

Modeling of dislocations and relaxation of functionals on 1-currents with discrete multiplicity

Sergio Conti · Adriana Garroni · Annalisa Massaccesi

Received: 29 November 2013 / Accepted: 31 January 2015
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Abstract In the modeling of dislocations one is led naturally to energies concentrated on lines, where the integrand depends on the orientation and on the Burgers vector of the dislocation, which belongs to a discrete lattice. The dislocations may be identified with divergence-free matrix-valued measures supported on curves or with 1-currents with multiplicity in a lattice. In this paper we develop the theory of relaxation for these energies and provide one physically motivated example in which the relaxation for some Burgers vectors is nontrivial and can be determined explicitly. From a technical viewpoint the key ingredients are an approximation and a structure theorem for 1-currents with multiplicity in a lattice.

Mathematics Subject Classification 49J45 · 49Q15 · 74G65

1 Introduction

Dislocations are topological singularities in crystals, which may be described by lines to which a lattice-valued vector, called Burgers vector, is associated. They may be identified with divergence-free matrix-valued measures supported on curves or equivalently with 1-currents with multiplicity in a lattice and without boundary. The energetic modeling of dislocations leads naturally to energies with linear growth concentrated on lines, where the integrand

Communicated by L. Ambrosio.

S. Conti
Institut für Angewandte Mathematik, Universität Bonn, 53115 Bonn, Germany

A. Garroni (✉)
Dipartimento di Matematica, Sapienza, Università di Roma, 00185 Rome, Italy
e-mail: garroni@mat.uniroma1.it

A. Massaccesi
Institut für Mathematik Universität Zürich, Zürich 8057, Switzerland
e-mail: annalisa.massaccesi@math.uzh.ch

depends on the orientation and on the Burgers vector of the dislocation. The energy of a dislocation supported on a line γ , with tangent vector $\tau : \gamma \rightarrow S^{n-1}$ and multiplicity $\theta : \gamma \rightarrow \mathbb{Z}^m$ takes the form

$$\int_{\gamma} \psi(\theta, \tau) d\mathcal{H}^1, \quad (1.1)$$

restricted to the set of dislocation density tensors $\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma$ which are divergence-free, see for example [13, 14]. In the two-dimensional case such divergence-free measures can be identified with gradients of characteristic functions in BV and the problem can be treated as a vector-valued partition problem [1, 2]; for a derivation of a line-tension energy of the type (1.1) from a Peierls–Nabarro model with linear elasticity see [7, 11]. The analysis in the three-dimensional case is substantially more subtle. A formulation of dislocations in terms of currents was considered also in [20].

The aim of this paper is to study the lower semicontinuity and relaxation of functionals of the type (1.1). One important question is whether sequences of measures with the given properties and bounded energy converge, upon taking a subsequence and in a suitable weak sense, to a measure in the same class. Without the divergence-free constraint this is, in general, not true. This can be solved by rephrasing the problem in terms of 1-rectifiable currents. The same tool is also helpful for proving density results and a structure theorem. However, the standard theory of currents deals with the scalar case [9, 12], whereas for dislocations lattice-valued currents are needed. Some statements, such as compactness, can be directly generalized from the scalar case working componentwise, this is however not always the case, as for example in the density result one must make sure that all components are approximated using the same polyhedral (or piecewise affine) curve. Therefore we revisit in Sect. 2 some of the classical proofs showing how they can be extended to the case of interest here.

Very general results for group-valued currents are available, but not all cases which are relevant for us are covered. The theory of group-valued currents was firstly developed by Fleming [10]. He considers so-called polyhedral chains with coefficients in a suitable abelian normed group G and then works in its closure, with respect to the flat norm. Essential results such as compactness and approximability were proved by White in [21, 22]. The approach we chose is quite different, relying on an explicit integral representation of group-valued 1-currents, matching with (1.1) (see [18] for a similar point of view). In Sect. 2 we rephrase our problem in terms of 1-currents, and we prove the polygonal approximation, density and structure theorems. In the rest of the paper, for notational simplicity, we use mostly the language of measures.

The relaxation of the functional (1.1) turns out to be an integral functional of the same form but with a different integrand, see Sect. 3. As in the case of the relaxation of partition problems [1, 2] the integrand in the relaxed functional, that we call the \mathcal{H}^1 -elliptic envelope, is obtained by a cell formula, given in (3.1) below. In Lemma 3.2 below we derive algebraic upper and lower bounds for the relaxation. We remark that in general the two bounds do not coincide, as was proven in the two-dimensional case in [2], see also [4]. For a specific problem of physical interest, namely, dislocations in a cubic crystal, we give in Sect. 4 an algebraic lower bound and an explicit expression for the \mathcal{H}^1 -elliptic envelope in the case of small Burgers vector. An application of the tools derived here to the study of dislocations in a three-dimensional discrete model of crystals, which has partly motivated the present work, will be discussed separately [5].

2 Preliminary results on \mathbb{Z}^m -valued 1-currents

2.1 Definitions and notation

A 1-current T is a functional on the space of smooth compactly supported 1-forms (vector fields in \mathbb{R}^n). We focus here on *rectifiable currents*, which are still a satisfying generalization of curves (or surfaces, in dimension greater than 1), but they are sufficiently regular to admit a handy representation as

$$\langle T, \varphi \rangle = \int_{\gamma} \theta(x) \langle \varphi(x); \tau(x) \rangle d\mathcal{H}^1(x) \in \mathbb{R}^m, \quad \forall \varphi \in C_c^\infty(\Omega, \mathbb{R}^n), \tag{2.1}$$

where $\Omega \subseteq \mathbb{R}^n$ is open, $\gamma \subset \Omega$ is a 1-rectifiable set and $\tau : \gamma \rightarrow \mathcal{S}^{n-1}$ is its tangent vector, \mathcal{H}^1 -almost everywhere. The multiplicity is an L^1 map

$$\theta : \gamma \rightarrow \mathbb{Z}^m.$$

Let us point out that, setting $m = 1$, we would recover the standard theory of rectifiable currents [9, 17, 19]; but, for our aims, we need an actual lattice $\mathbb{Z}^m \subseteq \mathbb{R}^m$. Nevertheless, a significant part of the theory of \mathbb{Z}^m -valued currents can be done componentwise, reducing to the classical theory. Notice that the results stated and proved in this section for \mathbb{Z}^m -valued rectifiable 1-currents can be actually given in the more general context of currents with multiplicity in a lattice \mathcal{L} , i.e., a discrete subgroup of \mathbb{R}^m spanning the whole of \mathbb{R}^m . Since we never use the specific Euclidean norm of \mathbb{Z}^m , the two formulations are completely equivalent, for notational simplicity we focus on \mathbb{Z}^m .

We will denote by $\mathcal{R}_1(\Omega, \mathbb{Z}^m)$ the set of rectifiable 1-currents and we will take (2.1) as a definition. Roughly speaking, one can imagine a rectifiable current as a countable sum of oriented simple Lipschitz curves with \mathbb{Z}^m -multiplicities (see Thm. 4.2.25 in [9] and its corollaries) and we will establish this remark precisely in Theorem 2.5. If the map θ is piecewise constant on the support of T , say $\theta|_{\gamma_i} \equiv \theta_i \in \mathbb{Z}^m$ with $\text{supp } T = \bigcup_i \gamma_i$ and γ_i the image of a function $\tilde{\gamma}_i \in \text{Lip}([0, 1]; \mathbb{R}^n)$, then for every $\varphi \in C_c^\infty(\Omega, \mathbb{R}^n)$

$$\langle T, \varphi \rangle = \sum_i \theta_i \int_{\gamma_i} \langle \varphi; \tau \rangle d\mathcal{H}^1 = \sum_i \theta_i \int_0^1 \varphi(\tilde{\gamma}_i(s)) \tilde{\gamma}'_i(s) ds. \tag{2.2}$$

The total variation of the rectifiable current in (2.1) is the measure $\|T\| = |\theta| \mathcal{H}^1 \llcorner \gamma$, its mass is

$$\mathbf{M}(T) = \|T\|(\Omega) = \int_{\gamma} |\theta| d\mathcal{H}^1,$$

and it gives the “weighted length” of the current T with respect to the Euclidean norm $|\cdot|$ on \mathbb{Z}^m . Indeed, in the piecewise constant multiplicities case (2.2) the mass of T is the sum

$$\mathbf{M}(T) = \sum_i |\theta_i| \mathcal{H}^1(\gamma_i). \tag{2.3}$$

Since we use the Euclidean norm on \mathbb{Z}^m , the mass of a vectorial current is not, in general, the sum of the masses of the components. Using a different norm on \mathbb{Z}^m would lead to an equivalent norm on \mathcal{R}_1 .

Consistently with Stokes’ Theorem, the boundary of a 1-current T is the 0-current

$$\langle \partial T, \psi \rangle = \langle T, d\psi \rangle \quad \forall \psi \in C_c^\infty(\Omega).$$

A current T is closed if $\partial T = 0$. If T is closed, then

$$\int_{\gamma} \theta(x) D_{\tau} \psi(x) d\mathcal{H}^1(x) = 0 \quad \forall \psi \in W_0^{1,\infty}(\Omega) \tag{2.4}$$

where γ , θ and τ are as in (2.1) and $D_{\tau} \psi(x)$ is the tangential derivative of ψ at x along γ . The integral is well defined since the Lipschitz function ψ has a Lipschitz trace on the rectifiable set γ , and therefore a tangential derivative \mathcal{H}^1 -almost everywhere on γ . Formally, and in analogy to (2.1), we can write (2.4) as $\langle T, d\psi \rangle = 0$ (the two expressions are indeed identical if $\psi \in C_c^1$). To prove (2.4) let $\psi_{\varepsilon} \in C_c^{\infty}(\Omega)$ be such that $\|D\psi_{\varepsilon}\|_{\infty} \leq 2\|D\psi\|_{\infty}$ and $\|\psi - \psi_{\varepsilon}\|_{\infty} \leq \varepsilon$. We claim that $D_{\tau} \psi_{\varepsilon}(x)$ converges weakly- $*$ in $L^{\infty}(\gamma, \mathcal{H}^1)$ to $D_{\tau} \psi(x)$. Indeed, $D_{\tau} \psi_{\varepsilon}(x)$ is uniformly bounded and therefore has a subsequence which converges weakly- $*$ to some $g \in L^{\infty}(\gamma)$. For every C^1 curve γ_j , the restriction to γ_j of ψ_{ε} converges uniformly, and hence weakly- $*$ in $W^{1,\infty}(\gamma_j)$, to the restriction of ψ . Therefore $g = D_{\tau} \psi$, \mathcal{H}^1 -almost everywhere on γ . Using $\theta \in L^1(\gamma, \mathcal{H}^1)$, $D_{\tau} \psi_{\varepsilon}(x) = \langle d\psi_{\varepsilon}(x), \tau(x) \rangle$ and $\langle T, d\psi_{\varepsilon} \rangle = 0$, it follows that

$$\int_{\gamma} \theta(x) D_{\tau} \psi(x) d\mathcal{H}^1(x) = \lim_{\varepsilon \rightarrow 0} \int_{\gamma} \theta(x) \langle d\psi_{\varepsilon}(x), \tau(x) \rangle d\mathcal{H}^1(x) = 0.$$

This proves (2.4).

If the multiplicity θ is piecewise constant as in (2.2), then

$$\langle \partial T, \psi \rangle = \sum_i \theta_i (\psi(\tilde{\gamma}_i(1)) - \psi(\tilde{\gamma}_i(0))) \quad \forall \psi \in C_c^{\infty}(\Omega).$$

We say that a rectifiable 1-current is polyhedral if its support γ is the union of finitely many segments and θ is constant on each of them. We denote by $\mathcal{P}_1(\Omega; \mathbb{Z}^m)$ the set of polyhedral 1-currents.

For a bi-Lipschitz map $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $f_{\#} T$ is the current

$$\langle f_{\#} T, \varphi \rangle = \int_{f(\gamma)} \theta(f^{-1}(y)) \langle \varphi(y), \tau'(y) \rangle d\mathcal{H}^1(y), \tag{2.5}$$

where τ' is the tangent to $f(\gamma)$ with the same orientation as τ , $\tau'(f(x)) = D_{\tau} f(x) / |D_{\tau} f(x)|$. As above, $D_{\tau} f(x)$ denotes the tangential derivative of f along γ , which exists \mathcal{H}^1 -almost everywhere on γ since f is Lipschitz on γ ; if f is differentiable in x then $D_{\tau} f(x) = Df(x)\tau(x)$.

Alternatively, one can interpret rectifiable 1-currents as measures. We say that a measure $\mu \in \mathcal{M}(\Omega; \mathbb{R}^{m \times n})$ is divergence free if

$$\int_{\Omega} \sum_{j=1}^n D\varphi_j d\mu_{ij} = 0 \quad \forall \varphi \in C_c^{\infty}(\Omega, \mathbb{R}^n), \quad i = 1, \dots, m$$

which we shorten to $\partial \mu = 0$. We denote by $\mathcal{M}_{\text{df}}^{(m)}(\Omega)$ the set of divergence-free measures $\mu \in \mathcal{M}(\Omega; \mathbb{R}^{m \times n})$ of the form

$$\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma,$$

where γ is a 1-rectifiable set contained in Ω , $\tau : \gamma \rightarrow \mathcal{S}^{n-1}$ its tangent vector, and $\theta : \gamma \rightarrow \mathbb{Z}^m$ is \mathcal{H}^1 -integrable. Such a measure is divergence-free if and only if the corresponding current defined by (2.1) is closed. We identify closed currents in $\mathcal{R}^1(\Omega; \mathbb{Z}^m)$ with measures in $\mathcal{M}_{\text{df}}^{(m)}(\Omega)$. With this identification the total variation of μ coincides with the mass of T , $\mathbf{M}(T) = |\mu|(\Omega)$.

