Effective cohesive behavior of layers of interatomic planes

Andrea Braides Adrian J. Lew Michael Ortiz

Abstract

A simple model of cleavage in brittle crystals consists of a layer of material containing N atomic planes separating in accordance with an interplanar potential under the action of an opening displacement δ prescribed on the boundary of the layer. The problem addressed in this work concerns the characterization of the constrained minima of the energy E_N of the layer as a function of δ as N becomes large. These minima determine the effective or macroscopic law of the crystal. The main results presented in this communication are: i) The computation of the Γ-limit E_0 of E_N as $N \to +\infty$; ii) The characterization of the minimum values of E_0 as a function of the opening displacement; iii) A proof of the uniform convergence of the values of E_N for the case of nearest-neighbor interactiond; iv) A proof of the uniform convergence of the derivatives of E_N (the tractions) in the same case. The scaling on which the present Γ-convergence analysis is based has the effect of separating the bulk and surface contributions to the energy. It differs crucially from other scalings employed in the past in that it renders both contributions of the same order.

1 Introduction

A simple model of cleavage in brittle crystals consists of a layer of material containing N atomic planes separating in accordance with an interplanar potential under the action of an opening displacement prescribed on the boundary of the layer. Let δ_j represent the opening displacement of the jth interatomic plane in the layer, $\delta = \sum_{j=1}^{N} \delta_j$ the prescribed total or *macroscopic* opening displacement, and $E_N(\delta_1, \ldots, \delta_N)$ the total energy *per unit* *area* of the layer as computed from the interplanar potential. Then, a central question is to characterize the constrained minima of E_N as a function of δ as N becomes large. This minimization process determines the effective or macroscopic cohesive law of the crystal.

Nguyen and Ortiz [10] and Hayes *et al.* [9] have investigated this problem using formal asymptotics, renormalization group techniques and first-principles calculations. Their work shows that the energy minimizers converge to a universal form independent of the interplanar potential when a certain scaling of the variables is introduced. The choice of scaling differs from the conventional scaling of bulk elasticity, and is instead tailored to the physics of cohesive behavior, which involves relations between *energy per unit area* and *opening displacement*. A striking demonstration of universality of the macroscopic cohesive law may be found in the recent work of Hayes *et al.* [9], who have computed the macroscopic cohesive law for three disparate materials: aluminum (a metal); alumina (Al_2O_3, a ceramic); and silicon (a semi-conductor) using density functional theory. When the energy and opening displacement are scaled appropriately with respect to N, all energy-displacement curves collapse onto a single universal curve. The work of Hayes *et al.* [9] also points to the importance of allowing for surface relaxation at newly created surfaces, an effect which is not within the scope of the nearest-neighbor analysis of Nguyen and Ortiz [10].

In the present communication we investigate the macroscopic limit $N \to \infty$ of a layer of interatomic planes by means of Γ-convergence. We consider a general class of interaction potentials with a range encompassing an arbitrary number of neighbors. The main results presented in this communication are:

i) The computation of $E_0 = \Gamma\text{-}\lim_{N\to\infty} E_N$ upon a suitable normalization that scales the macroscopic opening displacements and sets the absolute minimum of the energies at 0.
ii) The characterization of the minimum values of E_0 for each scaled macroscopic opening displacement, which are determined to be of the form: $\min\{\alpha\delta^2, \beta\}$, for $\delta \geq 0$, where α and β are constants.
iii) A proof of uniform convergence of the minima of the sequence E_N, as functions of δ, for the case of nearest-neighbor interactions.
iv) A proof of uniform convergence of the tractions for the case of nearest-neighbor interactions.

The rescaled macroscopic cohesive law $\min\{\alpha\delta^2, \beta\}$ for $\delta \geq 0$ is precisely of the universal form identified by Nguyen and Ortiz [10] and Hayes *et al.* [9], even for interactions involving an arbitrary number of neighbors. In particular, the macroscopic behavior depends only on the constants α and β. The constant α is related to the curvature, or stiffness, of the well of the interplanar potentials, whereas the constant β is twice the relaxed surface energy.

Useful intuition into the analysis and results of this article may be built from the following simple example. In the nearest-neighbor case, planes in-

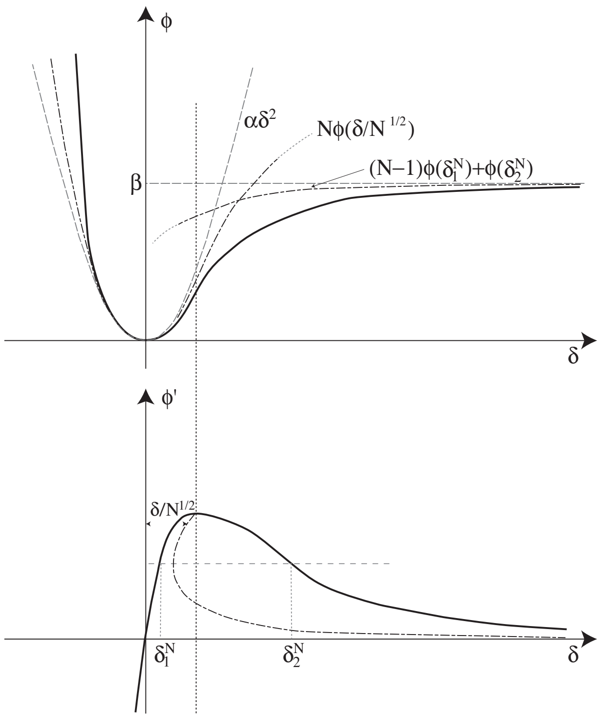

Fig. 1. Example of an interplanar potential of the Lennard-Jones type, which displays only one inflexion point separating convex and concave regions. For this simple case, a straightforward analysis proofs the uniform convergence of $P_N(\sqrt{N}\delta)$ and its derivative with respect to δ to the universal form $\min\{\alpha\delta^2, \beta\}$, for $\delta \geq 0$, and its derivative, respectively. A sketch of $P_N(\sqrt{N}\delta)$ for a particular value of N is shown in the top figure. Also shown is a graphical representation of the solution of equation (1.1). Given a value of $\delta/\sqrt{N}$, the values of δ_1^N and δ_2^N are determined by finding the horizontal line that leaves the point(s) in the dashed curve at a distance $\delta/\sqrt{N}$ from the $\delta = 0$ axis.

teract through a single interplanar potential $\phi(\delta_j)$, where δ_j is the separation between the two neighboring planes. Suppose, that $\phi(\delta_j)$ attains a minimum value of 0 at $\delta_j = 0$, and that $\phi(\delta_j)$ consists of convex and concave parts separated by a single inflection point, cf Figure 1. The total energy of the system in this case is: $E_N(\delta_1, \ldots, \delta_N) = \sum_i \phi(\delta_i)$. For given N and δ, the equilibrium configuration of the system is that which minimizes the total energy E_N subject to the constraint $\sum_i \delta_i = \delta$. The value of the energy at equilibrium, i. e., the *effective energy* of the layer, is, therefore,

$$P_N(\delta) = \min\Big\{\sum_{i=1}^{N} \phi(\delta_i) : \sum_i \delta_i = \delta\Big\}.$$

As $N \to +\infty$, a scaling of the macroscopic opening displacement with N must be introduced in order for the functions $P_N(\delta)$ to possess meaningful asymptotic behavior. The renormalization group approach of Nguyen and Ortiz [10] suggests that the correct scaling is to consider the sequence $P_N(\sqrt{N}\delta)$ for a fixed δ. With this scaling, the sequence of functions $P_N(\delta)$ converge uniformly, Theorem 1. In the case of a convex/concave potential such as shown in Figure 1, a study of local minima of the energy (cf, e. g., [4, 11, 10]) shows that two cases need only be considered: a) all opening displacements δ_i fall in the convex region of the interatomic potential, and hence are equal; and b) one single opening displacement falls in the concave region. Configurations of the first type correspond to an intact layer, whereas configurations of the second type correspond to a fractured layer. Accounting for cases (a) and (b), the scaled effective energy may be recast in the form

$$P_N(\sqrt{N}\delta) = \min\Big\{N\phi\Big(\frac{\delta}{\sqrt{N}}\Big), (N-1)\,\phi\big(\delta_1^N(\delta)\big) + \phi\big(\delta_2^N(\delta)\big)\Big\},$$

where $\delta_i^N(\delta)$ satisfy the following equilibrium equations and the boundary conditions

$$\begin{cases} \phi'(\delta_1^N(\delta)) = \phi'(\delta_2^N(\delta)), & \delta_1^N(\delta) < \delta_2^N(\delta) \\ (N-1)\delta_1^N(\delta) + \delta_2^N(\delta) = \sqrt{N}\,\delta \end{cases} . \tag{1.1}$$

A schematic of this system is shown in Figure 1. The functions $\delta_i^N(\delta)$ are then defined for $\delta \in [\delta_N, +\infty)$, δ_1^N is increasing, δ_2^N decreasing and $\delta_N \to 0$ when $N \to +\infty$. Therefore, the function $\widetilde{\phi}_N(\delta) = (N-1)\phi(\delta_1^N(\delta)) + \phi(\delta_2^N(\delta))$ is concave and converges to $\beta = \phi(+\infty)$ uniformly on $(w, +\infty)$ for all $w > 0$, whereas $\phi_N(\delta) = N\phi(\delta/\sqrt{N})$ converges locally uniformly on $\mathbb{R}$ to the quadratic approximation $\alpha\delta^2$ of ϕ at 0. We thus conclude that $P_N(\sqrt{N}\delta)$ converges to $\min\{\alpha\delta^2, \beta\}$ uniformly on $(w, +\infty)$ for all w. In addition, its derivative converges away from the point $\sqrt{\beta/\alpha}$. If ϕ does not have a simple convex/concave form, it is not possible to use the equilibrium equations as above. However, similar conclusions hold for very general potentials, as shown in Section 3. There, we use properties of the renormalization group in order to "sandwich" P_N between auxiliary upper and lower potentials. Using the ordering and monotonicity properties of the renormalization group we then show that the bounding potentials converge to the same universal limit as in he convex/concave case, and to establish the behavior of the derivatives.

In Section 4, the results for nearest-neighbor interactions are extended to a class of minimum problems of the general form

$$P_N(\sqrt{N}\delta) = \min\Big\{\sum_{i=1}^{N} \phi(\delta_i, \delta_{i+1}, \dots, \delta_{i+K-1}) : \sum_i \delta_i = \delta,\ i \mapsto \delta_i\ N\text{-periodic}\Big\},$$

where we allow interactions between $K+1$ neighboring planes. The properties that we require of the partial potentials ϕ are:

i) The existence of a unique ground state, together with the existence of second derivatives at that state.

ii) The validity of a Cauchy-Born hypothesis close to the ground state, namely, that for macroscopic opening displacements close to the ground state uniform interplanar separation is energetically favorable.
iii) An *impenetrability property.*
iv) Growth conditions at $+\infty$ that allow for detachments of planes.
v) The property that when two neighboring planes are completely detached the interactions of the remaining planes are decoupled.

For instance, these assumptions are satisfied by the superposition

$$\phi(\delta_1, \delta_2, \dots, \delta_K) = \sum_{n=1}^{K} \big(\phi_n(\delta_1) + \cdots + \phi_n(\delta_n)\big)$$

of K convex/concave potentials. The asymptotic form of P_N is as in the nearest-neighbor case, but the determination of the constant β requires the computation of the optimal energy of boundary layers that abut to pairs of detached planes. These boundary layers do not arise for nearest-neighbor interactions, and render the analysis of the general case comparatively much more challenging. The proof relies on Γ-convergence techniques recently developed for the passage from discrete to continuous variational problems. The Γ-limit result uses separation-of-scale arguments due to Chambolle [7] and Braides, Dal Maso and Garroni [4], and combines them with the analysis of internal boundary layers. It bears emphasis that whereas other scalings proposed in the past (Charlotte and Truskinovsky [8], Braides and Cicalese [3]) separate the bulk and surface contributions to the energy, for the scaling employed here both contributions have the same order.

