \begin{cases} \int_0^L \overline{F}(\dot{u}) \, dx + \sum_{S(u)} \overline{G}([u]) + \sigma Du_c^+(0, L) \\ & \text{if } u \in BV_{\text{loc}}(0, L) \ D_c u^- = 0 \ , \ and \ [u] > 0 \ on \ S(u) \\ & +\infty \qquad otherwise \ in \ L^1(0, L), \end{cases}$$

where  $\overline{F}$  and  $\overline{G}$  are defined by (for notation convenience we set G(0) = 0)

$$\overline{F}(z) := \inf\{F(z_1) + G^0(z_2) : z_1 + z_2 = z\},\$$
  
$$\overline{G}(z) := \inf\{F^{\infty}(z_1) + G(z_2) : z_1 + z_2 = z\},\$$

and  $\sigma := \overline{F}^{\infty}(1)$ .

**Proof.** Upon adding a fixed positive constant we may assume that all  $\psi_n^j$  are non negative. We begin by proving the limit inequality. We thus fix  $u_n, u \in L^1_{loc}(0, L)$  such that  $u_n \to u$  in measure and  $\sup_n E_n(u_n) < +\infty$ . Upon extracting a subsequence we may suppose that  $u_n \to u$  a.e. and that the limit  $\lim_n E_n(u_n)$  exists. By using (3.2) and reasoning as in the proof of Theorem 1.6 we get that  $u \in BV_{loc}(0, L)$  and  $u_n \to u$  weakly in  $BV_{loc}(0, L)$  (see [17] for details). It will be enough to show that for all 0 < a < b < L fixed we have

$$\int_{a}^{b} \overline{F}(\dot{u}(x)) \, dx + \sum_{t \in S(u) \cap (a,b)} \overline{G}([u](t)) + \sigma Du_{c}^{+}(a,b) \le \lim_{n} E_{n}(u_{n}). \tag{3.9}$$

As already mentioned, for all  $n \in \mathbb{N}$  we will estimate the energy  $E_n(u_n)$  with a 'nearest neighbour interaction' one, with energy density  $\psi_n$  and discretization step  $\varepsilon_n = \lambda_n N_n$ . Thus, with fixed  $N_n$ , we will choose  $w \in \{1, \ldots, N_n\}$  in such a way that we can find a suitable piecewise affine interpolation of  $u_n$  on the lattice  $(\lambda_n w + \varepsilon_n \mathbb{Z}) \cap (a, b)$ , call it  $v_n$ , so that  $v_n$  still converges to uin measure and  $E_n(u_n) = E_n^1(v_n) + o(1)$ .

For all  $w \in \{1, \ldots, N_n\}$  let

$$Z_n(w) = \{\ell \in w + N_n \mathbb{Z} : \lambda_n \ell \in (a, b)\}$$

$$\Phi_{n}(w) = \sum_{\ell \in Z_{n}(w)} \left( \sum_{j=1}^{K} \sum_{i=\ell-2K}^{\ell+2K-1} \lambda_{n} \psi_{n}^{j} \left( \frac{u_{n}(\lambda_{n}(i+j)) - u_{n}(\lambda_{n}i)}{j\lambda_{n}} \right) \right)$$

$$\sum_{s=\ell-2K}^{\ell+2K-1} |u_{n}(\lambda_{n}(s+1)) - u_{n}(\lambda_{n}s)| \qquad (3.10)$$

Note that  $\sum_{s=\ell-2K}^{\ell+2K-1} |u_n(\lambda_n(s+1)) - u_n(\lambda_n s)| = |Du_n|([(\ell-2K)\lambda_n, (\ell+2K)\lambda_n]))$ , where we consider the discrete function  $u_n$  identified with the  $L^1$  function piecewise constant. Since each interval  $[\lambda_n s, \lambda_n(s+1)]$  belongs at most to 4K interval of the type  $[\lambda_n(\ell-2K), \lambda_n(\ell+2K)]$  we have that

$$\sum_{w=1}^{N_n} \sum_{\ell \in Z_n(w)} \sum_{s=\ell-2K}^{\ell+2K-1} |u_n(\lambda_n(s+1)) - u_n(\lambda_n s)| \le 4K |Du_n|(a,b).$$

