Asymptotic analysis of Lennard-Jones systems beyond the nearest-neighbour setting: a one-dimensional prototypical case

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Abstract. We consider a one-dimensional system of Lennard-Jones nearest and next-to-nearest neighbour interactions. It is known that if a monotone parameterization is assumed then the limit of such a system can be interpreted as a Griffith fracture energy with an increasing condition on the jumps. In view of possible applications to a higher-dimensional setting, where an analogous parameterization seems not always reasonable, we remove the monotonicity assumption and describe the limit as a Griffith fracture energy where the increasing condition on the jumps is removed and is substituted by an energy that accounts for changes in orientation ('creases'). In addition, fracture may be generated by 'macroscopic' or 'microscopic' cracks.

1 Introduction

Atomistic energies often take into account pair potentials and the corresponding total internal energy, of the form

$$\sum_{i\neq j} J(|u_i - u_j|), \tag{1}$$

where i and j label the pair of atoms, and u_i and u_j denote the corresponding positions. Typical interatomic potentials are repulsive at small distances and (mildly) attractive at long distances, such as Lennard-Jones ones, which takes the form

$$J(z) = \frac{c_2}{z^{12}} - \frac{c_1}{z^6},$$

with $c_1, c_2 > 0$. The study of equilibrium configurations for such systems is a challenging problem. In dimension greater or equal than two even the arrangement of ground states has been described only for a class of energies (see Gardner and Radin [17], Theil [20]). In the two-dimensional case, ground states can be parameterized, up to rotations and translations, as the identity on a triangular lattice. The assumption that this reference parameterization is maintained under deformations allows to define scaled energies and prove the existence of a limit macroscopic energy (see e.g. [1, 9, 10]). Moreover, it also suggests that the effect of long-range interactions (i.e., between points that are distant in the reference lattice) can be somewhat neglected, and that by taking into account, e.g., only nearest-neighbour interactions in the lattice parameterization still gives a meaningful and more explicit approximate macroscopic energy. This can be done using a discrete-to-continuous approach by Γ-convergence for lattice energies, see [4, 5]. In order that the restriction to nearest neighbours do not introduce new ground states, technical restrictive hypotheses have to be added either on the topology of the interactions (typically, that the piecewise-affine deformations defined by the value on the nodes of the triangulation satisfy a positive-determinant constraint as done by Friesecke and Theil [16]) or on the convergence with respect to which the limit macroscopic energy is defined. In both cases the assumptions limit the range of the validity of the resulting macroscopic theory.

In the one-dimensional case monotonicity conditions are in a sense not restrictive, since indices can always be chosen in such a way that $u_i \geq u_j$ (in case of systems with finite Lennard-Jones energy, indeed $u_i > u_j$) if $i > j$. By scaling the reference lattice as $\varepsilon\mathbb{Z}$ and interpreting $u_i - u_j$ as a difference quotient in the reference (unscaled) lattice, we can consider the nearest-neighbour scaled energies

$$F_\varepsilon(u) = \sum_i J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big), \tag{2}$$

where the modulus appearing in (1) may be removed since $u_i - u_{i-1} > 0$. A 'linearization' argument around the ground state by Braides, Lew and Ortiz [8], who introduced a change of variables of the form $u = z^* id + \sqrt{\varepsilon} v$ (z^* is the minimizer for J), leads to the energies (with a slight abuse of notation)

$$F_\varepsilon(v) = \sum_i J\Big(\frac{v_i - v_{i-1}}{\sqrt{\varepsilon}} + z^*\Big).$$

These energies may be treated similarly to some functionals in Computer Vision (see Chambolle [13]). The limit of F_ε as $\varepsilon \to 0$ is a Griffith fracture energy, with the possibility of fracture only in tension, which can be written as

$$\alpha \int |v'|^2\,dx + \beta\#(S(v)), \qquad v^+ > v^-, \tag{3}$$

where $S(v)$ is the set of jump points of v, and v^+, v^- are the right-hand and left-hand limits of v. Using Braides and Truskinovsky's concept of equivalence by Γ-convergence [12] it can also be proved that Barenblatt's Fracture energy can be obtained as a first-order correction of this limit process in such a way that the behavior of local minimum problems is also accounted for (see [6]). If the monotonicity condition $u_i > u_{i-1}$ is not imposed then minimizers are all functions with $u_i - u_{i-1} = \pm\varepsilon z^*$, which give in the continuum all functions with $|u'| \leq z^*$ as minimizers of the limit energy. The linearization around $z^* id$ is then more arbitrary since this state is not an isolated minimizer, and it yields a model with no resistance to compression (while it maintains the form of a Griffith fracture energy in tension).

In this paper we consider the one-dimensional case, in which we do not impose a monotonicity condition on the parameterization but we keep long-range interactions (more precisely, we consider the effect of next-to-nearest neighbour interactions, and, more in general, of interactions in a finite range). Scope of this analysis is to single out relevant features, in view of the treatment of higher-dimensional cases when the positive-determinant constraint is removed. The limit description is more complex than the one given above when the monotonicity assumption is added: we do not have only one ground state $z^* id$ around which we may apply the linearization argument, but we may have varying orientations, and in a sense, locally we may apply either a linearization around $z^* id$ or $-z^* id$. The change in orientation is either due to the appearance of a crack, or of a 'crease' where the two orientations may interchange. In both cases, we have an additional surface energy which prevents the appearance of many changes of orientation. The limit description is of the form

$$\alpha \int |v'|^2 \, dx + \beta \#(S_v) + \gamma \#(P_v), \tag{4}$$

where now S_v is interpreted as the set of fracture points and P_v as the set of crease points. The underlying changes of orientation are determined by the partition given by $P_v \cup S_v$. The precise definition of v, S_v and P_v is given in Definition 2 and is justified by the compactness result in Proposition 4. Note that the surface energy is higher for cracks than for creases. It is also interesting to note that cracks can be subdivided into macroscopic cracks and microscopic ones. The latter ones cannot occur at places where we have a change of orientation. For simplicity we consider only nearest and next-to-nearest neighbour interactions, for which some homogenization formulas are more explicit. The analysis mixes the scaling arguments of Braides, Lew and Ortiz, and the description of internal interfacial energies of Braides and Cicalese [7] (see also [19] and the previous work on quadratic energies [14]). The lack of formulas to describe surface interactions seems to be the main technical difficulty in higher dimension (see [2, 21]), while compactness arguments seem possible to be exported to any dimension upon some hypothesis on the interactions, in the context of free-discontinuity problems (see [3]).

2 Statement of the problem

With the Lennard-Jones potential as a model, we consider a interaction potential $J : [0, +\infty) \to \mathbb{R} \cup \{+\infty\}$ with the following properties:

- $J(0) = +\infty$, J is of class C^2 in its domain
- $\lim\limits_{z \to +\infty} J(z) = 0$;
- $\min J = J(1) < 0$;
- J is convex in $[0, z_0]$ with $z_0 > 1$, concave in $[z_0, +\infty)$.