2. Problem definition and assumptions

We consider K partial interatomic potentials $\phi_n : \mathbb{R}^n \to (-\infty, +\infty]$ $(1 \le n \le K)$ such that, for each n:

i) ϕ_n is a C^2 function in its domain $\{x \in \mathbb{R} : \phi_n(x) < +\infty\}$
ii) We have:

$$\lim_{\inf t_i \to -\infty} \phi_n(t_1, \dots, t_n) = +\infty. \tag{2.1}$$

This condition may be regarded as requiring *impenetrability property.* In particular we may have $\phi_n(t_1, \dots, t_n) = +\infty$ if $t_i \le 0$ for some i.

iii) for all n and $0 \le j \le n$ there exist functions ψ_n^j such that

$$\phi_n(t_1, \dots, t_n) = \psi_n^{j-1}(t_1, \dots, t_{j-1}) + \psi_n^{n-j}(t_{j+1}, \dots, t_n) + o(1) \tag{2.2}$$

as $t_j \to +\infty$, uniformly in $t_1, \dots, t_{j-1}, t_{j+1}, \dots, t_n$ if all t_i are equi-bounded from below. This condition asserts that, when two planes detach completely, the interactions between the remaining planes are uncoupled. We assume that $\psi_n^0 = 0$ for definiteness and that for $j \ge 1$

$\psi_n^j : \mathbb{R}^j \to (-\infty, +\infty]$ themselves satisfy conditions (i)–(iii). The condition that $\psi_n^0 = 0$ can be regarded as a normalization assumption that implies that

$$\lim_{\inf t_i \to +\infty} \phi_n(t_1, \ldots, t_n) = 0; \tag{2.3}$$

i. e., the interaction energy between n planes is 0 when they are completely detached.

iv) $\min \phi_n < 0$. In view of (2.3), this condition implies that the complete detachment of all planes is not an absolute minimum for the energy.

Remark 1. (a) Since we consider energies of the form

$$\sum_{n=1}^{K} \sum_{j=1}^{N} \phi_n(\delta_j, \delta_{j+1}, \ldots, \delta_{j+n-1}) \tag{2.4}$$

in conditions (i)–(iii) above we are free to regroup some of the energy densities without changing the double sum in (2.4). Consider, by way of example, the case $K = 2$: for any $s \in (0,1)$ we may set $\widetilde{\phi}_1(t_1) = s\phi_1(t_1)$ and $\widetilde{\phi}_2(t_1, t_2) = \phi_2(t_1, t_2) + (1-s)(\phi_1(t_1) + \phi_1(t_2))$. Clearly the energy in (2.4) remains unchanged if we replace all ϕ_n by $\widetilde{\phi}_n$. In particular, this shows that in (iii) we may only require that each ψ_n^j be bounded from below, instead of (2.1), since we may always add to it (and, correspondingly, to ϕ_n) a term of the form $s_j(\phi_1(t_1) + \ldots + \phi_1(t_j))$.

(b) If $\phi_n(t_1, \ldots, t_n) = \phi_n(t_1 + \ldots + t_n)$ then conditions (ii) and (iii) may be replaced by

$$\lim_{s \to -\infty} \phi_n(s) = +\infty, \qquad \text{and} \qquad \lim_{s \to +\infty} \phi_n(s) = 0,$$

respectively.

(c) Conditions (i)–(iii) can be weakened somewhat without essential modification of the main conclusions of this work. In particular, condition (i) is necessary on a neighborhood of the ground state only; in (ii) we may require that the growth condition be satisfied for ϕ_1 only; whereas in (iii) we may require that each ψ_n^0 be a (possibly different) constant. However, these extensions will not be pursued here in the interest of simplicity.

We consider minimum problems of the form

$$P_N(\delta) = \min\Bigg\{ \sum_{n=1}^{K} \sum_{j=1}^{N} \phi_n(\delta_j, \delta_{j+1}, \ldots, \delta_{j+n-1}) : \\ j \mapsto \delta_j \ N\text{-periodic}, \ \sum_{j=1}^{N} \delta_j = \delta \Bigg\} \tag{2.5}$$

and analyze the behavior of $P_N(\delta)$ for N large and δ close to the ground state. In order to make the latter statement precise, we introduce certain comparison interplanar potentials that will also be used in the proofs of the theorems. To this end, we notice that $P_N(\delta)$ can be equivalently written as

$$P_N(\delta) = \min\left\{ \sum_{i=1}^{N} \sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_{i+j}, \dots, \delta_{i+j+n-1}) : \right.$$
$$\left. j \mapsto \delta_j \ N\text{-periodic}, \ \sum_{j=1}^{N} \delta_j = \delta \right\} \tag{2.6}$$

We define the lower-bound comparison potential as:

$$\Phi_-(\delta) = \inf\left\{ \sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j, \dots, \delta_{j+n-1}) : \sum_{i=1}^{K} \delta_i = K\delta \right\}. \tag{2.7}$$

In this formula all interactions of K consecutive planes are minimized at fixed total mean displacement δ and without additional constraints such as periodicity. Note the normalization factor $K-n+1$ that counts the number of n-interaction between $K+1$ neighboring planes.

We now append the following assumptions:

v) *Existence of a uniform ground state*: There exists a unique $\delta_{\min}$ such that
$$\min_\delta \Phi_-(\delta) = \Phi_-(\delta_{\min}) =: \Phi_{\min}; \tag{2.8}$$

vi) *Uniform Cauchy-Born hypothesis near the ground state*: There exist $\eta > 0$ and $C > 0$ such that
$$\sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j, \dots, \delta_{j+n-1}) \geq \sum_{n=1}^{K} \phi_n(\delta, \dots, \delta) + C \sum_{j=1}^{K} (\delta_j - \delta)^2 \tag{2.9}$$
whenever $\sum_{n=1}^{K} \delta_n = K\delta$ and $\sum_{n=1}^{K} |\delta_n - \delta| + |\delta - \delta_{\min}| \leq \eta$.

vii) *Non-degeneracy at the ground state*:
$$\Phi''_-(\delta_{\min}) = \sum_{n=1}^{K} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 \phi_n}{\partial \delta_i \partial \delta_j}(\delta_{\min}, \dots, \delta_{\min}) > 0; \tag{2.10}$$

viii) *Non-degeneracy at $+\infty$*:
$$\liminf_{\delta \to +\infty} \Phi_-(\delta) > \Phi_{\min}. \tag{2.11}$$

Remark 2. From the hypotheses above we have that, for $|\delta - \delta_{\min}| \leq \eta$,

$$\Phi_-(\delta) = \sum_{n=1}^{K} \phi_n(\delta, \dots, \delta), \tag{2.12}$$

corresponding to the uniform state $\delta_i = \delta$ for all i. This equality does not hold for δ far from the ground state, as may be verified explicitly, e. g., for Lennard-Jones potentials.

Remark 3. For $K = 1$ (nearest-neighbor interactions) the hypotheses above reduce to requirements on the sole energy density ϕ_1. For $K = 2$ and $\phi_2(\delta_1, \delta_2) = \phi_2(\delta_1 + \delta_2)$ assumptions (v) and (vi) are satisfied if there exists $\delta_{\min}$ such that

$$\phi_1(\delta_{\min}) + \phi_2(2\delta_{\min}) = \min \phi, \tag{2.13}$$

where

$$\phi(\delta) = \phi_2(2\delta) + \frac{1}{2} \min_t \{\phi_1(t) + \phi_1(2\delta - t)\}, \tag{2.14}$$

and the unique minimizer of the latter minimum problem for $\delta = \delta_{\min}$ is $t = \delta_{\min}$. It may readily be checked that commonly used potentials, such as the Lennard-Jones and Morse potentials, satisfy these assumptions.

Remark 4. From the assumptions above it follows, upon changing the value of C, that for η small enough

$$\sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j, \dots, \delta_{j+n-1}) - \varPhi_{\min} \geq C \sum_{n=1}^{K} (\delta_n - \delta_{\min})^2 \tag{2.15}$$

whenever $\sum_{n=1}^{K} |\delta_n - \delta_{\min}| \leq \eta$. To verify this inequality we use an argument by contradiction. Note that by (vi), the formula above holds for $\sum_n \delta_n = K\delta_{\min}$; hence to contradict it, with fixed $N \in \mathbb{N}$, we suppose that δ_n^k exist with $\sum_n \delta_n^k = K\delta^k \neq K\delta_{\min}$ and $\delta^k \to \delta_{\min}$, such that ($C$ as in (vi))

$$\sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j^k, \dots, \delta_{j+n-1}^k) - \varPhi_{\min} \leq \frac{C}{N} \sum_{n=1}^{K} (\delta_n^k - \delta_{\min})^2.$$

By using the triangular inequality and (v) we get

$$\begin{aligned}
&\sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j^k, \dots, \delta_{j+n-1}^k) - \varPhi_{\min} \\
&\quad \leq \frac{2C}{N} \sum_{n=1}^{K} (\delta_n^k - \delta^k)^2 + \frac{2KC}{N} (\delta^k - \delta_{\min})^2 \\
&\quad \leq \frac{2C}{N} \Big(\sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j^k, \dots, \delta_{j+n-1}^k) - \varPhi_{\min} \Big) \\
&\qquad + \frac{2KC}{N} (\delta^k - \delta_{\min})^2,
\end{aligned}$$

and hence

$$\begin{aligned}
&\varPhi_-(\delta^k) - \varPhi_-(\delta_{\min}) \\
&\quad \leq \sum_{n=1}^{K} \sum_{j=1}^{K-n+1} \frac{1}{K-n+1} \phi_n(\delta_j^k, \dots, \delta_{j+n-1}^k) - \varPhi_{\min} \\
&\quad \leq \frac{2KC}{N - 2C} (\delta^k - \delta_{\min})^2,
\end{aligned}$$

which contradicts condition (vii) in view of the arbitrariness of N.

3. Renormalization group (RG) and nearest–neighbor interactions

In this section, we start by analyzing here the case of nearest–neighbor interactions, $K = 1$, with the aid of a Renormalization Group (RG) iteration. The appeal of this approach is that it establishes a stronger convergence, namely, uniform convergence, of the effective energy than obtained from Γ-converge. In addition, the RG approach establishes the convergence of the derivatives of the energy, or tractions.

For the nearest–neighbor case hypotheses (i)–(viii) simplify to assumptions on the sole interplanar potential ϕ_1. In particular, (vi) is automatically satisfied, and the remaining assumptions reduce to:

i) ϕ_1 is a C^2 function in its domain $\{\phi_1 < +\infty\}$.
ii) $\lim_{t\to-\infty} \phi_1(t) = +\infty$.
iii) $\lim_{t\to+\infty} \phi_1(t) = 0$.
iv) There exists a unique minimizer $\delta_{\min}$ of ϕ_1 and $\min \phi_1 < 0$.
v) $\delta_{\min}$ is an interior point of $\{\phi_1 < +\infty\}$ and $\phi_1''(\delta_{\min}) > 0$.

In the interest of simplicity, in addition to these hypotheses in this section we suppose that $\{x \in \mathbb{R}: \phi_1(\delta) \neq +\infty\}$ is connected. In particular, this assumption implies that, if $\phi_1(\overline{\delta}) = +\infty$ for some $\overline{\delta} < \delta_{\min}$, then $\phi_1(\delta) = +\infty$ for all $\delta \leq \overline{\delta}$. Moreover, we note that by Taylor's theorem and the preceding assumptions there exists $C > 0$ and $\eta > 0$ such that

$$\phi_1(\delta) \geq \phi_1(\delta_{\min}) + C(\delta - \delta_{\min})^2, \tag{3.1}$$

whenever $\mid \delta - \delta_{\min} \mid < \eta$.

