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ESTRUCTURAS MINIMIZANTES PARA LA ENERGÍA ELÁSTICA EN TRANSICIONES DE FASE BAJO EL RÉGIMEN DE TEORÍA GEOMÉTRICA LINEAL EN PELÍCULA DELGADA

TESIS

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PRESENTA: LAURO MORALES MONTESINOS

TUTOR DE TESIS DR. ANTONIO CAPELLA KORT INSTITUTO DE MATEMÁTICAS - UNAM

MIEMBROS DEL COMITÉ TUTOR DRA. MARÍA DE LA LUZ JIMENA DE TERESA DE OTEYZA INSTITUTO DE MATEMÁTICAS - UNAM

DR. RAMÓN GABRIEL PLAZA VILLEGAS INSTITUTO DE INVESTIGACIONES EN MATEMÁTICAS APLICADAS Y SISTEMAS

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Abstract

This thesis aims to study weak limits of minimizing sequences for non-convex variational problems arising in two-dimensional linear elasticity. In certain type of crystals, it is common to observe periodic arrangements of grains along the sample when it is subjected to some stress. The existence of this "microstructure" in the material can be predicted by elasticity and the analysis of the energy stored in the sample. We work on the two-dimensional problem for linear elasticity. Given a sample $\Omega \subset \mathbb{R}^2$ distorted by a deformation $u: \Omega \to \mathbb{R}^2$, we have an energy density $\phi \ge 0$ that is a function of the linear strain $e(Du) := (Du + D^T u)/2$. This energy density vanishes if and only if the symmetric part of the argument belongs to a finite set of matrices $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$. This set is called the set of wells and the energy stored in the sample is given by

$$I(u) = \int_{\Omega} \phi(Du) \, dx,$$

Because of its multi-well structure the energy I is not weakly lower semicontinuous. The linear strains of minimizing sequences of I will typically oscillate among the \mathcal{U} 's elements. These oscillations are interpreted as microstructure. In order to study these minimizing sequences we consider \tilde{I} the quasiconvexification of I. The set of values taken by weak limits of minimizing sequences of \tilde{I} is known as the symmetric quasiconvex hull $Q^e(\mathcal{U})$ of the set \mathcal{U} . We are interested in determining explicitly $Q^e(\mathcal{U})$. In some cases we achieve this goal, whereas in other we are only able to produce explicit bounds. In our study we use the symmetric lamination convex hull $L^e(\mathcal{U})$, a well known inner bound of $Q^e(\mathcal{U})$.

In the first chapter, we present the problem, its physical origin, and we give a formal derivation of the mathematical model in nonlinear and linear elasticity. We also present our results that will be described in full in the later chapters. In the second chapter, we discuss the concept of compatibility and its geometrical interpretation in terms of an incompatible cone. We determine $L^e(\mathcal{U})$ for a three-well set \mathcal{U} and study the *polyconvex* biconjugate envelope f_C^{PP} of a particular function $f_C \geq 0$. This envelope is quasiconvex and by studying its zero-level set denoted by ker f_C^{PP} , we obtain an outer bound for $Q^e(\mathcal{U})$. Moreover, if there is a rank-one compatible pair in \mathcal{U} we show that $L^e(\mathcal{U}) = Q^e(\mathcal{U})$ and the outer bounds become optimal.

The third chapter is an extension of chapter two to the general n-well problem. We focus our analysis on the restriction that all wells belong to an affine space of codimension one in $\mathbb{R}^{2\times 2}_{sym}$. In the four-well case, we determine sufficient conditions to get the equality between $L^e(\mathcal{U})$ and $Q^e(\mathcal{U})$. One of this conditions is that there exist two rank-one compatible pair of wells in \mathcal{U} . With this prior knowledge, we define five configurations called *basic blocks* with three and four wells that can be glued together in a coplanar *basic configuration* that also satisfies $L^e(\mathcal{U}) = Q^e(\mathcal{U})$. These basic configurations can be constructed for any number of wells.

Finally, in the last chapter, we go back to study the three-well problem with a rank-one compatible pair in \mathcal{U} . Here we prove that triple junctions are rare, and they are obtained if and only if the three wells are pairwise compatible and the affine space of codimension one containing \mathcal{U} is tangent to the incompatible cone at any of them. We also prove a rigidity result. Namely, if e(Du) is a linear strain that takes value on the three-well set \mathcal{U} with its level sets given by a finite union of polygons, then u is (locally) a simple laminate.

Resumen

Esta tesis tiene como objetivo estudiar los límites débiles de sucesiones minimizantes para problemas variacionales no convexos que surgen en la elasticidad lineal bidimensional. En cierto tipo de cristales, es común observar arreglos periódicos de granos a lo largo de la muestra cuando esta es sometida a alguna tensión. La existencia de esta "microestructura" en el material se puede predecir mediante la elasticidad y el análisis de la energía almacenada en la muestra. Trabajamos en el problema bidimensional de la elasticidad lineal. Dada una muestra $\Omega \subset \mathbb{R}^2$ distorsionada por una deformación $u : \Omega \to \mathbb{R}^2$; Además, tenemos una densidad de energía $\phi \geq 0$ que es función de la deformación lineal $e(Du) := (Du + D^T u)/2$. Esta densidad de energía se anula si y solo si la parte simétrica del argumento pertenece a un conjunto finito de matrices $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$. Este conjunto se denomina conjunto de pozos y la energía almacenada en la muestra viene dada por

$$I(u) = \int_{\Omega} \phi(Du) \, dx,$$

Debido a la estructura multipozo, el funcional de energía I no es débilmente semicontinuo inferiormente. Las deformaciones lineales de sucesiones minimizantes de I normalmente oscilarán entre los elementos de \mathcal{U} , estas oscilaciones son interpretadas como la microestructura presente en el material. Para estudiar estas sucesiones minimizantes consideramos \tilde{I} la cuasiconvexificación de I; al conjunto de valores tomados por los límites débiles de dichas sucesiones de \tilde{I} se conoce como el casco simétrico cuasiconvexo $Q^e(\mathcal{U})$ del conjunto \mathcal{U} .

Estamos interesados en determinar explícitamente $Q^e(\mathcal{U})$. En algunos casos logramos este objetivo, mientras que en otros solo podemos producir cotas explícitas. En nuestro estudio usamos el *casco simétrico de laminación convexa* $L^e(\mathcal{U})$, una cota interna bien conocida de $Q^e(\mathcal{U})$.

En el primer capítulo, presentamos el problema, su origen físico y damos una derivación formal del modelo matemático en elasticidad lineal y no lineal. También presentamos nuestros resultados que se describirán en su totalidad en los capítulos posteriores. En el segundo capítulo, discutimos el concepto de compatibilidad y su interpretación geométrica en términos de un cono incompatible. Determinamos $L^e(\mathcal{U})$ para un conjunto de tres pozos \mathcal{U} y estudiamos la *envolvente biconjugada policonvexa* f_C^{pp} de una función particular $f_C \geq 0$. Esta envolvente es cuasiconvexa y al estudiar su conjunto de nivel cero denotado por ker f_C^{pp} obtenemos una cota exterior para $Q^e(\mathcal{U})$. Además, si hay un par de pozos compatibles por rango uno en \mathcal{U} , mostramos que $L^e(\mathcal{U}) = Q^e(\mathcal{U})$ y las cotas exteriores se vuelven óptimas.

El tercer capítulo es una extensión del capítulo dos al problema general de n-pozos. Centramos nuestro análisis en la restricción de que todos los pozos pertenecen a un espacio afín de codimensión uno en $\mathbb{R}^{2\times 2}_{sym}$. En el caso de cuatro pozos, determinamos condiciones suficientes para obtener la igualdad entre $L^e(\mathcal{U})$ y $Q^e(\mathcal{U})$; una de estas condiciones es que existan dos pares de pozos compatibles de rango uno en \mathcal{U} . Con este conocimiento previo, definimos cinco configuraciones llamadas *bloques básicos* con tres y cuatro pozos que se pueden pegar en una *configuración básica* coplanar que también satisface $L^e(\mathcal{U}) = Q^e(\mathcal{U})$. Estas configuraciones básicas se puede construir para cualquier número de pozos.

Finalmente, en el último capítulo, volvemos a estudiar el problema de tres pozos con un par compatible por rango uno en \mathcal{U} . Aquí demostramos que las uniones triples son raras, y se obtienen si y solo si los tres pozos son compatibles por pares y el espacio afín de codimensión uno que contiene \mathcal{U} es tangente al cono incompatible de uno de ellos. Por último probamos un resultado de rigidez. Es decir, si e(Du) es una deformación lineal que toma valores en el conjunto de tres pozos \mathcal{U} con sus conjuntos de niveles dados por uniones finitas de polígonos, entonces u localmente es un laminado simple.

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List of Symbols

The next list describes several symbols that will be later used within the body of the document

- ϕ Free energy density (nonlinear elasticity)
- Du Weak derivative of u
- $\operatorname{Ker} g \ \, \operatorname{Zero-level \ set \ of} \ g$

 $\operatorname{Ker}_{s} g$ Zero-level set of the restriction of g to the set of 2×2 symmetric matrices

 ψ Free energy density (linear elasticity)

Semiconvex notation

- $P\phi$ Polyconvex envelope of the function ϕ
- $Q\phi$ Quasiconvex envelope of the function ϕ
- $C(\mathcal{U})$ Convex hull of the set \mathcal{U}
- f^{pp} polyconvex biconjugate function of f
- f^p polyconvex conjugate function of f
- L(K) Lamination convex hull of the set K
- $L^{e}(\mathcal{U})$ Symmetric lamination convex hull of the set \mathcal{U}
- $L^{e,k}(\mathcal{U})$ k-degree symmetric lamination set of \mathcal{U}
- n_m Binomial coefficient between 2m and m minus 1
- P(K) Polconvex hull of the set K
- $P^{e}(\mathcal{U})$ Symmetric poleonvex hull of the set \mathcal{U}
- Q(K) Quasiconvex hull of the set K

- $Q^e(\mathcal{U})$ Symmetric quasiconvex hull of the set \mathcal{U}
- R(K) Rank-one convex hull of the set K
- $R^{e}(\mathcal{U})$ Symmetric rank-one convex hull of the set \mathcal{U}

Matrix notation

- $\langle \cdot, \cdot \rangle$ Frobenius inner product
- w_M Norm of the skew symmetric part of M
- (ξ,η) Representation of matrix $\xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$
- \mathcal{C}_V Set of matrices incompatible with V
- $\Pi_Q(V)$ Affine set orthogonal to Q that contains V
- $a \odot n~$ Symmetric part of the tensor product between vector a and n~
- $a \otimes n$ Tensor product between vector a and n
- $a^{\perp} = \pi/2$ counterclock wise rotation of $a \in \mathbb{R}^2$
- $e(\cdot)$ Symmetric part function
- Q Orthonormal matrix to Aff \mathcal{U}
- U_k Symmetric matrix that represents a well in \mathcal{U}
- $w(\cdot)$ Skew-symmetric part function

Set notation

 \mathcal{U} Set of symmetric matrices that represent linear elastic wells

 $\mathcal{U} \oplus \mathbb{R}^{2 \times 2}_{skew}$ Set of 2×2 matrices with their symmetric part in \mathcal{U} .

 $\mathbb{R}^{2\times 2}_{skew}$ Set of 2 × 2 skew-symmetric matrices

- $\operatorname{Aff}(L)$ Affine set of the set L
- $\mathbb{R}^{2\times 2}_{sym}$ Set of 2×2 symmetric matrices
- Ω Lipschitz Domain in \mathbb{R}^m
- ∂_{ri} relative boundary of a set
- K_{θ} Zero level set of the free energy density

Chapter 1

Mathematical Model and Summary of Results

1.1 The Physical Model

In daily life, we have learned from experiments and observations that some materials perform better than others at specific tasks. A mixture of some materials can improve some desired properties; for example, pure iron is a quite ductile material but not so resistant to oxidation; meanwhile, carbon is a brittle, oxidation-resistant material in ambient conditions. Steel, a *solid mixture* of iron and carbon, is both ductile and oxidation-resistant. A broad family of solid mixtures "remember" a prescribed shape. These mixtures are called shape memory alloys, or briefly SMA. It is possible to deform these alloys beyond the elastic regime, and by changing its internal energy (commonly by heating), the solid mixture recovers its prescribed shape. This property turns out to be extremely useful due to its medical and technological applications.

The shape memory effect can be explained from the study of phase transitions in the SMA's crystalline lattice. At a high temperature θ , the crystalline lattice of a SMA is highly symmetric. The high crystalline symmetry is preserved whenever the temperature is higher than a fixed temperature value M_s . This phase is known as the austenite phase, and the prescribed shape is fixed in this phase. If the temperature θ is below M_s and above a temperature M_f , the free energy in the SMA decreases and induces a reduction on the lattice symmetry in certain regions on the SMA, since it is a diffusionless transition that produces a new phase in the regions where the lattice symmetry is reduced. The new phase is called the martensitic phase. Due to the number of symmetries in the crystalline lattice of the austenite phase, a finite number of martensite phases exists. The martensite and austenite phase at this stage, and it can be handled and deformed easily. Due to the symmetry loss, it is remarkable that the sample's final volume is higher than its volume at the beginning of the process.

In order to recover the prescribed shape in the austenite phase, we reverse the process. As long as $\theta < A_s$, the whole material is in the martensitic phase. By heating up, the austenite-phase nucleation starts at a temperature A_s , and austenite and martensite phases coexist until the temperature reaches A_f . In sites where austenite exists, we recover the highly symmetric lattice, and the volume of those regions reduces. As $\theta > A_f$, the whole material is in the austenite phase, so the change in volume and symmetry imply that the SMA recovers its original shape. See Fig. 1.1 for a typical hysteresis diagram of the whole process and Fig. 1.2 for a two-dimensional picture of the change in the lattice structure.



Figure 1.1 Typical hysteresis diagram of the martensite concentration in a SMA. The blue curve represents the cooling process. Meanwhile, the red line represents the heating process.



Figure 1.2 Fig. (a) displays an austenite lattice configuration, Fig. (b) displays a martensite lattice configuration, and Fig. (c) shows a martensite lattice configuration after a deformation.

An interesting phenomenon occurs when the temperature $\theta < M_f$; SMA minimizes its free energy by creating microstructures among the different martensite variants. The transition between two different martensite variants is known as twins. Twinning is the cornerstone of microstructure.

1.1.1 Free Energy Model

From Atomistic Behavior to Continuum Model

Let us consider an alloy whose atoms are on a simple Bravais lattice, *i.e.*, the set of points $\mathcal{L}(e^1, e^2, e^3) = \{\nu_1 e^1 + \nu_2 e^2 + \nu_3 e^3 : \nu_i \in \mathbb{Z}, e^i \in \mathbb{R}^3 \text{ fixed}\}$ gives the mean position of an atom in the lattice. We want to quantify the energy stored in this lattice, more precisely

the free energy per unit volume ϕ , or simply the free energy density¹. This energy density is a function of the Bravais lattice and the temperature, but it does not depend on a particular choice of lattice vectors due to atoms' indistinguishability. Hence, if $\{\tilde{e}^1, \tilde{e}^2, \tilde{e}^3\}$ describe the same Bravais lattice $\mathcal{L}(e^1, e^2, e^3)$, then $\tilde{e}^i = \nu_j^i e^j$ and ν is an array of integer numbers. Moreover, ν^{-1} is also an array of integer numbers and $\nu \in GL(3, \mathbb{Z})$. Therefore, the free energy density ϕ must be invariant under this kind of transformation in the lattice. Also, the free energy an extra symmetry because it must be frame-invariant since the rotation of the entire Bravais lattice does not affect the energy, *i.e.*,

$$\phi(\mathcal{L}(e^1, e^2, e^3), \theta) = \phi(\mathcal{L}(Fe^1, Fe^2, Fe^3), \theta) \quad \text{for every } F \in SO(3).$$
(1.1)

This invariance is a global property that affects both the lattice and the entire material sample. We will assume from now on that the free energy density depends on the temperature, but it depends neither on $\partial \theta / \partial t$ nor $\partial (Dy) / \partial t$. This assumption is justified from a thermodynamical viewpoint, see for instance [13].

Assume that there is not hysteresis gap *i.e.*, $A_f = M_f := \theta_c$ and let $\mathcal{L}(e^1, e^2, e^3)$ be the lattice for austenite phase with temperature $\theta > \theta_c$. As we cool down the system fast enough, we avoid atom diffusion, but homogenous atom displacements are present. Those displacements induce a distortion of the lattice that is modeled by a linear transformation $F : \mathbb{R}^3 \to \mathbb{R}^3$ such that new lattice vectors are $\tilde{e}^i = Fe^i$ for $i \in \{1, 2, 3\}$. The free energy density becomes

$$\phi(\mathcal{L}(\tilde{e}^1, \tilde{e}^2, \tilde{e}^3), \theta) = (\det F) \, \phi(\mathcal{L}(Fe^1, Fe^2, Fe^3), \theta).$$

Notice that by fixing the reference lattice, the new lattice's free energy density is a function of the deformation gradient and the temperature. This deformation provokes a change in the sample's volume and density. The lattice can be observed with X-ray analysis. Cauchy-Born hypothesis relates lattice deformation with body deformation. This hypothesis states that if a continuum medium is located in a region Ω and undergoes a solid deformation $y : \Omega \to \mathbb{R}^3$, then the lattice vectors at a material point y(x) are given by the linear transformations Dy of the lattice vectors at the reference material point x. Therefore, the total free energy in a subset Ω' of the solid is

$$\Phi = \inf_{y \in \mathcal{K}} \int_{\Omega'} \phi(Dy, \theta) dx, \qquad (1.2)$$

where \mathcal{K} is the set of accesible thermodynamic states subject to some boundary conditions. The infimum is taken due to Gibbs' thermodynamical principle (see also Ericksen [13]).² This theory allows massive deformations that are not relevant for the analysis due to

¹This energy per unit volume is the free energy stored in a volume which is the smallest volume of a periodic cell in the lattice $\mathcal{L}(Fe^1, Fe^2, Fe^3)$.

²Gibbs' thermodynamical principle says that "for an equilibrium state of a thermodynamically isolated system, in contact with a heat bath at a constant temperature, it is necessary and sufficient that in all possible variations of the system, the variation of its ballistic free energy shall either vanish or be positive."

symmetry of the lattice behind $GL(3,\mathbb{Z})$, see [15] for more details. In order to fix this issue, Ericksen and Pitteri proposed that ϕ should be invariant under the following finite subset of $GL(3,\mathbb{Z})$,

$$S = \{Q \in SO(3) : Qe^{i} = \sum_{j=1}^{3} \mu_{j}^{i} e^{j}, i \in \{1, 2, 3\} \text{ and } \mu \in GL(3, \mathbb{Z})\},$$
(1.3)

where e^i are lattice vectors for the austenite phase. We interpret S as the set of rotations that preserve the unit cell in the austenite lattice. For instance, we consider the cubic-totetragonal phase transition. *i.e.*, the SMA is located in the region Ω in austenite phase with a body-center cubic lattice as in Fig. 1.3.(a). By cooling down the solid, we get a body-center tetragonal lattice for the martensite phase, see Fig. 1.3. (b), this change is represented by a deformation F in the y direction.

We see that some other lattice configurations have the same free energy, for instance, the structure in Fig. 1.3. (c). This configuration is obtained by a $\pi/2$ -rotation of the austenite lattice vectors in the xy-plane before applying the strain F. The first rotation costs no energy since the lattice remains unchanged, but it does change the directions of lattice vectors, see Fig. 1.3.(c). This feature holds for martensite phases that are considered stable states and for any other metastable state due to austenite phase symmetries. Summarizing,

$$\phi(PFQ,\theta) = \phi(F,\theta) \quad \text{for every} \quad Q \in S, \ P \in SO(3). \tag{1.4}$$

The zero-level set of the integrand in Eq. (1.2) for a fixed temperature θ is denoted by K_{θ} .



Figure 1.3 Atomic structure for austenitic and two different martensitic phases.

Rank-One Compatibility and the Hadamard Jump Condition.

We observe that if a continuous deformation $y : \mathbb{R}^m \to \mathbb{R}^m$ in a domain $\Omega \subset \mathbb{R}^m$ satisfies that there exists a smooth surface $\Sigma \subset \Omega$ such that Dy is continuous on either side of Σ , then the fibers along Σ should deform the same, and tangential derivatives on both sides must be equal. Thus, if $n \in S^{m-1}$ is the normal vector and τ is any tangent vector to Σ then,

$$[Dy^+ - Dy^-]\tau = 0$$
, with $Dy^{\pm} = \lim_{\epsilon \to 0^+} Dy(x \pm \epsilon n)$

Hence, the difference of deformation gradients is a rank-one tensor that depends on the normal direction

$$Dy^+ - Dy^- = a \otimes n, \tag{1.5}$$

for some $a \in \mathbb{R}^m$. We exclude the value a = 0 since it means that both gradients Dy^+ and Dy^- are the same, and no change on the deformation is present. Relation (1.5) is called *Hadamard jump condition*. The following result, due to Ball and James [2], generalizes the Hadamard jump condition:

Theorem 1.1 (Ball & James 1989). Let $\Omega \subset \mathbb{R}^l$ are open and connected. Assume Ω_A , Ω_B are two disjoint measurable sets with $\Omega = \Omega_A \cup \Omega_B$, $|\Omega_A| > 0$, and $|\Omega_B| > 0$. Then, $y \in W^{1,\infty}(\Omega, \mathbb{R}^m)$ satisfies

$$Dy(x) = \begin{cases} A & a.e. \ x \in \Omega_A, \\ B & a.e. \ x \in \Omega_B, \end{cases}$$

where $A, B \in \mathbb{R}^{m \times l}$, if and only if,

$$A - B = a \otimes n,$$

for some $a \in \mathbb{R}^m$, $n \in S^{l-1}$ and

$$y(x) = y_0 + Bx + \theta(x)a, \quad x \in \Omega, \tag{1.6}$$

where $y_0 \in \mathbb{R}^m$, $y_0 \cdot a = 0$, $\theta \in W^{1,\infty}(\Omega)$ satisfies $D\theta(x) = \chi_A n$ a.e., and χ_A denotes the characteristic function of Ω_A .

Moreover if $E \subset \Omega_A$ is convex, Eq. (1.6) has the form

$$y(x) = y_0 + Bx + f_E(x \cdot n)a, \quad x \in E,$$
 (1.7)

where f_E is Lipschitz with derivatives 0 or 1 a.e..

This theorem does not consider boundary conditions, but it allows the construction of layered structures between two phases whose difference is a rank-one matrix. This condition will be important in the rest of this work. We say that $A, B \in \mathbb{R}^{m \times m}$ are rank-one compatible if they satisfy that

$$A - B = a \otimes n,$$

for some $a \in \mathbb{R}^m$, $n \in S^{m-1}$. In Fig. 1.4, we show two laminated structures where Dy takes values A, B on layers perpendicular to the direction n.



Figure 1.4 Fig. (a) and (b) display a laminated structure of the same domain Ω , in both cases twinning is normal to direction n but the characteristic function χ_A is different.

Relaxed Problem and Generalized Hulls.

In the mathematical theory of elasticity, it is assumed that $y \in W^{1,p}(\Omega, \mathbb{R}^m)$ for p > 1. If there are no fractures in the material then y also needs to be bounded and continuous with bounded piecewise continuous first derivatives. Hence, we assume that $y \in W^{1,\infty}(\Omega, \mathbb{R}^m)$. We also consider affine boundary conditions since they represent traction on the boundary that can be manipulated in experiments. Thus the set \mathcal{K} in Eq. (1.2) is given by

$$\mathcal{K} = \{ y \in W^{1,p}(\Omega, \mathbb{R}^m) : y = Fx \in \partial \Omega \},\$$

where $F \in \mathbb{R}^{m \times m}$ is fixed and the problem (1.2) is written as

$$\inf_{\substack{y \in W^{1,p}(\Omega,\mathbb{R}^m) \\ y|_{\partial\Omega} = Fx}} I_{\theta}(y), \quad \text{where} \quad I_{\theta}(y) := \int_{\Omega} \phi(Dy,\theta) \, dx.$$
(1.8)

Notice that, although coercivity conditions are imposed on $I_{\theta}(y)$, the existence of nontrivial minimizers of (1.8) is not necessarily guaranteed. This functional does not have interfacial energy terms, and transitions between different gradient values are not penalized. Hence, if y satisfies (1.5) and $Dy \in K_{\theta}$ for a fixed temperature, then $y^k := y(kx)/k$ satisfies $Dy^k \in K_{\theta}$ for every $k \in \mathbb{N}$, but y^k has more interfaces than y. For instance, both structures given in Fig. 1.4 cost the same energy as long as both deformation gradients A and B belong to K_{θ} . Notice that coercivity conditions would imply that the sequence $\{y^k : k \in \mathbb{N}\}$ is uniformly bounded in $W^{1,p}(\Omega, \mathbb{R}^m)$ (see [9]) and by weak compactness $y^k \stackrel{w}{\longrightarrow} y$ in $W^{1,p}(\Omega, \mathbb{R}^m)$, but the rapidly oscillating character of Dy^k as k grows could imply that y is not a minimizer of $I_{\theta}(\cdot)$. Some other situations the weakly converge of minimizing sequences to minimizers is not guaranteed. For instance, ϕ may not meet the coercivity conditions, but it may satisfy some mild growth conditions, such as being bounded by a fixed positive constant when y is outside a given ball. An interesting example of this case is analyzed by James [15]. Therein, he assumes that the energy density $\phi \ge 0$, $K_{\theta} = \{U_1, U_2\} \subset \mathbb{R}^{3\times 3}$, the matrices U_1 and U_2 are rank-one compatible, and $F = \lambda U_1 + (1 - \lambda)U_2$ for a fixed and arbitrary $\lambda \in (0, 1)$. Since $I_{\theta}(\cdot)$ is not coercive, no $W^{1,p}(\Omega, \mathbb{R}^m)$ -boundedness is guaranteed on minimizing sequences. Nevertheless, after some analysis, it is possible to construct a minimizing sequence $\{y^k : k \in \mathbb{N}\}$ such that Dy^k is uniformly bounded in Ω and $Dy^k(x) \in K_{\theta}$ a.e. $x \in \Omega_k \subset \Omega$, with $\{\Omega_k : k \in \mathbb{N}\}$ an increasing sequence of sets such that $|\cup \Omega_k| = |\Omega|$. Hence the infimum of I_{θ} is zero. Also, by a contradiction argument, he proved that there are no minimizers. In materials science, the nonexistence of nontrivial minimizers implies the creation of microstructures in the sample.

To recover the existence of minimizers, we must pursuit (sequentially) weak lower semicontinuity on $I_{\theta}(\cdot)$. Morrey [20] and Ball & Murat [3] proved that when ϕ satisfies mild growth conditions³, (sequentially) weakly lower semicontinuity on $I_{\theta}(\cdot)$ is equivalent to *quasiconvexity* of the energy density $\phi(\cdot, \theta)$, that is

$$\phi(\eta,\theta)|D| \le \int_D \phi(\eta + D\psi(x),\theta) \, dx \text{ for every } \psi \in W^{1,\infty}_0(D,\mathbb{R}^m),$$

with $D \subset \Omega$ a bounded open set. This definition is independent of the domain D (see [3] for a scaling argument). Unfortunately, the quasiconvexity of $\phi(\cdot, \theta)$ is neither easy to prove nor satisfied in most cases.

Notice that SMA in open and bounded domains Ω with affine boundary conditions and a quasiconvex energy density ϕ present no microstructure. Therefore, if ϕ is not quasiconvex, the sample can present microstructure. With fixed affine boundary conditions, this phenomenon is analyzed with the *relaxed problem* [11, 17, 19], this is obtained by changing the energy density ϕ in Eq. (1.2) with its *quasiconvex envelope* $Q\phi(\cdot, \theta)$, given by

$$Q\phi(U,\theta) = \sup\{f(U) \mid f(U) \le \phi(U,\theta), \text{ and } f \text{ is quasiconvex}\}, \ \theta \text{ fixed.}$$

Dacorogna [10, 11] proved that quasiconvex envelopes have an integral representation in terms of $\phi(\cdot, \theta)$, as

$$Q\phi(\xi,\theta) \le \inf_{\psi \in W_0^{1,\infty}(\Omega,\mathbb{R}^m)} \frac{1}{|\Omega|} \int_{\Omega} \phi(\xi + D\psi,\theta) \, dx, \tag{1.9}$$

³For every $F \in \mathbb{R}^{m \times m} |\phi(F)| \le \beta |F|$, $\beta > 0$ when $p = \infty$, and

 $-\beta(1+|F|^q) \leq \phi(F)| < \beta(1+|F|^p), \ \beta > 0 \ \text{fixed and} \ 1 \leq q < p, \ \text{when} \ 1 < p < \infty.$

and that under certain growth conditions, minimizing sequences of the original problem (1.8) are minimizing sequences of the relaxed problem. The infimum coincides in both, but it is always attained due to quasiconvexity in the relaxed case. It can be proved that $Q\phi(\cdot,\theta)$ is continuous although $\phi(\cdot,\theta)$ is not, see [11]. The quasiconvex envelope $Q\phi(\cdot,\theta)$ represents the system's macroscopic energy, a kind of least averaged free energy needed to achieve a deformation-gradient ξ . For an excellent discussion about the meaning of quasiconvex envelopes, see Kohn and Vogelius [19].

Besides the notion of quasiconvex functions, polyconvex and rank-one convex functions are widely used in the study of polycrystals. Here we list the standard definitions from [11]. Let $n_m = C(2m, m) - 1$, and C(2m, m) is the binomial coefficient between 2m and m. We say that a function $f : \mathbb{R}^{n \times n} \to \mathbb{R}$ is *polyconvex* if there exists a convex function $G : \mathbb{R}^{n_m} \to \mathbb{R}$, such that

$$f(M) = G \circ T(M),$$

where $T : \mathbb{R}^{m \times m} \to \mathbb{R}^{n_m}$ is given by

$$T(M) = (M, adj_2(M), adj_3(M), \cdots, \det M).$$
 (1.10)

The notation $adj_k(M)$ stands for the matrix of all $k \times k$ minors of M. Also, a function $f : \mathbb{R}^{m \times m} \to \mathbb{R}$ is rank-one convex if for each pair of rank-one compatible matrices $M_1, M_2 \in \mathbb{R}^{m \times m}$,

$$f(\lambda M_1 + (1 - \lambda)M_2) \le \lambda f(M_1) + (1 - \lambda)f(M_2), \ \lambda \in [0, 1].$$

It can be proved that

$$f \text{ convex} \Rightarrow f \text{ polyconvex} \Rightarrow f \text{ quasiconvex} \Rightarrow f \text{ rank-one convex},$$

but the reverse implications are false in general [11, 25].