Our energies will be the *next-to-nearest neighbour* analogue of the nearest-neighbour energies (2); namely,

$$E_\varepsilon(u) = \sum_{i=1}^{N} \Bigg(J\Big(\frac{|u_i - u_{i-1}|}{\varepsilon}\Big) + J\Big(\frac{|u_{i+1} - u_{i-1}|}{\varepsilon}\Big) - \min J_{\text{eff}} \Bigg), \tag{5}$$

where we assume $N = N_\varepsilon = 1/\varepsilon \in \mathbb{N}$, $i \in \mathbb{Z} \cap [0, N]$ and u is identified with a function on $[0, 1]$ by $u(x) = u_{\lfloor x/\varepsilon \rfloor}$. Moreover, by simplicity we consider the *periodic boundary conditions* $u_N = u_0$ and $u_{N+1} = u_1$.

The *effective potential* J_{eff} is defined as

$$J_{\text{eff}}(z) = \frac{1}{2} \min\{J(|z_1|) + J(|z_2|) : z_1 + z_2 = 2z\} + J(2|z|). \tag{6}$$

This potential is obtained by integrating out the effect of nearest-neighbour interactions optimizing over atomic-scale oscillations. It highlights that we might have microscopic oscillations of period two at the lattice scale. In Fig. 1 we picture an example of such an effective potential, also highlighting the function $H(z)$ given by the minimum in (6).

In general, for next-to-nearest neighbour interactions in dimension one the convex envelope of this potential gives an energy function that describes at first-order the behaviour of energies E_ε (see [11, 4] and also [18, 14]). However, for our interactions this convex envelope is a constant, and a higher-order analysis is necessary.

Note that we can write

$$\begin{aligned} E_\varepsilon(u) &= \sum_{i=1}^{N} \Bigg(\frac{1}{2} J\Big(\frac{|u_{i+1} - u_i|}{\varepsilon}\Big) + \frac{1}{2} J\Big(\frac{|u_i - u_{i-1}|}{\varepsilon}\Big) + J\Big(\frac{|u_{i+1} - u_{i-1}|}{\varepsilon}\Big) - \min J_{\text{eff}} \Bigg) \\ &\geq \sum_{i=1}^{N} \Bigg(J_{\text{eff}}\Big(\frac{|u_{i+1} - u_{i-1}|}{2\varepsilon}\Big) - \min J_{\text{eff}} \Bigg), \end{aligned} \tag{7}$$

so that $E_\varepsilon \geq 0$. The hypothesis of having only up to next-to-nearest interactions is essentially used only in this estimate, which allows to obtain information on u with bounded energies through the properties of J_{eff}.

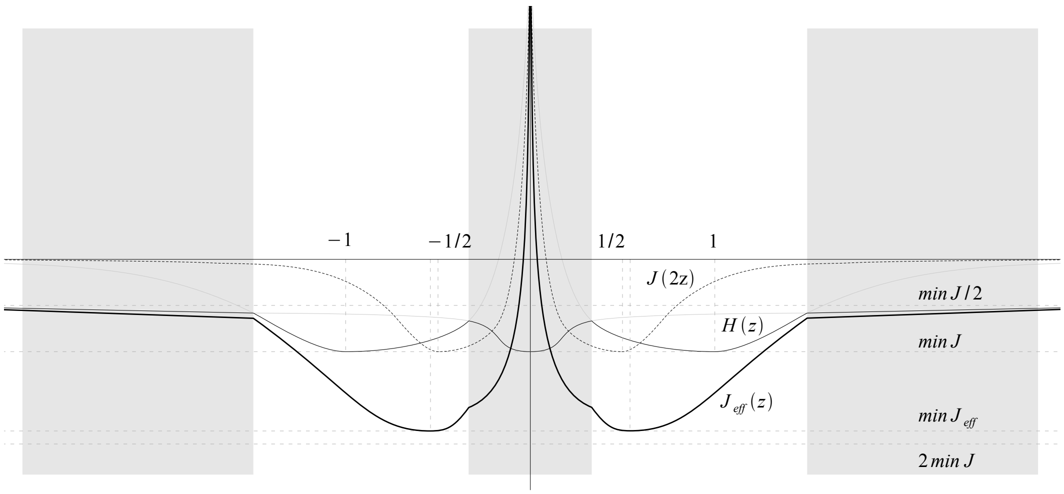

Figure 1: The effective potential J_{eff}

We make the following assumptions on J and J_{eff}, which are satisfied by the Lennard-Jones potential

• (uniqueness and non degeneracy of an increasing effective minimal state) there exist a unique minimizer $z^* > 0$ for J_{eff} on $[0, +\infty)$. Moreover, $J''_{\text{eff}}(z^*) > 0$ and $J''(z^*) > 0$;

• (uniform Cauchy-Born hypothesis) there exists a neighborhood of z^* such that for all z in such neighborhood the unique minimizing pair for the problem $J_{\text{eff}}(z)$ is $z_1 = z_2 = z$.

Under these hypotheses the restriction of the same functional to increasing functions has been studied by Braides and Cicalese [7], showing that it converges to a Griffith Fracture energy. Note that the hypotheses on J are not sufficient in general to guarantee the uniqueness of z^*, which has to be included as an assumption.

Remark 1. The properties of J and the uniform Cauchy-Born hypothesis ensure the following estimates.

a) there exits $\rho > 0$ such that if $(z_1 - z^*)^2 + (z_2 - z^*)^2 \leq \rho^2$ then

$$\frac{1}{2}\Big(J(z_1) + J(z_2)\Big) + J(z_1 + z_2) \geq \min J_{\text{eff}} + \frac{\lambda}{2}(z_1 - z^*)^2 + \frac{\lambda}{2}(z_2 - z^*)^2 \tag{8}$$

where $0 < \lambda < \min\left\{\frac{J''(z^*)}{2}, \frac{J''_{\text{eff}}(z^*)}{2}\right\}$. This is immediately obtained by computing the eigenvalues of the Hessian matrix of the function $(z_1, z_2) \mapsto \frac{1}{2}\big((J(z_1) + J(z_2)\big) + J(z_1 + z_2)$ at the minimum point $z_1 = z_2 = z^*$ taking into account the uniform Cauchy-Born hypothesis;

b) for all z_1, z_2 with $z_1 z_2 < 0$ we have

$$\frac{1}{2}\Big(J(|z_1|) + J(|z_2|)\Big) + J(|z_1 + z_2|) \geq C > \min J_{\text{eff}}. \tag{9}$$

This estimate follows after remarking that the function $\frac{1}{2}\big(J(|z_1|)+J(|z_2|)\big)+J(|z_1+z_2|)$ is continuous on the set $z_1 > 0$ and $z_2 < 0$, tends to $+\infty$ if either $z_1 \to 0$ or $z_2 \to 0$ and is larger than $\min J > \min J_{\text{eff}}$ if either $z_1 \to +\infty$ or $z_2 \to -\infty$, so that either is always larger than $\min J =: C$ or it achieves its minimum for some $z_1^* > 0$ and $z_2^* < 0$ and $C := \frac{1}{2}\big(J(|z_1^*|) + J(|z_2^*|)\big) + J(|z_1^* + z_2^*|) > \min J_{\text{eff}}$. Inequality (9) allows to avoid trivial non-monotone minimizers;

c) there exists $b > 0$ such that

$$\frac{1}{2}\big(J(z_1) + J(z_2)\big) + J(z_1 + z_2) - \min J_{\text{eff}} \geq \left(\frac{\lambda}{2}\left((z_1 - z^*)^2 + (z_2 - z^*)^2\right)\right) \wedge b \tag{10}$$

for all $z_1, z_2 > 0$. This estimate follows taking, e.g.,

$$b = \inf\Big\{\frac{1}{2}\big(J(z_1) + J(z_2)\big) + J(z_1 + z_2) - \min J_{\text{eff}} : (z_1 - z^*)^2 + (z_2 - z^*)^2 \geq \rho^2\Big\},$$

where ρ is such that (8) holds as in (a).

