



When Rank-One Convexity Meets Polyconvexity: An Algebraic Approach to Elastic Binodal

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Abstract

In the variational problems involving non-convex integral functionals, finding the *binodal*, the boundary of validity of the quasiconvexity of the energy density, is of central importance. We develop a systematic methodology for identifying a part of the binodal corresponding to simple laminates by showing that in this case the supporting null-Lagrangians, establishing polyconvexity, can be constructed explicitly. We present a nontrivial example from nonlinear elasticity where this approach allows one to obtain the entire quasiconvex envelope.

Keywords Quasiconvexity · Polyconvexity · Rank-one convexity · Jump set · Elastic stability · Binodal

Mathematics Subject Classification 74A50 · 74G65 · 49K40 · 49S05

1 Introduction

We consider the general problem of identifying strong local minimizers of an integral functional

$$E[y] = \int_{\Omega} L(x, y(x), \nabla y(x)) dx, \quad (1.1)$$

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where $\Omega \subset \mathbb{R}^n$ and $\mathbf{y} : \Omega \rightarrow \mathbb{R}^m$ satisfies prescribed boundary conditions; the term “strong” refers to local minima of $E[\mathbf{y}]$ in L^∞ topology. Such vectorial variational problems are encountered, for instance, in nonlinear elasticity (Truesdell 1952).

When the integrand $L(\mathbf{x}, \mathbf{y}, \mathbf{F})$ is not rank-one convex in the \mathbf{F} variable, as, for instance, in models of elastic phase transitions (Ericksen 1975; Ball and James 1987) and composite materials (Lurie 1963; Kohn and Strang 1982), Euler–Lagrange equations¹ may have a large set of solutions, most of which are unstable in L^∞ topology. The main distinguishing characteristic of strong local minimizers $\mathbf{y}(\mathbf{x})$ is the quasi-convexity of the integrand as a function of \mathbf{F} at $\mathbf{F} = \nabla \mathbf{y}(\mathbf{x})$, $\mathbf{x} \in \Omega$ (Morrey 1952; Meyers 1965). We recall that a function $W(\mathbf{F})$ is quasiconvex at $\mathbf{F} \in \mathbb{R}^{m \times n}$, if

$$\int_D W(\mathbf{F} + \nabla \phi(\mathbf{x})) d\mathbf{x} \geq W(\mathbf{F}) \quad (1.2)$$

for any² domain $D \subset \mathbb{R}^n$ and any $\phi \in C_0^\infty(D; \mathbb{R}^m)$, where f denotes the average.

Definition 1.1 The set of points \mathbf{F} , where quasiconvexity fails, will be called the QC binodal region \mathfrak{B} for the function $W(\mathbf{F})$ (Grabovsky and Truskinovsky 2013). The boundary of \mathfrak{B} will be called the QC binodal.

The QC binodal is one of the main tools in distinguishing local minima from saddle points in vectorial variational problems. For example, in the context of the study of stability of two-phase elastic solids in Eremeev et al. (2007) it would immediately rule out spherically-symmetric configurations in an annulus with more than one interface. For vectorial variational problems, identifying the QC binodal presents difficulties that are not present in the scalar ($\min(m, n) = 1$) case. Not only vectorial quasiconvexity lacks transparent geometric interpretation (Kristensen 1999) enjoyed by the analogous convexity condition for scalar variational problems, there seem to be no systematic methods for its verification (Schrüder and Neff 2010). The goal of this paper is to show that a part of the QC binodal is nonetheless accessible, providing at least some information about the relaxed energy. In the worst case scenario, this part is empty, and in the best it comprises the entire QC binodal.

This work is motivated by the question of stability of interfaces across which the deformation gradient is discontinuous. Such interfaces are observed in minimizers of non-quasiconvex functionals (1.1). For instance, in multi-well problems from elasticity theory such interfaces represents phase/domain boundaries. For minimizers of (1.1), when they exist, the deformation gradients at the two sides of these interfaces lay on the subset of the “jump set” (Grabovsky and Truskinovsky 2011, 2014) that belongs to the QC binodal. The jump set is a co-dimension 1 variety in the phase space of deformation gradients \mathbf{F} defined by the equations relating the values of the deformation gradient at the two sides of its jump discontinuity. The conventionally used system of relations on a jump discontinuity was recently found to be incomplete: An additional condition was necessary for interface stability (Grabovsky and Truskinovsky 2011).

¹ In nonlinear elasticity, the integrand cannot be regular for physical reasons and minimizers cannot be ascertained to satisfy Euler–Lagrange equations in general.

² If (1.2) holds for one D , then it will also hold for all others.

In scalar variational problems minimizers with discontinuous gradients are interpreted as having “corners,” whose shape and location are restricted by the Weierstrass–Erdmann (WE) corner conditions (Erdmann 1877). These necessary conditions can be used to prove (Giaquinta and Hildebrandt 1996) that jump discontinuities are forbidden, if an extremal lies in the interior of the region of convexity. This statement becomes apparent if we recall the geometric meaning of the scalar WE conditions (Gelfand and Fomin 1963): The values of the derivative of the minimizer on either side of the corner determine the pair of points where the tangent plane touches the graph of the Lagrangian. If this plane is supporting, i.e., lies below the graph of the Lagrangian, then the derivatives of minimizers at the corners must be on the C (convex) binodal.

The need of generalizing the Weierstrass–Erdmann corner conditions for the vectorial setting was understood in the studies of elastic phase transitions (Eshelby 1970; James 1981; Gurtin 1983; Šilhavý 1997). For instance, shifting the focus from the global behavior of minimizers to values of its gradient at points of jump discontinuity permitted modeling of the laminar microstructures observed in shape memory alloys (Ball and James 1987, 1992). The study of geometry in phase space of the generalized WE conditions was initiated in Freidin and Chiskis (1994a, b), and the question of stability of the surfaces of gradient jump discontinuity received much attention (Grinfeld 1980a, b; Šilhavý 2005; Kucher and Osmolovskii 2001; Osmolovskii 2004).

It was first thought that in the vectorial case the analog of the *necessary* WE conditions can be formulated in terms of rank-one convexity, whose geometric interpretation reduces to double-tangency of rank-one *lines*. However, even if such a line is supporting (lies below the graph of the Lagrangian), it no longer guarantees that the deformation gradients at the surface of jump discontinuity are on the QC binodal. In this paper, we propose a new generalization of the WE conditions that retains its *sufficiency* property from the scalar case. Specifically, we generalize the double-tangency (Maxwell) construction by delegating the role of affine functions, bounding the energy from below, to the quasi-affine functions. In this construction, the role of the convex envelope, built in the scalar case by supporting affine null-Lagrangians, is played by the polyconvex (PC) envelope defined in terms of supporting quasi-affine null-Lagrangians.

Polyconvexity, is a well-known sufficient condition for quasiconvexity (Dacorogna 2008). However, since polyconvex envelopes in vectorial problems are often strictly lower than the relaxed energy density, at the first glance they seem to be useless for identifying any points of the QC binodal. In this paper, we show that the generalized WE conditions emerge from the analysis of double-tangency of supporting null-Lagrangians, thereby guaranteeing that the relevant points must lie on the QC binodal, where it also coincides with PC and RC (rank-one) binodal. This leads to a constructive method of identifying points on the QC binodal where “polyconvexity (PC) meets rank-one convexity (RC).” A related approach that uses only quadratic null-Lagrangians, and known as the translation method, has been very effective in the study of composite media (Tartar 1979, 1985; Lurie et al. 1980b, 1982).

At the technical level, we essentially pursue what Carathéodory has called the “royal road” to Calculus of Variations (Young 1969), which is based on the idea of supporting null-Lagrangians. In the context of the variational problem (1.2), it translates to verifying polyconvexity (Dacorogna 2008). This approach is well known. However,

its effectiveness is often limited, since the resulting algebraic problem is usually too technically demanding to be practical. Moreover, establishing polyconvexity does not deliver the QC binodal directly. The situation, however, changes when points on a polyconvex binodal (boundary of validity of polyconvexity) can be shown to belong to a rank-one binodal because such points would have to belong to the QC binodal as well.

In this paper, we show that there is a special regime in which points on the polyconvex binodal must necessarily be a part of the *jump set* (Grabovsky and Truskinovsky 2011, 2014). This regime is characterized geometrically by double-tangency of supporting null-Lagrangians, which evokes the “common tangent” interpretation of the Weierstrass–Erdmann (WE) corner conditions. As we have already mentioned, while the latter naturally furnish the *convexification* of $W(\mathbf{F})$ via affine functions, their vectorial analogs, defining the jump set, do not automatically ensure *polyconvexification* of W by quasi-affine functions. The implied geometrical analogy is not direct since the space of null-Lagrangians is $\binom{m+n}{n}$ -dimensional and the boundary of validity of polyconvexity should be characterized by graphs of supporting quasi-affine functions touching the graph of $W(\mathbf{F})$ in $\binom{m+n}{n} - mn + 1$ points. This number is equal to 2 if and only if $\min(m, n) = 1$, explaining the importance of double-tangency in scalar variational problems. As we show, the role of the double-tangency condition in the general vectorial context, or equivalently, of the generalized WE conditions, is more subtle and is related to a nontrivial interplay between poly- and rank-one convexity.

Indeed, in Carathéodory’s approach the method of supporting null-Lagrangians, delivering *sufficient* conditions for a strong local minimum, is applicable whenever (a strengthened version of) *necessary* conditions holds. This connection breaks down for vectorial problems, since polyconvexity (sufficient condition) is not equivalent to quasiconvexity (necessary condition). In this paper, we identify a subset of the QC binodal where polyconvexity would necessarily collapse on rank-one convexity restoring the efficacy of Carathéodory’s approach. While this subset may or may not exist in particular problems, our method allows one to search for such subsets for general functions $W(\mathbf{F})$. As an illustration, we present a vectorial example where our method delivers the entire quasiconvexification of $W(\mathbf{F})$.