Moreover, we also have

$$\sum_{w=1}^{N_n} \sum_{\ell \in Z_n(w)} \sum_{j=1}^{K} \sum_{i=\ell-2K}^{\ell+2K-1} \lambda_n \psi_n^j \Big( \frac{u_n(\lambda_n(i+j)) - u_n(\lambda_n i)}{j\lambda_n} \Big)$$
  
= 
$$\sum_{i'=0}^{4K} \sum_{w=1}^{N_n} \sum_{\ell \in Z_n(w)} \lambda_n \psi_n^j \Big( \frac{u_n(\lambda_n(\ell-2K+j+i')) - u_n(\lambda_n(\ell-2K+i'))}{j\lambda_n} \Big)$$
  
$$\leq 5KE_n(u_n).$$
(3.11)

Hence,

$$\sum_{w=1}^{N_n} \Phi_n(w) \le 5KE_n(u_n) + 4K|Du_n|(a,b) \le c$$

and we can find  $w_n \in \{1, ..., N_n\}$  such that  $\Phi_n(w_n) \leq \frac{c}{N_n}$ . For all  $\ell \in Z_n(w_n)$  we define

$$z_n^{\ell} = \frac{u_n(\lambda_n(\ell + N_n - K)) - u_n(\lambda_n(\ell + K))}{\lambda_n(N_n - 2K)}$$

and  $\tilde{u}_n^\ell$  on  $\{0, \ldots, N_n\}$  by

$$\tilde{u}_{n}^{\ell}(i) = \begin{cases} \frac{1}{\lambda_{n}} (u_{n}(\lambda_{n}(\ell+i)) - u_{n}(\lambda_{n}(\ell+K))) + z_{n}^{\ell}K \\ & \text{if } i = K, \dots, N_{n} - K \\ z_{n}^{\ell}i & \text{otherwise.} \end{cases}$$

Finally, we define  $v_n$  as the continuous piecewise-affine interpolate function such that  $v_n(a) = u(a)$  and  $v'_n = z_n^{\ell}$  on  $(\lambda_n \ell, \lambda_n (\ell + N_n))$  for  $ell \in Z_n(w_n)$ . Note that  $v_n \to u$  in measure and  $\tilde{u}_n^{\ell}$  is a test function for the minimum problem defining  $\psi_n(z_n^{\ell})$ . We then have

$$E_{n}(u_{n}) \geq \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=\ell+K}^{\ell+N_{n}-K-j} \lambda_{n} \psi_{n}^{j} \Big( \frac{u_{n}(\lambda_{n}(i+j)) - u_{n}(\lambda_{n}i)}{j\lambda_{n}} \Big)$$
  

$$\geq \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=0}^{N_{n}-j} \lambda_{n} \psi_{n}^{j} \Big( \frac{\tilde{u}_{n}^{\ell}(i+j) - \tilde{u}_{n}^{\ell}(i)}{j} \Big)$$
  

$$- \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=0}^{K-1} \lambda_{n} \psi_{n}^{j} \Big( \frac{\tilde{u}_{n}^{\ell}(i+j) - \tilde{u}_{n}^{\ell}(i)}{j} \Big)$$
  

$$- \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=N_{n}-K-j+1}^{N_{n}-j} \lambda_{n} \psi_{n}^{j} \Big( \frac{\tilde{u}_{n}^{\ell}(i+j) - \tilde{u}_{n}^{\ell}(i)}{j} \Big).$$
(3.12)

As for the first term in (3.12), for any  $\ell \in Z_n(w_n)$ , we have

$$\sum_{j=1}^{K}\sum_{i=0}^{N_n-j}\psi_n^j\Big(\frac{\tilde{u}_n^\ell(i+j)-\tilde{u}_n^\ell(i)}{j}\Big) \ge N_n\psi_n(z_n^\ell),$$

so that, denoting  $Z_n = \{i \in \mathbb{Z} : \lambda_n w_n + \varepsilon_n i \in Z_n(w_n)\},\$ 

$$\sum_{\ell \in Z_n(w_n)} \sum_{j=1}^K \sum_{i=0}^{N_n-j} \lambda_n \psi_n^j \left( \frac{\tilde{u}_n^\ell(i+j) - \tilde{u}_n^\ell(i)}{j} \right) \ge \sum_{i \in Z_n} \varepsilon_n \psi_n \left( \frac{v_n(\varepsilon_n(i+1)) - v_n(\varepsilon_n i)}{\varepsilon_n} \right).$$
(3.13)