Definition 2 (convergence to a linearized state with jumps and creases)**.** *Given a sequence of periodic functions $u^\varepsilon \colon [0, N_\varepsilon] \to \mathbb{R}$; we say that u^ε converge to (v, S_v, P_v) where S_v and P_v are disjoint finite subsets of $[0,1)$ and $v \in H^1((0,1) \setminus (S_v \cup P_v))$ if*

(i) *there exists a piecewise-affine u with $u' \in BV((0,1); \{\pm z^*\})$ such that $u^\varepsilon \to u$ in L^1;*

(ii) *there exist $S = \{x_1, \dots, x_M\} \subset [0,1)$ with $x_1 < \cdots < x_M$ and sequences $(c_\varepsilon^j)_\varepsilon$ for $j = 1, \dots, M$ such that*

$$\frac{u^\varepsilon - u}{\sqrt{\varepsilon}} - c_\varepsilon^j \to v^j \quad \textit{weakly in } H^1_{\text{loc}}(x_{j-1}, x_j) \tag{11}$$

where u^ε is identified with its piecewise-affine interpolation, u is extended by periodicity and we set $x_0 = x_M - 1$.

Then we define v as

$$v(x) = \begin{cases} v^j(x) & \text{if } x \in (x_{j-1}, x_j) \cap (0,1) \text{ for } j = 1, \dots, M \\ v^1(x-1) & \text{if } x \in (x_M, 1), \end{cases}$$

$P_v = S(u') \setminus S(u)$, where $S(u)$ and $S(u')$ denote the points of essential discontinuity of u and u', respectively, in $[0,1)$ (u and u' are extended by periodicity to the whole $\mathbb{R}$) and S_v as the minimal subset of $[0,1) \setminus P_v$ such that (ii) *holds. Note that this is a good definition since if S and S' satisfy* (ii) *then also $S \cap S'$ does.*

Remark 3. Note that the sequences of constants c^j_ε and their limit are not uniquely determined. In particular, v^j are determined up to addition of a constant. The functions v^j are in a sense obtained as a linearization around the (unknown) function u, just as in the increasing case we had a linearization around z^*id. Note that in the set $P_v \cup S_v$ we have three types of points:

• points in $S(u')\setminus S(u)$; i.e, points where u is continuous but u' changes orientation (creases);

• points in $S(u)$ (macroscopic cracks);

• discontinuity points of v^j that are not in $S(u')\cup S(u)$ (microscopic cracks). Note that the functions v^j as defined are piecewise H^1 functions.

In principle, v^j may develop microscopic cracks also at points in $S(u')\setminus S(u)$, but we will see that energetically such points have to be considered as crease points.

The introduction of the previous definition is justified by the following proposition.

Proposition 4 (compactness)**.** *Let (u^ε) be a sequence such that $\sup_\varepsilon(E_\varepsilon(u^\varepsilon)+\|u^\varepsilon\|_\infty) < +\infty$. Then, up to subsequences, u^ε converge in the sense of Definition 2.*

Proof. For all $w\colon [0,N_\varepsilon]\cap\mathbb{Z}\to\mathbb{R}$ set

$$
\begin{aligned}
I^+(w) &= \bigcup\{[\varepsilon(i-1),\varepsilon i) : w_i - w_{i-1} > 0\} &\quad (12)\\
I^-(w) &= \bigcup\{[\varepsilon(i-1),\varepsilon i) : w_i - w_{i-1} < 0\}. &\quad (13)
\end{aligned}
$$

Note that $u^\varepsilon_i - u^\varepsilon_{i-1}\neq 0$ for all i by the assumption $J(0)=+\infty$.

We deduce from (9) that the number of connected components of $I^+(u^\varepsilon)$ and $I^-(u^\varepsilon)$ is equibounded.

Let C_ε be one of such connected components; e.g., of $I^+(u^\varepsilon)$. Up to subsequences, we may suppose that C_ε converge to an interval $I\subset[0,1]$ as $\varepsilon\to 0$.

Since $E_\varepsilon(u^\varepsilon)$ is uniformly bounded, estimate (10) ensures that except for a finite number of indices i

$$
\Bigl(\frac{u^\varepsilon_i - u^\varepsilon_{i-1}}{\varepsilon}\Bigr)^2 \vee \Bigl(\frac{u^\varepsilon_{i+1} - u^\varepsilon_{i}}{\varepsilon}\Bigr)^2 \le \frac{2b}{\lambda}.
$$

We can then consider intervals where this relation holds for all i. If we set

$$
\tilde v^\varepsilon_i = \frac{1}{\sqrt{\varepsilon}}\,(u^\varepsilon_i - z^*\varepsilon i)\,,
$$

in such intervals we have, thanks to (8),

$$
\begin{aligned}
\lambda\sum_i \varepsilon\Bigl(\frac{\tilde v^\varepsilon_i-\tilde v^\varepsilon_{i-1}}{\varepsilon}\Bigr)^2 &= \lambda\sum_i\Bigl(\frac{u^\varepsilon_i-u^\varepsilon_{i-1}}{\varepsilon}-z^*\Bigr)^2\\
&\le \frac{\lambda}{2}\sum_i\Bigl(\Bigl(\frac{u^\varepsilon_{i+1}-u^\varepsilon_{i}}{\varepsilon}-z^*\Bigr)^2+\Bigl(\frac{u^\varepsilon_i-u^\varepsilon_{i-1}}{\varepsilon}-z^*\Bigr)^2\Bigr)\\
&\le E_\varepsilon(u^\varepsilon).
\end{aligned}
$$

We then deduce that the gradients of the piecewise-affine interpolations of $\tilde v^\varepsilon_i$ are bounded in L^2 on each such interval. Hence there are constants c_ε depending on the interval such that, setting

$$v^\varepsilon_i = \frac{1}{\sqrt{\varepsilon}}\,(u^\varepsilon_i - z^*\varepsilon i) - c_\varepsilon,$$

such functions converge weakly in $H^1_{\rm loc}$.

Considering also the connected components of $I^-(u_\varepsilon)$ we deduce that up to subsequences there exists a finite subset of $[0,1]$ of points $0 = x_0 < x_1 < \cdots < x_{M+1} = 1$, $M+1$ sequences $\{c^k_\varepsilon\}$ and $M+1$ choices of minimizers of $J_{\rm eff}$ $z^*_k \in \{-z^*, z^*\}$ such that, setting

$$v^\varepsilon_i = \frac{1}{\sqrt{\varepsilon}}\,(u^\varepsilon_i - z^*_k\varepsilon i) - c^k_\varepsilon \qquad \text{for } \ \varepsilon i \in (x_{k-1}, x_k),$$

such functions converge to a limit v^k in $L^2_{\rm loc}(x_{k-1}, x_k)$ (or, equivalently, their piecewise-affine interpolations weakly converge to v^k in $H^1_{\rm loc}(x_{k-1}, x_k)$).

Note that this also implies that, up to subsequences and translations, u^ε converges to $z^*_k x$ in (x_{k-1}, x_k). By the uniform boundedness of u_ε this implies that $u_\varepsilon \to u$ in L^1, for some u with $u' = z^*_k$ in (x_{k-1}, x_k), and hence (i) in Definition 2 holds.

