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Explicit Relaxation of a Two-Well Hadamard Energy

Yury Grabovsky[1] · Lev Truskinovsky[2]

The paper is dedicated to the memory of W. Noll

Abstract We compute an explicit quasiconvex envelope for a subclass of double-well Hadamard energies which model materials undergoing isotropic-to-isotropic elastic phase transitions. The construction becomes possible because of stability of the entire jump set, representing points that can coexist at phase boundaries. To prove stability we apply a recently developed technique for establishing polyconvexity of points on the jump set.

Keywords Quasiconvexity · Polyconvexity · Rank-one convexity · Nonlinear elasticity · Hadamard material · Jump set · Elastic stability · Binodal

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

1 Introduction

The object of study of this paper is the behavior of Hadamard material [21], a term coined by F. John [22] for the nonlinear elasticity problem with the energy density

$$W(\boldsymbol{F}) = \frac{\mu}{2}|\boldsymbol{F}|^2 + h(\det \boldsymbol{F}), \quad \det \boldsymbol{F} > 0. \tag{1.1}$$

Specifically, we'll be interested in the case when $h(d)$ is a $C^2(0, +\infty)$ function with a double-well shape shown in Fig. 1; the precise technical definition will be given later. Such energies can be used to model materials undergoing isotropic-to-isotropic martensitic phase transitions which are the simplest transitions of this type [14, 26]. Even though the energy wells are described by a function of a single variable, $h(d)$, the results are nontrivial due to the incompatibility and nonlinearity of the energy wells [5].

The fundamental challenge in the theory of martensitic phase transitions is to construct the quasiconvex envelope of the elastic energy, and in this paper we solve this problem for

✉ Y. Grabovsky
  yury@temple.edu

[1] Temple University, Philadelphia, PA, USA
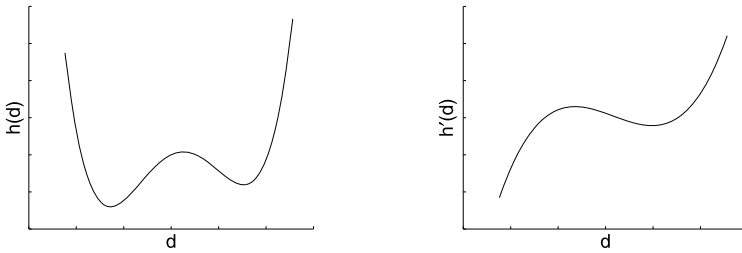
[2] ESPCI, Paris, France

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Fig. 1 Double-well structure of the energy density h

the Hadamard material (1.1), when the shear modulus μ is sufficiently large. It is well-known that $W(\boldsymbol{F})$, given by (1.1) is quasiconvex if and only if $h(d)$ is convex [6]. This statement may be thought of as a bit surprising, since it asserts failure of quasiconvexity of $W(\boldsymbol{F})$ for *any* non-convex $h(d)$, regardless of how large the coefficient μ in front of the quadratic term is. The reason is a highly anisotropic behavior of the determinant at infinity, where it can remain bounded, while $|\boldsymbol{F}|$ grows, and where small perturbations of $\boldsymbol{F}$, can lead to substantial variations of the determinant. This allows for variations that lower the energy due to the non-convexity of $h(d)$, while the increment of $\mu|\boldsymbol{F}|^2$ remains relatively small.

The relaxation of the Hadamard material with non-convex $h(d)$ is presently known only in the case $\mu = 0$, where $QW(\boldsymbol{F}) = h^{**}(\det \boldsymbol{F})$, [11]. This result may be taken as a hint that the quasiconvex envelope of (1.1) is

$$U(\boldsymbol{F}) = \frac{\mu}{2}|\boldsymbol{F}|^2 + h^{**}(\det \boldsymbol{F}), \tag{1.2}$$

where h^{**} denotes the convex hull of $h(d)$. However, this guess is wrong not just as a general statement but for every single non-convex function $h(d)$ of class C^1 with superlinear growth at infinity and/or blow-up at $d = 0$. To make our presentation self-contained, we supply the proof of this result in Appendix A even though this result is probably known to experts. Curiously, a version of formula (1.2) for linearized kinematics is, in fact, correct [20]. The effect of nonlinear kinematics is in the nontrivial coupling between $|\boldsymbol{F}|$ and $\det \boldsymbol{F}$, which is responsible for quasiconvexity of $W(\boldsymbol{F})$ at some $\boldsymbol{F}$ for which $h(\det \boldsymbol{F}) > h^{**}(\det \boldsymbol{F})$. By linearizing kinematics we effectively decouple the deviatoric part of $\boldsymbol{F}$ from its trace which can be then relaxed separately, see [20] for more details.

In this paper we present an explicit formula for $QW(\boldsymbol{F})$ in the case when $\mu > 0$ is sufficiently large and the quadratic term dominates. The formula couples $|\boldsymbol{F}|$ and $\det \boldsymbol{F}$, and $QW(\boldsymbol{F})$ is sandwiched between $W(\boldsymbol{F})$ above and $U(\boldsymbol{F})$, given by (1.2). Our constraint on μ is not a technical limitation, and as μ decreases our formula for $QW(\boldsymbol{F})$ ceases to be valid in some subsets of the binodal region. A preliminary study shows that in the range of small μ the relaxation of $W(\boldsymbol{F})$ goes through a complex chain of structural transitions whose nature will be revealed in a separate publication.

Our approach is rooted in the observation that in the course of a hard device loading program, the homogeneous deformation can become unstable in strong topology if the applied affine deformation crosses into the binodal region, where the quasi-convexity of the energy is lost. The instability manifests itself through a *strong bifurcation* [17], whereby a heterogeneous configuration with the same energy as the homogeneous one becomes available. In the case of materials supporting phase transitions, such inhomogeneous configurations will

feature smooth surfaces of jump discontinuity of the deformation gradient and the disjoint regions of the phase space between which the gradient jumps are regarded as phases. The set of such "broken extremals" is substantially larger than the set of smooth ones, and finding the location of jump discontinuities is usually a complex free-boundary problem, e.g., [1, 2, 8, 15, 27].

As in the case of quasiconvexification, there is no general algorithm for finding the boundary of the binodal region, known as the *binodal*. Nevertheless, in our prior work we have developed a general method for identifying its subset supporting the laminate type energy-minimizing configurations [16, 19, 20]. Behind this method is the study of stability of the jump set—a codimension one variety in the phase space that has a dual nature. On the one hand it determines the set of pairs $\boldsymbol{F}_{\pm}$ that could be the traces of the deformation gradient at the phase boundary in a stable configuration. On the other, the jump set must consist of points that are at most marginally stable in the sense that their every neighborhood contains points where quasiconvexity fails. Therefore, if one can prove quasiconvexity at a point on the jump set, then this point must lie on the binodal. Checking this is an algebraic problem posed in [20] for general $W(\boldsymbol{F})$ in any number of dimensions. In this paper we solve this problem for the Hadamard energy (1.1) in two space dimensions and with sufficiently large μ. We show that in this limit, the full jump set becomes stable which ensures that the method delivers the *entire* binodal. A natural consequence of this result is that all nontrivial energy-minimizing configurations are simple laminates.

2 Preliminaries

We begin by recalling the standard definitions.

Definition 2.1

(i) We say that $W(\boldsymbol{F})$ is quasiconvex at $\boldsymbol{F} \in \mathbb{M} = \mathbb{R}^{m \times n}$, if

$$\int_{\mathbb{R}^n} \left\{ W\left(\boldsymbol{F} + \nabla\boldsymbol{\phi}(z)\right) - W(\boldsymbol{F}) \right\} dz \geq 0 \tag{2.1}$$

for all $\boldsymbol{\phi} \in C_0^\infty(\mathbb{R}^n; \mathbb{R}^m)$.

(ii) The function $W(\boldsymbol{F})$ is called quasiconvex if it is quasiconvex at all points $\boldsymbol{F}$.

(iii) The quasiconvex envelope $QW(\boldsymbol{F})$ of $W(\boldsymbol{F})$ is the largest quasiconvex function satisfying $QW(\boldsymbol{F}) \leq W(\boldsymbol{F})$ for all $\boldsymbol{F} \in \mathbb{M}$.

(iv) The set of points $\boldsymbol{F}$, such that $QW(\boldsymbol{F}) < W(\boldsymbol{F})$ is called the binodal region $\mathfrak{B}$. The boundary of the binodal region is called the binodal, $\mathfrak{Bin} = \partial\mathfrak{B}$.

There is also a formula for the quasiconvex envelope

$$QW(\boldsymbol{F}) = \inf_{\boldsymbol{\phi} \in C_0^\infty(\Omega; \mathbb{R}^m)} \fint_\Omega W(\boldsymbol{F} + \nabla\boldsymbol{\phi}) dx, \tag{2.2}$$

due to Dacorogna [12].

We now describe our method from [20] for computing a subset of $\mathfrak{Bin}$, which in this paper will be shown to be the entire binodal. We start with the definition of the jump set, which lies in the closure of $\mathfrak{B}$.