Since a relaxed problem always attains its minima, we denote by $Q(K) \subset \mathbb{R}^{m \times m}$ the set of values taken by the deformation gradient of all minimizers of the relaxed problem, see Kinderlehrer and Pedregal [16]. Notice that $K \subset Q(K)$, since for each element $V \in K$ the function y = Vx is a solution of problem (1.8) with F = V. The set Q(K) is important in the calculus of variations since its elements correspond to (constant) weak limits of subsequences $\{Df_n : n \in \mathbb{N}\}$, where $\{f_n : n \in \mathbb{N}\}$ is a minimizing sequence of the functional (1.8). As $n \to \infty$, the sequence Df_n oscillates faster among the elements in Kto minimize the energy. These oscillations correspond to the observed microstructure, and $Q(K) \setminus K$ is related to the set of affine boundary conditions that generates microstructure.

For any compact set K, it is proved [1, 11, 19, 28] that

$$Q(K) = \left\{ \xi \in \mathbb{R}^{m \times m} \, \middle| \, f(\xi) \le \sup_{\eta \in K} f(\eta) \text{ for every } f : \mathbb{R}^{m \times m} \to \mathbb{R} \text{ quasiconvex} \right\}.$$
(1.11)

Analogously, with the notions of polyconvex and rank-one convex functions, we define the polyconvex hull P(K) and the rank-one convex hull R(K) as in Eq. (1.11), namely

$$R(K) = \left\{ \xi \in \mathbb{R}^{m \times m} \middle| f(\xi) \le \sup_{\eta \in K} f(\eta), \text{ for every } f : \mathbb{R}^{m \times m} \to \mathbb{R} \text{ rank-one convex} \right\},$$
$$P(K) = \left\{ \xi \in \mathbb{R}^{m \times m} \middle| f(\xi) \le \sup_{\eta \in K} f(\eta), \text{ for every } f : \mathbb{R}^{m \times m} \to \mathbb{R} \text{ polyconvex} \right\}.$$

It is clear that $R(K) \subset Q(K) \subset P(K) \subset C(K)$, where C(K) stands for the convex hull of K. Another useful semiconvex hull is the *lamination convex hull* of K. This hull is defined by $L(K) = \bigcup_{i=0}^{\infty} K^{(i)}$, where $K^{(i)}$ is the lamination of degree *i* of K given by

$$\begin{array}{ll} K^{(0)} & := & K, \\ K^{(i+1)} & := & \left\{ \lambda U + (1-\lambda)V \, \middle| \, \lambda \in [0,1] \text{ and } U, \, V \in K^{(i)} \text{ are rank-one compatible} \right\}. \end{array}$$

It is known that $L(K) \subset R(K)$, see [11, 24]. Under further hypothesis R(K) = Q(K) or R(K) = P(K), see [27].

1.1.2 The *n*-Well Problem in Nonlinear Elasticity

The Three-Dimensional Case

In the model, we assume that the zero-energy is attained by the austenitic or martensitic phase, whenever $\theta > \theta_c$, or $\theta_c > \theta$, respectively. Hence, if $U_1 \in \mathbb{R}^{3\times 3}$ is a fixed martensite phase, then, by Eq. (1.3), the set of martensite phases is given by,

$$\mathcal{V} = \{ Q^T U_1 Q \mid Q \in S \} = \{ U_1, U_2, \cdots, U_n \},\$$

and the kernel of ϕ is given by

$$K_{\theta} = \begin{cases} SO(3), & \text{if } \theta > \theta_c, \\ SO(3) \cup SO(3)U_1 \cup \dots \cup SO(3)U_n, & \text{if } \theta = \theta_c, \\ S0(3)U_1 \cup \dots \cup SO(3)U_n, & \text{if } \theta < \theta_c. \end{cases}$$
(1.12)

Although $K_{\theta} \subset \mathbb{R}^{m \times m}$, it only depends on the set \mathcal{V} since for every $M \in K_{\theta}$ there exist $U \in \mathcal{V}$ and $P \in SO(m)$ such that $\phi(M, \theta) = \phi(PU, \theta) = \phi(U, \theta)$. Indeed by polar decomposition and Eq. (1.1), $\phi(M, \theta)$ is a function of the term $(M^T M)^{1/2}$, hence

(

$$\phi(\cdot, \theta) : \mathbb{R}^{m \times m} \to \mathbb{R}^+ \cup \{0\},$$

$$M \mapsto \phi\left((M^T M)^{1/2}, \theta \right).$$
 (1.13)

In solid mechanics literature, the term $(D^T y D y)^{1/2}$ is known as the Cauchy-Green deformation tensor.

Rank-one compatibility among the elements in \mathcal{V} may or may not exist, but this condition can be weakened via the left symmetry of the functional $\phi(\cdot, \theta)$, see Eq. (1.1). Indeed, we say that two elements $U, V \in \mathbb{R}^{3\times 3}_{sym}$ are *compatible* if there exists $P \in SO(3)$ such that

$$PU - V = a \otimes n$$
, for some $a \in \mathbb{R}^3$, $n \in S^2$. (1.14)

This relation is known as twinning equation. Notice that if $U, V \in \mathcal{V}$ are compatible, by Theorem 1.1, we can construct a lamination $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that $Dy \in \{PM, N\}$. This lamination has zero elastic energy when the boundary conditions are properly chosen. Ball and James [2] found necessary and sufficient conditions for compatibility of two matrices M, N and an equivalent condition was given by Ericksen [12]. We summarize these conditions in the next result:

Proposition 1.2. Let $M, N \in \mathbb{R}^{3 \times 3}$ both with positive determinant and define $C^1 = M^T M$, and $C^2 = N^T N$. The following statements are equivalent:

- a) There exist $P \in SO(3)$, $n \in S^2$, and $a \in \mathbb{R}^3$ such that $QM N = a \otimes n$
- b) There exist $a \in \mathbb{R}^3$ and $n \in S^2$ such that $C^1 = C^2 + a \otimes n + n \otimes a$
- c) The three eigenvalues, λ_1, λ_2 and λ_3 , of $N^{-T}(C^1 C^2)N^{-1}$ satisfy $\lambda_1 \leq \lambda_2 = 1 \leq \lambda_3$.

The Two-Dimensional Case

For the two-dimensional problem, the set of martensite phases is assumed to be finite *i.e.*,

$$\mathcal{V} = \left\{ U_i \in \mathbb{R}_{sym}^{2 \times 2} \, \middle| \, i = 1, 2, \cdots, n \right\},\,$$

and the free energy density $\phi(\cdot, \theta) : \Omega \subset \mathbb{R}^{2 \times 2} \to \mathbb{R}$ satisfies the left frame invariance *i.e.*, $\phi(PF, \theta) = \phi(PF, \theta)$ for every $P \in SO(2)$ and some growth conditions can be imposed on ϕ . Finally the kernel of the energy density ϕ is given by:

$$K_{\theta} = \begin{cases} SO(2), & \text{if } \theta > \theta_c, \\ SO(2) \cup SO(2)U_1 \cup \dots \cup SO(2)U_n, & \text{if } \theta = \theta_c, \\ S0(2)U_1 \cup \dots \cup SO(2)U_n, & \text{if } \theta < \theta_c. \end{cases}$$
(1.15)

Additionally, the compatibility condition is inherited from Eq. (1.14) with the changes $P \in SO(2), a \in \mathbb{R}^2$ and $n \in S^1$. Analogously to Proposition 1.2, see [5], we have

Proposition 1.3. Let $M, N \in \mathbb{R}^{2 \times 2}$, both with positive determinant. Define $C^1 = M^T M$, and $C^2 = N^T N$. The following statements are equivalent:

- a') There exist $P \in SO(2)$, $n \in S^1$, and $a \in \mathbb{R}^2$ such that $QM N = a \otimes n$
- b') There exist $a \in \mathbb{R}^2$ and $n \in S^1$ such that $C^1 = C^2 + a \otimes n + n \otimes a$
- c') $\det(C^1 C^2) \le 0.$

1.1.3 The *n*-Well Problem in Linear Elasticity

In this section, we formally derive the setting for the *n*-well problem in geometrically linear elasticity. In this theory of elasticity, we focus on deformations $y: \Omega \subset \mathbb{R}^m \to \mathbb{R}^m$ close to the identity, so

$$y(x) = x + \epsilon u(x), \tag{1.16}$$

for some $\epsilon < 1$. The frame invariance for the free energy density is no longer preserved in the linear regime, but it is replaced by the invariance under the addition of skewsymmetric matrices in the argument. Indeed, if ψ stands for the linear version of the energy density, then

$$\psi(M,\theta) = \psi(M+S,\theta), {}^{4} \quad S \in \mathbb{R}^{m \times m}_{skew}.$$
(1.17)

This invariance implies a similar relation to Eq. (1.13). Thus, by decomposing every matrix $M \in \mathbb{R}^{m \times m}$ into its symmetric part e(M) and its skew-symmetric part w(M), we get

$$\psi(\cdot,\theta) : \mathbb{R}^{m \times m} \to \mathbb{R}^+ \cup \{0\},$$

$$M \mapsto \psi(e(M),\theta).$$
(1.18)

In the linear model, we also assume that there is a finite number of martensite phases, hence $\mathcal{U} = \{U_1, U_2, \cdots, U_n\}$. Due to (1.17), the kernel of the functional ψ is given by

$$K_{\theta} = \begin{cases} \mathbb{R}_{skew}^{m \times m}, & \text{if } \theta > \theta_{c}, \\ (\{0\} \cup \mathcal{U}) \oplus \mathbb{R}_{skew}^{m \times m}, & \text{if } \theta = \theta_{c}, \\ \mathcal{U} \oplus \mathbb{R}_{skew}^{m \times m}, & \text{if } \theta < \theta_{c}, \end{cases}$$
(1.19)

where the notation $K_{\theta} = \mathcal{U} \oplus \mathbb{R}^{m \times m}_{skew}$ indicates that the symmetric part of every element in K_{θ} belongs to \mathcal{U} . The set \mathcal{U} is widely known as the *set of wells* due to the invariance under skew-matrix addition. Lines below we will see that studying K_{θ} is equivalent to studying \mathcal{U} .

As in [7], we say that two matrices $M_1, M_2 \in \mathbb{R}^{m \times m}$ are *compatible* if and only if there exists a skew symmetric matrix W such that $\operatorname{Rank}(M_1 - M_2 + W) \leq 1$, otherwise M_1 and M_2 are *incompatible*. In the particular case where $\operatorname{Rank}(M_1 - M_2) \leq 1$, we also say that M_1 and M_2 are *rank-one compatible*. It is well known –see [11]– that this condition can be interpreted as $\det(M_1 - M_2) = 0$. Also, we denote the symmetric part of any matrix M by e(M). It readily follows that if M_1 and M_2 are compatible then

$$\phi(F) = \epsilon^2 \left\langle \alpha(e(G) - U_i), (e(G) - U_i) \right\rangle + o(\epsilon^3),$$

where α is a positive-defined linear map.

⁴A brief explanation of this symmetry if the following. Let ϕ be the nonlinear free energy density, and $\mathcal{V} = \{V_1, V_2, \cdots, V_n\} \subset \mathbb{R}_{sym}^{m \times m}$ be set of martensite phases. Since we assume linear elasticity, $V_i = \mathrm{Id} + \epsilon U_i$ for every $i = 1, 2, \cdots, n$. Hence, if $F = \mathrm{Id} + \epsilon G \in \mathbb{R}^{m \times m}$ is near to a martensite phase V_i , $\phi(F) = \phi\left((F^T F)^{1/2}\right) = \phi\left(\mathrm{Id} + \epsilon e(G) + O(\epsilon^2)\right)$. Hence, close to a martensite phase V_1 ,

 $M_1 - M_2 + W = a \otimes n$ for some $W \in \mathbb{R}^{m \times m}_{skew}$, $a \in \mathbb{R}^m$ and $n \in \mathbb{S}^{m-1}$, hence layered structures, or simple laminates, can be constructed and nontrivial minimizing sequences of the associated free energy emerged [7].

In order to analyze the pattern formation problem and the existence of minimizers in the geometrically linear regime, ideas from the nonlinear case can be pushed forward. Following Boussaid, Kreisbeck, and Sclömerkemper [8], we define a symmetric semi-convex function as:

Definition 1.4. The function $f : \mathbb{R}^{m \times m}_{sym} \to \mathbb{R}$ is symmetric polyconvex, quasiconvex or rank-one convex if $f(e(\cdot)) : \mathbb{R}^{m \times m} \to \mathbb{R}$ is polyconvex, quasiconvex or rank-one convex respectively.

As stated in [8, 32], it follows that $f : \mathbb{R}_{sym}^{m \times m} \to \mathbb{R}$ is symmetric quasiconvex if and only if for every $U \in \mathbb{R}_{sym}^{m \times m}$

$$f(U) \le \inf \left\{ \frac{1}{|\Omega|} \int_{\Omega} f(U + e(D\phi)) dx \, \middle| \, \phi \in C_0^{\infty}(\Omega, \mathbb{R}^m) \right\},$$

and it is symmetric rank-one convex if and only if for every two compatible matrices U_1 and $U_2 \in \mathbb{R}_{sym}^{m \times m}$ and $\lambda \in [0, 1]$,

$$f(\lambda U_1 + (1-\lambda)U_2) \le \lambda f(U_1) + (1-\lambda)f(U_2).$$

Characterization of symmetric polyconvexity for any dimension is rather challenging. Boussaid, Kreisbeck, and Sclömerkemper [8] gave explicit characterization for symmetric polyconvexity in the cases where m = 2 and m = 3. In the two-dimensional case, they proved that $f : \mathbb{R}_{sym}^{2\times 2} \to \mathbb{R}$ is symmetric polyconvex if and only if there exists $g : \mathbb{R}_{sym}^{2\times 2} \times \mathbb{R} \to \mathbb{R}$ convex and non-increasing on the second variable such that $f(\cdot) = g(\cdot, \det(\cdot))$.

Also, the symmetric polyconvex, quasiconvex and rank-one convex hull for a compact set $\mathcal{U} \in \mathbb{R}_{sym}^{m \times m}$ are defined respectively as, see [32],

$$P^{e}(\mathcal{U}) = \left\{ A \in \mathbb{R}^{m \times m}_{sym} \,|\, f(A) \le \sup_{B \in \mathcal{U}} f(B), \ f \text{ symmetric polyconvex} \right\}, \tag{1.20}$$

$$Q^{e}(\mathcal{U}) = \left\{ A \in \mathbb{R}^{m \times m}_{sym} \mid f(A) \leq \sup_{B \in \mathcal{U}} f(B), \ f \text{ symmetric quasiconvex} \right\},$$
(1.21)

$$R^{e}(\mathcal{U}) = \left\{ A \in \mathbb{R}^{m \times m}_{sym} \,|\, f(A) \le \sup_{B \in \mathcal{U}} f(B), \ f \text{ symmetric rank-one convex} \right\}.$$
(1.22)

The set $Q^e(\mathcal{U})$ is relevant [32] since it corresponds to the set of effective linear strains generated by the microstructures with symmetric deformation gradient in \mathcal{U} . As in the nonlinear case, determining the symmetric quasiconvex hull of a compact set \mathcal{U} is a challenging task [29, 32]. An inner approximation for the symmetric quasiconvex hull is given by $L^e(\mathcal{U})$, the symmetric lamination convex hull of \mathcal{U} , see [22, 32]. We define this set as the union of the symmetric lamination of any degrees, namely $L^{e}(\mathcal{U}) = \bigcup_{i=0}^{\infty} L^{e,i}(\mathcal{U})$, where $L^{e,0}(\mathcal{U}) = \mathcal{U}$, and

$$L^{e,i+1}(\mathcal{U}) = \{\lambda A + (1-\lambda)B \in \mathbb{R}^{m \times m}_{sym} \mid \lambda \in [0,1] \text{ and } A, B \in L^{e,i}(\mathcal{U}) \text{ are compatible} \}$$

It is also known [32] that for any compact set $\mathcal{U} \subset \mathbb{R}^{m \times m}_{sym}$,

$$\mathcal{U} \subset L^{e}(\mathcal{U}) \subset R^{e}(\mathcal{U}) \subset Q^{e}(\mathcal{U}) \subset P^{e}(\mathcal{U}) \subset C(\mathcal{U}).$$
(1.23)

Rank-one convex and quasiconvex hulls are generically very difficult (if not impossible) to compute for a particular choice of \mathcal{U} [14]. Explicit examples of quasiconvex functions [11, 26] and quasiconvex hulls [5, 7, 4, 31] are scarce and most of the nontrivial examples are not known explicitly.

Even in linear elasticity, phase transition problems are nonlinear, because we deal with characteristic functions, that is the location of the phases. Also, the location of the interfaces is not known. Under this regime, Kohn [17] found the symmetric quasiconvex envelope for a free energy given by a bilinear form with only two martensite wells and a periodic domain Ω . He also gave a characterization of all minimizing sequences in terms of H-measures and stated the issues of his method in the *n*-well problem. In the case where all the elements in \mathcal{U} are pairwise compatible, the symmetric quasiconvex set $Q^e(\mathcal{U}) = C(\mathcal{U})$, see [4, 23]. Zhang [32] proved a weaker version of the previous result, indeed he proved that $L^e(\mathcal{U}) = C(\mathcal{U})$ if and only if $qr^e(\mathcal{U}) = C(\mathcal{U})$, where $qr^e(K)$ is the quadratic rank-one convex hull obtained as in Eq. (1.22) when the class of functions used are quadratic and symmetric rank-one convex.

1.2 Summary of Results

In this section we summarize our results.

On the Quasiconvex Hull for a Two-Well Problem in 2D Linear Elasticity

In Chapter 2, we determine explicit outer bounds for the symmetric quasiconvex hull $Q^e(\mathcal{U})$ when $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ is a three-well set. Moreover, in the case when there is a rank-one compatible pair of wells in the set \mathcal{U} these bounds explicitly determine $Q^e(\mathcal{U})$. We study the three-well problem in terms of the number of compatibility relations among the elements in \mathcal{U} . If all of them are compatible, it is known that $Q^e(\mathcal{U}) = C(\mathcal{U})$, see [1, 23], and if all the wells in \mathcal{U} are incompatible, then $Q^e(\mathcal{U}) = \mathcal{U}$, see [7]. In this work we consider the remaining cases when there exist one or two incompatibility relations among the wells.

We begin Chapter 2 with some well known equivalences for the compatibility condition in two dimensions, see [7]. This result is analogous to Proposition 1.2 and Proposition 1.3. **Proposition** (Compatibility characterization). Let $M_1, M_2 \in \mathbb{R}^{2 \times 2}$ and $a \in S^1$. The following statements are equivalent:

- 1. There exist $v \in \mathbb{R}^2$ and $W \in \mathbb{R}^{2 \times 2}_{skew}$ such that $M_1 M_2 + W = a^{\perp} \otimes v$.
- 2. There exists $v \in \mathbb{R}^2$ such that $e(M_1) = e(M_2) + \frac{1}{2} \left(v \otimes a^{\perp} + a^{\perp} \otimes n \right)$.
- 3. The symmetric parts of M_1 and M_2 satisfy $\langle e(M_1) e(M_2), a \otimes a \rangle = 0$.
- 4. $\det(e(M_1) e(M_2)) \le 0.$

The last item turns to be important in our study since we exploit as much as possible the isomorphism between \mathbb{R}^3 and $\mathbb{R}^{2\times 2}_{sum}$ given by

$$M = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \mapsto \tilde{M} = \begin{pmatrix} x \\ y \\ z\sqrt{2} \end{pmatrix}, \qquad (1.24)$$

to give a geometrical representation of compatibility that will be used through all this manuscript. Namely, we show in Lemma 2.6 that if V and U are incompatible symmetric matrices, then V lies in the interior of the open cone

$$\mathcal{C}_U := \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \text{ such that } \|V - U\| < |\langle V - U, \operatorname{Id} \rangle| \right\}.$$

centered at the matrix V. We give a representation of C_U in \mathbb{R}^3 under the above isomorphism in Fig. 1.5.

From the isomorphism (1.24), it is straightforward that for every $\mathcal{U} = \{U_1, U_2, U_3\}$ there exists, up to a sign, a direction Q (*i.e.*, a symmetric matrix with norm one) normal to the affine space spanned by \mathcal{U} and if this direction Q is unique, then we call Π_Q to Aff(\mathcal{U}). Due to the structure of the *incompatible cone* \mathcal{C}_{U_1} , it is easy to see that if there exists a pair of incompatible elements in \mathcal{U} , then \mathcal{C}_{U_1} and Π_Q intersects along two rank-one lines spanned by two rank-one matrices and as a consequence det Q < 0.

In Section 2.2, we use the above characterization of compatibility to give explicit expressions for the symmetric lamination convex hull under the assumption that there are at least two incompatible wells in \mathcal{U} . This result is important because each element $M \in L^e(\mathcal{U})$ is the weak limit of a lamination of finite degree (at most two) where the proportion of each martensite phase remains constant [15].

Proposition (Symmetric lamination convex hull). Let $\mathcal{U} = \{U_1, U_2, U_3\} \subset \mathbb{R}^{2\times 2}_{sym}$ such that Aff(\mathcal{U}) has codimension one.

(a) If $\det(U_1 - U_2) > 0$, $\det(U_1 - U_3) > 0$ and $\det(U_2 - U_3) \le 0$, then

$$L^{e}(\mathcal{U}) = \{U_1\} \cup C(\{U_2, U_3\}).$$

(b) If $\det(U_1 - U_2) \leq 0$, $\det(U_1 - U_3) \leq 0$ and $\det(U_2 - U_3) > 0$, then

$$L^{e}(\mathcal{U}) = C(\{U_{0}, U_{1}, U_{2}\}) \cup C(\{U_{0}, U_{1}, U_{3}\}),$$



Figure 1.5 Figure 1.6 (a) shows the plane Π_Q and the incompatible cone at U. The matrix U is compatible with any other in the reddish sectors. Figure 1.6 (b) displays the case where det Q > 0 and every point in the plane is compatible with U.

where $U_0 \in C(\mathcal{U})$ is uniquely characterized by $\det(U_0 - U_3) = \det(U_0 - U_2) = 0$.

The proof of this result is based on the observation that, if two out of the three compatibility relations are missing, the set of laminations of degree one $L^{e,1}(\mathcal{U})$, and degree two $L^{e,2}(\mathcal{U})$ coincide. Meanwhile, if only one compatibility relation is missing, the set of laminations stabilizes at degree two *i.e.*, $L^{e,2}(\mathcal{U}) = L^{e,3}(\mathcal{U})$.

In our first main result in this chapter, we consider the symmetric quasiconvex hull of \mathcal{U} under the assumptions that there is an incompatible pair of wells, but there is not any rank-one compatible pair.

Theorem (Exterior bound for $Q^e(\mathcal{U})$). Let $\mathcal{U} = \{U_1, U_2, U_3\}$ represent a three-well set and assume that Aff(\mathcal{U}) has codimension one. Also, assume that (a) det $(U_1 - U_2) > 0$, det $(U_1 - U_3) > 0$, and det $(U_2 - U_3) < 0$, or (b) det $(U_1 - U_2) < 0$, det $(U_1 - U_3) < 0$, and det $(U_2 - U_3) > 0$, then

$$Q^{e}(\mathcal{U}) \subset \{U \in C(\mathcal{U}) \mid 0 \leq \hbar(U - U_0)\} \subsetneq C(\mathcal{U}),\$$

where $U_0 \in C(\mathcal{U})$ is uniquely characterized by $\det(U_0 - U_2) = \det(U_0 - U_3) = 0$, $\hbar : \mathbb{R}^{2 \times 2}_{sum} \to \mathbb{R}$ is given by

$$\hbar(V) = \langle C, V - (U_2 - U_0) \rangle \det(U_1 - U_0) - \langle C, U_1 - U_2 \rangle \det V_2$$

and

$$C = \frac{(U_2 - U_1) \langle U_3 - U_1, U_3 - U_2 \rangle + (U_3 - U_1) \langle U_2 - U_1, U_2 - U_3 \rangle}{\sqrt{\|U_2 - U_1\|^2 \|U_3 - U_1\|^2 - \langle U_2 - U_1, U_3 - U_1 \rangle}}$$

The second main result in Chapter 2 states the equality between the symmetric quasiconvex hull $Q^e(\mathcal{U})$ and the symmetric lamination convex hull $L^e(\mathcal{U})$ if there exists –at least– one pair of wells in \mathcal{U} that are rank-one compatible. More precisely,

Theorem (On equality between $L^e(K)$ and $Q^e(K)$). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a three-well set such that $\operatorname{Aff}(\mathcal{U})$ has codimension one. If there exist at least two rank-one compatible wells in \mathcal{U} , then

$$Q^e(\mathcal{U}) = L^e(\mathcal{U}).$$

Independently of the existence of a rank-one compatibility, Bhattacharya [4] – see also [22]– proved that $Q^e(\mathcal{U}) = L^e(\mathcal{U}) = C(\mathcal{U})$ if the wells are all pairwise compatible. On the other hand, Bhattacharya *et. al.* [7] showed that if the all the wells are pairwise incompatible, then $Q^e(\mathcal{U}) = L^e(\mathcal{U}) = \mathcal{U}$ and no microstructure can be formed. The novelty of Theorem 2.24 is to consider the intermediate cases when one or two pairs of wells in \mathcal{U} are compatible, and one of these compatibility relations is a rank-one compatibility.

Those main theorems are geometrically interpreted in terms of the isomorphism (1.24) as follows. If $\mathcal{U} = \{U_1, U_2, U_3\} \subset \mathbb{R}^{2\times 2}_{sym}$ satisfies that the points \tilde{U}_1, \tilde{U}_2 and \tilde{U}_3 are non-colinear, then there exists a symmetric matrix Q and a constant $\alpha \in \mathbb{R}$ such that $\langle Q, U_i \rangle = \alpha$. We define Π_Q as the affine span of the set \mathcal{U} . It is then straight forward that

$$\Pi_Q = \{ V \in \mathbb{R}^{2 \times 2}_{sum} \text{ such that } \langle Q, V - U_1 \rangle = 0 \}.$$

If $\mathcal{U} = \{U_1, U_2, U_3\} \subset \mathbb{R}^{2\times 2}_{sym}$ satisfies that $\operatorname{Aff}(\mathcal{U})$ has codimension one, then $\operatorname{Aff}(\{\tilde{U}_1, \tilde{U}_2, \tilde{U}_3\})$ defines a plane in \mathbb{R}^3 . Let $U_0 \in C(\mathcal{U})$ as in Lemma 2.9, then the intersection between \mathcal{C}_{U_0} and $\operatorname{Aff}(\mathcal{U})$ determines the set of incompatible wells with U_0 in $\operatorname{Aff}(\mathcal{U})$. Moreover, $\operatorname{Aff}(\mathcal{U}) \cap \partial \mathcal{C}_{U_0}$ consists of matrices U such that U and U_0 represent rank-one compatible wells, and due to the isomorphism (1.24), this set is identified with a pair of lines in \mathbb{R}^3 . Thus we shall say that $\operatorname{Aff}(\mathcal{U}) \cap \partial \mathcal{C}_{U_0}$ is a pair of rank-one lines, see Fig. 1.6. Additionally, if we assume that \mathcal{U} meets the conditions in Proposition 2.13, then the lamination convex hull is explicitly known and can be represented in the plane $\operatorname{Aff}(\{\tilde{U}_1, \tilde{U}_2, \tilde{U}_3\})$. Figures 1.6.(a) and 1.6.(c) display two configurations with two incompatibility relations between \mathcal{U} 's wells. Due to Proposition 2.13, the lamination convex hull equals the union between $\{U_1\}$ and the segment joining U_2 and U_3 . In the configuration presented in Fig. 1.6.(a), the outer bound given by Theorem 2.22 is the union of $\{U_1\}$ with the region bounded by the curve $\Gamma = \{U \in C(\mathcal{U}) \mid \hbar(U - U_0) = 0\}$ and the segment joining U_2 and U_3 . Additionally, the configuration shown in Fig. 1.6.(c) has a rank-one compatibility, and the set $Q^e(\mathcal{U})$ equals $L^e(\mathcal{U})$ by Theorem 2.24.

We present Fig. 1.6.(b) and Fig. 1.6.(d) to display the analogous configurations when only one pair of wells in \mathcal{U} is incompatible. In the configuration presented in Fig. 1.6.(b), $L^e(\mathcal{U})$ is the wedge-like region bounded by the polygon with vertices U_1, U_2, U_0 , and U_3 by Proposition 2.13, and the well $U_0 \in C(\mathcal{U})$ is rank-one compatible with U_2 and U_3 simultaneously. Theorem 2.22's outer bound correspond to the region bounded by the curve Γ and the two segments joining U_1 with U_2 and U_3 , respectively. The configuration



Figure 1.6 Four different three-well configurations related Theorem 2.24 and Theorem 2.22. Black and red dots represent the wells and U_0 , respectively. Solid lines represent compatibility between wells and dashed lines incompatibility. The gray planar cone represents $\operatorname{Aff}(\mathcal{U}) \cap \mathcal{C}_{U_0}$, namely the set of incompatible matrices with U_0 in $\operatorname{Aff}(\mathcal{U})$. Gray lines are the rank-one lines across U_0 . In Fig. (a) and (b), the blue regions are the outer bounds of $Q^e(\mathcal{U})$ in Theorem 2.22. Figures (c) and (d) represent two admissible configurations in Theorem 2.24, and blue regions are $Q^e(\mathcal{U}) = L^e(\mathcal{U})$.

presented in Fig. 1.6.(d) has a rank-one compatible pair, so $Q^e(\mathcal{U})$ equals $L^e(\mathcal{U})$ due to Theorem 2.24, and both sets equal the blue flag-like region.

