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Infinite-order laminates in a model in crystal plasticity

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We consider a geometrically nonlinear model for crystal plasticity in two dimensions, with two active slip systems and rigid elasticity. We prove that the rank-1 convex envelope of the condensed energy density is obtained by infinite-order laminates, and express it explicitly via the ${}_2F_1$ hypergeometric function. We also determine the polyconvex envelope, leading to upper and lower bounds on the quasiconvex envelope. The two bounds differ by less than 2%.

1. Introduction

Plastic deformation of single crystals leads to the spontaneous formation of microstructures, which largely influence the macroscopic material response. Possible origins for microstructure are both the interplay of different slip systems and the interplay of one slip system with rotations. Recent progress in the analysis of plastic microstructure has been largely based on variational formulations, starting from the work by Ortiz and Repetto [32] (see also [8, 26]). This is admissible if one assumes monotonicity, leading to the so-called *deformation theory of plasticity*. After discretization in time, monotonicity typically follows for sufficiently short time intervals. After minimizing in the internal variables, one obtains a variational integral of the form

$$\int_\Omega W(\nabla u)\,\mathrm{d}x,$$

possibly complemented by additional external forces and boundary conditions. Here W contains both energetic and dissipative terms (see [8, 28, 32] for details).

The discrete nature of crystalline slip systems makes the energy density W nonconvex, which in turn leads to the spontaneous formation of microstructures. The

theory of relaxation shows that the macroscopic material behaviour can be studied by replacing W with its quasiconvex envelope, which is defined as the largest quasiconvex function not larger than W,

$$W^{\mathrm{qc}}(F) = \sup\{V(F) : V \text{ quasiconvex},\ V(G) \leqslant W(G) \text{ for all } G \in \mathbb{R}^{n\times n}\}. \quad (1.1)$$

We recall that a function $W : \mathbb{R}^{n\times n} \to \mathbb{R} \cup \{\infty\}$ is quasiconvex if

$$W(F) \leqslant \frac{1}{|\Omega|}\int_\Omega W(F + \nabla\varphi)\,\mathrm{d}x \quad \text{for all } \varphi \in W_0^{1,\infty}(\Omega;\mathbb{R}^n) \quad (1.2)$$

(whenever the integral exists) for all bounded, open, non-empty sets $\Omega \subset \mathbb{R}^n$ such that $|\partial\Omega| = 0$ [4, 13, 16, 19, 29, 30]. This definition corresponds to optimizing locally (i.e. at any material point) over all possible microstructures, which are here described by all possible Lipschitz continuous functions φ which vanish on the boundary. The definition is hard to verify, since it involves an inequality on an infinite-dimensional function space; therefore, in practice it is often replaced by either of the two concepts of rank-1 convexity or polyconvexity. A function $W : \mathbb{R}^{n\times n} \to \mathbb{R}\cup\{\infty\}$ is rank-1 convex if it is convex along rank-1 lines, in the sense that $t \mapsto W(F + ta\otimes b)$ is convex for all $a, b \in \mathbb{R}^n$. A function $W : \mathbb{R}^{n\times n} \to \mathbb{R}\cup\{\infty\}$ is polyconvex if it can be written as a convex function of its argument and its minors, i.e. for $n = 2$, if there is a convex function $g : \mathbb{R}^5 \to \mathbb{R} \cup \{\infty\}$ such that $W(F) = g(F, \det F)$.

In a geometrically linear setting, quasiconvexity often reduces to the much simpler concept of convexity. Assuming convex potentials, a very satisfactory general theory can be obtained using methods from convex analysis and the theory of functions of bounded deformation (see, for example, [34]). Similar simplifications hold in the case of microstructure formation; indeed, for a model of crystal plasticity without hardening the quasiconvex envelope, W^{qc} turns out to be convex [10]. The analysis in [10] involved a realistic number of slip systems (e.g. the result included the case of the 12 slip systems with face-centred cubic symmetry, appropriate for many metals) but used in a substantial way the linear treatment of rotations, as well as the convexity of the relaxed problem.

In a finite-deformation context, it is well known that convexity contrasts with invariance under rotations. Whereas abstract theory shows that quasiconvexity is the appropriate concept, in practice this turns out to be much more difficult to handle. Ortiz and Repetto have shown that energy densities describing a system with a single slip system in finite deformation lack quasiconvexity, and therefore lead to spontaneous microstructure formation in the form of laminates, a fact known as geometric softening [32]. A two-dimensional energy density with a single slip system with linear hardening and with a polyconvex elastic part was proposed and shown also to lack quasiconvexity in [8]. In [11] an explicit formula for the quasiconvex envelope of a simplification of that model, based on rigid elasticity and no self-hardening, was obtained. Work has also been devoted to numerical approximations; in particular, in [6] the model from [8] was studied numerically. An approximate numerical relaxation for the same model was obtained and integrated in a macroscopic finite-element computation in [27]. A finer analysis of the quasiconvex envelope of the same energy density is now under way; preliminary results are pre-

sented in [7]. In all these works, containing a proper treatment of rotations, only a single slip system was considered.

We study here for the first time the interplay among several slip systems within a geometrically nonlinear model formulation. Precisely, we focus on a model with two slip systems in two dimensions, with rigid elasticity and no self-hardening. Our model,

$$W(F) = \begin{cases} |\gamma| & \text{if } F = Q(\mathrm{Id} + \gamma e_1 \otimes e_2) \text{ for some } \gamma \in \mathbb{R}, \quad Q \in \mathrm{SO}(2), \\ |\gamma| & \text{if } F = Q(\mathrm{Id} + \gamma e_2 \otimes e_1) \text{ for some } \gamma \in \mathbb{R}, \quad Q \in \mathrm{SO}(2), \\ \infty & \text{otherwise}, \end{cases} \tag{1.3}$$

is a direct generalization to two slip systems of the model considered in [11]. We explicitly determine the rank-1 convex envelope and the polyconvex envelope of W. The envelopes are defined in analogy to (1.1) as the largest rank-1 convex (polyconvex) functions not larger than W.

THEOREM 1.1. *The rank-1 convex envelope W^{rc} of W defined in (1.3) is given by*

$$W^{\mathrm{rc}}(F) = \begin{cases} (\lambda_2 - \lambda_1)(F) & \textit{if } \det F = 1, \quad \min\{|Fe_1|, |Fe_2|\} \leqslant 1, \\ \psi(|Fe_1|, |Fe_2|) & \textit{if } \det F = 1, \quad 1 \leqslant |Fe_1| \leqslant |Fe_2|, \\ \psi(|Fe_2|, |Fe_1|) & \textit{if } \det F = 1, \quad 1 \leqslant |Fe_2| \leqslant |Fe_1|, \\ \infty & \textit{if } \det F \neq 1, \end{cases} \tag{1.4}$$

where

$$\psi(\alpha, \beta) = \int_1^\alpha \frac{2s^2}{\sqrt{s^4 - 1}}\, \mathrm{d}s + \frac{1}{\alpha}(\sqrt{\alpha^2\beta^2 - 1} - \sqrt{\alpha^4 - 1}). \tag{1.5}$$

Here $\lambda_1(F)$ and $\lambda_2(F)$ denote the signed singular values of F, i.e. the ordered eigenvalues of U in the polar decomposition $F = QU$, $Q \in \mathrm{SO}(2)$, $U = U^{\mathrm{T}}$, where U^{T} denotes the transposed matrix. They are identified uniquely by the conditions

$$\lambda_1^2(F) + \lambda_2^2(F) = |F|^2, \qquad \lambda_1(F)\lambda_2(F) = \det F, \qquad \lambda_2 \geqslant |\lambda_1|. \tag{1.6}$$

Theorem 1.1 is proven in § 2 (upper bound) and § 3 (lower bound).

REMARK 1.2. Using standard formulae for hypergeometric functions (see, for example, [1, ch. 15]), one finds the following representation of the integral above in terms of Gauss's hypergeometric function ${}_2F_1$:

$$\psi(\alpha, \alpha) = \int_1^\alpha \frac{2s^2}{\sqrt{s^4 - 1}}\, \mathrm{d}s = 2\alpha\, {}_2F_1(-\tfrac{1}{4}, \tfrac{1}{2}; \tfrac{3}{4}; \alpha^{-4}) - \frac{2\sqrt{\pi}\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}.$$

The hypergeometric function ${}_2F_1$ is defined through its power series via the rising factorial $(k)_n = k(k+1)(k+2)\cdots(k+n-1)$ as

$${}_2F_1(a, b; c; z) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!}.$$

We also determine the polyconvex envelope, as given by the following theorem, which is proved in § 5.

THEOREM 1.3. *The polyconvex envelope W^{pc} of W defined in (1.3) is given by*

$$W^{\mathrm{pc}}(F) = \max_{\theta\in[0,\pi/2]} \sqrt{|F|^2 + 2|Fe_1 \cdot Fe_2| \sin(2\theta) + 2\cos(2\theta)} - 2\cos\theta. \tag{1.7}$$

Furthermore, we show that these two bounds give a bound on the quasiconvex envelope, in the sense that

$$W^{\mathrm{rc}}(F) \leqslant W^{\mathrm{qc}}(F) \leqslant W^{\mathrm{pc}}(F) \quad \text{for all } F \in \mathbb{R}^{2\times 2}. \tag{1.8}$$

The two bounds differ, however, even if the difference is quantitatively rather small; the details are discussed in § 6.

The proof of theorem 1.1 is as usual based on the construction of an appropriate laminate which realizes the relaxed energy; physically, this laminate gives an indication for the expected microstructure. Almost all examples of quasiconvex envelopes use the construction of suitable finite-order laminates (see, for example, [15,22–25]). In this case, however, not only is the appropriate laminate partially supported at infinity (if one considers an appropriate completion of the domain, as is usual in problems with linear growth), but it cannot be a finite-order laminate. Precisely, no finite-order lamination convex envelope $W^{\mathrm{lc},n}$ agrees with the rank-1 convex envelope W^{rc} (see § 4 for a precise definition of the lamination convex envelope $W^{\mathrm{lc},n}$).

THEOREM 1.4. *Let F be such that $\det F = 1 < \min\{|Fe_1|, |Fe_2|\}$. Then*

$$W^{\mathrm{rc}}(F) < W^{\mathrm{lc},n}(F)$$

for all $n \in \mathbb{N}$. For all other F and all $n \geqslant 1$, one has $W^{\mathrm{rc}}(F) = W^{\mathrm{lc},n}(F)$.

Physically, this means that slip concentration (a feature already observed in a geometrically linear context in [10]) is necessary, and that structures on many different scales will coexist. Analytically, analogous *unbounded laminates* have been used in [17, 18] for constructing critical solutions to elliptic equations and in [12] to give a rank-1 convex function on diagonal matrices with locally unbounded Hessian, as well as to obtain a simple derivation of a classical counter-example to Korn's inequality in L^1 by Ornstein.

2. Upper bound on the rank-1 convex envelope

In this section we prove the upper bound of theorem 1.1. Precisely, we prove the following lemma.