By plugging estimate (3.13) in (3.12) we get

$$E_n(u_n) \geq \sum_{i \in Z_n} \varepsilon_n \psi_n \Big( \frac{v_n(\varepsilon_n(i+1)) - v_n(\varepsilon_n i)}{\varepsilon_n} \Big)$$

$$-\sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=0}^{K-1} \lambda_{n} \psi_{n}^{j} \Big( \frac{\tilde{u}_{n}^{\ell}(i+j) - \tilde{u}_{n}^{\ell}(i)}{j} \Big)$$
$$-\sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i=N_{n}-K-j+1}^{N_{n}-j} \lambda_{n} \psi_{n}^{j} \Big( \frac{\tilde{u}_{n}^{\ell}(i+j) - \tilde{u}_{n}^{\ell}(i)}{j} \Big)$$
$$=: \sum_{i \in Z_{n}} \varepsilon_{n} \psi_{n} \Big( \frac{v_{n}(\varepsilon_{n}(i+1)) - v_{n}(\varepsilon_{n}i)}{\varepsilon_{n}} \Big) - I_{n}^{1} - I_{n}^{2}.$$
(3.14)

It remains to give an estimate of the terms  $I_n^1, I_n^2$ . We will confine ourselves to prove that  $I_n^1 = o(1)$ , the proof of the same estimate for  $I_n^2$  being analogous. Indeed, by using hypothesis (3.2), we have

$$I_n^1 \leq c_j^2 \sum_{\ell \in Z_n(w_n)} \sum_{j=1}^K \sum_{i=0}^{K-1} \left( \lambda_n \Psi \left( \frac{u_n(\lambda_n(\ell+i+j)) - u_n(\lambda_n(\ell+i)))}{j\lambda_n} \right) + \left| \frac{u_n(\lambda_n(\ell+i+j)) - u_n(\lambda_n(\ell+i)))}{j} \right| \right)$$

$$(3.15)$$

and, by convexity, we have also

$$\begin{aligned}
I_{n}^{1} \\
&\leq \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} c_{j}^{2} \sum_{i=0}^{K-1} \sum_{s=i}^{i+j-1} \frac{1}{j} \Big( \lambda_{n} \Psi \Big( \frac{u_{n}(\lambda_{n}(\ell+s+1)) - u_{n}(\lambda_{n}(\ell+s))}{j\lambda_{n}} \Big) \\
&+ |u_{n}(\lambda_{n}(\ell+s+1)) - u_{n}(\lambda_{n}(\ell+s))| \Big) \\
&\leq c \sum_{\ell \in Z_{n}(w_{n})} \sum_{j=1}^{K} \sum_{i>K-j}^{2K-j} \sum_{s=i}^{i+j-1} \frac{1}{j} \lambda_{n} \psi_{n}^{1} \Big( \frac{u_{n}(\lambda_{n}(\ell+s+1)) - u_{n}(\lambda_{n}(\ell+s))}{\lambda_{n}} \Big) \\
&+ \frac{c}{N_{n}} + \Phi_{n}(w_{n}).
\end{aligned}$$
(3.16)

By taking into account our choice of  $w_n$ , it follows

$$I_n^1 \le \frac{c}{N_n} \Big( 1 + \sum_{i \in Z_n} \varepsilon_n \psi_n \Big( \frac{v_n(\varepsilon_n(i+1)) - v_n(\varepsilon_n i)}{\varepsilon_n} \Big) \Big).$$
(3.17)

Eventually we get

$$E_n(u_n) \ge (1 - \frac{c}{N_n}) \sum_{i \in \mathbb{Z}_n} \varepsilon_n \psi_n \Big( \frac{v_n(\varepsilon_n(i+1)) - v_n(\varepsilon_n i)}{\varepsilon_n} \Big) - \frac{c}{N_n}$$

and it suffices to pass to the limit of and use Theorem 1.6 on the interval (a, b) to have the desired inequality.