Definition 2.2 The jump set $\mathfrak{J}$ is the closure of the set of points $\boldsymbol{F} \in \mathbb{M}$ for which there exists $\boldsymbol{a} \in \mathbb{R}^m \setminus \{0\}$ and a unit vector $\boldsymbol{n} \in \mathbb{R}^n$, such that

$$\begin{cases} (W_F(\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}) - W_F(\boldsymbol{F}))\boldsymbol{n} = 0, \\ (W_F(\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}) - W_F(\boldsymbol{F}))^T \boldsymbol{a} = 0, \\ W(\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}) - W(\boldsymbol{F}) = W_F(\boldsymbol{F})\boldsymbol{n} \cdot \boldsymbol{a}. \end{cases} \tag{2.3}$$

These equations have a dual nature. On the one hand they are necessary conditions on the surface of jump discontinuity of the gradient of any strong local minimizer of the energy $E[\boldsymbol{y}]$. On the other, these equations describe the set of homogeneous deformation gradients $\boldsymbol{F}$ that permit energy-neutral nucleation of layers of a new phase with a compatible deformation gradient $\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}$. If $\boldsymbol{F}$ is stable, i.e., if $QW(\boldsymbol{F}) = W(\boldsymbol{F})$, then such bifurcation property signals the boundary of stability, crossing which violates the quasiconvexity property. See [16] and [18] for the discussion.

We remark that if $\boldsymbol{F}$ solves (2.3), then $\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}$ also solves (2.3) with the same $\boldsymbol{n}$ and $\boldsymbol{a}$ replaced by $-\boldsymbol{a}$. This symmetry of the jump set makes it convenient to modify our notation and use $\boldsymbol{F}_-$ for $\boldsymbol{F}$ and $\boldsymbol{F}_+$ for $\boldsymbol{F} + \boldsymbol{a} \otimes \boldsymbol{n}$. We can also rewrite jump set equations in their canonical symmetric form

$$\begin{cases} \operatorname{rank}[\![\boldsymbol{F}]\!] = 1, \\ [\![W_F]\!][\![\boldsymbol{F}]\!]^T = 0, \\ [\![W_F]\!]^T[\![\boldsymbol{F}]\!] = 0, \\ [\![W]\!] - \langle W_F^{\pm}, [\![\boldsymbol{F}]\!] \rangle = 0, \end{cases} \tag{2.4}$$

where the last equation is a shorthand for a pair of equations for each choice of the sign. It is easy to see that one of these equations is a consequence of the rest of the system. However, even if one discards it (breaking the symmetry of the system), the remaining equations are still not independent, since the inner product of the second with $[\![\boldsymbol{F}]\!]$ equals to the inner product of the third with $[\![\boldsymbol{F}]\!]^T$. For this reason, we prefer to keep the symmetry at the price of some unavoidable redundancy.

Vectors $\boldsymbol{a}$ and $\boldsymbol{n}$ from (2.3) are then defined up to the $\mathbb{Z}_2$ symmetry $(\boldsymbol{a}, \boldsymbol{n}) \sim (-\boldsymbol{a}, -\boldsymbol{n})$ via the first equation in (2.4):

$$[\![\boldsymbol{F}]\!] = \boldsymbol{a} \otimes \boldsymbol{n}. \tag{2.5}$$

We also remark that if $\boldsymbol{F}$ solves (2.3), it is possible that it does so with several, or even infinitely many choices of $\boldsymbol{a} \otimes \boldsymbol{n}$. It follows that in general $\mathfrak{J}$ is not a submanifold in $\mathbb{M}$, but rather a codimension one variety with self-intersections and singularities.

Since $\mathfrak{J} \subset \overline{\mathfrak{B}}$ (under very mild non-degeneracy assumptions), establishing quasiconvexity at a point of $\mathfrak{J}$ implies that this point belongs to the binodal. Moreover, this also gives a formula for the quasiconvex hull along the rank-one lines joining $\boldsymbol{F}_\pm$ [18].

Theorem 2.3 *Suppose $\boldsymbol{F}_\pm$ is the corresponding pair of points on the jump set and*

$$QW(\boldsymbol{F}_\pm) = W(\boldsymbol{F}_\pm). \tag{2.6}$$

Then for any $\lambda \in [0, 1]$

$$QW\big(\lambda \boldsymbol{F}_+ + (1 - \lambda)\boldsymbol{F}_-\big) = \lambda W(\boldsymbol{F}_+) + (1 - \lambda)W(\boldsymbol{F}_-). \tag{2.7}$$

If we prove that the entire jump set is quasiconvex, then formula (2.7) gives the explicit form of the quasiconvex envelope of $W(F)$. For the energy (1.1) this formula produces our main result: formula (5.2).

Definition 2.4

(i) The function is called rank-one convex if it is convex along all rank-one lines, i.e., when $\phi(t) = W(F + ta \otimes n)$ is convex for all F, a and n.

(ii) The rank-one convex envelope RW of W is the largest rank-one convex function, such that $RW(F) \leq W(F)$ for all $F \in \mathbb{M}$.

(iii) We say that W is rank-one convex at F_0 if $W(F_0) = RW(F_0)$.

(iv) The set of points F, such that $RW(F) < W(F)$ is called the rank-one binodal region and its boundary is called the rank-one binodal.

It is well-known that every quasiconvex function is rank-one convex [23]. As a consequence we always have the implication

$$W(F_0) = QW(F_0) \quad \Rightarrow \quad W(F_0) = RW(F_0).$$

The converse is known to be false [25], when $n \geq 2$ and $m \geq 3$. However, it is not known if there is any difference between the two notions if $m = n = 2$. Since it is not known if $QW(F) = RW(F)$, we cannot conclude a priori that the binodal agrees with the rank-one binodal everywhere.

In the two-dimensional example ($m = n = 2$) we consider in this paper we are going to show that the entire jump set is polyconvex by applying the method from [20]. The idea is for a given F_0 to find a supporting null-Lagrangian $N(F)$, such that

(i) $N(F) \leq W(F)$ for all F,
(ii) $N(F_0) = W(F_0)$.

This implies that $QW(F_0) = W(F_0)$. In general, finding the set of points F_0, where such a null-Lagrangian exists is algebraically intractable for most nonlinear energies. However, and this is the main point of the method in [20], the search for such a null-Lagrangian simplifies to the point of feasibility in dimensions 2 and 3 when $F_0 = F_\pm \in \mathfrak{J}$. When $m = n = 2$ the desired null-Lagrangian has an explicit general formula, satisfying (ii). Stability of $F_\pm$ is then a corollary of (i), which has the form

$$W(F) \geq W(F_\pm) + \langle W_F(F_\pm), F - F_\pm \rangle + \frac{\langle [\![W_F]\!], \operatorname{cof} [\![F]\!] \rangle}{|[\![F]\!]|^2} \det(F - F_\pm), \qquad (2.8)$$

for every $F \in \mathbb{M}$. In other words, the energy is polyconvex at $F_\pm \in \mathfrak{J}$ if and only if the minimum value of

$$\Psi(F) = W(F) - W(F_\pm) - \langle W_F(F_\pm), F - F_\pm \rangle - \frac{\langle [\![W_F]\!], \operatorname{cof} [\![F]\!] \rangle}{|[\![F]\!]|^2} \det(F - F_\pm) \quad (2.9)$$

is 0 (achieved at $F = F_\pm$). Our notation emphasizes the fact that either choice of sign in $F_\pm$ results in one and the same function $\Psi(F)$.

3 The Jump Set

Failure of rank-one convexity implies that $W(\boldsymbol{F})$ has a non-trivial jump set. In [19] we have computed it and used our local bounds to identify an unstable portion of the jump set, when μ is not too large. Let us briefly recall its derivation. The simplest non-trivial case is when the non-convex function $h(d)$ is of "double-well" shape. The precise assumptions are not on the shape of the graph of $h(d)$ itself, but rather on the shape of the graph of $h'(d)$.

Definition 3.1 We will say that the function $h(d)$ has a double-well shape if the following 3 properties are satisfied.

  (i) There exists $d_0 > 0$, such that $h'(d)$ is concave on $(0, d_0)$ and has a strict local maximum there,
 (ii) $h'(d)$ is convex on $(d_0, +\infty)$ and has a strict local minimum there
(iii) $\lim_{d \to 0^+} h'(d) = -\infty$.

Condition (iii) is consistent with the requirement that infinite compression costs infinite energy

$$\lim_{d \to 0^+} h(d) = +\infty. \tag{3.1}$$

We start with the kinematic compatibility equation (2.5) and take the determinant of $\boldsymbol{F}_+ = \boldsymbol{F}_- + \boldsymbol{a} \otimes \boldsymbol{n}$ to obtain

$$d_+ = d_- + \operatorname{cof} \boldsymbol{F}_- \boldsymbol{n} \cdot \boldsymbol{a}, \qquad d_\pm = \det \boldsymbol{F}_\pm. \tag{3.2}$$

Using the formula

$$\boldsymbol{P}(\boldsymbol{F}) = \mu \boldsymbol{F} + h'(\det \boldsymbol{F}) \operatorname{cof} \boldsymbol{F}$$

for the Piola-Kirchhoff stress we compute

$$[\![\boldsymbol{P}]\!]\boldsymbol{n} = \mu \boldsymbol{a} + [\![h']\!] \operatorname{cof} \boldsymbol{F}_- \boldsymbol{n},$$

where we have used the well-known relation $\operatorname{cof}(\boldsymbol{F}_- + \boldsymbol{a} \otimes \boldsymbol{n})\boldsymbol{n} = (\operatorname{cof} \boldsymbol{F}_-)\boldsymbol{n}$. Similarly,

$$[\![\boldsymbol{P}]\!]^T \boldsymbol{a} = \mu |\boldsymbol{a}|^2 \boldsymbol{n} + [\![h']\!] \operatorname{cof} \boldsymbol{F}_-^T \boldsymbol{a}.$$