LEMMA 2.1. *Let W^{rc} be the rank-1 convex envelope of W defined in (1.3), and let*

$$\Phi(F) = \begin{cases} (\lambda_2 - \lambda_1)(F) & \text{if } \det F = 1, \quad \min\{|Fe_1|, |Fe_2|\} \leqslant 1, \\ \psi(|Fe_1|, |Fe_2|) & \text{if } \det F = 1, \quad 1 \leqslant |Fe_1| \leqslant |Fe_2|, \\ \psi(|Fe_2|, |Fe_1|) & \text{if } \det F = 1, \quad 1 \leqslant |Fe_2| \leqslant |Fe_1|, \\ \infty & \text{if } \det F \neq 1, \end{cases} \tag{2.1}$$

where

$$\psi(\alpha, \beta) = \int_1^\alpha \frac{2s^2}{\sqrt{s^4 - 1}}\, \mathrm{d}s + \frac{1}{\alpha}(\sqrt{\alpha^2\beta^2 - 1} - \sqrt{\alpha^4 - 1}).$$

Then $W^{\mathrm{rc}}(F) \leqslant \Phi(F)$ for all $F \in \mathbb{R}^{2\times 2}$.

We first prove that W^{rc} is finite on the smooth manifold $\Sigma = \{F \in \mathbb{R}^{2\times 2} : \det F = 1\}$ of matrices with determinant 1.

LEMMA 2.2. *Let W be given by (1.3). Then*

$$W^{\mathrm{rc}}(F) \leqslant |Fe_1| + |Fe_2| + 1 \quad \textit{for all } F \in \Sigma.$$

Proof. We use an approximation by two-well problems. Let $\gamma \in \mathbb{R}$, and define

$$K_\gamma = \mathrm{SO}(2)A_\gamma \cup \mathrm{SO}(2)B_\gamma, \quad A_\gamma = \mathrm{Id} + \gamma e_1 \otimes e_2, \quad B_\gamma = \mathrm{Id} + \gamma e_2 \otimes e_1.$$

The set K_γ corresponds to the well-studied 'two-well problem', and its rank-1 convex hull K_γ^{rc} is explicitly known [3, 33]. In order to characterize K_γ^{rc} it suffices to choose a pair $v, w \in \mathbb{R}^2$ of linearly independent vectors such that $|A_\gamma v| = |B_\gamma v|$, $|A_\gamma w| = |B_\gamma w|$; in our case, $v = (1,1)$, $w = (1,-1)$. Then

$$K_\gamma^{\mathrm{rc}} = \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ |Fv| \leqslant |A_\gamma v|, \ |Fw| \leqslant |A_\gamma w|\}.$$

This implies that

$$W^{\mathrm{rc}}(F) \leqslant W(A_\gamma) = W(B_\gamma) = |\gamma| \quad \text{for all } F \in K_\gamma^{\mathrm{rc}}.$$

Now let $F \in \Sigma$. We assert that if $\gamma = |Fe_1| + |Fe_2| + 1$, then $F \in K_\gamma^{\mathrm{rc}}$. Indeed, we have

$$\begin{aligned} |Fw|^2 &= |Fe_1 - Fe_2|^2 \leqslant (|Fe_1| + |Fe_2|)^2 \\ &= (\gamma - 1)^2 \leqslant (\gamma - 1)^2 + 1 = |A_\gamma w|^2, \end{aligned}$$

and, similarly,

$$\begin{aligned} |Fv|^2 &= |Fe_1 + Fe_2|^2 \leqslant (|Fe_1| + |Fe_2|)^2 \\ &= (\gamma - 1)^2 \leqslant (\gamma + 1)^2 + 1 = |A_\gamma v|^2, \end{aligned}$$

which proves the assertion. □

The proof of lemma 2.1 is based on proving a bound on the derivative of W^{rc} along certain lines. We start by proving that W^{rc} is locally Lipschitz on Σ, and hence that it is differentiable almost everywhere. This is well known for finite-valued rank-1 convex functions [5, 13]; we now show how the argument can be generalized to the case when W^{rc} is finite only on Σ. The key observation is that separately convex (i.e. convex independently in each variable) functions are locally Lipschitz. We report here this result in the quantitative version proven by Ball *et al.* [5, lemma 2.2].

LEMMA 2.3 (Ball *et al.* [5, lemma 2.2]). *Let $\xi_0 \in \mathbb{R}^n$ and $r > 0$. If $f : B_{2r}(\xi_0) \to \mathbb{R}$ is separately convex, then*

$$\mathrm{Lip}(f; B_r(\xi_0)) \leqslant \frac{n}{r} \operatorname{osc}(f; B_{2r}(\xi_0)),$$

where, for any $S \subset \mathbb{R}^n$,

$$\operatorname{osc}(f; S) = \sup\{|f(\xi) - f(\eta)| : \xi, \eta \in S\}.$$

Using this result, we show that W^{rc} is locally Lipschitz on Σ. Exactly the same argument applies to any rank-1 convex function which is finite valued on Σ.

LEMMA 2.4. *Let W be given as in (1.3), and let $F_0 \in \Sigma$. Then there exist $c, r > 0$ such that, for all $F_1, F_2 \in B_r(F_0) \cap \Sigma$,*

$$|W^{\mathrm{rc}}(F_1) - W^{\mathrm{rc}}(F_2)| \leqslant c|F_1 - F_2|.$$

Proof. Define the map $g : \mathbb{R}^3 \to \Sigma$ by

$$g(x, y, z) = F_0(\mathrm{Id} + xR_1)(\mathrm{Id} + yR_2)(\mathrm{Id} + zR_3),$$

where

$$R_1 = e_1 \otimes e_2, \qquad R_2 = e_2 \otimes e_1, \qquad R_3 = (e_1 + e_2) \otimes (e_1 - e_2),$$

and the map $f : \mathbb{R}^3 \to \mathbb{R}$ by $f = W^{\mathrm{rc}} \circ g$ (f is finite valued by lemma 2.2). Note that, for $x_1, x_2, y, z \in \mathbb{R}$,

$$\mathrm{rank}(g(x_1, y, z) - g(x_2, y, z)) \leqslant 1$$

and similarly in the other two coordinate directions. Since W^{rc} is rank-1 convex, f is separately convex.

Also note that g is a diffeomorphism in a neighbourhood of the origin. Indeed, the partial derivatives in x, y and z are F_0R_1, F_0R_2 and F_0R_3, respectively, and span the tangent plane to Σ at F_0. Thus, by the implicit function theorem, there exists an $r > 0$ such that g is invertible in $B_r(F_0) \cap \Sigma$ and on this set, $W^{\mathrm{rc}} = f \circ g^{-1}$.

Since W is non-negative, it follows that W^{rc} is also non-negative. On the bounded set $S = g^{-1}(B_r(F_0) \cap \Sigma)$, this observation, together with the inequality given in lemma 2.2, implies that the oscillation $\mathrm{osc}(f; S)$ is bounded. Thus, by lemma 2.3, f is Lipschitz in a neighbourhood of the origin. Near F_0, $W^{\mathrm{rc}}|_{\Sigma}$ is the composition of two Lipschitz functions and is therefore Lipschitz. □

Proof of lemma 2.1. If $\det F \neq 1$, there is nothing to prove; hence, we can assume $\det F = 1$. If $|Fe_1| \leqslant 1$, the result follows from [11]; for the convenience of the reader we give here a short, self-contained proof. The key observation is that the function

$$G \mapsto (\lambda_2 - \lambda_1)(G) = \sqrt{|G|^2 - 2\det G}$$

has a particularly simple form on rank-1 lines originating from the identity, namely, if $a \in \mathbb{R}^2$, $|a| = 1$, then

$$(\lambda_2 - \lambda_1)(\mathrm{Id} + ta^{\perp} \otimes a) = |t|$$

(henceforth, $a^{\perp} = (-a_2, a_1)$). Furthermore, for all matrices $G_\gamma = \mathrm{Id} + \gamma e_2 \otimes e_1$ we immediately obtain $(\lambda_2 - \lambda_1)(G_\gamma) = |\gamma| = W(G_\gamma)$. These two observations imply the assertion for all matrices of the form $F_t = Q(\mathrm{Id} + ta \otimes a^{\perp})$ with $Q \in \mathrm{SO}(2)$ and $|F_te_1| \leqslant 1$. It remains to show that any matrix F with $\det F = 1$ and $|Fe_1| \leqslant 1$ can be written in this form. In order to do so, fix $F \in \Sigma$ and let $a \in \mathbb{R}^2$ be such that $|a| = |Fa| = 1$. Such an a exists, since $\det F = 1$ and $|Fe_1| \leqslant 1$, implying $|Fe_2| \geqslant 1$. Let $Q \in \mathrm{SO}(2)$ be such that $Q^{\mathrm{T}}Fa = a$. Let $c_{1,2} \in \mathbb{R}$ be defined by $Q^{\mathrm{T}}Fa^{\perp} = c_1a + c_2a^{\perp}$. Since $1 = \det F = Q^{\mathrm{T}}Fa \wedge Q^{\mathrm{T}}Fa^{\perp}$, we have $c_2 = 1$ (we

identify $v \wedge w$ with the scalar $(v \wedge w) \cdot (e_1 \wedge e_2) = v_1 w_2 - v_2 w_1$, for any $v, w \in \mathbb{R}^2$). Hence, $Q^{\mathrm{T}} F = \mathrm{Id} + c_1 a \otimes a^{\perp}$, which proves the assertion with $t = c_1$. The case $|Fe_2| \leqslant 1$ is analogous.

Now we turn to the case of matrices in the set

$$\Sigma^+ = \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ |Fe_1| > 1, \ |Fe_2| > 1\}.$$

We first prove the following fact, which provides the basic step of our construction. Consider the rank-1 line along the coordinate axis $|Fe_1| = \text{const.}$ given by

$$F_t = F(\mathrm{Id} + te_1 \otimes e_2). \tag{2.2}$$

We assert that

$$W^{\mathrm{rc}}(F_t) \leqslant W^{\mathrm{rc}}(F) + |t||Fe_1| \quad \text{for all } t \in \mathbb{R} \tag{2.3}$$

and that the same statement holds after interchanging the indices. To prove (2.3) we remark that $F_t e_1 = Fe_1$ and $F_t e_2 = Fe_2 + tFe_1$, which implies that

$$|F_t e_2|^2 = |Fe_2|^2 + 2tFe_1 \cdot Fe_2 + t^2 |Fe_1|^2. \tag{2.4}$$

For $t \in \mathbb{R}$ and $k \in \mathbb{N} \setminus \{0\}$, the fact that W^{rc} is rank-1 convex implies that

$$W^{\mathrm{rc}}(F_t) \leqslant \frac{k-1}{k} W^{\mathrm{rc}}(F) + \frac{1}{k} W^{\mathrm{rc}}(F_{kt}). \tag{2.5}$$

In the limit as $k \to \infty$, $|F_{kt} e_1|/k = |Fe_1|/k \to 0$ and (2.4) shows that $|F_{kt} e_2|/k \to |t||Fe_1|$. Thus, by lemma 2.2, we have

$$\limsup_{k\to\infty} \frac{W^{\mathrm{rc}}(F_{kt})}{k} \leqslant \lim_{k\to\infty} \frac{|F_{kt} e_1| + |F_{kt} e_2| + 1}{k} = |t||Fe_1|.$$

Taking $k \to \infty$ in (2.5) proves (2.3). The analogous inequality follows when the roles of e_1 and e_2 are reversed.