The proof presented for this result uses convex analysis, more precisely polyconvex biconjugate functions (PBF). This idea is based in the following facts: First, any (symmetric) polyconvex function is also a (symmetric) quasiconvex function, hence the kernel of each nonnegative (symmetric) polyconvex function can be used to bound the set $Q^e(\mathcal{U})$, see Eq. (1.21). Second, since any polyconvex function, say $f : \mathbb{R}^{m \times m} \to \mathbb{R}$, is a composition of a convex function $G : \mathbb{R}^{n_m} \to \mathbb{R}$ with the function T(M), –see Eq. (1.10)– convex analysis techniques can be adapted to construct a polyconvex function f^{pp} known as the polyconvex biconjugate function of f, of briefly PBF of f. In few words, this polyconvex function is a generalization of the standard convex bidual function. These two facts are coupled in the following way: we propose a function f and we calculate its PBF. So, we get a bound on the set $Q^e(K)$ by looking at the level sets of the function f^{pp} . This technique is used to prove both main theorems in this chapter. It is not a new technique, see [18], but it has not been widely used to calculate bounds on the set $Q^e(K)$. Section 2.3 is devoted to develop these ideas. The function that we propose is

$$f(M) = \chi_B(e(M)) \left(|\det e(M)| + |\langle C, M \rangle | \right), \quad B = \mathbb{R}_{sum}^{2 \times 2} \setminus L^e(\mathcal{U}),$$

 $\chi_B : \mathbb{R}^{2\times 2}_{sym} \to \{0, 1\}$ is the indicator function of B, and C is properly chosen. We do not know whether our outer bounds on quasiconvex hull are sharp or not, but if they are not, we believe that better estimates can be obtained by considering extensions of the form

$$f(M) = \chi_{\bar{B}}(e(M)) \left(|\det e(M)|^q + |\langle C, M \rangle|^p \right),$$

where $p, q \in \mathbb{N}$. The computation in this case becomes cumbersome, and we do not pursuit it further. A similar bound was given by Tang & Zhang [30] for the case of a three dimensional three-well problem at an exposed edge of $C(\mathcal{U})$ where the wells at this edge were incompatible. In [30], the authors prove that one can chip a wedge-like slice off $C(\mathcal{U})$ without touching $Q^e(\mathcal{U})$. This estimate is independent of the diameter of the set \mathcal{U} , but it is neither explicit nor optimal.

At the end of Chapter 2, we prove that the bounds given in Theorem 2.22 determine $qP^e(\mathcal{U})$ the symmetric quadratic polyconvex hull of \mathcal{U} , namely

$$qP^{e}(\mathcal{U}) = \left\{ A \in \mathbb{R}_{sym}^{m \times m} \mid f(A) \leq \sup_{B \in \mathcal{U}} f(B), \ f \text{ symmetric quadratic polyconvex} \right\}$$

By definition, it follows that $Q^e(\mathcal{U}) \subseteq qP^e(\mathcal{U})$. Hence the bounds obtained are optimal in the set of symmetric quadratic polyconvex functions. With this in hand, we can readily conclude that if the three-well set \mathcal{U} has a rank-one compatible pair within, then $L^e(\mathcal{U}) = Q^e(\mathcal{U}) = qP^e(\mathcal{U}).$

The Symmetric Quasiconvex and Lamination Convex Hull for the Coplanar n-Well Problem

In Chapter 3 we find sufficient conditions on the set of *n*-wells \mathcal{U} such that $L^{e}(\mathcal{U}) = Q^{e}(\mathcal{U})$. One of these conditions is that the set $\mathcal{U} = \{U_1, U_2, \dots, U_n\} \subset \mathbb{R}^{2\times 2}_{sym}$ is coplanar, namely, there exist $Q \in \mathbb{R}^{2\times 2}_{sym}$ and $\delta \in \mathbb{R}$ fixed such that $\langle Q, U_i \rangle = \delta$ for every $i = 1, 2, \dots, n$. Also, for this set, we define the family of triplets in the coplanar set as $\mathcal{F} = \{\{U_i, U_j, U_k\} \mid i, j, k \in \{1, 2, \dots, n\}\}.$

The first of the results presented in this chapter is the explicit characterization of the symmetric lamination convex hull of an arbitrary coplanar set \mathcal{U} in terms of the symmetric lamination convex hull for every triplet $\mathcal{V} \in \mathcal{F}$.

Theorem (Laminar convex). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a finite coplanar set and define \mathcal{F} as above, then

$$L^{e}(\mathcal{U}) = \bigcup_{\mathcal{V}\in\mathcal{F}} L^{e}(\mathcal{V}).$$

This theorem combined with the characterization of the symmetric lamination convex hull for any three-well set –Proposition 2.13– fully describe the symmetric laminar convex hull for any number of coplanar wells. The proof of this result relays on showing that the symmetric lamination of degree n stabilizes for n = 2. Before we state our second result, we give a useful definition and identify a four-well configuration where our method does not apply. Since we assume det Q < 0, it is known that the affine set Π_Q and the incompatible cone C_{U_1} with $U_1 \in \mathcal{U}$ intersects along two rank-one lines. In this case, we define the planar compatible cone as $C_{U_1} = \Pi_Q \setminus C_{U_1}$. This planar compatible cone is divided into two sectors, called the upper and the lower parts of C_{U_1} , we precise these definitions in Chapter 3. Also, we say that the set $\mathcal{U} = \{U_0, U_1, U_2, U_3\} \subset \mathbb{R}^{2\times 2}_{sym}$ has a wedge configuration if there exists a subset of three wells, say $\mathcal{V} = \{U_1, U_2, U_3\}$, such that there is only one incompatible pair of wells in \mathcal{V} , and the remaining well $U_0 \in \text{rel int } C(\mathcal{V})$ is rank-one compatible with each element in the incompatible pair of wells in \mathcal{V} , see Fig. 1.7.



Figure 1.7 Four coplanar wells in a wedge configuration

In the following result, we prove that the laminar convex hull of \mathcal{U} equals $Q^e(\mathcal{U})$ for a family of four wells with two pairs of rank-one compatible wells. Moreover, these symmetric semi-convex hull are strictly contained in $C(\mathcal{U})$.

Theorem (Four coplanar wells). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a set of four coplanar wells such that all its elements have at least another compatible well in the set, its plane's normal satisfies det Q < 0, and \mathcal{U} is not in a wedge configuration. Furthermore, assume there exist two different subsets $\{V_1, V_2\}, \{W_1, W_2\} \subset \mathcal{U}$ of rank-one compatible pairs and let $D = C(\{W_1, W_2\}) \cup C(\{V_1, V_2\})$. If any of the following conditions holds,

- 1. The set D is disconnected,
- 2. D is a connected set and $\mathcal{U} \subset D$,
- 3. The intersection of the sets $\{V_1, V_2\}$ and $\{W_1, W_2\}$ has only one element, say V, and D is contained either in the upper or in the lower part of \mathcal{C}_V .

then $L^{e}(\mathcal{U}) = Q^{e}(\mathcal{U}).$

Theorem 3.10 extends the results for the three-well case. It is not a full characterization of the quasiconvex hull for the four-well problem, but in combination with Theorem 3.7 it lets us produce examples of sets with four and more wells, where we explicitly compute $L^e(\mathcal{U})$ and $Q^e(\mathcal{U})$. Besides the wedge configurations, we have only two cases that are



Figure 1.8 Images (a) to (c) show three different four-well sets configurations that satisfy conditions 1 to 3 in Theorem 3.10, respectively. Figure (d) shows a configurations where Theorem 3.10 does not apply since $T \subset \partial_{\rm ri}(\mathscr{C}_Q^+(V))$ but $\mathcal{U} \setminus \{V_1, V_2, W_1, W_2\} \subset \mathscr{C}_Q^-(V)$. Green dots represent the wells in \mathcal{U} , blue solid lines represent rank-one compatibility between wells, and dashed blue lines represent the rank-one directions.

not included in the statement of Theorem 3.10, see Fig. 1.8. In particular, when the intersection of the sets $\{V_1, V_2\}$ and $\{W_1, W_2\}$ has only one element V, and D is aligned to the left and right parts of the relative closure of $\Pi_Q \setminus \mathscr{C}_V$.

In our final main result, we give an algorithm for constructing sets with finitely many coplanar wells such that their symmetric laminar convex hull and symmetric quasiconvex hull are the same, but these sets are stricly contained in the convex hull. We set up these configurations in terms of five *basic blocks* with three or four wells. Three-well basic blocks have one compatible, one rank-one compatible, and one incompatible pair among its wells, see Fig. 1.9a, we also refer to this type of basic block as *flag configurations*. The four-well basic block corresponds to the case of Item 2 in Theorem 3.10, see Fig. 1.9b. Notice that in each basic block, the segment generated by a rank-one pair of wells contains a well U_0 that is rank-one compatible with any other element in the flag configuration. We called U_0 the *basic block's center*. By Theorem 2.24 and Theorem 3.10, if \mathcal{U} is a basic block, then $L^e(\mathcal{U}) = Q^e(\mathcal{U})$.



Figure 1.9 The five basic block configurations. Green dots represent the wells in \mathcal{U} while red dots represent the center of each basic block. To keep figures simple we assume that the angle between $a^{\perp} \otimes a^{\perp}$ and $n^{\perp} \otimes n^{\perp}$ directions is $\pi/2$.

The basic blocks can be stuck together to get other configurations with more than three wells where $L^e(\mathcal{U}) = Q^e(\mathcal{U}) \subsetneq C(\mathcal{U})$. We say \mathcal{U} is a *basic configuration* if there are no more than two collinear wells in the set, and it is the union of finitely many adjacent basic blocks where every pair of adjacent basic blocks share two compatible (but not rank-one compatible) wells. In Fig. 1.10 we show some examples of basic configurations. Notice that, if \mathcal{U} is a basic configuration, then $\mathcal{U} = \mathcal{U}_1 \cup \cdots \cup \mathcal{U}_n$, where \mathcal{U}_i is a basic block for every $i = 1, 2, \cdots, n$; and if $i \neq n$, then the set $\mathcal{U}_i \cap \mathcal{U}_{i+1} = \{V_i, W_i\}$ with $\det(V_i - W_i) < 0$. By Lemma 3.13 (see below), there are at most two three-wells basic blocks in any basic configuration. Furthermore, these three-well basic blocks appear only as the first one or the last one in \mathcal{U} . In the last result of the chapter, we show that the lamination convex hull of each finite and coplanar set with a basic configuration equals its symmetric quasiconvex hull.



Figure 1.10 Basic configurations obtained by sticking two basic blocks. The configurations presented in Fig. 1.10a are included in the conditions of Theorem 3.10.

Theorem (Basic configurations). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a finite coplanar set of wells. If \mathcal{U} is a basic configuration, then $L^{e}(\mathcal{U}) = Q^{e}(\mathcal{U})$.

In the proof of Theorem 3.16 we assume that many pairs of wells in \mathcal{U} are rank-one compatible. This condition is similar to those of Theorem 3.10.

Regarding our proof's methods, we combine three ideas. First, the symmetric quasiconvex hull is the set of wells that cannot be separated by symmetric quasiconvex functions. In particular, -det is symmetric quasiconvex. Second, by the characterization of the planar compatible cone \mathscr{C}_U at a well $U \in \Pi_Q$, we choose suitable translations of quasiconvex functions to identify wells in the convex hull that do not belong to the symmetric quasiconvex hull. Third, we know explicitly the symmetric lamination convex hull for finite coplanar set explicitly.

Finally but not least important, we provide some examples of coplanar well-sets where our main results apply.

Rigidity in Flag Configurations

In the final chapter we focus on proving that if $u \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ is a zero free energy deformation, namely $e(Du) \in \mathcal{U}$ a.e. in Ω , and the level sets of e(Du) are the union of finitely many polygons, then u is locally a simple lamination (*i.e.* for every $x_0 \in \Omega$ there exists r > 0 such that $u(x) = f(x \cdot n)$ in $B_r(x_0)$). This chapter follows up our study for the three-well problem where \mathcal{U} has a rank-one compatibility relation between a pair of wells in it and its elements are linearly independent.

To achieve this result, we need to study more complex structures than simple laminates, those structures are known as zero-homogeneous strains e(Du) that satisfy $e(Du(\lambda x)) = e(Du(x))$ for every $\lambda > 0$. The simplest of these structures are triple junctions and the deformations that produce these structures are piecewise affine functions $u : \mathbb{R}^2 \to \mathbb{R}^2$ such that $e(Du(x)) \in \mathcal{U}$ a.e. $x \in \mathbb{R}^2$. Moreover, e(Du) has exactly three level sets and u is a continuous function.



Figure 1.11 A triple junction.

Proposition. Let $\mathcal{U} = \{U_0, U_1, U_2\} \subset \mathbb{R}^{2 \times 2}_{sym}$ be as in the assumptions of Definition 4.1 and $Q \in \mathbb{R}^{2 \times 2}_{sym}$ such that $\langle Q, U \rangle = \alpha$ for some $\alpha \in \mathbb{R}$ and every $U \in \mathcal{U}$. The set $\{U_0, U_1, U_2\}$ admits a triple junction if and only if the matrix Q is non-invertible.

This proposition characterizes the existence of triple junctions on each set of three wells. Notice that if the set \mathcal{U} has a pair of incompatible wells in it, then it does not admit triple junctions since a necessary condition for the existence of triple junctions is that the elements in \mathcal{U} must be pairwise compatible. The proof of the previous proposition strongly relays on the isomorphism in Eq. (1.24), and the well-known fact that a plane in \mathbb{R}^3 is completely determined by three points on it.

The second main result of this section concerns a special family of three-well sets. We say that \mathcal{U} has a *P-configuration* if there exist a rank-one compatible pair of wells and an incompatible pair of wells in \mathcal{U} . It is easy to see that despite of the pairwise compatible or incompatible cases, any well-set considered in Theorem 2.24 has a P-configuration, and the flag configurations are considered therein. As we mentioned in Chapter 2, these well configurations satisfy that $L^e(\mathcal{U}) = Q^e(\mathcal{U})$. Moreover, \mathcal{U} does not admit triple junctions, see Theorem 2.24 and Proposition 4.4. Hence this type of sets seem to be very constraint. The following theorem makes this kind of rigidity precise.

Theorem. Let $\mathcal{U} = \{U_0, U_1, U_3\}$ have a *P*-configuration and Ω be a simply-connected bounded domain in \mathbb{R}^2 . Also assume $e(Du) \in L^{\infty}(\Omega, \mathcal{U})$ is such that its level sets are the union of finitely many polygons. Then, *u* is locally a lamination of degree one.

The proof of this result relays on a blow up technique at every inner point of the domain. In the blown up domain each point becomes a zero homogeneous strain that takes values on the set \mathcal{U} and since this set is very constrained, we can prove that simple laminations are the admissible configurations.

Chapter 2

On the Symmetric Quasiconvex Hull for the Three-Well Problem in 2D Linear Elasticity

Along this chapter we study the three-well problem in two-dimensional linear elasticity, more precisely we focus on the cases where not every pair of elements in \mathcal{U} are pairwise compatible. We begin by a characterization of the geometry of the incompatible cone. Next, we compute the lamination convex hull $L^e(\mathcal{U})$ when one or two wells in \mathcal{U} are incompatible. We also provide some results about polyconvex conjugate and biconjugate functions adapted to our three well problem setting. With these results at hand, we compute the exterior bound on $Q^e(\mathcal{U})$, the first main result on this chapter. In the case that there is at least one rank-one compatibility among the wells in \mathcal{U} , we show that $Q^e(\mathcal{U}) = L^e(\mathcal{U})$. In the final section, we show that the bound obtained for $Q^e(\mathcal{U})$ by means of the polyconvex conjugate and biconjugate method is optimal for quadratic polyconvex functions.

Before any calculation, theorem, or proof, we state the notation we use in the present chapter. In this regard we follow [22]. For every matrix $M \in \mathbb{R}^{2\times 2}$, e(M) and w(M)denote the symmetric and skew-symmetric part of M respectively. Also, for every $a, b \in \mathbb{R}^2$, the tensor product $a \otimes b \in \mathbb{R}^{2\times 2}$ is defined as $(a \otimes b)_{ij} = a_i b_j$ and its symmetric part is denoted by $a \odot b$. The 2×2 identity matrix is denoted by Id, and the bilinear form $\langle \cdot, \cdot \rangle : \mathbb{R}^{2\times 2} \times \mathbb{R}^{2\times 2} \to \mathbb{R}$ stands for the Frobenius inner product *i.e.*, $\langle A, B \rangle \mapsto Tr(A^T B)$, also $\| \cdot \|$ denotes the Frobenius norm. Since the space of skew-symmetric matrices has dimension one, we will use the following representation,

$$w(M) = w_M R$$
, where $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and $w_M = \frac{1}{2} \langle M, R \rangle$. (2.1)
2.1 Compatibility Characterization and the Incompatible Cone

We begin this section with some known equivalences for the compatibility relation.

Proposition 2.1 (Compatibility characterization). Let $M_1, M_2 \in \mathbb{R}^{2 \times 2}$. The following statements are equivalent:

- (a) There exist $v \in \mathbb{R}^2$, $a \in S^1$ and $W \in \mathbb{R}^{2 \times 2}_{skew}$ such that $M_1 M_2 + W = a^{\perp} \otimes v$.
- (b) There exist $v \in \mathbb{R}^2$ and $a \in S^1$ such that $e(M_1) = e(M_2) + v \odot a^{\perp}$.
- (c) There exists $a \in S^1$ such that $\langle e(M_1) e(M_2), a \otimes a \rangle = 0$.
- (d) $\det(e(M_1) e(M_2)) \le 0.$

Proof. That (a) implies (b) follows directly from the symmetric parts of the equation in the statement (a). Since a^{\perp} is orthogonal to a, we easily conclude that (b) implies (c). To show that (c) implies (d), we proceed by contradiction and assume $\det(e(M_1)-e(M_2)) > 0$, meanwhile (c) holds. Then it follows that $a \mapsto (e(M_1) - e(M_2))a \cdot a$ is either a positive or negative defined quadratic form. Thus, the unique solution to $(e(M_1) - e(M_2))a \cdot a = 0$ is a = 0, a contradiction to $a \in S^1$ by hypothesis.

Now, we show that (d) implies (a). Since det $M = \det(e(M)) + \det(w(M))$ for every $M \in \mathbb{R}^{2 \times 2}$ and (d) is assumed, we obtain

$$\det(M_1 - M_2 + \mu R) = \det(e(M_1) - e(M_2)) + \left(\frac{1}{2} \langle M_1 - M_2, R \rangle + \mu\right)^2.$$

Thus, the equation $\det(M_1 - M_2 + \mu R) = 0$ is satisfied by some $\mu^* \in \mathbb{R}$. So, the statement (a) follows, and the proof is finished.

Due to the isomorphism (1.24), we state the following

Definition 2.2. Let $\mathcal{U} = \{U_1, U_2, U_3\} \subset \mathbb{R}^{2 \times 2}_{sym}$, be such that $\operatorname{Aff}(\mathcal{U})$ has codimension one. We say that $Q \in \mathbb{R}^{2 \times 2}_{sym}$ is a normal matrix to the $\operatorname{Aff}(\mathcal{U})$ if $\langle Q, U - V \rangle = 0$ for every $U, V \in \mathcal{U}$ and ||Q|| = 1.

Notice that up to a sign, the matrix Q is unique for every admissible set \mathcal{U} . The following lemma states that if $Q \in \mathbb{R}^{2\times 2}_{sym}$ has non-positive determinant, then it is the symmetric part of a tensor product, this result will be helpful further in Lemma 2.5.

Lemma 2.3. Let $Q \in \mathbb{R}^{2\times 2}_{sym}$ be such that its determinant is non-positive. There exist $a, n \in S^1$ and $\nu \in \mathbb{R}$ such that $Q = \nu a \odot n$. Moreover, if det Q < 0, then $v_+ = a + n$, and $v_- = a - n$ are eigenvectors of Q with eigenvalues $\lambda_+ = \nu[a \cdot n + 1]/2$, and $\lambda_- = \nu[a \cdot n - 1]/2$, respectively, and det $Q = -\nu^2(a \cdot n^{\perp})^2/4$.

Proof. The existence of $a, n \in S^1$ and $\nu \in \mathbb{R}$ such that $Q = \nu a \odot n$ follows by setting $M_1 = Q$ and $M_2 = 0$ and the equivalence between Item (b) and Item (d) in Proposition 2.1. The statement concerning the eigenvalues and eigenvectors follows by a direct computation

$$Qv_{\pm} = \frac{\nu}{2}(a \otimes n + n \otimes a)(a \pm n) = \frac{\nu}{2}[(a \cdot n)(a \pm n) + (n \pm a)] = \frac{\nu}{2}[a \cdot n \pm 1](a \pm n).$$

Thus, det $Q = \lambda_+ \lambda_- = -\nu^2 [1 - (a \cdot n)^2]/4 = -\nu^2 (a \cdot n^\perp)^2/4.$

Remark 2.4. Let $S : \mathbb{R}^{2 \times 2} \to \mathbb{R}^{2 \times 2}$ stand for the linear map given by $M \mapsto RMR^T$. It is readily seen that S maps the symmetric (skew-symmetric) subspace into itself. Moreover, a simple calculation proves that adj(M) = SM for every $M \in \mathbb{R}^{2 \times 2}$. Hence, we have the following identities:

(a) $2 \det M = \langle SM, M \rangle$.

(b)
$$\det M = \det e(M) + \det w(M) = \det e(M) + w_M^2$$
.

- (c) $\det(N+M) = \det N + \det M + \langle SM, N \rangle, \quad N \in \mathbb{R}^{2 \times 2}.$
- (d) If $M = \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$ for some $a, n \in S^1$ and $\xi, \eta \in \mathbb{R}$, then

$$\det M = \xi \eta |a \times n|^2$$

The next lemma describes the coordinate system that will be used within the proofs of the main theorems. This system of coordinates is convenient and simplifies many of the computations.

Lemma 2.5. Let $V, Q \in \mathbb{R}^{2 \times 2}_{sym}$ such that det Q < 0 and denote by $\Pi_Q(V)$ the affine set of codimension one that contains V and is normal to Q, namely

$$\Pi_Q(V) = \{ U \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle Q, U - V \rangle = 0 \}.$$

Then, there exist two nonparallel vectors $a, n \in S^1$, such that

$$\Pi_Q(V) = \{ V + \xi \, a^\perp \otimes a^\perp + \eta \, n^\perp \otimes n^\perp \, | \, (\xi, \eta) \in \mathbb{R}^2 \}.$$

$$(2.2)$$

Also, $U \in \Pi_Q(V)$ and V are compatible if and only if $U = V + \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$ with $\xi \eta \leq 0$.

Proof. First, due to Lemma 2.3, we notice that there exist $a, n \in S^1$, and $\nu \in \mathbb{R} \setminus \{0\}$ such that $Q = \nu a \odot n$. Moreover, since det Q < 0, the vectors a and n are linearly independent. Also, by Proposition 2.1.(b) and (c), and the symmetric role between vectors a and n, we have that $a^{\perp} \otimes a^{\perp}$ and $n^{\perp} \otimes n^{\perp}$ are two linearly independent rank-one matrices such that

$$\left\langle Q, a^{\perp} \otimes a^{\perp} \right\rangle = \left\langle Q, n^{\perp} \otimes n^{\perp} \right\rangle = 0.$$

Thus, $\{a^{\perp} \otimes a^{\perp}, n^{\perp} \otimes n^{\perp}\}$ is a basis for the two-dimensional subspace $\Pi_Q(V) - V$ and (2.2) follows. Now, let $W \in \Pi_Q(V)$ so there exists $(\xi, \eta) \in \mathbb{R}^2$ such that

 $W - V = \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$, and $\det(W - V) = \xi \eta |a \times n|^2$.

The second part of the statement follows straight forward from Item (d) in Proposition 2.1.



Figure 2.1 shows the well V as a blue dot and the reddish region represents the elements in $\Pi_O(V)$ that are compatible with V given in Lemma 2.5.

Now, we characterize the set of symmetric matrices that are incompatible with U as elements in the interior of a solid cone. In particular, the set of symmetric matrices that are rank-one compatible with U is identified with the boundary of this cone.

Lemma 2.6. Let $M \in \mathbb{R}^{2 \times 2}_{sym}$, then det M = 0 if and only if $|\langle M, \mathrm{Id} \rangle| = ||M||$. Moreover, det M < 0 if and only if $|\langle M, \mathrm{Id} \rangle| < ||M||$.

Proof. Let $M \in \mathbb{R}^{2 \times 2}_{sym}$ be given by

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{pmatrix}$$

with $M_{11}, M_{12}, M_{22} \in \mathbb{R}$, and consider the square of its Frobenius norm

$$||M||^2 = M_{11}^2 + M_{22}^2 + 2M_{12}^2 = (M_{11} + M_{22})^2 + 2(M_{12}^2 - M_{11}M_{22}).$$

Hence, $||M||^2 = \langle M, \mathrm{Id} \rangle^2 - 2 \det M$, and the proof follows.

In view of Proposition 2.1 and Lemma 2.6, given a matrix $U \in \mathbb{R}^{2 \times 2}_{sym}$, the set of incompatible matrices therein is given by the interior of the cone

$$\mathcal{C}_{U} := \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \text{ such that } \|V - U\| < |\langle V - U, \operatorname{Id} \rangle| \right\}, \\ = \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \text{ such that } \frac{1}{\sqrt{2}} < \left| \left\langle \frac{V - U}{\|V - U\|}, \frac{1}{\sqrt{2}} \operatorname{Id} \right\rangle \right| \right\}$$
(2.3)

We notice that if e^1 , e^2 stand for the canonical vectors, then $e^1 \otimes e^1$ and $e^2 \otimes e^2$ belong to ∂C_0 , and the cone's aperture angle, 2θ , is $\pi/2$ due to $e^1 \otimes e^1$, $e^2 \otimes e^2$ and Id are coplanar, see Fig. 1.5.

In the following definitions, we classify any three-well set into two types based on the number of compatibility relationships among its elements.

Definition 2.7. Let \mathcal{U} be a three-well set such that $\operatorname{Aff}(\mathcal{U})$ has codimension one. We say that a \mathcal{U} is type one if up to a relabeling $\mathcal{U} = \{U_1, U_2, U_3\}$, where

$$\det(U_1 - U_2) > 0, \ \det(U_1 - U_3) > 0, \ \text{and} \ \det(U_2 - U_3) \le 0,$$
(2.4)

and \mathcal{U} is type two if up to a relabeling $\mathcal{U} = \{U_1, U_2, U_3\}$, where

$$\det(U_1 - U_2) \le 0, \ \det(U_1 - U_3) \le 0, \ \text{and} \ \det(U_2 - U_3) > 0.$$
(2.5)

Remark 2.8. We claim that if Q is normal to $\operatorname{Aff}(\mathcal{U})$ where \mathcal{U} has an incompatible pair of wells, then det Q < 0. The proof follows by contradiction. Indeed if det $Q \ge 0$, then U_1 is compatible with U_2 and U_3 since $\operatorname{Aff}(\mathcal{U}) \cap \mathcal{C}_{U_1} = \{U_1\}$, see Lemma 2.6. Arguing the same for the two remaining wells, we conclude that \mathcal{U} is pairwise compatible, but this is contradiction and the claim is proved. Particularly, if \mathcal{U} is either type one or type two, it follows that the normal to $\operatorname{Aff}(\mathcal{U})$ has negative determinant.

In the following lemma, we apply the coordinate system in Lemma 2.5 to the geometry of our three-well problem.

Lemma 2.9. Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a three-well set of either type one or type two. Then, there exist $U_2, U_3 \in \mathcal{U}$ and $U_0 \in C(\mathcal{U})$ such that $\det(U_2 - U_0) = \det(U_3 - U_0) = 0$.



Figure 2.2 Images (a) to (c) display three different three-well configurations where black dots represent the wells in \mathcal{U} and U_0 is represented with a red dot. Solid bluish segments and dashed bluish lines represent compatibility and incompatibility between the joint wells, respectively. Gray segments are the rank-one segments through the wells U_2 and U_3 , and their intersection determines $U_0 \in C(\mathcal{U})$. The well configurations in (a) and (b) are of type two and type one with $\det(U_2 - U_3) < 0$, respectively. In these cases, U_0 is uniquely determined. Meanwhile, $U_0 \in C(\mathcal{U})$ is not unique in the limiting case (c) where \mathcal{U} is of type one with $\det(U_2 - U_3) = 0$ because every element in the segment $C(\{U_2, U_3\})$ is rank-one compatible with U_2 and U_3 .

Proof. First, by Remark 2.8, we know that det Q < 0 and by Lemma 2.3, there exist two linearly independent vectors $a, n \in S^1$, such that $Q = \nu a \odot n$ for some $\nu \in \mathbb{R} \setminus \{0\}$. Moreover,

$$U_2 = U_1 + \xi_2 a^{\perp} \otimes a^{\perp} + \eta_2 n^{\perp} \otimes n^{\perp}, \quad \text{and} \quad U_3 = U_1 + \xi_3 a^{\perp} \otimes a^{\perp} + \eta_3 n^{\perp} \otimes n^{\perp}, \quad (2.6)$$

due to Lemma 2.5.

Second, we claim that

$$U_0 = U_1 + \alpha a^{\perp} \otimes a^{\perp} + \beta n^{\perp} \otimes n^{\perp}, \quad \text{with} \quad \begin{cases} \alpha = \arg\min\{|\xi| \mid \xi \in \{\xi_2, \xi_3\}\},\\ \beta = \arg\min\{|\eta| \mid \eta \in \{\eta_2, \eta_3\}\}, \end{cases}$$
(2.7)

is the desired matrix. If we consider (ξ_2, η_2) , (ξ_3, η_3) as vector in \mathbb{R}^2 , they must belong to the same quadrant no matter the type of \mathcal{U} ; otherwise, all of its elements are either pairwise compatible or pairwise incompatible, but these contradict Eq. (2.4) and Eq. (2.5).