2.2 Density

Our first result is an extension of the density theorem, as given in the scalar case for example in [9, Theorem 4.2.20], to vector-valued currents. We formulate the density result on \mathbb{R}^n , a local version can be easily deduced using the extension lemma discussed below. Although we find it more natural to phrase and prove the theorem in terms of 1-currents, the entire argument can be easily formulated in terms of measures supported on curves, with only notational changes.

Theorem 2.1 (Density) *Fix $\varepsilon > 0$ and consider a \mathbb{Z}^m -valued closed 1-current $T \in \mathcal{R}_1(\mathbb{R}^n, \mathbb{Z}^m)$. Then there exist a bijective map $f \in C^1(\mathbb{R}^n; \mathbb{R}^n)$, with inverse also C^1 , and a closed polyhedral 1-current $P \in \mathcal{P}_1(\mathbb{R}^n, \mathbb{Z}^m)$ such that*

$$\mathbf{M}(f_{\#}T - P) \leq \varepsilon$$

and

$$|Df(x) - \text{Id}| + |f(x) - x| \leq \varepsilon \quad \forall x \in \mathbb{R}^n.$$

Moreover, $f(x) = x$ whenever $\text{dist}(x, \text{supp } T) \geq \varepsilon$.

It is here important that a current T without boundary can be approximated by polyhedral currents without boundary. The proof cannot be done componentwise, since this would increase the total mass by a factor (depending on m), but follows closely the strategy used for currents with integer multiplicity [9]. For the sake of simplicity, we will prove the density result in the case of interest for this paper (1-dimensional currents without boundary), but the same proof can be performed for \mathbb{Z}^m -valued currents of generic dimension k .

Proof By standard arguments on rectifiable sets, there is a countable family \mathcal{F} of C^1 curves such that $\|T\|(\Omega \setminus \cup \mathcal{F}) = 0$. We denote by λ a real parameter in the interval $(0, 1)$, which will be chosen at the end of the proof.

Step 1 We fix a point $x_0 \in \gamma \in \mathcal{F}$ and assume that, for some $\theta_0 \in \mathbb{Z}^m \setminus \{0\}$,

$$\lim_{r \rightarrow 0} \frac{\|T - S\|(Q_r^{\tau}(x_0))}{r} = 0, \tag{2.6}$$

where S is the current defined by $\langle S, \varphi \rangle = \int_{\gamma} \theta_0 \langle \varphi(x), \tau(x) \rangle d\mathcal{H}^1(x)$, and $Q_r^{\tau}(x_0)$ is the cube of side $2r$, center in x_0 and one side parallel to the vector τ , which is the tangent to γ in x_0 .

Without loss of generality we can assume $x_0 = 0$ and $\text{Tan}_0 \gamma = \mathbb{R}e_1$, where e_1 is the first vector of the canonical basis of \mathbb{R}^n . We denote by Q_r the cube of center 0, side $2r$ and sides parallel to the coordinate directions. Let $\varepsilon' > 0$ be a small parameter chosen later. For r sufficiently small the set $\gamma \cap Q_r$ is the graph of a C^1 function $g : (-r, r) \rightarrow \mathbb{R}^{n-1}$ with $g(0) = 0$ and $\|g\|_{C^1} < \varepsilon'$. The function $\tilde{g} : (-r, r) \rightarrow \mathbb{R}^n$ defined as $\tilde{g}(x_1) = (0, g(x_1))$ obeys

$$\|D\tilde{g}\|_{L^{\infty}((-r,r))} < \varepsilon' \quad \text{and} \quad \|\tilde{g}\|_{L^{\infty}((-r,r))} < \varepsilon' r.$$

We define the function $f \in C^1(\mathbb{R}^n; \mathbb{R}^n)$ as

$$f(x) = x - \psi(x)\tilde{g}(x_1),$$

where $\psi \in C_c^{\infty}(Q_r; [0, 1])$ obeys $\psi \equiv 1$ on $Q_{\lambda r}$ and

$$\|D\psi\|_{L^{\infty}} \leq \frac{2}{(1-\lambda)r}.$$

For $2\varepsilon' < 1 - \lambda$ the function f is bi-Lipschitz and maps $\gamma \cap Q_{\lambda r}$ into the segment $(\mathbb{R}e_1) \cap Q_{\lambda r}$. Moreover for sufficiently small ε' (on a scale set by λ and ε) one has

$$\begin{aligned} |f(x) - x| + |Df(x) - \text{Id}| &\leq |\psi(x)\tilde{g}(x_1)| + |\psi(x)D\tilde{g}(x_1) \otimes e_1| \\ &\quad + |\tilde{g}(x_1) \otimes D\psi(x)| \\ &< \varepsilon' \left(r + 1 + \frac{2}{(1 - \lambda)} \right) < \varepsilon \end{aligned} \tag{2.7}$$

and

$$\|f^{-1}\|_{C^1} \leq 1 + \varepsilon. \tag{2.8}$$

Step 2 We let P be the polyhedral current defined by

$$\langle P, \varphi \rangle = \theta_0 \int_{(-\lambda r, \lambda r)e_1} \langle \varphi, e_1 \rangle d\mathcal{H}^1.$$

With S as in (2.6), by definition of P and f we have (see Fig. 1)

$$\mathbf{M}(S \llcorner Q_r - f_{\#}^{-1}P) = |\theta_0| \mathcal{H}^1(\gamma \cap (Q_r \setminus Q_{\lambda r})).$$

Since γ is a C^1 curve,

$$\lim_{r \rightarrow 0} \frac{\mathcal{H}^1(\gamma \cap (Q_r \setminus Q_{\lambda r}))}{2r} = (1 - \lambda).$$

Using a triangle inequality and (2.7) we obtain

$$\begin{aligned} \mathbf{M}(f_{\#}(T \llcorner Q_r) - P) &\leq \mathbf{M}(f_{\#}((T - S) \llcorner Q_r)) + \mathbf{M}(f_{\#}(S \llcorner Q_r - f_{\#}^{-1}P)) \\ &\leq (1 + \varepsilon)\mathbf{M}((T - S) \llcorner Q_r) + (1 + \varepsilon)\mathbf{M}(S \llcorner Q_r - f_{\#}^{-1}P) \end{aligned}$$

and, recalling (2.6),

$$\limsup_{r \rightarrow 0} \frac{\mathbf{M}(f_{\#}(T \llcorner Q_r) - P)}{2r} \leq (1 + \varepsilon)(1 - \lambda)|\theta_0|.$$

Since, again by (2.6), $\|T\|(Q_r)/(2r) \rightarrow |\theta_0|$, for r sufficiently small

$$\mathbf{M}(f_{\#}(T \llcorner Q_r) - P) < 2(1 - \lambda)\|T\|(Q_r). \tag{2.9}$$

Step 3 By [9, Th.4.3.17] for \mathcal{H}^1 -almost every point in the union of the curves in \mathcal{F} there is a θ_0 with the property (2.6), and therefore an $r_x \in (0, \varepsilon/\sqrt{n})$ satisfying the property (2.9) with Q_r replaced by $Q_{r_x}^{\tau(x)}$. Using Morse’s covering Theorem, we cover $\|T\|$ -almost all the set $\cup \mathcal{F}$ with a countable family of disjoint cubes $Q_{r_k}^{\tau_k}(x_k)$ with $\tau_k = \tau(x_k)$ and sides $2r_k$, with $r_k < r_{x_k}$. Then we have a polyhedral 1-current P_k with support in $Q_{r_k}^{\tau_k}(x_k)$ and a bi-Lipschitz map $f_k \in C^1(\mathbb{R}^n; \mathbb{R}^n)$ satisfying (2.7), (2.8) and (2.9).

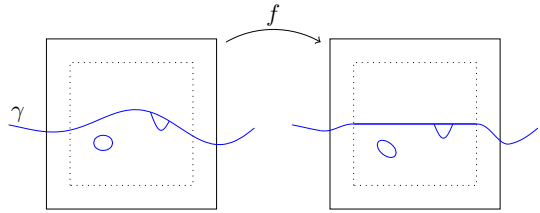
We choose a finite subfamily such that

$$\sum_{k=1}^{K(\lambda)} \|T\|(Q_{r_k}^{\tau_k}(x_k)) \geq \lambda \mathbf{M}(T) \tag{2.10}$$

and define

$$f = f_1 \circ \dots \circ f_{K(\lambda)}.$$

Fig. 1 The action of f on T in the proof of Theorem 2.1. The inner cube is $Q_{\lambda r}$, the outer one Q_r



Since $f_k(x) = x$ outside $Q_{r_k}^k(x_k)$ for all k and the cubes are disjoint the condition (2.7) still holds and $f(x) = x$ outside an ε -neighbourhood of $\text{supp } T$.

We define the polyhedral current

$$P^I = \sum_{k=1}^{K(\lambda)} P_k,$$

write

$$f_{\#}T - P^I = \sum_{k=1}^{K(\lambda)} (f_{\#}(T \llcorner Q_{r_k}^k(x_k)) - P_k) + f_{\#} \left(T \llcorner \bigcup_{k>K(\lambda)}^{\infty} Q_{r_k}^k(x_k) \right)$$

and, recalling (2.9) and (2.10), conclude that

$$\mathbf{M}(f_{\#}T - P^I) < 2(1 - \lambda)\mathbf{M}(T) + (1 - \lambda)\mathbf{M}(T) = 3(1 - \lambda)\mathbf{M}(T). \tag{2.11}$$

Step 4 We finally modify the polyhedral current P^I to make it closed.

The current $f_{\#}T - P^I$ has multiplicity in \mathbb{Z}^m and hence it can be decomposed in m rectifiable scalar 1-currents. Since $\partial f_{\#}T = 0$ and ∂P^I is a polyhedral current with finite mass (a finite sum of Diracs, actually) we can apply the Deformation Theorem in [9, Th. 4.2.9] to each component of $f_{\#}T - P^I$ in order to represent it as

$$f_{\#}T - P^I = P^O + Q + \partial S.$$

Here $P^O, Q \in \mathcal{P}_1(\mathbb{R}^n, \mathbb{Z}^m)$ are polyhedral 1-currents satisfying

$$\mathbf{M}(P^O) \leq \sqrt{m} c_O (\mathbf{M}(f_{\#}T - P^I) + \tilde{\varepsilon} \mathbf{M}(\partial P^I))$$

and

$$\mathbf{M}(Q) \leq \tilde{\varepsilon} \sqrt{m} c_Q \mathbf{M}(\partial P^I),$$

for some $\tilde{\varepsilon}$ arbitrarily small, where $c_O, c_Q > 0$ are geometric constants. The current Q is polyhedral by [9, Th. 4.2.9(8)]. Since $\partial(f_{\#}T - P^I)$ is polyhedral.

Then $P = P^I + P^O + Q$ is a closed polyhedral 1-current with

$$\begin{aligned} \mathbf{M}(f_{\#}T - P) &\leq \mathbf{M}(f_{\#}T - P^I) + \mathbf{M}(P - P^I) \\ &\leq 3(1 - \lambda)\mathbf{M}(T) + \mathbf{M}(P^O + Q) \\ &\leq 3(1 + \sqrt{m} c_O)(1 - \lambda)\mathbf{M}(T) + \tilde{\varepsilon} \sqrt{m} (c_O + c_Q) \mathbf{M}(\partial P^I). \end{aligned}$$

We first choose a $\lambda \in (0, 1)$ such that the first term is less than $\frac{1}{2}\varepsilon$, then $\tilde{\varepsilon}$ such that the second term is also less than $\frac{1}{2}\varepsilon$, and conclude. \square

As a consequence of Theorem 2.1 we easily prove that any closed current $T \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$ can be approximated by sequences of polyhedral currents P_k in the weak topology for currents, where

$$P_k \xrightarrow{*} T \iff \langle P_k, \varphi \rangle \xrightarrow{k \rightarrow +\infty} \langle T, \varphi \rangle \quad \forall \varphi \in C_c^\infty(\mathbb{R}^n; \mathbb{R}^n).$$

We recall that the currents P_k are supported on a finite number of segments.

Corollary 2.2 *For every $T \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$ with $\partial T = 0$ there is a sequence of polyhedral currents $P_k \in \mathcal{P}_1(\mathbb{R}^n; \mathbb{Z}^m)$ with $\partial P_k = 0$ such that*

$$P_k \xrightarrow{*} T \text{ and } \mathbf{M}(P_k) \rightarrow \mathbf{M}(T).$$

We conclude this section with an extension lemma, that can be found in various forms in the literature. We sketch here the argument for the case of interest, in which the closedness is preserved.