We apply this assertion once in each of the two directions $|Fe_i| = \text{const.}$ to a matrix of the form

$$G(F, s, t) = F(\mathrm{Id} + te_1 \otimes e_2)(\mathrm{Id} + se_2 \otimes e_1) \tag{2.6}$$

and obtain in view of

$$|F(\mathrm{Id} + te_1 \otimes e_2)e_2| = |Fe_2 + tFe_1| = \sqrt{|Fe_2|^2 + 2tFe_1 \cdot Fe_2 + t^2|Fe_1|^2}$$

that

$$W^{\mathrm{rc}}(G(F, s, t)) \leqslant W^{\mathrm{rc}}(F) + |t||Fe_1| + |s|\sqrt{|Fe_2|^2 + 2tFe_1 \cdot Fe_2 + t^2|Fe_1|^2}. \tag{2.7}$$

We use this estimate to show $W^{\mathrm{rc}} \leqslant \Phi$.

Case 1 (the columns of F have equal length). Let $F \in \Sigma$ with $|Fe_1| = |Fe_2| = \alpha > 1$. Fix $\varepsilon > 0$ and define $F_\varepsilon = G(F, s(\varepsilon), t(\varepsilon))$, where $s(\varepsilon)$ and $t(\varepsilon)$ are real numbers chosen so that

$$|F_\varepsilon e_1| = |F_\varepsilon e_2| = \alpha + \varepsilon.$$

That is, we choose t and s to solve

$$(1+st)^2\alpha^2 + 2s(1+st)Fe_1 \cdot Fe_2 + s^2\alpha^2 = (\alpha+\varepsilon)^2,$$
$$\alpha^2 + 2tFe_1 \cdot Fe_2 + t^2\alpha^2 = (\alpha+\varepsilon)^2.$$

Without loss of generality, we may assume that $Fe_1 \cdot Fe_2 \geqslant 0$ (otherwise take t and s negative in what follows). Then we take $t = t(\varepsilon)$ and $s = s(\varepsilon)$ as the positive roots of the polynomials above. By differentiating in ε, it follows that

$$t(\varepsilon) = \frac{\alpha}{\sqrt{\alpha^4-1}}\varepsilon + o(\varepsilon), \qquad s(\varepsilon) = \frac{\alpha}{\sqrt{\alpha^4-1}}\varepsilon + o(\varepsilon).$$

Then, by (2.7),

$$\begin{aligned} W^{\mathrm{rc}}(F_\varepsilon) &\leqslant W^{\mathrm{rc}}(F) + |t(\varepsilon)||Fe_1| + |s(\varepsilon)||Fe_2| + o(\varepsilon) \\ &= W^{\mathrm{rc}}(F) + \frac{2\alpha^2}{\sqrt{\alpha^4-1}}\varepsilon + o(\varepsilon). \end{aligned}$$

Taking ε to zero, we see that

$$\limsup_{\varepsilon\to 0^+} \frac{W^{\mathrm{rc}}(F_\varepsilon) - W^{\mathrm{rc}}(F)}{\varepsilon} \leqslant \frac{2\alpha^2}{\sqrt{\alpha^4-1}}. \tag{2.8}$$

It is now convenient to interpret the values of W^{rc} as a function of $\alpha = |Fe_1| = |Fe_2|$. We consider the case $Fe_1 \cdot Fe_2 \geqslant 0$; the remaining case is analogous. For $\alpha \geqslant 1$ we define

$$H(\alpha) = \begin{pmatrix} \sqrt{(\alpha^2+1)/2} & \sqrt{(\alpha^2-1)/2} \\ \sqrt{(\alpha^2-1)/2} & \sqrt{(\alpha^2+1)/2} \end{pmatrix}.$$

(In the case $Fe_1 \cdot Fe_2 \leqslant 0$, the off-diagonal elements are defined to be negative.) We define the function $f : [1,\infty) \to \mathbb{R}$ by $f(\alpha) = W^{\mathrm{rc}}(H(\alpha))$. We first show that $W^{\mathrm{rc}}(F) = f(|Fe_1|)$ for all $F \in \Sigma$ such that $|Fe_1| = |Fe_2|$ and $Fe_1 \cdot Fe_2 \geqslant 0$. To see this, it suffices to observe that, by polar decomposition, there exists a rotation $Q \in \mathrm{SO}(2)$ with $F = QH$. Since the two columns have equal length α, and since their scalar product is positive, H must coincide with $H(\alpha)$. By the rotational invariance of W, which implies the same invariance for W^{rc}, we obtain $W^{\mathrm{rc}}(F) = W^{\mathrm{rc}}(H) = f(\alpha)$.

It remains to determine the function f. By the definition of H and by lemma 2.4, f is locally Lipschitz on $(1,\infty)$ and is therefore almost everywhere differentiable. Note that $Fe_1 \cdot Fe_2 = He_1 \cdot He_2 = \sqrt{\alpha^4-1} > 0$, so, for sufficiently small $\varepsilon > 0$, the matrix F_ε in (2.8) satisfies $F_\varepsilon e_1 \cdot F_\varepsilon e_2 \geqslant 0$ and therefore $W^{\mathrm{rc}}(F_\varepsilon) = f(|F_\varepsilon e_1|) = f(\alpha+\varepsilon)$. Thus, (2.8) implies that

$$f'(\alpha) \leqslant \frac{2\alpha^2}{\sqrt{\alpha^4-1}} \quad \text{a.e. } \alpha \in (1,\infty).$$

Let $1 < \alpha_0 < \alpha$. By the fundamental theorem of calculus, we have

$$f(\alpha) = f(\alpha_0) + \int_{\alpha_0}^{\alpha} f'(\zeta)\,\mathrm{d}\zeta \leqslant f(\alpha_0) + \int_{\alpha_0}^{\alpha} \frac{2\zeta^2}{\sqrt{\zeta^4-1}}\,\mathrm{d}\zeta.$$

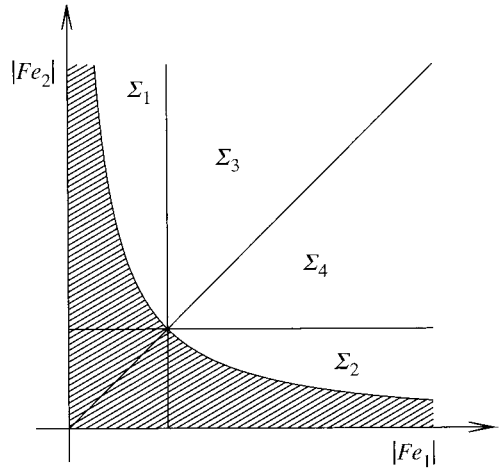

Figure 1. Decomposition of the domain in the proof of lemma 3.1.

But f is continuous on $[1,\infty)$ with $f(1) = W^{\mathrm{rc}}(\mathrm{Id}) = W(\mathrm{Id}) = 0$. Moreover, the integral on the right-hand side converges as $\alpha_0 \to 1$. Taking the limit $\alpha_0 \to 1$ in the foregoing inequality proves $W^{\mathrm{rc}} \leqslant \Phi$ for $F \in \Sigma^+ \cap \{F \in \mathbb{R}^{2\times 2} : |Fe_1| = |Fe_2|\}$.

CASE 2 (the columns of F have different length). Without loss of generality, we may assume that $1 < |Fe_1| = \alpha < \beta = |Fe_2|$. We estimate $W^{\mathrm{rc}}(F)$ by a lamination in the direction $e_1 \otimes e_2$ supported on one matrix with columns of equal length and the other at infinity, in the sense of (2.5). Define F_t as in (2.2). Then $|F_t e_1| = \alpha$ for all t and

$$|F_t e_2| = \sqrt{\beta^2 + 2tFe_1 \cdot Fe_2 + t^2\alpha^2}.$$

We choose t so that this quantity equals α. Again, we may assume that $Fe_1 \cdot Fe_2 \geqslant 0$ since otherwise we can change the sign of t. Thus, we choose

$$t = -\frac{1}{\alpha^2}(\sqrt{\alpha^2\beta^2 - 1} - \sqrt{\alpha^4 - 1}).$$

Applying (2.3) once again, we see that

$$W^{\mathrm{rc}}(F) \leqslant W^{\mathrm{rc}}(F_t) + |t||F_t e_2| \leqslant \psi(\alpha,\alpha) + |t|\alpha,$$

which implies that $W^{\mathrm{rc}}(F) \leqslant \psi(\alpha,\beta) = \Phi(F)$. □

3. Lower bound on the rank-1 convex envelope

In this section, we prove that the upper bound for W^{rc} derived in the previous section is actually rank-1 convex and is therefore a lower bound. This implies the desired characterization of W^{rc}.

LEMMA 3.1. *The function Φ given by (2.1) is rank-1 convex.*

Proof. We consider for fixed $F \in \mathbb{R}^{2\times 2}$ and $a, b \in \mathbb{R}^2$ the function

$$\phi(t) = \Phi(F_t), \qquad F_t = F + tFa \otimes b.$$

It suffices to show that for any F, a, b the function ϕ is convex in a neighbourhood of 0. Since

$$\det(F_t) = \det F(1 + ta \cdot b),$$

and Φ is finite only on Σ, we see that ϕ is either finite for all t or finite for at most one value of t. Thus, we may restrict our attention to the case where $\det F = 1$ and $b = a^{\perp}$.

We first consider separately the cases

$$\begin{aligned}
F \in \Sigma_1 &= \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ |Fe_1| < 1 < |Fe_2|\},\\
F \in \Sigma_2 &= \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ |Fe_2| < 1 < |Fe_1|\},\\
F \in \Sigma_3 &= \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ 1 < |Fe_1| < |Fe_2|\},\\
F \in \Sigma_4 &= \{F \in \mathbb{R}^{2\times 2} : \ \det F = 1, \ 1 < |Fe_2| < |Fe_1|\}
\end{aligned}$$

(see figure 1). Once we have done this, it will remain only to check smoothness across the shared boundaries of these sets. Suppose first that $F \in \Sigma_1 \cup \Sigma_2$. Then the same is true for F_t with t in a neighbourhood of 0. Since Φ coincides on this domain with the convex function

$$(\lambda_2 - \lambda_1)(F) = \sqrt{|F|^2 - 2\det F} = \sqrt{(F_{11} - F_{22})^2 + (F_{12} + F_{21})^2}, \tag{3.1}$$

we conclude that ϕ is convex on this set.

Consider next $F \in \Sigma_3$, $\theta \in \mathbb{R}$, $a = (\cos\theta, \sin\theta)$, $b = a^{\perp} = (-\sin\theta, \cos\theta)$. We shall show that, for any such matrix, ϕ is twice differentiable at the origin and $\phi''(t)|_{t=0} \geqslant 0$. If this holds for all $F \in \Sigma_3$, then ϕ necessarily has a non-negative second derivative in a neighbourhood of the origin and therefore it is convex in a neighbourhood of the origin.