Without loss of generality, we assume \mathcal{U} is type one. By the previous observation, we easily conclude that ξ_2, ξ_3, η_2 and η_3 have the same sign, thus $\alpha\beta \geq 0$. Hence, by the statement (d) in Remark 2.4 and relations (2.7) and (2.6), we get $\det(U_1 - U_0) = \alpha\beta|a\times n|^2 \geq 0$ and $\det(U_3 - U_0) = (\xi_3 - \alpha)(\eta_3 - \beta)|a\times n|^2$. Notice this expression is equal to zero since either $\alpha = \xi_3$ or $\beta = \eta_3$ because if this fails, then either $\xi_3 \leq \xi_2$ and $\eta_3 \leq \eta_2$ hold or $\xi_3 \geq \xi_2$ and $\eta_3 \geq \eta_2$ hold; both options contradict $\det(U_3 - U_2) = (\xi_3 - \xi_2)(\eta_3 - \eta_2) \leq 0$. An analog argument implies $\det(U_2 - U_0) = 0$. We can perform a similar analysis when \mathcal{U} is type two and conclude that $\det(U_2 - U_0) = \det(U_3 - U_0) = 0$, so we skip this part of the proof. Now let

$$\lambda_1 = \frac{(\alpha - \xi_2)(\beta - \eta_3) - (\alpha - \xi_3)(\beta - \eta_2)}{\xi_2 \eta_3 - \xi_3 \eta_2}, \ \lambda_2 = \frac{(\alpha - \xi_3)\beta - (\beta_- \eta_3)\alpha}{\xi_2 \eta_3 - \xi_3 \eta_2}, \ \text{and} \ \lambda_3 = \frac{(\beta - \eta_2)\alpha - (\alpha - \xi_2)\beta}{\xi_2 \eta_3 - \xi_3 \eta_2}$$

By a straight forward computation, we see that $\lambda_1, \lambda_2, \lambda_3 \in (0, 1)$, and $\lambda_1 + \lambda_2 + \lambda_3 = 1$; hence, $U_0 \in C(\mathcal{U})$ since $U_0 = \lambda_1 U_1 + \lambda_2 U_2 + \lambda_3 U_3$.

Corollary 2.10. Let $\mathcal{U} \subset \mathbb{R}^{2 \times 2}_{sym}$ be a three-well set of either type one or type two. Then, there exist $U_0 \in C(\mathcal{U})$, $a, n \in S^1$, and ξ , η , γ , $\zeta \in \mathbb{R}$ such that

$$U_1 = U_0 + \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}, \quad U_2 = U_0 + \gamma a^{\perp} \otimes a^{\perp}, \quad and \quad U_3 = U_0 + \zeta n^{\perp} \otimes n^{\perp}, \quad (2.8)$$

where

$$\begin{cases} \eta > 0 \ge \zeta, \quad \xi > 0 \ge \gamma \quad or \quad \zeta \ge 0 > \eta, \quad \gamma \ge 0 > \xi \quad if \ \mathcal{U} \ is \ type \ one, \\ \eta \ge 0 > \zeta, \quad \gamma > 0 \ge \xi \quad or \quad \zeta > 0 \ge \eta, \quad \xi \ge 0 > \gamma \quad if \ \mathcal{U} \ is \ type \ two. \end{cases}$$
(2.9)

Proof. First, we know there exists $U_0 \in C(\mathcal{U})$ that is rank-one compatible with U_2 and U_3 due to Lemma 2.9. Also, Remark 2.8 implies that det Q < 0, where Q is normal to Aff(\mathcal{U}). The relations in (2.8) readily follows from Lemma 2.3, Lemma 2.5, and that $\Pi_Q(U_0) = \text{Aff}(\mathcal{U})$ has codimension one.

Now we prove the inequalities in Eq. (2.9) and we assume that \mathcal{U} is type two. Then $\mathcal{U} = \{U_1, U_2, U_3\}$ and its elements satisfy $\det(U_2 - U_3) > 0$, and $\det(U_j - U_1) \leq 0$ for

j = 0, 2, 3. Therefore, by equation (2.8) and Item (d) in Remark 2.4,

$$-\gamma \zeta > 0, \quad \xi \eta \le 0, \quad (\xi - \gamma)\eta \le 0, \quad \text{and} \quad (\eta - \zeta)\xi \le 0,$$

and the second set of conditions in (2.9) follows. Finally, if \mathcal{U} is type one a similar argument can be pushed forward, so the proof is complete.

2.2 The Symmetric Lamination Convex Hull $L^{e}(\mathcal{U})$

In this section, we determine the symmetric lamination convex hull when \mathcal{U} is either type one or type two, *i.e.*, there is one out of the three wells in \mathcal{U} that is compatible with one of the two remaining wells and incompatible with the other. We start this section with a remark on the symmetric rank-one convexity of $-\det(\cdot)$, and then we proof a lemma that helps us to determine the symmetric lamination convex hull for the kind three-well set mentioned above.

Remark 2.11. It is well known, see [7, 11], that if $f : \mathbb{R}^{m \times m} \to \mathbb{R}$ is quadratic and $f(a \otimes n) \geq 0$ for every $a, n \in \mathbb{R}^m$ then f is rank-one convex. It is well known that $-\det(\cdot) : \mathbb{R}^{2\times 2}_{sym} \to \mathbb{R}$ is a symmetric rank-one convex function because Item (a) in Remark 2.4 implies that it is quadratic and the equivalence between items (b) and (d) in Proposition 2.1 implies that $f(a \otimes n) \geq 0$ for every $a, n \in \mathbb{R}^2$.

Lemma 2.12. Let $U, V, W \in \mathbb{R}^{2 \times 2}_{sym}$ such that V, W are compatible and U is incompatible with both of them. Then U is incompatible with any point in $C(\{U, V, W\}) \setminus \{U\}$.

Proof. Let $M \in C(\{U, V, W\}) \setminus \{U\}$. Hence, $M = \lambda_1 U + \lambda_2 V + \lambda_3 W$ for some $\lambda_1 \in [0, 1)$ and $\lambda_2, \lambda_3 \in [0, 1]$, such that $\lambda_1 + \lambda_2 + \lambda_3 = 1$. Since $\lambda_1 \neq 1$, we have that $\lambda_2 + \lambda_3 > 0$ and

$$M - U = (\lambda_2 + \lambda_3) (s(V - U) + (1 - s)(W - U)),$$

where $s = \lambda_2/(\lambda_2 + \lambda_3)$, and $(1 - s) = \lambda_3/(\lambda_2 + \lambda_3)$. Hence, $\det(M - U) = (\lambda_2 + \lambda_3)^2 \det(s(V - U) + (1 - s)(W - U))$. Now, since $-\det(e(\cdot))$ is a rank-one convex function, and $\{(V - U), (W - U)\}$ is a compatible set, we have that

$$\det(s(V-U) + (1-s)(W-U)) \ge s \det(V-U) + (1-s) \det(W-U) > 0$$

Therefore, U and M are incompatible and the proof is complete.

Proposition 2.13 (Symmetric lamination convex hull). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a three-well set such that $\operatorname{Aff}(\mathcal{U})$ has codimension one.

(a) If \mathcal{U} is type one, then up to a relabelling -see Definition 2.7-, we have

$$L^{e}(\mathcal{U}) = \{U_1\} \cup C(\{U_2, U_3\})$$

(b) If \mathcal{U} is type two, then up to relabelling as in Definition 2.7

$$L^{e}(\mathcal{U}) = C(\{U_0, U_1, U_2\}) \cup C(\{U_0, U_1, U_3\}),$$

where $U_0 \in C(\mathcal{U})$ is characterized by $\det(U_0 - U_3) = \det(U_0 - U_2) = 0$.



Figure 2.3 (a) and (b) show two three-well configuration of type one and two respectively and their symmetric lamination convex hull predicted by Proposition 2.13. The wells in these sets are labeled from U_1 to U_3 and they are represented with blue dots. The auxiliary well U_0 cited by Lemma 2.9 is displayed as a red dot. In Fig. (b), $L^e(\mathcal{U})$ is the yellow region, and in Fig. (a), $L^e(\mathcal{U})$ is union between \mathcal{U} and the yellow segment.

Remark 2.14. If the elements in the three-well set \mathcal{U} are pairwise compatible, $C(\mathcal{U}) = L^{e}(\mathcal{U})$, see [4, 22, 32]. Indeed, every $U \in C(\mathcal{U})$ is a lamination of degree two. This is readily proved by noticing that the parallel line to the segment $C(U_1, U_2)$ through U is a compatible line and it intersects the segments $C(U_2, U_3)$ and $C(U_3, U_1)$ at two compatible wells, say V and W respectively. Since $L^{e,1}(\mathcal{U})$ is the union of those three segments, we conclude that $U \in L^{e,2}(\mathcal{U})$. Moreover this affirmation holds for every three-well set; this follows directly from the proof of Proposition 2.13. Therefore, we conclude that if \mathcal{U} is any set of three wells, $L^{e,1}(\mathcal{U}) \subseteq \partial_{ri} L^{e,2}(\mathcal{U})$. We notice that the equality holds if either (a) the wells in \mathcal{U} are pairwise incompatible, (b) the wells in \mathcal{U} are pairwise compatible, or (c) there is only one compatible pair of wells in \mathcal{U} . In the case where there are two compatibility relations among the elements in \mathcal{U} , it follows that $L^{e,1}(\mathcal{U}) \subseteq \partial_{ri} L^{e,2}(\mathcal{U})$.

Proof. We prove item (a). By hypothesis, U_2 and U_3 are compatible and U_1 is incompatible with both. Then, $L^{e,1}(\mathcal{U}) = \{U_1\} \cup C(\{U_2, U_3\})$. By Lemma 2.12 it follows that there is not $U \in C(\mathcal{U})$ compatible with U_1 . Therefore, no laminate of degree two is admissible and $L^{e,2}(\mathcal{U}) = L^{e,1}(\mathcal{U})$. Moreover, the same argument yields $L^{e,n}(\mathcal{U}) = L^{e,1}(\mathcal{U})$ for every $n \geq 1$ and Item (a) follows from the definition of $L^e(\mathcal{U})$.

Now, we prove item (b). By the compatibility assumptions, the first symmetric lamination of \mathcal{U} is given by $L^{e,1}(\mathcal{U}) = C(\{U_1, U_2\}) \cup C(\{U_1, U_3\})$. Next we consider the laminations of degree greater than one; since \mathcal{U} is type two, the Lemma 2.9 implies the existence of $U_0 \in C(\mathcal{U})$ such that

$$\det(U_2 - U_0) = \det(U_3 - U_0) = 0, \qquad (2.10)$$



Figure 2.4 Configuration of the auxiliary well in the proof of Proposition 2.13. This figure shows a three-well set where both inequalities in Item (b) are strict. The shaded region is the incompatible cone of U_0 restricted to the plane defined by U_1 , U_2 , and U_3 . Notice that if $\det(U_1 - U_2) = 0$, then U_0 belongs to the segment $C(\{U_1, U_2\})$.

So in the rest of the proof, we assume that the wells in \mathcal{U} are given by Eq. (2.8) in Corollary 2.10. First, we assume that $\det(U_1 - U_2) < 0$ and $\det(U_1 - U_3) < 0$ and consider the continuous function

$$t \mapsto \det(tU_1 + (1-t)U_3 - U_0) = t^2 \det(U_1 - U_3) + t \left\langle \mathcal{S}(U_3 - U_1), U_3 - U_0 \right\rangle.$$

By Lemma 2.9,

$$\langle \mathcal{S}(U_3 - U_1), U_3 - U_0 \rangle = -\xi \zeta |n \times a|^2,$$

and from (2.9) item (b), we conclude that $\langle S(U_3 - U_1), U_3 - U_0 \rangle > 0$. Recalling that $\det(U_1 - U_3) < 0$, there exists $t_0 > 0$ such that $U_{1,3} = t_0U_1 + (1 - t_0)U_3 \in C(\{U_1, U_3\})$ and $\det(U_{1,3} - U_0) = 0$. Analogously, there exists $U_{1,2} \in C(\{U_1, U_2\})$ such that $\det(U_{1,2} - U_0) = 0$, see Fig. 2.4. With these new matrices, we define two triangles with vertices $K_2 = \{U_1, U_2, U_{1,3}\}$ and $K_3 = \{U_1, U_3, U_{1,2}\}$. Now, we divide the proof in three steps:

- (i) We claim that $C(K_2), C(K_3) \subset L^{e,2}(\mathcal{U})$. Indeed, if we assume that M belongs to the relative boundary of $C(K_2)$, then either $M \in C(\{U_1, U_2\})$ or $M \in C(\{U_2, U_{1,3}\}) \cup C(\{U_1, U_{1,3}\})$. Since $U_{1,3} \in L^{e,1}(\mathcal{U})$ and $C(\{U_1, U_2\}) \subset L^{e,1}(\mathcal{U})$ then $M \in L^{e,2}(\mathcal{U})$. If we assume M belongs to the relative interior of $C(K_2)$. In view of Lemma 2.6, by construction any two matrices on the line ℓ joining U_2 and $U_{1,3}$, or on any other line parallel to ℓ are rank-one compatible. Then, there exists a line ℓ_M parallel to ℓ and passing through M such that ℓ_M intersects $C(\{U_1, U_2\})$ and $C(\{U_1, U_{1,3}\})$ at some points V and W respectively; thus, $M \in C(\{V, W\})$, $\det(V W) = 0$, and $V, W \in L^{e,1}(\mathcal{U})$. Hence $M \in L^{e,2}(\mathcal{U})$. By a similar argument $C(K_3) \subset L^{e,2}(\mathcal{U})$ and the claim follows.
- (ii) Now, we claim $C(K_2) \cup C(K_3) = L^{e,2}(\mathcal{U})$. By contradiction, we assume that there exists $U \in L^{e,2}(\mathcal{U}) \setminus (C(K_2) \cup C(K_3))$ (see Fig. 2.4). The intersection between $\partial \mathcal{C}_U$ and the relative boundary of $C(\mathcal{U})$ yields the existence of $V_2, V_3 \in C(\{U_2, U_3\})$, $V_{1,2} \in C(\{U_1, U_2\})$, and $V_{1,3} \in C(\{U_1, U_3\})$ such that $\det(V_2 U) = \det(V_{1,2} U) =$

0 and det $(V_3 - U) = det(V_{1,3} - U) = 0$. Therefore, each matrix in the set \mathcal{U} that is compatible with U belongs to either the set $C_1 = C(\{U, V_{1,3}, U_1, V_{1,2}\})$ or the set $C_2 = C(\{U, V_2, V_3\})$. Now, since $U \in L^{e,2}(\mathcal{U})$, there exist two compatible matrices $V, W \in L^{e,1}(\mathcal{U})$ such that $U = \lambda V + (1 - \lambda)W$ for some $\lambda \in (0, 1)$. Notice that C_1 and C_2 are convex sets and $C_1 \cap C_2 = \{U\}$, so V and W cannot belong both to C_1 or C_2 simultaneously. The contradiction follows from the fact $C_2 \cap L^{e,1}(\mathcal{U}) = \emptyset$ since U_2 and U_3 are incompatible.

(iii) We claim $L^{e,2}(\mathcal{U}) = L^{e,3}(\mathcal{U})$. The proof follows by a contradiction argument similar to the one used before. Indeed, if there exists $U \in L^{e,3}(\mathcal{U}) \setminus L^{e,2}(\mathcal{U})$, then U is a convex combination of two compatible matrices $V, W \in L^{e,2}(\mathcal{U})$. Since $C_1 \cap C_2 = \{U\}, V$ and W cannot belong both to C_1 or C_2 . Again the contradiction emerged from the fact that $C_2 \cap L^{e,2}(\mathcal{U}) = \emptyset$. Hence, $L^{e,3}(\mathcal{U}) \subset L^{e,2}(\mathcal{U})$. The reverse inclusion follows from the definition of $L^{e,3}(\mathcal{U})$.

Second, we assume that there is only one rank-one compatibility among the elements of \mathcal{U} and without loss of generality, let $\det(U_1 - U_2) < 0$ and $\det(U_1 - U_3) = 0$. In this case, we define $K_2 = C(\{U_1, U_0, U_2\})$ and $K_3 = C(\{U_1, U_3\})$, and arguing as in step (i), we easily get that $K_2 \subset L^{e,2}(\mathcal{U})$. Also by definition $K_3 \subset L^{e,1}(\mathcal{U}) \subset L^{e,2}(\mathcal{U})$. The steps (ii) and (iii) are exactly the same.

Third, we assume that there are two rank-one compatible pairs in \mathcal{U} , so without loss of generality, det $(U_2 - U_1) = \det(U_3 - U_1) = 0$. For this case, we choose $K_2 = C(\{U_1, U_2\})$ and $K_3 = C(\{U_1, U_3\})$. Under these assumptions, $K_1 \cup K_2 = C(K_1) \cup C(K_2) = L^{e,1}(\mathcal{U})$. Hence, by step (ii), $L^{e,1}(\mathcal{U}) = L^{e,2}(\mathcal{U})$.

Finally, due to $L^{e,3}(\mathcal{U}) = L^{e,2}(\mathcal{U})$ in all case, we get that $L^{e,n}(\mathcal{U}) = L^{e,2}(\mathcal{U})$ for every $n \geq 2$ and Item (b) follows from the definition of $L^e(\mathcal{U})$.

2.3 Results on Polyconvex Conjugate and Biconjugate Functions

2.3.1 General Results in $\mathbb{R}^{2 \times 2}$

Since there are few known examples of quasiconvex functions, we will estimate the set Q(K) by means of non-negative polyconvex functions that vanish on K. One way to construct these functions is by considering the polyconvex conjugate and biconjugate functions $f^p(\xi^*) : \mathbb{R}^{n_m} \to \mathbb{R} \cup \{\pm \infty\}$ and $f^{pp}(\xi) : \mathbb{R}^{m \times m} \to \mathbb{R} \cup \{\pm \infty\}$, respectively, of a given $f : \mathbb{R}^{m \times m} \to \mathbb{R}$. Those are defined as

$$f^{p}(\xi^{*}) := \sup\{(T(\eta), \xi^{*}) - f(\eta) \mid \eta \in \mathbb{R}^{m \times m}\}, \text{ and } f^{pp}(\xi) := (f^{p})^{*}(T(\xi)),$$

where $T : \mathbb{R}^{m \times m} \to \mathbb{R}^{n_m}$ is given by (1.10), and $(f^p)^* : \mathbb{R}^{n_m} \to \mathbb{R} \cup \{\pm \infty\}$ is the dual convex of f^p , which is given by $(f^p)^*(\eta) := \sup\{(\eta, \xi^*) - f^p(\xi^*) | \xi^* \in \mathbb{R}^{n_m}\}$. The following theorem was proved by Kohn and Strang [18], also see [11].

Theorem 2.15. Let $f : \mathbb{R}^{m \times m} \to \mathbb{R}$ and $f^{pp}(M) := (f^p)^* \circ T(M)$. If there exist $g : \mathbb{R}^{m \times m} \to \mathbb{R}$ is a polyconvex function such that $f(\xi) \ge g(\xi)$ for every $\xi \in \mathbb{R}^{m \times m}$, then $f^{pp} = Pf$, the polyconvex envelope of f.

We recall that $Pf(x) = \sup\{g(x) | g \leq f, \text{ and } g \text{ is polyconvex}\}$, see [11]. In the two-dimensional framework, $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$, the expressions for polyconvex conjugate and biconjugate functions become

$$f^{p}(M^{*}, \delta^{*}) = \sup_{M \in \mathbb{R}^{2 \times 2}} \langle M^{*}, M \rangle + \delta^{*} \det M - f(M), \quad \text{with} \quad M^{*} \in \mathbb{R}^{2 \times 2} \text{ and } \delta^{*} \in \mathbb{R},$$
(2.11)

and $f^{pp}(M) = (f^p)^*(M, \det M)$, where

$$(f^p)^*(M,\lambda) = \sup_{\substack{\delta^* \in \mathbb{R} \\ M^* \in \mathbb{R}^{2\times 2}}} \left(\langle M, M^* \rangle + \delta^* \lambda - f^p(M^*,\delta^*) \right), \quad \text{for } M \in \mathbb{R}^{2\times 2} \text{ and } \lambda \in \mathbb{R}.$$

In the proof of Theorem 2.24 and Theorem 2.22, we strongly use the existence of the matrix U_0 given in Lemma 2.9 and due to self-similarity of the incompatible cone and Lemma 2.5, we set U_0 as the center of coordinates. The following lemma allows us to do that.

Proposition 2.16. Let $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$ and $g(M) = f(M - M_0)$, then $g^{pp}(M) = f^{pp}(M - M_0)$.

Proof. From relation (2.11),

$$g^{p}(M^{*}, \delta^{*}) = \sup_{\substack{M \in \mathbb{R}^{2 \times 2}}} \left(\langle M^{*}, M \rangle + \delta^{*} \det M - f(M - M_{0}) \right)$$
$$= \sup_{\bar{M} \in \mathbb{R}^{2 \times 2}} \left(\langle M^{*}, \bar{M} + M_{0} \rangle + \delta^{*} \det(\bar{M} + M_{0}) - f(\bar{M}) \right).$$

The last expression for $g^p(M^*, \delta^*)$ is easily simplified by Item (c) in Remark 2.4. Hence

$$g^{p}(M^{*},\delta^{*}) = \langle M^{*}, M_{0} \rangle + \delta^{*} \det M_{0} + f^{p}(M^{*} + \delta^{*} \mathcal{S} M_{0}, \delta^{*})$$

Moreover,

$$(g^{p})^{*}(M,\delta) = \sup_{\substack{M^{*} \in \mathbb{R}^{2 \times 2} \\ \delta^{*} \in \mathbb{R}}} \left\{ \langle M - M_{0}, M^{*} \rangle + \delta^{*}(\delta - \det M_{0}) - f^{p}(M^{*} + \delta^{*}SM_{0}, \delta^{*}) \right\},\$$
$$= \sup_{\substack{\bar{M} \in \mathbb{R}^{2 \times 2} \\ \delta^{*} \in \mathbb{R}}} \left\{ \langle M - M_{0}, \bar{M} \rangle + \delta^{*}(\delta - \det M_{0} - \langle M - M_{0}, SM_{0} \rangle) - f^{p}(\bar{M}, \delta^{*}) \right\}$$

Thus, $(g^p)^*(M, \delta) = (f^p)^*(M - M_0, \delta - \det M_0 - \langle M - M_0, \mathcal{S}M_0 \rangle)$. Finally, the affirmation readily follows from $g^{pp}(M) = (g^p)^*(M, \det M)$, and $\langle M - M_0, \mathcal{S}M_0 \rangle = -2 \det M_0 + \langle \mathcal{S}M_0, M \rangle$.

The next proposition determines the polyconvex conjugate function of $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$ when it depends on the symmetric part of the argument. **Proposition 2.17.** Let $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$ be such that f(M) = f(e(M)) for every $M \in \mathbb{R}^{2 \times 2}_{sym}$. Then the polyconvex conjugate function of f is given by

$$f^{p}(M^{*},\delta^{*}) = \begin{cases} \infty, & \text{if } \delta^{*} > 0, \text{ or } \delta^{*} = 0 \text{ and } w_{M^{*}} \neq 0, \\ -\frac{w_{M^{*}}^{2}}{\delta^{*}} + \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(e(M^{*}),\delta^{*},U), & \text{if } \delta^{*} < 0, \\ \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(e(M^{*}),0,U), & \text{if } \delta^{*} = w_{M^{*}} = 0, \end{cases}$$

$$(2.12)$$

where $w_M \in \mathbb{R}$ satisfies $w(M) = w_M R$ and

$$\mathcal{L}(V,\delta,U) := \langle V, U \rangle + \delta \det U - f(U).$$
(2.13)

Proof. From relation (2.11) and statement (b) in Remark 2.4, we get

$$f^{p}(M^{*}, \delta^{*}) = \sup_{\substack{M \in \mathbb{R}^{2 \times 2}}} \left[\langle M^{*}, M \rangle + \delta^{*} \det M - f(e(M)) \right] \\ = \sup_{\substack{M \in \mathbb{R}^{2 \times 2}}} \left[2w_{M}w_{M^{*}} + \delta^{*}w_{M}^{2} + \langle e(M^{*}), e(M) \rangle + \delta^{*} \det e(M) - f(e(M)) \right]$$

Since w_M and e(M) are independent, we conclude that

$$f^{p}(M^{*}, \delta^{*}) = \sup_{w \in \mathbb{R}} \left(2ww_{M^{*}} + \delta^{*}w^{2} \right) + \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(e(M^{*}), \delta^{*}, U).$$
(2.14)

It is not difficult to see that $f^p(M^*, \delta^*) = \infty$ if either $\delta^* > 0$ or $\delta^* = 0$, and $w_{M^*} \neq 0$. Moreover, from standard calculus, if $\delta^* < 0$, the first suprema in the right hand side of relation (2.14) is attained at $w = -w_{M^*}/\delta^*$. Thus

$$f^p(M^*, \delta^*) = -\frac{w_{M^*}^2}{\delta^*} + \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(e(M^*), \delta^*, U).$$

The expression for the third condition in (2.12) readily follows from (2.14), and this finishes the proof.

The following proposition characterizes the polyconvex biconjugate function of every function of the form f(M) = f(e(M)).

Proposition 2.18. Let $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$. If f(M) = f(e(M)) for every $M \in \mathbb{R}^{2 \times 2}$, then $f^{pp}(M) = f^{pp}(e(M))$ and

$$f^{pp}(M) = \sup_{V \in \mathbb{R}^{2 \times 2}_{sym}, \ \delta^* \le 0} \left\{ \langle e(M), V \rangle + \delta^* \det e(M) - \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(V, \delta^*, U) \right\}.$$

Proof. Since f(M) = f(e(M)), $f^p(M^*, \delta^*)$ is given by (2.12). Hence,

$$(f^p)^*(M,\delta) = \max\{g_1(M), g_2(M,\delta)\}$$

where

$$g_1(M) = \sup_{\substack{V \in \mathbb{R}^{2\times 2}_{sym}}} \left\{ \langle e(M), V \rangle - \sup_{\substack{U \in \mathbb{R}^{2\times 2}_{sym}}} \mathcal{L}(V, 0, U) \right\}, \text{ and}$$
$$g_2(M, \delta) = \sup_{\substack{w \in \mathbb{R}, \delta \ast < 0\\ V \in \mathbb{R}^{2\times 2}_{sym}}} \left\{ \langle e(M), V \rangle + 2w_M w + \frac{w^2}{\delta^*} + \delta\delta^* - \sup_{\substack{U \in \mathbb{R}^{2\times 2}_{sym}}} \mathcal{L}(V, \delta^*, U) \right\},$$

with $\mathcal{L}(V, \delta^*, U)$ as in Proposition 2.17. Now, the function

$$w \mapsto \langle e(M), V \rangle + 2w_M w + \frac{w^2}{\delta^*} + \delta \delta^* - \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(V, \delta^*, U)$$

is concave in w for every $\delta^* < 0$. Thus,

$$2w_M w + \frac{w^2}{\delta^*} + \langle e(M), V \rangle + \delta\delta^* - \sup_{\substack{U \in \mathbb{R}^{2\times 2}_{sym}}} \mathcal{L}(V, \delta^*, U) \leq \langle e(M), V \rangle + (\delta - w_M^2)\delta^* - \sup_{\substack{U \in \mathbb{R}^{2\times 2}_{sym}}} \mathcal{L}(V, \delta^*, U),$$

with equality at $w = -\delta^* w_M$. Therefore,

$$(f^p)^*(M,\delta) = \sup_{V \in \mathbb{R}^{2 \times 2}_{sym}, \delta^* \le 0} \left\{ \langle e(M), V \rangle + (\delta - w_M^2) \delta^* - \sup_{U \in \mathbb{R}^{2 \times 2}_{sym}} \mathcal{L}(V,\delta^*,U) \right\}$$

Next, we notice that $w_M^2 = \det w(M)$, thus by Item (b) in Remark 2.4 we obtain

$$f^{pp}(M) = \sup_{\substack{V \in \mathbb{R}^{2\times 2}_{sym}, \delta^* \leq 0 \\ V \in \mathbb{R}^{2\times 2}_{sym}, \delta^* \leq 0}} \left\{ \langle e(M), V \rangle + (\det M - w_M^2) \delta^* - \sup_{\substack{U \in \mathbb{R}^{2\times 2}_{sym}}} \mathcal{L}(V, \delta^*, U) \right\},\$$

Hence, $f^{pp}(M) = (f^p)^*(e(M), \det e(M)) = f^{pp}(e(M))$ as claimed.

2.3.2 Polyconvex Conjugate and Biconjugate Functions of f_C

In this section we specialize our results to a particular function f that is instrumental in our proofs. Let $f : \mathbb{R}^{2 \times 2} \to \mathbb{R}$ be such that

$$f(M) = \chi_{\bar{B}}(e(M)) \left(|\det e(M)| + |\langle C, M \rangle | \right),$$
(2.15)

where $C \in \mathbb{R}^{2 \times 2}_{sym}$ with negative determinant, and

$$\chi_{\bar{B}}(U) = \begin{cases} 1 & \text{if } U \in \mathbb{R}^{2 \times 2}_{sym} \setminus L^{e}(\mathcal{U}) \\ 0 & \text{otherwise.} \end{cases}$$

The function f is chosen in this manner because (a) it needs to be a non negative and real valued function to ensure that it is bounded from below by a polyconvex function, namely g = 0, see Theorem 2.15. (b) We use the function $\chi_{\bar{B}}$ to guarantee that f vanishes at least on $L^e(\mathcal{U}) \supset \mathcal{U}$, this way, \mathcal{U} belongs to $\{M \in \mathbb{R}^{2\times 2}_{sym} \mid f^{pp}(M) \leq 0\}$ and this set contains $Q^e(\mathcal{U})$ if f^{pp} is polyconvex, see Eq. (1.23). (c) Finally, the function f must involve $|\det(e(M))|$ to simplify the computations but the disadvantage of this term is that it also vanishes on the cone \mathcal{C}_0 , thus, we add the term $|\langle C, M \rangle|$ to reduce the size of the zero-level set of f and to get a better outer bound on $Q^e(\mathcal{U})$.

The following lemmas will be used to determine the polyconvex conjugate and biconjugate functions of f given as in Eq. (2.15). Notice that f, restricted to Aff(\mathcal{U}), vanishes on $L^e(\mathcal{U})$. From now on, we denote by \mathcal{V} any three-well where Aff(\mathcal{V}) is a two-dimensional subspace, and by \mathcal{U} any three-well where Aff(\mathcal{U}) has codimension one. This notation makes the proof of Theorem 2.24 and Theorem 2.22 shorter.