The set $S = \{x_1, \dots, x_M\} \cup \{0\}$ satisfies (ii) in Definition 2, with v defined as v^k on (x_{k-1}, x_k). $\square$

The following theorem is the main result of the paper, and gives an energetic description of the energy E_ε in terms of the parameters given by Definition 2.

Theorem 5. *The sequence (E_ε) Γ-converges with respect to the convergence in Definition 2 to the functional*

$$F(v, S_v, P_v) = \alpha \int_{(0,1)} |v'|^2\,dx + \beta\#S_v + \gamma\#P_v \tag{14}$$

where

$$\alpha = \frac{1}{2}J''_{\rm eff}(z^*) \tag{15}$$

$$\beta = 2\inf\Big\{\sum_{i=1}^{+\infty}\big(J(|z_i|) + J(|z_i + z_{i+1}|) - \min J_{\rm eff}\big) : z_i = z^* \textit{ for } i \geq K, K \in \mathbb{N}\Big\} - 2\min J_{\rm eff} + J(z^*) \tag{16}$$

$$\gamma = \inf\Big\{\sum_{i=-\infty}^{+\infty}\big(J(|z_i|) + J(|z_i + z_{i+1}|) - \min J_{\rm eff}\big) : z_i = {\rm sgn}(i)z^* \textit{ for } |i| \geq K, K \in \mathbb{N}\Big\}. \tag{17}$$

Note that the definition of β and γ actually involve only finite sums.

The proof of the theorem is the content of the rest of the paper.

We now prove some properties of β and γ which might be of independent interest.

Remark 6 (surface relaxation)**.** We note that β is not trivially obtained by taking $z_i = z^*$ for all i; i.e., that

$$\inf\Big\{\sum_{i=1}^{+\infty}\big(J(|z_i|)+J(|z_i+z_{i+1}|)-\min J_{\rm eff}\big):\ z_i=z^* \text{ for } i\ge K, K\in\mathbb{N}\Big\}<0.$$

Indeed, take $z_i = z^*$ for $i \geq 2$ as a test function. For $z_1 > 0$ we have

$$\sum_{i=1}^{+\infty}\big(J(|z_i|)+J(|z_i+z_{i+1}|)-\min J_{\rm eff}\big)=G(z_1)-\min J_{\rm eff},$$

where $G(t) = J(t) + J(t + z^*)$. Note that $G'(z^*) = J'(z^*) + J'(2z^*) = -J'(2z^*) < 0$, so that there exists $\tau > z^*$ such that $G(\tau) < G(z^*) = \min J_{\rm eff}$. Choosing $z_1 = \tau$ we get the estimate.

The next result allows to relax the boundary condition as a condition at infinity in the definition of β and γ.

Proposition 7. *We have*

$$\begin{aligned}\beta = &\ 2\inf\Big\{\sum_{i=1}^{+\infty}\big(J(|z_i|)+J(|z_i+z_{i+1}|)-\min J_{\rm eff}\big):\lim_{i\to+\infty} z_i=z^*\Big\}\\ &\qquad -2J_{\rm eff}(z^*)+J(z^*),\end{aligned} \tag{18}$$

$$\gamma = \inf\Big\{\sum_{i=-\infty}^{+\infty}\big(J(|z_i|)+J(|z_i+z_{i+1}|)-\min J_{\rm eff}\big):\lim_{i\to\pm\infty}\operatorname{sgn}(i)\, z_i=z^*\Big\}. \tag{19}$$

Note that the infinite sums are well defined since they involve only non-negative terms.

Proof. We only treat the formula for γ, the formula for β being dealt with in the same way. Let z_i be a test function for (19). With fixed $\eta > 0$, let K_η be such that $|z_i - \operatorname{sign}(i)z^*| < \eta$ for $|i| \geq K_\eta$, and define

$$z_i^\eta=\begin{cases} z_i & \text{if } |i|\le K_\eta\\ \operatorname{sign}(i)z^* & \text{if } |i|>K_\eta.\end{cases}$$

Then we have

$$
\begin{aligned}
& \sum_{i=-\infty}^{+\infty} \big(J(|z_i^\eta|) + J(|z_i^\eta + z_{i+1}^\eta|) - \min J_{\mathrm{eff}}\big) \\
= & \sum_{i=-\infty}^{+\infty} \Big(\frac{1}{2}(J(|z_i^\eta|) + J(|z_{i+1}^\eta|)) + J(|z_i^\eta + z_{i+1}^\eta|) - \min J_{\mathrm{eff}}\Big) \\
= & \sum_{i=-K_\eta-1}^{K_\eta} \Big(\frac{1}{2}(J(|z_i^\eta|) + J(|z_{i+1}^\eta|)) + J(|z_i^\eta + z_{i+1}^\eta|) - \min J_{\mathrm{eff}}\Big) \\
= & \sum_{i=-K_\eta}^{K_\eta-1} \Big(\frac{1}{2}(J(|z_i|) + J(|z_{i+1}|)) + J(|z_i + z_{i+1}|) - \min J_{\mathrm{eff}}\Big) \\
& + \frac{1}{2}(J(|z_{K_\eta}|) + J(|z^*|)) + J(|z_{K_\eta} + z^*|) - \min J_{\mathrm{eff}} \\
& + \frac{1}{2}(J(|-z^*|) + J(|z_{-K_\eta}|)) + J(|-z^* + z_{-K_\eta}|) - \min J_{\mathrm{eff}} \\
\le & \sum_{i=-\infty}^{+\infty} \Big(\frac{1}{2}(J(|z_i|) + J(|z_{i+1}|)) + J(|z_i + z_{i+1}|) - \min J_{\mathrm{eff}}\Big) + 2\,\omega(\eta),
\end{aligned}
$$

where

$$
\omega(\eta) := \max\Big\{\frac{1}{2}(J(|z|) + J(|z^*|)) + J(|z+z^*|) - \min J_{\mathrm{eff}} : |z - z^*| \le \eta\Big\}
$$

is infinitesimal as $\eta \to 0$. This proves that the value of γ is not greater than the one in (19). Since the converse inequality is trivial, we have the thesis. $\square$

3 Proof of Theorem 5

In this section we will prove Theorem 5 by making use of some arguments close to those of Braides, Lew and Ortiz [8] and Braides and Cicalese [7]. In particular, we use a result from [8] that we state in our notation as follows.

Theorem 8 (Braides, Lew and Ortiz)**.** *Let (v^ε) be a sequence of functions such that $z^*\mathrm{id} + \sqrt{\varepsilon} v^\varepsilon$ are increasing on a subset (a,b) of $(0,1)$ and such that, if we set*

$$
F_\varepsilon(v,(a,b)) = \sum_i \Big(J\Big(z^* + \sqrt{\varepsilon}\frac{v_i - v_{i-1}}{\varepsilon}\Big) + J\Big(2z^* + \sqrt{\varepsilon}\frac{v_{i+1} - v_{i-1}}{\varepsilon}\Big) - \min J_{\mathrm{eff}}\Big), \tag{20}
$$

where the sum is taken over all i with $\varepsilon i \in (a,b)$, then we have $\sup_\varepsilon F_\varepsilon(v^\varepsilon,(a,b)) < +\infty$. Suppose furthermore that $v^\varepsilon(a)$ and $v^\varepsilon(b)$ converge. Then the sequence v^ε weakly *converges up to a subsequence to a piecewise-$H^1(a,b)$ function v and we have*

$$\liminf_{\varepsilon\to 0} F_\varepsilon(v^\varepsilon,(a,b)) \ge \alpha \int_a^b |v'|^2\,dx + \beta\,\#S(v).$$

The following proposition will allow us to distinguish energetically between points in S_v and points in P_v.