To prove the assertion it is useful to introduce the variables

$$\xi(t) = |F_t e_1|^2, \qquad \eta(t) = |F_t e_2|^2.$$

Starting from $\phi(t) = \psi(\xi^{1/2}(t), \eta^{1/2}(t))$, we compute

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{\partial\psi}{\partial\alpha}\frac{1}{2\xi^{1/2}}\frac{\mathrm{d}\xi}{\mathrm{d}t} + \frac{\partial\psi}{\partial\beta}\frac{1}{2\eta^{1/2}}\frac{\mathrm{d}\eta}{\mathrm{d}t},$$

with $\nabla\psi$ evaluated at $\alpha = \xi^{1/2}(t)$, $\beta = \eta^{1/2}(t)$. Differentiating a second time, and rearranging terms,

$$\begin{aligned}
\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2} = {} & \left(\frac{1}{4\alpha^2}\frac{\partial^2\psi}{\partial\alpha^2} - \frac{1}{4\alpha^3}\frac{\partial\psi}{\partial\alpha}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}t}\right)^2 + \left(\frac{1}{4\beta^2}\frac{\partial^2\psi}{\partial\beta^2} - \frac{1}{4\beta^3}\frac{\partial\psi}{\partial\beta}\right)\left(\frac{\mathrm{d}\eta}{\mathrm{d}t}\right)^2\\
& + \left(\frac{1}{2\alpha\beta}\frac{\partial^2\psi}{\partial\alpha\partial\beta}\right)\left(\frac{\mathrm{d}\xi}{\mathrm{d}t}\frac{\mathrm{d}\eta}{\mathrm{d}t}\right) + \left(\frac{1}{2\alpha}\frac{\partial\psi}{\partial\alpha}\right)\left(\frac{\mathrm{d}^2\xi}{\mathrm{d}t^2}\right) + \left(\frac{1}{2\beta}\frac{\partial\psi}{\partial\beta}\right)\left(\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2}\right).
\end{aligned}$$

Again, derivatives of ψ are evaluated at $\alpha = \xi^{1/2}(t)$, $\beta = \eta^{1/2}(t)$.

From the definition of ξ we obtain

$$\left.\frac{\mathrm{d}\xi}{\mathrm{d}t}\right|_{t=0} = 2(Fe_1 \cdot Fa)(a^\perp \cdot e_1) = -2|Fe_1|^2 \cos\theta \sin\theta - 2(Fe_1 \cdot Fe_2)\sin^2\theta,$$

$$\begin{aligned}\left.\frac{\mathrm{d}^2\xi}{\mathrm{d}t^2}\right|_{t=0} &= 2|Fa|^2(a^\perp \cdot e_1)^2 \\ &= 2|Fe_1|^2\cos^2\theta\sin^2\theta + 4(Fe_1 \cdot Fe_2)\cos\theta\sin^3\theta + 2|Fe_2|^2\sin^4\theta.\end{aligned}$$

Analogously,

$$\left.\frac{\mathrm{d}\eta}{\mathrm{d}t}\right|_{t=0} = 2|Fe_2|^2\cos\theta\sin\theta + 2(Fe_1 \cdot Fe_2)\cos^2\theta,$$

$$\left.\frac{\mathrm{d}^2\eta}{\mathrm{d}t^2}\right|_{t=0} = 2|Fe_1|^2\cos^4\theta + 4(Fe_1 \cdot Fe_2)\cos^3\theta\sin\theta + 2|Fe_2|^2\cos^2\theta\sin^2\theta.$$

From (1.5) we compute

$$\frac{\partial\psi}{\partial\alpha} = \delta + \frac{1}{\alpha^2\gamma}, \qquad \frac{\partial\psi}{\partial\beta} = \frac{\alpha\beta}{\gamma}, \tag{3.2}$$

where $\gamma = (\alpha^2\beta^2 - 1)^{1/2}$ and $\delta = (1 - \alpha^{-4})^{1/2}$. Differentiating once again,

$$\frac{\partial^2\psi}{\partial\alpha^2} = \frac{2}{\alpha^5\delta} - \frac{3\alpha^2\beta^2 - 2}{\alpha^3\gamma^3}, \qquad \frac{\partial^2\psi}{\partial\beta^2} = -\frac{\alpha}{\gamma^3}, \qquad \frac{\partial^2\psi}{\partial\alpha\partial\beta} = -\frac{\beta}{\gamma^3}.$$

At this point we have all the ingredients with which to evaluate $\mathrm{d}^2\phi/\mathrm{d}t^2|_{t=0}$. By the above expressions it is clear that it is a homogeneous polynomial of fourth order in $\cos\theta$ and $\sin\theta$; therefore, one only has to evaluate the five coefficients. The coefficients can be expressed in terms of $|Fe_1| = \alpha$, $|Fe_2| = \beta$, $Fe_1 \cdot Fe_2 = \gamma$ and $(1 - \alpha^{-4})^{1/2} = \delta$. A direct computation that uses $\gamma^2 = \alpha^2\beta^2 - 1$ shows that

$$\left.\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2}\right|_{t=0} = \frac{\sin^2\theta}{|Fe_1|^5\sqrt{|Fe_1|^4 - 1}}(c_1\cos^2\theta + c_2\cos\theta\sin\theta + c_3\sin^2\theta), \tag{3.3}$$

where

$$\begin{aligned}c_1 &= 2|Fe_1|^4, \\ c_2 &= 4|Fe_1|^2(\sqrt{|Fe_1|^2|Fe_2|^2 - 1} - \sqrt{|Fe_1|^4 - 1}), \\ c_3 &= (\sqrt{|Fe_1|^2|Fe_2|^2 - 1} - \sqrt{|Fe_1|^4 - 1})(2\sqrt{|Fe_1|^2|Fe_2|^2 - 1} - \sqrt{|Fe_1|^4 - 1}).\end{aligned}$$

Rearranging terms and minimizing the parenthesis over θ we obtain

$$\begin{aligned}\left.\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2}\right|_{t=0} &= \frac{\sin^2\theta}{2|Fe_1|^5\sqrt{|Fe_1|^4 - 1}}((c_1 - c_3)\cos 2\theta + c_2\sin 2\theta + c_1 + c_3) \\ &\geqslant \frac{\sin^2\theta}{2|Fe_1|^5\sqrt{|Fe_1|^4 - 1}}\left(c_1 + c_3 - \sqrt{c_2^2 + (c_1 - c_3)^2}\right) \\ &= \frac{\sin^2\theta}{2|Fe_1|^5\sqrt{|Fe_1|^4 - 1}}\left(c_1 + c_3 - \sqrt{(c_1 + c_3)^2 - (4c_1c_3 - c_2^2)}\right).\end{aligned}$$

Since $|Fe_2| > |Fe_1|$, each $c_i > 0$. Moreover,

$$4c_1c_3 - c_2^2 = 8|Fe_1|^4\sqrt{|Fe_1|^4 - 1}(\sqrt{|Fe_1|^2|Fe_2|^2 - 1} - \sqrt{|Fe_1|^4 - 1}) > 0,$$

so $\phi''(t)|_{t=0} \geqslant 0$ and we have proved that Φ is locally rank-1 convex in Σ_3. The case $F \in \Sigma_4$ is analogous and follows by interchanging indices. For later reference we observe that all inequalities are strict, unless $\sin\theta = 0$, i.e. $F_t = F(\mathrm{Id} + te_1 \otimes e_2)$, and in particular that

$$\text{if } F \in \Sigma_3 \text{ and } \sin\theta \neq 0, \text{ then } \left.\frac{\mathrm{d}^2\phi}{\mathrm{d}t^2}\right|_{t=0} > 0. \tag{3.4}$$

To finish the proof that Φ is rank-1 convex, we need to check the following remaining cases on Σ corresponding to the intersection of the boundaries of different domains:

$$F \in (\partial\Sigma_1 \cap \partial\Sigma_3) \cup (\partial\Sigma_3 \cap \partial\Sigma_4) \cup (\partial\Sigma_4 \cap \partial\Sigma_2)$$

(see figure 1). In fact, we will show that Φ is C^1 in the set

$$\{F \in \mathbb{R}^{2\times 2} : \det F = 1,\ F \notin \mathrm{SO}(2)\}.$$

A final calculation for $F = \mathrm{Id}$ completes the proof.

To check the smoothness, it is convenient to use, as before, the variables $\alpha = |Fe_1|$, $\beta = |Fe_2|$. First consider the intersection $(\partial\Sigma_1 \cap \partial\Sigma_3) \setminus \mathrm{SO}(2)$. By construction, Φ is continuous on Σ. Moreover, the normal derivative to the boundary in Σ_1 is

$$\left.\frac{\partial}{\partial\alpha}\sqrt{\alpha^2 + \beta^2 - 2}\right|_{\alpha=1} = \frac{1}{\sqrt{\beta^2 - 1}},$$

while in Σ_3, recalling (3.2), the normal derivative is

$$\left.\frac{\partial}{\partial\alpha}\psi(\alpha,\beta)\right|_{\alpha=1} = \left.\frac{1}{\alpha^2}\left(\frac{1}{\sqrt{\alpha^2\beta^2 - 1}} + \sqrt{\alpha^4 - 1}\right)\right|_{\alpha=1} = \frac{1}{\sqrt{\beta^2 - 1}}.$$

A similar computation shows smoothness at the intersection $(\partial\Sigma_2 \cap \partial\Sigma_4) \setminus \mathrm{SO}(2)$. The smoothness across $(\partial\Sigma_3 \cap \partial\Sigma_4) \setminus \mathrm{SO}(2)$ follows again from (3.2) since

$$\left.\frac{\partial}{\partial\alpha}\psi(\alpha,\beta)\right|_{\alpha=\beta} = \frac{\alpha^2}{\sqrt{\alpha^4 - 1}} = \left.\frac{\partial}{\partial\beta}\psi(\alpha,\beta)\right|_{\alpha=\beta}.$$

Finally, we need to check rank-1 convexity in the case $F \in \mathrm{SO}(2)$, so $F_t = R(\mathrm{Id} + ta \otimes a^\perp)$ for some $R \in \mathrm{SO}(2)$. Then for $i = 1, 2$,

$$|F_te_i|^2 = |e_i + t(a^\perp \cdot e_i)a|^2 = 1 + 2t(a^\perp \cdot e_i)(a \cdot e_i) + t^2(a^\perp \cdot e_i)^2.$$

Since the coefficient of the linear term $(a^\perp \cdot e_i)(a \cdot e_i)$ is the product of two factors with opposite signs for $i = 1, 2$, it follows that for t sufficiently small $\min\{|F_te_1|, |F_te_2|\} \leqslant 1$, and hence $F_t \in \overline{\Sigma_1 \cup \Sigma_2}$. Hence, $\phi(t) = \Phi(F_t)$ is defined through the convex function in (3.1) and thus is convex on this interval. □

Proof of theorem 1.1. Lemma 2.1 proves that $W^{\mathrm{rc}} \leqslant \Phi$. To prove the converse inequality, we observe that by lemma 3.1 Φ is rank-1 convex, and by construction $\Phi \leqslant W$; hence, $\Phi \leqslant W^{\mathrm{rc}}$. This concludes the proof. □

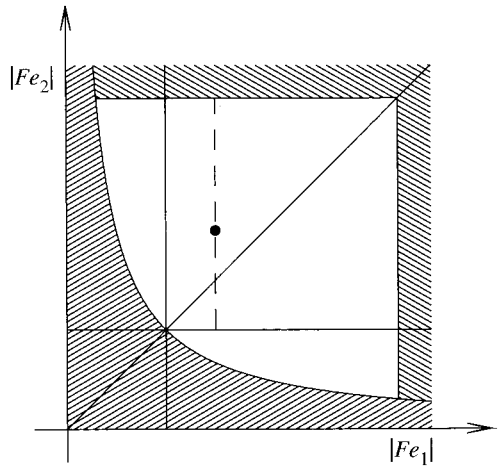

Figure 2. Restriction to a compact domain as in (4.2). The dashed line represents the vertical rank-1 line in the proof of lemma 4.2.