Lemma 2.3 (Extension) *Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz open set. For every closed rectifiable 1-current defined in Ω , $T \in \mathcal{R}_1(\Omega; \mathbb{Z}^m)$, there is a closed rectifiable 1-current $\mathcal{E}T \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$ with $\mathcal{E}T \llcorner \Omega = T$ and $\mathbf{M}(\mathcal{E}T) \leq c\mathbf{M}(T)$. The constant depends only on Ω . Further, $\lim_{\delta \rightarrow 0} \mathbf{M}(\mathcal{E}T \llcorner (\Omega_\delta \setminus \Omega)) = 0$, where $\Omega_\delta = \{x : \text{dist}(x, \Omega) < \delta\}$.*

Proof Step 1. We first extend T to a neighbourhood of Ω .

Choose a function $N \in C^1(\partial\Omega; \mathcal{S}^{n-1})$ such that $N(x) \cdot \nu(x) \geq \alpha > 0$ for almost all $x \in \partial\Omega$, where ν is the outer normal to $\partial\Omega$ and \mathcal{S}^{n-1} is the unit sphere in \mathbb{R}^n . For $\rho > 0$ sufficiently small the function $g : \partial\Omega \times (-\rho, \rho) \rightarrow \mathbb{R}^n$, $g(x, t) = x + tN(x)$, is bi-Lipschitz. Let $D_\rho = g(\partial\Omega \times (-\rho, \rho))$ and $f : D_\rho \rightarrow D_\rho$ be defined by $f(g(x, t)) = g(x, -t)$. Then f is bi-Lipschitz and coincides with its inverse.

We define $\tilde{T} = T - f_{\#}(T \llcorner (D_\rho \cap \Omega))$. Let $\varphi \in C_c^1(\Omega \cup D_\rho)$. Then, recalling (2.4) and interpreting the duality in that sense,

$$\langle \tilde{T}, D\varphi \rangle = \langle T, D\varphi \rangle - \langle f_{\#}(T \llcorner (D_\rho \cap \Omega)), D\varphi \rangle = \langle T, D\varphi - D((\varphi \chi_{D_\rho \setminus \Omega}) \circ f) \rangle = 0$$

since $\varphi - (\varphi \chi_{D_\rho \setminus \Omega}) \circ f \in W_0^{1,\infty}(\Omega)$, and T is closed.

Step 2. Let $\tilde{\gamma}$ and $\tilde{\theta}$ be the support and the multiplicity of \tilde{T} , defined as in (2.1). We can slice the outer tubular neighborhood $D_\rho \setminus \Omega = g(\partial\Omega \times [0, \rho))$ through the family of sets $\partial(\Omega_s)$ with $s \in [0, \rho)$. More precisely, we slice (see [9, Section 4.3] or [17]) the current $\tilde{T} \llcorner (D_\rho \setminus \Omega)$ with the distance function from $\partial\Omega$. By slicing, we get that

$$\mathbf{M}(\tilde{T}) \geq \int_0^\rho \left(\sum_{x \in \tilde{\gamma} \cap \partial(\Omega_s)} |\tilde{\theta}(x)| \right) ds.$$

Moreover, we can choose $s \in (0, \rho)$ such that

$$\sum_{x \in \tilde{\gamma} \cap \partial(\Omega_s)} |\tilde{\theta}(x)| \leq c\mathbf{M}(T),$$

with a constant depending only on Ω , and the sum runs over finitely many points x_1, \dots, x_M . Let us point out that the set of points $\{x_1, \dots, x_M\}$, with multiplicity $\tilde{\theta}(x_1), \dots, \tilde{\theta}(x_M)$ and positive orientation if $\tilde{\gamma}$ exits Ω_s at x_i , are the boundary of $\tilde{T} \llcorner \Omega_s$. For each $i = 2, \dots, M$, let γ_i be a Lipschitz curve in $\mathbb{R}^n \setminus \Omega_s$ which joins x_1 with x_i and has length bounded by $C(\Omega)$. Let τ_i be the tangent vector, with the same orientation as $\tilde{\gamma}$ in x_i . We set

$$\langle \mathcal{E}T, \varphi \rangle = \langle \tilde{T} \llcorner \Omega_s, \varphi \rangle + \sum_{i=2}^M \tilde{\theta}(x_i) \int_{\gamma_i} \langle D\varphi, \tau_i \rangle d\mathcal{H}^1 \quad \forall \varphi \in C_c^\infty(\mathbb{R}^n, \mathbb{R}^n).$$

Since T was closed one can see that $\mathcal{E}T$ is also closed. To conclude the proof it is enough to note that, by construction, $\mathbf{M}(\mathcal{E}T \llcorner \partial\Omega) = 0$ and hence $\lim_{\delta \rightarrow 0} \mathbf{M}(\mathcal{E}T \llcorner (\Omega_\delta \setminus \Omega)) = 0$. \square

2.3 Compactness and structure

In this section we characterize the support of rectifiable 1-currents without boundary as a countable union of loops. This characterization is known in the theory of one dimensional integral currents (i.e. with scalar multiplicity). In the latter case the result is stated in [9], subsection 4.2.25, where a quick sketch of the proof is also given. Here, for the convenience of the reader, we will give a complete proof.

We start with the compactness statement, which is also used in proving the Structure Theorem 2.5.

Theorem 2.4 (Compactness) *Let $(T_k)_{k \in \mathbb{N}}$ be a sequence of rectifiable 1-currents without boundary in $\mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$. If*

$$\sup_{k \in \mathbb{N}} \mathbf{M}(T_k) < \infty$$

then there are a current $T \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$ without boundary and a subsequence $(T_{k_j})_{j \in \mathbb{N}}$ such that

$$T_{k_j} \xrightarrow{*} T.$$

Proof This follows from the result on scalar currents [9, Theorems 4.2.16] working componentwise. \square

Theorem 2.5 (Structure) *Let $T \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$ with $\partial T = 0$ and $\mathbf{M}(T) < \infty$. Then there are countably many oriented Lipschitz closed curves γ_i with tangent vector fields $\tau_i : \gamma_i \rightarrow S^{n-1}$ and multiplicities $\theta_i \in \mathbb{Z}^m$ such that*

$$\langle T, \varphi \rangle = \sum_{i \in \mathbb{N}} \theta_i \int_{\gamma_i} \langle \varphi, \tau_i \rangle d\mathcal{H}^1.$$

Further,

$$\sum_i |\theta_i| \mathcal{H}^1(\gamma_i) \leq \sqrt{m} \mathbf{M}(T).$$

Proof Since each current in $\mathcal{R}_1(\Omega; \mathbb{Z}^m)$ can be seen as the sum of m rectifiable 1-currents with scalar integer multiplicity, it suffices to prove the statement in the scalar case $m = 1$. From the density of polyhedral currents (see Corollary 2.2) there is a sequence of polyhedral currents without boundary $P_k \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z})$ such that

$$P_k \xrightarrow{*} T \text{ and } \mathbf{M}(P_k) \rightarrow \mathbf{M}(T).$$

Each P_k can be decomposed into the sum of finitely many polyhedral loops,

$$P_k = \sum_{j=1}^{J_k} L_{j,k},$$

such that

$$\sum_{j=1}^{J_k} \mathbf{M}(L_{j,k}) = \mathbf{M}(P_k) \leq M, \tag{2.12}$$

for some $M > 0$.

We can assume these loops $L_{j,k}$ to be ordered by mass, starting with the biggest one. Moreover we can assume (up to extracting a subsequence) that the currents $L_{j,k}$ have multiplicity 1 and that for every j they weakly converge to some closed rectifiable 1-current L_j . Let us denote by \tilde{T} the current

$$\tilde{T} = \sum_{j=1}^{\infty} L_j.$$

We need to show that $\tilde{T} = T$. If $\mathbf{M}(T) = 0$ there is nothing to prove. Otherwise we fix $\delta > 0$ and observe that by (2.12) we have $\mathbf{M}(L_{i,k}) < \delta$ for all $i > M/\delta$. We write

$$\langle P_k, \varphi \rangle = \sum_{i \leq \frac{M}{\delta}} \langle L_{i,k}, \varphi \rangle + \sum_{i > \frac{M}{\delta}} \langle L_{i,k}, \varphi \rangle. \tag{2.13}$$

In the first sum of the right hand side we can take the limit as $k \rightarrow \infty$ and get $\sum_{i \leq \frac{M}{\delta}} \langle L_i, \varphi \rangle$. Parametrizing each polyhedral curve by arc length, and possibly passing to a further subsequence, we see that each polyhedral curve converges to a closed Lipschitz curve.

The second sum in (2.13) can be estimated as follows. For every $i > M/\delta$ and for every k we fix a point $x_i^k \in \text{supp } L_{i,k} = \gamma_{i,k}$ and using the fact that $\gamma_{i,k}$ is a closed curve we have

$$\begin{aligned} \left| \sum_{i > \frac{M}{\delta}} \langle L_{i,k}, \varphi \rangle \right| &= \left| \sum_{i > \frac{M}{\delta}} \int_{\gamma_{i,k}} \langle \varphi - \varphi(x_i^k), \tau_i^k \rangle d\mathcal{H}^1 \right| \\ &\leq \sum_{i > \frac{M}{\delta}} \sup_{\gamma_{i,k}} |\varphi - \varphi(x_i^k)| \mathbf{M}(L_{i,k}) \\ &\leq \delta \|\varphi\|_{\text{Lip}} \sum_{i > \frac{M}{\delta}} \mathbf{M}(L_{i,k}) \leq \delta M \|\varphi\|_{\text{Lip}}. \end{aligned} \tag{2.14}$$

Then we get

$$\left| \langle T - \sum_{i \leq \frac{M}{\delta}} \langle L_i, \varphi \rangle \right| \leq o(1) + \left| \langle P_k - \sum_{i \leq \frac{M}{\delta}} \langle L_{i,k}, \varphi \rangle \right| \leq o(1) + \delta M \|\varphi\|_{\text{Lip}}$$

which implies $T = \tilde{T}$ and hence

$$T = \sum_{j=1}^{\infty} \tau_j \mathcal{H}^1 \llcorner \gamma_j,$$

with $\gamma_j = \text{supp } L_j$ and τ_j the corresponding tangent vector. □

3 Relaxation

3.1 Main result

In this section we consider the relaxation of functionals of the form

$$E(\mu) = \begin{cases} \int_{\gamma} \psi(\theta, \tau) d\mathcal{H}^1 & \text{if } \mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma \in \mathcal{M}_{\text{df}}^{(m)}(\Omega), \\ +\infty & \text{otherwise.} \end{cases}$$

We shall show that the relaxation is

$$\bar{E}(\mu) = \begin{cases} \int_{\gamma} \bar{\psi}(\theta, \tau) d\mathcal{H}^1 & \text{if } \mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma \in \mathcal{M}_{\text{df}}^{(m)}(\Omega), \\ +\infty & \text{otherwise,} \end{cases}$$

where $\bar{\psi}$ is defined by solving for any $b \in \mathbb{Z}^m$ and $t \in S^{n-1}$ a cell problem, namely,

$$\bar{\psi}(b, t) = \inf \left\{ \int_{\gamma} \psi(\theta, \tau) d\mathcal{H}^1 : \mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma \in \mathcal{M}_{\text{df}}^{(m)}(B_{1/2}), \right. \\ \left. \text{supp}(\mu - b \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t \cap B_{1/2})) \subset B_{1/2} \right\} \tag{3.1}$$

where $B_{1/2}$ denotes a ball of radius 1/2 and center 0. The condition on the support in (3.1) fixes the boundary values of μ , in the sense that it requires the existence of a ball $B' \subset\subset B_{1/2}$ with $\mu = b \otimes t \mathcal{H}^1 \llcorner \mathbb{R}t$ on $B_{1/2} \setminus B'$. We call the function $\bar{\psi}$ the \mathcal{H}^1 -elliptic envelope of ψ and say that ψ is \mathcal{H}^1 -elliptic if $\bar{\psi} = \psi$. It is easy to see that $\bar{\psi}(b, t) \leq \psi(b, t)$, and our result implies that $\bar{\psi}$ is the largest \mathcal{H}^1 -elliptic function below ψ .

For any open set $\omega \subset \Omega$, we write

$$E(\mu, \omega) = \int_{\gamma \cap \omega} \psi(\theta, \tau) d\mathcal{H}^1$$

where $\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma \in \mathcal{M}_{\text{df}}^{(m)}(\Omega)$, and the same for \bar{E} .

Theorem 3.1 (Relaxation) *Let $\psi : \mathbb{Z}^m \times S^{n-1} \rightarrow [0, \infty)$ be Borel measurable with $\psi(b, t) \geq c_0|b|$ and $\psi(0, \cdot) = 0$; define $\bar{\psi}$ as in (3.1). Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz set. Then \bar{E} is the lower semicontinuous envelope of E with respect to the weak convergence in $\mathcal{M}_{\text{df}}^{(m)}(\Omega)$, in the sense that*

$$\bar{E}(\mu) = \inf \left\{ \liminf_{j \rightarrow \infty} E(\mu_j) : \mu_j \in \mathcal{M}_{\text{df}}^{(m)}(\Omega), \mu_j \xrightarrow{*} \mu \right\}.$$

In particular, \bar{E} is lower semicontinuous.

A key ingredient in the proof of the relaxation is to use the deformation theorem to reduce to the case that the limit is polyhedral. The continuity of \bar{E} under deformations follows from the Lipschitz continuity of the integrand $\bar{\psi}$, see Lemma 3.3. In turn, the Lipschitz continuity of $\bar{\psi}$ is proven via a series of constructions in Lemma 3.2. The upper bound is then obtained covering the polyhedral with balls and using the definition of $\bar{\psi}$. For the lower bound instead we need to show that \bar{E} is lower semicontinuous on polyhedrals, which can be done locally assuming that the limit is a straight line. The most involved part of the proof deals with the relation between minimization with boundary data and without boundary data, and is discussed in Lemma 3.5 below.