Thus, the first two equations in (2.3) imply

$$\boldsymbol{a} = -\frac{[\![h']\!]}{\mu} \operatorname{cof} \boldsymbol{F}_- \boldsymbol{n}, \qquad [\![h']\!]^2 \operatorname{cof}(\boldsymbol{C}_-)\boldsymbol{n} = \mu^2 |\boldsymbol{a}|^2 \boldsymbol{n}, \tag{3.3}$$

where $\boldsymbol{C}_\pm = \boldsymbol{F}_\pm^T \boldsymbol{F}_\pm$ is the Cauchy-Green strain tensor. We conclude that $\boldsymbol{n}$ must be an eigenvector of $\boldsymbol{C}_-$. Equations (3.3) permit us to find a relation between the two Cauchy-Green tensors $\boldsymbol{C}_\pm$. Using the kinematic compatibility equation we compute

$$\boldsymbol{C}_+ = \boldsymbol{C}_- + \boldsymbol{F}_-^T \boldsymbol{a} \otimes \boldsymbol{n} + \boldsymbol{n} \otimes \boldsymbol{F}_-^T \boldsymbol{a} + |\boldsymbol{a}|^2 \boldsymbol{n} \otimes \boldsymbol{n}.$$

Applying $\boldsymbol{F}_-^T$ to the first equation in (3.3) we obtain $\boldsymbol{F}_-^T \boldsymbol{a} = -([\![h']\!]/\mu)d_- \boldsymbol{n}$, so that

$$[\![\boldsymbol{C}]\!] = \left(|\boldsymbol{a}|^2 - \frac{2[\![h']\!]d_-}{\mu} \right) \boldsymbol{n} \otimes \boldsymbol{n}. \tag{3.4}$$

It follows that the Cauchy-Green tensors C_+ and C_- are simultaneously diagonalizable, since, by (3.3) n is an eigenvector of C_-. According to Eq. (3.4) C_+ and C_- have the same eigenvectors and the same eigenvalues corresponding to all eigenvectors orthogonal to n. Hence $F_\pm$ would have singular values $(\varepsilon_\pm, \varepsilon_2, \ldots, \varepsilon_n)$, the first one corresponding to the eigenvector n of $C_\pm$. Substituting the first equation in (3.3) into (3.2) we obtain

$$d_+ = d_- - \frac{[\![h']\!]}{\mu} \operatorname{cof} C_- n \cdot n = d_- - \frac{[\![h']\!] d_-^2}{\mu \varepsilon_-^2},$$

which can be written in the more symmetric form as

$$\mu \frac{[\![d]\!]}{[\![h']\!]} = -\prod_{j=2}^{n} \varepsilon_j^2 = -\frac{d_\pm^2}{\varepsilon_\pm^2}. \tag{3.5}$$

This will be the equation for the jump set, when we determine d_+ as a function of d_- from the Maxwell relation (the last equation in (2.4), which hasn't been used so far). It is well-known that the Maxwell relation does not change if we add any quadratic function in F to the energy. Thus, the term $\mu|F|^2/2$ can be disregarded and the Maxwell relation becomes

$$[\![h]\!] = \{h' \operatorname{cof} F\} n \cdot a.$$

Recalling that due to (3.2) $(\operatorname{cof} F_+) n \cdot a = (\operatorname{cof} F_-) n \cdot a = [\![d]\!]$ we obtain

$$[\![h]\!] = \{h'\}[\![d]\!]. \tag{3.6}$$

Equation (3.6) can be written in such a way as to highlight its geometric meaning. Observe that the straight line with equation

$$y = h'(d_-) + \frac{[\![h']\!]}{[\![d]\!]}(x - d_-)$$

is the secant line joining $(d_-, h'(d_-))$ and $(d_+, h'(d_+))$. Then the Maxwell relation (3.6) is equivalent to

$$\int_{d_-}^{d_+} \{h'(x) - y(x)\} dx = 0. \tag{3.7}$$

Now the relation (3.7) can be interpreted geometrically as equality of areas between the secant line and the graph of $h'(d)$. Hence, according to (3.5), the slope of the straight line orthogonal to the secant is the single common eigenvalue of $\operatorname{cof} C_+$ and $\operatorname{cof} C_-$, implying that the secant line has a negative slope.

It is now easy to show that under assumptions (i)–(iii) in Definition 3.1 there exists a single interval (d_1, d_2) on which $h(d)$ differs from its convex hull, which on (d_1, d_2) agrees with the common tangent line at d_1 and d_2 to the graph of $h(d)$. In terms of $h'(d)$ this double-tangency can also be interpreted geometrically as the horizontal "Maxwell line" with the equal area property. Then $d_- \in (d_1, d_0)$ and $d_+ \in (d_0, d_2)$. For every $d_- \in (d_1, d_0)$ there is a unique $d_+ = D(d_-)$ with equal area property (3.7) (see Fig. 2). (By continuity we can set $D(d_0) = d_0$.) For example if $h(d)$ is a quartic polynomial $(d - d_1)^2 (d - d_2)^2$, then $D(d) = d_1 + d_2 - d$, and $d_0 = (d_1 + d_2)/2$. Regarding the function $D(d)$ as known, we obtain the explicit description of the jump set in terms of the singular values of F. It can be viewed as

Fig. 2 The map $d_\pm = D(d_\mp)$ is defined by the equal area condition (3.6)
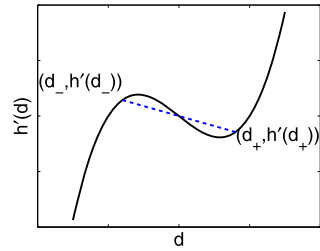
a parametric hypersurface in $\mathbb{R}^n$ parametrized by $n-1$ parameters $d, \varepsilon_3, \ldots, \varepsilon_n$ via (3.5). Explicitly, choosing the ordering of eigenvalues where $\boldsymbol{n} = \boldsymbol{e}_1$ we obtain

$$\begin{cases} \varepsilon_1 = d\sqrt{-\dfrac{h'(D(d)) - h'(d)}{\mu(D(d) - d)}}, \\ \varepsilon_2 = \left(\displaystyle\prod_{j=3}^{n} \dfrac{1}{\varepsilon_j}\right)\sqrt{-\dfrac{\mu(D(d) - d)}{h'(D(d)) - h'(d)}}, \\ \varepsilon_3 = \varepsilon_3, \ldots, \varepsilon_n = \varepsilon_n. \end{cases} \tag{3.8}$$

The entire jump set is therefore a set of $\boldsymbol{F}$, whose singular values have the ordering, which satisfies (3.8). We note that the hypersurface (3.8) is invariant under all permutations of $(\varepsilon_2, \ldots, \varepsilon_n)$. Therefore, the entire jump set is the union of n components: surface (3.8) and the ones obtained from it by swapping ε_1 and ε_k in (3.8). When $n = 2$ we have

$$\begin{cases} \varepsilon_1 = d\sqrt{-\dfrac{h'(D(d)) - h'(d)}{\mu(D(d) - d)}}, \\ \varepsilon_2 = \sqrt{-\dfrac{\mu(D(d) - d)}{h'(D(d)) - h'(d)}}, \end{cases} \tag{3.9}$$

with the second component given by interchanging ε_1 and ε_2. Let us now restrict our attention to the 2D case. When μ is sufficiently large the jump set is a connected embedded submanifold of $\mathbb{R}^{2\times 2}$. For smaller values of μ the two symmetry-related components of the jump set in $(\varepsilon_1, \varepsilon_2)$ plane intersect and the jump set is no longer a manifold, as it has self-intersections. Since, the pair $(\varepsilon_1, \varepsilon_2)$ determines parameter $d = \varepsilon_1 \varepsilon_2$ uniquely, the self-intersection happens only at the solutions of the equation $\varepsilon_1(d) = \varepsilon_2(d)$. Thus, if

$$\mu > \max_{d \in [d_1, d_2]} -d\frac{h'(D(d)) - h'(d)}{D(d) - d}, \tag{3.10}$$

then the jump set has no self-intersections (see Fig. 3).

If $\boldsymbol{F}_\pm$ is a corresponding pair on the jump set (i.e., the pair satisfying (2.4)), then there are frames in which both $\boldsymbol{F}_\pm$ are diagonal. The rank-1 lines connecting $\boldsymbol{F}_+$ and $\boldsymbol{F}_-$, i.e., the lines along the direction $\boldsymbol{n}$ are horizontal lines in representation (3.9).

Remark 3.2 In [19] we have found necessary conditions for the points on the jump set to be stable. Using our formula from [19] we have the lower bound

$$\mu_*^2 = \max_{d \in [d_1, d_2]} R^4(d)\left(\frac{(D(d) - d)^2 R^2(d)}{R^2(d) + h''(d)} - d^2 + 2dD(d)\right), \tag{3.11}$$

Fig. 3 The jump set for the non-convex Hadamard material when μ satisfies (3.10)
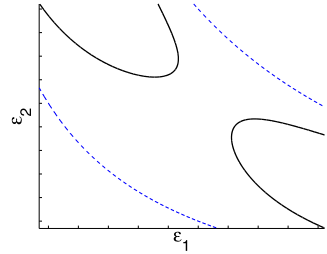
where $R(d)^2 = -[\![h']\!]/[\![d]\!]$. If $\mu < \mu_*$ there will be a part of the jump set which fails rank-one convexity.

4 Polyconvexity

In this section we are going to prove that for sufficiently large $\mu > 0$ the function $\Psi(F)$, given by (2.9) is minimized only at $F = F_\pm$ for every corresponding pair $F_\pm$ on the jump set.

The isotropy of the energy implies that it is sufficient to verify non-negativity of $\Psi(F)$ when $F_\pm$ are both diagonal

$$F_\pm = \begin{bmatrix} \varepsilon_\pm & 0 \\ 0 & \varepsilon_0 \end{bmatrix}, \tag{4.1}$$

where we have chosen the representative of the symmetry class on the jump set, given by (3.9), so that $n = e_1$ and therefore, $F_\pm e_2 = \varepsilon_0 e_2$.