Proposition 9. *We have $0<\gamma<\beta$.*

Proof. With fixed $\eta>0$ let $\{z_i^\eta\}$ be an η-minimizer for the problem defining β. With fixed $M>0$, we may take as a test function in the minimum problem defining γ the function

$$z_i^M = \begin{cases} z_i^\eta & \text{for } i\ge 1\\ M & \text{for } i=0\\ -z_{-i}^\eta & \text{for } i\le -1.\end{cases}$$

We then have

$$\begin{aligned}
&\sum_{i=-\infty}^{+\infty}\big(J(|z_i^M|)+J(|z_i^M+z_{i+1}^M|)-\min J_{\rm eff}\big)\\
=\ &\sum_{i=1}^{K-1}\big(J(|z_i^M|)+J(|z_i^M+z_{i+1}^M|)-\min J_{\rm eff}\big)\\
&+J(|z_0^M|)+J(|z_{-1}^M+z_0^M|)-\min J_{\rm eff}\\
&+\sum_{i=-K}^{-2}\big(J(|z_i^M|)+J(|z_i^M+z_{i+1}^M|)-\min J_{\rm eff}\big)\\
&+J(|z_{-1}^M|)+J(|z_{-1}^M+z_0^M|)-\min J_{\rm eff}
\end{aligned}$$

$$\begin{aligned}
=\ &2\sum_{i=1}^{K-1}\big(J(|z_i^\eta|)+J(|z_i^\eta+z_{i+1}^\eta|)-\min J_{\rm eff}\big)-2\min J_{\rm eff}+J(|z_k^\eta|)\\
&+J(|M|)+J(|M-z_1^\eta|)+J(|z_1^\eta+M|)\\
=\ &2\sum_{i=1}^{\infty}\big(J(|z_i^\eta|)+J(|z_i^\eta+z_{i+1}^\eta|)-\min J_{\rm eff}\big)-2\min J_{\rm eff}+J(z^*)\\
&+J(|M-z_1^\eta|)+J(M)+J(|M+z_1^\eta|)\\
\le\ &\beta+\eta+J(|M-z_1^\eta|)+J(M)+J(|M+z_1^\eta|).
\end{aligned}$$

Note that z_1^η remain bounded; hence, for M large enough independent of η we have $J(|z_1^\eta+M|)<0$ and $J(|M-z_1^\eta|)<0$; then, by the arbitrariness of η,

$$\gamma\le\beta+J(M)<\beta.$$

The estimate $\gamma > 0$ follows immediately from the fact that the unique minimizers in the definition of J_{eff} are the pairs (z^*, z^*) and $(-z^*, -z^*)$. $\square$

The following remark will be useful in the construction of recovery sequences.

Remark 10. For all η we may construct functions $w_i^{\beta,\eta}$ such that

$$w_i^{\beta,\eta} = z^* i$$

for $i \geq T^{\beta,\eta}$, and

$$z_i = w_i^{\beta,\eta} - w_{i-1}^{\beta,\eta}$$

is an η-minimizer for the problem defining β. This is just a translation argument, upon noticing that, if z_i is admissible for the problem defining β, then we have

$$Mz^* - \sum_{i=1}^{M} z_i = c$$

constant for $M \geq K$.

Similarly, we may construct functions $w_i^{\gamma,\eta}$ such that

$$w_i^{\gamma,\eta} = z^* |i|$$

for $|i| \geq T^{\gamma,\eta}$ large enough, and

$$z_i = w_i^{\gamma,\eta} - w_{i-1}^{\gamma,\eta}$$

is an η-minimizer for the problem defining γ. Indeed a translation argument as above gives a function $\{w_i\}$ with $w_i = z^* i$ for $i \geq K$ and $w_i = -z^* i + c$ for $i \leq -K$. For $M \in \mathbb{N}$ fixed, we can then define

$$w_i^{\gamma,\eta} = \begin{cases} w_i & \text{for } i \geq -K \\ w_i + \frac{c}{M}(i+K) & \text{for } -K-M \leq i < -K-1 \\ z^*|i| & \text{for } i \leq -K-M-1. \end{cases}$$

Taking into account the Cauchy-Born hypothesis on J, the extra energy due to the correction for $-K - M \leq i \leq -K - 1$ can be estimated by

$$\begin{aligned} & (M-1)\Big(J\Big(z^* - \frac{c}{M}\Big) + J\Big(2z^* - 2\frac{c}{M}\Big) - \min J_{\text{eff}}\Big) \\ & \quad +2\Big(\frac{1}{2}J\Big(z^* - \frac{c}{M}\Big) + \frac{1}{2}J(z^*) + J\Big(2z^* - \frac{c}{M}\Big)\Big) - \min J_{\text{eff}}\Big) \\ = \; & (M-1)\Big(J_{\text{eff}}\Big(z^* + \frac{c}{M}\Big) - \min J_{\text{eff}}\Big) + o(1)_{M\to\infty} \\ = \; & \frac{1}{2}J''_{\text{eff}}(z^*)\frac{c^2(M-1)}{M^2} + o\Big(\frac{1}{M}\Big)_{M\to\infty} + o(1)_{M\to\infty}, \end{aligned}$$

which gives the thesis for M large enough.

The same argument above shows that we may require that $w_i^{\gamma,\eta}$ satisfy

$$w_i^{\gamma,\eta} = z^* i + c_+^\eta, \qquad w_i^{\gamma,\eta} = -z^* i + c_-^\eta$$

for $i \geq T^{\gamma,\eta}$ and $i \leq -T^{\gamma,\eta}$, respectively. Here $c_\pm^\eta$ are any two constants that remain bounded with η.

Proof of Theorem 5. We first prove the lower bound. Let (u^ε) be a sequence converging to (v, S_v, P_v) in the sense of Definition 2. By the periodicity condition, we may assume, without loss of generality, that $0 \notin S_v \cup P_v$.

We fix $\eta > 0$ and subdivide the contribution of u^ε inside each $x_j + (-\eta, \eta)$ and outside their union. Setting

$$v^\varepsilon = \frac{u^\varepsilon - u}{\sqrt{\varepsilon}} - c_\varepsilon^j$$

on $(x_{j-1}+\eta, x_j-\eta)$, we have $v^\varepsilon \to v^j$ in $H^1(x_{j-1}+\eta, x_j-\eta)$. Upon further subdividing our interval, we may suppose that $z^*\mathrm{id} + \sqrt{\varepsilon}v^\varepsilon$ are increasing on $(x_{j-1}+\eta, x_j-\eta)$ (or $-z^*\mathrm{id} + \sqrt{\varepsilon}v^\varepsilon$ are decreasing). We can then apply Theorem 8 with $(a,b) = (x_{j-1} + \eta, x_j - \eta)$ to get

$$\liminf_{\varepsilon \to 0} F_\varepsilon(v^\varepsilon, (x_{j-1}+\eta, x_j-\eta)) \geq \alpha \int_{(x_{j-1}+\eta, x_j-\eta)} |(v^j)'|^2 \, dt. \tag{21}$$