3.2 Proof of the upper bound

We start by proving the Lipschitz continuity of $\bar{\psi}$. As a side product we also show that $\bar{\psi}$ (and hence any \mathcal{H}^1 -elliptic function), much like the case of BV -elliptic integrands, is subadditive and convex.

Lemma 3.2 (Cell problem) *Let $\psi, \bar{\psi}$ be as in Theorem 3.1. Then:*

- (i) *For every polyhedral measure $\mu = \sum_{i=1}^N b_i \otimes t_i \mathcal{H}^1 \llcorner \gamma_i \in \mathcal{M}_{\text{df}}^{(m)}(B_{1/2})$ such that $\gamma_i \subset B_{1/2}$ are disjoint segments (up to the endpoints) and $\text{supp}(\mu - b \otimes t \mathcal{H}^1 \llcorner (t\mathbb{R} \cap B_{1/2})) \subset B_{1/2}$ one has*

$$\bar{\psi}(b, t) \leq \sum_{i=1}^N \mathcal{H}^1(\gamma_i) \bar{\psi}(b_i, t_i) = \bar{E}(\mu, B_{1/2}).$$

- (ii) *The function*

$$t \mapsto \bar{\psi}\left(b, \frac{t}{|t|}\right) |t| \tag{3.2}$$

is convex in $t \in \mathbb{R}^n$. In particular, $\bar{\psi}$ is continuous.

- (iii) *The function $\bar{\psi}$ is subadditive in its first argument, i.e.,*

$$\bar{\psi}(b + b', t) \leq \bar{\psi}(b, t) + \bar{\psi}(b', t).$$

- (iv) *The function $\bar{\psi}$ obeys*

$$\frac{1}{c} |b| \leq \bar{\psi}(b, t) \leq c |b|$$

for all $b \in \mathbb{Z}^m, t \in S^{n-1}$.

- (v) *The function $\bar{\psi}$ is Lipschitz continuous in the sense that*

$$|\bar{\psi}(b, t) - \bar{\psi}(b', t')| \leq c |b - b'| + c |b| |t - t'|.$$

with c depending only on ψ .

Proof (i) Let B' be a ball such that $\text{supp}(\mu - b \otimes t \mathcal{H}^1 \llcorner (t\mathbb{R} \cap B_{1/2})) \subset B' \subset\subset B_{1/2}$. We cover $\gamma = \cup_{i=1}^N \gamma_i \cap B'$ with a countable number of balls $\{B^k\}_{k \in \mathbb{N}}$ such that: the balls are disjoint and contained in B' ; $\gamma \cap B^k$ is a diameter of B^k , $\mu \llcorner B^k = b_{i_k} \otimes t_{i_k} \mathcal{H}^1 \llcorner (\gamma \cap B^k)$ for some $i_k \in \{1, \dots, N\}$, $\mathcal{H}^1(\gamma \setminus \cup_{k \in \mathbb{N}} B^k) = 0$. Let $\varepsilon > 0$. By the definition of $\bar{\psi}$, for every k we can find a measure $\mu_k \in \mathcal{M}_{\text{df}}^{(m)}(B^k)$ with $\text{supp}(\mu_k - (\mu \llcorner B^k)) \subset B^k$ such that

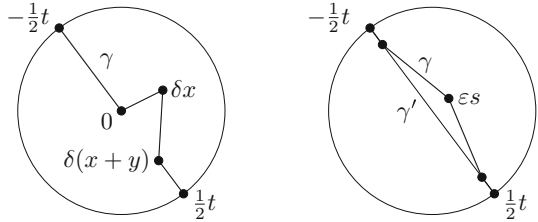
$$E(\mu_k, B^k) \leq \text{diam}(B^k) \bar{\psi}(b_{i_k}, t_{i_k}) + \frac{\varepsilon}{2^k}.$$

We define $\nu = \sum_k \mu_k + \mu \llcorner (B_{1/2} \setminus B')$. Then $\nu \in \mathcal{M}_{\text{df}}^{(m)}(B_{1/2})$ and $\text{supp}(\nu - b \otimes t \mathcal{H}^1 \llcorner (t\mathbb{R} \cap B_{1/2})) \subset B_{1/2}$, therefore

$$\begin{aligned} \bar{\psi}(b, t) &\leq E(\nu, B_{1/2}) = \sum_{k \in \mathbb{N}} E(\mu_k, B^k) + E(\mu, B_{1/2} \setminus B') \\ &\leq \sum_{i=1}^N \mathcal{H}^1(\gamma_i) \bar{\psi}(b_i, t_i) + \psi(b, t) \mathcal{H}^1(r\mathbb{R} \cap B_{1/2} - B') + \varepsilon. \end{aligned}$$

We conclude by the arbitrariness of B' and ε .

Fig. 2 Constructions used in the proof of Lemma 3.2(ii) (left) and Lemma 3.2(iii) (right)



(ii) We extend $\bar{\psi}$ to $\mathbb{Z}^m \times \mathbb{R}^n$ to be one-homogeneous in the last argument [i.e., to be the function given in (3.2)]. Let $\tilde{x}, \tilde{y} \in \mathbb{R}^n, \lambda \in (0, 1)$. We want to show that

$$\bar{\psi}(b, \lambda\tilde{x} + (1 - \lambda)\tilde{y}) \leq \lambda\bar{\psi}(b, \tilde{x}) + (1 - \lambda)\bar{\psi}(b, \tilde{y}).$$

By the definition of the extension of $\bar{\psi}$, defining $x = \lambda\tilde{x}$ and $y = (1 - \lambda)\tilde{y}$ it suffices to show that

$$\bar{\psi}(b, x + y) \leq \bar{\psi}(b, x) + \bar{\psi}(b, y).$$

If $x + y = 0$ then $\bar{\psi}(b, x + y) = 0$ and the statement holds. If not, we choose $\delta > 0$ such that $\delta x, \delta x + \delta y \in B_{1/2}$ and define $t = (x + y)/|x + y|$. Let γ be the polyhedral curve that joins (in this order) the points

$$-\frac{1}{2}t, \quad 0, \quad \delta x, \quad \delta x + \delta y, \quad \frac{1}{2}t,$$

see Fig. 2. Notice that the first and last segment belong to the line $t\mathbb{R}$ and that $\gamma \subset \bar{B}_{1/2}$. We apply (i) to the measure $\mu = b \otimes \tau \mathcal{H}^1 \llcorner \gamma$, where τ is the tangent to γ , and obtain

$$\bar{\psi}(b, t) \leq (1 - \delta|x + y|)\bar{\psi}(b, t) + \delta|x|\bar{\psi}\left(b, \frac{x}{|x|}\right) + \delta|y|\bar{\psi}\left(b, \frac{y}{|y|}\right).$$

Rearranging terms this gives $\bar{\psi}(b, x + y) \leq \bar{\psi}(b, x) + \bar{\psi}(b, y)$, as desired.

(iii) Fix $\varepsilon > 0$ and a vector $s \in S^{n-1}$ not parallel to t . Let γ be the curve that joins the points

$$-\frac{1}{2}t, \quad \left(-\frac{1}{2} + \varepsilon\right)t, \quad \varepsilon s, \quad \left(\frac{1}{2} - \varepsilon\right)t, \quad \frac{1}{2}t,$$

see Fig. 2. We define the polyhedral measure

$$\mu_\varepsilon = b \otimes t \mathcal{H}^1 \llcorner (t\mathbb{R} \cap B_{1/2}) + b' \otimes \tau \mathcal{H}^1 \llcorner \gamma,$$

where τ is the tangent vector to γ . Notice that the supports of the two components overlap on the two segments of length ε close to $\partial B_{1/2}$. By (i) we obtain

$$\bar{\psi}(b + b', t) \leq (1 - 2\varepsilon)\bar{\psi}(b, t) + 2\varepsilon\bar{\psi}(b + b', t) + \frac{1}{2}\bar{\psi}(b', t'_\varepsilon) + \frac{1}{2}\bar{\psi}(b', t''_\varepsilon).$$

Since $\bar{\psi}$ is continuous in the second argument, taking $\varepsilon \rightarrow 0$ proves the assertion.

(iv) The lower bound is immediate from the definition of $\bar{\psi}$ and the growth of ψ . To prove the upper bound, we deduce from (iii)

$$\bar{\psi}(b, t) \leq \sum_{j=1}^n |b \cdot e_j| (\bar{\psi}(e_j, t) + \bar{\psi}(-e_j, t))$$

and observe that, since $\bar{\psi}$ is continuous,

$$\max_{j=1,\dots,n} \max_{t \in \mathcal{S}^{n-1}} (\bar{\psi}(e_j, t) + \bar{\psi}(-e_j, t)) < \infty.$$

(v) From (iii) and (iv) we obtain

$$\bar{\psi}(b, t) \leq \bar{\psi}(b', t) + c|b - b'|,$$

while by (ii) and (iv) we deduce that

$$\bar{\psi}(b, t) \leq \bar{\psi}(b, t') + |t - t'| \bar{\psi}\left(b, \frac{t - t'}{|t - t'|}\right) \leq \bar{\psi}(b, t') + c|b| |t - t'|.$$

□

We now show that the continuity of $\bar{\psi}$ proven in (v) gives continuity of E under deformations.

Lemma 3.3 *Assume that $\psi : \mathbb{Z}^m \times \mathcal{S}^{n-1} \rightarrow [0, \infty)$ is Borel measurable, obeys $\psi(0, t) = 0$, $\psi(b, t) \geq c|b|$ and*

$$|\psi(b, t) - \psi(b', t')| \leq c|b - b'| + c|b| |t - t'|.$$

Let $\mu, \mu' \in \mathcal{M}_{\text{df}}^{(m)}(\Omega)$. Then for any open set $\omega \subset \Omega$ we have

$$|E(\mu, \omega) - E(\mu', \omega)| \leq c|\mu - \mu'|(\omega).$$

Further, if $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is bi-Lipschitz then for any open set $\omega \subset \mathbb{R}^n$

$$|E(\mu, \omega) - E(f_{\#}\mu, f(\omega))| \leq cE(\mu, \omega) \|Df - \text{Id}\|_{L^\infty}.$$

We recall that in this paper $f_{\#}$ denotes the action of f on the current associated to μ , see (2.5). In particular, if $\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma$, then

$$f_{\#}\mu = \theta \circ f^{-1} \otimes \tilde{\tau} \mathcal{H}^1 \llcorner f(\gamma), \quad \tilde{\tau} = \frac{D_{\tau} f}{|D_{\tau} f|} \circ f^{-1}$$

where $D_{\tau} f$ denotes as in (2.5) the tangential derivative.

Proof Let $\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma$, $\mu' = \theta' \otimes \tau' \mathcal{H}^1 \llcorner \gamma'$. To prove the first estimate we observe that $\tau = \pm \tau' \mathcal{H}^1$ -a.e. on $\gamma \cap \gamma'$. Changing the sign of θ' and τ' on the set where $\tau = -\tau'$ we compute

$$\int_{(\gamma \cup \gamma') \cap \omega} |\psi(\theta, \tau) - \psi(\theta', \tau')| d\mathcal{H}^1 \leq c \int_{(\gamma \cup \gamma') \cap \omega} |\theta - \theta'| d\mathcal{H}^1 \leq c|\mu - \mu'|(\omega),$$

where we defined $\theta = 0$, $\tau = \tau'$ on $\gamma' \setminus \gamma$ and $\theta' = 0$, $\tau' = \tau$ on $\gamma \setminus \gamma'$.

To prove the second statement in the theorem we write, by the area formula,

$$E(f_{\#}\mu, f(\omega)) = \int_{f(\gamma) \cap f(\omega)} \psi(\theta \circ f^{-1}, \tilde{\tau}) d\mathcal{H}^1 = \int_{\gamma \cap \omega} \psi(\theta, \tilde{\tau} \circ f) |Df \tau| d\mathcal{H}^1$$

and observe that $|\tilde{\tau} \circ f - \tau| \leq |Df - \text{Id}|$.

□

At this point we give the proof of the upper bound.