3.1. Renormalization group transformation

The renormalization group transformation R is defined on an interplanar potential through a two–step process, namely *relaxation* and *renormalization.* The relaxation of an interplanar potential ϕ_1 is given by another interplanar potential $\overline{\phi_1}$ defined as

$$\overline{\phi_1}(\delta) = \inf_{\overline{\delta}\in\mathbb{R}} [\phi_1(\overline{\delta}) + \phi_1(\delta - \overline{\delta})], \tag{3.2}$$

The interplanar potential $R\phi_1$ then follows by renormalization, i. e.,

$$(R\phi_1)(\delta) = \overline{\phi_1}(\sqrt{2}\delta). \tag{3.3}$$

Evidently, R is well–defined for all functions bounded from below, and, in particular, for all interplanar potentials. For $2^n + 1$ atomic planes, problem (2.5) can be equivalently stated in terms of the renormalization group transformation as

$$\begin{aligned} P_{2^n}(\delta) &= \min\Big\{\sum_{j=1}^{2^{n-1}} R\phi_1(\delta_j) \colon \sum_{j=1}^{2^{n-1}} \delta_j = \delta/\sqrt{2}\Big\} \\ &= \min\Big\{\sum_{j=1}^{2^{n-2}} R^2\phi_1(\delta_j) \colon \sum_{j=1}^{2^{n-2}} \delta_j = \delta/\sqrt{2^2}\Big\} \\ &\ \vdots \qquad\qquad\qquad \vdots \\ &= \min\Big\{R^{n-1}\phi_1(\delta_1) + R^{n-1}\phi_1(\delta_2) \colon \delta_1 + \delta_2 = \delta/\sqrt{2^{n-1}}\Big\} \\ &= R^n\phi_1(\delta/\sqrt{2^n}). \end{aligned} \tag{3.4}$$

For purposes of the present analysis, it is simpler to redefine ϕ_1 such that 0 is its absolute minimum point and $\Phi_{\min} = 0$, i. e., we define a function $\psi^1(\delta) = \phi_1(\delta + \delta_{\min}) - \Phi_{\min}$. Then, $\lim_{\delta\to+\infty} \psi^1(\delta) = -\Phi_{\min}$ and $\lim_{\delta\to-\infty} \psi^1(\delta) = +\infty$.

The following remark summarizes the properties of interplanar potentials that are preserved under recursive application of the renormalization group transformation.

Remark 5. (a) Let $\psi : \mathbb{R} \to (-\infty, +\infty]$ be an interplanar potential such that

1. ψ is a C^0 function in its domain, which contains 0 in its interior.
2. ψ has a unique minimum at 0, $\psi(0) = 0$.
3. ψ satisfies

$$\lim_{\delta\to-\infty} \psi(\delta) = +\infty, \qquad \lim_{\delta\to+\infty} \psi(\delta) = -\Phi_{\min} \tag{3.5}$$

and

$$\lim_{\delta\to 0} \frac{\psi(\delta)}{\delta^2} = C. \tag{3.6}$$

Then $R\psi$ has these properties as well. It is straightforward to verify that $R\psi$ is a C^0 function and that

$$\lim_{\delta\to+\infty} R\psi(\delta) = -\Phi_{\min}, \qquad \lim_{\delta\to-\infty} R\psi(\delta) = +\infty. \tag{3.7}$$

It is also clear that $R\psi(0) \geq 0$, that $R\psi(\delta) = 0$ if and only if $\delta = 0$, and that $\delta = 0$ is in the interior of the domain of $R\psi$. Therefore, there remains to prove only that equation (3.6) holds for $R\psi$. To verify this property, note that for $\varepsilon > 0$ there exists $\xi > 0$ such that

$$(C - \varepsilon)\delta^2 \leq \psi(\delta) \leq (C + \varepsilon)\delta^2, \tag{3.8}$$

whenever $|\delta| < 2\xi$, and, therefore,

$$(C - \varepsilon)\left[\overline{\delta}^2 + (\delta - \overline{\delta})^2\right] \leq \psi(\overline{\delta}) + \psi(\delta - \overline{\delta}) \leq (C + \varepsilon)\left[\overline{\delta}^2 + (\delta - \overline{\delta})^2\right], \tag{3.9}$$

whenever $|\overline{\delta}|, |\delta| < \xi$. Note also that for $|\delta|$ small enough

$$\overline{\psi}(\delta) = \min_{|\overline{\delta}| \leq \xi} \left[\psi(\overline{\delta}) + \psi(\delta - \overline{\delta})\right]. \tag{3.10}$$

Since inequality (3.9) holds when $|\overline{\delta}| < \xi$, it also holds for the corresponding minima. Then, in conjunction with (3.10) we obtain

$$\frac{C-\varepsilon}{2} \leq \lim_{\delta \to 0} \frac{\overline{\psi}(\delta)}{\delta^2} \leq \frac{C+\varepsilon}{2}, \tag{3.11}$$

which holds for all $\varepsilon > 0$, and (3.6) follows after renormalization.

(b) We note, for subsequent reference, that hypotheses (i)-(vii) imply that for all $\varepsilon > 0$

$$\inf_{|\delta| > \varepsilon} \psi^1(\delta) > 0. \tag{3.12}$$

(c) Since ψ^1 is C^2, and $(\psi^1)''(0) > 0$, we have that

$$\lim_{\delta \to 0} \frac{\psi^1(\delta)}{\delta^2} = C, \tag{3.13}$$

where $0 < C < +\infty$, whence we conclude that ψ^1 satisfies hypotheses 1-3 in part (a) of this remark.

We proceed to establish a monotonicity property of R. Consider two interplanar potentials ψ_1 and ψ_2, not necessarily continuous, such that $\psi_1(\delta) \leq \psi_2(\delta)$ for all $\delta \in \mathbb{R}$. Then, $(R\psi_1)(\delta) \leq (R\psi_2)(\delta)$ for all $\delta \in \mathbb{R}$. The property follows directly by noting, for all $\overline{\delta} \in \mathbb{R}$,

$$\psi_1(\overline{\delta}) + \psi_1(\delta - \overline{\delta}) \leq \psi_2(\overline{\delta}) + \psi_2(\delta - \overline{\delta}). \tag{3.14}$$

Therefore, $\overline{\psi_1}(\delta) \leq \overline{\psi_2}(\delta)$ and $(R\psi_1)(\delta) \leq (R\psi_2)(\delta)$, for any $\delta \in \mathbb{R}$.

Next, we prove a property of the derivative of $R\psi$ to be used subsequently to prove the convergence of tractions.

Proposition 1. *Let* $w = \inf\{x \in \mathbb{R} \colon \psi(x) < +\infty\}$. *If* $\psi \in W^{1,\infty}(w, +\infty)$ *then* $R\psi \in W^{1,\infty}(\sqrt{2}w, +\infty)$. *Furthermore, there exists a function* $y : \mathbb{R} \to \mathbb{R}$ *such that*

$$\psi(y(x)) + \psi(x - y(x)) = \overline{\psi}(x) = \inf_{\delta \in \mathbb{R}} \left[\psi(\delta) + \psi(x - \delta)\right], \tag{3.15}$$

for which the following identity holds

$$(R\psi)'(x) = \sqrt{2}\ \psi'(y(\sqrt{2}x)), \tag{3.16}$$

for almost every $x \in (\sqrt{2}w, +\infty)$.

Proof. We begin by noting that, since $\lim_{\delta\to-\infty}\psi=+\infty$, the $y(x)$ satisfying equation (3.15) exists for all $x\in\mathbb{R}$. Without loss of generality, we assume $y(x)\le x-y(x)$ for all x, or $y(x)\le x/2$. If $x\in(\sqrt{2}w,+\infty)$ we additionally have $\overline{\psi}(\sqrt{2}x)\le 2\psi(x/\sqrt{2})<+\infty$, and, consequently, $w\le y(\sqrt{2}x)$ and $w<\sqrt{2}x-y(\sqrt{2}x)$.

Next we prove that $R\psi$ is absolutely continuous in every bounded interval $[a,b]\in(\sqrt{2}(w+\varepsilon),+\infty)$, for all $\varepsilon>0$. To this end, consider a collection of non-overlapping intervals $\{[a_i,b_i]\}$ of $[a,b]$. Then, for any $[a_i,b_i]$ such that $0<b_i-a_i<\varepsilon/\sqrt{2}$ there are two cases. One possibility is

$$\begin{aligned}0\le R\psi(b_i)-R\psi(a_i)&\le\psi(\sqrt{2}b_i-y(\sqrt{2}a_i))-\psi(\sqrt{2}a_i-y(\sqrt{2}a_i))\\&\le\|\psi'\|_{L^\infty(w,+\infty)}\sqrt{2}\,(b_i-a_i),\end{aligned}\tag{3.17}$$

since $\sqrt{2}b_i-y(\sqrt{2}a_i)=\sqrt{2}(b_i-a_i)+(\sqrt{2}a_i-y(\sqrt{2}a_i))>w$. Here we have used the fact that $\psi\in W^{1,\infty}(w,+\infty)$ is Lipschitz with Lipschitz constant $\|\psi'\|_{L^\infty(w,+\infty)}$. The second case is

$$\begin{aligned}0>R\psi(b_i)-R\psi(a_i)&\ge\psi(\sqrt{2}b_i-y(\sqrt{2}b_i))-\psi(\sqrt{2}a_i-y(\sqrt{2}b_i))\\&\ge-\|\psi'\|_{L^\infty(w,+\infty)}\sqrt{2}\,(b_i-a_i).\end{aligned}\tag{3.18}$$

In arriving at this inequality we have used the bound $\sqrt{2}a_i-y(\sqrt{2}b_i)>w$. To proof this bound, assume otherwise. Then,

$$\sqrt{2}a_i-w\le y(\sqrt{2}b_i)\le\frac{b_i}{\sqrt{2}}\Longrightarrow\sqrt{2}a_i-\frac{b_i}{\sqrt{2}}\le w.\tag{3.19}$$

But

$$\sqrt{2}a_i-\frac{b_i}{\sqrt{2}}\ge\sqrt{2}a_i-\frac{a_i}{\sqrt{2}}+\left(\frac{a_i}{\sqrt{2}}-\frac{b_i}{\sqrt{2}}\right)\ge w+\varepsilon-\frac{\varepsilon}{2}\ge w+\frac{\varepsilon}{2},\tag{3.20}$$

which contradicts (3.19). Then, from (3.17) and (3.18) we have

$$\sum_i|R\psi(b_i)-R\psi(a_i)|\le\|\psi'\|_{L^\infty(w,+\infty)}\sqrt{2}\,\sum_i(b_i-a_i),\tag{3.21}$$

for $\sum_i(b_i-a_i)$ small enough. This proves that $R\psi$ is absolutely continuous in every interval $(\sqrt{2}(w+\varepsilon),+\infty)$ for all $\varepsilon>0$, whence we conclude that $(R\psi)'$ exists almost everywhere in $(w,+\infty)$ and is the distributional derivative of $R\psi$. Finally, equation (3.16), which we prove next, allows us to conclude that $R\psi\in W^{1,\infty}(\sqrt{2}w,+\infty)$. Begin by noting that

$$\begin{aligned}&\frac{1}{h}\left[R\psi(x+h)-R\psi(x)\right]\\&\quad\le\frac{1}{h}\left[\psi(\sqrt{2}x-y(\sqrt{2}x))+\psi(y(\sqrt{2}x)+\sqrt{2}h)-R\psi(x)\right]\\&\quad\le\frac{1}{h}\left[\psi\left(y(\sqrt{2}x)+\sqrt{2}h\right)-\psi\left(y(\sqrt{2}x)\right)\right],\end{aligned}$$

for all $h > 0$ small enough, from where we conclude that

$$(R\psi)'(x) \leq \sqrt{2}\ \psi'\big(y(\sqrt{2}x),\big) \tag{3.22}$$

for almost every $x > \sqrt{2}w$. Similarly, from

$$\begin{aligned} &\frac{1}{h}\left[R\psi(x) - R\psi(x-h)\right] \\ &\geq \frac{1}{h}\Big[R\psi(x) - \psi(\sqrt{2}x - y(\sqrt{2}x)) - \psi(y(\sqrt{2}x) - \sqrt{2}h)\Big], \end{aligned}$$

for all $h > 0$ small enough we obtain

$$(R\psi)'(x) \geq \sqrt{2}\ \psi'\big(y(\sqrt{2}x)\big), \tag{3.23}$$

for almost every $x > \sqrt{2}w$, and equation (3.16) follows. □

3.2. Coarse-graining of interplanar potentials

Successive coarse-grainings of the interplanar potentials may be achieved by recursive application of R. More precisely, the transformation R^n, $n \in \mathbb{N}_0$, is defined inductively as $R^n = R \circ R^{n-1}$ for $n \geq 1$, with R^0 being just the identity. The **n**-th coarse-grained interplanar potential corresponding to an initial interplanar potential ψ is defined as $\psi_n = R^n\psi$. It is clear that $R^n\psi$ is well–defined. Specifically, we endeavor to characterize the limit of $R^n\psi$ as $n \to +\infty$, which defines the effective or macroscopic cohesive potential.