4. Infinite-order laminates

Given a function $V : \mathbb{R}^{2\times 2} \to [0,\infty]$, its nth lamination convex envelope $V^{\mathrm{lc},n}$ is defined inductively by $V^{\mathrm{lc},0} = V$, and

$$V^{\mathrm{lc},n+1}(F) = \inf\{\lambda V^{\mathrm{lc},n}(F_1) + (1-\lambda)V^{\mathrm{lc},n}(F_2) : \\ \lambda \in [0,1],\ \operatorname{rank}(F_1 - F_2) \leqslant 1,\ \lambda F_1 + (1-\lambda)F_2 = F\}. \quad (4.1)$$

The lamination envelopes are often used as approximations to the rank-1 convex envelope (and, as a consequence, of the quasiconvex one); in many cases it turns out that a lamination envelope of relatively low order coincides with the rank-1 and quasiconvex envelopes. We show that this is not the case here, and that no finite-order lamination-convex envelope coincides with the rank-1 convex envelope, in the sense that

$$W^{\mathrm{rc}}(F) < W^{\mathrm{lc},n}(F)$$

for all matrices F with $\det F = 1 < \min\{|Fe_1|, |Fe_2|\}$ (see theorem 1.4). The key difficulty in the proof is that the set over which the infimum in (4.1) is taken is unbounded, and the construction of § 2 shows that exactly those pairs (F_1, F_2) are relevant, for which one component diverges to infinity. We restrict our attention to a compact set by introducing a cut-off M, which will then be chosen large enough. Given $M > 1$ we define

$$V_M(F) = \begin{cases} W(F) & \text{if } \det F = 1,\ \max\{|Fe_1|, |Fe_2|\} < M, \\ W^{\mathrm{rc}}(F) & \text{if } \det F = 1,\ \max\{|Fe_1|, |Fe_2|\} = M, \\ \infty & \text{otherwise} \end{cases} \quad (4.2)$$

(see figure 2). We observe that V_M is finite only on a compact set, and that it is lower semicontinuous. We first show that these properties are stable under the passage to the lamination envelopes.

LEMMA 4.1. *Let $\Psi : \mathbb{R}^{2\times 2} \to [0,\infty]$ be lower semicontinuous and such that $K_\Psi = \Psi^{-1}([0,\infty[)$ is compact. Then all its lamination convex envelopes $\Psi^{\mathrm{lc},n}$ have the same property, i.e. $K_n = (\Psi^{\mathrm{lc},n})^{-1}([0,\infty[)$ is compact and $\Psi^{\mathrm{lc},n}$ is lower semicontinuous for all n. Furthermore, all infima in the definition of the lamination convex envelopes $\Psi^{\mathrm{lc},n}$ are minima.*

Proof. It clearly suffices to prove the assertion for $n = 1$, and then proceed by induction. Let $\Phi = \Psi^{\mathrm{lc},1}$. By definition,

$$\Phi(F) = \inf\{\lambda\Psi(F_1) + (1-\lambda)\Psi(F_2) : \\ \lambda \in [0,1],\ \operatorname{rank}(F_1 - F_2) \leqslant 1,\ \lambda F_1 + (1-\lambda)F_2 = F\}.$$

There is nothing to show if $\Phi(F) = \infty$. Assume thus that $\Phi(F) < \infty$, i.e. $F \in K_1 = K_\Phi$. Then we can assume $F_{1,2} \in K_\Psi$ in the infimum above. By compactness of $[0,1] \times K_\Psi \times K_\Psi$, and lower semicontinuity, the infimum is actually a minimum.

We now show that if $F^i \to F$, and $F^i \in K_\Phi$, then

$$F \in K_\Phi \quad \text{and} \quad \Phi(F) \leqslant \liminf_{i\to\infty} \Phi(F^i).$$

This will imply that K_Φ is closed and that Φ is lower semicontinuous on it. Let F^i be a sequence with the foregoing properties and let $F^i_{1,2}$, λ^i be such that

$$\Phi(F^i) = \lambda^i\Psi(F^i_1) + (1-\lambda^i)\Psi(F^i_2) \tag{4.3}$$

and

$$\lambda^i \in [0,1], \quad \operatorname{rank}(F^i_1 - F^i_2) \leqslant 1, \quad \lambda^i F^i_1 + (1-\lambda^i)F^i_2 = F^i. \tag{4.4}$$

By compactness we can, after extracting a subsequence, assume that $F^i_1 \to F_1 \in K_\Psi$, $F^i_2 \to F_2 \in K_\Psi$, $\lambda^i \to \lambda \in [0,1]$; all conditions in (4.4) automatically hold for the limit. In particular, $\Phi(F) \leqslant \lambda\Psi(F_1) + (1-\lambda)\Psi(F_2) < \infty$ and $F \in K_\Phi$. Passing to the limit in (4.3) we obtain $\Phi(F) \leqslant \liminf \Phi(F^i)$. This proves the assertion.

Finally, observe that if $F \in K_\Phi$ and F_1, F_2 are as above, then

$$|F| \leqslant \max\{|F_1|, |F_2|\};$$

hence, K_Φ is bounded and compact. □

LEMMA 4.2. *Let $M > 1$, V_M as in (4.2). Then for all $n \in \mathbb{N}$ and all $F \in \Sigma$ such that $1 < |Fe_1|, |Fe_2| < M$ one has*

$$W^{\mathrm{rc}}(F) < V^{\mathrm{lc},n}_M(F).$$

Proof. For simplicity we write V for V_M in this proof. Since $W^{\mathrm{rc}} \leqslant V$ and W^{rc} is rank-1 convex, it is clear that $W^{\mathrm{rc}} \leqslant V^{\mathrm{rc}} \leqslant V^{\mathrm{lc},n}$ everywhere.

To prove that the inequality is strict, we proceed by contradiction. Let n be the smallest number such that there is an F satisfying the assumptions in the lemma with $W^{\mathrm{rc}}(F) = V^{\mathrm{lc},n}(F)$, and assume without loss of generality that $|Fe_1| \leqslant |Fe_2|$ (i.e. $F \in \bar{\Sigma}_3$ in the notation of § 3). Since $V^{\mathrm{lc},0}(F) = V(F) = \infty$, obviously $n > 0$. Then $V^{\mathrm{lc},n}$ is defined by (4.1). By lemma 4.1 the infimum is actually a minimum. Let F_1, F_2, λ be such that

$$V^{\mathrm{lc},n}(F) = \lambda V^{\mathrm{lc},n-1}(F_1) + (1-\lambda)V^{\mathrm{lc},n-1}(F_2)$$

with $\lambda \in [0,1]$, $\operatorname{rank}(F_1 - F_2) = 1$, $\lambda F_1 + (1-\lambda)F_2 = F$. By minimality of n, it follows that $\lambda \in (0,1)$. Since $W^{\mathrm{rc}}(F)$ is rank-1 convex, we obtain

$$\begin{aligned} V^{\mathrm{lc},n}(F) &= W^{\mathrm{rc}}(F) \\ &\leqslant \lambda W^{\mathrm{rc}}(F_1) + (1-\lambda)W^{\mathrm{rc}}(F_2) \\ &\leqslant \lambda V^{\mathrm{lc},n-1}(F_1) + (1-\lambda)V^{\mathrm{lc},n-1}(F_2) \\ &= V^{\mathrm{lc},n}(F). \end{aligned}$$

Therefore, all inequalities must be equalities. By (3.4) the first inequality can be an equality only if $\sin\theta = 0$ in the rank-1 direction, i.e. if $|F_1 e_1| = |Fe_1| = |F_2 e_1|$. Furthermore, by the same argument, the segment $[F_1, F_2]$ cannot cross the set $\{G : |Ge_1| = |Ge_2|\}$. At the same time, by minimality of n the second inequality is strict if $1 < |F_{1,2}e_2| < M$. They cannot both equal M, since ψ is strictly increasing in its arguments. Analogously, the case $|F_{1,2}e_2| \leqslant 1$ is ruled out since by convexity the same would hold for $|Fe_2|$. Therefore, possibly after relabelling,

$$|F_1 e_2| \leqslant 1 < M = |F_2 e_2|.$$

By continuity, this implies that $[F_1, F_2] \cap \{G : |Ge_1| = |Ge_2|\}$ is non-empty: a contradiction (see figure 2). □

Proof of theorem 1.4. Let F_0 be a matrix as given in the statement, and let $M = |F_0| + 1$. We first assert that

$$V_M^{\mathrm{lc},n}(F) \leqslant W^{\mathrm{lc},n}(F) \tag{4.5}$$

for all n and all $F \in S$, where $S = \{F : 1 < |Fe_1| < M,\ 1 < |Fe_2| < M\}$. The assertion is proven by induction. For $n = 0$, both equal ∞. Assume the inequality to hold for n. For notational convenience we rewrite the definition of the lamination convex envelope as

$$\begin{aligned} V^{\mathrm{lc},n+1}(F) = \inf\{\ell(F) \mid \ell : \mathbb{R}^{2\times 2} \to \mathbb{R} \text{ affine, there are } F_1, F_2 \in \mathbb{R}^{2\times 2} \\ \text{such that } \ell(F_1) = V^{\mathrm{lc},n}(F_1),\ \ell(F_2) = V^{\mathrm{lc},n}(F_2), \\ \operatorname{rank}(F_1 - F_2) \leqslant 1,\ F \in [F_1, F_2]\} \end{aligned} \tag{4.6}$$

and similarly for W (with the convention $\inf\emptyset = \infty$). Fix one matrix $F \in S \cap \Sigma$. If $W^{\mathrm{lc},n+1}(F) = \infty$, there is nothing to prove. Otherwise, let ℓ, F_1, F_2 be as in the definition of $W^{\mathrm{lc},n+1}$; clearly $F_{1,2} \in \Sigma$. It remains to show that

$$V_M^{\mathrm{lc},n+1}(F) \leqslant \ell(F). \tag{4.7}$$

The key property will be that $V_M = W^{\mathrm{rc}}$ on $\Sigma \cap \partial S$, which immediately implies that $V_M^{\mathrm{lc},n} = W^{\mathrm{rc}}$ on $\Sigma \cap \partial S$ for all n.