Let $\overline{x} \in P_v$. We suppose without loss of generality that $\lim_{x \to \overline{x}^+} u'(x) = z^*$. Up to changing the functions u^ε sufficiently far from $\overline{x}$, we may also suppose that

$$\frac{u_i^\varepsilon - u_{i-1}^\varepsilon}{\varepsilon} = z^*$$

for $\varepsilon i \geq \overline{x} + \frac{3\eta}{4}$ and

$$\frac{u_i^\varepsilon - u_{i-1}^\varepsilon}{\varepsilon} = -z^*$$

for $\varepsilon i \geq \overline{x} - \frac{3\eta}{4}$. Indeed, for any i we set

$$w_i^\varepsilon = \frac{v_i^\varepsilon - v_{i-1}^\varepsilon}{\varepsilon}$$

where v^ε is defined as above; since v_ε weakly converges in $H^1\big(\overline{x} + \frac{\eta}{4}, \overline{x} + \frac{3\eta}{4}\big)$, it follows that there exists an index $i(\varepsilon)$ with $\overline{x} + \frac{\eta}{4} < \varepsilon i(\varepsilon) < \overline{x} + \frac{3\eta}{4}$ such that $(w_{i(\varepsilon)}^\varepsilon)^2 \leq C/\eta$ with C independent on ε. Then, setting for $\varepsilon i \in (\overline{x}, \overline{x} + \eta)$

$$z_i^\varepsilon = \begin{cases} \dfrac{u_i^\varepsilon - u_{i-1}^\varepsilon}{\varepsilon} & \text{if } i \leq i(\varepsilon) \\ z^* & \text{if } i > i(\varepsilon) \end{cases}$$

we have, since $\lim_{\varepsilon\to 0}\sqrt{\varepsilon}w^\varepsilon_{i(\varepsilon)}=0$, that the extra energy due to the modification of u^ε_i is negligible; that is,

$$\begin{aligned}&\lim_{\varepsilon\to 0}\left(\frac{1}{2}\Big(J(z^\varepsilon_{i(\varepsilon)+1})+J(z^\varepsilon_{i(\varepsilon)})\Big)+J(z^\varepsilon_{i(\varepsilon)+1}+z^\varepsilon_{i(\varepsilon)})-\min J_{\rm eff}\right)\\ &\qquad=\lim_{\varepsilon\to 0}\left(\frac{1}{2}\Big(J(z^*)+J(z^*+\sqrt{\varepsilon}w^\varepsilon_{i(\varepsilon)})\Big)+J(2z^*+\sqrt{\varepsilon}w^\varepsilon_{i(\varepsilon)})-\min J_{\rm eff}\right)=0.\end{aligned}$$

The corresponding construction for $\varepsilon i\in(\overline{x}-\eta,\overline{x})$ gives a sequence $\{z^\varepsilon_i\}$ admissible for the problem defining γ, so that we get that

$$\liminf_{\varepsilon\to 0}E_\varepsilon(u^\varepsilon,(\overline{x}-\eta,\overline{x}+\eta))\geq\gamma.$$

We now consider $x=x^j\in S_v$. Note that there are indices i_ε such that $\varepsilon i_\varepsilon\to x^j$ and

$$\liminf_{\varepsilon\to 0}\frac{|u^\varepsilon_{i_\varepsilon+1}-u^\varepsilon_{i_\varepsilon}|}{\varepsilon}=+\infty. \tag{22}$$

This is trivial if $x^j\in S(u)$. Otherwise, since $x^j\not\in S(u')$, we may suppose that $u'=z^*$ on $(x^j-\eta,x^j+\eta)$. If (22) does not hold then the L^2-norm of the gradient of the piecewise-affine interpolation of v^ε is bounded, and, upon translation by constants, we have that

$$v^\varepsilon_i=\frac{1}{\sqrt{\varepsilon}}(u^\varepsilon_i-z^*\varepsilon i)$$

weakly converge in $H^1(x^j-\eta,x^j+\eta)$. This contradicts the minimality of S_v. The same argument shows that we can suppose that

$$\liminf_{\varepsilon\to 0}\frac{|u^\varepsilon_{i_\varepsilon+1}-u^\varepsilon_{i_\varepsilon-1}|}{\varepsilon}=\liminf_{\varepsilon\to 0}\frac{|u^\varepsilon_{i_\varepsilon+2}-u^\varepsilon_{i_\varepsilon}|}{\varepsilon}=+\infty. \tag{23}$$

We now estimate the energy as follows. If $x^j\not\in S(u')$, we can modify u^ε as in the case $\overline{x}\in P_v$ obtaining $\tilde u^\varepsilon$ such that

$$\frac{\tilde u^\varepsilon_i-\tilde u^\varepsilon_{i-1}}{\varepsilon}=z^* \tag{24}$$

holds outside $(x^j-\frac{3\eta}{4},x^j+\frac{3\eta}{4})$. We can then take as test functions for the computation of the minimum problem in β

$$z^+_i=\frac{\tilde u^\varepsilon_{i+i_\varepsilon+1}-\tilde u^\varepsilon_{i+i_\varepsilon}}{\varepsilon},$$

and

$$z^-_i=\frac{\tilde u^\varepsilon_{i_\varepsilon-i}-\tilde u^\varepsilon_{i_\varepsilon-i+1}}{\varepsilon}.$$

We then obtain

$$
\begin{aligned}
&E_\varepsilon(\tilde u^\varepsilon,(x_j-\eta,x_j+\eta))\\
&= \sum_{i=-\infty}^{i_\varepsilon-1}\left(\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_i|}{\varepsilon}\Big)+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)+J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)-\min J_{\rm eff}\right)\\
&\quad+\sum_{i=i_\varepsilon}^{i_\varepsilon+1}\left(\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_i|}{\varepsilon}\Big)+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)+J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)-\min J_{\rm eff}\right)\\
&\quad+\sum_{i=i_\varepsilon+2}^{+\infty}\left(\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_i|}{\varepsilon}\Big)+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)+J\Big(\frac{|\tilde u^\varepsilon_{i+1}-\tilde u^\varepsilon_{i-1}|}{\varepsilon}\Big)-\min J_{\rm eff}\right)\\
&= \sum_{i=1}^{+\infty}\Big(\frac12(J(|z^-_{i+1}|)+J(|z^-_i|))+J(|z^-_i+z^-_{i+1}|)-\min J_{\rm eff}\Big)\\
&\quad+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon+1}-\tilde u^\varepsilon_{i_\varepsilon}|}{\varepsilon}\Big)+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon}-\tilde u^\varepsilon_{i_\varepsilon-1}|}{\varepsilon}\Big)+J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon+1}-\tilde u^\varepsilon_{i_\varepsilon-1}|}{\varepsilon}\Big)-\min J_{\rm eff}\\
&\quad+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon+2}-\tilde u^\varepsilon_{i_\varepsilon+1}|}{\varepsilon}\Big)+\frac12 J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon+1}-\tilde u^\varepsilon_{i_\varepsilon}|}{\varepsilon}\Big)+J\Big(\frac{|\tilde u^\varepsilon_{i_\varepsilon+2}-\tilde u^\varepsilon_{i_\varepsilon}|}{\varepsilon}\Big)-\min J_{\rm eff}\\
&\quad+\sum_{i=1}^{+\infty}\Big(\frac12(J(|z^+_{i+1}|)+J(|z^+_i|))+J(|z^+_i+z^+_{i+1}|)-\min J_{\rm eff}\Big)\\
&= \sum_{i=1}^{+\infty}\Big(\frac12(J(|z^-_{i+1}|)+J(|z^-_i|))+J(|z^-_i+z^-_{i+1}|)-\min J_{\rm eff}\Big)+\frac12 J(|z^-_1|)-2\min J_{\rm eff}\\
&\quad+\sum_{i=1}^{+\infty}\Big(\frac12(J(|z^+_{i+1}|)+J(|z^+_i|))+J(|z^+_i+z^+_{i+1}|)-\min J_{\rm eff}\Big)+\frac12 J(|z^+_1|)+o(1)_{\varepsilon\to0}
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{i=1}^{+\infty}\Big(J(|z^-_i|)+J(|z^-_i+z^-_{i+1}|)-\min J_{\rm eff}\Big)+J(|z^*|)-2\min J_{\rm eff}\\
&\quad+\sum_{i=1}^{+\infty}\Big(J(|z^+_i|)+J(|z^+_i+z^+_{i+1}|)-\min J_{\rm eff}\Big)+o(1)_{\varepsilon\to0},
\end{aligned}
$$