Theorem 1. *Let ψ be an interplanar potential, such that the hypotheses of Remark 5 are satisfied. Then $R^n\psi = \psi^n \to \psi^\infty$ uniformly in $(z, +\infty)$, for all $z \in \mathbf{R}$. Here,*

$$\psi^\infty(\delta) = \begin{cases} C\delta^2 & \text{if } \delta < 0 \\ \min\{C\delta^2, -\Phi_{\min}\} & \text{if } \delta \geq 0. \end{cases} \tag{3.24}$$

In terms of the minimum problem (2.5), we have

$$\lim_{n\to+\infty} P_{2^n}(\sqrt{2^n}\delta + 2^n\delta_{\min}) - 2^n\Phi_{\min} = \psi^\infty(\delta) \tag{3.25}$$

uniformly in $(z, +\infty)$.

Remark 6. For the sake of simplicity, in the proof we consider only interplanar potentials ψ with convex growth to $-\infty$. Thus, we suppose that there exists a convex function ψ_{convex} and $\delta_0 < 0$ such that $\psi_{\text{convex}}(\delta) \leq \psi(\delta)$ for all $\delta < \delta_0$. It follows from the monotonicity of R that $R^n\psi$ has the same property. In general, the theorem is valid for potentials that satisfy hypothesis (ii), e. g., potentials with logarithmic growth to $-\infty$.

Convergence of tractions. The uniform convergence of the interplanar potentials stated in Theorem 1 also implies the strong convergence in L^∞ of the renormalized traction, defined as the distributional derivative of the interplanar potential.

Theorem 2. *Let $t_n(\delta)$ and $t_\infty(\delta)$ denote the distributional derivatives of $R^n\psi(\delta)$ and $\psi^\infty(\delta)$ respectively. Then*

$$t_n \to t_\infty \qquad \text{in } L^\infty((z, x_c - \varepsilon) \cup (x_c + \varepsilon, +\infty)), \tag{3.26}$$

where $x_c = \sqrt{-\frac{\Phi_{\min}}{C}}$ for any $z \in \mathbf{R}$ and any $\varepsilon > 0$. Additionally, $t_n \overset{*}{\rightharpoonup} t_\infty$ in $L^\infty(z, +\infty)$, for any $z \in \mathbf{R}$.

Remark 7. (a) The failure to obtain uniform convergence close to x_c is not surprising, since the limit t_∞ is discontinuous at that point.

(b) With reference to the minimum problem (2.5), let T_{2^n} be the distributional derivative of P_{2^n} with respect to its argument, i. e.,

$$T_{2^n}(\varDelta) = P'_{2^n}(\varDelta). \tag{3.27}$$

Then, from Theorem 2 we have that

$$\sqrt{2^n}\; T_{2^n}(\sqrt{2^n}\delta + 2^n\delta_{\min}) \to t_\infty(\delta), \tag{3.28}$$

in $L^\infty((z, x_c - \varepsilon) \cup (x_c + \varepsilon, +\infty))$ for any $z \in \mathbf{R}$ and any $\varepsilon > 0$. Note that the convergence is attained for a precisely scaled value of δ.

Remark 8. In [10] potentials of the type

$$\phi_0(\delta) = \begin{cases} \varphi(\delta) & \text{if } \delta \geq 0 \\ +\infty & \text{otherwise,} \end{cases} \tag{3.29}$$

where $\varphi(\delta)$ has a unique minimum at $\varphi(0) = 0$, $\lim_{\delta \to +\infty} \varphi(\delta) = -\Phi_{\min} > 0$, and it is C^2 in $[0, +\infty)$. All results and proofs proceed *mutatis mutandis* in the general case. In this case we have that $R^n\phi_0(\delta) \to \min\{C\delta^2, -\Phi_{\min}\}$ uniformly in $[0, +\infty)$, and $R^n\phi_0(\delta) = +\infty$ for $\delta < 0$. An analogous result for the tractions holds as well.

Proof (Theorem 1).

1. Action of R on special potentials. Let $\Theta : \mathbf{R} \to (-\infty, +\infty]$ be an interplanar potential of the form

$$\Theta(\delta) = \begin{cases} \varphi(\delta) & \text{if } \delta < \delta^c \\ H & \text{if } \delta \geq \delta^c, \end{cases} \tag{3.30}$$

where $\varphi : \mathbf{R} \mapsto (-\infty, +\infty]$ is a convex function, continuous for all $\delta \geq 0$, with a unique minimum at $\delta = 0$, $\varphi(0) = 0$, $0 < H < +\infty$. Here $\delta^c > 0$ denotes the only nonnegative solution of $\varphi(\delta^c) = H$.Then,

$$R^n\Theta(\delta) = \begin{cases} 2^n\varphi(\delta/\sqrt{2^n}) & \text{if } \delta < \delta^c_n \\ H & \text{if } \delta \geq \delta^c_n, \end{cases} \tag{3.31}$$

where $\delta^c_n > 0$ denotes the single nonnegative solution of $2^n\varphi(\delta^c_n/\sqrt{2^n}) = H$.

To prove the previous statement, we compute first $R\Theta$. We begin by noting that since φ is convex we have

$$2\varphi(\delta/2) = \min_{\overline{\delta}\in\mathbf{R}} \left[\varphi(\delta-\overline{\delta}) + \varphi(\overline{\delta})\right]. \tag{3.32}$$

Then,

$$\begin{aligned} R\Theta(\delta/\sqrt{2}) &= \min\{\inf_{\frac{\delta}{2}\leq\overline{\delta}<\delta^c} \left[\varphi(\overline{\delta}) + \varphi(\delta-\overline{\delta})\right], \inf_{\overline{\delta}\geq\delta^c} \left[H + \Theta(\delta-\overline{\delta})\right]\} \\ &= \begin{cases} \min\{2\varphi(\delta/2), H + \inf_{\overline{\delta}\geq\delta^c}\varphi(\delta-\overline{\delta})\} & \text{if } \delta < 2\delta^c \\ H & \text{if } \delta \geq 2\delta^c. \end{cases} \end{aligned} \tag{3.33}$$

Next, assume that $\delta \leq 0$. Then, if $\overline{\delta} \geq \delta^c$ we have $\delta - \overline{\delta} \leq \delta - \delta^c \leq 0$, and consequently $\varphi(\delta-\overline{\delta}) \geq \varphi(\delta-\delta^c)$, since $\varphi(\delta)$ is decreasing when $\delta < 0$. From here we conclude that $H + \varphi(\delta-\overline{\delta}) \geq \varphi(\delta^c) + \varphi(\delta-\delta^c) \geq 2\varphi(\delta/2)$, and therefore $R\Theta(\delta/\sqrt{2}) = 2\varphi(\delta/2)$ for $\delta \leq 0$. If $0 < \delta < \sqrt{2}\delta_1^c$, then $2\varphi(\delta/2) < H$, and $R\Theta(\delta/\sqrt{2}) = 2\varphi(\delta/2)$. Finally, in the case $\sqrt{2}\delta_1^c \leq \delta$ note that the convexity of φ implies that

$$2\varphi(\delta^c/2) \leq \varphi(\delta^c) + \varphi(0) = H = 2\varphi(\delta_1^c/\sqrt{2}) \tag{3.34}$$

and, since $\varphi(\delta)$ is increasing for $\delta > 0$, we obtain that $\delta^c \leq \sqrt{2}\delta_1^c \leq \delta$. In this case, by choosing $\overline{\delta} = \delta$ in (3.33) we it follows that $R\Theta(\delta/\sqrt{2}) = H$. Summarizing,

$$R\Theta(\delta) = \begin{cases} 2\varphi(\delta/\sqrt{2}) & \text{if } \delta < \delta_1^c \\ H & \text{if } \delta \geq \delta_1^c. \end{cases} \tag{3.35}$$

Formula (3.31) follows by recursively applying the last result. Consider next the interplanar potential

$$\theta^1(\delta; H, h, \zeta) = \begin{cases} +\infty & \text{if } \delta < 0 \\ 0 & \text{if } \delta = 0 \\ H & \text{if } 0 < \delta \leq \zeta \\ h & \text{if } \zeta < \delta, \end{cases} \tag{3.36}$$

where $0 < h \leq H$, and $\zeta \geq 0$. By direct computation, it is straightforward to verify that

$$R\theta^1(\delta; H, h, \zeta) = \theta^1(\delta; H, h, \zeta/\sqrt{2}), \tag{3.37}$$

and, by recursion,

$$R^n\theta^1(\delta; H, h, \zeta) = \theta^1(\delta; H, h, \zeta/\sqrt{2^n}). \tag{3.38}$$

2. Equivalent upper and lower potentials. Given the interplanar potential ψ, we have that for all $\varepsilon > 0$ and every $w \in \mathbf{R}$ there exist $N_\varepsilon \in \mathbf{N}$ and interplanar potentials ψ_ε^- and ψ_ε^+ such that

$$\psi_\varepsilon^- \leq \psi \leq \psi_\varepsilon^+ \qquad \forall\delta \in \mathbf{R}, \tag{3.39}$$

In addition, there exists a constant M such that

$$0 \le \psi^\infty - R^n \psi_\varepsilon^- < \varepsilon M \tag{3.40}$$

and

$$0 \le R^n \psi_\varepsilon^+ - \psi^\infty < \varepsilon M, \tag{3.41}$$

for all $n > N_\varepsilon$, for all $\delta \in (w, +\infty)$. The proof of this statement is given next.

3. Existence of upper potential ψ_ε^+. Choose $\zeta > 0$ such that

$$(C+\varepsilon)\delta^2 \ge \psi(\delta) \text{ if } \mid \delta \mid < \zeta, \tag{3.42}$$

and $\lambda > 0$ such that

$$\psi(\delta) < -\Phi_{\min} + \varepsilon \qquad \forall \delta > \lambda. \tag{3.43}$$

Let $\Psi_{\max} = \max_{\delta > \delta_{\min}} \psi(\delta)$; clearly $\Psi_{\max} < +\infty$. Set

$$\theta^2(\delta) = \begin{cases} +\infty & \text{if } \delta \le -\zeta \\ \Psi(\delta) & \text{if } -\zeta < \delta < \zeta \\ \Psi_{\max} & \text{if } \delta \ge \zeta, \end{cases} \tag{3.44}$$

where $\Psi(\delta)$ is a convex function that satisfies $\Psi(\delta) = (C+\varepsilon)\delta^2$ whenever $\delta < \zeta/2$, and $\Psi(\zeta) = \Psi_{\max}$. From the previous computation, for n large enough we have that

$$R^n\theta^2(\delta) = \begin{cases} +\infty & \text{if } \delta \le -\zeta\sqrt{2^n} \\ (C+\varepsilon)\delta^2 & \text{if } -\zeta\sqrt{2^n} < \delta < \sqrt{\frac{H}{C+\varepsilon}} \\ \Psi_{\max} & \text{if } \delta \ge \sqrt{\frac{H}{C+\varepsilon}}. \end{cases} \tag{3.45}$$

Define

$$\psi_\varepsilon^+ = \min\left\{\theta^1(\delta; \Psi_{\max}, -\Phi_{\min} + \varepsilon, \lambda), \theta^2(\delta)\right\}. \tag{3.46}$$

Clearly $\psi \le \psi_\varepsilon^+$. By the monotonicity of R we get

$$R^n\psi_\varepsilon^+(\delta) < \min\left\{R^n\theta^1(\delta; \Psi_{\max}, -\Phi_{\min} + \varepsilon, \lambda), R^n\theta^2(\delta)\right\}, \tag{3.47}$$

which for n large enough reduces to

$$R^n\psi_\varepsilon^+(\delta) < \begin{cases} +\infty & \text{if } \delta \le -\zeta\sqrt{2^n} \\ (C+\varepsilon)\delta^2 & \text{if } -\zeta\sqrt{2^n} < \delta < \sqrt{\frac{H}{C+\varepsilon}} \\ -\Phi_{\min} + \varepsilon & \text{if } \delta \ge \sqrt{\frac{H}{C+\varepsilon}}, \end{cases} \tag{3.48}$$

whence (3.41) follows immediately.