In general, the application of the method (in the context of two- and three-dimensional elasticity) may require analysis of minima of a function of a small number of variables, which may be somewhat technically involved, if one aims to obtain explicit analytic results. We therefore have chosen an example, where the answer is available by other means and the calculations will not obscure the theoretical thrust of the paper. Full-scale application of the proposed method to the analysis of non-quasiconvex Hadamard materials will be done in our forthcoming work.

The paper is organized as follows. In Sect. 2, we discuss the two main ingredients of our approach: the idea of a supporting null-Lagrangian and the concept of a jump set. In Sect. 3, we study the PC binodal and identify conditions when it (partially) overlaps with the jump set. In Sect. 4, we show how to reconstruct the quasiconvex envelope for points of quasiconvexity on the jump set. In Sect. 5, we present an analytically transparent and yet nontrivial example, where our method is particularly effective delivering the whole relaxed energy. We close the discussion with some conclusions in Sect. 6. Our “Appendix A” contains proofs of two technical Lemmas. In “Appendix B,”

we show that if the goal is to locate the limits of validity of rank-one convexity (RC binodal instead of QC binodal), the proposed approach is even more effective. The reason is that, in contrast to QC binodal, RC binodal is insensitive to modifications of $W(\mathbf{F})$ outside the binodal region. Finally, in ‘‘Appendix C’’ we provide an alternative path to finding the relaxed energy in our example.

2 Preliminaries

In this section, we recall the two key elements of our approach: the supporting null-Lagrangians and the jump set.

2.1 Supporting Null-Lagrangians

We recall that a function $N(\mathbf{F})$ is called a null-Lagrangian if $\int_D N(\nabla \mathbf{y}) dx$ depends only on the values of $\mathbf{y}(\mathbf{x})$ on ∂D . A null-Lagrangian must be a linear combination of minors of \mathbf{F} (Ericksen 1962; Edelen 1962). We say that $N(\mathbf{F})$ is a supporting null-Lagrangian at $\mathbf{F}_0 \in \mathbb{R}^{m \times n}$ if

- (A) $N(\mathbf{F}_0) = W(\mathbf{F}_0)$
- (B) $N(\mathbf{F}) \leq W(\mathbf{F})$ for all $\mathbf{F} \in \mathbb{R}^{m \times n}$.

If such a null-Lagrangian exists, then for every domain $D \subset \mathbb{R}^n$ and every $\phi \in C_0^\infty(D; \mathbb{R}^m)$

$$\int_D W(\mathbf{F}_0 + \nabla \phi) dx \geq \int_D N(\mathbf{F}_0 + \nabla \phi) dx = N(\mathbf{F}_0) = W(\mathbf{F}_0).$$

Hence, $W(\mathbf{F})$ is quasiconvex at \mathbf{F}_0 . This simple observation is a starting point of the classical approach of Carathéodory’s known as the ‘‘royal road’’ in Calculus of Variations (Young 1969). If $W(\mathbf{F})$ has a supporting null-Lagrangian at \mathbf{F}_0 , we will say that $W(\mathbf{F})$ is polyconvex at \mathbf{F}_0 . The calculation above shows that polyconvexity at \mathbf{F}_0 implies quasiconvexity. The converse is false, unless $\min(m, n) = 1$.

Definition 2.1 The set of points \mathbf{F} , where $W(\mathbf{F})$ is not polyconvex, is called the PC binodal region. The boundary of this region is called the PC binodal.

We remark that the method of supporting null-Lagrangians was applied in the theory of composites under the name of translation method (see Milton 2002 and references therein). The double-tangency trick we are exploiting below was also noted there and is responsible for the optimality of translation bounds in particular regimes (Grabovsky 1996; Chenchiah and Bhattacharya 2008).

Let us examine the implications of existence of a supporting null-Lagrangian at a fixed $\mathbf{F}_0 \in \mathbb{R}^{m \times n}$. Let $\mathfrak{M}(\mathbf{F})$ denote a list of all minors of \mathbf{F} of degree at least 2. Their ordering can be arbitrary, but fixed once chosen. We search for constants $H_0, \mathbf{T}_0, \mathfrak{M}_0$, such that

$$W(\mathbf{F}) \geq N(\mathbf{F}) = H_0 + \langle \mathbf{T}_0, \mathbf{F} \rangle + \langle \mathfrak{M}_0, \mathfrak{M}(\mathbf{F}) \rangle, \tag{2.1}$$

for every $\mathbf{F} \in \mathbb{R}^{m \times n}$, with equality reached at $\mathbf{F} = \mathbf{F}_0$. Here, $\langle \cdot, \cdot \rangle$ denotes the Frobenius inner product of matrices or dot product of vectors. We have written null-Lagrangians of degree 0 and 1 explicitly in (2.1) because their coefficients can be eliminated due to properties (A) and (B). Indeed, condition (A) implies

$$H_0 = W(\mathbf{F}_0) - \langle \mathbf{T}_0, \mathbf{F}_0 \rangle - \langle \mathfrak{M}_0, \mathfrak{M}(\mathbf{F}_0) \rangle.$$

It also follows from (A) and (B) that \mathbf{F}_0 is a global minimizer of the nonnegative smooth function $W(\mathbf{F}) - N(\mathbf{F})$. Therefore,

$$\mathbf{T}_0 = W_{\mathbf{F}}(\mathbf{F}_0) - \mathfrak{M}_{\mathbf{F}}(\mathbf{F}_0)^{\mathbf{T}} \mathfrak{M}_0,$$

where the subscript \mathbf{F} denotes the array of partial derivatives with respect to components of \mathbf{F} and $\mathfrak{M}_{\mathbf{F}}(\mathbf{F}_0)^{\mathbf{T}} \mathfrak{M}_0$ is a $m \times n$ matrix whose (ij) th component is $\mathfrak{M}_{F_{ij}}^{\alpha}(\mathbf{F}_0) \mathfrak{M}_0^{\alpha}$, assuming summation over the repeated index α .

The remaining task is to find constants \mathfrak{M}_0 from the condition

$$\Psi(\mathbf{F}; \mathfrak{M}_0) = \tilde{W}(\mathbf{F}_0, \mathbf{F}) - \langle \mathfrak{M}_0, \tilde{\mathfrak{M}}(\mathbf{F}_0, \mathbf{F}) \rangle \geq 0, \quad (2.2)$$

where

$$\begin{aligned} \tilde{W}(\mathbf{F}, \mathbf{G}) &= W(\mathbf{G}) - W(\mathbf{F}) - \langle W_{\mathbf{F}}(\mathbf{F}), \mathbf{G} - \mathbf{F} \rangle, \\ \tilde{\mathfrak{M}}(\mathbf{F}, \mathbf{G}) &= \mathfrak{M}(\mathbf{G}) - \mathfrak{M}(\mathbf{F}) - \mathfrak{M}_{\mathbf{F}}(\mathbf{F})(\mathbf{G} - \mathbf{F}). \end{aligned}$$

In other words, we need to find a list of constants \mathfrak{M}_0 , such that $\mathbf{F} = \mathbf{F}_0$ is a point of global minimum of $\Psi(\mathbf{F}; \mathfrak{M}_0)$. A necessary condition for (2.2) to hold is the requirement that $\mathbf{F} = \mathbf{F}_0$ is a point of *local* minimum of $\Psi(\mathbf{F}; \mathfrak{M}_0)$. By construction, $\Psi_{\mathbf{F}}(\mathbf{F}_0; \mathfrak{M}_0) = 0$, and therefore it is necessary that

$$\Psi_{\mathbf{F}\mathbf{F}}(\mathbf{F}_0; \mathfrak{M}_0) \geq 0 \quad (2.3)$$

in the sense of quadratic forms.

2.2 The Jump Set

One of the consequences of quasiconvexity at a point (1.2) is rank-one convexity at a point:

$$\tilde{W}(\mathbf{F}_0, \mathbf{F}_0 + \mathbf{a} \otimes \mathbf{n}) \geq 0 \quad (2.4)$$

for every $\mathbf{a} \in \mathbb{R}^m$ and $\mathbf{n} \in \mathbb{R}^n$ (without loss of generality, we can take \mathbf{n} to be a unit vector). Following (Grabovsky and Truskinovsky 2016), we can describe the jump set as the boundary of validity of (2.4). Let us briefly recall the argument.

Condition (2.4) can be restated as the property that

$$w(\mathbf{a}, \mathbf{n}) = \tilde{W}(\mathbf{F}_0, \mathbf{F}_0 + \mathbf{a} \otimes \mathbf{n})$$

has a minimal value 0 (achieved at $\mathbf{a} \otimes \mathbf{n} = 0$). At the boundary of validity of (2.4), the function $w(\mathbf{a}, \mathbf{n})$ will also be minimized at $(\mathbf{a}_0, \mathbf{n}_0) \neq 0$, which leads to equations

$$\begin{cases} w(\mathbf{a}_0, \mathbf{n}_0) = 0, \\ \nabla_{\mathbf{a}} w(\mathbf{a}_0, \mathbf{n}_0) = 0, \\ \nabla_{\mathbf{n}} w(\mathbf{a}_0, \mathbf{n}_0) = 0. \end{cases} \tag{2.5}$$

If we eliminate variables \mathbf{a}_0 and \mathbf{n}_0 from these equations, we obtain a scalar constraint on \mathbf{F}_0 , describing the surface $\mathfrak{J} \subset \mathbb{R}^{m \times n}$, which we call the *jump set*. This name comes from a different way in which the jump set equations arise.