Proof of the upper bound in Theorem 3.1 We only need to deal with the case $\bar{E}(\mu, \Omega) < \infty$. Let $\mu \in \mathcal{M}_{\text{df}}^{(m)}(\Omega)$. We need to construct a sequence of measures $\mu_k \in \mathcal{M}_{\text{df}}^{(m)}(\Omega)$ such that $\mu_k \xrightarrow{*} \mu$ and

$$\limsup_{k \rightarrow \infty} E(\mu_k, \Omega) \leq \bar{E}(\mu, \Omega).$$

By Lemma 2.3 we can extend μ to a measure $\mathcal{E}\mu \in \mathcal{M}_{\text{df}}^{(m)}(\mathbb{R}^n)$, with

$$\lim_{\delta \rightarrow 0} |\mathcal{E}\mu|(\Omega_\delta \setminus \Omega) = 0$$

(we recall that $\Omega_\delta = \{x : \text{dist}(x, \Omega) < \delta\}$). By Theorem 2.1 there are a sequence of polyhedral measures $\mu_k \in \mathcal{M}_{\text{df}}^{(m)}(\mathbb{R}^n)$ and a sequence of C^1 and bi-Lipschitz maps f_k such that

$$|\mu_k - (f_k)_\# \mathcal{E}\mu|(\mathbb{R}^n) \rightarrow 0, \quad \|f_k - x\|_{L^\infty} \rightarrow 0, \quad \|Df_k - \text{Id}\|_{L^\infty} \rightarrow 0.$$

This implies $\mu_k \xrightarrow{*} \mathcal{E}\mu$. By Lemma 3.3 and Lemma 3.2(v) one obtains

$$\begin{aligned} \bar{E}(\mu_k, \Omega) &\leq \bar{E}((f_k)_\# \mathcal{E}\mu, \Omega) + c\|\mu_k - (f_k)_\# \mathcal{E}\mu\| \\ &\leq \bar{E}(\mathcal{E}\mu, \Omega_{\delta_k})(1 + c\|Df_k - \text{Id}\|_{L^\infty}) + c\|\mu_k - (f_k)_\# \mathcal{E}\mu\|, \end{aligned}$$

where $\delta_k = \|f_k - x\|_{L^\infty} \rightarrow 0$. Taking the limit we conclude

$$\limsup_{k \rightarrow \infty} \bar{E}(\mu_k, \Omega) \leq \bar{E}(\mu, \Omega).$$

Therefore it suffices to prove the upper bound for polyhedral measures (since we are dealing with bounded subsets of $\mathcal{M}_{\text{df}}^{(m)}(\mathbb{R}^n)$, weak convergence is metrizable).

Let $\mu = \sum_{i=1}^N b_i \otimes t_i \mathcal{H}^1 \llcorner \gamma_i \in \mathcal{M}_{\text{df}}^{(m)}(\mathbb{R}^n)$ be a polyhedral measure, in the sense that the γ_i are disjoint segments, $b_i \in \mathbb{Z}^m$, $t_i \in S^{n-1}$, for $i = 1, \dots, N$. Let $\gamma = \cup_{i=1}^N \gamma_i$. We choose $\varepsilon > 0$ and cover $\gamma \cap \Omega$, up to an \mathcal{H}^1 -null set, with a countable number of disjoint balls $\{B^k = B_{r_k}(x_k)\}_{k \in \mathbb{N}}$ with $r_k < \varepsilon$, which are contained in Ω and have the property that $\gamma \cap B^k$ is a diameter of B^k and $\mu \llcorner B^k = b_{i_k} \otimes t_{i_k} \mathcal{H}^1 \llcorner (\gamma \cap B^k)$ for some $i_k \in \{1, \dots, N\}$ (this is similar to the proof of Lemma 3.2(i), but here we take small balls to ensure weak convergence). By the definition of $\bar{\psi}$, for every k we can find a measure $\mu_k \in \mathcal{M}_{\text{df}}^{(m)}(B^k)$ with $\text{supp}(\mu_k - b_{i_k} \otimes t_{i_k} \mathcal{H}^1 \llcorner (x_k + \mathbb{R}t_{i_k} \cap B^k)) \subset B^k$ such that

$$E(\mu_k, B^k) \leq \text{diam}(B^k) \bar{\psi}(b_{i_k}, t_{i_k}) + \frac{\varepsilon}{2^k}.$$

Finally, define $\nu_\varepsilon = \sum_k \mu_k$. We have

$$E(\nu_\varepsilon, \Omega) \leq \bar{E}(\mu, \Omega) + \varepsilon$$

and the desired recovery sequence is then obtained by letting $\varepsilon \rightarrow 0$. □

We remark that an additional application of the density result from Theorem 2.1, if appropriate care is taken around the boundary and on segments with large multiplicity, permits to obtain polygonal approximating sequences, see [5, Lemma 6.4].

3.3 Proof of the lower bound

In order to prove the lower bound, we need to show that the boundary conditions in the definition of $\bar{\psi}$ can be substituted with an asymptotic condition. We start by working on a rectangle and showing that the energy is concentrated on the line.

Lemma 3.4 *Let ψ and E be as in Theorem 3.1. Given $b \in \mathbb{Z}^m$ and $t \in \mathcal{S}^{n-1}$, we choose a rotation $Q_t \in \text{SO}(n)$ with $Q_t e_1 = t$ and for $h, \ell > 0$ we define the parallelepiped $R_{\ell,h}^t = Q_t \left[\left(-\frac{\ell}{2}, \frac{\ell}{2}\right) \times \left(-\frac{h}{2}, \frac{h}{2}\right)^{n-1} \right]$ and the energy on the parallelepiped*

$$\varphi(b, t, \ell, h) = \inf \left\{ \liminf_{k \rightarrow \infty} \frac{1}{\ell} E(\mu_k, R_{\ell,h}^t) : \mu_k \in \mathcal{M}_{\text{df}}^{(m)}(R_{\ell,h}^t), \mu_k \xrightarrow{*} b \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t \cap R_{\ell,h}^t) \right\}. \tag{3.3}$$

Then φ does not depend on ℓ and h . We write $\varphi(b, t, \ell, h) = \varphi(b, t)$.

Proof The statement is obtained through the following remarks. We work here at fixed b and t and write for simplicity $\phi(\ell, h) = \varphi(b, t, \ell, h)$.

(i) With a rescaling argument we get that

$$\phi(\ell, h) = \phi(\lambda \ell, \lambda h) \quad \forall \lambda > 0. \tag{3.4}$$

(ii) It is also immediate to notice that

$$\phi(\ell, h) \leq \phi(\ell, H) \quad \text{whenever } h \leq H, \tag{3.5}$$

by definition.

(iii) Moreover

$$\phi\left(\frac{\ell}{p}, h\right) \leq \phi(\ell, h) \quad \forall p \in \mathbb{N} \setminus \{0\} \tag{3.6}$$

by a selection argument. For example, if $p = 2$, then (3.6) is obtained choosing for each k the half of $R_{\ell,h}^t$ with energy less than $\frac{1}{2} E(\mu_k, R_{\ell,h}^t)$.

Thus our claim is proved, because by the previous three steps we have, for all $h, \ell > 0$ and all $p \in \mathbb{N} \setminus \{0\}$,

$$\phi\left(\frac{\ell}{p}, h\right) \leq \phi(\ell, h) = \phi\left(\frac{\ell}{p}, \frac{h}{p}\right) \leq \phi\left(\frac{\ell}{p}, h\right)$$

hence equality holds throughout. □

The next lemma shows that φ , which was defined using weak convergence instead of boundary values, is the same as $\bar{\psi}$. This is the key step in which we show that the natural upper and lower bounds coincide.

Lemma 3.5 *Let $\psi, \bar{\psi}$ and \bar{E} be as in Theorem 3.1, φ as in Lemma 3.4. Then we have:*

(i) *For every sequence $\mu_k \in \mathcal{M}_{\text{df}}^{(m)}(B_{1/2})$ with $\mu_k \xrightarrow{*} \mu = b \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t \cap B_{1/2})$ weakly in $\mathcal{M}_{\text{df}}^{(m)}(B_{1/2})$ one has*

$$\varphi(b, t) \leq \liminf_{k \rightarrow \infty} \bar{E}(\mu_k, B_{1/2}).$$

(ii) $\bar{\psi}(b, t) = \varphi(b, t)$.

Proof (i) We can assume the liminf to be a limit and to be finite. We first pass from \bar{E} to E on the right-hand side. By the upper bound proven in the previous section, for every k there is a sequence $v_h^{(k)} \xrightarrow{*} \mu_k$ in $\mathcal{M}_{df}^{(m)}(B_{1/2})$ such that

$$\limsup_{h \rightarrow \infty} E(v_h^{(k)}, B_{1/2}) \leq \bar{E}(\mu_k, B_{1/2}).$$

Since the weak convergence is metrizable on bounded sets we can take a diagonal subsequence and obtain a sequence $\tilde{\mu}_k$ which converges weakly to μ in $\mathcal{M}_{df}^{(m)}(B_{1/2})$, with

$$\lim_{k \rightarrow \infty} E(\tilde{\mu}_k, B_{1/2}) \leq \lim_{k \rightarrow \infty} \bar{E}(\mu_k, B_{1/2}).$$

Therefore it suffices to show that $\varphi(b, t) \leq \liminf_{k \rightarrow \infty} E(\tilde{\mu}_k, B_{1/2})$.

We fix $\ell \in (0, 1)$ and then choose $h \ll 1$ such that $R_{\ell, h}^t \subset B_{1/2}$. Then $E(\tilde{\mu}_k, R_{\ell, h}^t) \leq E(\tilde{\mu}_k, B_{1/2})$ and, using Lemma 3.4,

$$\ell\varphi(b, t) \leq \liminf_{k \rightarrow \infty} E(\tilde{\mu}_k, R_{\ell, h}^t) \leq \liminf_{k \rightarrow \infty} E(\tilde{\mu}_k, B_{1/2}).$$

Since $\ell \in (0, 1)$ was arbitrary, the proof is concluded.

(ii) We choose $b \in \mathbb{Z}^m, t \in \mathcal{S}^{n-1}$, and set $\mu = b \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t \cap R_{1,1}^t)$. We start by defining a version of $\tilde{\psi}$ where the ball is replaced by a cube,

$$\tilde{\psi}(b, t) = \inf \left\{ E(\tilde{\mu}, R_{1,1}^t) : \tilde{\mu} \in \mathcal{M}_{df}^{(m)}(R_{1,1}^t), \text{ supp}(\tilde{\mu} - \mu) \subset R_{1,1}^t \right\}.$$

It suffices to show that $\varphi \leq \tilde{\psi}, \bar{\psi} \leq \tilde{\psi}$ and $\tilde{\psi} \leq \varphi$.

To prove $\varphi \leq \tilde{\psi}$ let $\mu^* = \theta^* \otimes \tau^* \mathcal{H}^1 \llcorner \gamma^*$ be one of the measures entering (3.1). We fill $R_{1,1}^t$ by $2k + 1$ scaled-down copies of μ^* , for all $k \in \mathbb{N}$. Precisely, let $f_j^k(x) = \frac{1}{(2k+1)}(x + jt)$ and set $\mu^k = \sum_{j=-k}^k (f_j^k)_\# \mu^*$. Since $Df_j^k = \frac{1}{2k+1} \text{Id}$, for any test function $\varphi \in C_c^0(\mathbb{R}^n)$ we have

$$\int \varphi d[(f_j^k)_\# \mu^*] = \frac{1}{2k+1} \int (\varphi \circ f_j^k) d\mu^* = \frac{1}{2k+1} \int \varphi \left(\frac{jt+x}{2k+1} \right) d\mu^*(x).$$

Then $\mu^k \in \mathcal{M}_{df}^{(m)}(R_{1,1})$, $\mu^k \xrightarrow{*} \mu$, and $E(\mu^k, R_{1,1}^t) = E(\mu^*, B_{1/2})$. Since μ^* was arbitrary, we obtain $\varphi \leq \tilde{\psi}$.

By covering most of the diameter of $B_{1/2}$ with small squares one can easily see that $\bar{\psi} \leq \tilde{\psi}$.

We now show $\tilde{\psi} \leq \varphi$. Choose a sequence $\mu_k \xrightarrow{*} \mu$ in $\mathcal{M}_{df}^{(m)}(R_{1,1}^t)$ such that

$$\lim_{k \rightarrow \infty} E(\mu_k, R_{1,1}^t) = \varphi(b, t). \tag{3.7}$$

By Lemma 3.4, for any $h \in (0, 1)$ we have

$$\varphi(b, t) \leq \liminf_{k \rightarrow \infty} E(\mu_k, R_{1,h}^t).$$

In particular,

$$\limsup_{k \rightarrow \infty} E(\mu_k, R_{1,1}^t \setminus R_{1,h}^t) = 0. \tag{3.8}$$

By the structure theorem (Theorem 2.5) the measure μ_k has the form $\sum_i \theta_{k,i} \otimes \tau_{k,i} \mathcal{H}^1 \llcorner \gamma_{k,i}$, with $\theta_{k,i} \in \mathbb{Z}^m$ and $\gamma_{k,i}$ Lipschitz curves, each either closed or with endpoints in $\partial R_{1,1}^t$. We

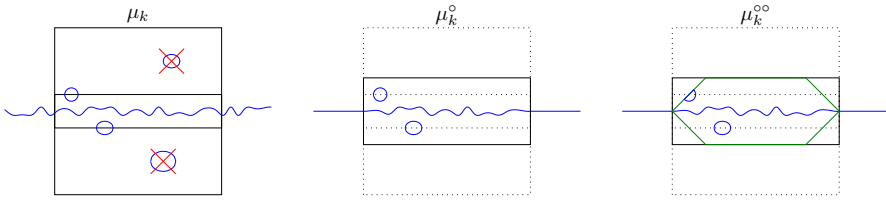


Fig. 3 Passing from μ_k to μ_k° . The squares represent $R_{1,1}^t$, the rectangles $R_{1,h}^t$ and $R_{1,2h}^t$

denote by J_k the set of i for which the curve $\gamma_{k,i}$ intersects $R_{1,h}^t$, and we define $\gamma_k^{\circ} = \cup_{i \in J_k} \gamma_{k,i}$ and $\mu_k^{\circ} = \sum_{i \in J_k} \theta_{k,i} \otimes \tau_{k,i} \mathcal{H}^1 \llcorner \gamma_{k,i}$. By construction $\partial \mu_k^{\circ} = 0$. By (3.8) we have

$$\mathcal{H}^1(\gamma_k \cap R_{1,1}^t \setminus R_{1,h}^t) \rightarrow 0 \text{ as } k \rightarrow \infty,$$

therefore $\gamma_k^{\circ} \subset R_{1,2h}^t$ for k sufficiently large. In summary, we have constructed a new sequence of vector-valued measures μ_k° which satisfies

$$\mu_k^{\circ} \xrightarrow{*} \mu$$

with $\text{supp} \mu_k^{\circ} \subset R_{1,2h}^t$ and $\partial \mu_k^{\circ} = 0$ in $R_{1,1}^t$ (see Fig. 3).