4. Existence of lower potential ψ_ε^-. Choose $\zeta > 0$ such that

$$(C-\varepsilon)\delta^2 \le \psi(\delta) \qquad \text{if } \mid \delta \mid < \zeta, \tag{3.49}$$

and $\lambda > 0$ such that

$$\psi(\delta) > -\Phi_{\min} - \varepsilon \qquad \text{if } \delta > \lambda. \tag{3.50}$$

Next, consider the interplanar potential

$$\psi_\varepsilon^-(\delta) = \begin{cases} \Psi(\delta) & \text{if } \delta < \lambda \\ -\Phi_{\min} - \varepsilon & \text{if } \delta \geq \lambda, \end{cases} \tag{3.51}$$

where $\Psi(\delta)$ is a convex function such that $\Psi(\delta) = (C - \varepsilon)\delta^2$ if $|\delta| < \zeta$, $\Psi(\lambda) = -\Phi_{\min} - \varepsilon$, and $\Psi(\delta) < \psi(\delta)$ for all $\delta \in \mathbf{R}$. That such a function exists follows from Remark 5, part (b), by choosing ζ small enough and λ large enough. Note that $\psi_\varepsilon^- < \psi$. From the previous computation, for n large enough we have

$$R^n\psi_\varepsilon^-(\delta) = \begin{cases} 2^n\Psi(\delta/\sqrt{2^n}) & \text{if } \delta \leq -\zeta\sqrt{2^n} \\ (C-\varepsilon)\delta^2 & \text{if } -\zeta\sqrt{2^n} < \delta < \sqrt{\frac{H}{C-\varepsilon}} \\ -\Phi_{\min} - \varepsilon & \text{if } \delta \geq \sqrt{\frac{H}{C-\varepsilon}}, \end{cases} \tag{3.52}$$

whence (3.40) follows immediately. A schematic representation of the upper and lower potentials is shown in Figure 2.

5. Convergence. Let $\varepsilon > 0$ and $z \in \mathbf{R}$. Because of (3.39) and the monotonicity of R, we have

$$R^n\psi_\varepsilon^- \leq R^n\psi \leq R^n\psi_\varepsilon^+, \tag{3.53}$$

for all $n \in \mathbf{N}$ and for all $\delta \in (z, +\infty)$. In particular, if $n > N_\varepsilon$

$$-\varepsilon M < R^n\psi_\varepsilon^- - \psi^\infty \leq R^n\psi - \psi^\infty \leq R^n\psi_\varepsilon^+ - \psi^\infty < \varepsilon M, \tag{3.54}$$

whence it follows that

$$\lim_{n\to+\infty} |R^n\psi - \psi^\infty| < \varepsilon M \qquad \forall\delta > z. \tag{3.55}$$

Since this holds for any $\varepsilon > 0$, the uniform convergence in $(z, +\infty)$ follows. To prove (3.25) it suffices to note that

$$R^n\phi_1(\delta + \sqrt{2^n}\delta_{\min}) = R^n\psi(\delta) + 2^n\Phi_{\min}, \tag{3.56}$$

which together with (3.4) gives the desired result. □

Proof (Theorem 2).

1. Asymptotic structure of minimizers. Let $\psi^n = R^n\psi$, and define the function $y_n(x)$ such that $|y_n(x)| \leq |x - y_n(x)|$ and

$$\overline{\psi}^n(x) = \inf_{\delta\in\mathbf{R}} [\psi^n(\delta) + \psi^n(x-\delta)] = \psi^n(y_n(x)) + \psi^n(x - y_n(x)), \tag{3.57}$$

which is well-defined since $\lim_{\delta\to-\infty}\psi^n(\delta) \to +\infty$, and ψ^n is continuous (it may, however, not be uniquely defined). We seek to characterize the values

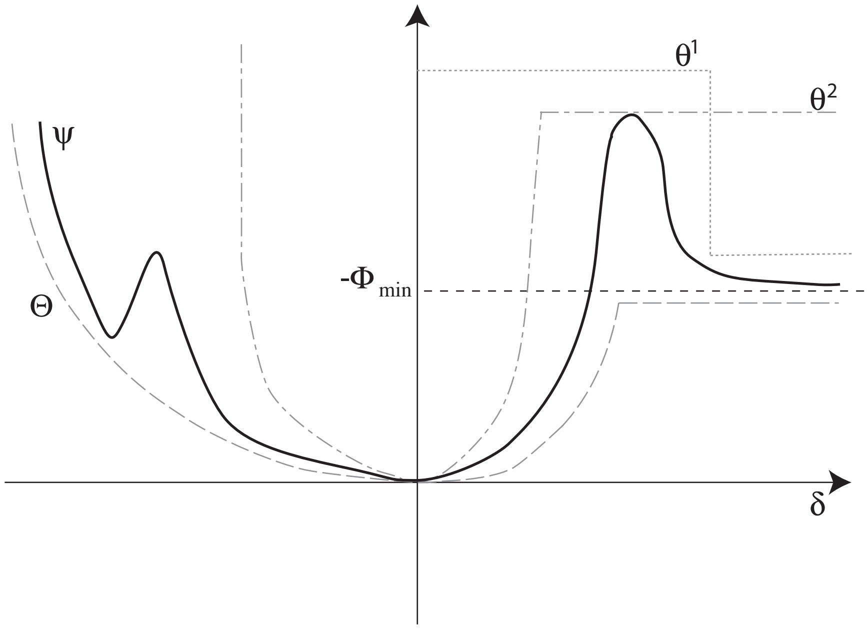

Fig. 2. Schematic representation of the construction of upper and lower potentials. A typical interplanar potential is shown in a solid line. Note the asymptotic behavior as $\delta \to +\infty$ and the possibility of having multiple inflexion points, local minima and maxima. Possible choices of upper and lower potentials are shown in dashed lines.

of $y_n(x)$. Let $x_0 < z < 0$ be such that $\psi^\infty(x) > -\Phi_{\min}$ for all $x < z$, which implies that $\psi^\infty(z) > \psi^\infty(x)$ for $x \in (z, +\infty)$. For all $\varepsilon > 0$ there exists $n_\varepsilon \in \mathbf{N}$ such that, for all $n > n_\varepsilon$, $|\psi^n(x) - \psi^\infty(x)| < \varepsilon$ whenever $x \in (x_0, +\infty)$ and $\psi^n(x) > \psi^\infty(x_0) - \varepsilon$ whenever $x \in (-\infty, x_0)$. The existence of n_ε such that the last condition is satisfied is guaranteed by the shape of the lower potential (3.51). Additionally, we take ε small enough such that $\psi^\infty(z) + \varepsilon \le \psi^\infty(x_0) - \varepsilon$.

We proceed to show that $y_n(x) > x_0$ and $x - y_n(x) > x_0$ for all $x > z$ and $n > n_\varepsilon$. Assume otherwise. Then, for some $n > n_\varepsilon$,

$$\overline{\psi}^n(x) > \psi^\infty(x_0) - \varepsilon, \tag{3.58}$$

But, by definition,

$$\overline{\psi}^n(x) \le \psi^n(x) \le \psi^\infty(x) + \varepsilon \le \psi^\infty(z) + \varepsilon \le \psi^\infty(x_0) - \varepsilon, \tag{3.59}$$

which contradicts the assumption. Next, consider the function $\phi(y, x) = \psi^\infty(y) + \psi^\infty(x - y)$, whose minimum for every x is attained at $y_\infty(x)$, where

$$y_\infty(x) = \begin{cases} \frac{x}{2} & \text{if } x \le \sqrt{2}\, x_c \\ 0 & \text{if } x \ge \sqrt{2}\, x_c \end{cases} \tag{3.60}$$

is bi–valued at $\sqrt{2}\ x_c = \sqrt{\frac{-2\Phi_{\min}}{C}}$. We have that for $x > z$ and $n > n_\varepsilon$

$$\begin{aligned}\phi(y_n(x), x) - 2\varepsilon &\leq \psi^n(y_n(x)) + \psi^n(x - y_n(x)) \\ &\leq \psi^n(y_\infty(x)) + \psi^n(x - y_\infty(x)) \\ &\leq \phi(y_\infty(x), x) + 2\varepsilon,\end{aligned}$$

or, equivalently,

$$0 \leq \phi(y_n(x), x) - \phi(y_\infty(x), x) \leq 4\varepsilon. \tag{3.61}$$

Let $\mathcal{A} = \{(y_\infty(x), x) : x \in \mathbf{R}\}$. Then, it is straightforward to verify that there exists $c_1, c_2 > 0$ such that

$$c_1\ d_{\mathcal{A}}\,(y, x)^2 \wedge c_2 \leq \phi(y, x) - \phi(y_\infty(x), x), \tag{3.62}$$

whenever $|y| \leq |x - y|$, where $d_{\mathcal{A}}$ is the Euclidean distance from a point in $\mathbf{R}^2$ to the set $\mathcal{A}$. It follows from (3.61) and (3.62) that $y_n(x) \to y_\infty(x)$ uniformly in any set of the form $(z, \sqrt{2}\ x_c - \varepsilon) \cup (\sqrt{2}\ x_c + \varepsilon, +\infty)$, for any $\varepsilon > 0$, and by the arbitrariness of z, pointwise for all $x \in \mathbf{R} \setminus \{\sqrt{2}\ x_c\}$.

2. Uniform convergence of tractions. We begin by considering the behavior of $(R^n\psi)'(x)$ in a neighborhood of $x = 0$. With reference to Remark 5, part b, and hypotheses (i) and (vii), we can construct a continuous function $\Theta(x)$ as in equation (3.30), such that $\Theta(x) = \psi(x)$ in an open neighborhood of $x = 0$ in which $\psi''(x) > 0$, and $\Theta(x) \leq \psi(x)$ for all x. Then, for $\eta > 0$ small enough, equation (3.31) gives

$$R^n\psi(x) \leq 2^n\psi\left(\frac{x}{\sqrt{2^n}}\right) = 2^n\Theta\left(\frac{x}{\sqrt{2^n}}\right) = R^n\Theta(x) \leq R^n\psi(x), \tag{3.63}$$

or

$$R^n\psi(x) = 2^n\psi\left(\frac{x}{\sqrt{2^n}}\right), \tag{3.64}$$

for all $x \in (-\eta, \eta)$ and all $n \in \mathbf{N}$. Also, by Taylor's theorem we have that

$$\psi'(x) = (C + \xi(x))\,x, \tag{3.65}$$

for all $x \in (-\eta, \eta)$, with $\lim_{x\to 0}\xi(x) \to 0$. Therefore,

$$(R^n\psi)'(x) = \sqrt{2^n}\psi'\left(\frac{x}{\sqrt{2^n}}\right) = (C + \xi(x/\sqrt{2^n}))x \tag{3.66}$$

whence it follows that

$$\lim_{n\to+\infty}(R^n\psi)'(x) = Cx, \tag{3.67}$$

uniformly in $(-\eta, \eta)$.

In the more general case of $x \in (z, +\infty)$, we know from Proposition 1 that for $n, m \in \mathbf{N}$, $m \leq n$, and for almost all $x \in \mathbf{R}$

$$\begin{aligned}(R^n\psi)'(x) &= \sqrt{2}(R^{n-1}\psi)'(y_{n-1}(\sqrt{2}\ x)) \\ &= \sqrt{2^2}(R^{n-2}\psi)'(y_{n-2}(\sqrt{2}\ y_{n-1}(\sqrt{2}\ x))) \\ &\ \vdots \\ &= \sqrt{2^m}(R^{n-m}\psi)'(\beta_m^n(x)),\end{aligned} \tag{3.68}$$

where $\beta_0^n(x) = x$ and $\beta_i^n(x) = y_{n-i}(\sqrt{2}\ \beta_{i-1}^n(x))$, for all $i \leq n$.