Let us now examine minima of the functions $\Psi(F)$, given by (2.9) when μ is sufficiently large. For the Hadamard material

$$\Psi(F) = \Psi(F; F_\pm)$$
$$= \frac{\mu}{2}|F - F_\pm|^2 + h(\det F) - h_\pm - h'_\pm \langle \text{cof} \, F_\pm, F - F_\pm \rangle - m_0 \det(F - F_\pm),$$

where

$$m_0 = \frac{\langle [\![W_F]\!], \text{cof}[\![F]\!] \rangle}{|[\![F]\!]|^2} = \frac{[\![h'd]\!]}{[\![d]\!]}. \tag{4.2}$$

If F is a critical point of $\Psi(F; F_\pm)$, then

$$\mu F + \lambda \, \text{cof} \, F = \mu \begin{bmatrix} \varepsilon_\pm & 0 \\ 0 & \varepsilon_0 \end{bmatrix} + \lambda_\pm \begin{bmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_\pm \end{bmatrix}, \tag{4.3}$$

$$\lambda = h'(\det F) - m_0, \qquad \lambda_\pm = h'_\pm - m_0.$$

In components we have

$$\mu F_{12} - \lambda F_{21} = 0, \qquad \mu F_{21} - \lambda F_{12} = 0, \qquad \mu F_{11} + \lambda F_{22} = \mu \varepsilon_\pm + \lambda_\pm \varepsilon_0,$$
$$\mu F_{22} + \lambda F_{11} = \mu \varepsilon_\pm + \lambda_\pm x_\pm.$$

Using (4.2) we get

$$\lambda_{\pm} = h'_{\pm} - \frac{[\![h'd]\!]}{[\![d]\!]} = -\frac{[\![h']\!]}{[\![d]\!]} d_{\mp} = \mu \frac{d_{\mp}}{\varepsilon_0^2} = \mu \frac{\varepsilon_{\mp}}{\varepsilon_0}, \tag{4.4}$$

where the penultimate equality is due to (3.5).

If $\lambda \neq \pm\mu$, then F must also be diagonal. This is our main case. Before considering it, let us rule out the exceptional cases. If $\lambda = -\mu$ then $(\varepsilon_{\pm} + \varepsilon_0)(\mu + \lambda_{\pm}) = 0$, which is impossible, since $\varepsilon_{\pm} > 0$ and $\varepsilon_0 > 0$ and $\lambda_{\pm} > 0$, due to (4.4). If $\lambda = \mu$, then $(\varepsilon_{\pm} - \varepsilon_0)(\mu - \lambda_{\pm}) = 0$ and either $\varepsilon_{\pm} = \varepsilon_0$ or $\lambda_{\pm} = \mu$. However, according to (4.4), equation $\lambda_{\pm} = \mu$ implies $\varepsilon_{\mp} = \varepsilon_0$. Hence, if $\lambda = \mu$, then either F_+ or F_- is a point of self-intersection of the jump set. If μ is sufficiently large, as to satisfy (3.10), then such points are not present, and in particular, combining inequality (3.10) with jump set equation (3.5) we obtain

$$\varepsilon_{\pm} < \varepsilon_0. \tag{4.5}$$

We now consider the only remaining possibility $\lambda \neq \pm\mu$. Then any critical point F of Ψ must necessarily be diagonal in the frame in which $F_{\pm}$ are diagonal. Denoting by x and y the two diagonal entries of F we obtain

$$\Psi(F) = \Phi(x, y) + \text{const},$$

where

$$\Phi(x, y) = \frac{\mu}{2}\left(x^2 + y^2\right) + h(xy) - m_0 xy - \alpha x - \beta y, \quad x > 0, \ y > 0. \tag{4.6}$$

$$\alpha = \mu \varepsilon_{\pm} + \lambda_{\pm} \varepsilon_0 > 0, \qquad \beta = \mu \varepsilon_0 + \lambda_{\pm} \varepsilon_{\pm} > 0. \tag{4.7}$$

Emphasizing explicit dependence on μ the jump set equations (3.9) will be written as follows:

$$\begin{cases} \varepsilon_{\pm} = \dfrac{d_{\pm} R}{\sqrt{\mu}}, \\[2mm] \varepsilon_0 = \dfrac{\sqrt{\mu}}{R}, \end{cases} \qquad R = \sqrt{-\frac{[\![h']\!]}{[\![d]\!]}}. \tag{4.8}$$

In this notation parameters (4.7) are:

$$\alpha = 2\sqrt{\mu} R\{d\}, \qquad \beta = \frac{\mu^2 + R^4 d_+ d_-}{R\sqrt{\mu}}. \tag{4.9}$$

We compute

$$\beta - \alpha = \frac{(\mu - R^2 d_+)(\mu - R^2 d_-)}{R\sqrt{\mu}} > 0,$$

due to (3.10).

We are now ready to examine global minima of $\Phi(x, y)$. We begin by first minimizing $\Phi(x, y)$ over all pairs (x, y), satisfying $xy = d$ for each fixed $d > 0$, and then minimizing

$$\phi(d) = h(d) - m_0 d + \phi_0(d), \qquad \phi_0(d) = \min_{xy=d} \Phi_0(x, y)$$

in $d > 0$, where m_0 is given in (4.2) and

$$\Phi_0(x, y) = \frac{\mu}{2}(x^2 + y^2) - \alpha x - \beta y.$$

As shown in Appendix B, the minimum of $\Phi_0(x, y)$ is achieved at $(d/y(d), y(d))$, where $y(d)$ is the largest root of

$$q(y, d) = \mu y^4 - \beta y^3 + d\alpha y - \mu d^2 = 0. \qquad (4.10)$$

The function $y(d)$ is analytic in d, regarded as a complex variable. Singularities of such a function occur at values of d for which $q_y(y(d), d) = 0$. It is a routine algebraic calculation (solving the system $q = 0$, $q_y = 0$) to show than none of the singularities of $y(d)$ lie on the real d-axis.

Using formulas (4.9) we compute

$$y(d_\pm) = \frac{\sqrt{\mu}}{R}.$$

Hence,

$$z(d) = \frac{(y(d) - \sqrt{\mu}/R)\mu^{3/2}}{(d - d_-)(d - d_+)}, \qquad (4.11)$$

is analytic in the same complex domain as $y(d)$, and in particular on the real d-axis. The factor $\mu^{3/2}$ in the numerator in (4.11) is for convenience, since as is easy to show

$$\lim_{\mu \to \infty} z(d) = R^3, \qquad (4.12)$$

and convergence is uniform in d on compact subsets of $\mathbb{R}$. When $d_\pm$ varies in (d_1, d_2), the parameter $R = R(d_\pm)$ varies in $(0, \sqrt{-h''(d_0)}]$. Thus, $z(d) = z(d; \mu)$ is uniformly bounded, as $\mu \to +\infty$. Therefore, the asymptotics of $y(d) = y(d; \mu)$ as $\mu \to +\infty$ can be read off the representation

$$y(d; \mu) = \frac{\sqrt{\mu}}{R} + \mu^{-3/2}(d - d_-)(d - d_+)z(d; \mu). \qquad (4.13)$$

It is a calculation best done using computer algebra system, such as Maple, to show that

$$\phi_0'(d) = \frac{\mu y(d)^2 - \beta y(d)}{d}.$$

In a similar fashion one verifies that $\phi_0''(d)$ cannot vanish on $d > 0$. Thus, $\phi_0'(d)$ is an increasing function of d on $(0, +\infty)$, and the minima of $\phi(d)$ occur at critical points of $\phi(d)$, since $\phi(d) \to +\infty$, when $d \to +\infty$. Then, minimizers of $\phi(d)$ satisfy

$$\phi'(d) = \frac{\mu y(d)^2 - \beta y(d)}{d} + (h'(d) - m_0) = 0. \qquad (4.14)$$

This implies that there is a compact interval $[d_{\min}, d_{\max}] \subset (0, +\infty)$, where all solutions of (4.14) lie. Indeed, $d_{\min}$ (respectively $d_{\max}$), chosen to be independent of $d_\pm \in (d_1, d_2)$, is found from the condition that both terms in (4.14) are negative (respectively positive). The details are in Appendix B.

We note that $\phi(d_+) = \phi(d_-)$ due to (3.6). Our goal is to prove that

$$\psi(d) = \phi(d) - \phi(d_\pm) \geq 0, \quad \forall d > 0.$$

We compute (using Maple)

$$\lim_{\mu \to \infty} \psi(d) = \psi_\infty(d) = h(d) - \{h\} - \{h'\}\big(d - \{d\}\big) + \frac{R^2}{2}(d - d_+)(d - d_-).$$

The function $\psi_\infty(d)$ satisfies $\psi_\infty(d_\pm) = 0$ (due to (3.6)) and $\psi'_\infty(d_\pm) = 0$ (due to the value of R, given in (4.8)). We observe that if $h(d)$ is *any* quartic polynomial with leading coefficient a, then

$$\psi_\infty(d) = a(d - d_+)^2(d - d_-)^2. \tag{4.15}$$

The geometric meaning of $\psi'_\infty(d)$ is the difference between $h'(d)$ and the equal-area secant line passing through $(d_\pm, h'(d_\pm))$ (see Fig. 2). The assumption of the double-well shape of $h(d)$ implies that there are exactly 3 points of intersection of this secant line with the graph of $h'(d)$, unless $d_+ = d_- = d_0$. In every case (including the limiting one) the points $d_\pm$ correspond to local (and hence global) minima of $\psi_\infty(d)$, while the third point is a point of local maximum.