from which we deduce that

$$\liminf_{\varepsilon\to0} E_\varepsilon(u^\varepsilon,(x^j+\eta,x^j-\eta))\geq\beta.$$

The case $x^j\in S(u')$ can be treated in a completely similar way, by considering a modified sequence with

$$\frac{\tilde u^\varepsilon_i-\tilde u^\varepsilon_{i-1}}{\varepsilon}=-z^*$$

for $\varepsilon i \le x^j - \frac{3\eta}{4}$ and by defining

$$z_i^- = \frac{\tilde{u}^\varepsilon_{i_\varepsilon - i+1} - \tilde{u}^\varepsilon_{i_\varepsilon - i}}{\varepsilon}.$$

We take now (v, P_v, S_v) as in Definition 2, and construct a recovery sequence for the upper bound. As above, we may assume, without loss of generality, that $0 \notin S_v \cup P_v$.

By a density and translation argument we may suppose that $v \in C^2[0,1]$ and that v is 0 on a neighbourhood of $P_v \cup S_v$. We then choose any function u such that $u' \in BV((0,1);\{\pm z^*\})$, that $S(u) \subset S_v$ and that $P_v = S(u') \setminus S(u)$ (for example we may take a function $u' \in BV((0,1);\{\pm z^*\})$ with $S(u) = \emptyset$ and $S(u') = P_v$). The result will be independent of this choice.

Note that by the periodicity of u there exists $\overline{x} \in S(u) \cup S(u') \neq \emptyset$, and we define $\overline{u}^\varepsilon$ by setting

$$D\overline{u}^\varepsilon = Du + \sum_{x \in S_v \setminus S(u)} \sqrt{\varepsilon}\,\mathrm{sgn}(u'(x))\delta_x - \sum_{x \in S_v \setminus S(u)} \sqrt{\varepsilon}\,\mathrm{sgn}(u'(x))\delta_{\overline{x}}.$$

In this way we have inserted small jumps on the points of S_v where u does not jump, that preserve the monotonicity of u. We have also modified u at $\overline{x}$ in order to preserve the periodicity of $\overline{u}^\varepsilon$. Note that this modification may insert a jump of vanishing size at a crease point. This point must nevertheless be regarded as a crease point at a slightly misplaced location $\overline{x}_\varepsilon$. The situation is the one pictured in Fig. 2. For simplicity of notation we will suppose that $\overline{x}_\varepsilon = \overline{x}$.

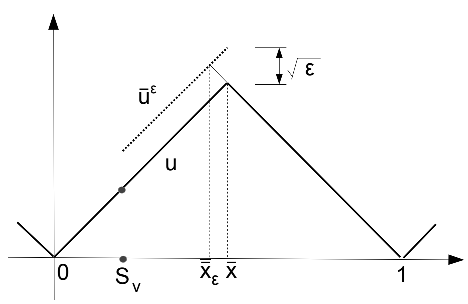

Figure 2: Perturbation of the function u

Note that we may suppose that $x/\varepsilon \in \mathbb{Z}$, upon taking its integer part. For any fixed $\eta > 0$, we consider sequences $(w_i^{\gamma,\eta})_{i\in\mathbb{Z}}$ and $(w_i^{\beta,\eta})_{i\ge 0}$ given by Remark 10 satisfying the following properties

• $w_i^{\gamma,\eta} = z^*|i|$ for $|i| \ge T^{\gamma,\eta}$ and $(z_i^{\gamma,\eta})_{i\in\mathbb{Z}} = (w_i^{\gamma,\eta} - w_{i-1}^{\gamma,\eta})_{i\in\mathbb{Z}}$ is an η-minimizing sequence for the problem defining γ;

• $w_i^{\beta,\eta} = z^* i$ for $i \geq T^{\beta,\eta}$ and $(z_i^{\beta,\eta})_{i\geq 1} = (w_i^{\beta,\eta} - w_{i-1}^{\beta,\eta})_{i\geq 1}$ is an η-minimizing sequence for the problem defining β.

We can then define the recovery sequence (u^ε) in a neighborhood of $x \in P_v$ by setting

$$u_i^\varepsilon = \overline{u}^\varepsilon(x) + \varepsilon \frac{u'(x+) - u'(x-)}{2z^*} w_{i-x/\varepsilon}^{\gamma,\eta} \quad \text{if } \ |i - x/\varepsilon| \leq T^{\gamma,\eta};$$

for $x \in S(\overline{u}^\varepsilon)$ we define, for $|i - x/\varepsilon| \leq T^{\gamma,\eta}$

$$u_i^\varepsilon = \begin{cases} \overline{u}^\varepsilon(x+) + \varepsilon \dfrac{u'(x+)}{z^*} w_{i-x/\varepsilon-1}^{\beta,\eta} & \text{if } 1 \leq i - x/\varepsilon \leq T^{\beta,\eta} \\ \\ \overline{u}^\varepsilon(x-) - \varepsilon \dfrac{u'(x-)}{z^*} w_{x/\varepsilon - i}^{\beta,\eta} & \text{if } -T^{\beta,\eta} \leq i - x/\varepsilon \leq 0. \end{cases}$$

Moreover we set

$$u_i^\varepsilon = \overline{u}_i^\varepsilon + \sqrt{\varepsilon} v_i \quad \text{otherwise},$$

where $v_i = v(\varepsilon i)$. Note that the sequence (u^ε) converges to (v, P_v, S_v) in the sense of Definition 2.