Lemma 2.19. Let $\mathcal{V} = \{V_1, V_2, V_3\} \subset \mathbb{R}^{2 \times 2}_{sym}$ such that $\det(V_2) = \det(V_3) = 0$, and $\operatorname{Aff}(\mathcal{V}) \subset \mathbb{R}^{2 \times 2}_{sym}$ is a two-dimensional subspace. Also, assume that either \mathcal{V} is type one or \mathcal{V} is type two and $0 \in C(\mathcal{V})$. Additionally, let f be defined as in Eq. (2.15) for a fixed $C \in \mathbb{R}^{2 \times 2}_{sym}$ with negative determinant, and $\mathcal{L}(V, \delta, U)$ be defined as in Eq. (2.13). Then

$$\sup_{U \in \mathbb{R}^{2\times 2}_{sym}} \mathcal{L}(V, \delta^*, U) = \begin{cases} \infty & \text{if } (V, \delta^*) \in \mathcal{N}^c, \\ \max_{U \in \mathcal{V} \cup \{0\}} (k \langle C, U \rangle + \delta^* \det U) & \text{if } (V, \delta^*) \in \mathcal{N}, \end{cases}$$
(2.16)

where \mathcal{N} and \mathcal{N}^c are subsets of $\mathbb{R}^{2\times 2}_{sym} \times (-\infty, 0]$ given by

$$\mathcal{N} = \{ (kC, \delta^*) \mid -1 < k < 1, \ -1 \le \delta^* \le 0 \} \quad and \quad \mathcal{N}^c = \left(\mathbb{R}^{2 \times 2}_{sym} \times (-\infty, 0] \right) \setminus \mathcal{N}.$$

Proof. We start the proof by noticing that $\operatorname{Aff}(\mathcal{V}) = \prod_Q(0)$, for some $Q \in \mathbb{R}^{2\times 2}_{sym}$ with negative determinant, since $0 \in \operatorname{Aff}(\mathcal{V})$, see Lemma 2.5. This proof is divided into two parts corresponding to the following claims. First, we claim that

$$\sup_{U \in \mathbb{R}^{2 \times 2}_{sym} \setminus L^{e}(\mathcal{V})} \mathcal{L}(V, \delta^{*}, U) = \begin{cases} 0 & \text{if } (V, \delta^{*}) \in \mathcal{N}, \\ \infty & \text{otherwise.} \end{cases}$$
(2.17)

Second, we claim that if $(V, \delta^*) \in \mathcal{N}$, then

$$\sup_{U \in L^{e}(\mathcal{V})} \mathcal{L}(kC, \delta^{*}, U) = \begin{cases} \max_{U \in \mathcal{V}} (k \langle C, U \rangle + \delta^{*} \det U) & \text{if } \mathcal{U} \text{ is type one,} \\ \max_{U \in \mathcal{V} \cup \{0\}} (k \langle C, U \rangle + \delta^{*} \det U) & \text{if } \mathcal{U} \text{ is type two.} \end{cases}$$
(2.18)

Assuming the claims, we prove Eq. (2.16). Indeed, we are interested in $L := \sup \{ \mathcal{L}(V, \delta^*, U) \mid U \in \mathbb{R}^{2 \times 2}_{sym} \}$ for each $(V, \delta^*) \in \mathbb{R}^{2 \times 2}_{sym} \times (-\infty, 0] = \mathcal{N} \cup \mathcal{N}^c$. Hence if $(V, \delta^*) \in \mathcal{N}^c$, then $L = \infty$ by Eq. (2.17), and if $(V, \delta^*) \in \mathcal{N}$, then

$$L = \max\left\{\sup\{\mathcal{L}(V,\delta^*,U) \mid U \in L^e(\mathcal{V})\}, \sup\{\mathcal{L}(V,\delta^*,U) \mid U \in \mathbb{R}^{2\times 2}_{sym} \setminus L^e(\mathcal{V})\}\right\}.$$

So, the second part of Eq. (2.16) follows from Eq. (2.17) and Eq. (2.18). Now we present the proof of the claims in the following two parts.

Part 1: We will prove Eq. (2.17). Since $U \notin L^e(\mathcal{V})$, then

$$\mathcal{L}(e(M^*), \delta^*, U) = \min\{(\delta^* - 1) \det U, (\delta^* + 1) \det U\} + \min\{\langle e(M^*) - C, U \rangle, \langle e(M^*) + C, U \rangle\}$$

We notice that

$$\mathcal{N}^c = \{ (V, \delta^*) \in \mathbb{R}^{2 \times 2}_{sym} \times (-\infty, 0] \mid \delta^* < -1 \text{ or } V \not\models C \text{ or } V = kC, \ |k| > 1 \},$$

we inspect each option for $(V, \delta^*) \in \mathcal{N}^c$.

(i) Assume that $\delta^* < -1$. Since $(\delta^* - 1), (\delta^* + 1) < 0$, we choose $U(t) = t\overline{U}$ for a fixed $\overline{U} \in \mathbb{R}^{2\times 2}_{sum} \setminus L^e(\mathcal{V})$ with det $\overline{U} < 0$ and $t \in \mathbb{R}$, then we find

$$\mathcal{L}(e(M^*), \delta^*, U(t)) = t^2(\delta^* - 1) \det \overline{U} + t \min\{\left\langle e(M^*) - C, \overline{U} \right\rangle, \left\langle e(M^*) + C, \overline{U} \right\rangle\}.$$

Hence by letting $t \to \infty$ the claim follows.

- (ii) Now we assume $e(M^*)$ and C to be linearly independent. Thus, there exists $V \in \mathbb{R}^{2 \times 2}_{sym}$ with $\langle V, C \rangle = 0$ such that $e(M^*) = \alpha V + kC$ for some $\alpha, k \in \mathbb{R}$; so, $V \in \Pi_C(0)$. Due to det C < 0 and Lemma 2.9, the boundary of $\Pi_C(0) \cap \mathcal{C}_0$ consist of two nonparallel rank-one lines, say $\ell_1 = \{tu_1 \otimes u_1 | t \in \mathbb{R}\}$ and $\ell_2 = \{tu_2 \otimes u_2 | t \in \mathbb{R}\}$ for some $u_1, u_2 \in S^1$. So we choose $\overline{U} \in \{u_1 \otimes u_1, -u_1 \otimes u_1, u_2 \otimes u_2, -u_2 \otimes u_2\}$ such that $\alpha \langle V, \overline{U} \rangle > 0$. By construction, det $\overline{U} = 0$ and $\langle C, \overline{U} \rangle = 0$, hence $\mathcal{L}(e(M^*), \delta^*, t\overline{U}) = t\alpha \langle V, \overline{U} \rangle$ and by letting $t \to \infty$ we get the desired result.
- (iii) If $e(M^*) = kC$ with |k| > 1, then we choose $\overline{U} \in \mathcal{C}_0 \setminus \Pi_C(0)$ such that $k \langle C, \overline{U} \rangle > 0$ and det $\overline{U} = 0$. Hence $\mathcal{L}(e(M^*), \delta^*, t\overline{U}) = \min\{t(k-1) \langle C, \overline{U} \rangle, t(k+1) \langle C, \overline{U} \rangle\}$. Clearly, $(k-1) \langle C, \overline{U} \rangle > 0$, and $(k+1) \langle C, \overline{U} \rangle > 0$, so by letting $t \to \infty$ the result follows.

From those steps, we conclude that $\sup \{ \mathcal{L}(V, \delta^*, U) \mid U \in \mathbb{R}^{2 \times 2}_{sym} \setminus L^e(\mathcal{V}) \} = \infty$, if $(V, \delta^*) \in \mathcal{N}^c$.

Now, we assume $(V, \delta^*) \in \mathcal{N}$, and we prove that $\sup \{\mathcal{L}(e(M^*), \delta^*, U) \mid U \in \mathbb{R}^{2 \times 2}_{sym} \setminus L^e(\mathcal{V})\} = 0$. Indeed, we have that

$$\mathcal{L}(kC,\delta^*,U) = \min\{(\delta^*-1)\det U, (\delta^*+1)\det U\} + \min\{(k-1)\langle C,U\rangle, (k+1)\langle C,U\rangle\} \le 0.$$
(2.19)

The last inequality follows since both terms on the right hand side of (2.19) are nonpositive. Thus if $\overline{U} \in \mathcal{C}_0 \setminus \Pi_Q(0)$ is fixed and det $\overline{U} = 0$, then we get

$$\mathcal{L}(kC,\delta^*,t\bar{U}) = \min\{t(k-1)\left\langle C,\bar{U}\right\rangle,t(k+1)\left\langle C,\bar{U}\right\rangle\} \to 0, \quad \text{as} \quad t \to 0.$$

Therefore the affirmation follows and Eq. (2.17) is proved.

Part 2: we consider the optimization problem of \mathcal{L} for $U \in L^{e}(\mathcal{V})$. By Lemma 2.9, for every $U \in L^{e}(\mathcal{V}) \subset \Pi_{Q}(0)$ there exist $\xi, \eta \in \mathbb{R}$ such that $U = \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$, and

$$\mathcal{L}(kC,\delta^*,U) = k \langle C,U \rangle + \delta^* \det U = \xi \eta \,\delta^* |n \times a|^2 + \xi C a^{\perp} \cdot a^{\perp} + \eta C n^{\perp} \cdot n^{\perp}.$$
(2.20)

The level sets of (2.20) as function of ξ and η are hyperbolae (or straight lines). Hence, the supremum of $\mathcal{L}(kC, \delta^*, U)$ in $L^e(\mathcal{V})$ is attained at some point \overline{U} on the relative boundary of $L^e(\mathcal{V})$, denoted by $\partial_{\mathrm{ri}} L^e(\mathcal{V})$, and by Proposition 2.13 this relative boundary depends on the type of \mathcal{V} .

$$\partial_{\mathrm{ri}} L^{e}(\mathcal{V}) = \begin{cases} L^{e}(\mathcal{V}) & \text{if } \mathcal{V} \text{ is type one,} \\ C(\{V_1, V_2\}) \cup C(\{V_2, 0\}) \cup C(\{0, V_3\}) \cup C(\{V_3, V_1\}) & \text{if } \mathcal{V} \text{ is type two,} \end{cases}$$

Now, we assume that \mathcal{V} is type two. If $\overline{U} \in C(\{V_2, 0\}) \cup C(\{0, V_3\})$, then det $\overline{U} = 0$ and the equation (2.20) becomes linear. Hence, the maximum of $\mathcal{L}(kC, \delta^*, U)$ in $C(\{V_2, 0\}) \cup C(\{0, V_3\})$ is attained at either 0, V_2 or V_3 . Now, if $U \in C(\{V_1, V_2\})$, then $U = [\lambda \xi + (1 - \lambda)\gamma]a^{\perp} \otimes a^{\perp} + \lambda \eta n^{\perp} \otimes n^{\perp}$ for some $\lambda \in [0, 1]$ due to Corollary 2.10, and (2.20) becomes a polynomial of degree two in λ . It is readily seen that

$$\frac{d^2 \mathcal{L}(kC, \delta^*, U(\lambda))}{d\lambda^2} = 2\delta^* \eta(\xi - \gamma) |n \times a|^2 \ge 0.$$

Thus, either $\mathcal{L}(kC, \delta^*, U(\lambda))$ is linear in λ if $\xi = \gamma$ or it is quadratic in λ with a minimum if $\xi \neq \gamma$. Therefore, the maximum value of $\mathcal{L}(kC, \delta^*, U)$ on $C(\{V_1, V_2\})$ is always attained at the extremal points $\{V_1, V_2\}$. With a similar argument, the supremum of $\mathcal{L}(kC, \delta^*, U)$ on $C(\{V_1, V_3\})$ is attained on either V_1 or V_3 . Therefore, we conclude that the supremum of $\mathcal{L}(kC, \delta^*, U)$ in $L^e(\mathcal{V})$ is attained at some matrix $\overline{U} \in \{0, V_1, V_2, V_3\}$ as claimed.

When \mathcal{V} is type one, the maximum value of $\mathcal{L}(kC, \delta^*, U)$ is attained either in V_1 or in $C(\{V_2, V_3\})$, if the second option happens then we can be argued analogously since $d^2\mathcal{L}/d\lambda^2 = -2\delta^*\gamma\zeta |n \times a|^2 \ge 0$, and the result follows straight forward. So the supremum of $\mathcal{L}(kC, \delta^*, U)$ in $L^e(\mathcal{V})$ is attained at some matrix $\overline{U} \in \{V_1, V_2, V_3\}$ and Eq. (2.18) is proved. This completes the proof.

The last result of this section, Lemma 2.20, gives explicit bounds for Ker $f^{pp} \subset \mathbb{R}^{2\times 2}$, the zero-level set of the polyconvex biconjugate function of the function $f : \mathbb{R}^{2\times 2} \to \mathbb{R}$, when the matrix C satisfies appropriate conditions. From now on, if $g : \mathbb{R}^{2\times 2} \to \mathbb{R}$ is any function that satisfies g(M) = g(e(M)) for every $M \in \mathbb{R}^{2\times 2}_{sym}$, we denote the zero-level set of $g|_{\mathbb{R}^{2\times 2}_{sym}}$ as

$$Ker_{s} g := \{ V \in \mathbb{R}^{2 \times 2}_{sym} \, | \, g(V) = 0 \}.$$

Indeed notice Ker $g = \{M \in \mathbb{R}^{2 \times 2} | e(M) \in \text{Ker}_{s} g\}$. Particularly, if we study Ker f^{pp} , we can focus on Ker_s f^{pp} and no information is missing.

Lemma 2.20. Let $\mathcal{V} = \{V_1, V_2, V_3\} \subset \mathbb{R}^{2\times 2}_{sym}$ be either type one or two such that $\operatorname{Aff}(\mathcal{V}) \subset \mathbb{R}^{2\times 2}_{sym}$ is a two-dimensional subspace with $\det V_2 = \det V_3 = 0$. Let $C \in \mathbb{R}^{2\times 2}_{sym}$ with negative determinant and define f(M) as in Eq. (2.15). If C is normal to $\operatorname{Aff}(\mathcal{V})$, then $f^{pp}(M) \geq 0$ for every $M \in \mathbb{R}^{2\times 2}$, and

$$\operatorname{Ker}_{s} f^{pp} = \begin{cases} \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \middle| V \in \operatorname{Aff}(\mathcal{V}), \, \det V_{1} \leq \det V \right\}, & \text{if } \mathcal{V} \text{ is type two,} \\ \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \middle| V \in \operatorname{Aff}(\mathcal{V}), \, 0 \leq \det V \right\}, & \text{if } \mathcal{V} \text{ is type one,} \end{cases}$$

$$(2.21)$$

Also, if $0 \in C(\mathcal{V})$, C satisfies $\langle C, V_1 \rangle \leq 0 < \langle C, V_3 \rangle = \langle C, V_2 \rangle$, and

(i) \mathcal{V} is type one, then

$$\operatorname{Ker} f^{pp} \subset \{ M \in \mathbb{R}^{2 \times 2} | \langle C, e(M) - V_2 \rangle \leq 0 \leq \langle C, e(M) - V_1 \rangle, \\ 0 \leq \det e(M) \quad and \quad 0 \leq \hbar(M) \},$$

$$(2.22)$$

(ii) \mathcal{V} is type two, then

$$\operatorname{Ker} f^{pp} \subset \{ M \in \mathbb{R}^{2 \times 2} | \langle C, e(M) - V_2 \rangle \leq 0 \leq \langle C, e(M) - V_1 \rangle, \\ \det V_1 \leq \det e(M) \quad and \quad 0 \leq \hbar(M) \}.$$

$$(2.23)$$

where

$$\hbar(M) = \langle C, e(M) - V_2 \rangle \det V_1 - \langle C, V_1 - V_2 \rangle \det e(M).$$
(2.24)

Moreover, f^{pp} is a non negative real-valued function and $\mathcal{V} \subset \operatorname{Ker}_{s} f^{pp}$.

Proof. We notice that Proposition 2.18 and Lemma 2.19 readily imply

$$f^{pp}(M) = f^{pp}(e(M)) = \sup_{(k,\delta^*)\in\mathcal{E}} \left(k \langle e(M), C \rangle + \delta^* \det e(M) - \max_{U\in\mathcal{V}\cup\{0\}} (k \langle C, U \rangle + \delta^* \det U) \right),$$
(2.25)

where $\mathcal{E} := [-1, 1] \times [-1, 0]$. Due to Proposition 2.18, we focus on bounding Ker_s f^{pp} .

First, we assume that C is normal to $Aff(\mathcal{V})$ and we prove relation (2.21) from Eq. (2.25). Under these assumptions the latter equations reduces to

$$f^{pp}(V) = \begin{cases} \sup_{\substack{(k,\delta^*)\in\mathcal{E}\\ \sup_{\substack{(k,\delta^*)\in\mathcal{E}}}} (k \langle V, C \rangle + \delta^* (\det V - \det V_1)), & \text{if } \mathcal{V} \text{ is type two,} \\ \sup_{\substack{(k,\delta^*)\in\mathcal{E}}} (k \langle V, C \rangle + \delta^* \det V), & \text{if } \mathcal{V} \text{ is type one.} \end{cases}$$

because $0 \in Aff(\mathcal{V})$. By computing the supremum, we get

$$f^{pp}(V) = \begin{cases} |\langle V, C \rangle| + \max\{0, \det V_1 - \det V\}, & \text{if } \mathcal{V} \text{ is type two,} \\ |\langle V, C \rangle| + \max\{0, -\det V\}, & \text{if } \mathcal{V} \text{ is type one.} \end{cases}$$
(2.26)

The first term on the right hand side of (2.26) penalizes the distance to the plane $\operatorname{Aff}(\mathcal{V})$, meanwhile the second term is an in-plane condition. Moreover, f^{pp} is non negative and

$$\operatorname{Ker}_{s} f^{pp} = \begin{cases} \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \middle| V \in \operatorname{Aff}(\mathcal{V}), \, \det V_{1} \leq \det V \right\}, & \text{if } \mathcal{V} \text{ is type two,} \\ \\ \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \middle| V \in \operatorname{Aff}(\mathcal{V}), \, 0 \leq \det V \right\}, & \text{if } \mathcal{V} \text{ is type one,} \end{cases}$$

as claimed. Second, we assume $\langle C, V_1 \rangle \leq 0 < \langle C, V_2 \rangle = \langle C, V_3 \rangle$. A simple computation lead us to

$$k \langle C, V_2 \rangle > \delta^* \det V_1 + k \langle C, V_1 \rangle$$
, for $\frac{\det V_1}{\langle C, V_2 - V_1 \rangle} \delta^* \le k \le 1$.

This observation implies

,

$$\max_{i=0,1,2,3} \{k \langle C, V_i \rangle + \delta^* \det V_i\} = \begin{cases} k \langle C, V_2 \rangle, & \text{if } \frac{\det V_1}{\langle C, V_2 - V_1 \rangle} \delta^* \leq k \leq 1, \\ \delta^* \det V_1 + k \langle C, V_1 \rangle, & \text{otherwise.} \end{cases}$$

$$(2.27)$$

Now, we define the sets $\mathcal{D} = \{(k, \delta^*) \in \mathcal{E} : \det V_1 / \langle C, V_2 - V_1 \rangle \delta^* \leq k \leq 1\}$, and $\mathcal{E} \setminus \mathcal{D}$, see Fig. 2.5, and we define $\chi_{\mathcal{D}} : \mathcal{E} \to \{0, 1\}$ and $\chi_{\mathcal{E} \setminus \mathcal{D}} : \mathcal{E} \to \{0, 1\}$ as the characteristic functions of \mathcal{D} and $\mathcal{E} \setminus \mathcal{D}$ respectively. By Proposition (2.18) and the symmetry of the Frobenius inner product,

$$f^{pp}(V) = \sup\{\bar{f}_1(V, k, \delta^*) + \bar{f}_2(V, k, \delta^*) \,|\, (k, \delta^*) \in \mathcal{E}\},\$$

where

$$\begin{cases} \bar{f}_1(V,k,\delta^*) = \chi_{\mathcal{D}}\left(k\left\langle C, V - V_2\right\rangle + \delta^* \det V\right), \\ \bar{f}_2(V,k,\delta^*) = \chi_{\mathcal{E}\setminus\mathcal{D}}\left(k\left\langle C, V - V_1\right\rangle + \delta^* (\det V - \det V_1)\right). \end{cases}$$
(2.28)

Since \mathcal{D} and $\mathcal{E} \setminus \mathcal{D}$ are disjoint sets, we readily see that

$$f^{pp}(V) = \max\{f_1(V), f_2(V)\}, \text{ where } \begin{cases} f_1(V) = \sup_{\substack{(k,\delta^*) \in \mathcal{D}}} \bar{f}_1(V, k, \delta^*), \\ f_2(V) = \sup_{\substack{(k,\delta^*) \in \mathcal{E} \setminus \mathcal{D}}} \bar{f}_2(V, k, \delta^*). \end{cases}$$



Figure 2.5 Figures a) and b) represent the two possible subdivisions of the set \mathcal{E} , the former of these pictures is related to the condition $\langle C, V_2 - V_1 \rangle < -\det V_1$ and the latter picture remains for the reverse condition.

Notice that \bar{f}_1 is linear in (k, δ^*) ; thus, its supremum in \mathcal{D} is attained on $\partial \mathcal{D}$ for each $V \in \mathbb{R}^{2 \times 2}_{sym}$. Analogously, the supremum of \bar{f}_2 in $\mathcal{E} \setminus \mathcal{D}$ is attained on $\partial(\mathcal{E} \setminus \mathcal{D})$.

The computation of f_1 and f_2 strongly depend on the \mathcal{D} and $\mathcal{E} \setminus \mathcal{D}$ respectively. Thus, these functions depend on det V_1 because it determines part of $\partial \mathcal{D}$ and $\partial(\mathcal{E} \setminus \mathcal{D})$, see Eq. (2.27). Since $0 \in C(\mathcal{V})$ and det $V_2 = \det V_3 = 0$, Corollary 2.10 implies that det $V_1 > 0$ if \mathcal{V} is type one and det $V_1 \leq 0$ if \mathcal{V} is type two. In the sequel, we assume the latter option *i.e.*, det $V_1 \leq 0$. The computation of f_1 is divided in four cases:

- (a) Assume $0 < \langle C, V V_2 \rangle$ and $0 < \det V$, then the supremum is attained at $(k, \delta^*) = (1, 0)$, and $f_1(V) = \langle C, V V_2 \rangle > 0$.
- (b) Assume $0 < \langle C, V V_2 \rangle$ and det $V \leq 0$. Notice that det $V_1 < 0$ implies the supremum of $\overline{f_1}$ is attained at $(k, \delta^*) = (1, \max\{-1, -\langle C, V_1 V_2 \rangle / \det V_1\})$, and if det $V_1 = 0$ the supremum of $\overline{f_1}$ is attained at $(k, \delta^*) = (1, -1)$, in any case,

$$f_1(V) = \langle C, V - V_2 \rangle - \frac{1}{\max\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\}} \det V > 0.$$

(c) Assume $\langle C, V - V_2 \rangle \leq 0$ and det $V \leq 0$. In this case, the supremum of \bar{f}_1 is attained on the line segment

$$\left\{ \left(-\frac{\det V_1}{\langle C, V_1 - V_2 \rangle} \delta^*, \delta^* \right) \in \mathcal{E} \, \middle| \, \delta^* \in [-1, 0] \right\}.$$

The function \bar{f}_1 evaluated at this segment is

$$\bar{f}_1\left(V, -\frac{\det V_1}{\langle C, V_1 - V_2 \rangle} \delta^*, \delta^*\right) = -\frac{\hbar(V)}{\langle C, V_1 - V_2 \rangle} \delta^*.$$

The last equation is linear in δ^* and increasing or decreasing depending on the sign of $\hbar(V)/\langle C, V_1 - V_2 \rangle$. Hence, if $\hbar(V)$ is non negative, $f_1(V) = 0$, meanwhile for

 $\hbar(V) < 0,$

$$f_1(V) = \min\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\} \langle C, V - V_2 \rangle - \frac{1}{\max\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\}} \det V.$$

Inserting the definition of $\hbar(V)$ in the last equation we get

$$f_1(V) = \frac{\hbar(V)}{p} > 0, \quad \text{where} \quad p = \begin{cases} \det V_1, & \text{if } 1 \le \det V_1 / \langle C, V_1 - V_2 \rangle, \\ \langle C, V_1 - V_2 \rangle, & \text{otherwise.} \end{cases}$$

(d) Now assume $\langle C, V - V_2 \rangle \leq 0$ and $0 < \det V$, so the supremum is attained at $(k, \delta^*) = (0, 0)$ and $f_1(V) = 0$. In this case, we also have that $\hbar(V) > 0$.

Summarizing the analysis above we conclude that

$$\operatorname{Ker}_{s} f_{1} = \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_{2} \rangle \leq 0 \text{ and either } \det V \leq 0 \leq \hbar(V), \text{ or } 0 < \det V \},$$

and we easily conclude

$$\operatorname{Ker}_{s} f_{1} \subset \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_{2} \rangle \leq 0 \leq \hbar(V) \}.$$

$$(2.29)$$

Next, we compute f_2 . We notice that

$$\mathcal{E} \setminus \mathcal{D} = \left\{ (k, \delta^*) \in \mathcal{E} \, \middle| \, -1 \le k \le \min \left\{ 1, \frac{-\delta^* \det V_1}{\langle C, V_1 - V_2 \rangle} \right\}, \quad -1 \le \delta^* \le 0 \right\}.$$

In this case, we also have four possible further cases:

- (a) If $\langle C, V V_1 \rangle < 0$ and $0 \leq \det V \det V_1$, the supremum is attained at $(k, \delta^*) = (-1, 0)$ and $f_2(V) = -\langle C, V V_1 \rangle > 0$.
- (b) If $\langle C, V V_1 \rangle \leq 0$ and det $V \det V_1 < 0$, then the supremum is attained at $(k, \delta^*) = (-1, -1)$ and $f_2(V) = -\langle C, V V_1 \rangle \det V + \det V_1 > 0$.
- (c) If $0 < \langle C, V V_1 \rangle$ and $\det V \det V_1 < 0$, the supremum is attained at $(k, \delta^*) = (\min \{1, \det V_1 / \langle C, V_1 V_2 \rangle\}, -1)$ and

$$f_2(V) = \min\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\} \langle C, V - V_1 \rangle - \det V + \det V_1 > 0.$$

(d) If $0 \leq \langle C, V - V_1 \rangle$ and $0 \leq \det V - \det V_1$, then the supremum is attained at a point on the segment

$$\left\{ \left(\frac{-\det V_1}{\langle C, V_1 - V_2 \rangle} \delta^*, \delta^* \right) \in \mathcal{E} \, \middle| \, \delta^* \in [-1, 0] \right\}, \quad \text{and} \quad \bar{f}_2 \left(V, \frac{-\det V_1}{\langle C, V_1 - V_2 \rangle} \delta^*, \delta^* \right) = \frac{-\hbar(V)}{\langle C, V_1 - V_2 \rangle} \delta^*.$$

By linearity in k, if $-\hbar(V)/\langle C, V_1 - V_2 \rangle \ge 0$, then $f_2(V) = 0$; meanwhile for $\hbar(V) < 0$,

$$f_2(V) = \min\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\} \langle C, V - V_1 \rangle - \frac{1}{\max\left\{1, \frac{\det V_1}{\langle C, V_1 - V_2 \rangle}\right\}} (\det V - \det V_1).$$

From the definition of $\hbar(M)$, we get

$$f_2(M) = \frac{\hbar(V)}{p}, \quad \text{where} \quad p = \begin{cases} \det V_1, & \text{if} \quad 1 \le \det V_1 / \langle C, V_1 - V_2 \rangle, \\ \langle C, V_1 - V_2 \rangle, & \text{otherwise.} \end{cases}$$

We notice that in any of these cases $f_2 > 0$.

Hence, the four previous items imply

$$\operatorname{Ker}_{s} f_{2} = \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid 0 \le \langle C, V - V_{1} \rangle, \, \det V_{1} \le \det V, \, 0 \le \hbar(V) \}.$$

$$(2.30)$$

From the analysis above, we conclude that f_C^{pp} is nonnegative and Ker_s $f^{pp} = \text{Ker}_s f_1 \cap \text{Ker}_s f_2$. Hence, by (2.29) and (2.30) we get

$$\operatorname{Ker}_{s} f^{pp} \subset \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_2 \rangle \le 0 \le \langle C, V - V_1 \rangle, \, \det V_1 \le \det V, \, 0 \le \hbar(V) \},$$

and Item (ii) follows straight forward.

In the case where \mathcal{V} is type one *i.e.*, det $V_1 > 0$ the functions f_1 and f_2 can be computed analogously but we must be aware that \mathcal{D} and $\mathcal{E} \setminus \mathcal{D}$ are different due to the sign of det V_1 , see Fig. 2.6. In fact, f_1 and f_2 are real-valued functions, such that



Figure 2.6 Two possible subdivisions of the set \mathcal{E} when det $V_1 > 0$, the former of these pictures is related to the condition $\langle C, V_2 - V_1 \rangle < \det V_1$ and the latter picture remains for the reverse condition.

$$f_1 \ge 0$$
, and $\operatorname{Ker}_{s} f_1 = \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_2 \rangle \le 0, 0 \le \det V, 0 \le \hbar(V) \},$

meanwhile,

$$f_2 \ge 0$$
, and $\operatorname{Ker}_{\mathrm{s}} f_2 \subset \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid 0 \le \langle C, V - V_1 \rangle \ 0 \le \hbar(V) \}.$

These equations imply f^{pp} is a real-valued function such that $f^{pp} \ge 0$ and

 $\operatorname{Ker}_{s} f^{pp} \subset \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_{2} \rangle \le 0 \le \langle C, V - V_{1} \rangle, \ 0 \le \det V, \ 0 \le \hbar(V) \right\}$

So, Item (i) follows and the proof is complete.

2.4 The Quasiconvex Hull $Q^e(\mathcal{U})$

In this section we provide the bounds for the quasiconvex hull of \mathcal{U} for the general three-well problem, and we show its equality with the symmetric lamination convex hull if two of the wells are rank-one connected.