Lemma 4.1 *There exists $c_0 > 0$, such that for all $d_- \in (d_1, d_2)$ (setting $d_+ = D(d_-)$) and for all $d \in [d_{\min}, d_{\max}]$ we have*

$$\frac{\psi_\infty(d; d_-)}{(d - d_+)^2(d - d_-)^2} \geq c_0. \tag{4.16}$$

Proof If inequality (4.16) fails, then there exist sequences $d_-^{(n)}$ and $d_n \in [d_{\min}, d_{\max}]$ such that

$$\lim_{n \to \infty} \frac{\psi_\infty(d_n; d_-^{(n)})}{(d_n - d_+^{(n)})^2(d_n - d_-^{(n)})^2} = 0. \tag{4.17}$$

Since both sequences are bounded we can extract convergent subsequences, not relabeled:

$$d_-^{(n)} \to d_-^\infty, \qquad d_+^{(n)} \to d_+^\infty = D\big(d_-^\infty\big), \qquad d_n \to d_\infty.$$

Since denominator in (4.17) is uniformly bounded we conclude that $\psi_\infty(d_\infty; d_-^\infty) = 0$. Thus, d_∞ is either d_-^∞ or d_+^∞. To fix notation we assume that $d_\infty = d_-^\infty$.

If $d_-^\infty \neq d_0$ then $d_+^\infty \neq d_-^\infty$ and we conclude that

$$\lim_{n \to \infty} \frac{\psi_\infty(d_n; d_-^{(n)})}{(d_n - d_+^{(n)})^2(d_n - d_-^{(n)})^2} = \frac{\psi''_\infty(d_-^\infty; d_-^\infty)}{2[\![d^\infty]\!]^2} = \frac{h''(d_-^\infty) + R^2(d_-^\infty)}{2[\![d^\infty]\!]^2} > 0,$$

contradicting (4.17). The only possibility is therefore $d_\infty = d_-^\infty = d_+^\infty = d_0$. In this case

$$\lim_{n \to \infty} \frac{\psi_\infty(d_n; d_-^{(n)})}{(d_n - d_+^{(n)})^2(d_n - d_-^{(n)})^2} = \frac{h^{(4)}(d_0)}{24} > 0, \tag{4.18}$$

since for sufficiently large n all sequences d_n and $d_\pm^{(n)}$ lie in any arbitrarily small neighborhood of $d = d_0$. In that neighborhood the function $h(d)$ will be indistinguishable from its

quartic Taylor polynomial with leading coefficient $h^{(4)}(d_0)/24 > 0$. The value of the limit in (4.18) then follows from (4.15). □

In order to show that $d_{\pm}$ are the only minimizers of $\psi(d; \mu)$ we use representation (4.13) for $y(d; \mu)$ and obtain (via a Maple calculation)

$$\lim_{\mu \to \infty} \mu^2 \frac{\psi(d; \mu) - \psi_{\infty}(d)}{(d - d_+)^2 (d - d_-)^2} = -\frac{R^6}{2},$$

where the limit is uniform in $d \in [d_{\min}, d_{\max}]$ and in $d_- \in (d_1, d_2)$.

Now, recalling that $R^2 \leq -h''(d_0)$ for all $d_- \in (d_1, d_2)$, we have for sufficiently large μ

$$\mu^2 \frac{\psi(d; \mu) - \psi_{\infty}(d)}{(d - d_+)^2 (d - d_-)^2} \geq h''(d_0)^3$$

for all $d \in [d_{\min}, d_{\max}]$ and all $d_- \in (d_1, d_2)$. Applying Lemma 4.1 we have

$$\frac{\psi(d; \mu)}{(d - d_+)^2 (d - d_-)^2} \geq c_0 + \mu^{-2} h''(d_0)^3 > 0$$

when μ is sufficiently large, and where the lower bound on μ does not depend on neither d, nor d_-. We conclude that $\psi(d; \mu)$ is minimized only at $d_{\pm}$, since $\psi(d_{\pm}; \mu) = 0$. Therefore, the entire jump set satisfies the polyconvexity condition.

Remark 4.2 The lowest value of μ for which the entire jump set becomes polyconvex is not given explicitly here. In our numerical calculations we observed that if the point on the jump set corresponding to $d_+ = d_- = d_0$ is polyconvex, then the entire jump set is polyconvex, at least when $h(d)$ is a quartic polynomial. We can then write equations corresponding to the appearance of d_*, such that $\phi(d_*) = \phi(d_0)$ and $\phi'(d_*) = \phi'(d_0) = 0$. This leads to explicit but very cumbersome equation in the single variable d, whose solution is $d = d_*$. To give a rough idea of the strength of our results we have evaluated this value of μ for $h(d) = (d - 1)^2 (d - 3)^2$. In this case the entire jump set is polyconvex if and only if $\mu \geq 10.53$. Inequality (3.10) says that the jump set has no self-intersections, when $\mu > 8.45$ and inequality (3.11) implies that the jump set does not capture the entire binodal if $\mu < 9.98$. Thus, there is a small interval of values [9.98, 10.53] of the parameter μ for which the jump set contains a region whose stability status is unknown. This interval represents the gap between necessary and sufficient conditions.
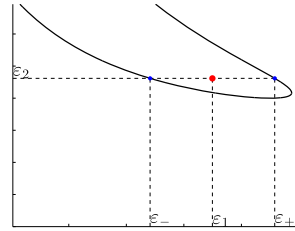
5 The Quasiconvex Envelope

We have now proved that when μ is sufficiently large, the entire jump set satisfies the quasiconvexity condition. As a consequence, we obtain an explicit rule for finding $QW(F)$ for the two-well Hadamard energy (1.1).

We recall a theorem from [13] that the quasiconvex envelope of the objective isotropic energy is also objective and isotropic. Therefore, $QW(F)$ depends on F only through its singular values $0 < \varepsilon_1(F) \leq \varepsilon_2(F)$. In order to describe $QW(\varepsilon_1, \varepsilon_2)$, for $d \in (d_1, d_2)$, let

$$R(d) = \sqrt{-\frac{h'(D(d)) - h'(d)}{D(d) - d}}.$$

Fig. 4 The convex combination rule (2.7) for computing the quasiconvex hull

Then,

$$\mathcal{B}_\mu = \left\{(\varepsilon_1, \varepsilon_2) : \varepsilon_1 > 0, \ d_1 < \varepsilon_1\varepsilon_2 < d_2, \ \varepsilon_2 R(\varepsilon_1\varepsilon_2) > \sqrt{\mu}\right\}$$

describes the region inside the curve in Fig. 4. If $(\varepsilon_1, \varepsilon_2) \in \mathcal{B}_\mu$, then there exists a uniquely determined pair $\varepsilon_-(\varepsilon_2) < \varepsilon_+(\varepsilon_2)$, such that $(\varepsilon_\pm, \varepsilon_2) \in \partial\mathcal{B}_\mu$ (see Fig. 4). Algebraically, $\varepsilon_\pm(\varepsilon_2)$ are found as the two solutions $\varepsilon = \varepsilon_\pm$ of

$$\varepsilon_2 R(\varepsilon\varepsilon_2) = \sqrt{\mu}. \tag{5.1}$$

We observe that for $(\varepsilon_1, \varepsilon_2) \in \mathcal{B}_\mu$ we always have

$$\varepsilon_-(\varepsilon_2) < \varepsilon_1 < \varepsilon_+(\varepsilon_2).$$

For any $\boldsymbol{F} \in \mathbb{R}_+^{2\times 2}$, let $0 < \varepsilon_1(\boldsymbol{F}) \le \varepsilon_2(\boldsymbol{F})$ be the ordered pair of its singular values. Then, according to (2.7)

$$QW(\varepsilon_1, \varepsilon_2) = \begin{cases} W(\varepsilon_1, \varepsilon_2), & (\varepsilon_1, \varepsilon_2) \notin \mathcal{B}_\mu, \\ \frac{\varepsilon_1 - \varepsilon_-}{\varepsilon_+ - \varepsilon_-} W(\varepsilon_+, \varepsilon_2) + \frac{\varepsilon_+ - \varepsilon_1}{\varepsilon_+ - \varepsilon_-} W(\varepsilon_-, \varepsilon_2), & (\varepsilon_1, \varepsilon_2) \in \mathcal{B}_\mu, \end{cases} \tag{5.2}$$

where $\varepsilon_\pm = \varepsilon_\pm(\varepsilon_2)$.

Let us examine the structure of QW and how it is related to W. We first note that

$$\varepsilon_\pm(\varepsilon_2) = \frac{\varepsilon'_\pm(\frac{\varepsilon_2}{\sqrt{\mu}})}{\sqrt{\mu}},$$

where $\varepsilon'_\pm(\varepsilon'_2)$ are the two solutions of $\varepsilon'_2 R(\varepsilon'\varepsilon'_2) = 1$. Therefore,

$$\mathcal{B}_\mu = \left\{\left(\frac{\varepsilon'_1}{\sqrt{\mu}}, \varepsilon'_2\sqrt{\mu}\right) : (\varepsilon'_1, \varepsilon'_2) \in \mathcal{B}_1\right\}.$$

In other words $\mathcal{B}_\mu$ is a hyperbolic rotation of $\mathcal{B}_1$:

$$\mathcal{B}_\mu = \mathcal{R}_\mu \mathcal{B}_1, \qquad \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{\mu}} & 0 \\ 0 & \sqrt{\mu} \end{bmatrix} \begin{bmatrix} \varepsilon'_1 \\ \varepsilon'_2 \end{bmatrix}.$$

We can describe $\mathcal{B}_1$ more explicitly in terms of functions $\varepsilon'_\pm(\varepsilon'_2)$:

$$\mathcal{B}_1 = \left\{(\varepsilon'_1, \varepsilon'_2) : \varepsilon'_2 > \frac{1}{\sqrt{-h''(d_0)}}, \ \varepsilon'_-(\varepsilon'_2) < \varepsilon'_1 < \varepsilon'_+(\varepsilon'_2)\right\}, \tag{5.3}$$

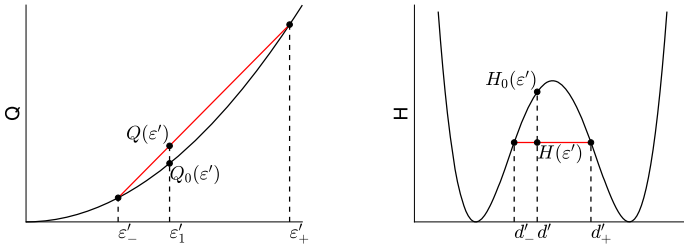where $d_0 \in (d_1, d_2)$ is the unique fixed point of the map $D(d)$.