Next, we analyze the asymptotic behavior of the sequence $\beta_m^n(x)$ as $n \to +\infty$. Given $\varepsilon > 0$, and $\zeta > 0$ sufficiently small, there exists n_ζ such that

$$\zeta > \left| y_{n-m}(\sqrt{2}\beta_{m-1}^n(x)) - y_\infty(\sqrt{2}\beta_{m-1}^n(x)) \right| = \left| \beta_m^n(x) - \frac{\beta_{m-1}^n(x)}{\sqrt{2}} \right|, \tag{3.69}$$

for all $x \in (z, x_c - \varepsilon)$, whenever $0 < m < n - n_\zeta$. Equation (3.69) is a consequence of the uniform convergence of $\{y_n(x)\}$. It follows by induction on m after noticing that ζ can be chosen small enough such that if $\beta_{m-1}^n(x) \in (z, x_c - \varepsilon)$ then $\beta_m^n(x) \in (z, x_c - \varepsilon)$, whenever $0 < m < n - n_\zeta$. By recursive application of (3.69) and the triangular inequality it is straightforward to verify that

$$\left| \beta_m^n(x) - \frac{x}{\sqrt{2^m}} \right| < \zeta^*, \tag{3.70}$$

for all m such that $0 \leq m < n - n_\zeta$ and all $x \in (z, x_c - \varepsilon)$, where $\zeta^* = \zeta\sqrt{2}/(\sqrt{2} - 1)$. Similarly, if $x > x_c + \varepsilon$, it follows from the uniform convergence of $\{y_n\}$ that

$$|\beta_1^n(x)| < \zeta, \tag{3.71}$$

and by using (3.70)

$$|\beta_m^n(x)| < (1 + 1/\sqrt{2^{m-1}})\zeta^*, \tag{3.72}$$

for all m such that $1 \leq m < n - n_\zeta$. With η as in equation (3.67), choose ζ such that $2\zeta^* < \eta$, and $m \geq 1$ such that $x/\sqrt{2^m} \in (-\eta + \zeta^*, \eta - \zeta^*)$ for all $x \in (z, x_c - \varepsilon)$. Then for n large enough we have

$$\left| (R^{n-m}\psi)'(\beta_m^n(x)) - C\beta_m^n(x) \right| < C\zeta^*, \tag{3.73}$$

for all $x \in (z, x_c - \varepsilon) \cup (x_c + \varepsilon, +\infty)$, where we have used equations (3.70) and (3.72) and replaced n for $n - m$ and x for $\beta_m^n(x)$ in equation (3.67). In particular, for $x \in (z, x_c - \varepsilon)$, it follows from equation (3.70) that

$$\left| (R^{n-m}\psi)'(\beta_m^n(x)) - C\frac{x}{\sqrt{2^m}} \right| < 2C\zeta^*, \tag{3.74}$$

or, equivalently by using equation (3.68)

$$|(R^n\psi)'(x) - Cx| < \sqrt{2^{m+2}}C\zeta^*. \tag{3.75}$$

Similarly, if $x > x_c + \varepsilon$ we have from equations (3.68), (3.72) and (3.73) that

$$|(R^n\psi)'(x)| < 3\sqrt{2^m}C\zeta^*. \tag{3.76}$$

Therefore, it follows that the tractions converge uniformly in any set $(z, x_c - \varepsilon) \cup (x_c + \varepsilon, +\infty)$, for all $z \in \mathbf{R}$, and for any $\varepsilon > 0$. Finally, if $x \in (x_c - 2\varepsilon, x_c + 2\varepsilon)$ we have from equation (3.62) that, for n large enough, either $|\beta_1^n(x) - x_c/\sqrt{2}| < \zeta$ or $|\beta_1^n(x)| < \zeta$. In either case, by using equations (3.70) and (3.68) we conclude that the tractions are uniformly bounded in $(z, +\infty)$, for any $z \in \mathbf{R}$, whence the weak* convergence of the tractions in the same interval follows. □

4. Γ-limit of the energy functional

Under assumptions (i)-(viii) of Section 2, in this section we prove the following:

Theorem 3. *There exist constants α and β such that for $\delta \geq 0$*

$$P_N(N\delta_{\min} + \sqrt{N}\,\delta) = N\Phi_{\min} + \min\{\alpha\delta^2, \beta\} + o(1). \tag{4.1}$$

The constants $\Phi_{\min}$ and α are simply given by

$$\Phi_{\min} = \sum_{n=1}^{K} \phi_n(\delta_{\min}, \ldots, \delta_{\min}),\ \ \alpha = \frac{1}{2}\sum_{n=1}^{K}\sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2\phi_n}{\partial\delta_i\partial\delta_j}(\delta_{\min}, \ldots, \delta_{\min}), \tag{4.2}$$

while $\beta = 2B - K\Phi_{\min}$, where B is the (free) boundary-layer energy

$$\begin{aligned} B = \inf_{R\in\mathbf{N}} \min\Big\{ &\sum_{j\geq 0}\Big(\sum_{n=1}^{K}\sum_{j=0}^{K-n} \frac{1}{K-n+1}\phi_n(\delta_{i+j}, \ldots, \delta_{i+j+n-1}) - \Phi_{\min}\Big) \\ &+ \sum_{n=1}^{K-1}\sum_{j=0}^{n-1} \frac{K-n-j}{K-n+1}\,\phi_n(\delta_j, \ldots, \delta_{j+n-1}) \\ &+ \sum_{n=1}^{K}\sum_{i=1}^{n-1} \psi_n^i(\delta_0, \ldots, \delta_{i-1}) : \delta_j = \delta_{\min} \text{ for } j \geq R\Big\}. \end{aligned} \tag{4.3}$$

If $K = 1$ (nearest-neighbor interactions) *and $\phi_1 = \phi$, then $\Phi_{\min} = \phi(\delta_{\min})$, $\alpha = \frac{1}{2}\phi''(\delta_{\min})$, and $B = 0$ so that $\beta = -\Phi_{\min}$.*

The behavior of minimum problems may be turned into the computation of a Γ-limit on a metric (more precisely, metrizable) space. To this end, we may identify each discrete function $j \mapsto \delta_j$ with a function on the continuum. One way to do this is simply by identifying it with the piecewise-constant function

$$\delta(t) = \sqrt{N}\,(\delta_i - \delta_{\min}) \text{ if } \frac{i-1}{N} < t \leq \frac{i}{N}.$$

In this way the domain of our energies may be interpreted as a subset of $L^1(0,1)$ (more precisely, as a subset of $L^1_{\rm loc}(\mathbf{R})$ with a periodicity constraint). However, our energies are be coercive on these sets: minimizers are not compact in $L^1(0,1)$. Therefore, we have to further view $L^1(0,1)$ as a subset of the set of measures on $\mathcal{M}([0,1])$, where we eventually obtain compactness and hence convergence of the minimum problem. Moreover, in this framework that sequences δ_N with an energy of the same order as that of minimizers may converge to measures μ whose singular part is composed of a finite number of Dirac deltas.

In order to have a more direct connection with known results, we additionally use an equivalent identification. Instead of identifying each $\{\delta_j\}$ with a piecewise-constant function we interpret our energies as defined on the space of piecewise-H^1 functions, i. e., functions u which are H^1 outside a finite number of points of discontinuity. This discontinuity set is denoted by $S(u)$. The results thus obtained may readily be recast in the framework of $\mathcal{M}([0,1])$ by interpreting μ as the derivative of u, and hence each discontinuity of u as a Dirac mass of μ.

The identification is obtained by making the following changes in notation. We set $\varepsilon_N=\frac{1}{N}$ and, for given $\{\delta_j\}$ we define the function $u:\varepsilon_N\mathbf{Z}\to\mathbf{R}$ given by

$$u_0=u(0)=0,\qquad u_j=u(j\varepsilon_N)=u((j-1)\varepsilon_N)+\sqrt{\varepsilon_N}(\delta_j-\delta_{\rm min}).\quad (4.4)$$

Every such u is understood to represent a piecewise affine function with $\mathbf{R}$ as domain given by

$$u(t)=\Big(1-\frac{t}{\varepsilon_N}+j\Big)u_j+\Big(\frac{t}{\varepsilon_N}-j\Big)\,u_{j+1}\qquad\text{if } j\varepsilon_N\le t\le (j+1)\varepsilon_N,\quad (4.5)$$

so that the convergence of the discrete functions can be interpreted in terms of that of the corresponding interpolations.

We introduce the space $\mathcal{A}_N(\delta)$ as the set of functions $u:\varepsilon_N\mathbf{Z}\to\mathbf{R}$ such that $u((i+N)\varepsilon_N)=\delta+u(i\varepsilon_N)$ (1-periodicity of $u(t)-\delta t$). We then have

$$\begin{aligned}
&P_N(N\delta_{\rm min}+\sqrt{N}\,\delta)-N\varPhi_{\rm min}\\
&=P_N(N\delta_{\rm min}+\sqrt{N}\,\delta)-N\sum_{n=1}^K\phi_n(\delta_{\rm min},\dots,\delta_{\rm min})\\
&=\min\Big\{\sum_{n=1}^K\sum_{j=1}^N\Big(\phi_n(\delta_j,\delta_{j+1},\dots,\delta_{j+n-1})-\phi_n(\delta_{\rm min},\dots,\delta_{\rm min})\Big):\\
&\qquad\qquad j\mapsto\delta_j\text{ is N-periodic and }\sum_{j=1}^N\delta_j=N\delta_{\rm min}+\sqrt{N}\,\delta\Big\}\\
&=\min\Big\{\sum_{n=1}^K\sum_{j=1}^N\Big(\phi_n\Big(\sqrt{\varepsilon}_N\Big(\frac{u_{j+1}-u_j}{\varepsilon_N}\Big)+\delta_{\rm min},\dots
\end{aligned}$$

$$\dots, \sqrt{\varepsilon}_N\Big(\frac{u_{j+n}-u_{j+n-1}}{\varepsilon_N}\Big)+\delta_{\min}\Big)$$
$$-\phi_n(\delta_{\min},\dots,\delta_{\min})\Big): u\in\mathcal{A}_N(\delta)\Big\}.$$

Theorem 3 in turn follows as a consequence of the following Γ-convergence result for the functionals defined on $\mathcal{A}_N(\delta)$ by

$$E_N(u)=\sum_{n=1}^{K}\sum_{j=1}^{N}\varepsilon_N\phi_n^N\Big(\frac{u_{j+1}-u_j}{\varepsilon_N},\dots,\frac{u_{j+n}-u_{j+n-1}}{\varepsilon_N}\Big), \tag{4.6}$$

where

$$\phi_n^N(z_1,\dots,z_n)=\frac{1}{\varepsilon_N}\Big(\phi_n\Big(\sqrt{\varepsilon}_N z_1+\delta_{\min},\dots,\sqrt{\varepsilon}_N z_n+\delta_{\min}\Big) -\phi_n(\delta_{\min},\dots,\delta_{\min})\Big). \tag{4.7}$$

Theorem 4. *Let α and β be the constants defined above. Then the functionals E_N Γ-converge with respect to the L^1-convergence to the functional E_0 defined on piecewise-H^1 functions such that $u-\delta x$ is 1-periodic by*

$$E_0(u)=\begin{cases}\alpha\displaystyle\int_0^1|u'|^2\,dt+\beta\#(S(u)\cap(0,1]) & \textit{if } u^+>u^- \textit{ on } S(u)\\ +\infty & \textit{otherwise}\end{cases} \tag{4.8}$$

Moreover, if $\delta>0$ the minimum values above converge to the minimum value

$$\min E_0=\min\{\alpha\delta^2,\beta\}. \tag{4.9}$$

Remark 9. Γ-limits of functionals of the form (4.6) and their multidimensional analogs when ϕ_n^N depend on $z_1+\dots+z_n$ have been extensively studied in recent times (see e. g. [7,4–6,1]). The choice of notation in terms of difference quotients is made in order to facilitate usage of–and comparison with–those results.