As a consequence of the definition of the truncated energy in Lemma 3.4 we get

$$(1 - 2h)\varphi \leq \liminf_{k \rightarrow \infty} E(\mu_k^{\circ}, R_{1-2h,2h}^t),$$

thus the endstrips $S_h^t = R_{1,2h}^t \setminus R_{1-2h,2h}^t$ contain little energy, in the sense that

$$\limsup_{k \rightarrow \infty} E(\mu_k^{\circ}, S_h^t) \leq 2h\varphi. \tag{3.9}$$

As we drew in Fig. 3, we head to the conclusion squeezing the measure μ_k° through the projection $f^t : R_{1,2h}^t \rightarrow R_{1,2h}^t$, defined by $f^t(x) = x$ for $x \in R_{1-2h,2h}^t$ and $f^t(x) = Q_t f(Q_t^{-1}x)$ in S_h^t , where Q_t is a rotation such that $Q_t e_1 = t$ and f is defined as

$$f(x_1, x') = \left(x_1, \left(\frac{1}{2h} - \frac{1}{h}|x_1| \right) x' \right) \text{ for } x = (x_1, x') \in S_h^{e_1}.$$

Let us define

$$\mu_k^{\circ\circ} = f_{\#}^t(\mu_k^{\circ}).$$

Thus

$$E(\mu_k^{\circ\circ}, S_h^t) \leq cE(\mu_k^{\circ}, S_h^t),$$

and therefore by (3.7) and (3.9)

$$\limsup_{k \rightarrow \infty} E(\mu_k^{\circ\circ}, R_{1,2h}^t) \leq \varphi + ch\varphi. \tag{3.10}$$

Finally we deal with the boundary. By the definition of $\mu_k^{\circ\circ}$,

$$\partial \mu_k^{\circ\circ} = \theta'(\delta_{1/2e_1} - \delta_{-1/2e_1}). \tag{3.11}$$

The measure

$$\mu_k^{\circ\circ\circ} = \mu_k^{\circ\circ} + \theta' \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}e_1 \setminus R_{1,h}^t)$$

satisfies $\partial\mu_k^{\circ\circ} = 0$, but, at the same time,

$$\mu_k^{\circ\circ} \xrightarrow{*} b \otimes t\mathcal{H}^1 \llcorner (\mathbb{R}e_1 \cap R'_{1,h}) + \theta' \otimes t\mathcal{H}^1 \llcorner (\mathbb{R}e_1 \setminus R'_{1,h}),$$

thus $\theta' = b$. Thus, (3.11) together with (3.10) implies $\tilde{\psi} \leq \varphi$. □

We are now ready for proving the lower bound.

Proof of the lower bound in Theorem 3.1 Fix $\mu \in \mathcal{M}_{df}^{(m)}(\Omega)$ and consider a sequence $\mu_k \xrightarrow{*} \mu$. Since $\bar{E} \leq E$, it suffices to prove that

$$\bar{E}(\mu, \Omega) \leq \liminf_{k \rightarrow \infty} \bar{E}(\mu_k, \Omega)$$

(this means, it suffices to show that \bar{E} is lower semicontinuous). Passing to a subsequence we can assume that the sequence $\bar{E}(\mu_k, \Omega)$ converges. We can assume that the limit is finite, and therefore that $\sup_k |\mu_k|(\Omega) < \infty$. We extend each of the measures μ_k to $\mathcal{E}\mu_k \in \mathcal{M}_{df}^{(m)}(\mathbb{R}^n)$ using Lemma 2.3. The sequence $\mathcal{E}\mu_k$ is uniformly bounded, extracting a subsequence we can assume that $\mathcal{E}\mu_k$ has a weak limit, which is automatically an extension of μ . With a slight abuse of notation we denote the limit by $\mathcal{E}\mu$. We identify $\mathcal{E}\mu$ and $\mathcal{E}\mu_k$ with the corresponding closed currents $T, T_k \in \mathcal{R}_1(\mathbb{R}^n; \mathbb{Z}^m)$.

We fix $\varepsilon > 0$ and apply the Deformation Theorem to $\mathcal{E}\mu$ (Theorem 2.1). Let f and P be the resulting C^1 bi-Lipschitz map and polyhedral measure such that

$$\|f_{\#}\mathcal{E}\mu - P\| < \varepsilon \text{ and } |f(x) - x| + |Df(x) - \text{Id}| < \varepsilon.$$

We define

$$\tilde{\mu}_k = f_{\#}(\mathcal{E}\mu_k - \mathcal{E}\mu) + P = f_{\#}\mathcal{E}\mu_k - (f_{\#}\mathcal{E}\mu - P).$$

Clearly $\partial\tilde{\mu}_k = 0$; from $\mathcal{E}\mu_k \xrightarrow{*} \mathcal{E}\mu$ we deduce $\tilde{\mu}_k \xrightarrow{*} P$. From Lemma 3.3 we get, for $\omega_\varepsilon = \{x \in \Omega : \text{dist}(x, \partial\Omega) > \varepsilon\}$,

$$\bar{E}(\tilde{\mu}_k, \omega_\varepsilon) \leq (1 + c\|Df - \text{Id}\|_{L^\infty})\bar{E}(\mu_k, \Omega) + c\|f_{\#}\mathcal{E}\mu - P\|. \tag{3.12}$$

Since P is polyhedral, we can find finitely many disjoint balls $B_i = B(x_i, r_i) \subset \omega_\varepsilon$ such that $P \llcorner B_i = b_i \otimes t_i \mathcal{H}^1 \llcorner (x_i + t_i \mathbb{R} \cap B_i)$ and $|P|(\omega_{2\varepsilon} \setminus \cup B_i) \leq \varepsilon$. For each ball, by Lemma 3.5, we have

$$\bar{E}(P, B_i) = 2r_i \bar{\psi}(b_i, t_i) \leq \liminf_{k \rightarrow \infty} \bar{E}(\tilde{\mu}_k, B_i).$$

Summing over the balls we conclude that

$$\bar{E}(P, \omega_{2\varepsilon}) \leq \sum_i \bar{E}(P, B_i) + c|P|(\omega_{2\varepsilon} \setminus \cup B_i) \leq \liminf_{k \rightarrow \infty} \bar{E}(\tilde{\mu}_k, \omega_\varepsilon) + c\varepsilon.$$

By (3.12) we then get

$$\bar{E}(P, \omega_{2\varepsilon}) \leq (1 + c\varepsilon) \liminf_{k \rightarrow \infty} \bar{E}(\mu_k, \Omega) + c\varepsilon.$$

Since another application of Lemma 3.3 gives

$$\bar{E}(\mu, \omega_{3\varepsilon}) \leq \bar{E}(P, \omega_{2\varepsilon})(1 + c\varepsilon) + c\varepsilon,$$

the conclusion follows by the arbitrariness of ε . □

4 Explicit relaxation for dislocations in cubic crystals

We consider here the energy density $\psi : \mathbb{Z}^n \times \mathcal{S}^{n-1} \rightarrow \mathbb{R}$

$$\psi(b, t) = |b|^2 + \eta(b \cdot t)^2 \quad (4.1)$$

which arises in the modeling of dislocations in crystals. Focusing on the case $\eta \in [0, 1]$ which arose in previous works [3, 7, 11], we determine here the relaxation $\bar{\psi}(b, t)$ for the (most relevant) small values of b and in particular show that complex structures may arise, in which different values of b and of t interact.

4.1 Line-energy of dislocations

A dislocation is a line singularity in a crystal which may be described by a divergence-free measure of the form $\theta \otimes \tau \mathcal{H}^1 \llcorner \gamma$, as studied in the previous sections, where θ physically represents the components of the Burgers vector in a lattice basis [13, 14]. In the case that dislocations are restricted to a plane, $\gamma \subset \mathbb{R}^2 \times \{0\}$ and $\theta \in \mathbb{Z}^2$, a model of this form was derived from linear three-dimensional elasticity in [7, 11] using the tools of Γ -convergence, building mathematically upon the concept of BV -elliptic envelope and physically upon a generalization of the Peierls–Nabarro model introduced by Koslowski, Cuitiño and Ortiz [15, 16]. One key observation was that the (unrelaxed) energy per unit length of a dislocation is given by a specific function $\psi^c(b, t)$, which can be computed from the elastic constants of the solid. Assuming a cubic kinematics for the dislocations and isotropic elastic constants and writing $t = (\cos \alpha, \sin \alpha) \in \mathcal{S}^1$, the energy density takes the form (see [3, Eq. (51)] or [7, Eq.(1.8)]),

$$\psi^c(b, t) = \frac{\mu a_0^2}{4\pi(1-\nu)} b \begin{pmatrix} 2 - 2\nu \cos^2 \alpha & -2\nu \sin \alpha \cos \alpha \\ -2\nu \sin \alpha \cos \alpha & 2 - 2\nu \sin^2 \alpha \end{pmatrix} b,$$

where the parameter $\nu \in [-1, 1/2]$ represents the material's Poisson ratio, μ the shear modulus of the crystal, a_0 the length of the Burgers vector (i.e., the lattice spacing). Straightforward manipulations permit to rewrite this expression as

$$\psi^c(b, t) = \frac{\mu a_0^2}{4\pi(1-\nu)} \left(2(1-\nu)|b|^2 + 2\nu(b^\perp \cdot t)^2 \right) = \frac{\mu a_0^2}{2\pi} \psi(b^\perp, t), \quad (4.2)$$

where ψ was defined in (4.1), $\eta = \frac{\nu}{1-\nu} \leq 1$, and $b^\perp = (-b_2, b_1)$. Without loss of generality we can assume $\eta \in [0, 1]$: indeed, if $\nu < 0$, we can rewrite (4.2) as $\psi^c(b, t) = \frac{\mu a_0^2}{2\pi(1-\nu)} \psi'(b, t)$ where $\psi'(b, t) = |b|^2 + \eta'(b \cdot t)^2$ contains the constant $\eta' = -\nu \in [0, 1]$.

The expression (4.1) is invariant under rotations, and indeed the above discussion can be immediately generalized to the three-dimensional case, resulting (at least in the somewhat academic case $\nu < 0$) in the same formula, see, e.g., [14, Sect. 4.4] or [15, Eq.(51)].

4.2 Lower bound on the relaxation

We now start the analysis of the energy density (4.1). The key idea is to decompose the set γ on which the measure is concentrated into sets on which θ is constant. Each component is then replaced by a segment with the same end-to-end span, an operation which by convexity does not increase the energy (here we use Lemma 4.2 below). This involves an implicit rearrangement, which one can expect to be sharp since γ is one dimensional. In a second step we show that only small multiplicities are relevant in the definition of the relaxation,

due to the quadratic growth of ψ (here we use Lemma 4.3 below). A similar procedure is also helpful to characterize the relaxation in a total-variation model for the reconstruction of optical flow in image processing [6].

Proposition 4.1 *Let $\eta \in [0, 1]$, ψ be as in (4.1). For $n \leq 9$ its \mathcal{H}^1 -elliptic envelope obeys*

$$\bar{\psi}(b, t) \geq \min \left\{ \sum_{\alpha \in \{-1, 0, 1\}^n} \psi_e(\alpha, T_\alpha) : T \in \mathbb{R}^{n \times 3^n}, \sum_{\alpha \in \{-1, 0, 1\}^n} \alpha \otimes T_\alpha = b \otimes t \right\}, \tag{4.3}$$

where ψ_e denotes the positively one-homogeneous extension of ψ ,

$$\psi_e(b, t) = |t| \psi \left(b, \frac{t}{|t|} \right). \tag{4.4}$$

For $n \geq 10$ Eq. (4.3) holds with $T \in \mathbb{R}^{n(4n+1)^n}$ and both sums running over all α in $[-2n, 2n]^n \cap \mathbb{Z}^n$.

Proof Step 1 We fix b and t . Let $\mu = \theta \otimes \tau \mathcal{H}^1 \llcorner \gamma$ be any of the measures entering (3.1). We decompose its support γ depending on the value of θ . For any $\alpha \in \mathbb{Z}^n$ we set

$$\gamma_\alpha = \{x \in \gamma : \theta(x) = \alpha\}.$$

These countably many 1-rectifiable sets are pairwise disjoint and cover γ . Since $\partial(\mu - b \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t \cap B_{\frac{1}{2}})) = 0$ we have

$$b \otimes t = \int_\gamma \theta \otimes \tau d\mathcal{H}^1 = \sum_{\alpha \in \mathbb{Z}^n} \alpha \otimes T_\alpha,$$

where we defined

$$T_\alpha = \int_{\gamma_\alpha} \tau d\mathcal{H}^1.$$

An analogous decomposition of the energy gives

$$E(\theta \otimes \tau \mathcal{H}^1 \llcorner \gamma) = \sum_\alpha \int_{\gamma_\alpha} \psi(\alpha, \tau) d\mathcal{H}^1 \geq \sum_\alpha \psi_e(\alpha, T_\alpha),$$

where in the second step we used Lemma 4.2 below. In particular, if the energy is finite then $\sum_\alpha |T_\alpha| < \infty$.