Fig. 5 Geometric interpretation of functions $Q(\varepsilon')$ and $H(\varepsilon')$

Denoting $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2)$ and $\boldsymbol{\varepsilon}' = (\varepsilon_1', \varepsilon_2')$ we can also write

$$W(\boldsymbol{\varepsilon}) = \frac{\mu \varepsilon_2^2}{2} + \Psi_0\big(\mathcal{R}_\mu^{-1}\boldsymbol{\varepsilon}\big), \qquad QW(\boldsymbol{\varepsilon}) = \frac{\mu \varepsilon_2^2}{2} + \Psi\big(\mathcal{R}_\mu^{-1}\boldsymbol{\varepsilon}\big),$$

where

$$\Psi_0\big(\boldsymbol{\varepsilon}'\big) = Q_0\big(\boldsymbol{\varepsilon}'\big) + H_0\big(\boldsymbol{\varepsilon}'\big), \qquad \Psi\big(\boldsymbol{\varepsilon}'\big) = Q\big(\boldsymbol{\varepsilon}'\big) + H\big(\boldsymbol{\varepsilon}'\big).$$

For $\boldsymbol{\varepsilon}' \notin \mathcal{B}_1$

$$Q\big(\boldsymbol{\varepsilon}'\big) = Q_0\big(\boldsymbol{\varepsilon}'\big) = \frac{(\varepsilon_1')^2}{2}, \qquad H\big(\boldsymbol{\varepsilon}'\big) = H_0\big(\boldsymbol{\varepsilon}'\big) = h\big(\varepsilon_1'\varepsilon_2'\big).$$

For $\boldsymbol{\varepsilon}' \in \mathcal{B}_1$ Q_0 and H_0 retain their form above, while

$$Q\big(\boldsymbol{\varepsilon}'\big) = \frac{\varepsilon_1' - \varepsilon_-'}{\varepsilon_+' - \varepsilon_-'} \frac{(\varepsilon_+')^2}{2} + \frac{\varepsilon_+' - \varepsilon_1'}{\varepsilon_+' - \varepsilon_-'} \frac{(\varepsilon_-')^2}{2},$$

$$H\big(\boldsymbol{\varepsilon}'\big) = \frac{\varepsilon_1' - \varepsilon_-'}{\varepsilon_+' - \varepsilon_-'} h\big(\varepsilon_+'\varepsilon_2'\big) + \frac{\varepsilon_+' - \varepsilon_1'}{\varepsilon_+' - \varepsilon_-'} h\big(\varepsilon_-'\varepsilon_2'\big).$$

These formulas are deceptively messy. Functions Q and H have a simple geometric interpretation shown in Fig. 5. Denoting

$$d' = \varepsilon_1'\varepsilon_2', \qquad d_\pm' = \varepsilon_\pm'\varepsilon_2'.$$

The point $(d', H(\boldsymbol{\varepsilon}'))$ lies on the chord connecting points $(d_\pm', h(d_\pm'))$, while the point $(\varepsilon_1', Q(\boldsymbol{\varepsilon}'))$ lies on the chord connecting points $(\varepsilon_\pm', (\varepsilon_\pm')^2/2)$. Comparing this formula to the naive first guess (1.2) we can write $U(\boldsymbol{\varepsilon})$ in the exact same form

$$U(\boldsymbol{\varepsilon}) = \frac{\mu \varepsilon_2^2}{2} + Q_0\big(\mathcal{R}_\mu^{-1}\boldsymbol{\varepsilon}\big) + \widetilde{H}\big(\mathcal{R}_\mu^{-1}\boldsymbol{\varepsilon}\big),$$

where the point $(d', \widetilde{H}(\boldsymbol{\varepsilon}'))$ lies on the Horizontal chord (common tangent) connecting points $(d_1, h(d_1))$ and $(d_2, h(d_2))$ in Fig. 5. We can have an idea of the relation between $W(\boldsymbol{\varepsilon})$, $QW(\boldsymbol{\varepsilon})$ and $U(\boldsymbol{\varepsilon})$ by observing that

$$U(\boldsymbol{\varepsilon}) \leq QW(\boldsymbol{\varepsilon}) \leq W(\boldsymbol{\varepsilon}).$$

Both inequalities above are strict when $\boldsymbol{\varepsilon} \in \mathcal{B}_\mu$. When $\varepsilon_1\varepsilon_2 \notin (d_1, d_2)$, then both inequalities become equalities, and when $\boldsymbol{\varepsilon} \notin \mathcal{B}_\mu$, but $\varepsilon_1\varepsilon_2 \in (d_1, d_2)$, then the left inequality remains

strict, while the right inequality turns into equality. We note that the above analysis used simplified notation, where ε_2 denoted the larger of the two singular values of $\boldsymbol{F}$ and ε_1, the smaller.

6 Conclusions

The problem of computing quasi-convex envelopes for non-rank one convex energies is notoriously complex and only very few explicit constructions of this type are known in the literature [7, 24]. In this paper we presented a new explicit construction of this type for a subclass of double-well Hadamard energies which model materials undergoing isotropic-to-isotropic elastic phase transitions. The explicit calculations are performed in two space dimensions, but the technique works in 3D, as well, producing analogous results. Our example is non-trivial because the energy wells are not rank one connected and the construction does not reduce to convexification of any auxiliary energy. The possibility to obtain the explicit result is due to the fact that in the range of the dominance of the quadratic term in the Hadamard energy, the energy-minimizing microstructures are simple laminates which we prove by showing stability of the entire jump set representing deformation gradients that can coexist at jump discontinuities. When the relative size of the quadratic convex term decreases, the non-convex term in the Hadamard energy starts to dominate and the microstructures get more and more complex in some regions of the binodal. Yet, our method of identifying a laminate subset of the binodal remains effective, even though it no longer captures the entire binodal. When the rigidity modulus μ tends to zero and the material progressively fluidizes, the relaxation of Hadamard material should involve laminates of infinite rank, since the part of the binodal that is not captured by our method cannot be captured by laminates of any finite rank. We believe that such situations where either simple or infinite rank laminates are optimal must be generic, notwithstanding examples to the contrary for very special energies [3, 4, 9, 10].

Appendix A

Theorem A.1 *Suppose that $W(\boldsymbol{F})$ is given by* (1.1) *and that $h(d)$ is of class C^1, non-convex, has superlinear growth as $d \to +\infty$, and $h(d) = h^{**}(d)$ for all d outside of a finite interval. Then $QW(\boldsymbol{F})$ cannot be written in the form $\mu'|\boldsymbol{F}|^2/2 + H(d)$ for any function H and $\mu' > 0$.*

Let d_0 be such that $h^{**}(d_0) = h(d_0)$. Then for any $\boldsymbol{F}_0$, such that $\det \boldsymbol{F}_0 = d_0$ we have $QW(\boldsymbol{F}_0) = W(\boldsymbol{F}_0)$. Indeed, we have $W(\boldsymbol{F}_0) = U(\boldsymbol{F}_0)$, where $U(\boldsymbol{F})$ is defined in (1.2). But $U(\boldsymbol{F})$ is polyconvex and therefore quasiconvex, while satisfying $U(\boldsymbol{F}) \leq W(\boldsymbol{F})$. It follows that

$$U(\boldsymbol{F}) \leq QW(\boldsymbol{F}) \leq W(\boldsymbol{F}). \tag{A.1}$$

Thus, $QW(\boldsymbol{F}_0) = W(\boldsymbol{F}_0)$ for any $\boldsymbol{F}_0$, such that $W(\boldsymbol{F}_0) = U(\boldsymbol{F}_0)$.

Theorem [A.1] is proved by contradiction. Hence we assume that there exists a number μ' and a function $H(d)$, such that

$$QW(\boldsymbol{F}) = \frac{\mu'}{2}|\boldsymbol{F}|^2 + H(d). \tag{A.2}$$

We fix d_0, such that $h(d_0) = h^{**}(d_0)$. Then for diagonal $\boldsymbol{F}$ with components f and d_0/f on the diagonal we must have

$$\frac{\mu'}{2}\left(f^2 + \frac{d_0^2}{f^2}\right) + H(d_0) = \frac{\mu}{2}\left(f^2 + \frac{d_0^2}{f^2}\right) + h(d_0),$$

for every $f > 0$. It follows that $\mu = \mu'$ and $H(d) = h(d)$ for any d for which $h(d) = h^{**}(d)$. But then inequality [(A.1)] implies $h^{**}(d) \leq H(d) \leq h(d)$ for all $d > 0$. However quasiconvexity of [(A.2)] implies that $H(d)$ has to be convex [6]. It follows that $H(d) = h^{**}(d)$ and we must conclude that if [(A.2)] is true then

$$QW(\boldsymbol{F}) = \frac{\mu}{2}|\boldsymbol{F}|^2 + h^{**}(d). \tag{A.3}$$

Showing that [(A.3)] is impossible is the main technical difficulty to be overcome. The idea is to prove that there exists $\boldsymbol{F}_0$, such that $h^{**}(\det \boldsymbol{F}_0) < h(\det \boldsymbol{F}_0)$, yet $W(\boldsymbol{F}_0) = QW(\boldsymbol{F}_0)$, which would contradict [(A.3)].