We define $F_1' = F_1$ if $F_1 \in \bar{S}$, and F_1' to be one element of $\partial S \cap [F, F_1]$ otherwise, and we define F_2' analogously. Let $k : \mathbb{R}^{2\times 2} \to \mathbb{R}$ be affine and such that $k(F_i') = V_M^{\mathrm{lc},n}(F_i')$, for $i = 1, 2$. It suffices to show that

$$k(F_i') = V_M^{\mathrm{lc},n}(F_i') \leqslant \ell(F_i'), \quad i = 1, 2. \tag{4.8}$$

Indeed, if (4.8) holds, then by linearity the same holds in the segment $[F_1', F_2']$ which contains F; hence $V_M^{\mathrm{lc},n+1}(F) \leqslant k(F) \leqslant \ell(F)$, and (4.7) follows.

To prove (4.8), we distinguish two cases. If $F_i' \in S$, then $F_i' = F_i$ and this follows from the inductive assumption. Otherwise, $F_i' \in \partial S \cap [F_1, F_2]$ and therefore

$$k(F_i') = V_M^{\mathrm{lc},n}(F_i') = W^{\mathrm{rc}}(F_i') = V_M^{\mathrm{lc},n+1}(F_i') \leqslant \ell(F_i').$$

This proves the assertion (4.8) and therefore (4.5).

Recalling lemma 4.2, we obtain

$$W^{\mathrm{rc}}(F_0) < V_M^{\mathrm{lc},n}(F_0) \leqslant W^{\mathrm{lc},n}(F_0),$$

which concludes the proof. □

5. Polyconvex envelope

In this section, we prove theorem 1.3 by constructing the polyconvex envelope W^{pc} of the energy W defined in (1.3). The polyconvex envelope of a function W is defined by

$$W^{\mathrm{pc}}(F) = \sup\{V(F) : V \text{ polyconvex},\ V(G) \leqslant W(G) \text{ for all } G \in \mathbb{R}^{n\times n}\}. \tag{5.1}$$

It is well known that for finite-valued energy densities W it suffices to take the supremum over polyaffine functions V (see, for example, [13, § 5.1.1.2]). We first verify that the same is true in the case of interest here, where V is finite only on Σ. The following lemma shows that it suffices to consider the smaller class of all affine functions. We state the result in a more general setting which does not rely on special properties of W.

LEMMA 5.1. *Let $V : \mathbb{R}^{2\times 2} \to [0,\infty]$ be such that $V^{\mathrm{pc}}(F) < \infty$ if and only if $\det F = 1$. Then for all F with $\det F = 1$ we have*

$$V^{\mathrm{pc}}(F) = \sup\{\ell(F) : \ell \in \mathcal{A},\ \ell(G) \leqslant V(G) \textit{ for all } G \in \mathbb{R}^{2\times 2}\}, \tag{5.2}$$

where $\mathcal{A}$ denotes the class of affine functions

$$\mathcal{A} = \{\ell : \mathbb{R}^{2\times 2} \to \mathbb{R} \textit{ such that } \ell(F) = F : G + \beta,\ G \in \mathbb{R}^{2\times 2},\ \beta \in \mathbb{R}\}.$$

We recall that $F : G = \operatorname{Tr} F^{\mathrm{T}} G = \sum_{ij} F_{ij} G_{ij}$.

Proof. Since affine functions are polyconvex, the supremum in (5.2) is taken over a smaller class than in (5.1); hence, it is less than or equal to V^{pc}. Therefore, we only need to show that for any $F \in \Sigma$ there exists an $\ell \in \mathcal{A}$ with $\ell(F) = V^{\mathrm{pc}}(F)$, $\ell \leqslant V$.

Let $\psi : \mathbb{R}^5 \to [0,\infty]$ be defined by

$$\psi(x) = \sup\{g(x), g : \mathbb{R}^5 \to [0,\infty],\ g \text{ convex},\ g(F, \det F) \leqslant V(F) \text{ for all } F\}$$

(we identify $\mathbb{R}^{2\times 2} \times \mathbb{R}$ with $\mathbb{R}^5$). As the pointwise supremum over a class of convex functions, ψ is convex, and $\psi(F, \det F) = V^{\mathrm{pc}}(F)$. We show next that there is a convex function $h : \mathbb{R}^{2\times 2} \to \mathbb{R}$ such that the function ψ can be represented as

$$\psi(F,t) = \begin{cases} h(F) & \text{if } t = 1, \\ \infty & \text{otherwise} \end{cases}$$

for all $F \in \mathbb{R}^{2\times 2}$, $t \in \mathbb{R}$. The fact that $\psi(F,t) = \infty$ for $t \neq 1$ follows from the fact that

$$g_d(F,t) = \begin{cases} 0 & \text{if } t = 1, \\ \infty & \text{otherwise} \end{cases}$$

belongs to the class of functions in the definition of ψ; hence, $\psi \geqslant g_d$. To prove the existence of h we define

$$h(F) = \psi(F,1).$$

The convexity of h follows from the convexity of ψ, and it remains to show that h is finite valued. Since $h(F) = V^{\mathrm{pc}}(F) < \infty$ for all matrices F with $\det F = 1$, it suffices to prove that the convex hull of $\Sigma = \{F \in \mathbb{R}^{2\times 2} : \det F = 1\}$ coincides with $\mathbb{R}^{2\times 2}$. To do this, fix $F \in \mathbb{R}^{2\times 2}$. If $\det F < 1$, we consider the line $t \mapsto F_t = F + t\,\mathrm{Id}$. Obviously, $\det F_t$ is continuous, and $\lim_{t\to\pm\infty} \det F_t = \infty$. Therefore, there are two values $t_- < 0 < t_+$ such that $\det F_{t_\pm} = 1$. This implies that F belongs to the convex hull of $\{F_{t_-}, F_{t_+}\} \subset \Sigma$. If $\det F > 1$, one proceeds analogously with $\tilde{F}_t = F + t(e_1 \otimes e_1 - e_2 \otimes e_2)$. This concludes the proof of the assertion.

Now let $F \in \Sigma$. Since $h : \mathbb{R}^4 \to \mathbb{R}$ is convex, and $h(F) \in \mathbb{R}$, there is an affine function $\ell \in \mathcal{A}$ such that $\ell(F) = h(F) = V^{\mathrm{pc}}(F)$, and $\ell \leqslant h$ on $\mathbb{R}^4$. The latter implies that

$$\ell(G) \leqslant h(G) = \psi(G,1) \leqslant \psi(G, \det G) = V^{\mathrm{pc}}(G)$$

for all $G \in \mathbb{R}^{2\times 2}$. This concludes the proof. □

We now turn to the specific problem at hand. We first recall the well-known fact that for any $F \in \mathbb{R}^{2\times 2}$ one has

$$\max_{G\in \mathrm{SO}(2)} F : G = (\lambda_2 + \lambda_1)(F). \tag{5.3}$$

Here λ_1 and λ_2 are the signed singular values of F, defined as in (1.6). We further observe that if $F = QH$, with $Q \in \mathrm{SO}(2)$ and $H = H^{\mathrm{T}}$, then

$$(\lambda_2 + \lambda_1)(F) = |\operatorname{Tr} H|.$$

Multiplying both F and G in (5.3) by $e_1 \otimes e_1 - e_2 \otimes e_2$, we obtain

$$\max_{G\in \mathrm{O}(2)\setminus \mathrm{SO}(2)} F : G = (\lambda_2 - \lambda_1)(F). \tag{5.4}$$

LEMMA 5.2. *The polyconvex envelope W^{pc} of the function W defined in (1.3) satisfies*

$$W^{\mathrm{pc}}(F) = \begin{cases} \max\{\varphi_F(G) : G \in \mathbb{R}^{2\times 2},\ |Ge_1| \leqslant 1,\ |Ge_2| \leqslant 1\} & \textit{if } \det F = 1, \\ \infty & \textit{otherwise}, \end{cases} \tag{5.5}$$

where

$$\varphi_F(G) = F : G - (\lambda_1 + \lambda_2)(G). \tag{5.6}$$

Proof. We start from (5.2), with $V = W$. Choose G, β such that the corresponding affine function ℓ satisfies $\ell \leqslant W$. Then, necessarily for all $F = Q(\mathrm{Id} + \gamma e_i \otimes e_i^{\perp})$, $i \in \{1,2\}$ one has

$$F : G + \beta \leqslant |\gamma|.$$

In other words,

$$Q : G + \gamma Q e_i \cdot G e_i^{\perp} + \beta \leqslant |\gamma| \tag{5.7}$$

for all $Q \in \mathrm{SO}(2)$, $\gamma \in \mathbb{R}$, $i \in \{1, 2\}$. Considering the limits $\gamma \to \pm\infty$, we see that (5.7) implies that $|Qe_i \cdot Ge_i^{\perp}| \leqslant 1$ for all $Q \in \mathrm{SO}(2)$, $i \in \{1, 2\}$. This is equivalent to the conditions

$$|Ge_1| \leqslant 1, \qquad |Ge_2| \leqslant 1. \tag{5.8}$$

For $\gamma = 0$, (5.7) instead reduces to

$$\beta + \max_{Q \in \mathrm{SO}(2)} Q : G \leqslant 0, \tag{5.9}$$

which by (5.3) is equivalent to $\beta \leqslant -\sqrt{|G|^2 + 2\det G} = -(\lambda_1 + \lambda_2)(G)$. By linearity, it may immediately be seen that (5.8) and (5.9) are equivalent to (5.7). Furthermore, it is clear that it suffices to consider the largest value of β compatible with (5.9), i.e. $-(\lambda_1 + \lambda_2)(G)$. This concludes the proof. □

LEMMA 5.3. *The result of lemma 5.2 is equivalent to*

$$W^{\mathrm{pc}}(F) = \begin{cases} \max\{\varphi_F(G) : G \in \mathbb{R}^{2\times 2}, |Ge_1| = |Ge_2| = 1\} & \textit{if } \det F = 1, \\ \infty & \textit{otherwise.} \end{cases} \tag{5.10}$$

Proof. We need only to show that we can restrict the class of matrices in the maximum to those for which both columns have length 1. Fix $F \in \Sigma$. We must show that the maximum of φ_F on the set

$$K = \{G \in \mathbb{R}^{2\times 2} : |Ge_1| \leqslant 1, |Ge_2| \leqslant 1\} \tag{5.11}$$

is attained on the set $K' = \{G \in \mathbb{R}^{2\times 2} : |Ge_1| = |Ge_2| = 1\} \subset K$.

Recalling (5.3) and (5.4), we see that

$$\max_{G \in \mathrm{O}(2)\setminus\mathrm{SO}(2)} \varphi_F(G) = (\lambda_2 - \lambda_1)(F) \geqslant 0. \tag{5.12}$$

In order to conclude the proof, we note first that by continuity there exists $G \in K$ such that $\varphi_F(G) = \max\{\varphi_F(H), H \in K\}$. In the following argument we distinguish several cases depending on properties of G.

If $\varphi_F(G) = 0$, then by (5.12) there also exists a matrix with the asserted properties that realizes the maximum. This, in particular, treats the case when $G = 0$.