Before the proof of Theorem 2.24, we make the following

Remark 2.21. We observe that the intersection between $C(\mathcal{V})$ and $\operatorname{Ker}_{s} f^{pp}$, see Lemma 2.20, is bounded by

$$\operatorname{Ker} f^{pp} \cap C(\mathcal{V}) \subset \{ M \in C(\mathcal{V}) | \langle C, e(M) - V_2 \rangle \le 0 \le \langle C, e(M) - V_1 \rangle, 0 \le \hbar(M) \},\$$

and the type of \mathcal{V} does not matter. We can prove that the first condition on det V, namely $0 \leq \det V$ or $\det V_1 \leq \det V$ in cases 2.20(i) and 2.20(ii) respectively, is readily implied by $\hbar \geq 0$. We claim that positiveness of \hbar is equivalent to the relation $\theta_1 \det V_1 \leq \det V$ for some $\theta_1 \in [0, 1]$. We proceed with the requested proof by assuming the claim. If \mathcal{V} is type one then det $V_1 > 0$, an the inequality $0 \leq \det V$ follows. Also, if \mathcal{V} is type two, then det $V_1 \leq 0$ and since $0 \leq \theta \leq 1$, it also follows that det $V_1 \leq \det V$.

Now we prove the claim. Since $\langle C, V_1 - V_2 \rangle \neq 0$, $\hbar \geq 0$ is easily written as

$$\frac{\langle C, V - V_2 \rangle}{\langle C, V_1 - V_2 \rangle} \det V_1 \le \det V, \tag{2.31}$$

so, it is enough to show the equivalence between Eq. (2.31) and $\theta_1 \det V_1 \leq \det V$ for some $\theta_1 \in [0,1]$. First, we assume Eq. (2.31). Since $V \in C(\mathcal{V})$, then there exist $\theta_1, \theta_2, \theta_3 \in [0,1]$ such that $\theta_1 + \theta_2 + \theta_3 = 1$ and $V = \theta_1 V_1 + \theta_2 V_2 + \theta_3 V_3$. Thus, if we take the inner product with C, we have $\langle C, V \rangle = \theta_1 \langle C, V_1 \rangle + (1 - \theta_1) \langle C, V_2 \rangle$. Therefore $\langle C, V - V_2 \rangle = \theta_1 \langle C, V_1 - V_2 \rangle$, and the inequality $\theta_1 \det V_1 \leq \det V$ follows. Second, the reverse implication follows by simple algebra manipulation, and the previous arguments, so we will omit it.

2.4.1 Exterior Bound on $Q^e(\mathcal{U})$

Theorem 2.22. Let $\mathcal{U} = \{U_1, U_2, U_3\}$ represent a three-well set and assume that $\operatorname{Aff}(\mathcal{U})$ has codimension one. Also, assume that (a) $\det(U_1 - U_2) > 0$, $\det(U_1 - U_3) > 0$, and $\det(U_2 - U_3) < 0$, or (b) $\det(U_1 - U_2) < 0$, $\det(U_1 - U_3) < 0$, and $\det(U_2 - U_3) > 0$, then

$$Q^{e}(\mathcal{U}) \subset \{U \in C(\mathcal{U}) \mid 0 \leq \hbar(U - U_0)\} \subsetneq C(\mathcal{U}),\$$

C

where $U_0 \in C(\mathcal{U})$ is uniquely characterized by $\det(U_0 - U_2) = \det(U_0 - U_3) = 0$, $\hbar : \mathbb{R}^{2 \times 2}_{sum} \to \mathbb{R}$ is given by

$$\hbar(V) = \langle C, V - (U_2 - U_0) \rangle \det(U_1 - U_0) - \langle C, U_1 - U_2 \rangle \det V,$$

and

$$=\frac{(U_2-U_1)\langle U_3-U_1, U_3-U_2\rangle + (U_3-U_1)\langle U_2-U_1, U_2-U_3\rangle}{\sqrt{\|U_2-U_1\|^2\|U_3-U_1\|^2 - \langle U_2-U_1, U_3-U_1\rangle}}$$

Proof. We notice that under the assumptions of Theorem 2.22, Lemma 2.9 guarantees the existence of $U_0 \in C(\mathcal{U})$ such that $\det(U_2 - U_0) = \det(U_3 - U_0) = 0$ and $\det(V_1 - U_0) \neq 0$, hence the translated set $\mathcal{V} = \{V_1, V_2, V_3\} := \mathcal{U} - U_0$ satisfies that $0 \in C(\mathcal{V})$, $\det(V_2) = \det(V_3) = 0$, and $\operatorname{Aff}(\mathcal{V})$ is a two dimensional subspace. Moreover, Lemma 2.20 can be applied, to obtain an explicit bound for Ker_s f^{pp} for certain matrices C. Then by Proposition 2.16 and Eq. (1.23),

$$Q^{e}(\mathcal{U}) \subset (\operatorname{Ker}_{s} f^{pp} + U_{0}) \cap C(\mathcal{U}), \qquad (2.32)$$

where $\operatorname{Ker}_{s} f^{pp} + U_{0}$ stands for the translated set $\{U_{0} + V \mid V \in \operatorname{Ker}_{s} f^{pp}\}$.

Also by Remark 2.8, if $Q \in \mathbb{R}^{2 \times 2}_{sym}$ is orthogonal to Aff \mathcal{V} , then det Q < 0. Moreover, due to Corollary 2.10, we recall that

$$V_1 = \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}, \quad V_2 = \gamma a^{\perp} \otimes a^{\perp}, \quad \text{and} \quad V_3 = \zeta n^{\perp} \otimes n^{\perp}, \tag{2.33}$$

for some linearly independent $a, n \in S^1$ and constants $\xi, \eta, \gamma, \zeta \in \mathbb{R}$ that satisfy (2.9).

First, we define a matrix C_0 that will be crucial to determine the matrix C. We choose $C_0 \in \text{Aff } V$ normal to the vector $V_3 - V_2$. We can easy construct it with the isomorphism Eq. (1.24). Indeed if $Q \in \mathbb{R}^{2 \times 2}_{sym}$, with ||Q|| = 1, is normal to Aff \mathcal{V} and \tilde{Q} is its \mathbb{R}^3 representation then

$$\tilde{Q} = \frac{(\tilde{V}_2 - \tilde{V}_1) \times (\tilde{V}_3 - \tilde{V}_1)}{\|(\tilde{V}_2 - \tilde{V}_1) \times (\tilde{V}_3 - \tilde{V}_1)\|}, \text{ and } \tilde{C}_0 = \tilde{Q} \times (\tilde{V}_2 - \tilde{V}_3).$$

Due to vector algebra and the equality

$$P^{2} := \|(\tilde{V}_{2} - \tilde{V}_{1}) \times (\tilde{V}_{3} - \tilde{V}_{1})\|^{2} = \|\tilde{V}_{2} - \tilde{V}_{1}\|^{2}\|\tilde{V}_{3} - \tilde{V}_{1})\|^{2} - \left\langle\tilde{V}_{2} - \tilde{V}_{1}, \tilde{V}_{3} - \tilde{V}_{1}\right\rangle^{2}, \quad (2.34)$$

we achieve that

$$\tilde{C}_0 = \frac{(\tilde{V}_3 - \tilde{V}_1) \|\tilde{V}_2 - \tilde{V}_1\|^2 + (\tilde{V}_2 - \tilde{V}_1) \|\tilde{V}_3 - \tilde{V}_1\|^2 - (\tilde{V}_3 + \tilde{V}_2 - 2\tilde{V}_1) \left\langle \tilde{V}_2 - \tilde{V}_1, \tilde{V}_3 - \tilde{V}_1 \right\rangle}{|P|}.$$

Since the isomorphism Eq. (1.24) preserves inner product, we can simply drop the tildes out. Now, by the relations in (2.33),

$$P^{2} = (\eta \gamma + \xi \zeta - \gamma \zeta)^{2} (1 - (a \cdot n)^{4}),$$

and

$$C_0 = -\left(\frac{\left[\left(\zeta - \gamma(a \cdot n)^2\right)a^{\perp} \otimes a^{\perp} + \left(\gamma - \zeta(a \cdot n)^2\right)n^{\perp} \otimes n^{\perp}\right]}{\sqrt{1 - (a \cdot n)^4}}\right)\operatorname{sign}(\eta\gamma + \xi\zeta - \gamma\zeta).$$

Due to the relations in (2.9), and Corollary 2.10,

$$\operatorname{sign}(\eta\gamma + \xi\zeta - \gamma\zeta) = \begin{cases} -1 & \mathcal{U} \text{ is type one,} \\ 1 & \mathcal{U} \text{ is type two.} \end{cases}$$

Thus

$$\det C_0 = \frac{\gamma \zeta (1 + (a \cdot n)^2)^2 - (\gamma + \zeta)^2 (a \cdot n)^2}{1 + (a \cdot n)^2}.$$

Second, we assume \mathcal{U} is type two. This assumption readily implies \mathcal{V} is also type two. Also, we assume $C = \frac{1}{\sqrt{1 - (a \cdot n)^4}} C_0$. This special selection satisfies det C < 0, and $\Pi_C \cap \operatorname{Aff}(\mathcal{V})$ is a line, parallel to $V_2 - V_3$. Indeed

$$\langle C, V_2 \rangle = \langle C, V_3 \rangle = -\zeta \gamma > 0 \ge -(\xi \zeta + \eta \gamma) = \langle C, V_1 \rangle.$$
 (2.35)

Therefore, the set \mathcal{V} and the matrix C meet necessary conditions to apply Lemma 2.20 part (ii) and Remark 2.21. Thus, we have

$$\operatorname{Ker}_{s} f^{pp} = \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C, V - V_{2} \rangle \le 0 \le \langle C, V - V_{1} \rangle, \quad 0 \le \hbar(V) \}.$$

By relation Eq. (2.32), we are interested in Ker_s $f^{pp} \cap C(\mathcal{V})$, but the sets $\{V \in \operatorname{Aff}(\mathcal{V}) \mid \langle C, V - V_2 \rangle = 0\}$ and $\{V \in \operatorname{Aff}(\mathcal{V}) \mid \langle C, V - V_3 \rangle = 0\}$ are supporting lines of $C(\mathcal{V})$ on V_2 and V_1 respectively. Thus, by Eq. (2.32),

$$Q^{e}(\mathcal{V}) \subset \operatorname{Ker}_{s} f^{pp} \cap C(\mathcal{V}) = \{ V \in C(\mathcal{V}) \, | \, 0 \le \hbar(V) \},$$
(2.36)

with

 $\hbar(V) = \langle C, V - V_2 \rangle \det V_1 - \langle C, V_1 - V_2 \rangle \det V.$ (2.37)

Thus, Theorem 2.22 follows from the definition $V_i = U_i - U_0$ and $V = U - U_0$.

Finally, we assume \mathcal{U} is type one. As before, \mathcal{V} is type one. If we assume that $Q \in \mathbb{R}^{2\times 2}_{sym}$ is orthogonal to Aff (\mathcal{V}) , then we define $C(t) \in \mathbb{R}^{2\times 2}_{sym}$ for each $t \in (-\pi, \pi]$ as

$$C(t) = Q\cos t + C\sin t,$$

Where C is chosen as before. We can readily see that

$$\langle C(t), V_2 \rangle = \langle C(t), V_3 \rangle = \zeta \gamma \sin t$$
, and $\langle C(t), V_1 \rangle = (\xi \zeta + \eta \gamma) \sin t$

Thus, due to the continuity of $t \mapsto \det C(t)$ and Remark 2.8, we there exists $t_0 > 0$ small enough such that $\det C(t_0) < 0$ and $\langle C(t_0), V_1 \rangle \leq 0 < \langle C(t_0), V_3 \rangle = \langle C(t_0), V_2 \rangle$. Hence, by Lemma 2.20 (i) and Remark 2.21, we have that

$$\operatorname{Ker}_{s} f^{pp} = \{ V \in \mathbb{R}^{2 \times 2}_{sym} \mid \langle C(t_{0}), V - V_{2} \rangle \le 0 \le \langle C(t_{0}), V - V_{1} \rangle, \quad 0 \le \kappa(V) \},$$

where $\kappa(V) = \langle C(t_0), V - V_2 \rangle \det V_1 - \langle C(t_0), V_1 - V_2 \rangle \det V$. By a similar argument as before, we conclude that

$$Q^{e}(\mathcal{V}) \subset \operatorname{Ker}_{s} f^{pp} \cap C(\mathcal{V}) = \{ V \in C(\mathcal{V}) \mid 0 \le \kappa(V) \}.$$

Next, since $V \in C(\mathcal{V})$, it follows that $\kappa(V) = \sin t_0 \hbar(V)$ where \hbar is defined by Eq. (2.37). Therefore, we conclude that

$$Q^{e}(\mathcal{V}) \subset \{ V \in C(\mathcal{V}) \mid 0 \le \hbar(V) \},$$
(2.38)

and Theorem 2.22 follows from Eq. (2.32). This finishes the proof of our theorem.

Remark 2.23. The component-wise representation of relations Eq. (2.36) and Eq. (2.38) can be easily found. Indeed if $V \in \operatorname{Aff}(\mathcal{V})$, then $V = xa^{\perp} \otimes a^{\perp} + yn^{\perp} \otimes n^{\perp}$ for some real x, y, and $\hbar(V) = |n \times a|^2 h(x, y)$, where

$$h(x,y) = xy(\eta\gamma + (\xi - \gamma)\zeta) - \xi\eta(\gamma y + (x - \gamma)\zeta).$$
(2.39)

Therefore, Eq. (2.36) is rewritten as

$$Q^{e}(\mathcal{V}) \subset \left\{ V \in C(\mathcal{V}) \,|\, V = xa^{\perp} \otimes a^{\perp} + yn^{\perp} \otimes n^{\perp}, \ 0 \le h(x, y) \right\}.$$
(2.40)

Meanwhile, Eq. (2.38) is rewritten as

$$Q^{e}(\mathcal{V}) \subset \left\{ V \in C(\mathcal{V}) \,|\, U = xa^{\perp} \otimes a^{\perp} + yn^{\perp} \otimes n^{\perp}, \ h(x,y) \le 0 \right\}.$$
(2.41)

2.4.2 On the Equality Between $L^{e}(\mathcal{U})$ and $Q^{e}(\mathcal{U})$

Now, we prove the theorem concerning the equality between the symmetric lamination convex hull and the symmetric quasiconvex hull when there exists a rank-one compatibility among the elements in \mathcal{U} .

Theorem 2.24 (On the equality between $L^e(K)$ and $Q^e(K)$). Let $\mathcal{U} = \{U_1, U_2, U_3\}$ be a set of 2 × 2 linearly independent symmetric matrices. If there are two wells in \mathcal{U} that are rank-one compatible, then

$$Q^e(\mathcal{U}) = L^e(\mathcal{U}).$$

Proof. We consider three cases:

(a) If all the wells in \mathcal{U} are pairwise compatible Bhattacharya [4] proved that $Q^e(\mathcal{U}) = L^e(\mathcal{U}) = C(\mathcal{U})$, and there is nothing to prove.

(b) Let us assume that \mathcal{U} is of type two, so there exists a rank-one compatible pair of wells. Without loss of generality, we assume that

$$\det(U_1 - U_2) = 0, \det(U_1 - U_3) \le 0 \text{ and } \det(U_2 - U_3) > 0.$$
(2.42)

Hence by Lemma 2.9, there exists $U_0 \in C(\mathcal{U})$ such that $\det(U_2 - U_0) = \det(U_3 - U_0) = 0$. Moreover, $\det(U_1 - U_0) = 0$ since U_2 and U_1 are rank-one compatible. So the translated set $\mathcal{V} = \mathcal{U} - U_0$ satisfies that $\operatorname{Aff}(\mathcal{V}) \subset \mathbb{R}^{2 \times 2}_{sym}$ is a two-dimensional subspace, where $\det(V_i) = 0$ for i = 1, 2, 3. Hence by Eq. (2.21) and the first part of Lemma 2.20, we conclude that if f is given as in Eq. (2.15), then f^{pp} is a non negative polyconvex function such that $\mathcal{V} \subset \operatorname{Kers} f^{pp}$, hence

$$L^{e}(\mathcal{V}) \subset Q^{e}(\mathcal{V}) \subset \operatorname{Ker}_{s} f^{pp} \cap C(\mathcal{V}) = \left\{ V \in \mathbb{R}^{2 \times 2}_{sym} \, \middle| \, V \in C(\mathcal{V}), \, 0 \le \det V \right\} = C(\mathcal{V}) \cap \overline{\mathcal{C}_{0}},$$

where the notation $\overline{\mathcal{C}_0}$ stands for the closure of the incompatible cone at 0. Moreover, by Proposition 2.13, we have that $L^e(\mathcal{V}) = C(\{0, V_2\}) \cup C(\{0, V_1, V_3\}) = C(\mathcal{V}) \cap \overline{\mathcal{C}_0}$. and the proof follows.

(c) Now, we assume that there is only one compatible pair in \mathcal{U} and it is a rank-one compatibility. Without loss of generality, we assume that

$$\det(U_2 - U_3) > 0, \det(U_1 - U_3) > 0 \text{ and } \det(U_1 - U_2) = 0.$$
(2.43)

Now we claim that there exist $U_0 \notin C(\mathcal{U})$ such that

$$\det(U_0 - U_1) = \det(U_0 - U_2) = \det(U_0 - U_3) = 0.$$
(2.44)





This claim readily follows by noticing that

$$t \mapsto \det(tU_1 + (1-t)U_2 - U_3) = \det(U_2 - U_3) + t \left\langle \mathcal{S}(U_1 - U_2), U_2 - U_3 \right\rangle,$$

is linear in t, and $\langle \mathcal{S}(U_1 - U_2), U_2 - U_3 \rangle$ does not vanish since Aff(\mathcal{U}) has codimension two. Thus, there exists $t_0 \in \mathbb{R}$ such that (2.44) holds. Moreover, we have that $t_0 \notin [0,1]$ and $U_0 = t_0 U_1 + (1-t_0) U_2 \notin C(\mathcal{U})$ due to (2.43) see Fig. 2.7. Proceeding as before, we define $\mathcal{V} = \{V_1, V_2, V_3\} = \mathcal{U} - U_0$ where $V_i = U_i - U_0$ and det $V_i = 0$

for $i \in \{1, 2, 3\}$. Hence by Eq. (2.21) and the first part of Lemma 2.20, we conclude that if f is given as in Eq. (2.15), then f^{pp} is a non negative polyconvex function such that $\mathcal{V} \subset \operatorname{Ker}_{s} f^{pp}$, and

$$L^{e}(\mathcal{V}) \subset Q^{e}(\mathcal{V}) \subset \operatorname{Ker}_{\mathrm{s}} f^{pp} \subset \left(C(\mathcal{V}) \cap \overline{\mathcal{C}_{0}}\right),$$

but $(C(\mathcal{V}) \cap \overline{\mathcal{C}_0}) = \{V_3\} \cup C(\{V_1, V_2\}) = L^e(\mathcal{V})$, by Proposition 2.13.(a), and the proof is complete.

2.5 Optimality of the Bound for $Q^e(\mathcal{U})$ by Symmetric Quadratic Polyconvex Functions

We finish this chapter with a brief comment about the optimality of the bounds in Theorem 2.22. By the characterization of symmetric quadratic polyconvex functions given by Boussaid, Kreisbeck, and Sclömerkemper [8] we can prove that our outer bound for $Q^e(\mathcal{U})$ is optimal when we restrict the analysis to quadratic functions. By Proposition 4.5 in [8], $f: \mathbb{R}^{2\times 2}_{sym} \to \mathbb{R}$ is symmetric quadratic polyconvex if and only if it has the form $f(\cdot) = g(\cdot) - \alpha \det(\cdot)$ for some convex function $g: \mathbb{R}^{2\times 2}_{sym} \to \mathbb{R}$ and $\alpha > 0$. In this case, f is also symmetric quasiconvex.

It is well-known, see [2], that a uniformly bounded minimizing sequence of linear strains $\{e(Du_k)\}$ has a subsequence $\{e(Du_{k_j})\}$ that generates a family of probability measures ν_x in $\mathbb{R}^{2\times 2}_{sym}$, indexed by $x \in \Omega$ and supported on \mathcal{U} , such that for every continuous function $\Psi : \mathbb{R}^{2\times 2}_{sym} \to \mathbb{R}$, the sequence $\{\Psi(e(Du_k))\}$ weakly converges to $\int_{\mathbb{R}^{2\times 2}_{sym}} \Psi(A) d\nu_x(A)$. Moreover this family of measures satisfies that if Ψ is quasiconvex then $\Psi(\int_{\mathbb{R}^{2\times 2}_{sym}} A d\nu_x(A)) \leq \int_{\mathbb{R}^{2\times 2}_{sym}} \Psi(A) d\nu_x(A)$ a.e. $x \in \Omega$, see [16]. Therefore, if ν is a homogeneous Young measure limit of linear strains supported on $\mathcal{V} = \mathcal{U} - U_0$, *i.e.*, $\nu_x = \theta_1 \delta_{V_1} + \theta_2 \delta_{V_2} + \theta_3 \delta_{V_3}$ with barycenter V, it follows that $V = \theta_1 V_1 + \theta_2 V_2 + \theta_3 V_3$ and

$$g(V) - \alpha \det(V) \le \sum_{i=1}^{3} \theta_i g(V_i) - \alpha \sum_{i=1}^{3} \theta_i \det(V_i).$$

Since any (symmetric) quadratic polyconvex function is (symmetric) quasiconvex, and we are interested in a bound on $Q^e(\mathcal{V})$, it follows that if $V \in Q^e(\mathcal{V})$, then

$$\det(V) - \theta_1 \det(V_1) \ge \sup\left\{ \frac{1}{\alpha} \left(g(V) - \sum_{i=1}^3 \theta_i g(V_i) \right) \mid g \text{ is convex}, \alpha > 0 \right\}$$
(2.45)

Notice that the terms $\theta_2 \det V_2$ and $\theta_3 \det V_3$ vanish since $\det V_i = U_i - U_0 = 0$ for i = 2 and i = 3. Due to the convexity of g, the supremum in Eq. (2.45) is upperly bounded

by 0; indeed it is attained since g = 0 is convex. Therefore, the best bound on $Q^e(\mathcal{V})$ obtained by symmetric and quadratic polyconvex functions is given by

$$\left\{ V = \theta_1 V_1 + \theta_2 V_2 + \theta_3 V_3 \ \left| \ \det(V) \ge \theta_1 \det(V_1), \ (\theta_1, \theta_2, \theta_3) \in [0, 1]^3, \ \sum_{i=1}^3 \theta_i = 1 \right\}$$
(2.46)

This set is equivalent to the one presented in Theorem 2.22, and the optimality is proved.

This analysis suggest that better bounds in $Q^e(\mathcal{U})$ could be obtained only for symmetric polyconvex functions that are not quadratic, and the method based on convex analysis presented above could be applied to non-quadratic functions f_C for providing better outer bounds on $Q^e(\mathcal{U})$.

Chapter 3

The Symmetric Quasiconvex and Lamination Convex Hull for the Coplanar n-Well Problem

In this chapter, we study the coplanar n-well problem in 2D linear elasticity and we explicitly determine the symmetric lamination convex hull for this type of sets. In the coplanar four-well problem, we show that under appropriate conditions $L^e(\mathcal{U}) = Q^e(\mathcal{U}) \neq$ $C(\mathcal{U})$. Finally, we extend this result to some particular configurations of n wells. Most of the proofs are constructive, and we also present explicit examples. Along this chapter, we will assume that a normal matrix Q for each set of coplanar wells has negative determinant, since in the case where this does not hold $L^e(\mathcal{U}) = C(\mathcal{U})$, see [22, 4].

It is well known that, if all the elements of a finite symmetric set of wells \mathcal{U} are compatible, then its symmetric lamination convex hull $L^e(\mathcal{U})$ and its convex hull $C(\mathcal{U})$ coincide, see for instance [22, 4]. Moreover, in the three-well case a complete characterization of the lamination convex hull is known, see Proposition 2.13 in Chapter 2. We begin by defining precisely the notion of coplanar wells.

Definition 3.1. We say that $\{U_1, U_2, \dots, U_n\} \subset \mathbb{R}^{2 \times 2}_{sym}$ is a set of *n* coplanar wells if there exists $Q \in \mathbb{R}^{2 \times 2}_{sym}$ and $\delta \in \mathbb{R}$ fixed such that $\langle Q, U_i \rangle = \delta$ for every $i = 1, 2, \dots, n$. Also we define the family of triplets \mathcal{F} contained in \mathcal{U} as

$$\mathcal{F} = \{\{U_i, U_j, U_k\} \mid i, j, k \in \{1, 2, \dots, n\} \text{ are different indexes}\}.$$
(3.1)

Since $\mathcal{V} \subset \mathcal{U}$ for every $\mathcal{V} \in \mathcal{F}$, it follows that $L^{e,i}(\mathcal{V}) \subset L^{e,i}(\mathcal{U})$ for each $i \in \mathbb{N}$, and

$$\bigcup_{\mathcal{V}\in\mathcal{F}} L^{e,i}(\mathcal{V}) \subset L^{e,i}(\mathcal{U}).$$
(3.2)

We introduce some notations before presenting our next result. First, for any coplanar set \mathcal{U} we denote by $\mathscr{C}_Q(U) = \mathcal{C}_U^c \cap \Pi_Q$ the planar compatible cone of U. With this at

hand, we define the upper and lower parts of $\mathscr{C}_Q(U)$ as

$$\mathscr{C}_{Q}^{+}(U) = \{ V \in \mathbb{R}^{2 \times 2}_{sum} \text{ such that } V = U + \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}, \text{ for some } \xi \ge 0 \ge \eta \}$$

and

 $\mathscr{C}_Q^-(U) = \{ U \in \mathbb{R}^{2 \times 2}_{sym} \text{ such that } V = U + \xi a^\perp \otimes a^\perp + \eta n^\perp \otimes n^\perp, \text{ for some } \eta \ge 0 \ge \xi \},$

respectively.

Remark 3.2. Since we will be frequently using matrices of the for $M = N + \xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$, we adopt the notation (ξ, η) for the matrix $\xi a^{\perp} \otimes a^{\perp} + \eta n^{\perp} \otimes n^{\perp}$, where $a, n \in S^1$ and $\xi, \eta \in \mathbb{R}$.

3.1 The Symmetric Lamination Convex Hull for the Coplanar *n*-Well Problem

This section is devoted to prove the equality in Eq. (3.2). To this end, we must show the reverse inclusion, namely

$$L^{e,i}(\mathcal{U}) \subset \bigcup_{\mathcal{V}\in\mathcal{F}} L^{e,i}(\mathcal{V}).$$

Before doing this, we prove some auxiliary lemmas that make this process smooth.

3.1.1 Preliminary Lemmas

The following lemma states that *being in the upper compatible cone of* is a transitive relation.

Lemma 3.3. Let U, V and $W \in \mathbb{R}^{2 \times 2}_{sym}$ such that $V \in \mathscr{C}^+_Q(U)$ and $W \in \mathscr{C}^-_Q(U)$, then $V \in \mathscr{C}^+_Q(W)$.

Proof. Let a and n be the unitary vectors associated with Q as in the definition of $\mathscr{C}_Q(U)$. The result is straight forward, since

 $V = U + (\xi, \eta)$, with $\xi \ge 0 \ge \eta$ and $W = U + (\gamma, \delta)$, with $\delta \ge 0 \ge \gamma$,

imply that $V = W + (\xi - \gamma, \eta - \delta)$, where $\xi - \gamma \ge 0 \ge \eta - \delta$ and we have used the notation introduced in Remark 3.2.

We say that the matrices of a coplanar set $\mathcal{U} = \{U_1, \dots, U_n\}$ are labeled in increasing order if at any edge of $C(\mathcal{U})$ the corresponding vertices are U_i and U_{i+1} for $i \in \{1, \dots, n\}$ in cyclic order.

Lemma 3.4. Let $\mathcal{L} := \{U_1, U_2, U_3, U_4\} \subset \mathbb{R}^{2 \times 2}_{sym}$ be a coplanar set such that its convex hull $C(\mathcal{L})$ is a quadrilateral labeled in increasing order. If there are three values for $i \in \{1, 2, 3, 4\}$ such that the pairs $\{U_i, U_{i+1}\}$ are compatible, then either $\{U_1, U_3\}$ or $\{U_2, U_4\}$ are compatible.

Proof. Without loss of generality, we assume $U_1 = 0$. By Lemma 2.5 and Remark 2.4, there exist $b, c, d, f, g, h \in \mathbb{R}$ such that

$$U_1 = (0,0), \quad U_2 = (b,c), \quad U_3 = (d,f), \text{ and } U_4 = (g,h).$$

Without loss of generality, we assume that for each $i \in \{1, 2, 3\}$ the wells U_i, U_{i+1} are compatible but U_1, U_4 are incompatible wells, see Fig. 3.1. Hence, we get (up to a common factor $|a \times n|^2$) the following set of equations

$$0 \ge \det(U_2 - U_1) = bc, \tag{3.3}$$

$$0 \ge \det(U_3 - U_2) = (d - b)(f - c), \tag{3.4}$$

$$0 \ge \det(U_4 - U_3) = (g - d)(h - f), \tag{3.5}$$

$$gh = \det(U_4 - U_1) > 0.$$
 (3.6)

From Eq. (3.3) we have two options. First, we assume that $c \le 0 \le b$. Due to Eq. (3.4), we have two more cases, either

(I)
$$(f-c) \le 0 \le (d-b)$$
 or (II) $(d-b) \le 0 \le (f-c)$.

If (I) holds, it follows that $U_3 \in \mathscr{C}_Q^+(U_2)$ and $U_1 \in \mathscr{C}_Q^-(U_2)$. Then, by Lemma 3.3, the wells U_1 and U_3 are compatible. Now, if (II) holds, then $U_2 = U_3 + (b - d, c - f)$, and $U_2 \in \mathscr{C}_Q^+(U_3)$. We notice that U_3 satisfies either 0 < fb - cd and the set \mathcal{L} is clockwise oriented, or fb - cd < 0 and the set \mathcal{L} is counterclockwise oriented. To preserve the vertex orientation and relations (3.5) and (3.6), it follows that $U_4 \in \mathscr{C}_Q^-(U_3)$ in either case. Hence, by Lemma 3.3, the wells U_4 and U_2 are compatible.