Indeed, in Grabovsky and Truskinovsky (2011) we identified constraints on the traces \mathbf{F}_{\pm} of $\nabla \mathbf{y}(\mathbf{x})$ at a surface of the jump discontinuity of $\nabla \mathbf{y}(\mathbf{x})$, provided $\mathbf{y}(\mathbf{x})$ is a strong local minimizer of an integral functional $E[\mathbf{y}]$. In that context, we can identify \mathbf{F}_- with \mathbf{F}_0 and \mathbf{F}_+ with $\mathbf{F}_0 + \mathbf{a}_0 \otimes \mathbf{n}_0$. Noting that equations of the jump set, found in Grabovsky and Truskinovsky (2011), are invariant with respect to the interchange of \mathbf{F}_+ and \mathbf{F}_- , we can rewrite them in a ‘‘canonical’’ (symmetric) form³

$$\text{rank}[\mathbb{F}] = 1, \tag{2.6}$$

$$\llbracket W_{\mathbf{F}} \rrbracket \llbracket \mathbb{F} \rrbracket^T = 0, \tag{2.7}$$

$$\llbracket W_{\mathbf{F}} \rrbracket^T \llbracket \mathbb{F} \rrbracket = 0, \tag{2.8}$$

$$\llbracket W \rrbracket - \langle W_{\mathbf{F}}^{\pm}, \llbracket \mathbb{F} \rrbracket \rangle = 0. \tag{2.9}$$

where we use the notation $\llbracket A \rrbracket = A_+ - A_-$. In the context of nonlinear elasticity equation (2.6) is the kinematic compatibility condition, arising due to the continuity of the deformation $\mathbf{y}(\mathbf{x})$ across, say, a martensitic phase boundary. Equation (2.7) expresses traction continuity across such interface. Equation (2.9) is known as the Maxwell condition of phase equilibrium (Eshelby 1970).

It is straightforward to show that (2.7)–(2.9) is equivalent to (2.5). Moreover, one can also easily recognize that (2.7)–(2.9) is a vectorial generalization of the well-known Weierstrass–Erdmann corner conditions (Erdmann 1877; Gelfand and Fomin 1963). The fact that the first Weierstrass–Erdmann condition generalizes not to (2.7), but to a pair of equations (2.7), (2.8) is rather remarkable. The variational meaning of (2.8) was elucidated in Grabovsky and Truskinovsky (2011) where it was shown that it is related to a roughening instability of an interface.

For our purposes, we will only need the fact that that all points $\mathbf{F}_{\pm} \in \mathfrak{J}$ belong to the boundary of validity of rank-one convexity (2.4). Then, if $W(\mathbf{F})$ is quasiconvex at \mathbf{F}_{\pm} , these points also lie on the QC binodal. The main idea of our approach is that quasiconvexity at such points \mathbf{F}_{\pm} can be proved by establishing a more transparent property: the polyconvexity.

³ The canonical form of the jump set equations not only highlights the symmetry between phases $\mathbf{F}_+ \leftrightarrow \mathbf{F}_-$, but also emphasizes the symmetry between the strain and the stress.

3 PC Binodal

We now return to the inequality (2.2) that guarantees polyconvexity at F_0 and examine the boundary of its validity. As we cross such boundary, two things may happen. Either $F = F_0$ ceases to be a point of local minimum, which could be detected by the quadratic form in (2.3) becoming degenerate, or it may stop being a global minimum before it stops being a local minimum.

We focus on the latter possibility, since, by analogy with the convex envelope, it should be the primary mode of polyconvexity failure for non-polyconvex energies. Let us consider the case where on the PC binodal there appears a single additional global minimizer $F^* \neq F_0$ of $\Psi(F; \mathfrak{M}_0)$. Then, we must have

$$\Psi(F^*; \mathfrak{M}_0) = 0, \quad \Psi_F(F^*; \mathfrak{M}_0) = 0, \quad (3.1)$$

Let us assume, in addition to (3.1), that

$$\Psi_{FF}(F_0; \mathfrak{M}_0) > 0, \quad \Psi_{FF}(F^*; \mathfrak{M}_0) > 0, \quad (3.2)$$

which is sufficient to ensure that F_0 and F^* are local minima of $\Psi(F; \mathfrak{M}_0)$. We also assume that $\Psi(F; \mathfrak{M}_0) > 0$ for every $F \notin \{F_0, F^*\}$, guaranteeing that F_0 and F^* are the only global minimizers of $\Psi(F; \mathfrak{M}_0)$.

Now, for the sake of the foregoing argument we assume that $W(F)$ has very rapid growth at infinity, say $W(F)/|F|^{\min(m,n)} \rightarrow \infty$, when $|F| \rightarrow \infty$. We will then derive a set of equations to be satisfied by the unknowns F_0 , F^* and \mathfrak{M}_0 . We emphasize that our method consists of choosing these parameters according to the derived constraints for *all* smooth functions $W(F)$, regardless of their growth at infinity, since the success or failure of the method consists entirely in the outcome of establishing inequality (2.2) for the chosen values of the parameters.

Assuming sufficiently fast growth of $W(F)$ at infinity, we can conclude that $\Psi(F; \mathfrak{M}_0) \rightarrow \infty$, when $|F| \rightarrow \infty$ uniformly in \mathfrak{M}_0 on compact sets.

Lemma 3.1 *Suppose that $W(F)$ is of class C^3 and*

$$\lim_{|F| \rightarrow \infty} \frac{W(F)}{|F|^{\min(m,n)}} = +\infty$$

Suppose that for a particular choice of parameters F_0 , F^ and \mathfrak{M}_0 , we have*

- (i) $\Psi(F^*, \mathfrak{M}_0) = 0$
- (ii) $\Psi(F, \mathfrak{M}_0) > 0$, $\forall F \notin \{F^*, F_0\}$
- (iii) $\Psi_{FF}(F_0, \mathfrak{M}_0) > 0$ and $\Psi_{FF}(F^*, \mathfrak{M}_0) > 0$ in the sense of quadratic forms.

Suppose further that

$$\Psi_{\mathfrak{M}_0}(F^*; \mathfrak{M}_0) \neq 0.$$

Then, there exists $\delta > 0$, so that for all $\hat{F}_0 \in B(F_0, \delta)$ there exist constants $\widehat{\mathfrak{M}}_0$ for which $\hat{\Psi}(F; \widehat{\mathfrak{M}}_0) \geq 0$ for all $F \in \mathbb{R}^{m \times n}$, where $\hat{\Psi}$ is defined in (2.2) with F_0 , replaced by \hat{F}_0 .

The proof of this lemma is given in ‘‘Appendix A.’’ However, it is easy to explain why it should be true. Indeed, if $\Psi_{\mathfrak{M}_0}(F^*; \mathfrak{M}_0) \neq 0$, then we can always choose constants $\widehat{\mathfrak{M}}_0$, sufficiently close to \mathfrak{M}_0 for which $\Psi(F^*; \widehat{\mathfrak{M}}_0) > 0$. By continuity, $\hat{\Psi}(F; \widehat{\mathfrak{M}}_0) > 0$ for all \hat{F}_0 sufficiently close to F_0 and all F sufficiently close to F^* , as well as for all F away from F_0 and F^* . By continuity of second derivatives, $\hat{\Psi}(F; \widehat{\mathfrak{M}}_0)$ would still have a local minimum at $F = \hat{F}_0$, showing that F_0 is in the interior of the region of polyconvexity of $W(F)$. Hence, Lemma 3.1 implies that for F_0 to lie on the PC binodal we must require that

$$\widetilde{\mathfrak{M}}(F_0, F^*) = \Psi_{\mathfrak{M}_0}(F^*; \mathfrak{M}_0) = 0. \tag{3.3}$$

It remains to observe that Eq. (3.3) is equivalent to

$$\text{rank}(F^* - F_0) = 1. \tag{3.4}$$

Indeed, if $M(F)$ is a 2×2 minor of F , then it is quadratic and homogeneous and therefore

$$\widetilde{M}(F_0, F^*) = M(F^* - F_0) = 0,$$

which implies (3.4). Conversely, (3.4) implies (3.3). Indeed, the ‘‘Weierstrass operator’’ $U \mapsto \widetilde{U}$ annihilates all affine functions of F . But every minor of F is quasi-affine, i.e., affine along rank-one directions. Therefore, $\widetilde{\mathfrak{M}}(F_0, F^*) = 0$, provided (3.4) holds. This argument explains why similar observation could be made in the study of energy-minimizing composites (Grabovsky 1996; Chenchiah and Bhattacharya 2008; Antimonov et al. 2016), where the choice of $W(F)$ was particular (minimum of two linearly elastic wells).

The rank-one relation (3.4) suggests a link with the jump set. For this reason, we change notations

$$F_- = F_0, \quad F_+ = F^*, \quad P_{\pm} = W_F(F_{\pm}), \tag{3.5}$$

so that (3.4) coincides with (2.6). We will now show that Eq. (3.1) implies (2.7)–(2.9). The first equation in (3.1) becomes

$$\widetilde{W}(F_-, F_+) = \llbracket W \rrbracket - \langle P_-, \llbracket F \rrbracket \rangle = 0, \tag{3.6}$$

since $\widetilde{\mathfrak{M}}(F_0, F^*) = 0$. Given that $N(F)$ is a null-Lagrangian, $N(F + \llbracket F \rrbracket)$ must also be null-Lagrangian. Hence, Eq. (3.6) must also hold if we switch the plus and the minus subscripts in F . In other words, (3.6) must have a symmetric counterpart

$$\widetilde{W}(F_+, F_-) = -\llbracket W \rrbracket + \langle P_+, \llbracket F \rrbracket \rangle = 0. \tag{3.7}$$

This establishes (2.9).