Assume next that $G \neq 0$, with both columns of length less than 1 and $\varphi_F(G) \neq 0$. By continuity, there exists a $t > 1$ such that $tG \in K$. But, since

$$\varphi_F(tG) = t\varphi_F(G),$$

it follows that the maximum was not attained at G: a contradiction.

We finally consider the case when only one of the columns of G has length less than 1, i.e. we assume that

$$|Ge_1| < 1 = |Ge_2|.$$

We consider the polar decomposition of G, i.e. choose a symmetric matrix H and $Q \in \mathrm{SO}(2)$ such that $G = QH$. The (signed) singular values of G are the eigenvalues

of H, up to a global sign, and therefore $(\lambda_1 + \lambda_2)(G) = (\lambda_1 + \lambda_2)(H) = |\operatorname{Tr} H|$. Consider, for $t \in \mathbb{R}$, the matrices

$$G_t = QH_t = Q(H + te_1 \otimes e_1).$$

It is clear that $|G_t e_2| = |Ge_2|$ for all $t \in \mathbb{R}$; hence, by continuity for small t we have $G_t \in K$. Consider now the function $t \mapsto \varphi_F(G_t)$. Since $H_t = H + te_1 \otimes e_1$ is symmetric, and $Q \in \mathrm{SO}(2)$, we have

$$(\lambda_1 + \lambda_2)(QH_t) = (\lambda_1 + \lambda_2)(H_t) = |\operatorname{Tr} H_t| = |\operatorname{Tr} H + t|.$$

We now distinguish two cases. If $\operatorname{Tr} H = 0$, then the fact that $|He_2| = 1$ and $H^{\mathrm{T}} = H$ implies necessarily that $H \in \mathrm{O}(2) \setminus \mathrm{SO}(2) \subset K'$. Otherwise, there is a (maximal) closed segment $I \subset \mathbb{R}$, $0 \in I$, such that $G_t \in K$ for all $t \in I$ and $t \mapsto \varphi_F(G_t)$ is affine on I; its end points satisfy either $|G_t e_1| = 1$ or $\operatorname{Tr} H_t = 0$. If φ_F attains its maximum in the interior of the interval, the coefficient of the linear term must vanish and the function $\varphi(G_t)$ is constant for $t \in I$. The end points belong to K' and hence in any case the maximum on K coincides with the maximum on K'. This concludes the proof. □

Proof of theorem 1.3. Consider in lemma 5.3 a generic G with $|Ge_1| = |Ge_2| = 1$, and let $G = QH$ be its polar decomposition. Since H is a symmetric matrix with both columns of length 1, it necessarily has the form

$$H = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \quad \text{or} \quad H = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

In the first case, $H \in \mathrm{O}(2)$. Recalling (5.3) and (5.4), together with the fact that $\det F = 1$ implies $\lambda_1(F) > 0$, we see that the supremum over all H of the first form is $(\lambda_2 - \lambda_1)(F)$. It remains to treat the second case. Since $(\lambda_1 + \lambda_2)(G) = |\operatorname{Tr} H| = 2|\cos\theta|$, we need to consider

$$\begin{aligned} \max_{Q \in \mathrm{SO}(2)} F : (QH) - 2|\cos\theta| &= \max_{Q \in \mathrm{SO}(2)} \operatorname{Tr} Q^{\mathrm{T}} FH - 2|\cos\theta| \\ &= (\lambda_1 + \lambda_2)(FH) - 2|\cos\theta|. \end{aligned}$$

Thus,

$$\begin{aligned} (\lambda_1 + \lambda_2)(FH) &= \sqrt{|FH|^2 + 2\det(FH)} \\ &= \sqrt{|FHe_1|^2 + |FHe_2|^2 + 2\det H} \\ &= \sqrt{|Fe_1|^2 + |Fe_2|^2 + 2Fe_1 \cdot Fe_2 \sin(2\theta) + 2\cos(2\theta)}. \end{aligned}$$

Therefore, $F : (QH) - |\operatorname{Tr} H|$ for the matrix under consideration coincides with

$$\tilde{\psi}(\theta) = \sqrt{|F|^2 + 2Fe_1 \cdot Fe_2 \sin(2\theta) + 2\cos(2\theta)} - 2|\cos\theta|.$$

Finally, we compute

$$\tilde{\psi}(\tfrac{1}{2}\pi) = \sqrt{|F|^2 - 2} = \lambda_2(F) - \lambda_1(F),$$

which proves that the maximum of $\tilde{\psi}$ is always larger than $\lambda_2(F) - \lambda_1(F)$; hence, the matrices in $\mathrm{O}(2)$ can also be neglected. Since $\tilde{\psi}$ is π-periodic, we can take

$\theta \in [-\frac{1}{2}\pi, \frac{1}{2}\pi]$ and drop the absolute value on the last cosine. Since $\sin 2\theta$ is odd, and all other terms are even, we can take $\theta \in [0, \frac{1}{2}\pi]$ if we put replace $\sin 2\theta$ by $|\sin 2\theta|$. This concludes the proof. □

6. Bounds on the quasiconvex envelope

We address here bounds on the quasiconvex envelope W^{qc}, which are non-trivial since W takes the value ∞ on a large set, and for extended-valued functions quasiconvexity does not automatically imply rank-1 convexity. We also investigate numerically the quality of the approximations we have derived.

6.1. Analytical bounds

In the situation at hand it turns out that the rank-1 convex envelope does give a bound on the quasiconvex one.

PROPOSITION 6.1. *For all matrices $F \in \mathbb{R}^{2\times 2}$, and with the notation above, we have*

$$W^{\mathrm{pc}}(F) \leqslant W^{\mathrm{qc}}(F) \leqslant W^{\mathrm{rc}}(F).$$

Proof. The lower bound $W^{\mathrm{pc}} \leqslant W^{\mathrm{qc}}$ holds for generic extended-valued functions [30, lemma 4.3]; hence, there is nothing to prove.

The upper bound $W^{\mathrm{qc}}(F) \leqslant W^{\mathrm{rc}}(F)$ holds in general for finite-valued functions W, but not necessarily for extended-valued ones (see, for example, [4] for an example where it does not).

We show next that $W^{\mathrm{qc}}(F) < \infty$ for all matrices F with $\det F = 1$. If the assertion holds, then [9, theorem 1.1] implies that W^{qc} is rank-1 convex. Since obviously $W^{\mathrm{qc}} \leqslant W$, we obtain that W^{qc} constitutes a lower bound on W^{rc} and the statement follows.

The assertion can be proven using the method of convex integration for Lipschitz mappings developed by Müller and Šverák [31], which is based on the construction of a suitable in-approximation (see [31] for the precise statements and the definition of an in-approximation and [2, 11, 15] for similar applications). Here, we shall argue that it suffices to apply two known consequences of the result by Müller and Šverák.

We use different constructions in the different parts of the domain. If $|Fe_1| \leqslant 1$, then the assertion follows from [11, theorem 1], and analogously if $|Fe_2| \leqslant 1$. Consider now a matrix F with $\det F = 1$ and $|Fe_1|, |Fe_2| > 1$. Then, arguing as in the proof of lemma 2.1, we find $\gamma \in \mathbb{R}$ such that F is in the rank-1 convex hull of the set

$$K_\gamma = \mathrm{SO}(2)A_\gamma \cup \mathrm{SO}(2)B_\gamma, \quad A_\gamma = \mathrm{Id} + \gamma e_1 \otimes e_2, \quad B_\gamma = \mathrm{Id} + \gamma e_2 \otimes e_1.$$

By [31, corollary 1.4] there is a Lipschitz mapping $u \in W^{1,\infty}((0,1)^2; \mathbb{R}^2)$ such that $\nabla u \in K$ a.e. and $u(x) = Fx$ on the boundary. Therefore, $W^{\mathrm{qc}}(F) \leqslant |\gamma|$, and the assertion is proven. □

We remark that, even if one knew the quasiconvex envelope, this would not immediately prove that $\int W^{\mathrm{qc}}(Du)\,\mathrm{d}x$ is the relaxation of $\int W(Du)\,\mathrm{d}x$. Indeed, standard theorems apply only for finite-valued energy densities with p-growth conditions, $p > 1$. In the case of linear growth $p = 1$, the variational integral needs

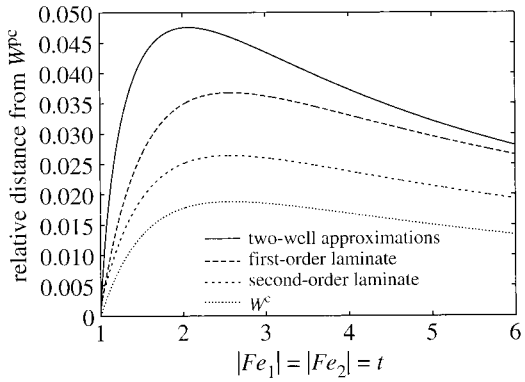

Figure 3. A comparison between four upper bounds for W^{qc} and the lower bound W^{pc} on matrices $|Fe_1| = |Fe_2|$. The curves represent the relative distance between a given upper bound and the lower bound. From highest to lowest, the curves correspond to: a bound using an estimate by the two-well problem, a bound based on a simple laminate with one support at infinity, a bound based on a second-order laminate whose support contains two matrices at infinity in the sense of (2.5), and the rank-1 convex envelope W^{rc} generated by infinite-rank laminates with support on SO(2) and at ∞.

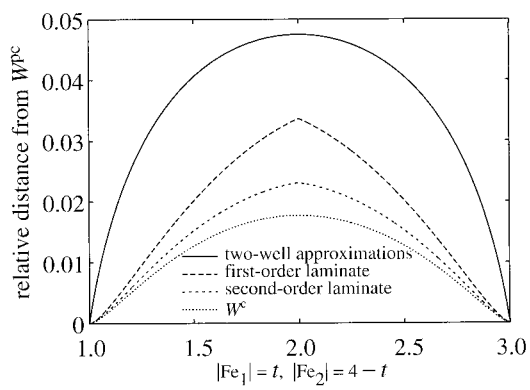

Figure 4. A comparison between the bounds, as in figure 3, but along the line $\{|Fe_1| + |Fe_2| = 4\}$. The midpoint corresponds to the point at $t = 2$ of figure 3; the end points belong to the set where $W = W^{rc}$.

to be augmented by additional terms involving the recession function of W^{qc} and the singular part of the distributional gradient Du, in the sense of functions of bounded variation [14, 20, 21]. In this case additional difficulties are expected from the constraint on the determinant.

6.2. Numerical approximations to the quasiconvex envelope

We discuss in this section the numerical difference between several approximations to W^{qc} we have obtained. Since plotting the absolute values would result in indistinguishable curves, we display instead the relative distance from the lower

bound W^{pc}, defined, in the case of W^{rc}, for example, as

$$\frac{W^{\mathrm{rc}}(F) - W^{\mathrm{pc}}(F)}{W^{\mathrm{pc}}(F)}.$$

We consider two different directions in the plane in figures 3 and 4. The first one considers matrices in Σ with columns of equal lengths, the second one considers matrices such that the sum of the lengths of the columns is fixed.