Second, we assume $b \le 0 \le c$. The arguments in this case follows the same lines as the previous case and we skip the proof.

Lemma 3.5. Let $\mathcal{L} := \{U_{v,1}, U_{v,2}, U_{w,1}U_{w,2}\} \subset \mathbb{R}^{2\times 2}_{sym}$ be coplanar four-well set with $\det(U_{v,1} - U_{v,2}) \leq 0$ and $\det(U_{w,1} - U_{w,2}) \leq 0$. Also let \mathcal{F} as in Eq. (3.1) and assume there exist $u \in C(\mathcal{L}), v \in L^{e,1}(\{U_{v,1}, U_{v,2}\})$, and $w \in L^{e,1}(\{U_{w,1}, U_{w,2}\})$ such that $u \in L^{e,1}(\{v, w\})$. Then, $u \in L^{e,2}(\mathcal{V})$ for some $\mathcal{V} \in \mathcal{F}$.

Proof. We consider three different cases depending on the number of extreme points (or vertices) of $C(\mathcal{L})$.

First, if the set of extreme points of $C(\mathcal{L})$ consists of two points, \mathcal{L} is contained in a compatible line, and the affirmation follows trivially. Second, we assume that $C(\{U_{v,1}, U_{v,2}, U_{w,1}, U_{w,2}\})$ has exactly three extremal points. Without loss of generality, let

$$U_{w,2} \in C(\{U_{v,1}, U_{v,2}, U_{w,1}\}).$$
(3.7)

By Lemma 2.12, either $U_{v,1}$ or $U_{v,2}$ are compatible with $U_{w,1}$, otherwise $U_{w,2}$ would be incompatible with $U_{w,1}$. Hence, there exist at least two compatibility relations between the extreme points $U_{v,1}, U_{v,2}$, and $U_{w,1}$. By Proposition 2.13, since $U_{w,2}$ and $U_{w,1}$ are compatible, the whole segment $\{tU_{w,1}+(1-t)U_{w,2}|t \in [0,1]\}$ is contained in $L^{e,2}(\{U_{v,1}, U_{v,2}, U_{w,1}\})$. Therefore $v, w \in L^{e,2}(\{U_{v,1}, U_{v,2}, U_{w,1}\})$ and $u \in L^{e,3}(\{U_{v,1}, U_{v,2}, U_{w,1}\})$. Due to Proposition 2.13 and Remark 2.14, $L^{e,2}(\{U_{v,1}, U_{v,2}, U_{w,1}\}) = L^e(\{U_{v,1}, U_{v,2}, U_{w,1}\})$. Hence, $u \in L^{e,2}(\{U_{v,1}, U_{v,2}, U_{w,1}\})$ and the lemma follows.

Third, we assume that all wells in \mathcal{L} are the extremal points of $C(\mathcal{L})$. Since \mathcal{L} is coplanar, the set $C(\mathcal{L})$ is a quadrilateral, and there exist six segments joining the wells in \mathcal{L} . The boundary $\partial_{\mathrm{ri}} C(\mathcal{L})$ is given by four segments on the boundary of the quadrilateral. The two remaining segments connect the opposite wells of \mathcal{L} diagonally. Now, we split our analysis into three cases that depend on how many compatible segments are on $\partial_{\mathrm{ri}} C(\mathcal{L})$.

- a) If all four segments in $\partial_{\mathrm{ri}} C(\mathcal{L})$ are compatible, then either $U_{w,1}$ and $U_{v,2}$ or $U_{w,2}$ and $U_{v,1}$ are compatible. This follows from the assignment $(U_{v,1}, U_{v,2}, U_{w,2}, U_{w,1}) \mapsto$ (U_1, U_2, U_3, U_4) and Lemma 3.4. Hence, a diagonal in $C(\mathcal{L})$ is a compatible segment, and every point in $C(\mathcal{L})$ belongs to a triangle with pairwise compatible vertices and $u \in L^{e,2}(\mathcal{V})$ for some $\mathcal{V} \in \mathcal{F}$.
- b) We assume that only one out of the four segments in $\partial_{\mathrm{ri}} C(\mathcal{L})$ is not a compatible segment. By assignment $(U_{v,1}, U_{v,2}, U_{w,2}, U_{w,1}) \mapsto (U_1, U_2, U_3, U_4)$ and Lemma 3.4, at least one of the diagonal segments is compatible, see Fig. 3.1.



Figure 3.1 A four-well configuration where one the boundary segments is not a compatible one.

Thus, $C(\mathcal{L}) = T_1 \cup T_2$, where T_1 and T_2 are two triangles such that $\partial_{\mathrm{ri}}(T_1)$ and $\partial_{\mathrm{ri}}(T_2)$ consist of three and only two compatible segments, respectively. If $u \in T_1$ then $u \in L^{e,2}(\mathcal{V})$ for some $\mathcal{V} \in \mathcal{F}$ and the lemma follows. Hence, let $u \in T_2$ and, without loss of generality, assume that the set of extreme points of T_2 is $\mathcal{L}_T = \{U_{v,1}, U_{w,1}, U_{w,2}\}$ with the incompatible line segment $\{tU_{v,1} + (1-t)U_{w,1} \mid t \in [0,1]\}$. Notice that u is a convex combination of two compatible wells $v \in L^{e,1}(\{U_{v,1}, U_{v,2}\})$ and $w \in L^{e,1}(\{U_{w,1}, U_{w,2}\})$, hence there exists $v' \in L^{e,1}(\{U_{v,1}, U_{w,2}\})$ such that u also is a convex combination of v' and w, due to $\mathcal{L}_T \subset \mathcal{L}$. Moreover v' and w are compatible since they belong to the compatible segment $\{tv + (1-t)w \mid t \in [0,1]\}$, so we conclude that $u \in L^{e,2}(\mathcal{L}_T)$.

c) We assume there are only two compatible segments on the boundary of $C(\mathcal{L})$. We claim that there exists a compatible diagonal segment. If the claim holds, we let $\{tU_{v,1} + (1-t)U_{w,2} | t \in [0,1]\}$ be the compatible diagonal segment without loss of generality. Hence, $C(\mathcal{L}) = T_1 \cup T_2$ where $T_1 = C(\{U_{v,1}, U_{w,2}, U_{v,2}\})$ and $T_2 =$

 $C(\{U_{v,1}, U_{w,1}, U_{w,2}\})$ are triangles such that $\partial_{\mathrm{ri}} T_1$ and $\partial_{\mathrm{ri}} T_2$ have two compatible segments, see Fig. 3.2a. We have that either $u \in T_1$ or $u \in T_2$. In both cases, we argue as in the second part of b) to prove that $u \in L^{e,2}(\mathcal{V})$ where either $\mathcal{V} = \{U_{v,1}, U_{w,1}, U_{w,2}\}$ or $\mathcal{V} = \{U_{v,1}, U_{w,2}, U_{v,2}\}$ and the lemma follows.



Figure 3.2 Images (a) and (b) show four-well configurations where two of the boundary segments are incompatible segments. The configuration in Fig. (b) is not considered in the statement of Lemma 3.5 since there is not a well $C(\mathcal{L})$ that meets the conditions in Lemma 3.5.

Finally, we prove the claim in part c). By contradiction, we assume that there are no compatible diagonal segments, namely $\{U_{w,1}, U_{v,2}\}$ and $\{U_{w,2}, U_{v,1}\}$ are incompatible. By Lemma 2.12, it follows that $U_{v,1}$ and $U_{v,2}$ are incompatible with every element in $\{sU_{w,1} + (1-s)U_{w,2} | s \in [0,1]\}$. Hence, on the one hand, for every $s \in [0,1]$, we have that

$$\det(sU_{w,1} + (1-s)U_{w,2} - U_{v,1}) > 0 \text{ and } \det(sU_{w,1} + (1-s)U_{w,2} - U_{v,2}) > 0.$$

On the other hand, if $t \in [0, 1]$, the rank-one convexity of $-\det(e(\cdot))$ and the compatibility of $U_{v,1}$ and $U_{v,2}$ implies that

$$det(w - v) = det(sU_{w,1} + (1 - s)U_{w,2} - tU_{v,1} - (1 - t)U_{v,2})$$

= det[t(sU_{w,1} + (1 - s)U_{w,2} - U_{v,1}) + (1 - t)(sU_{w,1} + (1 - s)U_{w,2} - U_{v,2})]
\geq t det(sU_{w,1} + (1 - s)U_{w,2} - U_{v,1}) + (1 - t) det(sU_{w,1} + (1 - s)U_{w,2} - U_{v,2})
> 0.

Since by assumption there exists $u \in L^{e,1}(\{v, w\})$ and v and w are compatible, $det(v - w) \leq 0$, a contradiction, and we finish the proof.

Lemma 3.6. Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a set of n coplanar wells and \mathcal{F} as in Eq. (3.1). Also let $\mathcal{V}_1, \mathcal{V}_2$ be two different sets in \mathcal{F} . If there exists $U \in \mathbb{R}^{2\times 2}_{sym}$ such that U is a symmetric lamination of degree one of two compatible wells, $V \in L^{e,2}(\mathcal{V}_1)$ and $W \in L^{e,2}(\mathcal{V}_2)$. Then, U is a symmetric lamination of degree one of two compatible wells, $V' \in L^{e,1}(\mathcal{V}_1)$ and $W' \in L^{e,1}(\mathcal{V}_2)$.

Proof. We notice that if $U \in L^{e,2}(\mathcal{V}_1) \cup L^{e,2}(\mathcal{V}_2)$ there is nothing to prove, hence we focus on the case $U \notin L^{e,2}(\mathcal{V}_1) \cup L^{e,2}(\mathcal{V}_2)$.

We claim that there exists $W' \in L^{e,1}(\mathcal{V}_2)$ such that $U \in L^{e,1}(\{V, W'\})$. Notice that by the assignment $V \mapsto W$ and $W' \mapsto V$, the claim implies that there exists $V' \in L^{e,1}(\mathcal{V}_1)$ such that $U \in L^{e,1}(\{V', W'\})$ and the result follows.

Now we prove the claim. If $W \in L^{e,1}(\mathcal{V}_2)$, by letting W' = W the affirmation follows straight forward. Hence, we assume that $W \in L^{e,2}(\mathcal{V}_2) \setminus L^{e,1}(\mathcal{V}_2)$. Let ℓ_0, ℓ_1 and ℓ_2 denote line segments that make up the boundary $\partial_{\mathrm{ri}} C(\mathcal{V}_2)$ and \mathcal{L} be the compatible line through V and W. Since W and V belong to the relative interior and exterior of $C(\mathcal{V}_2)$, respectively, \mathcal{L} intersects two of the line segments ℓ_0, ℓ_1 and ℓ_2 . Now, by Remark 2.14 and Proposition 2.13 it follows that

$$L^{e,1}(\mathcal{V}_2) = \begin{cases} \partial_{\mathrm{ri}} C(\mathcal{V}_2) & \text{if the wells in } \mathcal{V}_2 \text{ are pairwise compatible} \\ \ell_i \cup \ell_{i+1}, \text{ for some } i = 1, 2, 3 & \text{if there is an incompatible pair in } \mathcal{V}_2. \end{cases}$$

Therefore, $\mathcal{L} \cap L^{e,1}(\mathcal{V}_2) \neq \emptyset$, and the claim follows by choosing

$$W' = rg \max \left\{ \operatorname{dist}(V, Z) \, | \, Z \in L^{e,1}(\mathcal{V}_2) \cap \mathcal{L} \right\}.$$

3.1.2 The Symmetric Lamination Convex Hull

Now we prove the characterization of the symmetric lamination convex hull of a finite coplanar set of wells.

Theorem 3.7 (Laminar convex). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a finite coplanar set and define \mathcal{F} as in Eq. (3.1), then

$$L^{e}(\mathcal{U}) = \bigcup_{\mathcal{V}\in\mathcal{F}} L^{e}(\mathcal{V}).$$

Proof of Theorem 3.7. By definition of $L^{e,1}(\mathcal{U})$ and the equality $L^{e,0}(\mathcal{U}) = \mathcal{U}$, it follows that

$$L^{e,1}(\mathcal{U}) = \bigcup_{\mathcal{V}\in\mathcal{F}} L^{e,1}(\mathcal{V}).$$
(3.8)

Now, we claim that

$$\bigcup_{\mathcal{V}\in\mathcal{F}} L^{e,2}(\mathcal{V}) = L^{e,2}(\mathcal{U}).$$

By contradiction, we assume that there exists

$$u \in L^{e,2}(\mathcal{U}) \setminus \bigcup_{\mathcal{V} \in \mathcal{F}} L^{e,2}(\mathcal{V}).$$
(3.9)

So u is a convex combination of two elements in the set of laminations of degree one $v, w \in L^{e,1}(\mathcal{U})$. Due to (3.8) $v \in L^{e,1}(\mathcal{V}_1)$ and $w \in L^{e,1}(\mathcal{V}_2)$ for some $\mathcal{V}_1, \mathcal{V}_2 \in \mathcal{F}$. We

assume that $\mathcal{V}_1 \neq \mathcal{V}_2$, otherwise u would belong to $L^{e,2}(\mathcal{V}_1)$, a contradiction. Moreover, if $v \in \mathcal{V}_1$ or $w \in \mathcal{V}_2$, then there exists $\mathcal{V} \in \mathcal{F}$ such that $u \in L^{e,2}(\mathcal{V})$, again a contradiction. Hence, there are four wells $U_{v,1}, U_{v,2} \in \mathcal{V}_1$ and $U_{w,1}, U_{w,2} \in \mathcal{V}_2$ such that v and w belong to the compatible segments $L^{e,1}(\{U_{v,1}, U_{v,2}\})$ and $L^{e,1}(\{U_{w,1}, U_{w,2}\})$, respectively, and $u \in C(\{U_{v,1}, U_{v,2}, U_{w,1}, U_{w,2}\})$. By Lemma 3.5, $u \in L^{e,2}(\mathcal{V})$ for some $\mathcal{V} \in \mathcal{F}$, a contradiction, and the claim follows. Thus, by Remark 2.14 $L^{e,2}(\mathcal{V}) = L^e(\mathcal{V})$ for every three-well set \mathcal{V} and

$$L^{e,2}(\mathcal{U}) = \bigcup_{\mathcal{V}\in\mathcal{F}} L^{e,2}(\mathcal{V}) = \bigcup_{\mathcal{V}\in\mathcal{F}} L^e(\mathcal{V}).$$
(3.10)

Next, prove that

$$L^{e,3}(\mathcal{U}) = L^{e,2}(\mathcal{U}).$$

We proceed again by contradiction. Assume that $u \in L^{e,3}(\mathcal{U}) \setminus L^{e,2}(\mathcal{U}) \neq \emptyset$, so it is a convex combination of two compatible wells, say $v, w \in L^{e,2}(\mathcal{U})$, and by the first equality in Eq. (3.10), $v \in L^{e,2}(\mathcal{V}_1)$ and $w \in L^{e,2}(\mathcal{V}_2)$ for some $\mathcal{V}_1, \mathcal{V}_2 \in \mathcal{F}$. Due to the last equality in Eq. (3.10) we also have that $\mathcal{V}_1 \neq \mathcal{V}_2$. Thus, by Lemma 3.6, u is a convex combination of two compatible wells $v' \in L^{e,1}(\mathcal{V}_1)$ and $w' \in L^{e,1}(\mathcal{V}_1)$, where $\mathcal{V}_1 \neq \mathcal{V}_2$. So, there exist two pair of compatible wells $U_{v,1}, U_{v,2} \in \mathcal{V}_1$ and $U_{w,1}, U_{w,2} \in \mathcal{V}_1$ such that v' and w' are convex combinations of the former and latter pairs, respectively, and by Lemma 3.5, $u \in L^{e,2}(\mathcal{V})$ for some $\mathcal{V} \in \mathcal{F}$, a contradiction. Therefore $L^{e,3}(\mathcal{U}) = L^{e,2}(\mathcal{U})$ and the proof is complete.

3.2 The Quasiconvex Hull for the Coplanar *n*-Well Problem.

The symmetric quasiconvex hull $Q^e(\mathcal{U})$ is the set of wells that cannot be separated from the set \mathcal{U} by symmetric quasiconvex functions, see Eq. (1.21). The next lemma gives a manner to exclude matrices that do not belong to $Q^e(\mathcal{U})$.

Lemma 3.8. Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a finite coplanar set of wells contained in the affine space Π_Q . Assume there exists $U_0 \in \Pi_Q$ such that $\det(V - U_0) \ge 0$ for every $V \in \mathcal{U}$. If $U \in C(\mathcal{U})$ and $\det(U - U_0) < 0$, then $U \notin Q^e(\mathcal{U})$.

Proof. We proceed by contradiction and assume that $U \in Q^e(\mathcal{U})$. From Remark 2.11, the function $-\det : \mathbb{R}^{2\times 2}_{sym} \to \mathbb{R}$ and its translation $f(\cdot) = -\det((\cdot) - U_0)$ are both symmetric quasiconvex. Due to Eq. (1.21), U satisfies $-\det(U - U_0) \leq \sup\{-\det(V - U_0) \mid V \in \mathcal{U}\}$, but this is a contradiction to the statement, so $U \notin Q^e(\mathcal{U})$.

3.2.1 The four-well case

Before stating the theorem, we make the following definition:

Definition 3.9. we say that the set $\mathcal{U} = \{U_0, U_1, U_2, U_3\} \subset \mathbb{R}^{2 \times 2}_{sym}$ has a wedge configuration if there exists a subset of three wells, say $\mathcal{V} = \{U_1, U_2, U_3\}$, such that there is

only one incompatible pair of wells in \mathcal{V} , and the remaining well $U_0 \in \operatorname{rel} \operatorname{int} C(\mathcal{V})$ is rank-one compatible with each element in the incompatible pair of wells in \mathcal{V} , see Fig. 1.7 in Section 1.2 for an example of this well configuration.

Now, we prove that the laminar convex hull of \mathcal{U} equals $Q^e(\mathcal{U})$ for a family of four wells with two pairs of rank-one compatible wells.

Theorem 3.10 (Four coplanar wells). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a set of four coplanar wells such that all its elements have at least another compatible one, its plane's normal satisfies det Q < 0, and \mathcal{U} is not in a wedge configuration. Furthermore, assume there exist two different subsets $\{V_1, V_2\}, \{W_1, W_2\} \subset \mathcal{U}$ of rank-one compatible pairs and let $D = C(\{W_1, W_2\}) \cup C(\{V_1, V_2\})$. If any of the following conditions holds,

- 1. the set D is disconnected;
- 2. D is a connected set and $\mathcal{U} \subset D$;
- 3. the intersection of the sets $\{V_1, V_2\}$ and $\{W_1, W_2\}$ has only one element, say V, and D is contained either in the upper or in the lower part of $\partial(\mathscr{C}_Q(V))$,

then $L^{e}(\mathcal{U}) = Q^{e}(\mathcal{U}).$



Figure 3.3 Images (a) to (c) show three different four-well sets configurations that satisfy conditions 1 to 3 in Theorem 3.10, respectively. Green dots are the wells in \mathcal{U} , blue solid lines represent rank-one compatibility between the joint wells. Dashed blue lines represent the rank-one directions through W_2 .

We must point out that $\{V_1, V_2\} \neq \{W_1, W_2\}$, and this condition holds although they have a common well for example $V_1 = W_2$. Item 3 in Theorem 3.10 takes into account this situation. Meanwhile, Item 2 considers that $V_i \neq W_j$ for every i, j = 1, 2.

Proof of Theorem 3.10. Let Π_Q be the affine space generated by \mathcal{U} , see Lemma 2.5. Notice that, since $\{V_1, V_2\}$ and $\{W_1, W_2\}$ are rank-one compatible pairs, there are only two possibilities, either the corresponding rank-one lines generated by them are parallel or not. We warn the reader that we frequently use the notation introduced in Remark 3.2 throughout the proof. We divide the proof into three steps.

STEP 1 We assume that $D = C(\{V_1, V_2\}) \cup C(\{W_1, W_2\})$ is a disconnected set (Item 1 in Theorem 3.10). The compatible planar cones $\mathscr{C}_Q(W_1)$ and $\mathscr{C}_Q(W_2)$ determine a division of the plane Π_Q into three disjoint sets (see Fig. 3.4), namely

$$\Pi_Q = A \cup B \cup C,$$

where $A = \mathscr{C}_Q(W_1) \cap \mathscr{C}_Q(W_2)$, $B = \mathscr{C}_Q(W_1) \triangle \mathscr{C}_Q(W_2)$, and $C = (\prod_Q \setminus \mathscr{C}_Q(W_1)) \cap (\prod_Q \setminus \mathscr{C}_Q(W_2))$.



Figure 3.4 The plane Π_Q divided into three sets for item 1. This division is naturally determined by the rank-one lines through W_1 and W_2 .

Notice that, A is the set of all matrices compatible with W_1 and W_2 simultaneously, namely

$$A = \left[\mathscr{C}_{Q}^{-}(W_{1}) \cap \mathscr{C}_{Q}^{-}(W_{2})\right] \cup \left[\mathscr{C}_{Q}^{+}(W_{1}) \cap \mathscr{C}_{Q}^{+}(W_{2})\right] \cup C(\{W_{1}, W_{2}\}).$$
(3.11)

Since D is disconnected, V_1 and V_2 do not belong to $C(\{W_1, W_2\})$. Also V_1 and V_2 cannot lie in different connected components of $A \setminus C(\{W_1, W_2\})$ because they are rank-one compatible and the rank-one line throughout $C(\{W_1, W_2\})$ is a supporting line of the two connected components of $A \setminus C(\{W_1, W_2\})$. The same affirmations on V_1 and V_2 holds for different connected components of B, and C with a similar argument. Next, we consider the remaining four possible cases.

Now, because $\{V_1, V_2\}$ is a rank-one compatible pair, if $V_1, V_2 \in A$, both belong to $\mathscr{C}_Q^-(W_1) \cap \mathscr{C}_Q^-(W_2)$ or $\mathscr{C}_Q^+(W_1) \cap \mathscr{C}_Q^+(W_2)$. Therefore, all wells in $\mathcal{U} = \{W_1, W_2, V_1, V_2\}$ are pairwise compatible and $L^e(\mathcal{U}) = C(\mathcal{U})$. If one of the wells in $\{V_1, V_2\}$ belongs to A and the other belongs to B, we obtain the same conclusion.

We assume the case when $V_1 \in A$ and $V_2 \in C$. Thus, W_1, W_2 , and V_2 belong all to $\mathscr{C}_Q(V_1)$'s upper or lower parts by definition of A (see Eq. (3.11)). Without loss of generality, we assume that $W_1, W_2, V_2 \in \mathscr{C}_Q^+(V_1)$, and let W_2 the furthest well in $\{W_1, W_2\}$ from V_1 . By construction, $W_2 = V_1 + (\xi, \eta)$, and $W_1 = V_1 + (\xi', \eta)$ for some $\xi \geq 0 \geq \eta$, and $\xi \geq \xi' \geq 0$, respectively. Now, we assume that $C(\{V_1, V_2\})$ and $C(\{W_1, W_2\})$ are non parallel segments, and $V_2 = V_1 + (0, \gamma)$ for some $\gamma \leq 0$. In this case, by computation, $U_0 = V_1 + (0, \eta)$ is such that $\det(U - U_0) \leq 0$ for every $U \in \{W_1, W_2, V_1, V_2\}$. Now, let $M \in C(\mathcal{U}) \setminus L^e(\mathcal{U})$. As a consequence of Theorem 3.7 and Proposition 2.13, $M \in \text{relint } C(\{W_2, U_0, V_2\}) \cup C(\{W_2, V_2\})$. Thus, $M = U_0 + (\alpha', \beta')$ for some $\beta' > 0 > \alpha'$ and $\det(M - U_0) < 0$. From Lemma 3.8 we conclude that $M \notin Q^e(\mathcal{U})$. If $C(\{V_1, V_2\})$ and $C(\{W_1, W_2\})$ are parallel segments, letting $U_0 = V_1 + (\xi, 0)$, we can repeat the argument to get the result.

Let V_1 and V_2 belong to B. By definition of B, V_1 and V_2 are compatible with only one of the wells W_1 or W_2 . The result follows by replacing wells $\{V_1, V_2\}$ with $\{W_1, W_2\}$ and arguing as in the previous paragraph.
Next, we assume that $V_1 \in B$ and $V_2 \in C$. By definition of B, only one wells in $\{W_1, W_2\}$ is compatible with V_1 , say W_1 . Then, we have that

$$\det(W_1 - W_2) = 0, \quad \det(W_2 - V_1) > 0, \quad \det(V_1 - W_1) \le 0, \\ \det(V_1 - V_2) = 0, \quad \det(V_2 - W_1) > 0, \quad \det(W_1 - V_1) \le 0.$$

$$(3.12)$$

Thus, by Theorem 3.7, $L^{e}(\mathcal{U}) = L^{e}(\{V_{2}, V_{1}, W_{1}\}) \cup L^{e}(\{V_{1}, W_{1}, W_{2}\})$, and by Proposition 2.13,

$$L^{e}(\{V_{2}, V_{1}, W_{1}\}) = C(\{U_{0}, V_{1}, W_{1}\}) \cup C(\{U_{0}, V_{2}\})$$

and

$$L^{e}(\{V_{1}, W_{1}, W_{2}\}) = C(\{U'_{0}, V_{1}, W_{1}\}) \cup C(\{U'_{0}, W_{2}\})$$

where $U_0 \in C(\{V_1, V_2\})$ and $U'_0 \in C(\{W_1, W_2\})$ are such that $\det(W_1 - U_0) = 0$ and $\det(V_1 - U'_0) = 0$, respectively. Hence, $C(\mathcal{U}) = L^e(\mathcal{U}) \cup L_1 \cup L_2$ where $L_1 =$ rel int $C(\{V_1, V_2, W_1\}) \cup C(\{V_2, W_1\})$ and $L_2 =$ rel int $C(\{V_1, W_1, W_2\}) \cup C(\{V_1, W_2\})$. By construction, every $M \in L_1$ and $N \in L_2$ satisfy that $\det(M - U_0) < 0$ and $\det(N - U'_0) < 0$. From last inequalities, Eq. (3.12), and Lemma 3.8, we conclude $M, N \notin Q^e(\mathcal{U})$ as claimed.



Figure 3.5 Figures (a) and (b) are two four-well configurations considered in step 1 where two wells are incompatible with the remaining pair

Assume $V_1, V_2 \in C$. Since D is disconnected, by Theorem 3.7, $L^e(\mathcal{U}) = D$. First, we assume that $C(\{V_1, V_2\})$ and $C(\{W_1, W_2\})$ are non parallel segments, see Fig. 3.5b. Let U_0 be the intersection point of the rank-one lines $\{tV_1 + (1-t)V_2 | t \in \mathbb{R}\}$ and $\{tW_1 + (1-t)W_2 | t \in \mathbb{R}\}$. We assume that $W_1 - U_0 = (\alpha, 0)$ and $V_1 - U_0 = (0, \beta)$ for some $\alpha, \beta \in \mathbb{R}$ such that $\alpha\beta < 0$, since V_1 and W_1 are incompatible. In this case $C(\mathcal{U}) \subset \{U_0 + t(W_1 - U_0) + s(V_1 - U_0) | t, s \in \mathbb{R}^+ \cup \{0\}\}$, see Fig. 3.5b. As before, we conclude that $\det(U - U_0) = 0$ for every $U \in \mathcal{U}$. Hence, if $M \in C(\mathcal{U}) \setminus D$, $\det(M - U_0) < 0$ and by Lemma 3.8, $M \notin Q^e(\mathcal{U})$.

Second, we assume that $C(\{V_1, V_2\})$ and $C(\{W_1, W_2\})$ are parallel segments, see Fig. 3.5a. Without loss of generality, let $V_2 = V_1 + (\xi, 0)$ for some $\xi \neq 0$ and let V_1, W_2 be the closest wells between $\{V_1, V_2\}$ and $\{W_1, W_2\}$, then $W_2 = V_1 + (\alpha, \beta)$ where $\alpha\beta > 0$ and $(\alpha - \xi)\beta > 0$ since $V_1, V_2 \in C$. Moreover, $W_1 = V_1 + (\alpha + \gamma, \beta)$ where $\gamma\alpha > 0$ since W_2 is closer to V_1 than W_1 . Now, let $U_0 = V_1 + (\alpha, 0)$ and $U'_0 = V_1 + (0, \beta)$. A calculation yields,

$$\det(U - U_0) \ge 0$$
, and $\det(U - U'_0) \ge 0$ (3.13)

for every $U \in \mathcal{U}$. If $M \in \operatorname{relint} \mathscr{C}^+_Q(U'_0) \setminus D$, $\det(M - U'_0) > 0$. Thus, last inequality, (3.13), and Lemma 3.8 yields $M \notin Q^e(\mathcal{U})$. Analogously, if $M \in \operatorname{relint} \mathscr{C}^-_Q(U_0) \setminus D$ then $\det(M - U_0) > 0$ and we conclude that $M \notin Q^e(\mathcal{U})$. Finally, we notice that

$$C(\{V_1, W_1, W_2\}) \subset \mathscr{C}_Q^+(U'_0) \text{ and } C(\{W_2, V_1, V_2\}) \subset \mathscr{C}_Q^-(U_0),$$

and $C(\mathcal{U}) = C(\{V_1, W_1, W_2\}) \cup C(\{W_2, V_1, V_2\})$. Hence, if $M \in C(\mathcal{U}) \setminus D$, then $M \notin Q^e(\mathcal{U})$ and the result follows.