Recalling that v vanishes in a neighborhood of P_v, we obtain for any $x \in P_v$

$$\sum_{|i-x/\varepsilon|\leq T^{\gamma,\eta}} \left(\frac{1}{2} J\left(\frac{|u_{i+1}^\varepsilon - u_i^\varepsilon|}{\varepsilon}\right) + \frac{1}{2} J\left(\frac{|u_i^\varepsilon - u_{i-1}^\varepsilon|}{\varepsilon}\right) + J\left(\frac{|u_{i+1}^\varepsilon - u_{i-1}^\varepsilon|}{\varepsilon}\right) - \min J_{\mathrm{eff}} \right)$$
$$\leq \gamma + \eta.$$

For any $x \in S_v$ it follows that, setting $s_\varepsilon = \overline{u}_\varepsilon(x+) - \overline{u}_\varepsilon(x-)$

$$\sum_{|i-x/\varepsilon|\leq T^{\beta,\eta}} \left(\frac{1}{2} J\left(\frac{|u_{i+1}^\varepsilon - u_i^\varepsilon|}{\varepsilon}\right) + \frac{1}{2} J\left(\frac{|u_i^\varepsilon - u_{i-1}^\varepsilon|}{\varepsilon}\right) + J\left(\frac{|u_{i+1}^\varepsilon - u_{i-1}^\varepsilon|}{\varepsilon}\right) - \min J_{\mathrm{eff}} \right)$$

$$\begin{aligned} &= 2 \sum_{k=1}^{T^{\beta,\eta}} \Big(J(|z_k^{\beta,\eta}|) + J(|z_k^{\beta,\eta} + z_{k+1}^{\beta,\eta}|) - \min J_{\mathrm{eff}} \Big) + J(|z^*|) - 2 \min J_{\mathrm{eff}} \\ &\quad + J\Big(\Big| \frac{u'(x+) + u'(x-)}{z^*} w_0^{\beta,\eta} + \frac{s_\varepsilon}{\varepsilon} \Big| \Big) + J\Big(\Big| \frac{u'(x+) + u'(x-)}{z^*} w_1^{\beta,\eta} + \frac{s_\varepsilon}{\varepsilon} \Big| \Big) \\ &\quad + J\Big(\Big| \frac{u'(x-)}{z^*} w_1^{\beta,\eta} + \frac{u'(x+)}{z^*} w_0^{\beta,\eta} + \frac{s_\varepsilon}{\varepsilon} \Big| \Big) \\ &\leq \beta + \eta + o(1)_{\varepsilon\to 0} \end{aligned}$$

since $|s_\varepsilon/\varepsilon| \geq 1/\sqrt{\varepsilon}$ and v vanishes in a neighborhood of P_v.

We now consider the set I_ε^η of the indices i such that εi lie between $x_j + \eta$ and $x_{j+1} - \eta$ with η small enough so that v vanishes in the η-neighbourhood of $S_v \cup P_v$ and ε small enough so that $\varepsilon T^{\beta,\eta}$ and $\varepsilon T^{\gamma,\eta}$ are smaller than η.

Since v' is C^1 we can write

$$\frac{v_{i+1}-v_{i-1}}{2\varepsilon}=\frac{v_{i+1}-v_i}{\varepsilon}+O(\varepsilon)_{\varepsilon\to0}.$$

Noting that J is Lipschitz continuous on a neighbourhood of z^*, using the Taylor expansion of $J_{\rm eff}$ at z^*, we then deduce that

$$\begin{aligned}
&\sum_{i\in I_\varepsilon^\eta}\left(\frac12 J\left(\frac{|u^\varepsilon_{i+1}-u^\varepsilon_i|}{\varepsilon}\right)+\frac12 J\left(\frac{|u^\varepsilon_i-u^\varepsilon_{i-1}|}{\varepsilon}\right)+J\left(\frac{|u^\varepsilon_{i+1}-u^\varepsilon_{i-1}|}{\varepsilon}\right)-\min J_{\rm eff}\right)\\
&\quad=\sum_{i\in I_\varepsilon^\eta}\Big(\frac12 J\left(z^*+\sqrt{\varepsilon}\frac{v_{i+1}-v_i}{\varepsilon}\right)+\frac12 J\left(z^*+\sqrt{\varepsilon}\frac{v_i-v_{i-1}}{\varepsilon}\right)\\
&\qquad+J\left(2z^*+\sqrt{\varepsilon}\frac{v_{i+1}-v_{i-1}}{\varepsilon}\right)-\min J_{\rm eff}\Big)\\
&\quad=\sum_{i\in I_\varepsilon^\eta}\left(\frac12 J\left(z^*+\sqrt{\varepsilon}\frac{v_{i+1}-v_i}{\varepsilon}\right)+\frac12 J\left(z^*+\sqrt{\varepsilon}\frac{v_i-v_{i-1}}{\varepsilon}\right)\right.\\
&\qquad\left.+J\left(2z^*+2\sqrt{\varepsilon}\frac{v_{i+1}-v_i}{\varepsilon}\right)-\min J_{\rm eff}\right)+o(1)_{\varepsilon\to0}\\
&\quad=\sum_{i\in I_\varepsilon^\eta}\left(J\left(z^*+\sqrt{\varepsilon}\frac{v_{i+1}-v_i}{\varepsilon}\right)+J\left(2z^*+2\sqrt{\varepsilon}\frac{v_{i+1}-v_i}{\varepsilon}\right)-\min J_{\rm eff}\right)+o(1)_{\varepsilon\to0}\\
&\quad=\sum_{i\in I_\varepsilon^\eta}\left(\frac{J''_{\rm eff}(z^*)}{2}\varepsilon\Big(\frac{v_{i+1}-v_i}{\varepsilon}\Big)^2+o(\varepsilon)_{\varepsilon\to0}\right)+o(1)_{\varepsilon\to0}\\
&\quad=\alpha\int_{I_\eta}|v'|^2\,dx+o(1)_{\varepsilon\to0},
\end{aligned}$$

where $I_\eta=(x_j+\eta,x_{j+1}-\eta)$.

We then have

$$\limsup_{\varepsilon\to0}E_\varepsilon(u^\varepsilon)\le F(v,P_v,S_v)+\eta\#(P_v\cup S_v),$$

and the limsup inequality by the arbitrariness of η. □

4 Wider range of interactions

For interactions beyond next-to-nearest neighbours (but with a finite range of interactions M) the potential $J_{\rm eff}$ may be defined as

$$J_{\rm eff}(z)=\min\Big\{\sum_{j=1}^{M}\sum_{i=1}^{M-j}\frac{1}{M-j+1}J(|z_i+\cdots+z_{i+j-1}|):z_1+\cdots+z_M=Mz\Big\}.$$

Note that in general such type of potentials do not describe the Γ-limit if $M > 2$ due to possible oscillations at a larger scale than M. However, if we assume that $J_{\rm eff}$ satisfies the analog of the hypotheses for $M = 2$ then the properties of Remark 1 hold with the obvious changes and the same result as above can be proved. We refer to [8] (see in particular Remark 1) for details and more general potentials.

5 Conclusions

We have examined the effect of second-neighbor interactions on the asymptotic behaviour of an atomistic chain subject to Lennard-Jones interactions, showing that to some extent this may replace the assumption of a monotone parameterization of the atoms in the chain, and, in perspective, the positive-determinant constraint that is often assumed in order to derive limiting continuum theories in higher dimension. As in the monotonically parameterized case, we deduce a limiting theory of Griffith brittle-fracture type, the main difference being that the atoms may change from an increasingly to a decreasingly parameretized chain. The number of such changes is limited due to a positive energy of such 'creases'. From a mechanical point of view, allowing changes of orientation at crease points which do not coincide with fracture points is questionable, and this model should be understood, in the perspective of an application to higher-dimensional case, as a way to allow for a failure of the positive-determinant constraint in small zones. Note that the model does not prevent large portions of the chain to interpenetrate each other, a property that should be instead deduced from the optimality of monotone states. The main analytic contribution of the paper is the definition of convergence of discrete functions to a linearized state with jumps and creases, which the authors found more subtle than anticipated.

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