Let us consider the set

$$\mathcal{C} = \{d : h(d) > h^{**}(d)\},$$

which is open and bounded. In particular $\mathcal{C}$ is an at most countable union of finite intervals. Let (d_*, d^*) be one such interval. Let us prove a geometrically "obvious" statement that the tangent line to the graph of $h(d)$ at d_* must also be tangent to it at d^*.

Lemma A.2 *Suppose that $h(d)$ is of class C^1 and has superlinear growth. Suppose that $h(d) > h^{**}(d)$ for all $d \in (d_*, d^*)$ and $h(d_*) = h^{**}(d_*)$ and $h(d^*) = h^{**}(d^*)$. Then $h'(d_*) = h'(d^*)$ and $h(d^*) - h(d_*) = h'(d_*)(d^* - d_*)$.*

Proof We assume, without loss of generality, that

$$h(d^*) = h'(d^*) = 0.$$

We will now show that $h(d_*) = h'(d_*) = 0$. It is enough to show that $h'(d_*) = 0$, since the graph of $h(d)$ can not be below the tangent line at either d^* or d_*, we will then conclude (since both tangent lines are horizontal) that $h(d_*) = h(d^*) = 0$.

From the inequalities

$$0 = h(d^*) \geq h(d_*) + h'(d_*)(d^* - d_*) \geq h'(d_*)(d^* - d_*)$$

we conclude that $h'(d_*) < 0$, if it is not equal to 0. Now consider supporting lines to the graph of $h(d)$ with small and negative slope. In other words, for all $0 < \epsilon < -h'(d_*)$ we consider

$$\phi(\epsilon) = \min_d\big(h(d) + \epsilon d\big).$$

Let d_ϵ denote a minimizer, which must exist, since $h(d)$ has a superlinear growth. This minimizer must satisfy $h^{**}(d_\epsilon) = h(d_\epsilon)$, so that $d_\epsilon \notin (d_*, d^*)$. It is easy to see that d_ϵ cannot be larger than d^*. Indeed, if $d_\epsilon > d^*$

$$0 = h(d^*) \geq h(d_\epsilon) + h'(d_\epsilon)(d^* - d_\epsilon) = h(d_\epsilon) + \epsilon(d_\epsilon - d^*) \geq \epsilon(d_\epsilon - d^*) > 0,$$

which is a contradiction. Let us show that d_ϵ cannot be smaller that d_* either. If $d_\epsilon < d_*$ then we have

$$h(d_\epsilon) \geq h(d_*) + h'(d_*)(d_\epsilon - d_*)$$

and

$$h(d_*) \geq h(d_\epsilon) - \epsilon(d_* - d_\epsilon) \geq h(d_*) - \big(h'(d_*) + \epsilon\big)(d_* - d_\epsilon) > h(d_*),$$

which is a contradiction. □

We will now show that for all sufficiently small $\epsilon > 0$ we must have $QW(F) = W(F)$ for any F with $\det F = d^* - \epsilon$. This would contradict formula (A.3).

Lemma A.3 *For $\delta \in (d_*, d^*)$ we define*

$$\mathcal{D}(\delta) = \big\{d : h(d) < h(\delta) + h'(\delta)(d - \delta)\big\} \neq \emptyset,$$

and $\theta(\delta) = \inf \mathcal{D}(\delta)$. Then there exists $\delta_n \to d_*$, such that $\theta(\delta_n) \to d^*$, as $n \to \infty$.

Proof In our case $h(d) > 0$ for all $d \in (d_*, d^*)$, while $h(d_*) = h(d^*) = 0$. For any $\epsilon > 0$ let $E_\epsilon = \{d \in (d_*, d^*) : h(d) < \epsilon\}$. Let

$$d^\epsilon = \inf\left\{d \in E_\epsilon : d > \frac{d_* + d^*}{2}\right\}, \qquad d_\epsilon = \sup\left\{d \in E_\epsilon : d < \frac{d_* + d^*}{2}\right\}$$

Then $h(d_\epsilon) = h(d^\epsilon) = \epsilon$, $h(d) > \epsilon$ for all $d \in (d_\epsilon, d^\epsilon)$ and $d_\epsilon \to d_*$ and $d^\epsilon \to d^*$, as $\epsilon \to 0$. Now consider the function

$$\phi_\epsilon(d) = h(d) - \frac{\epsilon(d - d_*)}{d^\epsilon - d_*}.$$

Let d_ϵ^* be a minimizer of ϕ_ϵ:

$$\phi_\epsilon(d_\epsilon^*) = \min_{d \in [d_*, d^\epsilon]} \phi_\epsilon(d) = m_\epsilon.$$

We observe that $m_\epsilon < 0$. Indeed,

$$0 = h'(d_*) = \lim_{d \to d_*} \frac{h(d)}{d - d_*}.$$

Thus, for all $d > d_*$ sufficiently close to d_* we have

$$\frac{h(d)}{d - d_*} < \frac{\epsilon}{d^\epsilon - d_*}.$$

Therefore, $d_\epsilon^* \in (d_*, d_\epsilon)$. Indeed, for all $d \in (d_\epsilon, d^\epsilon)$ we have

$$\phi_\epsilon(d) \geq \epsilon - \frac{\epsilon(d - d_*)}{d^\epsilon - d_*} = \frac{\epsilon(d^\epsilon - d)}{d^\epsilon - d_*} > 0.$$

We conclude that $d_\epsilon^* \to d_*$, as $\epsilon \to 0$ and $\phi_\epsilon'(d_\epsilon^*) = 0$, i.e.,

$$h'(d_\epsilon) = \frac{\epsilon}{d^\epsilon - d_*} > 0.$$

In addition we have $\phi_\epsilon(d) \geq \phi_\epsilon(d_\epsilon^*)$, i.e.,

$$h(d) \geq \frac{\epsilon(d - d_\epsilon^*)}{d^\epsilon - d_*} + h(d_\epsilon^*) = h(d_\epsilon^*) + h'(d_\epsilon^*)(d - d_\epsilon^*),$$

for all $d \in [d_*, d^\epsilon]$. This inequality will also hold for $d < d_*$. Indeed, since $\phi_\epsilon(d_\epsilon^*) < 0$ we have

$$h(d_\epsilon^*) < \frac{\epsilon(d_\epsilon^* - d_*)}{d^\epsilon - d_*}.$$

Therefore,

$$\frac{\epsilon(d - d_\epsilon^*)}{d^\epsilon - d_*} + h(d_\epsilon^*) < \frac{\epsilon(d - d_*)}{d^\epsilon - d_*} < 0 \leq h(d),$$

when $d < d_*$. We conclude that

$$d^* \in \mathcal{D}(d_\epsilon^*) \subset (d^\epsilon, +\infty). \qquad \square$$

Now, let δ_n be as in the lemma. The superlinear growth of $h(d)$ implies that there exists $\beta > 0$ so that $\mathcal{D}(\delta_n) \subset (\theta(\delta_n), \beta)$ for all sufficiently large n. Hence,

$$\lim_{n \to \infty} \sup_d \{h(\delta_n) + h'(\delta_n)(d - \delta_n) - h(d)\} = 0.$$

Let $\boldsymbol{F}_n = \sqrt{\delta_n}\boldsymbol{I}_2$. Then,

$$\lim_{n \to \infty} \inf_{\{\boldsymbol{F}:\det \boldsymbol{F} \in \mathcal{D}(\delta_n)\}} |\boldsymbol{F} - \boldsymbol{F}_n| \geq \mathrm{dist}\left(\sqrt{d_*}\boldsymbol{I}_2, \{\boldsymbol{F} : \det \boldsymbol{F} \geq d^*\}\right) > 0.$$

It follows that there exists $N > 0$, such that

$$\sup_d \{h(\delta_N) + h'(\delta_N)(d - \delta_N) - h(d)\} < \frac{\mu}{2}|\boldsymbol{F} - \boldsymbol{F}_N|^2$$

for every $\boldsymbol{F}$ with $\det \boldsymbol{F} \in \mathcal{D}(\delta_N)$. Then, for any $\boldsymbol{F}$, either $\det \boldsymbol{F} \notin \mathcal{D}(\delta_N)$ and hence

$$h(\det \boldsymbol{F}) - h(\delta_N) - h'(\delta_N)(\det \boldsymbol{F} - \delta_N) \geq 0,$$

or $\det \boldsymbol{F} \in \mathcal{D}(\delta_N)$ and thus

$$h(\delta_N) + h'(\delta_N)(\det \boldsymbol{F} - \delta_N) - h(\det \boldsymbol{F}) \leq \frac{\mu}{2}|\boldsymbol{F} - \boldsymbol{F}_N|^2.$$

In either case

$$\frac{\mu}{2}|\boldsymbol{F} - \boldsymbol{F}_N|^2 + h(\det \boldsymbol{F}) - h(\delta_N) - h'(\delta_N)(\det \boldsymbol{F} - \delta_N) \geq 0. \qquad (A.4)$$

We observe that the function

$$\mathcal{N}(\boldsymbol{F}) = h(\delta_N) + h'(\delta_N)(\det \boldsymbol{F} - \delta_N)$$

is a null-Lagrangian and satisfies $W(\boldsymbol{F}) \geq \mathcal{N}(\boldsymbol{F})$ for all $\boldsymbol{F}$ and $W(\boldsymbol{F}_N) = \mathcal{N}(\boldsymbol{F}_N)$. Thus, since $\mathcal{N}(\boldsymbol{F})$ is quasiconvex, we have

$$W(\boldsymbol{F}) \leq QW(\boldsymbol{F}) \leq \mathcal{N}(\boldsymbol{F}),$$

which implies that $QW(\boldsymbol{F}_N) = W(\boldsymbol{F}_N)$, as desired, while $h^{**}(\delta_N) < h(\delta_N)$, since $\delta_N \in (d_*, d^*)$. Theorem A.1 is proved now.