In the proof of this theorem we make repeated use of the following results on the energies

$$G_N(u)=\sum_{j=1}^{N-1}\Psi_N\Big(\frac{u_{j+1}-u_j}{\varepsilon_N}\Big), \tag{4.10}$$

where

$$\Psi_N(z)=\begin{cases}(\varepsilon_N c_1 z^2)\wedge c_2 & \text{if } z\ge 0\\ (\varepsilon_N c_1 z^2)\wedge c_3 & \text{if } z<0,\end{cases} \tag{4.11}$$

with $c_i>0$ (see e.g. [2] Section 8.3):

1) G_N Γ-converge to

$$c_1\int_0^1|u'|^2\,dt+c_2\#\{t\in(S(u)):u^+>u^-\}+c_3\#\{t\in(S(u)):u^+<u^-\}. \tag{4.12}$$

2) The functionals G_N are equicoercive on bounded sets of $L^1(0,1)$. Moreover, if (u_N) is a bounded sequence in $L^1(0,1)$ and $\sup_N G_N(u_N) < +\infty$ then, there exists a finite set S such that (u_N) is precompact in $H^1((0,1)\setminus S)$.

3) If $\sup_N G_N(u_N) < +\infty$ and $\eta > 0$ is fixed then the number of indices j such that

$$\frac{u_{j+1}-u_j}{\varepsilon_N} > \frac{\eta}{\sqrt{\varepsilon_N}} \tag{4.13}$$

is equibounded.

The proof of Theorem 4 consists of four steps. First, we prove that the sequence E_N is equicoercive, i. e., that from every sequence (u_N) bounded in $L^1(0,1)$ and with $\sup_N E_N(u_N) < +\infty$ we may extract a converging subsequence. The proof follows by remarking that we may obtain a lower bound of E_N with an energy of the form (4.10), for which this property already holds. The second step is to provide a lower bound for the limit energy. This step is in turn divided into two parts: First we locally minimize the interaction of each group of $K+1$ neighboring planes (with the proper 'multiplicities' giving the factor $K-n+1$ in the definition of Φ_-), thus obtaining an estimate of the energy in terms of a sum of nearest-neighbor energies with a proper scaling of $\Phi_- - \Phi_{\min}$ as an energy density. The Γ-limit of this simpler energy is standard and provides a lower bound outside $S(u)$. A bound on the energy of a discontinuity between u^- and u^+ is then obtained by minimization among all discrete transitions between these two values. In this step, hypothesis (iii) plays a crucial role in establishing that the final energy necessary to create a discontinuity does not depend on the values of $u^\pm$. The third step consists of showing that these bounds are optimal by exhibiting a recovery sequence for each piecewise-H^1 u. In this step the hypothesis of the validity of the Cauchy-Born rule close to the ground state is used to ensure that, away from jump points, we may take recovery sequences simply as interpolations of the target function. Finally, we obtain the convergence of minima by explicitly computing the values of the minima of the Γ-limit.

It is convenient to rewrite our energies taking into account the form in (2.6) of problem $P_N(\delta)$. To this end we introduce the energy

$$\Phi(\delta_1,\dots,\delta_K) = \sum_{n=1}^{K}\sum_{j=1}^{K-n+1}\frac{1}{K-n+1}\phi_n(\delta_j,\dots,\delta_{j+n-1}). \tag{4.14}$$

Note that

$$\Phi_-(\delta) = \min\Big\{\Phi(\delta_1,\dots,\delta_K) : \sum_{i=1}^{K}\delta_i = K\delta\Big\},$$

and in particular that $\Phi(\delta_1,\dots,\delta_K) \geq \Phi_{\min}$, the equality holding only for $\delta_1 = \dots = \delta_K = \delta_{\min}$. As in (2.6) the energy E_N can be rewritten as

$$E_N(u) = \sum_{i=1}^{N}\varepsilon_N \Psi_N\Big(\frac{u_{i+1}-u_i}{\varepsilon_N},\dots,\frac{u_{i+K}-u_{i+K-1}}{\varepsilon_N}\Big), \tag{4.15}$$

where

$$\Psi_N(z_1,\dots,z_K) = \frac{1}{\varepsilon_N}\Big(\Phi\Big(\sqrt{\varepsilon_N}z_1+\delta_{\min},\dots,\sqrt{\varepsilon_N}z_K+\delta_{\min}\Big)-\Phi_{\min}\Big)\,. \tag{4.16}$$

Proof. Throughout the proof we identify $(0,1)$ with the torus; i. e., the points 0 and 1 are identified and jumps at 0 are taken into account in the limit energies.

1. Coerciveness. We note that, from (vi) and Remark 4, it follows that there exist constants $K_1, K_2 > 0$ such that

$$\sum_{n=1}^{K}\sum_{j=1}^{K-n+1}\frac{1}{K-n+1}\phi_n(\delta_j,\dots,\delta_{j+n-1})-\Phi_{\min} \ge K_1\sum_{n=1}^{K}(\delta_n-\delta_{\min})^2\wedge K_2. \tag{4.17}$$

We then have

$$\begin{aligned}
E_N(u) &= \sum_{j=1}^{N}\varepsilon_N\Psi_N\Big(\frac{u_{j+1}-u_j}{\varepsilon_N},\dots,\frac{u_{j+K}-u_{j+K-1}}{\varepsilon_N}\Big)\\
&\ge \sum_{j=1}^{N}\varepsilon_N\sum_{n=1}^{K}\Big(K_1\Big(\frac{u_{j+n+1}-u_{j+n}}{\varepsilon_N}\Big)^2\Big)\wedge\frac{K_2}{\varepsilon_N}\\
&= K\sum_{j=1}^{N}\Big(\varepsilon_N K_1\Big(\frac{u_{j+1}-u_j}{\varepsilon_N}\Big)^2\Big)\wedge K_2.
\end{aligned}$$

By Remark 9(2) we then conclude that, given a sequence (u_N) with equibounded energy ($\sup_N E_N(u_N) < +\infty$), upon addition of a constant the sequence is compact in $L^1(0,1)$, and, upon a finite set $S \subset (0,1]$ it is also locally weakly compact in $H^1((0,1)\setminus S)$.

2. Lower bound. We have to prove the 'liminf inequality'

$$E_0(u) \le \liminf_N E_N(u_N) \qquad \text{for all } u_N \to u.$$

The lower bound needs to be proved only for sequences (u_N) converging in L^1 and with $\sup_N E_N(u_N) < +\infty$. This implies that (we can assume that) the sequence also converges locally weakly in H^1 away from the set S in the sense of Step 1.

We begin by remarking that, from the growth conditions on ϕ_n and the hypotheses on Φ_-, we have

$$\liminf_{\delta\to+\infty}\Phi_-(\delta) > \Phi_{\min} \qquad \liminf_{\delta\to-\infty}\Phi_-(\delta) = +\infty. \tag{4.18}$$

We then infer (similarly to the the proof of the existence of lower potentials in the previous section) that there exist constants $C_1, C_2, C_3 > 0$ such that

$$\Phi_-(\delta)-\Phi_{\min} \ge \Psi(\delta-\delta_{\min}) := \begin{cases} C_1(\delta-\delta_{\min})^2\wedge C_2 & \text{if } \delta\ge\delta_{\min}\\ C_1(\delta-\delta_{\min})^2\wedge C_3 & \text{if } \delta\le\delta_{\min}\end{cases} \tag{4.19}$$

Moreover, note that

$$\sup\{C_1 :\ (4.19) \text{ holds}\} = \frac{1}{2}\sum_{n=1}^{K}\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial^2\phi_n}{\partial\delta_i\partial\delta_j}(\delta_{\min},\dots,\delta_{\min}) \tag{4.20}$$

by hypothesis (vii) and

$$\sup\{C_3 :\ (4.19) \text{ holds for some } C_1 \text{ and } C_2\} = +\infty \tag{4.21}$$

by (4.18).

We can then estimate

$$\begin{aligned} E_N(u) &= \sum_{j=1}^{N}\varepsilon_N\sum_{n=1}^{K}\phi_n^N\Big(\frac{u_{j+1}-u_j}{\varepsilon_N},\dots,\frac{u_{j+n}-u_{j+n-1}}{\varepsilon_N}\Big) \\ &\geq \sum_{j=1}^{N}\Big(\varPhi_-\Big(\delta_{\min}+\sqrt{\varepsilon_N}\cdot\frac{u_{j+K}-u_j}{K\varepsilon_N}\Big)-\varPhi_{\min}\Big) \\ &\geq \sum_{j=1}^{N}\varPsi\Big(\frac{u_{j+K}-u_j}{K\sqrt{\varepsilon_N}}\Big). \end{aligned} \tag{4.22}$$

Let (u_N) converge to u in L^1. We then obtain

$$\begin{aligned} \liminf_N E_N(u_N) \geq C_1\int_0^1 |u'|^2\,dt + C_2\#\{t\in S(u) : u^+ > u^-\} \\ +C_3\#\{t\in S(u) : u^+ < u^-\} \end{aligned} \tag{4.23}$$

by Remark 9(1). By using (4.20) and (4.21) we finally get

$$\liminf_N E_N(u_N) \geq \alpha\int_0^1 |u'|^2\,dt + C_2\#S(u) \tag{4.24}$$

and the constraint that $u^+ > u^-$ on $S(u)$.

Next, we need to compute the contribution of the discontinuity. If we optimize the constant C_2 we find the value

$$\sup\{C_2 :\ (4.19) \text{ holds for some } C_1 \text{ and } C_3\} = \liminf_{\delta\to+\infty}\varPhi_-(\delta)-\varPhi_{\min}.$$

This estimate is sharp if $K = 1$; in general, this is only a lower bound, and a finer analysis is needed to describe the optimal transition between u^- and u^+. This is explained by the fact that the minimization process giving $\varPhi_-(\delta)$ may be incompatible with the minimal configuration giving $\varPhi_{\min}$.

We now give a sharp estimate for the energy that concentrates at a point $t \in S(u)$. Without loss of generality we may suppose that $t = 0$, and that $w := u^+(0) - u^-(0) > 0$. Note that there exist indices j_N such that $\varepsilon_N j_N \to 0$ and

$$\lim_N \frac{u_N((j_N+1)\varepsilon_N) - u_N(j_N\varepsilon_N)}{\sqrt{\varepsilon}_N} = +\infty, \tag{4.25}$$

otherwise u_N would be equibounded in H^1 of a neighborhood of 0 (to this end, remark that if $|u_N'|_\infty \le \eta/\sqrt{\varepsilon_N}$ on some interval $(-\xi,\xi)$ for some $\eta>0$ then, following Step 1 we obtain $\int_{-\xi}^{\xi}|u_N'|^2\,dt \le C'\,E_N(u_N)$ for some constant C').

Again, it is not restrictive to suppose that $j_N=0$ for all N. By the equiboundedness of $E_N(u_N)$ and the growth condition (ii) we have

$$\inf_{N,j}\frac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\sqrt{\varepsilon}_N}>-\infty;$$

hence by (iii), if $j\le 0$ and $j+n\ge 1$ then, upon setting

$$w_j^N=\frac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\sqrt{\varepsilon}_N},$$

we have

$$\begin{aligned}\phi_n\big(\delta_{\min}+w_j^N,\dots,\delta_{\min}+w_{j+n-1}^N\big)&=\psi_n^j\big(\delta_{\min}+w_j^N,\dots,\delta_{\min}+w_{-1}^N\big)\\ +\psi_n^{j+n-1}\big(\delta_{\min}+w_1^N,\dots,\delta_{\min}+w_{j+n-1}^N\Big)&+o(1)\end{aligned}\tag{4.26}$$

uniformly as $N\to+\infty$ by hypothesis (iii).