The second equation in (3.1) can be written as

$$\llbracket P \rrbracket = \llbracket \mathfrak{M}_F^T \rrbracket \mathfrak{M}_0. \tag{3.8}$$

We will now show that Eq. (3.8) implies both (2.7) and (2.8). Indeed, (3.8) is a linear system for constants \mathfrak{M}_0 . By the Fredholm alternative, Eq. (3.8) is solvable if and only if

$$\langle \llbracket P \rrbracket, K \rangle = 0, \quad \forall K : \llbracket \mathfrak{M}_F \rrbracket K = 0. \tag{3.9}$$

Suppose that $N(F)$ is an arbitrary null-Lagrangian. Then,

$$N(F + u \otimes v) = N(F) + \langle N_F(F), u \otimes v \rangle, \tag{3.10}$$

for all u and v . Differentiating (3.10) with respect to u and v , we obtain

$$\langle (N_F(F + u \otimes v) - N_F(F)), \dot{u} \otimes v + u \otimes \dot{v} \rangle = 0,$$

where $\dot{u} \in \mathbb{R}^m$ and $\dot{v} \in \mathbb{R}^n$ can be arbitrary. It is evident now that all K of the form $K = b \otimes n + a \otimes m$, $b \in \mathbb{R}^m$, $m \in \mathbb{R}^n$, where $\llbracket F \rrbracket = a \otimes n$ satisfy $\llbracket \mathfrak{M}_F \rrbracket K = 0$. Hence, according to (3.9), solvability of (3.8) implies

$$\begin{cases} \llbracket P \rrbracket n = 0, \\ \llbracket P \rrbracket^T a = 0. \end{cases} \tag{3.11}$$

The first equation in (3.11) is equivalent to (2.7), while the second, to (2.8).

In particularly important cases $m = n = 2$ or 3 , we can describe the set of solutions of (3.8) explicitly. When $m = n = 2$,

$$\Psi(F; m_0) = \tilde{W}(F_0, F) - m_0 \det(F - F_0). \tag{3.12}$$

where

$$m_0 = \frac{\langle \llbracket P \rrbracket, \text{cof} \llbracket F \rrbracket \rangle}{|\llbracket F \rrbracket|^2}. \tag{3.13}$$

In addition, inequalities (3.2) become

$$\langle W_{FF}(F_{\pm}) \xi, \xi \rangle - 2m_0 \det \xi > 0 \tag{3.14}$$

for all 2×2 matrices ξ . The points F_{\pm} where at least one of them fails the non-strict version of (3.14) must lie in the interior of the binodal region. Inequalities (3.14) are equivalent to the Legendre–Hadamard conditions for two-phase configurations (Grabovsky and Truskinovsky 2016).

If $m = n = 3$

$$\Psi(F; \mathbf{b}_0, \mathbf{m}_0, m_0) = \tilde{W}(F_0, F) - \langle \text{cof}(F - F_0), M_0 \rangle - m_0 \det(F - F_0), \tag{3.15}$$

where

$$M_0 = \frac{(\nabla \text{cof} \llbracket F \rrbracket) \llbracket P \rrbracket}{\|\llbracket F \rrbracket\|^2} + a \otimes m_0 + b_0 \otimes n, \tag{3.16}$$

where $\llbracket F \rrbracket = F^* - F_0 = a \otimes n$, while $b_0 \in \mathbb{R}^3$, $m_0 \in \mathbb{R}^3$ and $m_0 \in \mathbb{R}$ are free parameters. Inequalities (3.2) become

$$\begin{cases} \langle W_{FF}(F_-)\xi, \xi \rangle - 2\langle \text{cof} \xi, M_0 \rangle > 0, \\ \langle W_{FF}(F_+)\xi, \xi \rangle - 2\langle \text{cof} \xi, M_0 + m_0 \llbracket F \rrbracket \rangle > 0 \end{cases} \tag{3.17}$$

and provide restrictions on the possible values of the free parameters, which need to be determined from the condition

$$\min_F \Psi(F; b_0, m_0, m_0) = 0. \tag{3.18}$$

If (3.18) is impossible to satisfy, then polyconvexity at F_0 fails.

4 Relaxed Energy

There is an additional “bonus” for proving quasiconvexity of $W(F)$ at $F_{\pm} \in \mathfrak{J}$ in the form of the explicit formula for $QW(F)$ —the quasiconvex envelope of $W(F)$ (Dacorogna 1982) as described by the theorem below (Grabovsky and Truskinovsky 2014).

Theorem 4.1 *Suppose F_{\pm} is the corresponding pair of points on the jump set and $W(F)$ is quasiconvex at F_+ (or F_-). Then, $W(F)$ is quasiconvex at F_- (or F_+) and for any $\lambda \in [0, 1]$*

$$QW(\lambda F_+ + (1 - \lambda)F_-) = \lambda W(F_+) + (1 - \lambda)W(F_-). \tag{4.1}$$

Of course, under the assumptions of Theorem 4.1 equality $QW(F_0) = RW(F_0)$ holds at all $F_0 = \lambda F_+ + (1 - \lambda)F_-$.

We can also use the right-hand side of (4.1) to define a function $\overline{W}(F)$ for all pairs F_{\pm} , without verifying quasiconvexity. $\overline{W}(F)$ can be called simple laminate-relaxation of $W(F)$. Its QC (and RC) binodal contains points on the binodal of $W(F)$, not described by Theorem 4.1. Hence, applying our method to \overline{W} can reveal other common parts of the QC and RC binodals, corresponding to higher-order laminate-relaxations of $W(F)$. However, one would have to confront increasingly more complex algebraic problems.

One drawback of the method is that establishing (2.2) may depend on $W(F)$ outside of the binodal region. However, if we change our goal from proving $W(F_0) = QW(F_0)$ to proving $W(F_0) = RW(F_0)$, where RW is the rank-one convex envelope of $W(F)$, then the method can be applied to a modified energy density $\widehat{W}(F)$, which is set to $+\infty$ in regions where we already know that $RW(F) = W(F)$. Theorem B.2

in “Appendix B” shows that such modifications do not affect the rank-one convex envelope, and therefore, if the method is successful for $\widehat{W}(\mathbf{F})$ at \mathbf{F}_0 , then

$$RW(\mathbf{F}_0) = R\widehat{W}(\mathbf{F}_0) = Q\widehat{W}(\mathbf{F}_0) = \widehat{W}(\mathbf{F}_0) = W(\mathbf{F}_0),$$

even if the method fails for the original energy density. The modification trick does not work for the quasiconvex envelopes because of the inherent “non-locality” of the quasiconvexity condition (Kristensen 1999, 2000). An effective numerical algorithm to compute the rank-one convexification of $W(\mathbf{F})$ was recently developed in Oberman and Ruan (2017). Both the new and the older algorithm (Dolzmann 1999) implement a similar iterative procedure numerically.

5 Example

To illustrate the effectiveness of the proposed method, consider a simple example of “geometrically linearized” Hadamard material (Hadamard 1903; John 1966). Starting with $W(\mathbf{F}) = h(\det \mathbf{F}) + \mu|\mathbf{F}|^2$, we can use the “geometric” approximation $\det \mathbf{F} \approx 1 + \text{Tr}(\mathbf{F} - \mathbf{I})$, which is valid in the limit $\mathbf{F} \rightarrow \mathbf{I}$; however, the formal asymptotic expansion with respect to a small parameter would also induce physical linearization and would trivialize the problem. For rigorous linearization of multi-well energies, see (Schmidt 2008; Agostiniani et al. 2015; Alicandro et al. 2017). To avoid this, we view the Hadamard material only as a motivation and study below the ad hoc energy

$$W(\mathbf{F}) = f(\theta) + \mu|\boldsymbol{\varepsilon}|^2 + \mu'|\boldsymbol{\Omega}|^2, \quad \mu > 0, \mu + \mu' > 0, \quad (5.1)$$

where

$$\theta = \text{Tr} \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} = \frac{1}{2}(\mathbf{F} + \mathbf{F}^T), \quad \boldsymbol{\Omega} = \frac{1}{2}(\mathbf{F} - \mathbf{F}^T). \quad (5.2)$$

To ensure the existence of a QC binodal, we assume that the function $f(\theta)$ has a double-well shape, illustrated in Fig. 1a.

Remark 5.1 Usually, geometrically linear but physically nonlinear theory of elasticity deals with the energies of form $W(\mathbf{F}) = \widehat{W}(\boldsymbol{\varepsilon})$; see for instance (Khachaturyan 1983; Budiansky et al. 1983; Kaganova and Roytburd 1988; Abeyaratne and Guo-Hua 1989a,b). In the case of Hadamard material, the term $\mu|\mathbf{F}|^2$ is already quadratic and applying geometric linearization only to the nonlinear term, we obtain the model (5.1) with $\mu' = \mu$. In the absence of rigorous derivation of such model we have no compelling reason to set $\mu' = 0$. Therefore, we study (5.1) in the entire range of parameters μ, μ' which obviously includes sub-cases $\mu' = 0$ and $\mu' = \mu$.