Appendix B: Minimization of $\Phi_0(x, y)$ over $xy = d$

We use the method of Lagrange multipliers to minimize

$$\Phi_0(x, y) = \frac{\mu}{2}(x^2 + y^2) - \alpha x - \beta y,$$

subject to the constraints $x > 0$, $y > 0$, $xy = d$. We note that $\Phi_0(x, y) \to +\infty$ when $x^2 + y^2 \to +\infty$, since $\mu > 0$. Therefore, the minimum of $\Phi_0(x, y)$ is achieved at a critical point on the branch of the hyperbola $xy = d$, $x > 0$. This critical point satisfies the following linear the system of equations:

$$\begin{cases} \mu x - \lambda y = \alpha, \\ \mu y - \lambda x = \beta. \end{cases}$$

Its solution is

$$x = x(\lambda) = \frac{\lambda\beta + \alpha\mu}{\mu^2 - \lambda^2}, \qquad y = y(\lambda) = \frac{\lambda\alpha + \beta\mu}{\mu^2 - \lambda^2}. \tag{B.1}$$

These equations describe both branches of the hyperbola

$$\mu(y^2 - x^2) + \alpha x - \beta y = 0. \tag{B.2}$$

The minimum value of $\Phi_0(x, y)$, subject to the constraints $x > 0$, $y > 0$, $xy = d$ is achieved at a point of intersection of the hyperbola (B.1), shown as a thick solid line on Fig. 6 with the hyperbola $xy = d$, shown as a dashed line. The x and y coordinates of these points of intersection solve the quartic equations

$$\mu x^4 - \alpha x^3 + d\beta x - \mu d^2 = 0, \qquad \mu y^4 - \beta y^3 + d\alpha y - \mu d^2 = 0, \tag{B.3}$$

respectively. When d is very small there are 3 points of intersection of the two hyperbolas in the first quadrant and one in the third, as shown in Fig. 6. There is a critical value $d_* > 0$,

Fig. 6 Critical points of $\Phi_0(x, y)$ subject to the constraint $xy = d$
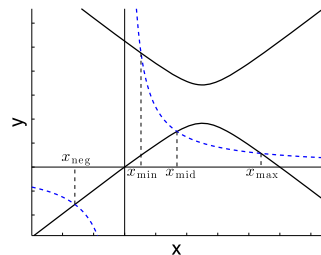
such that for $d > d_*$ there will be only one point of intersection of the two hyperbolas in the first quadrant, located on the upper branch of the hyperbola (B.2). In this case this point must be the minimizer, since the minimum is achieved at a critical point on $xy = d$, $x > 0$. When $0 < d < d_*$, the other three points of intersection will lie on the lower branch of (B.2). Let us show that in this case the point of intersection with the upper branch corresponds to the minimizer. Let

$$x_{\text{neg}} < 0 < x_{\min}(d) < x_{\text{mid}}(d) < x_{\max}(d)$$

denote the 4 roots of (B.3). They are critical points of $f(x; d) = \Phi_0(x, d/x)$. Since $f(x, d) \to +\infty$ when $x \to 0^+$ and $x \to +\infty$, we conclude that $x_{\min}(d)$ and $x_{\max}(d)$ are points of local minimum, while $x_{\text{mid}}(d)$ is a point of local maximum of $f(x; d)$. It will also be convenient to denote $y_\gamma = d/x_\gamma$, where γ is one of 'neg', 'min', 'mid' or 'max'. We note that

$$\lim_{d \to 0^+} \left(x_{\min}(d), y_{\min}(d)\right) = \left(0, \frac{\beta}{\mu}\right), \qquad \lim_{d \to 0^+} \left(x_{\max}(d), y_{\max}(d)\right) = \left(\frac{\alpha}{\mu}, 0\right).$$

Thus,

$$\lim_{d \to 0^+} f\left(x_{\min}(d); d\right) = -\frac{\beta^2}{2\mu} < -\frac{\alpha^2}{2\mu} = \lim_{d \to 0^+} f\left(x_{\max}(d); d\right).$$

This shows that

$$\Delta(d) = f\left(x_{\max}(d); d\right) - f\left(x_{\min}(d); d\right) > 0$$

when d is sufficiently small. In order to prove that $\Delta(d) > 0$ for all $d \leq d_*$ we note that

$$f\left(x_\gamma(d); d\right)' = \frac{\partial f}{\partial d}\left(x_\gamma(d); d\right), \quad \gamma \in \left\{\text{'neg', 'min', 'mid', 'max'}\right\}.$$

Then, after a straightforward calculation, we find that

$$\Delta'(d) = \left[f\left(x_{\max}(d); d\right) - f\left(x_{\min}(d); d\right)\right]' = \mu \frac{x_{\max} - x_{\min}}{x_{\max} x_{\min}} \left(\frac{\beta}{\mu} - (y_{\min} + y_{\max})\right).$$

Finding one more term of the asymptotic expansion of the roots of (B.3) in powers of d we compute

$$\lim_{d \to 0^+} \Delta'(d) = \frac{\mu(\alpha^2 - \beta^2)}{\alpha\beta} < 0.$$

Thus, $\Delta(d)$ is positive and decreasing when d is sufficiently small. The decrease of $\Delta(d)$ will continue either until d reaches d_* or a value at which $\Delta'(d) = 0$, whichever occurs first. Let us show that $\Delta'(d) \neq 0$ for any $d \in [0, d_*]$. Indeed, if $\Delta'(d) = 0$ then we must have

$$y_{\min} + y_{\max} = \frac{\beta}{\mu}.$$

However, since the y's are roots of the y-quartic in (B.3) we also have

$$y_{\text{neg}} + y_{\min} + y_{\text{mid}} + y_{\max} = \frac{\beta}{\mu}.$$

Hence, if $\Delta'(d) = 0$ we must have $y_{\text{mid}} = -y_{\text{neg}}$. However, if for some $y > 0$ both y and $-y$ solve (B.3), then such y must satisfy

$$\mu y^4 - \mu d^2 = 0, \qquad -\beta y^3 + d\alpha y = 0,$$

resulting in the consistency requirement $\alpha = \beta$, which is not true at all points satisfying (4.5). Thus, $\Delta(d)$ achieves its smallest value at $d = d_*$. However, at $d = d_*$ the function $f(x; d_*)$ has only one local minimum at $x_{\text{min}}(d_*)$, while it is an increasing function in the neighborhood of $x_{\text{min}}(d_*) = x_{\text{mid}}(d_*)$. Thus, $\Delta(d_*) > 0$, and therefore, $\Delta(d) > 0$ for all $d \in [0, d_*]$. We conclude that for all $d > 0$

$$\phi(d) = \min_{xy=d} \Phi(x, y) = \Phi_0\big(x_{\text{min}}(d), y_{\text{min}}(d)\big) + h(d) - m_0 d, \tag{B.4}$$

where $x_{\text{min}}(d)$ is the smallest positive root of the x-quartic in (B.3). ($y_{\text{min}}(d) = d/x_{\text{min}}(d)$ will be the largest root of the y-quartic in (B.3).) Moreover, Maple calculation shows

$$\phi'(d) = \frac{\mu y_{\text{min}}(d)^2 - \beta y_{\text{min}}(d)}{d} + h'(d) - m_0. \tag{B.5}$$

When d is sufficiently large $\phi'(d) > 0$ and therefore the minimum of $\phi(d)$ is attained at a critical point of $\phi(d)$. We note that $y_{\text{min}}(d)$ is an decreasing function of d on $(0, d_{\text{min}})$ and an increasing function on $(d_{\text{min}}, +\infty)$, which is geometrically obvious, since hyperbola (B.2) is independent of d. The value of d_{min} is easily found from the condition that the hyperbola $xy = d$ passes through the upper vertex of hyperbola (B.2). Another observation is that

$$y_{\text{min}}\left(\frac{\alpha\beta}{\mu^2}\right) = \frac{\beta}{\mu}.$$

The immediate consequence of this observation is that

$$\begin{cases} \phi'(d) > 0, & \text{if } h'(d) > m_0 \text{ and } d > \delta_{\text{max}}(\mu) = \dfrac{\alpha\beta}{\mu^2}, \\ \phi'(d) < 0, & \text{if } h'(d) < m_0 \text{ and } d < \delta_{\text{min}}(\mu) = \dfrac{\alpha(\beta + \sqrt{\beta^2 - \alpha^2})}{4\mu^2}. \end{cases}$$

We easily compute

$$\lim_{\mu \to \infty} \delta_{\text{max}}(\mu) = 2\{d\}, \qquad \lim_{\mu \to \infty} \delta_{\text{min}}(\mu) = \{d\}.$$

It follows that there exist $0 < d_{\text{min}} < d_{\text{max}}$ and $M_0 > 0$ that depend only on the choice of $h(d)$, so that for all $\mu > M_0$ all critical points of $\phi(d)$ are confined to the interval $(d_{\text{min}}, d_{\text{max}})$.

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