Fix $M\in\mathbf{N}$. Let S be a finite set such that $u_N\to u$ locally weakly in $H^1((0,1)\setminus S)$ and $|u_N'|\le 1/(M\sqrt{\varepsilon_N})$ for large enough N on each compact set of $(0,1)\setminus S$ (by Remark 9(3)). Fix $\eta>0$ such that $S\cap(-4\eta,4\eta)=\{0\}$. Note that we have that

$$|u_N'|\le\frac{1}{M\sqrt{\varepsilon_N}}\ \text{on } (-3\eta,-\eta)\text{ and }(\eta,3\eta),\tag{4.27}$$

and that $u_N\to u$ uniformly in $(-3\eta,-\eta)$ and $(\eta,3\eta)$. Let

$$J_\eta^N=\{j\in\mathbf{Z}:\varepsilon_N j\in(-2\eta,2\eta)\}=:\{-j_\eta^N,\dots,j_\eta^N\}.\tag{4.28}$$

We can then write

$$\begin{aligned}\sum_{j\in J_\eta^N}\varepsilon_N\Psi_N\Big(\tfrac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N},\dots,\tfrac{u_N((j+K)\varepsilon_N)-u_N((j+K-1)\varepsilon_N)}{\varepsilon_N}\Big)&\\ =I_1^N+I_0^N+I_2^N,&\end{aligned}\tag{4.29}$$

where (w_j^N as above)

$$\begin{aligned}I_0^N=\sum_{n=1}^{K}\sum_{j\le 0,j+n\ge 1}\Big(&\phi_n\big(\delta_{\min}+w_j^N,\dots,\delta_{\min}+w_{j+n-1}^N\big)\\ &-\psi_n^{j+n-1}\big(\delta_{\min}+w_j^N,\dots,\delta_{\min}+w_{-1}^N\big)\\ &-\psi_n^j\big(\delta_{\min}+w_1^N,\dots,\delta_{\min}+w_{j+n-1}^N\big)\Big)-K\Phi_{\min},\end{aligned}$$

$$
\begin{aligned}
I_1^N = & \sum_{j\in J_\eta^N,\ j\geq 1} \varepsilon_N \Psi_N\Big(\tfrac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N},\dots,\tfrac{u_N((j+K)\varepsilon_N)-u_N((j+K-1)\varepsilon_N)}{\varepsilon_N}\Big)\\
& + \sum_{n=1}^{K-1}\sum_{j=1}^{n} \frac{K-n-j+1}{K-n+1}\,\phi_n\big(\delta_{\min}+w_j^N,\dots,\delta_{\min}+w_{j+n-1}^N\big)\\
& + \sum_{n=1}^{K}\sum_{j=1}^{n-1} \psi_n^j\big(\delta_{\min}+w_1^N,\dots,\delta_{\min}+w_j^N\big),
\end{aligned}
$$

$$
\begin{aligned}
I_2^N = & \sum_{j\in J_\eta^N,\ j\leq -K} \varepsilon_N \sum_{n=1}^{K} \Psi_N\Big(\tfrac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N},\dots,\tfrac{u_N((j+K)\varepsilon_N)-u_N((j+K-1)\varepsilon_N)}{\varepsilon_N}\Big)\\
& + \sum_{n=1}^{K-1}\sum_{j=0}^{n-1} \frac{K-n+j}{K-n+1}\,\phi_n\big(\delta_{\min}+w_{-j-n}^N,\dots,\delta_{\min}+w_{-j-1}^N\big)\\
& + \sum_{n=1}^{K}\sum_{j=1}^{n-1} \psi_n^j\big(\delta_{\min}+w_{-j}^N,\dots,\delta_{\min}+w_{-1}^N\big).
\end{aligned}
$$

By (4.26) we have

$$
\lim_N I_0^N = -K\,\Phi_{\min}. \tag{4.30}
$$

Note the factor K that derives from the decomposition of the K terms involving Ψ_N labeled by $j \in \{1-K,\dots,0\}$ into the three sums involving the ϕ_ns.

We now compute the limit of I_1^N, that of I_2^N being completely analogous. Let $v_N : \mathbf{Z} \to \mathbf{R}$ be the function defined by

$$
v_N(j) = \begin{cases} u_N(j\varepsilon_N) & \text{if } -j_\eta^N \leq j \leq j_\eta^N + K \\ u_N(-j_\eta^N\varepsilon_N) & \text{if } j < -j_\eta^N \\ u_N(j_\eta^N\varepsilon_N) & \text{if } j > j_\eta^N + K. \end{cases} \tag{4.31}
$$

Upon setting

$$
z_j^N = \frac{v_N((j+1)\varepsilon_N) - v_N(j\varepsilon_N)}{\sqrt{\varepsilon}_N},
$$

we may write

$$
\begin{aligned}
I_1^N = & \sum_{j\geq 1} \varepsilon_N \Psi_N\Big(\frac{v_N(j+1)-v_N(j)}{\varepsilon_N},\dots,\frac{v_N(j+K)-v_N(j+K-1)}{\varepsilon_N}\Big)\\
& - \sum_{j=j_\eta^N+1}^{j_\eta^N+K} \varepsilon_N \Psi_N\Big(\frac{v_N(j+1)-v_N(j)}{\varepsilon_N},\dots,\frac{v_N(j+K)-v_N(j+K-1)}{\varepsilon_N}\Big)\\
& + \sum_{n=1}^{K-1}\sum_{j=1}^{n} \frac{K-n-j+1}{K-n+1}\,\phi_n\big(\delta_{\min}+z_j^N,\dots,\delta_{\min}+z_{j+n-1}^N\big)
\end{aligned}
$$

$$+\sum_{n=1}^{K}\sum_{j=1}^{n-1}\psi_n^j\big(\delta_{\min}+z_1^N,\dots,\delta_{\min}+z_j^N\big) \tag{4.32}$$

We can estimate

$$\begin{aligned}
&\sum_{j=j_\eta^N+1}^{j_\eta^N+K}\varepsilon_N\Psi_N\Big(\frac{v_N(j+1)-v_N(j)}{\varepsilon_N},\dots,\frac{v_N(j+K)-v_N(j+K-1)}{\varepsilon_N}\Big)\\
&\le\sum_{j=j_\eta^N+1}^{j_\eta^N+K}\sup\Big\{\Phi(z_1+\delta_{\min},\dots,z_K+\delta_{\min})-\Phi_{\min}:|z_i|\le 1/M\Big\}\\
&\le K\sup\Big\{\Phi(z_1+\delta_{\min},\dots,z_K+\delta_{\min})-\Phi_{\min}:|z_j|\le 1/M\Big\}\\
&=:\omega\Big(\frac{1}{M}\Big),
\end{aligned}$$

with $\lim_{x\to 0}\omega(x)=0$.

We now define the boundary-layer energy of the discrete system as

$$\begin{aligned}
B=\inf_{R\in\mathbf{N}}\inf\Big\{&\sum_{j\ge 0}(\Phi_n(z_j+\delta_{\min},\dots,z_{j+K}+\delta_{\min})-\Phi_{\min})\\
&+\sum_{n=1}^{K-1}\sum_{j=0}^{n-1}\frac{K-n-j}{K-n+1}\,\phi_n(\delta_{\min}+z_j,\dots,\delta_{\min}+z_{j+n-1})\\
&+\sum_{n=1}^{K}\sum_{i=1}^{n-1}\psi_n^i(z_0+\delta_{\min}\dots,z_{i-1}+\delta_{\min}):z_j=0\text{ if }j\ge R\Big\}.
\end{aligned} \tag{4.33}$$

We then obtain (taking $z_j=\frac{1}{\sqrt{\varepsilon_N}}(v_N(j+1)-v_N(j))$)

$$\liminf_N I_1^N\ge B-\omega\Big(\frac{1}{M}\Big), \tag{4.34}$$

and, by the arbitrariness of M and a symmetric argument,

$$\liminf_N I_1^N\ge B,\qquad \liminf_N I_2^N\ge B. \tag{4.35}$$

Since the estimates concerning u' and $S(u)$ may be decoupled, we may sum up the previous inequalities to obtain

$$\liminf_N E_N(u_N)\ge\alpha\int_0^1|u'|^2\,dt+(2B-K\,\Phi_{\min})\,\#(S(u)) \tag{4.36}$$

with the constraint $u^+>u^-$ on $S(u)$.

3. Upper bound. We have to prove the 'limsup inequality': that for every u and for every $r>0$ there exists a sequence (u_N) (called a recovery sequence) converging to u and such that

$$\limsup_N E_N(u_N)\le E_0(u)+r.$$

First, note that it is sufficient to check this property for piecewise H^1-functions that are sufficiently smooth and locally constant on both sides of $S(u)$, by a density argument (see, e. g., [2] Section 1.7.1).

We confine our analysis to $u \in C^2(0,1)$ with a discontinuity in 0 and such that $u = u^+(0)$ on $(0,\eta)$ and $u = u^-(0)(= u^-(1)) < u^+(0)$ on $(-\eta, 0]$. Let $M \in \mathbf{N}$, $R \in \mathbf{N}$ and let $z : \mathbf{Z} \to \mathbf{R}$ be such that $z_j = 0$ for $j \geq R$, and

$$\begin{aligned}&\sum_{j\geq 0}(\Phi_n(z_j+\delta_{\min},\dots,z_{j+K}+\delta_{\min})-\Phi_{\min})\\&+\sum_{n=1}^{K-1}\sum_{j=0}^{n-1}\frac{K-n-j}{K-n+1}\,\phi_n(\delta_{\min}+z_j,\dots,\delta_{\min}+z_{j+n-1})\\&+\sum_{n=1}^{K}\sum_{i=1}^{n-1}\psi_n^i(z_0+\delta_{\min}\dots,z_{i-1}+\delta_{\min})\leq B+\frac{1}{M}.\end{aligned}\tag{4.37}$$

We then define u_N as follows:

$$u_N(j\varepsilon_N)=\begin{cases}\sqrt{\varepsilon}_N(\sum_{i=0}^{j-1}z_i-\sum_{i=0}^{R}z_i)+u(j\varepsilon_N) & \text{if } j\geq 0\\ \sqrt{\varepsilon}_N(\sum_{i=-R}^{0}z_i-\sum_{i=-j}^{0}z_i)+u(j\varepsilon_N) & \text{if } j<0.\end{cases}\tag{4.38}$$

Note that this definition makes sense since $u_N(j\varepsilon_N) = u(j\varepsilon_N)$ for $|j| > R$. It can be easily checked now that (u_N) is a recovery sequence for u. In fact, by the definition of (z_j) we deduce that

$$\sum_{|j|<\eta/(2\varepsilon_N)}\varepsilon_N\Psi_N\Big(\tfrac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N},\dots,\tfrac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N}\Big)\leq B+\tfrac{1}{M},$$

while, using Taylor's expansion of Φ at $(\delta_{\min},\dots,\delta_{\min})$ we obtain

$$\begin{aligned}&\sum_{|j|>\eta/(2\varepsilon_N)}\varepsilon_N\Psi_N\Big(\frac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N},\dots,\frac{u_N((j+1)\varepsilon_N)-u_N(j\varepsilon_N)}{\varepsilon_N}\Big)\\&=\sum_{|j|>\eta/(2\varepsilon_N)}\varepsilon_N\Psi_N\Big(\frac{u((j+1)\varepsilon_N)-u(j\varepsilon_N)}{\varepsilon_N},\dots,\frac{u((j+1)\varepsilon_N)-u(j\varepsilon_N)}{\varepsilon_N}\Big)\\&\leq\sum_{|j|>\eta/(2\varepsilon_N)}(\Phi(\delta_{\min}+\sqrt{\varepsilon_N}(u'(j\varepsilon_N)+o(1)),\dots\\&\qquad\qquad\dots,\delta_{\min}+\sqrt{\varepsilon_N}(u'(j\varepsilon_N)+o(1)))-\Phi_{\min})\\&\leq\sum_{|j|>\eta/(2\varepsilon_N)}\alpha\,\varepsilon_N|u'(j\varepsilon_N)|^2+o(1)\leq\alpha\int_0^1|u'|^2\,dt+o(1).\end{aligned}$$

4. Convergence of minimum problems. The convergence of minimum problems now follows immediately from the Γ-convergence of the functionals. It remains to verify that

$$\min\{E_0(u) : u-\delta t \text{ 1-periodic}\}=\min\{\alpha\delta^2, 2B-K\Phi_{\min}\},\tag{4.39}$$

if $\delta > 0$. This is a simple computation, minimizers being given by $u(t) = \delta t$ or $u(t) = 0$ (in this case with $S(u) = \mathbf{Z}$). □

Acknowledgements

AB is grateful to Caltech for the hospitality. MO and AL are grateful to the Department of Energy for support provided through Caltech's ASCI/ASAP Center for the Simulation of the Dynamic Response of Materials.

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Dipartimento di Matematica
Università di Roma "Tor Vergata"
00133 Rome, Italy

and

Department of Mechanical Engineering
Stanford University
Stanford, CA 94305

and

Division of Engineering and Applied Science
California Institute of Technology
Pasadena, CA 90025