The first step of the method is to characterize the jump set by solving (2.6)–(2.9). Given that $\llbracket \mathbf{F} \rrbracket = \mathbf{a} \otimes \mathbf{n}$ and

$$W_{\mathbf{F}}(\mathbf{F}) = f'(\text{Tr} \boldsymbol{\varepsilon})\mathbf{I} + 2\mu\boldsymbol{\varepsilon} + 2\mu'\boldsymbol{\Omega},$$

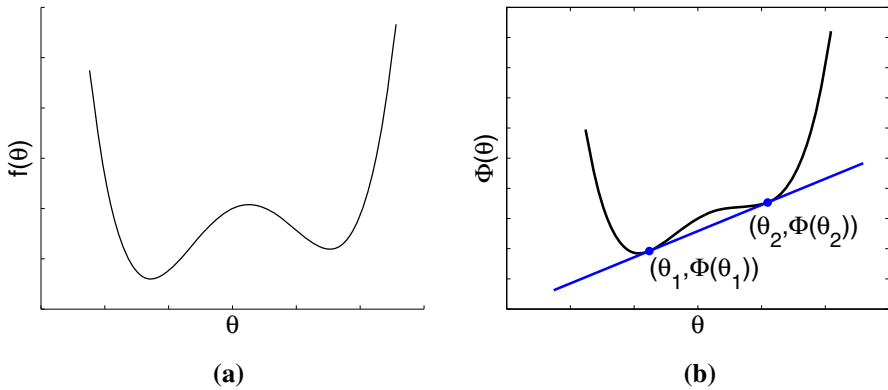


Fig. 1 **a** Double-well nonlinearity in a geometrically linear Hadamard material; **b** common tangent to the graph of $\Phi(\theta)$

we obtain

$$\llbracket W_F \rrbracket = \llbracket f' \rrbracket \mathbf{I} + \mu(\mathbf{a} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{a}) + \mu'(\mathbf{a} \otimes \mathbf{n} - \mathbf{n} \otimes \mathbf{a}). \tag{5.3}$$

Equations (2.7) and (2.8) take the form

$$\begin{cases} \langle \llbracket f' \rrbracket + (\mu - \mu') \langle \mathbf{a}, \mathbf{n} \rangle \rangle \mathbf{n} + (\mu + \mu') \mathbf{a} = 0 \\ \langle \llbracket f' \rrbracket + (\mu - \mu') \langle \mathbf{a}, \mathbf{n} \rangle \rangle \mathbf{a} + |\mathbf{a}|^2 (\mu + \mu') \mathbf{n} = 0. \end{cases}$$

Since $\mu + \mu' > 0$, we can conclude that $\mathbf{a} = \alpha \mathbf{n}$ for some $\alpha \neq 0$. Therefore, $\alpha = -\llbracket f' \rrbracket / 2\mu$.

Now, taking the trace of $\llbracket \mathbf{F} \rrbracket = \alpha \mathbf{n} \otimes \mathbf{n}$ we obtain that $\alpha = \llbracket \theta \rrbracket$. Equations (2.6)–(2.8) can be summarized as follows

$$\begin{cases} \llbracket f' + 2\mu\theta \rrbracket = 0, \\ \llbracket \mathbf{F} \rrbracket = \llbracket \theta \rrbracket \mathbf{n} \otimes \mathbf{n}, \\ \llbracket W_F \rrbracket = -2\mu \llbracket \theta \rrbracket (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}). \end{cases} \tag{5.4}$$

In order to simplify the Maxwell relation (2.9), we take the average⁴ of the two equations in (2.9) to obtain

$$\llbracket W \rrbracket - \langle \llbracket W_F \rrbracket, \llbracket \mathbf{F} \rrbracket \rangle = 0,$$

where $\llbracket A \rrbracket = \frac{1}{2}(A^+ + A^-)$. The advantage for writing the Maxwell condition in this way is that it annihilates all polynomial contributions of up to degree 2 in \mathbf{F} .

⁴ Since the two equations in (2.9) are equivalent, we can use only one or only the other or an arbitrary linear combination of the two.

Therefore, we obtain

$$\llbracket f \rrbracket - \{ f' \} \llbracket \theta \rrbracket = 0. \quad (5.5)$$

Note that neither μ nor μ' enters this equation, since they are contained in the quadratic term of the energy. We can use the degree 2 polynomial annihilation property again in order to see the geometric meaning of the first equation in (5.4) coupled with (5.5). Defining

$$\Phi(\theta) = f(\theta) + \mu\theta^2, \quad (5.6)$$

we can now rewrite the entire jump set system in the form

$$\begin{cases} \llbracket \Phi' \rrbracket = 0, \\ \llbracket \Phi \rrbracket - \{ \Phi' \} \llbracket \theta \rrbracket = 0, \\ \llbracket \mathbf{F} \rrbracket = \llbracket \theta \rrbracket \mathbf{n} \otimes \mathbf{n}, \\ \llbracket W_{\mathbf{F}} \rrbracket = -2\mu \llbracket \theta \rrbracket (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}). \end{cases} \quad (5.7)$$

The first two equations in (5.7) are scalar, and they imply that $\theta_- = \theta_1$ and $\theta_+ = \theta_2$, where θ_1 and θ_2 are the two points of common tangency to the graph of $\Phi(\theta)$, shown in Fig. 1b. The conclusion is that the jump set \mathfrak{J} for the energy (5.1) is the union of two disjoint hyperplanes

$$\mathfrak{J}_- = \{ \mathbf{F} \in \mathbb{M} : \text{Tr } \mathbf{F} = \theta_1 \}, \quad \mathfrak{J}_+ = \{ \mathbf{F} \in \mathbb{M} : \text{Tr } \mathbf{F} = \theta_2 \}.$$

We recall (Grabovsky and Truskinovsky 2011) that the region

$$\mathcal{B}_0 = \{ \mathbf{F} \in \mathbb{M} : \theta_1 < \text{Tr } \mathbf{F} < \theta_2 \}$$

bounded by jump set always fails the Weierstrass positivity condition (2.4).

We are now in a position to establish polyconvexity for the entire jump set \mathfrak{J} in two space dimensions. Formulas (3.13) and (5.7) give $m_0 = -2\mu$, and hence (3.12) becomes

$$\Psi_{\pm}(\mathbf{F}) = \tilde{f}(\theta_{\pm}, \gamma) + \mu |\boldsymbol{\varepsilon}|^2 + 2\mu' \omega^2 + 2\mu(\det \boldsymbol{\varepsilon} + \omega^2),$$

where

$$\mathbf{F} = \mathbf{F}_{\pm} + \boldsymbol{\varepsilon} + \omega \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \gamma = \text{Tr } \mathbf{F}.$$

By assumption, $\mu + \mu' > 0$, and therefore $\Psi_{\pm}(\mathbf{F})$ is minimized when $\omega = 0$. We also have (for any symmetric matrix $\boldsymbol{\varepsilon}$)

$$|\boldsymbol{\varepsilon}|^2 + 2 \det \boldsymbol{\varepsilon} = (\text{Tr } \boldsymbol{\varepsilon})^2 = (\gamma - \theta_{\pm})^2.$$

Hence,

$$\min_{\mathbf{F}} \Psi_{\pm}(\mathbf{F}) = \min_{\gamma} \tilde{\Phi}(\theta_{\pm}, \gamma) = 0,$$

and the common tangent to the graph of $\Phi(\theta)$ at θ_{\pm} is a supporting line, as shown in Fig. 1b. The polyconvexity of the jump set is now established.

Consider next the three-dimensional case. Formulas (3.16) and (5.7) give

$$M_0 = -2\mu(I_3 - n \otimes n) + n \otimes m_0 + b_0 \otimes n, \tag{5.8}$$

and hence (3.15) becomes

$$\Psi_{\pm}(F; b_0, m_0) = \tilde{f}(\theta_{\pm}, \gamma) + \mu|\boldsymbol{\varepsilon}|^2 + \mu'|\boldsymbol{\Omega}|^2 - \langle M_0, \text{cof}(F - F_{\pm}) \rangle - m_0 \det(F - F_{\pm}).$$

From this form, it is immediately clear that we must choose $m_0 = 0$, since $\det F$ has cubic growth at infinity, even if we fix $\gamma = \text{Tr } F$. This will make $\min_F \Psi_{\pm} = -\infty$, if $m_0 \neq 0$. Using the orthogonal decomposition

$$F - F_{\pm} = D + \frac{\eta}{3}I_3 + \boldsymbol{\Omega}, \quad D = \boldsymbol{\varepsilon} - \frac{1}{3}(\text{Tr } \boldsymbol{\varepsilon})I_3, \quad \eta = \gamma - \theta_{\pm},$$

we can conclude that $\Psi_{\pm}(F; b_0, m_0)$ is quadratic in D and $\boldsymbol{\Omega}$. We can therefore minimize Ψ_{\pm} in D and $\boldsymbol{\Omega}$ (constraining free parameters b_0 and m_0 so that the minimum value is not $-\infty$).