To prove the limsup inequality we will first prove that

$$\Gamma - \limsup_{n} E_n(u) \le \int_0^L F(\dot{u}(x)) \, dx + \sum_{t \in S(u)} G([u](t))$$

on the functions  $u \in SBV(0, L)$  with  $\#S(u) < +\infty$  and then we will use a relaxation argument. For the sake of simplicity as a first step we provide a recovery sequence for functions of the form  $u(x) = \xi x + z\chi_{(x_0,L)}$ . Thus, let us consider the case of  $u(x) = \xi x$ . By proceeding as in the proof of Theorem 1.6 (for details see [17]) we can find  $\xi_n^1, \xi_n^2 \in \mathbb{R}$  and a set of indices  $J_n \subset \{0, \ldots, \left\lfloor \frac{L}{\varepsilon_n} \right\rfloor\}$  such that, set  $\beta_n := \#(J_n)$  and  $M_n := \lfloor L/\varepsilon_n \rfloor$ , there holds

$$\varepsilon_n \beta_n \xi_n^1 + \varepsilon_n (M_n - \beta_n) \xi_n^2 = L\xi + o(1)$$
  

$$\varepsilon_n \beta_n \psi_n (\xi_n^1) + \varepsilon_n (M_n - \beta_n) \psi_n (\xi_n^2) = LF(\xi) + o(1)$$
(3.18)

For s = 1, 2, let  $v_n^s$  be a minimum point for the problem defining  $\psi_n(\xi_n^i)$ , and define  $u_n$  as

$$u_n(i\lambda_n) := \lambda_n v_n^s(i-\ell) + \xi_n^2 \ell \lambda_n + \sum_{j=1}^{\ell} (\xi_n^1 - \xi_n^2) \chi_{J_n}(j) N_n \lambda_n$$

if  $i \in [\ell, \ell + N_n)$ . It can be proved that  $u_n \to u$  in  $L^1(0, L)$  and

$$E_n(u_n) \leq \varepsilon_n \beta_n \psi_n(\xi_n^1) + \varepsilon_n (M_n - \beta_n) \psi_n(\xi_n^2) + \sum_{\ell \in Z_n(0)} \sum_{j=1}^K \sum_{i=0}^{K-1} \lambda_n \psi_n^j \Big( \frac{u_n((i+j+\ell)\lambda_n) - u_n((i+\ell)\lambda_n)}{j\lambda_n} \Big) + \sum_{i=N_n-K-j+1}^{N_n-j} \lambda_n \psi_n^j \Big( \frac{u_n((i+j+\ell)\lambda_n) - u_n((i+\ell)\lambda_n)}{j\lambda_n} \Big).$$

Since by (3.18)  $\lim_{n} \varepsilon_{n} \beta_{n} \psi_{n}(\xi_{n}^{1}) + \varepsilon_{n} (M_{n} - \beta_{n}) \psi_{n}(\xi_{n}^{2}) = LF(\xi)$ , it remains to prove that the second terms in (3.19) tend to 0. To do this we will proceed exactly as in the estimate of the terms  $I_{n}^{1}, I_{n}^{2}$  in the limit inequality, by taking into account hypothesys (3.2) and using the convexity of  $\Psi(z) + |z|$  to consider only interactions of order one. Thus, it holds

$$E_{n}(u_{n}) \leq LF(\xi) + o(1) + c \sum_{\ell \in Z_{n}(0)} \sum_{j=1}^{K} \sum_{i=0}^{K} \sum_{s=0}^{j-1} \frac{1}{j} \lambda_{n} \psi_{n}^{1} \Big( \frac{u_{n}(\lambda_{n}(\ell+i+s+1)) - u_{n}(\lambda_{n}(\ell+i+s))}{\lambda_{n}} \Big) + c \sum_{\ell \in Z_{n}(0)} \sum_{j=1}^{K} \sum_{i=N_{n}-K-j}^{N_{n}-K} \sum_{s=0}^{j-1} \frac{1}{j} \lambda_{n} \psi_{n}^{1} \Big( \frac{u_{n}(\lambda_{n}(\ell+i+s+1)) - u_{n}(\lambda_{n}(\ell+i+s))}{\lambda_{n}} \Big) + \frac{c}{N_{n}} (1 + \varepsilon_{n}(\beta_{n}|\xi_{n}^{1}| + (M_{n} - \beta_{n})|\xi_{n}^{2}|)) \\ \leq \frac{c}{N_{n}} (F(\xi) + 1 + \varepsilon_{n}(\beta_{n}|\xi_{n}^{1}| + (M_{n} - \beta_{n})|\xi_{n}^{2}|)). \quad (3.19)$$

By the growth condition on  $\Psi$  (and then on  $\psi_n, F$ ) the terms  $\varepsilon_n(\beta_n |\xi_n^1| + (M_n - \beta_n) |\xi_n^2|)$  are equibounded. Then it suffices to take the limsup as n goes to  $+\infty$ .