Step 2 Assume first $n \leq 9$. Let $T : \mathbb{Z}^n \rightarrow \mathbb{R}^n$ be as above, $\alpha^* \in \mathbb{Z}^n$ be such that $|\alpha_i^*| > 1$ for some i and $T_{\alpha^*} \neq 0$. Let $a \in \mathbb{Z}^n$ be as in Lemma 4.3(i) below, so that

$$\psi_e(\alpha^* - a, T_{\alpha^*}) + \psi_e(a, T_{\alpha^*}) \leq \psi_e(\alpha^*, T_{\alpha^*}).$$

By the subadditivity in Lemma 4.2,

$$\psi_e(a, T_a + T_{\alpha^*}) \leq \psi_e(a, T_{\alpha^*}) + \psi_e(a, T_a)$$

and the same for $\alpha^* - a$. We set $T'_{\alpha^*} = 0, T'_a = T_a + T_{\alpha^*}, T'_{\alpha^* - a} = T_{\alpha^* - a} + T_{\alpha^*}, T'_\alpha = T_\alpha$ for the other values. Then $\sum_\alpha \alpha \otimes T'_\alpha = \sum_\alpha \alpha \otimes T_\alpha$ and

$$\sum_\alpha \psi_e(\alpha, T'_\alpha) \leq \sum_\alpha \psi_e(\alpha, T_\alpha).$$

Let $M > 2$. Finitely many iterations of this step produce a T^M with $T_\alpha^M = 0$ for all α with $\max_i |\alpha_i| \in [2, M]$. Taking the limit $M \rightarrow \infty$ gives a T^∞ with $T_\alpha^\infty = 0$ whenever $\max_i |\alpha_i| \geq 2$. This concludes the proof for $n \leq 9$.

If $n \geq 9$ we use the same procedure with Lemma 4.3(ii) instead of (i). □

One key ingredient in the above proof was the subadditivity of ψ_e .

Lemma 4.2 *The function ψ_e defined in (4.4) is subadditive in the second argument, in the sense that for any $b \in \mathbb{Z}^n$ and any set of vectors $T_1, \dots, T_N \in \mathbb{R}^n$ we have*

$$\psi_e\left(b, \sum_i T_i\right) \leq \sum_i \psi_e(b, T_i).$$

Analogously, if γ is 1-rectifiable and τ its tangent,

$$\psi_e\left(b, \int_\gamma \tau d\mathcal{H}^1\right) \leq \int_\gamma \psi_e(b, \tau) d\mathcal{H}^1.$$

Proof For brevity we prove only the first formula, the differences are purely notational. We can assume $b \neq 0$. We set $\tau_i = T_i/|T_i|$, $L = \sum_i |T_i|$, and write $\psi_e(b, T_i) = |T_i|\varphi(\tau_i)$ where $\varphi(\tau) = |b|^2 + \eta(b \cdot \tau)^2$, $\tau \in \mathbb{R}^n$. Since φ is convex we obtain

$$|b|^2 + \eta(b \cdot \hat{\tau})^2 = \varphi(\hat{\tau}) \leq \sum_i \frac{|T_i|}{L} \varphi(\tau_i) = \frac{1}{L} \sum_i \psi_e(b, T_i),$$

where

$$\hat{\tau} = \sum_i \frac{|T_i|}{L} \tau_i = \frac{1}{L} \sum_i T_i.$$

Set now $h(\ell) = \ell|b|^2 + \ell^{-1}\eta(b \cdot \hat{\tau})^2$. The function h has a global minimum at $\ell_0 = \sqrt{\eta} \frac{|b \cdot \hat{\tau}|}{|b|} \leq |\hat{\tau}|$ and is increasing afterwards. Since $\hat{\tau}$ is an average of unit vectors, $|\hat{\tau}| \leq 1$. We obtain

$$\psi_e(b, \hat{\tau}) = h(|\hat{\tau}|) \leq h(1) = \varphi(\hat{\tau}),$$

and therefore the desired inequality

$$\psi_e\left(b, \sum_i T_i\right) = \psi_e(b, L\hat{\tau}) = L\psi_e(b, \hat{\tau}) \leq L\varphi(\hat{\tau}) \leq \sum_i \psi_e(b, T_i).$$

□

Lemma 4.3 (i) *Let $n \in \{2, \dots, 9\}$, $b \in \mathbb{Z}^n$. If $\beta = \max_i |b_i| > 1$ then there is a vector $a \in \mathbb{Z}^n$ such that $\max_i |a_i| = 1$, $\max_i |b_i - a_i| = \beta - 1$, and*

$$\psi(b - a, t) + \psi(a, t) \leq \psi(b, t) \text{ for all } t \in S^{n-1}. \tag{4.5}$$

(ii) *Let $b \in \mathbb{Z}^n$. If $|b| \geq 4\sqrt{n}$ then there is a vector $a \in \mathbb{Z}^n$ such that $\max_i |a_i| < \max_i |b_i|$, $\max_i |b_i - a_i| < \max_i |b_i|$, and (4.5) holds.*

(iii) *If $a, b \in \mathbb{Z}^n$, $a \cdot b = 0$ and $|b| \leq |a|\sqrt{2}$, then*

$$\psi(b, t) \leq \psi(a + b, t) \text{ for all } t \in S^{n-1}.$$

We observe that the construction in (i) does not work for $n \geq 10$. Indeed, if we take $n = 10$, $\eta = 1$, $b = 2e_1 + \sum_{i=2}^{10} e_i$, $t = \frac{1}{2}e_1 - (12)^{-1/2} \sum_{i=2}^{10} e_i$ then a short computation shows that $\psi(b, t) < \psi(b - e_1, t) + \psi(e_1, t)$.

Proof (i) We need to choose a such that the quantity

$$\xi = \psi(b, t) - \psi(a, t) - \psi(b - a, t) = 2(b - a) \cdot a + 2\eta((b - a) \cdot t)(a \cdot t)$$

is nonnegative. We set

$$a = \sum_{i:|b_i|=\beta} \operatorname{sgn}(b_i)e_i,$$

so that $\max_i |a_i| = 1$, $\max_i |b_i - a_i| = \beta - 1$, $b = \beta a + b'$ and $a \cdot b' = 0$. Then

$$\begin{aligned} \xi &= 2(\beta - 1)|a|^2 + 2\eta(\beta - 1)(a \cdot t)^2 + 2\eta(b' \cdot t)(a \cdot t) \\ &\geq 2(\beta - 1)|a|^2\eta \left[1 + x^2 - \frac{|b'|}{|a|(\beta - 1)}x\sqrt{1 - x^2} \right], \end{aligned}$$

where we set $x = |a \cdot t|/|a|$ and used that, since a and b' are orthogonal, $|b' \cdot t| \leq |b'|\sqrt{1 - x^2}$. Since b' has at most $n - 1$ non-zero components, each of them has length at most $\beta - 1$, and $|a| \geq 1$ we have $\frac{|b'|}{|a|(\beta - 1)} \leq \sqrt{n - 1} \leq \sqrt{8} = 2\sqrt{2}$. The conclusion follows from the fact that $2\sqrt{2}x\sqrt{1 - x^2} \leq (\sqrt{2}x)^2 + (1 - x^2) = 1 + x^2$.

(ii) We set $a = \sum_i \operatorname{sgn}(b_i)[|b_i|/2]e_i$, $f = b - 2a$, and compute, with ξ as above,

$$\xi = 2(|a|^2 + f \cdot a + \eta(a \cdot t)^2 + \eta(a \cdot t)(f \cdot t)) \geq 2(|a|^2 - 2|a||f|).$$

The conclusion follows from $|f| \leq \sqrt{n}$ and $|a| \geq |b|/2 \geq 2\sqrt{n}$.

(iii) We write

$$\begin{aligned} \psi(a + b, t) - \psi(b, t) &= |a|^2 + |b|^2 + \eta(t \cdot a + t \cdot b)^2 - (|b|^2 + \eta(t \cdot b)^2) \\ &= |a|^2 + \eta[(t \cdot a + t \cdot b)^2 - (t \cdot b)^2] \\ &\geq \eta[|a|^2 + (t \cdot a)^2 + 2(t \cdot a)(t \cdot b)]. \end{aligned}$$

As in the previous case we set $x = |a \cdot t|/|a|$ and use orthogonality to write

$$\psi(a + b, t) - \psi(b, t) \geq \eta|a|^2 \left[1 + x^2 - \frac{2|b|}{|a|}x\sqrt{1 - x^2} \right].$$

The conclusion follows, using $|b| \leq |a|\sqrt{2}$, with the same inequality as in (i). □

4.3 Explicit relaxation for special b

Lemma 4.4 *For $n \leq 9$ and all $i \in \{1, \dots, n\}$, $\beta \in \mathbb{Z}$ we have*

$$\bar{\psi}(\beta e_i, t) = |\beta|\psi(e_i, t).$$

Proof The inequality $\bar{\psi}(\beta e_i, t) \leq |\beta|\psi(e_i, t)$ follows from subadditivity. To prove the converse inequality, we first observe that

$$\psi(e_i, t) \leq \psi(\alpha, t) \text{ whenever } \alpha_i \in \{-1, 1\}.$$

Indeed, it suffices to apply Lemma 4.3(iii) with $b = \alpha_i e_i$, and $a = \alpha - b$, which is admissible because $|b| = 1$ and $|a| \geq 1$ (unless $a = 0$, but in this case there is nothing to prove).

Let T be a minimizer in the lower bound (4.3). We estimate, using the above observation and then Lemma 4.2,

$$\sum_{\alpha:\alpha_i \neq 0} \psi_e(\alpha, T_\alpha) \geq \sum_{\alpha:\alpha_i \neq 0} \psi_e(e_i, T_\alpha) \geq \psi_e(e_i, \sum_{\alpha:\alpha_i \neq 0} \alpha_i T_\alpha) = \psi_e(e_i, z),$$

where we defined $z = \sum_{\alpha:\alpha_i \neq 0} \alpha_i T_\alpha$. The i -th row of the condition $\sum_\alpha \alpha \otimes T_\alpha = b \otimes t$ gives then $z = \beta t$. We conclude that

$$\bar{\psi}(\beta e_i, t) \geq \psi_e(e_i, \beta t) = |\beta| \psi(e_i, t)$$

and therefore the statement. □

Lemma 4.5 For $n \leq 9$ and all $\beta \in \mathbb{Z}$, $t \in \mathcal{S}^{n-1}$, $i \neq j \in \{1, \dots, n\}$ we have

$$\begin{aligned} \bar{\psi}(\beta(e_i + e_j), t) = |\beta| \min & \left\{ \psi_e(e_i, z_1) + \psi_e(e_j, z_2) \right. \\ & \left. + \psi_e\left(e_i - e_j, \frac{z_2 - z_1}{2}\right) + \psi_e\left(e_i + e_j, t - \frac{z_1 + z_2}{2}\right) : z_1, z_2 \in \mathbb{R}^n \right\} \end{aligned}$$

and correspondingly for $\beta(e_i - e_j)$.

Proof Step 1 Lower bound. For ease of notation we focus on the case $i = 1, j = 2$. Let T be a minimizer in the lower bound (4.3) corresponding to $\beta(e_1 + e_2)$. We define

$$\begin{aligned} T_1 &= \sum_{\alpha_1 \neq 0, \alpha_2 = 0} \alpha_1 T_\alpha, & T_2 &= \sum_{\alpha_1 = 0, \alpha_2 \neq 0} \alpha_2 T_\alpha, \\ T_+ &= \sum_{\alpha_1 = \alpha_2 \neq 0} \alpha_1 T_\alpha, & T_- &= \sum_{\alpha_1 = -\alpha_2 \neq 0} \alpha_1 T_\alpha. \end{aligned}$$

The sets over which these sums run are disjoint, and $\alpha_1 = \alpha_2 = 0$ on all other values of α . Therefore the first two rows of $\sum_\alpha \alpha \otimes T_\alpha = \beta(e_1 + e_2) \otimes t$ give

$$T_1 + T_+ + T_- = \beta t \quad \text{and} \quad T_2 + T_+ - T_- = \beta t. \tag{4.6}$$

In particular, $T_1 - T_2 + 2T_- = 0$. We decompose the sum of the $\psi(\alpha, T_\alpha)$ in (4.3) into the same four parts as above.