It will be convenient to parametrize 3×3 antisymmetric matrices by vectors $\boldsymbol{\omega} \in \mathbb{R}^3$, so that $\boldsymbol{\Omega}u = \boldsymbol{\omega} \times u$ and in what follows we will use for this mapping the notation $\boldsymbol{\Omega} = \boldsymbol{\Omega}(\boldsymbol{\omega})$. Then,

$$\Psi_{\pm}(H; b_0, m_0) = \tilde{f}(\theta_{\pm}, \gamma) + \mu|\boldsymbol{\varepsilon}|^2 + 2\mu'|\boldsymbol{\omega}|^2 - \langle M_0, \text{cof } \boldsymbol{\varepsilon} + \boldsymbol{\omega} \otimes \boldsymbol{\omega} + \boldsymbol{\Omega}(\boldsymbol{\varepsilon}\boldsymbol{\omega}) \rangle.$$

Now, we see that using formula (5.8) for M_0 is less convenient than separating its symmetric and antisymmetric parts:

$$M_0 = -2\mu(I_3 - n \otimes n) + n \odot u + \boldsymbol{\Omega}(n \times \boldsymbol{\varepsilon}), \quad n \odot u = \frac{1}{2}(n \otimes u + u \otimes n).$$

It is evident that we can set $\boldsymbol{\varepsilon} = 0$ because (setting $\gamma = \theta_{\pm}$) the nonnegativity of the quadratic forms $\mu|D|^2 + \langle M_0, \text{cof } D \rangle$ and $2\mu'|\boldsymbol{\omega}|^2 + \langle M_0\boldsymbol{\omega}, \boldsymbol{\omega} \rangle$ is already necessary. The nonnegativity of the latter form is equivalent to

$$\langle u, n \rangle \leq 2\mu'. \tag{5.9}$$

Hence, we obtain

$$\Psi_{\pm}(F; u) = \tilde{f}(\theta_{\pm}, \gamma) + \mu|\boldsymbol{\varepsilon}|^2 + 2\mu\langle I_3 - n \odot v, \text{cof } \boldsymbol{\varepsilon} \rangle, \quad v = \frac{u}{2\mu} + n,$$

where the constraint (5.9) becomes

$$\langle v, n \rangle \leq \frac{\mu + \mu'}{\mu}. \tag{5.10}$$

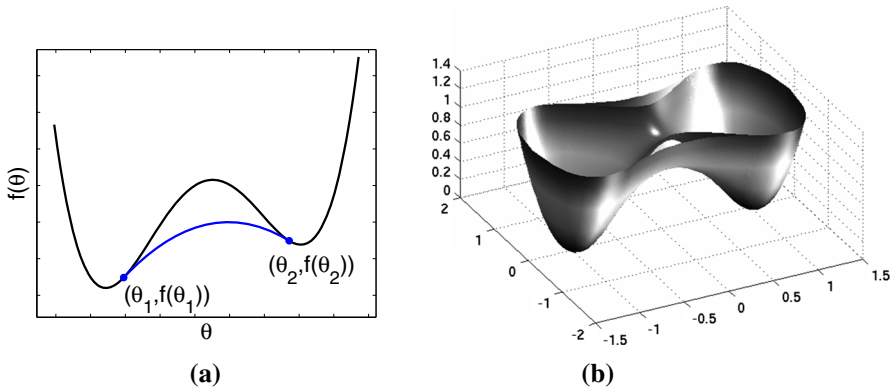


Fig. 2 **a** The graph of $f^{qc}(\theta)$ for the example; **b** relaxed energy $QW(F)$ restricted to diagonal 2×2 matrices F in the (F_{11}, F_{22}) -plane

If we decompose $\boldsymbol{\varepsilon} = \mathbf{D} + (\eta/3)\mathbf{I}_3$, we can use the relations

$$|\boldsymbol{\varepsilon}|^2 = |\mathbf{D}|^2 + \frac{\eta^2}{3}, \quad \text{cof} \boldsymbol{\varepsilon} = \text{cof} \mathbf{D} - \frac{\eta}{3} \mathbf{D} + \frac{\eta^2}{9} \mathbf{I}_3.$$

Observing that for symmetric trace-free 3×3 matrices $\text{Tr} \text{cof} \mathbf{D} = -|\mathbf{D}|^2/2$, we can write

$$\Psi_{\pm}(\mathbf{H}; \mathbf{u}) = \tilde{f}(\theta_{\pm}, \gamma) + \mu\eta^2 - 2\mu \left\langle \mathbf{n} \odot \mathbf{v}, \text{cof} \mathbf{D} - \frac{\eta}{3} \mathbf{D} + \frac{\eta^2}{9} \mathbf{I}_3 \right\rangle.$$

Since

$$\tilde{f}(\theta_{\pm}, \gamma) + \mu\eta^2 = \tilde{\Phi}(\theta_{\pm}, \gamma) \geq 0,$$

we see that setting $\mathbf{v} = 0$ [which satisfies (5.10)] completes the proof of polyconvexity at \mathbf{F}_{\pm} .

As we have already mentioned, polyconvexity and a fortiori quasiconvexity at \mathbf{F}_{\pm} implies a simple formula (4.1) for the quasiconvex envelope of W . In the case of the energy density (5.1), we obtain

$$QW(\mathbf{F}) = f^{qc}(\text{Tr} \mathbf{F}) + \mu|\boldsymbol{\varepsilon}|^2 + \mu'|\boldsymbol{\Omega}|^2, \tag{5.11}$$

where

$$f^{qc}(\theta) = \begin{cases} f(\theta), & \mathbf{F} \notin \mathcal{B}_0, \\ \{\{ f' \}\}(\theta - \{\{ \theta \}\}) + \{\{ f \}\} + \mu(\theta - \theta_1)(\theta_2 - \theta), & \mathbf{F} \in \mathcal{B}_0, \end{cases} \tag{5.12}$$

where $\{\{ f \}\}, \{\{ \theta \}\}$ are constants, independent of θ .

In conclusion, we note that we can write the energy (5.1) as

$$W(\mathbf{F}) = g(\theta) + \mu |\operatorname{dev}(\boldsymbol{\epsilon})|^2 + \mu' |\boldsymbol{\Omega}|^2,$$

where $g(\theta) = f(\theta) + \theta^2/n$, where $n = 2$ or 3 is the space dimension. In this form, the *convexification* of $W(\mathbf{F})$ is obviously

$$CW(\mathbf{F}) = Cg(\theta) + \mu |\operatorname{dev}(\boldsymbol{\epsilon})|^2 + \mu' |\boldsymbol{\Omega}|^2,$$

where $Cg(\theta)$ is the convexification of $g(\theta)$. By contrast [see (C.4)]

$$QW(\mathbf{F}) = g^{\text{qc}}(\theta) + \mu |\operatorname{dev}(\boldsymbol{\epsilon})|^2 + \mu' |\boldsymbol{\Omega}|^2,$$

where

$$g^{\text{qc}}(\theta) = C\Phi(\theta) - \frac{n-1}{n}\theta^2.$$

Hence, $g^{\text{qc}}(\theta)$ is quadratic in θ on $[\theta_1, \theta_2]$, see a double-tangent downward-facing parabola in Fig. 2a. By contrast, convexification of $W(\mathbf{F})$ would be represented by a double-tangent straight line on the graph of $g(\theta)$. Behind this purely vectorial effect is the fact that we had to replace affine functions by quasi-affine functions in (2.1). The supporting quasi-affine function used in our method is necessarily quadratic because of the quadratic rate of growth of the energy at infinity in all directions perpendicular to multiples of the identity. The same structure of $QW(\mathbf{F})$ is obtained in the case of piece-wise quadratic double-well energy in Kohn (1991) and for the same reason.

The graphs of the entire energies $W(\mathbf{F})$ and $QW(\mathbf{F})$, restricted to diagonal matrices, are shown in Fig. 2b.

Remark 5.2 For our geometrically linear example (5.1), the quasiconvexification of $W(\mathbf{F})$ can be also computed directly; see “Appendix C.” However, in the nontrivial case of a geometrically nonlinear Hadamard material with double-well dependence on the determinant, the shortcut discussed in “Appendix C” won’t work, while the general method developed in this paper is still applicable. A preliminary study suggests that our approach allows one to fully characterize the function $QW(\mathbf{F})$ for such materials when the parameter μ is sufficiently large.

6 Conclusions

The proposed approach is based on a simple observation that the part of the PC binodal, characterized by double-tangency of supporting null-Lagrangians, must necessarily belong to the jump set, and therefore to the QC binodal. While the jump set and PC binodal are known to provide bounds from the inside and from the outside for the QC binodal, the general nature of bound collapse was not noticed before.

The main advantage of the proposed approach is that it is fully algebraic and therefore constructive. The first step of the method is to compute the jump set \mathfrak{J} by solving

algebraic equations (2.6)–(2.9). Then, for each point $F_0 \in \mathfrak{J}$ the point of second tangency F^* is uniquely determined. Next, one needs to verify algebraic conditions (2.2), where the constants \mathfrak{M}_0 satisfy (3.8). In the special case $m = n = 2$, the method delivers explicit values for \mathfrak{M}_0 , while when $m = n = 3$ the method determines 4 out of 10 constants \mathfrak{M}_0 ; see (3.15), (3.16). For large values of m and n , the number of constants in \mathfrak{M}_0 is vastly larger than mn , and hence the practical value of the method rapidly diminishes with growth of the dimensions.

Nevertheless, in the important case of nonlinear elasticity with $m = n \leq 3$ the method can be very effective. We illustrated the workings of the method on a nontrivial model example, where it produced optimal answers, in the sense that the whole quasiconvex envelope could be reconstructed analytically. The generality of the algorithm allows the method to be applied systematically to problems for which finding directly the quasiconvexification of the energy is currently beyond reach.

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A Proof of Lemma 3.1

Lemma A.1 *Suppose $f(x, \mathbf{m})$ is a smooth (C^2 is enough) function on $\mathbb{R}^d \times B(0, 1)$, where $B(0, 1)$ is a unit ball in \mathbb{R}^N . We assume that $f(x, \mathbf{m}) > 1$ for all $|x| > R$ and all $\mathbf{m} \in B(0, 1)$ for some uniform constant R . Suppose that there exists $x_0 \neq 0$, such that $x = 0$ and $x = x_0$ are the only global minimizers of $f(x, 0)$. Specifically,*

- (i) $f(0, 0) = f(x_0, 0) = 0$,
- (ii) $f_{xx}(0, 0) > 0$ and $f_{xx}(x_0, 0) > 0$ in the sense of quadratic forms
- (iii) $f(0, \mathbf{m}) = 0$, $f_x(0, \mathbf{m}) = 0$, $\mathbf{m} \in B(0, 1)$,

Suppose that $f_{\mathbf{m}}(x_0, 0) \neq 0$. Then, for any $\delta \in (0, 1)$ there exists $\mathbf{m} \in B(0, \delta)$ so that $f(x, \mathbf{m}) > 0$ for all $x \neq 0$.