Let us come now to the case  $u(x) = \xi x + z \chi_{(x_o,L)}(x)$  with  $z \neq 0$  and  $G(z) < +\infty$ . Analogously to the proof of Theorem 1.6 we can find natural numbers  $L_n \in \mathbb{N}$  and real numbers  $z_n^s \in [0, +\infty)$ for  $s = \{1, \ldots, L_n\}$  with the following properties

$$\lim_{n} L_n \varepsilon_n = 0, \qquad \lim_{n} \sum_{s=1}^{L_n} z_n^s = z, \qquad G(z) = \lim_{n} \sum_{s=1}^{L_n} G_n(z_n^s).$$
(3.20)

Let  $\ell_o \in Z_n(0)$  be such that  $x_o \in [\ell_o \lambda_n, (\ell_o + N_n)\lambda_n)$ . If  $v_n^s$  is a minimum point for the problem defining  $\psi_n(z/\varepsilon_n)$  for  $s = 1, \ldots, L_n$  and  $u_n$  is the recovery sequence for  $\xi x$  previously defined, we set for  $i \in [\ell \lambda_n, (\ell + N_n)\lambda_n)$  with  $\ell \in Z_n(0)$ 

$$w_n(i\lambda_n) = \begin{cases} u_n(i\lambda_n) & \text{if } \ell < \ell_o \\\\ \lambda_n v_n^s(i-\ell) + u_n(\ell_0\lambda_n) + \sum_{s'=1}^s z_n^s & \text{if } \ell \in [\ell_o, \ell_o + L_nN_n) \\\\ u_n(i\lambda_n + (\ell_o + L_nN_n)\lambda_n) + \sum_{s=1}^{L_n} z_n^s & \text{if } \ell \ge \ell_o + L_nN_n. \end{cases}$$

By using (3.20) it can be easily checked that  $w_n$  converges to u in  $L^1(0, L)$  and, by proceeding as above,

$$E_n(u_n) = LF(\xi) + G(z) + o(1).$$

This procedure can be applied, up to slight modifications, to any function in SBV(0, L), piecewise affine and with a finite number of jumps. So the thesis follows by usual density and relaxation arguments (see e.g. [11]).

**Remark 3.3 (next-to-nearest neighbour interactions)** In the case that  $\psi_n^j = 0$  for all j > 2 then we can equivalently take in place of  $\psi_n$  the function  $\tilde{\psi}_n$  defined as in the Sobolev case, by

$$\tilde{\psi}_n(z) = \psi_n^2(z) + \frac{1}{2} \min\{\psi_n^1(z_1) + \psi_n^1(z_2) : z_1 + z_2 = 2z\}$$

With the previous remark in mind, we can examine the behaviour of next-to-nearest neighbour systems for Lennard-Jones potentials.

**Example 3.4 (next-to-nearest neighbour Lennard Jones interactions)** Let  $\psi$  be as in Remark 3.1, for any n let  $\psi_n^1(z) = \psi(z)$ ,  $\psi_n^2(z) = \psi(2z)$  and  $\psi_n^j = 0$  for  $j \ge 3$ . By using the previous remark, we obtain

$$\overline{F}(z) = \begin{cases} +\infty & \text{if } z \leq 0\\ \frac{1+2^{-12}}{z^{12}}k_1 - \frac{1+2^{-6}}{z^6}k_2 & \text{if } 0 < z \leq z_{\min}\\ -\frac{k_2^2}{4k_1}(1+2^{-12})(1+2^{-6})^2 =: m_{\overline{F}} & \text{if } z > z_{\min}, \end{cases}$$

where

$$z_{\min} = \left(2\frac{(1+2^{-12})k_1}{(1+2^{-6})k_2}\right)^{1/6}$$

is the minimum point for  $\tilde{\psi} = \tilde{\psi}_n$  given by the previous remark. The two values  $z_{\min}$  and  $m_{\overline{F}}$  can be compared to the corresponding minimum point and minimum value for  $\tilde{\psi}$ , that are  $(2k_1/k_2)^{1/6}$  and  $-k_2^2/4k_1$ , respectively. It is also interesting to note that

$$\lim_{w \to +\infty} \tilde{\psi}(w) = -\frac{k_2^2}{8k_1} = \frac{1}{2}\min\psi.$$

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