Let us start with the part with $\alpha_1 = \alpha_2 \neq 0$. For each α with this property we consider $b = \alpha_1(e_1 + e_2)$ and $a = \alpha - b$. Then $a \cdot b = 0$ and, recalling that $|\alpha_1| = 1$, we have $\sqrt{2} = |b| \leq |a|\sqrt{2}$ (unless $a = 0$, but in this case there is nothing to prove). By Lemma 4.3(iii) we obtain $\psi_e(e_1 + e_2, t) \leq \psi_e(\alpha, t)$ for all t . Therefore

$$\sum_{\alpha_1 = \alpha_2 \neq 0} \psi_e(\alpha, T_\alpha) \geq \sum_{\alpha_1 = \alpha_2 \neq 0} \psi_e(e_1 + e_2, \alpha_1 T_\alpha) \geq \psi_e(e_1 + e_2, T_+),$$

where in the last step we used the subadditivity of Lemma 4.2. The case $\alpha_1 \neq 0 = \alpha_2$ is similar and has already been treated in the proof of Lemma 4.4,

$$\sum_{\alpha_1 \neq 0, \alpha_2 = 0} \psi_e(\alpha, T_\alpha) \geq \sum_{\alpha_1 \neq 0, \alpha_2 = 0} \psi_e(e_1, \alpha_1 T_\alpha) \geq \psi_e(e_1, T_1).$$

The other two cases are almost identical. Therefore we have shown that

$$\bar{\psi}(\beta(e_1 + e_2), t) \geq \psi_e(e_1, T_1) + \psi_e(e_2, T_2) + \psi_e(e_1 + e_2, T_+) + \psi_e(e_1 - e_2, T_-).$$

We set $z_1 = T_1/\beta$, $z_2 = T_2/\beta$. By (4.6) one has $T_- = \beta(z_2 - z_1)/2$ and $T_+ = \beta(t - (z_1 + z_2)/2)$. Since ψ_e is positively 1-homogeneous in the second argument,

$$\begin{aligned} \bar{\psi}(\beta(e_1 + e_2), t) &\geq |\beta| \psi_e(e_1, z_1) + |\beta| \psi_e(e_2, z_2) \\ &\quad + |\beta| \psi_e\left(e_1 + e_2, t - \frac{z_1 + z_2}{2}\right) + |\beta| \psi_e\left(e_1 - e_2, \frac{z_2 - z_1}{2}\right). \end{aligned}$$

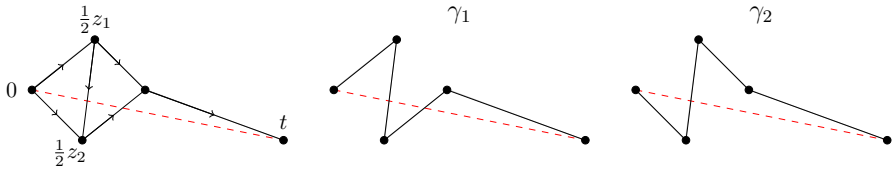


Fig. 4 Sketch of the construction used in the upper bound of Lemma 4.5. The *left panel* shows the support of the measure, the *central* one the part on which $\alpha_1 \neq 0$, the *right* one the part on which $\alpha_2 \neq 0$. The *red dashed line* is t

Step 2 Upper bound. It suffices to consider $\beta = 1$, the other cases follow by subadditivity. The construction is illustrated in Fig. 4. Precisely, we let γ_1 be the polygonal curve that joins (in this order) the points

$$(0, 0), \quad \frac{1}{2} z_1, \quad \frac{1}{2} z_2, \quad \frac{1}{2} (z_1 + z_2), \quad t,$$

and τ_1 its tangent vector. Analogously, let γ_2 be the curve that joins

$$(0, 0), \quad \frac{1}{2} z_2, \quad \frac{1}{2} z_1, \quad \frac{1}{2} (z_1 + z_2), \quad t,$$

and τ_2 its tangent. Then we set

$$\mu = e_1 \otimes \tau_1 \mathcal{H}^1 \llcorner \gamma_1 + e_2 \otimes \tau_2 \mathcal{H}^1 \llcorner \gamma_2.$$

One can then extend μ t -periodic and rescale to get a sequence $\mu_k \rightarrow (e_1 + e_2) \otimes t \mathcal{H}^1 \llcorner (\mathbb{R}t)$ and prove the upper bound. □

The following, more explicit result in two dimensions was mentioned without proof in [7]. It shows that in this case the relaxation is obtained first by making the integrand subadditive in the first argument than taking the (one-homogeneous) convex envelope in the second argument of the result, corresponding to the upper bound given in [3]. In particular, the minimum is not always trivial. For example, for $t = e_2$ it is easy to see that whenever $\eta > 0$ the minimizer obeys $z \cdot e_1 > 0$. The resulting microstructure is illustrated in Fig. 5. The relation of this explicit relaxation formula to dislocation models in three dimensions is treated in [5]. A similar result for dislocations restricted to two planes is discussed in [8].

Lemma 4.6 *For $n = 2$ and all $\beta \in \mathbb{Z}$, $t \in \mathcal{S}^1$ we have*

$$\bar{\psi}(\beta(e_1 + e_2), t) = |\beta| \min \{ \psi_e(e_1, z) + \psi_e(e_2, z) + \psi_e(e_1 + e_2, t - z) : z \in \mathbb{R}^2 \}.$$

Proof We just need to show that minimum in the formula of Lemma 4.5 is attained at $z_1 = z_2$. This is equivalent to the statement that

$$\psi_e(e_1, m - d) + \psi_e(e_2, m + d) + \psi_e(e_1 - e_2, d) - \psi_e(e_1, m) - \psi_e(e_2, m) \geq 0$$

for all $m, d \in \mathbb{R}^2$ (we set $z_1 = m - d, z_2 = m + d$). Explicitly, this expression is

$$|m - d| + |m + d| + 2|d| + \eta \frac{(m_1 - d_1)^2}{|m - d|} + \eta \frac{(m_2 + d_2)^2}{|m + d|} + \eta \frac{(d_1 - d_2)^2}{|d|} - 2|m| - \eta \frac{m_1^2 + m_2^2}{|m|}.$$

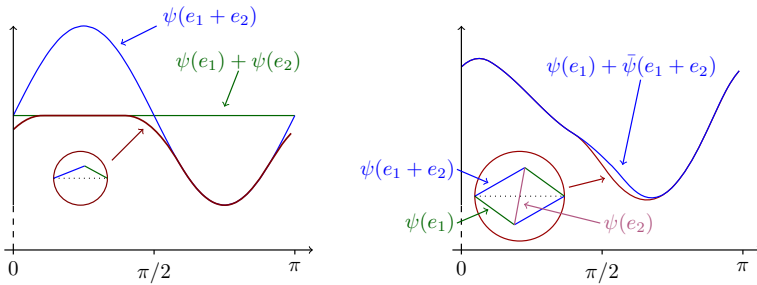


Fig. 5 *Left panel* $\bar{\psi}(e_1 + e_2, t)$ as given in Lemma 4.6 as a function of α , for $\eta = 1, t = (\cos \alpha, \sin \alpha)$. The two one-dimensional options $\psi(e_1, t) + \psi(e_2, t) = 2 + \eta$ and $\psi(e_1 + e_2, t) = 2 + \eta(1 + 2t_1 t_2)$ are optimal for different orientations. Close to the intersection a mixture of the two options is optimal, as sketched in the inset. *Right panel* corresponding plot for $\bar{\psi}(2e_1 + e_2, t)$ (different vertical scale). For most values of t the optimal energy is obtained using $\psi(e_1, t) + \bar{\psi}(e_1 + e_2, t)$. The latter is the convex, subadditive envelope of ψ , see discussion at the end of Sect. 4.3. However, there is a region in which a more complex structure develops (sketched in the inset), leading to a lower energy. The latter construction bears similarity to the examples given in [2,4]

Clearly $|m + d| + |m - d| \geq 2|m|$, $(d_1 - d_2)^2 \geq 0$ and $2|d| \geq 2\eta|d|$. Therefore it suffices to show that

$$\xi = 2|d| + \frac{(m_1 - d_1)^2}{|m - d|} + \frac{(m_2 + d_2)^2}{|m + d|} - |m| \geq 0$$

for all $m, d \in \mathbb{R}^2$. We set $m - d = r(\cos \theta, \sin \theta)$, $m + d = s(\cos \varphi, \sin \varphi)$, with $r, s \in (0, \infty)$, $\theta, \varphi \in \mathbb{R}$. From $2m = (m + d) + (m - d)$ we obtain $|m| \leq (r + s)/2$, and with $2d = (m + d) - (m - d)$ we have $\xi \geq \zeta$, where

$$\begin{aligned} \zeta &= \sqrt{r^2 + s^2 - 2rs \cos(\varphi - \theta)} + r \cos^2 \theta + s \sin^2 \varphi - \frac{1}{2}(r + s) \\ &= \sqrt{r^2 + s^2 - 2rs \cos(\varphi - \theta)} + \frac{1}{2}r \cos(2\theta) - \frac{1}{2}s \cos(2\varphi) \end{aligned}$$

since $\frac{1}{2} \cos 2\theta = \cos^2 \theta - \frac{1}{2} = \frac{1}{2} - \sin^2 \theta$. We change variables again, and write $2\theta = \gamma - \delta$, $2\varphi = \gamma + \delta$. Then

$$2\zeta = r \cos(\gamma - \delta) - s \cos(\gamma + \delta) + 2\sqrt{r^2 + s^2 - 2rs \cos \delta}.$$

With $\cos(\gamma - \delta) = \cos \gamma \cos \delta + \sin \gamma \sin \delta$ we obtain

$$2\zeta = (r - s) \cos \gamma \cos \delta + (r + s) \sin \gamma \sin \delta + 2\sqrt{r^2 + s^2 - 2rs \cos \delta}.$$

The first two terms are the scalar product of $(\cos \gamma, \sin \gamma)$ with another vector, which is bounded by the length of the vector. Therefore

$$\begin{aligned} 2\zeta &\geq 2\sqrt{r^2 + s^2 - 2rs \cos \delta} - \sqrt{(r - s)^2 \cos^2 \delta + (r + s)^2 \sin^2 \delta} \\ &= 2\sqrt{r^2 + s^2 - 2rs \cos \delta} - \sqrt{(r + s)^2 - 4rs \cos^2 \delta}. \end{aligned}$$

Squaring, the last expression is nonnegative iff

$$4r^2 + 4s^2 - 8rs \cos \delta \geq (r + s)^2 - 4rs \cos^2 \delta,$$

which in turn is equivalent to

$$3r^2 + 3s^2 - 2rs + 4rs(\cos^2 \delta - 2 \cos \delta) \geq 0,$$

which is true since $x^2 - 2x \geq -1$ and $r^2 + s^2 \geq 2rs$. □

In closing, we remark that the relaxation for other values of b is more complex and includes other microstructures. To see this, we define ψ^* by

$$\psi^*(b, t) = \min \left\{ \sum_{i=1}^N \bar{\psi}(z^i, t) : N \in \mathbb{N}, z^i \in \{-1, 0, 1\}^2, \sum_{i=1}^N z^i = b \right\}. \tag{4.7}$$

The values of $\bar{\psi}$ entering this expression are characterized in Lemmas 4.4 and 4.6. The function ψ^* is by definition subadditive in b , existence of the minimum follows from growth and continuity. We now show that a sequence $\{z^1, \dots, z^N\}$ which contains a pair (z, z') with $z_1 = -z'_1 = 1$ cannot be optimal. If $z + z' = 0$, it suffices to remove both of them. If $z + z' = \pm e_2$, replacing the pair by $\pm e_2$ reduces the energy, since $\bar{\psi}(e_2) \leq \bar{\psi}(e_1) + \bar{\psi}(e_1 \pm e_2)$. If $z + z' = \pm 2e_2$ then replacing the pair with $(\pm e_2, \pm e_2)$ reduces the energy, since $2\bar{\psi}(e_2) \leq \bar{\psi}(e_1 + e_2) + \bar{\psi}(e_1 - e_2)$. Therefore the sign of all z^i_1 is the same. Analogously for the z^i_2 , and one concludes that

$$\begin{aligned} \psi^*(b, t) = \min\{&|b_1|, |b_2|\} \bar{\psi}(e_1 + \text{sgn}(b_1 b_2) e_2, t) \\ &+ (|b_2| - |b_1|)_+ \psi(e_2, t) + (|b_1| - |b_2|)_+ \psi(e_1, t). \end{aligned}$$

This expression is clearly convex in t . Finally, we show that $\psi^* \leq \psi$. This is immediate if $|b| \leq \sqrt{2}$, and follows from quadratic growth of ψ for larger b . In particular, if $|b_1|$ and $|b_2|$ are not 1 then from $\psi(e_1, t) \leq 2$ we obtain $\psi^*(b, t) \leq 2|b_1| + 2|b_2| \leq b_1^2 + b_2^2 \leq \psi(b, t)$. If $|b_1| = 1$ and $|b_2| \geq 3$, a similar computation holds since $2|b_1| + 2|b_2| \leq 1 + 3|b_2| \leq |b|^2$. It remains to deal with the case $b = (1, 2)$ (up to signs and permutations). In this case, from $\eta|2t_1 t_2| \leq |t|^2 = 1$ we obtain

$$\psi^*((1, 2), t) \leq 3 + \eta(t_1^2 + 2t_2^2) \leq 5 + \eta(t_1^2 + 4t_2^2 + 4t_1 t_2) = \psi((1, 2), t).$$

Therefore $\psi^* \leq \psi$. We conclude that ψ^* is the convex subadditive envelope of ψ .

In Fig. 5 we investigate the case $b = (2, 1)$ in more detail. The lower bound (4.3) is (numerically) attained by a microstructure in which $\alpha = (1, 1)$, $\alpha = (1, 0)$ and $\alpha = (0, 1)$ play a role, and is smaller than ψ^* . Therefore in this case $\bar{\psi} < \psi^*$.

Acknowledgments We thank Giovanni Alberti and Camillo De Lellis for fruitful discussions and useful suggestions. This work was partially supported by the Deutsche Forschungsgemeinschaft through the Sonderforschungsbereich 1060 “The mathematics of emergent effects”, project A5.

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