Proof Let us first examine what happens in the neighborhoods of 0 and x_0 . Near $x = 0$, we have

$$\begin{aligned} f(x, \mathbf{m}) &= f(0, \mathbf{m}) + \langle f_x(0, \mathbf{m}), x \rangle + \frac{1}{2} \langle f_{xx}(0, \mathbf{m})x, x \rangle + o(|x|^2) \\ &= \frac{1}{2} \langle f_{xx}(0, \mathbf{m})x, x \rangle + o(|x|^2). \end{aligned}$$

By continuity of second derivatives, there exist $\delta_0 > 0$ and $c_0 > 0$, so that $f(x, \mathbf{m}) \geq c_0|x|^2$ for all $|x| < \delta_0$, $|\mathbf{m}| < \delta_0$. In the neighborhood of x_0 , we have

$$\begin{aligned} f(x, \mathbf{m}) &= f(x, 0) + \langle f_{\mathbf{m}}(x, 0), \mathbf{m} \rangle + O(|\mathbf{m}|^2) \\ &= f(x, 0) + \langle f_{\mathbf{m}}(x_0, 0), \mathbf{m} \rangle + O(|x - x_0||\mathbf{m}|) + O(|\mathbf{m}|^2). \end{aligned}$$

By assumption, there exists $\delta_0 > 0$ and $c_0 > 0$ (we are using the same notation each time instead of δ_1, c_1, \dots , ultimately choosing the smallest δ_j and c_j), such that $f(x, 0) \geq c_0|x - x_0|^2$ for all $|x - x_0| < \delta_0$. Thus, there exists $C > 0$, so that

$$f(x, \mathbf{m}) \geq c_0|x - x_0|^2 + \langle f_{\mathbf{m}}(x_0, 0), \mathbf{m} \rangle - C(|x - x_0||\mathbf{m}| + |\mathbf{m}|^2),$$

for all $|\mathbf{m}| < \delta_0$ and $|x - x_0| < \delta_0$. Using the inequality

$$2|x - x_0||\mathbf{m}| \leq k|x - x_0|^2 + \frac{|\mathbf{m}|^2}{k}$$

with $k = c_0/(2C)$ we conclude that

$$f(x, \mathbf{m}) \geq \frac{c_0}{2}|x - x_0|^2 + \langle f_{\mathbf{m}}(x_0, 0), \mathbf{m} \rangle - C|\mathbf{m}|^2,$$

If $f_{\mathbf{m}}(x_0, 0) \neq 0$, then we can choose a unit vector $u_0 \in \mathbb{R}^N$, such that $\langle f_{\mathbf{m}}(x_0, 0), u_0 \rangle > 0$. Therefore, there exists $\delta_0 > 0$, so that for all $|x - x_0| < \delta_0$ and all $\delta \in (0, \delta_0)$

$$f(x, \delta u_0) \geq \frac{c_0}{8}|x - x_0|^2 + \frac{\delta}{2}\langle f_{\mathbf{m}}(x_0, 0), u_0 \rangle$$

This shows that $f(x, \delta u_0) > 0$ for all $\delta \in (0, \delta_0)$ and all $|x - x_0| < \delta_0$.

By our assumption $f(x, 0) > \gamma_0 > 0$ for all x outside of $B(0, \delta_0) \cup B(x_0, \delta_0)$. By smoothness, there is a constant $C > 0$, so that

$$|f(x, \delta u_0) - f(x, 0)| < C\delta$$

for all $|x| < R$, and therefore, $f(x, \mathbf{m}) > \gamma_0/2 > 0$ for all $|\mathbf{m}| < \delta$ and all x outside of $B(0, \delta_0) \cup B(x_0, \delta_0)$, if we choose $\delta < \gamma_0/(2C)$. The lemma is proved now. \square

This lemma shows that if $\Psi(F, \mathfrak{M}_0)$ attains its minimum value 0 at exactly two points F_0 and F^* and $\Psi_{\mathfrak{M}_0}(F^*, \mathfrak{M}_0) \neq 0$, then it is possible to modify \mathfrak{M}_0 , so that $\Psi(F, \mathfrak{M}_0)$ attains its minimum value 0 only at F_0 . We now show that if F_0 is the unique minimizer of $\Psi(F, \mathfrak{M}_0)$, satisfying (2.3), then this will also be true for all other F_0 that are sufficiently close to the original F_0 , where the constants \mathfrak{M}_0 are kept fixed. Hence, we now regard Ψ as a function of F and F_0 , keeping \mathfrak{M}_0 fixed. The conclusion of Lemma 3.1 follows from the lemma below.

Lemma A.2 *Suppose that $f \in C^2(\mathbb{R}^d \times B(0, 1))$ satisfies*

- (i) $f(x, 0) > 0$ for all $x \neq 0$
- (ii) $f_{xx}(0, 0) > 0$
- (iii) $f(a, a) = 0$ and $f_x(a, a) = 0$ for all $a \in B(0, 1)$
- (iv) $f(x, a) > 1$ for all $|x - a| > R$ and all $a \in B(0, 1)$.

Then, there exists $\delta > 0$, so that $f(x, a) > 0$ for all $x \neq a$ and $|a| < \delta$.

Proof By implicit function theorem, there exists $\delta_1 > 0$, such that the equation $f_x(x, a) = 0$ has a unique solution $x = a$ on a neighborhood of 0, provided $|a| < \delta_1$. By continuity, $f_{xx}(a, a) > 0$ when $|a| < \delta_1$. Hence, $x = a$ is also a point of local minimum of $x \mapsto f(x, a)$, while $f(a, a) = 0$. Hence, $f(x, a) > 0$, whenever $|x| < \delta_1$, $|a| < \delta_1$ and $x \neq a$. By assumption

$$\min_{|x| \geq \delta_1} f(x, 0) = \gamma > 0.$$

Hence, by condition (iv), there exists $0 < \delta < \delta_1$, so that

$$\min_{|x| \geq \delta_1} f(x, a) = \min_{\delta_1 \leq |x| \leq R+1} f(x, a) > \frac{\gamma}{2} > 0,$$

provided $|a| < \delta$. But then for any $|a| < \delta$, we have $f(x, a) > 0$, whenever $|x| < \delta_1$ and $x \neq a$, and $f(x, a) > 0$, when $|x| \geq \delta_1$. The lemma is now proved. \square

B The Robustness of Rank-One Convex Envelopes

In this section, we will show that the rank-one convex envelope is insensitive (robust) to certain “safe” modifications of the energy density. Specifically, let $W^{(1)}, W^{(2)} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ be of class C^1 and satisfy the mild growth conditions required to ensure that $RW^{(1)}$ and $RW^{(2)}$ are of class C^1 via a theorem of Ball et al. (2000). Let

$$\mathcal{B}_j = \{\mathbf{F} : RW^{(j)}(\mathbf{F}) < W^{(j)}(\mathbf{F})\}, \quad j = 1, 2$$

be their rank-one convex binodal regions. The intuition is that since rank-one convexity, just as convexity, can be locally defined, the binodal region of $W(\mathbf{F})$ can be regarded as a set of all points lacking rank-one convexity, while its complement consists of “rank-one convex points.” According to that image, any modification of $W(\mathbf{F})$ outside of rank-one binodal that does not destroy rank-one convexity should not affect neither the binodal region, nor the rank-one convex envelope inside the binodal region. In order to formulate our intuition as a theorem, we need to make precise what we mean by rank-one convexity at a point for C^1 functions.

Definition B.1 We say that a C^1 function $W(\mathbf{F})$ satisfies the Legendre–Hadamard (LH) condition at a point \mathbf{F}_0 if there exists $\delta > 0$ so that

$$W(\mathbf{F}_0 + t\mathbf{u} \otimes \mathbf{v}) \geq W(\mathbf{F}_0) + t\langle W_{\mathbf{F}}(\mathbf{F}_0), \mathbf{u} \otimes \mathbf{v} \rangle$$

for all $|t| < \delta$ and all unit vectors \mathbf{u} and \mathbf{v} .

It is easy to see that if $W(\mathbf{F})$ is of class C^2 , then the above definition implies the classical LH condition at a point $\langle W_{\mathbf{F}\mathbf{F}}(\mathbf{F}_0)(\mathbf{u} \otimes \mathbf{v}), \mathbf{u} \otimes \mathbf{v} \rangle \geq 0$. The converse implication is also true on open subsets. We will use the fact that a C^1 function $W(\mathbf{F})$ is rank-one convex if and only if it satisfies the LH condition at every \mathbf{F} . This statement is referred to as “locality” of rank-one convexity.

Theorem B.2 Suppose $W^{(1)}, W^{(2)}, RW^{(1)}$ and $RW^{(2)}$ are of class C^1 . Assume that

- (a) $W^{(1)}(\mathbf{F}) = W^{(2)}(\mathbf{F})$ for all $\mathbf{F} \in \mathcal{B}_1$
- (b) $W^{(2)}(\mathbf{F})$ satisfies the LH condition for all $\mathbf{F} \notin \mathcal{B}_1$.

Then

- (i) $\mathcal{B}_2 = \mathcal{B}_1 = \mathcal{B}$
- (ii) $RW^{(1)}(\mathbf{F}) = RW^{(2)}(\mathbf{F})$ for all $\mathbf{F} \in \mathcal{B}$.