We now discuss the different upper bounds to W^{qc}, starting from the worst one (i.e. from the highest to the lowest).

The worst approximation, labelled 'two-well approximation', is an upper bound based on a refinement of lemma 2.2. In the notation of the proof of lemma 2.2, we determine for each F the smallest γ such that $F \in K_\gamma^{\mathrm{rc}}$ (which amounts to solving a quadratic equation), and then estimate $W^{\mathrm{rc}}(F) \leqslant |\gamma|$. This simple computation results in a maximum relative error on W^{qc} of less than 5%.

The next bound is derived directly from (2.3). Given F, we define F_t as in (2.2) and find the parameter t with smallest magnitude such that $|F_t e_2| = 1$ (again, t is the solution of a quadratic equation). This gives the bound $W^{\mathrm{rc}}(F) \leqslant W(F_t) + |t||Fe_1|$. The minimum between this bound and the one obtained by swapping the indices 1 and 2 is labelled 'first-order laminate' in the figure.

The third bound, labelled 'second-order laminate', arises from (2.7). Given F, let $\theta \in [0, \infty)$ and define

$$F_\theta = \begin{pmatrix} 1 & \pm\theta \\ 0 & 1 \end{pmatrix},$$

where the sign in front of θ is chosen to the same as that of $Fe_1 \cdot Fe_2$. Since any $F \in \Sigma$ is uniquely determined, up to left-multiplication by a rotation, by the lengths of its columns and the sign of the inner product of its columns, it is not difficult to show that there exists a rotation $Q \in \mathrm{SO}(2)$ and numbers $s, t \in \mathbb{R}$ such that $F = G(QF_\theta, s, t)$. Then, by (2.7) and the rotational invariance of W, we find

$$W^{\mathrm{rc}}(F) \leqslant W(F_\theta) + |t| + |s|\sqrt{(\theta^2+1)^2 \pm 2t\theta + t^2}.$$

By choosing s and t to have the smallest magnitude when solving the associated quadratic equations, we arrive at an upper bound for $W^{\mathrm{rc}}(F)$ for every θ. We report the best of these bounds, obtained from numerically optimizing in θ.

The lowest curve in the figure is the rank-1 convex envelope, W^{rc}. Observe that, as estimates of W^{qc}, W^{rc} and W^{pc} have a maximum relative error of about 1.7%.

From the given formulae for the energy it is easy to derive expressions for the deviatoric stress (which, in two dimensions, has two independent components). Precisely, given a curve $F : \mathbb{R} \to G \in \mathbb{R}^{2\times 2} : G^{\mathrm{T}} = G, \det G = 1$, we can compute the stress component along the curve resulting from the rank-1 convex envelope of W by

$$\sigma(t) = \left|\frac{\mathrm{d}}{\mathrm{d}t}F(t)\right|^{-1} \frac{\mathrm{d}}{\mathrm{d}t}W^{\mathrm{rc}}(F(t)) = \nabla W^{\mathrm{rc}}(F(t))\frac{F'(t)}{|F'(t)|}. \tag{6.1}$$

Analogous expressions hold for W^{pc}. It is easy to check from the formulae given in § 2 that for the curve corresponding to figure 3 one obtains $\sigma = \sqrt{2}$ independently of t. Numerical results obtained with W^{rc}, with W^{pc} and with the approximation

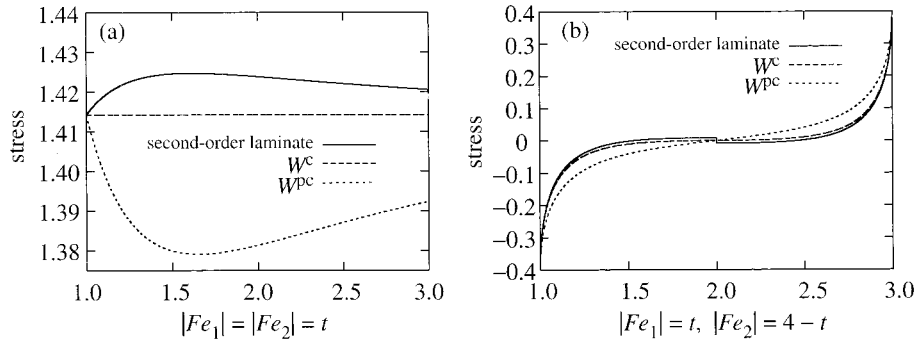

Figure 5. Estimate of the stress obtained in the relaxed model. We plot the component of the stress along the lines used (a) in figure 3 and (b) in figure 4. The 'diagonal' component of the stress, corresponding to figure 3, is very similar for the rank-1 convex and the polyconvex envelope (the difference being about 2%); whereas in the 'off-diagonal' component there is a significant relative difference.

with second-order laminates are illustrated in figure 5. As may be expected from the energy plots, second-order laminates give a very good approximation to the rank-1 convex envelope; the difference from the polyconvex envelope is somewhat larger, especially in the component corresponding to figure 4.

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References

1 M. Abramowitz and I. A. Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, National Bureau of Standards Applied Mathematics Series, vol. 55 (Washington, DC: US Government Printing Office, 1964).

2 J. Adams, S. Conti, A. DeSimone and G. Dolzmann. Relaxation of some transversally isotropic energies and applications to smectic A elastomers. *Math. Models Meth. Appl. Sci.* **18** (2008), 1–20.

3 J. M. Ball and R. D. James. Proposed experimental tests of a theory of fine microstructure and the two-well problem. *Phil. Trans. R. Soc. Lond.* A **338** (1992), 389–450.

4 J. M. Ball and F. Murat. $W^{1,p}$-quasiconvexity and variational problems for multiple integrals. *J. Funct. Analysis* **58** (1984), 225–253.

5 J. M. Ball, B. Kirchheim and J. Kristensen. Regularity of quasiconvex envelopes. *Calc. Var. PDEs* **11** (2000), 333–359.

6 S. Bartels, C. Carstensen, K. Hackl and U. Hoppe. Effective relaxation for microstructure simulations: algorithms and applications. *Computat. Meth. Appl. Mech. Engng* **193** (2004), 5143–5175.

7 C. Carstensen, S. Conti and A. Orlando. Mixed analytical–numerical relaxation in finite single-slip crystal plasticity. *Continuum Mech. Thermodyn.* **20** (2008), 275–301.

8 C. Carstensen, K. Hackl and A. Mielke. Nonconvex potentials and microstructure in finite-strain plasticity. *Proc. R. Soc. Lond.* A **458** (2002), 299–317.

9 S. Conti. Quasiconvex functions incorporating volumetric constraints are rank-1 convex. *J. Math. Pures Appl.* **90** (2008), 15–30.

10 S. Conti and M. Ortiz. Dislocation microstructures and the effective behavior of single crystals. *Arch. Ration. Mech. Analysis* **176** (2005), 103–147.

11 S. Conti and F. Theil. Single-slip elastoplastic microstructures. *Arch. Ration. Mech. Analysis* **178** (2005), 125–148.

12 S. Conti, D. Faraco and F. Maggi. A new approach to counterexamples to L^1 estimates: Korn's inequality, geometric rigidity, and regularity for gradients of separately convex functions. *Arch. Ration. Mech. Analysis* **175** (2005), 287–300.

13 B. Dacorogna. *Direct methods in the calculus of variations* (Springer, 1989).

14 G. Dal Maso. Integral representation on $\mathrm{BV}(\Omega)$ of Γ-limits of variational integrals. *Manuscr. Math.* **30** (1979), 387–416.

15 A. DeSimone and G. Dolzmann. Macroscopic response of nematic elastomers via relaxation of a class of SO(3)-invariant energies. *Arch. Ration. Mech. Analysis* **161** (2002), 181–204.

16 G. Dolzmann. *Variational methods for crystalline microstructure: analysis and computation*, Lecture Notes in Mathematics, vol. 1803 (Springer, 2003).

17 D. Faraco. Milton's conjecture on the regularity of solutions to isotropic equations. *Annales Inst. H. Poincaré* **20** (2003), 889–909.

18 D. Faraco. Tartar conjecture and Beltrami operators. *Michigan Math. J.* **52** (2004), 83–104.

19 I. Fonseca. The lower quasiconvex envelope of the stored energy function for an elastic crystal. *J. Math. Pures Appl.* **67** (1988), 175–195.

20 I. Fonseca and S. Müller. Quasi-convex integrands and lower semicontinuity in L^1. *SIAM J. Math. Analysis* **23** (1992), 1081–1098.

21 I. Fonseca and S. Müller. Relaxation of quasiconvex functionals in $\mathrm{BV}(\Omega, \mathbb{R}^p)$ for integrands $f(x, u, \nabla u)$. *Arch. Ration. Mech. Analysis* **123** (1993), 1–49.

22 R. V. Kohn and G. Strang. Optimal design and relaxation of variational problems. I. *Commun. Pure Appl. Math.* **39** (1986), 113–137.

23 R. V. Kohn and G. Strang. Optimal design and relaxation of variational problems. II. *Commun. Pure Appl. Math.* **39** (1986), 139–182.

24 R. V. Kohn and G. Strang. Optimal design and relaxation of variational problems. III. *Commun. Pure Appl. Math.* **39** (1986), 353–377.

25 H. Le Dret and A. Raoult. The quasiconvex envelope of the Saint Venant–Kirchhoff stored energy function. *Proc. R. Soc. Edinb.* A **125** (1995), 1179–1192.

26 C. Miehe, J. Schotte and M. Lambrecht. Homogeneization of inelastic solid materials at finite strains based on incremental minimization principles: application to the texture analysis of polycrystals. *J. Mech. Phys. Solids* **50** (2002), 2123–2167.

27 C. Miehe, M. Lambrecht and E. Gürses. Analysis of material instabilities in inelastic solids by incremental energy minimization and relaxation methods: evolving deformation microstructures in finite plasticity. *J. Mech. Phys. Solids* **52** (2004), 2725–2769.

28 A. Mielke. Energetic formulation of multiplicative elasto-plasticity using dissipation distances. *Continuum Mech. Thermodyn.* **15** (2003), 351–382.

29 C. B. Morrey. Quasi-convexity and the lower semicontinuity of multiple integrals. *Pac. J. Math.* **2** (1952), 25–53.

30 S. Müller. Variational models for microstructure and phase transitions. In *Calculus of variations and geometric evolution problems* (ed. F. Bethuel *et al.*), Springer Lecture Notes in Mathematics, vol. 1713, pp. 85–210 (Springer, 1999).

31 S. Müller and V. Šverák. Convex integration with constraints and applications to phase transitions and partial differential equations. *J. Eur. Math. Soc.* **1** (1999), 393–442.

32 M. Ortiz and E. A. Repetto. Nonconvex energy minimization and dislocation structures in ductile single crystals. *J. Mech. Phys. Solids* **47** (1999), 397–462.

33 V. Šverák. On the problem of two wells. In *Microstructure and phase transition*, IMA Volumes in Mathematics and Its Applications, vol. 54, pp. 183–189 (Springer, 1993).

34 R. Temam. *Mathematical problems in plasticity* (Paris: Bordas, 1985).

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