Proof The idea is to show that $RW^{(1)}(\mathbf{F}) \leq RW^{(2)}(\mathbf{F})$ and $RW^{(2)}(\mathbf{F}) \leq RW^{(1)}(\mathbf{F})$ for every $\mathbf{F} \in \mathcal{B}_1$. For this reason, we define

$$\widehat{W}^{(1)}(\mathbf{F}) = \begin{cases} W^{(1)}(\mathbf{F}), & \mathbf{F} \notin \mathcal{B}_1, \\ RW^{(2)}(\mathbf{F}), & \mathbf{F} \in \mathcal{B}_1, \end{cases}, \quad \widehat{W}^{(2)}(\mathbf{F}) = \begin{cases} W^{(2)}(\mathbf{F}), & \mathbf{F} \notin \mathcal{B}_1, \\ RW^{(1)}(\mathbf{F}), & \mathbf{F} \in \mathcal{B}_1, \end{cases}.$$

Let us examine $\widehat{W}^{(2)}$. We note that for all $\mathbf{F} \in \partial\mathcal{B}_1$, we have

$$W^{(2)}(\mathbf{F}) = W^{(1)}(\mathbf{F}) = RW^{(1)}(\mathbf{F}), \quad W_{\mathbf{F}}^{(2)}(\mathbf{F}) = W_{\mathbf{F}}^{(1)}(\mathbf{F}) = RW_{\mathbf{F}}^{(1)}(\mathbf{F}).$$

Thus, $\widehat{W}^{(2)}$ is of class C^1 and satisfies the LH condition at all \mathbf{F} . We conclude that $\widehat{W}^{(2)}$ is rank-one convex. Also, $\widehat{W}^{(2)}(\mathbf{F}) = W^{(2)}(\mathbf{F})$ for all $\mathbf{F} \notin \mathcal{B}_1$ and $\widehat{W}^{(2)}(\mathbf{F}) = RW^{(1)}(\mathbf{F}) \leq W^{(1)}(\mathbf{F}) = W^{(2)}(\mathbf{F})$, for all $\mathbf{F} \in \mathcal{B}_1$. Hence, $\widehat{W}^{(2)}$ is a rank-one convex function, such that $\widehat{W}^{(2)} \leq W^{(2)}$. Therefore,

$$\widehat{W}^{(2)}(\mathbf{F}) \leq RW^{(2)}(\mathbf{F}), \quad \forall \mathbf{F}. \tag{B.1}$$

In particular, for all $\mathbf{F} \notin \mathcal{B}_1$

$$W^{(2)}(\mathbf{F}) = \widehat{W}^{(2)}(\mathbf{F}) \leq RW^{(2)}(\mathbf{F}) \leq W^{(2)}(\mathbf{F}).$$

We conclude that $RW^{(2)}(\mathbf{F}) = W^{(2)}(\mathbf{F})$ for all $\mathbf{F} \notin \mathcal{B}_1$ and hence, $\mathcal{B}_2 \subset \mathcal{B}_1$. It follows that

$$\widehat{W}^{(1)}(\mathbf{F}) = \begin{cases} W^{(1)}(\mathbf{F}), & \mathbf{F} \notin \mathcal{B}_2, \\ RW^{(2)}(\mathbf{F}), & \mathbf{F} \in \mathcal{B}_2. \end{cases}$$

Indeed, for every $\mathbf{F} \in \mathcal{B}_1 \setminus \mathcal{B}_2$ the left-hand side has the value $RW^{(2)}(\mathbf{F}) = W^{(2)}(\mathbf{F}) = W^{(1)}(\mathbf{F})$, agreeing with the right-hand side. But then we can repeat the same argument where the roles of $W^{(1)}$ and $W^{(2)}$ are interchanged, proving that $\mathcal{B}_1 \subset \mathcal{B}_2$ and, hence $\mathcal{B}_1 = \mathcal{B}_2 = \mathcal{B}$, and

$$\widehat{W}^{(1)} \leq RW^{(1)}(\mathbf{F}), \quad \forall \mathbf{F}. \tag{B.2}$$

But then for $\mathbf{F} \in \mathcal{B}$ inequality (B.1) says $RW^{(1)}(\mathbf{F}) \leq RW^{(2)}(\mathbf{F})$, while inequality (B.2) says $RW^{(2)}(\mathbf{F}) \leq RW^{(1)}(\mathbf{F})$, proving the theorem. \square

C Direct Calculation of the Quasiconvex Envelope of (5.1)

The quasiconvexification of $W(\mathbf{F})$ in the example (5.1) is actually easier to compute using formula

$$QW(\mathbf{F}) = \inf_{\phi \in C_0^\infty(D; \mathbb{R}^m)} \int_D W(\mathbf{F} + \nabla \phi) dx, \quad (\text{C.1})$$

due to Dacorogna (1982), if one can guess that for any matrix \mathbf{F} we have

$$|\boldsymbol{\varepsilon}|^2 = \theta^2 + |\boldsymbol{\Omega}|^2 - 2J_2(\mathbf{F}), \quad (\text{C.2})$$

where θ , $\boldsymbol{\varepsilon}$ and $\boldsymbol{\Omega}$ are defined in (5.2) and

$$J_2(\mathbf{F}) = \frac{1}{2}((\text{Tr } \mathbf{F})^2 - \text{Tr } (\mathbf{F}^2))$$

is a null-Lagrangian. Decomposition (C.2) amounts to a direct guess of the supporting null-Lagrangian in our method. Applying the decomposition (C.2) and recalling definition (5.6) of Φ , we obtain

$$\int_D W(\mathbf{F} + \nabla \phi) dx = \int_D \left\{ \Phi(\theta + \nabla \cdot \phi) + (\mu' + \mu)|\boldsymbol{\Omega} + \nabla \phi - (\nabla \phi)^T|^2 \right\} dx - 2\mu J_2(\mathbf{F})$$

Using the Jensen's inequality (recalling that $\mu + \mu' > 0$), we obtain

$$\int_D W(\mathbf{F} + \nabla \phi) dx \geq C\Phi(\theta) + (\mu' + \mu)|\boldsymbol{\Omega}|^2 - 2\mu J_2(\mathbf{F}), \quad (\text{C.3})$$

where $C\Phi(\theta)$ is the convex hull of $\Phi(\theta)$, which agrees with $\Phi(\theta)$, when $\theta \notin (\theta_1, \theta_2)$ and agrees with the common tangent in Fig. 1b, when $\theta \in (\theta_1, \theta_2)$. Thus, if $\theta = \text{Tr } \mathbf{F} \notin (\theta_1, \theta_2)$ the right-hand side of (C.3) is exactly $W(\mathbf{F})$. If $\theta \in (\theta_1, \theta_2)$, then we need to look for ϕ that achieves equality in (C.3). Such ϕ must necessarily satisfy $\nabla \phi - (\nabla \phi)^T = 0$. Hence, $\phi = \nabla \psi$. In addition, $\nabla \cdot \phi$ must take values $\theta_1 - \theta$ and $\theta_2 - \theta$. These constraints can all be met for D —a unit ball in \mathbb{R}^n and $\psi(\mathbf{x}) = \psi(|\mathbf{x}|)$:

$$\psi(r) = \begin{cases} \frac{\theta_2 - \theta}{2n} \left(r^2 + \frac{2}{(n-2)r^{n-2}} \right), & 1 < r < r^*, \\ \frac{\theta_1 - \theta}{2n} r^2 + c, & r^* \leq r \leq 0, \end{cases}$$

where c is chosen to ensure that $\psi(r)$ is continuous, and r^* is chosen to ensure that $\psi'(r)$ is on continuous $0 \leq r \leq 1$. It is easy to check that $\nabla \psi$ vanishes when $r = 1$ and that $\nabla \cdot \psi \in \{\theta_1 - \theta, \theta_2 - \theta\}$. This implies that $\phi = \nabla \psi$ attains equality in (C.3), thereby proving that the right-hand side of (C.3) is $QW(\mathbf{F})$ for all \mathbf{F} .

Using formula (C.2), we can rewrite the right-hand side of (C.3) as follows

$$QW(\mathbf{F}) = C\Phi(\theta) - \mu\theta^2 + \mu|\boldsymbol{\varepsilon}|^2 + \mu'|\boldsymbol{\Omega}|^2. \quad (\text{C.4})$$

It remains to observe that when $\theta \notin (\theta_1, \theta_2)$, we have

$$C\Phi(\theta) - \mu\theta^2 = \Phi(\theta) - \mu\theta^2 = f(\theta).$$

When $\theta \in (\theta_1, \theta_2)$, then $C\Phi(\theta)$ is affine and hence $C\Phi(\theta) - \mu\theta^2$ must agree with $f^{\text{qc}}(\theta)$, given by (5.12), since $f^{\text{qc}}(\theta) + \mu\theta^2$ is affine on (θ_1, θ_2) , agrees with $\Phi(\theta)$ outside (θ_1, θ_2) and is of class C^1 , so that the graph of the affine function $f^{\text{qc}}(\theta) + \mu\theta^2$ must be tangent to the graph of $\Phi(\theta)$ at θ_1 and θ_2 . Such an affine function is unique and agrees with $C\Phi(\theta)$ on (θ_1, θ_2) .

We note that the direct calculation of the quasiconvex envelope is based on subtracting the right null-Lagrangian $-2\mu J_2(F)$ from $W(F)$. This gives us immediate formulas for the translation constants \mathfrak{m}_0 , \mathfrak{b}_0 and \mathfrak{m}_0 . Formulas (3.13) and (3.16) show that our method can recover these values without having to guess the right null-Lagrangian in (2.1).

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