STEP 2 We assume that the intersection of the sets $\{V_1, V_2\}$ and $\{W_1, W_2\}$ has only one element, say V, and D is contained either in the upper or in the lower part of $\mathscr{C}_Q(V)$ (Item 3 in Theorem 3.10). Let $\mathcal{U} = \{U_1, U_2, U_3, U_4\}$, assume $V = U_2, U_4 \notin \{V_1, V_2\} \cup$ $\{W_1, W_2\}$, and $D \subset \mathscr{C}_Q^+(U_2)$ (see Fig. 3.6). Thus, $U_1 = U_2 + (\alpha, 0), U_3 = U_2 + (0, \beta)$, and $U_4 = U_2 + (l, m)$ for some $\beta < 0 < \alpha$ and $l, m \in \mathbb{R}$. Notice that $U_4 \notin \mathscr{C}_Q^-(U_2)$, otherwise l < 0 < m and \mathcal{U} would be a wedge configuration. Now, we split $\Pi_Q \setminus \mathscr{C}_Q^-(U_2)$ into five regions by the rank-one lines passing through U_1, U_2 and U_3 , see Fig. 3.6. Namely, $\Pi_Q \setminus \mathscr{C}_Q^-(U_2) = A \cup B \cup C \cup D \cup E$, where

$$\begin{split} A &= \{ U \in \Pi_Q \setminus \mathscr{C}_Q^-(U_2) \, | \, U \in \mathscr{C}_Q^+(U_2) \cap \mathscr{C}_Q(U_1) \cap \mathscr{C}_Q(U_3) \} \\ B &= \{ U \in \Pi_Q \setminus \mathscr{C}_Q^-(U_2) \, | \, U \in \mathscr{C}_Q^+(U_2) \cap \mathscr{C}_Q(U_1) \triangle \mathscr{C}_Q(U_3) \} \\ C &= \{ U \in \Pi_Q \setminus \mathscr{C}_Q^-(U_2) \, | \, U \in \mathscr{C}_Q^c(U_2) \cap \mathscr{C}_Q(U_1) \triangle \mathscr{C}_Q(U_3) \} \\ D &= \{ U \in \Pi_Q \setminus \mathscr{C}_Q^-(U_2) \, | \, U \in \mathscr{C}_Q^+(U_2) \cap \mathscr{C}_Q^c(U_1) \cap \mathscr{C}_Q^c(U_3) \} \\ E &= \{ U \in \Pi_Q \setminus \mathscr{C}_Q^-(U_2) \, | \, U \in \mathscr{C}_Q^c(U_2) \cap \mathscr{C}_Q^c(U_1) \cap \mathscr{C}_Q^c(U_3) \} \end{split}$$

and every complement set operation considers $\Pi_Q \setminus \mathscr{C}_Q^-(U_2)$ as the universe.



Figure 3.6 This figure shows the splitting of Π_Q used in item 3.

Next, we explore U_4 's five different possibilities. If $U_4 \in A$, all wells are pairwise compatible and $L^e(\mathcal{U}) = Q^e(\mathcal{U}) = C(\mathcal{U})$ (see Remark 2.14). By hypothesis, $U_4 \notin E$ otherwise it will be incompatible with the remaining wells in \mathcal{U} .

Assume $U_4 \in B$, thus it is incompatible with either U_1 or U_3 . Without loss of generality, let $det(U_4 - U_3) > 0$, that is $l(m - \beta) > 0$. Hence by Theorem 3.7, $L^e(\mathcal{U}) = L^e(\{U_4, U_2, U_3\}) \cup L^e(\{U_4, U_2, U_1\})$. Also by Proposition 2.13, we accomplish that $L^e(\{U_4, U_2, U_1\}) = C(\{U_1, U_2, U_4\})$, and $L^e(\{U_4, U_2, U_3\}) = C(\{U_2, U_3\}) \cup U_3$.

 $C(\{U_4, U_2, U_0\})$. Here, $U_0 = U_2 + (0, m)$ for some $\beta \leq m \leq 0 < l$ is the flag's center of $\{U_2, U_3, U_4\}$. Thus, $\det(U - U_0) = 0$ for $U \in \{U_2, U_3, U_4\}$, and $\det(U_1 - U_0) = -\alpha m |a \times n|^2 \geq 0$ (see Remark 2.4).

Now, since $C(\mathcal{U}) = C(\{U_1, U_2, U_4\}) \cup C(\{U_2, U_3, U_4\})$ it follows that $C(\mathcal{U}) = L^e(\mathcal{U}) \cup L$, where

$$L = \{\lambda_1 U_0 + \lambda_2 U_4 + \lambda_3 U_3 \mid \lambda_1 \in [0, 1), \ \lambda_2, \lambda_3 \in (0, 1), \ \text{and} \ \lambda_1 + \lambda_2 + \lambda_3 = 1\}.$$

If $U \in L$, $U = U_0 + (\lambda_2 l, \lambda_3(\beta - m))$ for $\lambda_2, \lambda_3 \in (0, 1)$, and $\det(U - U_0) < 0$ by Remark 2.4. Therefore, by Lemma 3.8, $U \notin Q^e(\mathcal{U})$ as claimed.

Let $U_4 \in C$. Then, $\det(U_2 - U_4) > 0$ and without loss of generality, we assume $\det(U_4 - U_3) > 0 \ge \det(U_4 - U_1)$. By Theorem 3.7, we get $L^e(U) = L^e(\{U_1, U_2, U_3\}) \cup L^e(\{U_1, U_2, U_4\})$. Due to Proposition 2.13 and the compatibility relations among \mathcal{U} 's wells, we have that $L^e(\{U_1, U_2, U_3\}) = C(\{U_1, U_2\}) \cup C(\{U_2, U_3\})$ and $L^e(\{U_1, U_2, U_4\}) = C(\{U_0, U_1, U_4\}) \cup C(\{U_0, U_2\})$, where $U_0 \in C(\{U_1, U_2\})$ is the flag's center of $\{U_1, U_2, U_4\}$. Hence, $C(\mathcal{U}) = L^e(\mathcal{U}) \cup L_1 \cup L_2$, where

$$L_{1} = \{\lambda_{1}U_{1} + \lambda_{2}U_{2} + \lambda_{3}U_{3} | \lambda_{1}, \lambda_{3} \in (0, 1), \lambda_{2} \in [0, 1) \text{ and } \lambda_{1} + \lambda_{2} + \lambda_{3} = 1\}, L_{2} = \{\lambda_{1}U_{0} + \lambda_{2}U_{2} + \lambda_{3}U_{4} | \lambda_{2}, \lambda_{3} \in (0, 1), \lambda_{1} \in [0, 1) \text{ and } \lambda_{1} + \lambda_{2} + \lambda_{3} = 1\}.$$

If $M \in L_1$, then $M = U_2 + (\lambda_1 \alpha, \lambda_3 \beta)$, and $\det(U - U_2) = \lambda_1 \lambda_2 \alpha \beta |a \times n|^2 < 0$. Thus, recalling that $\det(U - U_2) \ge 0$ for every $U \in \mathcal{U}$, we get $M \notin Q^e(\mathcal{U})$ by Lemma 3.8. Now, if $M \in L_2$, we can prove by the same arguments that $\det(M - U_0) < 0$.

Finally, let $U_4 \in D$. In this case, U_4 is compatible only with U_2 , and, by Theorem 3.7, $L^e(\mathcal{U}) = L^e(\{U_2, U_3, U_4\}) \cup L^e(\{U_1, U_2, U_4\})$, and by Proposition 2.13,

$$L^{e}(\{U_{2}, U_{3}, U_{4}\}) = C(\{U_{0}, U_{2}, U_{4}\}) \cup C(\{U_{0}, U_{3}\}), \text{ and } L^{e}(\{U_{1}, U_{2}, U_{4}\}) = C(\{U_{0}', U_{2}, U_{4}\}) \cup C(\{U_{0}', U_{1}\}),$$

where $U_0 \in C(\{U_2, U_3\}), U'_0 \in C(\{U_1, U_2\})$, and $\det(U_4 - U_0) = \det(U_4 - U'_0) = 0$. It follows that $U_0 = U_2 + (0, m)$ and $U'_0 = U_2 + (l, 0)$ for some $l, m \in \mathbb{R}$ such that lm < 0. Due to the location of $U_4, C(\mathcal{U})$ is either a quadrilateral or a triangle. In the former case, $C(\mathcal{U}) = C(\{U_1, U_2, U_4\}) \cup C(\{U_2, U_3, U_4\})$, so $C(\mathcal{U}) = L^e(\mathcal{U}) \cup L_1 \cup L_2$, where

$$L_{1} = \{\theta_{0}U_{0} + \theta_{3}U_{3} + \theta_{4}U_{4} | \theta_{3}, \theta_{4} \in (0, 1), \theta_{0} \in [0, 1) \text{ and } \theta_{0} + \theta_{3} + \theta_{4} = 1\},\$$

$$L_{2} = \{\lambda_{1}U_{1} + \lambda_{0}U_{0}' + \lambda_{4}U_{4} | \lambda_{1}, \lambda_{4} \in (0, 1), \lambda_{0} \in [0, 1) \text{ and } \lambda_{0} + \lambda_{1} + \lambda_{4} = 1\}.$$

If $M \in L_1$, then $\det(M - U'_0) < 0$ since $M = U'_0 + (\lambda_1(\alpha - l), \lambda_4 m)$ and $m(\alpha - l) < 0$, due to the incompatibility between U_4 and U_1 . Thus, by Lemma 3.8, $L_1 \cap Q^e(\mathcal{U}) = \emptyset$. The same result follows for $U \in L_2$ by a similar argument.

Now we assume that C(U) is a triangle, hence $U_4 \in C(\{U_1, U_2, U_3\})$. As before, we let $U_0 = U_2 + (0, m)$ and $U'_0 = U_2 + (l, 0)$, and we define $U'_1, U'_3 \in C(\{U_1, U_3\})$ such that $U'_1 = U_2 + (t, m)$ and $U'_3 = U_2 + (l, s)$ for some $t, s \in \mathbb{R}$, see Fig. 3.7. By construction, it

follows that $C(\mathcal{U}) \subset L^e(\mathcal{U}) \cup \tilde{L}_1 \cup \tilde{L}_2$, where

$$\tilde{L}_1 = \{\theta_0 U_0 + \theta_1 U_1' + \theta_3 U_3 \mid \theta_1, \theta_3 \in (0, 1), \theta_0 \in [0, 1) \text{ and } \theta_0 + \theta_1 + \theta_3 = 1\},\$$

$$L_2 = \left\{ \lambda_0 U_0' + \lambda_1 U_1 + \lambda_3 U_3' \,|\, \lambda_1, \lambda_3 \in (0, 1), \lambda_0 \in [0, 1) \text{ and } \lambda_0 + \lambda_1 + \lambda_3 = 1 \right\}.$$

The result follows as in the quadrilateral case by replacing U_4 with U'_1 and U_4 by U'_3 in the sets L_1 , and L_2 , respectively.



Figure 3.7 This figure shows a four-well configuration considered in step 2, when $U_4 \in D$ and $C(\mathcal{U})$ is a triangle.

STEP 3: We assume D is a connected set and $\mathcal{U} \subset D$ (Item 2 in Theorem 3.10). In this case, the rank-one segments $C(\{V_1, V_2\})$ and $C(\{W_1, W_2\})$ intersects at a point, say U_0 . Without loss of generality, assume that $U_0 = W_1 + (-\alpha, 0)$ for some $\alpha > 0$. Hence, by Lemma 2.5, we get

$$W_1 = U_0 + (\alpha, 0), \quad W_2 = U_0 + (\beta, 0), \quad V_1 = U_0 + (0, \gamma), \text{ and } V_2 = U_0 + (0, \eta)$$

where $\alpha\beta \leq 0$ and $\gamma\eta \leq 0$. Due to Remark 2.4 we conclude that W_1 is compatible with either V_1 or V_2 . Assume $\det(W_1 - V_1) \leq 0$ and $\det(W_2 - V_2) \leq 0$, then $L^e(\mathcal{U}) = L^e(\{W_1, W_2, V_1\}) \cup L^e(\{W_1, W_2, V_2\})$ by Theorem 3.7. Moreover, from Proposition 2.13, $L^e(\{W_1, W_2, V_1\}) = C(\{W_1, V_1, U_0\}) \cup C(\{W_2, U_0\})$ and $L^e(\{W_1, W_2, V_2\}) = C(\{W_2, V_2, U_0\}) \cup C(\{W_1, U_0\})$. Thus, $C(\mathcal{U}) = L^e(\mathcal{U}) \cup L_1 \cup L_2$ where

$$L_1 = \{\theta_0 U_0 + \theta_1 V_1 + \theta_3 W_2 \mid \theta_1, \theta_3 \in (0, 1), \theta_0 \in [0, 1) \text{ and } \theta_0 + \theta_1 + \theta_3 = 1\}, \text{ and}$$

$$L_{2} = \{\lambda_{0}U_{0} + \lambda_{1}W_{1} + \lambda_{3}V_{2} \mid \lambda_{1}, \lambda_{3} \in (0, 1), \lambda_{0} \in [0, 1) \text{ and } \lambda_{0} + \lambda_{1} + \lambda_{3} = 1\}$$

As before, a calculation yields $\det(U - U_0) < 0$ for every $U \in L_1 \cup L_2$, but $\det(V - U_0) = 0$ for all $V \in \mathcal{U}$. Therefore, $(L_1 \cup L_2) \cap Q^e(\mathcal{U}) = \emptyset$ and the result follows.

As we have considered all admissible configurations, this concludes the theorem's proof. $\hfill\blacksquare$

3.2.2 The *n*-Well Problem (Basic Configurations)

In this final section, we prove that if \mathcal{U} is a finite coplanar set of wells in a basic configuration (see Definition 3.12), then $Q^e(\mathcal{U}) = L^e(\mathcal{U})$, see Theorem 3.16. Here, we also

warn the reader that we frequently use the notation introduced in Remark 3.2 throughout the proof. We begin this subsection by formalizing two definitions given in Section 1.2.

Definition 3.11. We say that set of wells $\mathcal{U} \subset \mathbb{R}^{2 \times 2}_{sym}$ is a *basic block* if

- 1. either \mathcal{U} is a three-well set if it has one compatible, one rank-one compatible, and one incompatible pair of wells,
- 2. or \mathcal{U} is a four-well set that satisfies the condition 2 in Theorem 3.10.

It is readily seen that in each basic block, the segment that joins a rank-one pair of wells contains a well U_0 that is rank-one compatible with any other element in the basic block, see Fig. 3.8. We called U_0 the *basic block's center*. By Theorem 2.24 and Theorem 3.10, if \mathcal{U} is a basic block, then $Q^e(\mathcal{U}) = L^e(\mathcal{U})$.



Figure 3.8 displays the five basic block configurations. Green dots represent the wells in \mathcal{U} while red dots represent the center of each basic block. Blue lines between two wells means compatibility between them and the union of yellow region and blue lines depict $L^e(\mathcal{U})$. To keep figures simple we assume that the angle between $a^{\perp} \otimes a^{\perp}$ and $n^{\perp} \otimes n^{\perp}$ directions is $\pi/2$.

The basic blocks can be stuck together to get other configurations with more than three wells.

Definition 3.12. We say \mathcal{U} is a *basic configuration* if (a) there are no more than two collinear wells in the set, (b) $\mathcal{U} = \mathcal{U}_1 \cup \cdots \cup \mathcal{U}_n$, where \mathcal{U}_i is a basic block for every $i = 1, 2, \cdots, n$, and (c) $\mathcal{U}_i \cap \mathcal{U}_{i+1} = \{V_i, W_i\}$ with $\det(V_i - W_i) < 0$ for every i < n.

In Fig. 1.10 we show some examples of basic configurations. The following lemma characterizes basic configurations in terms of the basis $\{a^{\perp} \otimes a^{\perp}, n^{\perp} \otimes n^{\perp}\}$. Also it states that there are, at most, two three-wells basic blocks in any basic configuration, and these three-well basic blocks appear only as the first one or the last one in \mathcal{U} .

Lemma 3.13. A finite coplanar set \mathcal{U} is a basic configuration made of n basic blocks if and only if there exist $M_0 \in \Pi_Q$, and α_i, β_i for $i = 1, 2, \dots n + 1$ positive constants such that if

$$V_{i} = M_{0} + \sum_{j < i} (\alpha_{j}, \beta_{j}) + (\alpha_{i}, 0), \quad and \quad W_{i} = M_{0} + \sum_{j < i} (\alpha_{j}, \beta_{j}) + (0, \beta_{i}), \quad (3.14)$$

then
$$\left(\bigcup_{i=1}^{n+1} \{V_i, W_i\}\right) \setminus \mathcal{U} \subset \{A, B\}$$
, where $A \in \{V_1, W_1\}$ and $B \in \{V_{n+1}, W_{n+1}\}$.

Remark 3.14. We emphasize that $\bigcup_{i=1}^{n+1} \{V_i, W_i\}$ can be equal to \mathcal{U} , or their set difference has at most two wells.

Proof. We assume \mathcal{U} is a basic configuration to prove the result by induction on the number of basic blocks in \mathcal{U} . The induction's base is for n = 1. Let \mathcal{U} be a basic block with center at $U_0 = (0,0)$ (see Fig. 1.9a and Fig. 1.9b). First, we assume that \mathcal{U} is a four-well basic block. Since all wells in \mathcal{U} are rank-one compatible with U_0 , by Lemma 2.5, $\mathcal{U} = \{(\alpha, 0), (0, \beta), (\alpha', 0), (0, \beta')\}$ for some $\alpha > 0 > \alpha'$ and $\beta > 0 > \beta'$. By letting

$$M_0 = (\alpha', \beta'), \quad V_1 = (0, \beta'), \quad W_1 = (\alpha', 0), \quad V_2 = (\alpha, 0), \text{ and } W_2 = (0, \beta),$$

we have that $\mathcal{U} = \{V_1, W_1, V_2, W_2\}$, and Eq. (3.14) holds for the positive constants $\alpha_1 = -\alpha', \beta_1 = -\beta', \alpha_2 = \alpha$ and $\beta_2 = \beta$. Second, assume \mathcal{U} is a three-well basic block. Since all wells in \mathcal{U} are rank one compatible with the flag's center $U_0 = (0, 0)$, we have that $\mathcal{U} = \{(\alpha, 0), (0, \beta), \alpha'(\chi, 1 - \chi)\}$, for some $\chi \in \{0, 1\}$ and, $\alpha\beta > 0 > \alpha\alpha'$. Next, if β' is such that $\beta\beta' < 0$, then the set $\mathcal{U}' = \mathcal{U} \cup \{\beta'(1 - \chi, \chi)\}$ is a four-well basic block. Now, the result follows by the above argument for the four-well case.

For the induction step, we assume that the result holds for every basic configuration made of n basic blocks and we will prove that it is still valid for a basic configuration \mathcal{U} with n + 1 basic blocks. Indeed $\mathcal{U} = \mathcal{U}' \cup \mathcal{U}_{n+1}$, where \mathcal{U}' is a n basic block configuration. Thus, by the induction hypothesis, $\bigcup_{i=1}^{n+1} \{V_i, W_i\} \setminus \mathcal{U}' \subset \{A, B\}$. By construction, the set \mathcal{U}_n has two adjacent basic blocks, $(\mathcal{U}_{n-1} \text{ and } \mathcal{U}_{n+1})$, and it has two different compatible, but not rank-one compatible, pairs of wells. Since, only four-well basic block has this property, we have that $\bigcup_{i=1}^{n+1} \{V_i, W_i\} \setminus \mathcal{U}' \subset \{A\}$.

Next, since no more than two wells in \mathcal{U} are collinear, \mathcal{U}_{n+1} is either a four-well or three-well basic block. In the former case, the set $\mathcal{U}_{n+1} = \{V_{n+1}, W_{n+1}, V_{n+2}, W_{n+2}\}$ where V_{n+1} , W_{n+1} satisfies Eq. (3.14) and

$$V_{n+2} = \sum_{i=1}^{n+1} (\alpha_i, \beta_i) + (\alpha_{n+2}, 0), \text{ and } W_{n+2} = \sum_{i=1}^{n+1} (\alpha_i, \beta_i) + (0, \beta_{n+2})$$

for some positive α_{n+2} and β_{n+2} as claimed. If \mathcal{U}_{n+1} is a three-well basic block, then $\mathcal{U}_{n+1} = M_0^{n+1} + \{(-\alpha_{n+1}, 0), (0, -\beta_{n+1}), \alpha'(\chi, 1-\chi)\}$ with $\alpha' > 0$ and $M_0^{n+1} = \sum_{i=1}^{n+1} (\alpha_i, \beta_i)$. As in the proof of the induction basis, we complete the set \mathcal{U}_{n+1} to form a four-well basic

As in the proof of the induction basis, we complete the set \mathcal{U}_{n+1} to form a four-well basic block, and we conclude by the four-well case.

Notice that if we prove that $\mathcal{U}_i = \{V_i, W_i, V_{i+1}, W_{i+1}\}$ is a basic block for $i = 1, 2, 3, \dots, n$, the reverse implication, namely $\bigcup_{i=1}^{n+1} \{V_i, W_i\} \setminus \mathcal{A}$ is a basic configuration for each set $\mathcal{A} \subset \{A, B\}$, follows straight forward since $\mathcal{U}_1 \setminus \{A\}$ and $\mathcal{U}_n \setminus \{B\}$ also are three-well basic blocks.

Hence, we prove that \mathcal{U}_i is a basic block for $i = 1, 2, 3, \cdots, n$. Indeed, since $W_{i+1} - V_i = (0, \beta_i + \beta_{i+1})$ and $V_{i+1} - W_i = (\alpha_i + \alpha_{i+1}, 0)$, see Eq. (3.14), we have that $\{V_i, W_{i+1}\}$ and $\{V_{i+1}, W_i\}$ are both rank-one compatible pairs. Moreover, the well $M_0 + \sum_{i \in I} (\alpha_i, \beta_i)$

belongs to both $C(\{V_i, W_{i+1}\})$ and $C(\{V_{i+1}, W_i\})$. Hence, \mathcal{U}_i satisfies the conditions of Item 2 Theorem 3.10, and it is a four-well basic block and the proof is complete.

Lemma 3.15. Let \mathcal{U} be a basic configuration such that $\mathcal{U} = \bigcup_{i=1}^{n} \mathcal{U}_{i}$ where \mathcal{U}_{i} is a basic block for every $i = 1, 2, \dots, n$. Then there exist two compatible wells $P_{1}, Q_{1} \in \mathcal{U}_{1}$, and two compatible wells $P_{n}, Q_{n} \in \mathcal{U}_{n}$ such that $\operatorname{Aff}(\{P_{1}, Q_{1}\})$ and $\operatorname{Aff}(\{P_{n}, Q_{n}\})$ are two supporting lines of $C(\mathcal{U})$.

Proof. To keep the proof simple, let $M_0 = 0$. We know that $\mathcal{A} = \bigcup_{i=1}^{n+1} \{V_i, W_i\} \setminus \mathcal{U}$ is empty or it has at most two elements. We assume either $\mathcal{A} = \{A\}$ or $\mathcal{A} = \emptyset$. In the latter case, we let $(P_1, Q_1) = (V_1, W_1)$, and define the linear functional $\ell(U) := \nu_1 \alpha + \nu_2 \beta$, where $\nu_1 = 1/\alpha_1, \nu_2 = 1/\beta_1$, and $U = (\alpha, \beta)$. Thus,

$$C(\{P_1, Q_1\}) \subset \operatorname{Aff}(\{P_1, Q_1\}) = \{U \in \Pi_Q \,|\, \ell(U) = 1\}.$$

Next, since every α_i, β_i in (3.14) are positive numbers,

$$1 = \ell(V_1) \le \ell(V_i), \text{ and } 1 = \ell(W_1) \le \ell(W_i),$$
 (3.15)

for $i = 1, 2, \dots, n + 1$. Thus, all wells in \mathcal{U} are on one side of the line $\ell(U) = 1$, and $\operatorname{Aff}(\{P_1, Q_1\})$ is a supporting line of $C(\mathcal{U})$. Assuming $\mathcal{A} = \{A\}$, we have two further cases, either $A = V_1$ or $A = W_1$. We let $(P_1, Q_1) = (V_2, W_1)$ with $\nu_1 = 0$, $\nu_2 = 1/\beta_1$ and $(P_1, Q_1) = (V_1, W_2)$ with $\nu_1 = 1/\alpha_1$, $\nu_2 = 0$, respectively. Now the proof follows exactly as above.

In the case of $\mathcal{A} = \emptyset$, we also let $(P_n, Q_n) = (V_{n+1}, W_{n+1})$ and $\tilde{\ell}(U) = \tilde{\nu}_1 \alpha + \tilde{\nu}_2 \beta$ with $\tilde{\nu}_1 = \beta_{n+1}/\kappa$ and $\tilde{\nu}_2 = \alpha_{n+1}/\kappa$, where $\kappa = \alpha_{n+1}\beta_{n+1} + \sum_{i=1}^n \alpha_{n+1}\beta_i + \beta_{n+1}\alpha_i$. Thus,

$$C(\{P_n, Q_n\}) \subset \operatorname{Aff}(\{P_n, Q_n\}) = \{U \in \Pi_Q \,|\, \tilde{\ell}(U) = 1\},\$$

and

$$\tilde{\ell}(V_i) \le \tilde{\ell}(V_n) = 1$$
, and $\tilde{\ell}(W_i) \le \tilde{\ell}(W_n) = 1$, (3.16)

for $i = 1, 2, \dots, n + 1$. Arguing as before, we find that $\operatorname{Aff}(\{P_n, Q_n\})$ is a supporting line of $C(\mathcal{U})$. Assuming $\mathcal{A} = \{B\}$, we have two cases, either $B = V_{n+1}$ or $B = W_{n+1}$. If

 $B = V_{n+1}$, we let $(P_n, Q_n) = (V_n, W_{n+1})$ with $\tilde{\nu}_1 = 1/\sum_{j \le n} \alpha_j$ and $\tilde{\nu}_2 = 0$. If $B = W_{n+1}$, then we let $(P_n, Q_n) = (V_{n+1}, W_n)$ with $\tilde{\nu}_1 = 0$ and $\tilde{\nu}_2 = 1/\sum_{j \le n} \beta_j$. In both cases the result follows as before. Finally, the case $\mathcal{A} = \{A, B\}$ follows as combination of above cases, and the proof is concluded.

Theorem 3.16 (Basic configurations). Let $\mathcal{U} \subset \mathbb{R}^{2\times 2}_{sym}$ be a finite coplanar set of wells. If \mathcal{U} is a basic configuration, then $L^{e}(\mathcal{U}) = Q^{e}(\mathcal{U})$.

Proof of Theorem 3.16. Since \mathcal{U} is a basic configuration, $\mathcal{U} \subset \bigcup_{i=1}^{n+1} \{V_i, W_i\}$ for V_i and W_i given by Eq. (3.14) in Lemma 3.13. Let α_i, β_i for $i = 1, 2, \dots, n+1$ be the corresponding positive constants, and let

$$U_0^i := M_0 + \sum_{j \le i} (\alpha_j, \beta_j) \text{ for } i \in \{1, \dots, n\}.$$
(3.17)

First, we claim that $\det(U - U_0^i) \ge 0$ for every $U \in \mathcal{U}$. Indeed, by Eq. (3.14),

$$U_0^i - V_k = \left(\sum_{j \le i} \alpha_j - \sum_{j \le k} \alpha_j, \sum_{j \le i} \beta_j - \sum_{j < k} \beta_j\right) = \begin{cases} \sum_{k < j \le i} (\alpha_j, \beta_j) & \text{if } k < j, \\ (0, \beta_k) & \text{if } k = j, \\ -\sum_{i < j \le k} (\alpha_j, \beta_j) & \text{if } k < j, \end{cases}$$

and

$$U_0^i - W_k = \left(\sum_{j \le i} \alpha_j - \sum_{j < k} \alpha_j, \sum_{j \le i} \beta_j - \sum_{j \le k} \beta_j\right) = \begin{cases} \sum_{k \le j \le i} (\alpha_j, \beta_j) & \text{if } k < j, \\ (\alpha_k, 0) & \text{if } k = j, \\ -\sum_{i < j < k} (\alpha_j, \beta_j) & \text{if } k < j. \end{cases}$$

Hence, $\det(U_0^i - V_k) \ge 0$ and $\det(U_0^i - W_k) \ge 0$ for every $i \in \{1, 2, \dots, n\}$ and $k \in \{1, 2, \dots, n+1\}$ by Remark 2.4, and the claim follows.

Second, we show next that if $U \in C(\mathcal{U})$ and it does not belong to the lamination convex hull of any basic block, then $U \notin Q^e(\mathcal{U})$. If \mathcal{U}_i for i = 0, ..., n are the basic blocks of $\mathcal{U} = \bigcup_{i=1}^n \mathcal{U}_i$, then,

$$\bigcup_{i=1}^{n} L^{e}(\mathcal{U}_{i}) \subset L^{e}(\mathcal{U}) \subset Q^{e}(\mathcal{U}) \subset C(\mathcal{U}) \subset \Pi_{Q}.$$
(3.18)

Now, we assume that $U \in C(\mathcal{U}) \setminus \bigcup_{i=1}^{n} L^{e}(\mathcal{U}_{i}) = \bigcap_{i=1}^{n} (C(\mathcal{U}) \setminus L^{e}(\mathcal{U}_{i}))$. For the sets in the latter intersection we have

$$C(\mathcal{U}) \setminus L^{e}(\mathcal{U}_{i}) = \mathcal{A}_{i} \cup \mathcal{B}_{i}, \text{ with } \qquad \begin{array}{l} \mathcal{A}_{i} = \{U \in C(\mathcal{U}) \mid \det(U - U_{0}^{i}) < 0\}, \\ \mathcal{B}_{i} = \{U \in C(\mathcal{U}) \mid \det(U - U_{0}^{i}) \geq 0, U \notin L^{e}(\mathcal{U}_{i})\}, \end{array}$$

where $U_0^i \in C(\mathcal{U}_i)$ (see (3.17)) is the center of the basic block \mathcal{U}_i . We claim that $\bigcap_{i=1}^n \mathcal{B}_i = \emptyset$. Assuming the claim, by simple algebra, we have that

$$\bigcap_{i=1}^{n} \left(C(\mathcal{U}) \setminus L^{e}(\mathcal{U}_{i}) \right) = \bigcup_{i=1}^{n} \left(\bigcap_{j=1}^{i} \mathcal{A}_{j} \bigcap_{k>i}^{n} \mathcal{B}_{k} \right).$$

Thus, there exists $i \in \{1, 2, \dots, n\}$ such that $\det(U - U_0^i) < 0$. Hence, by the first claim and Lemma 3.8, the result follows and the proof is complete.

Finally, we prove the claim. By Lemma 3.15 there exist two compatible wells $P_1, Q_1 \in \mathcal{U}_1$, and another pair of compatible wells $P_n, Q_n \in \mathcal{U}_n$ such that $\operatorname{Aff}\{P_1, Q_1\}$ and $\operatorname{Aff}\{P_n, Q_n\}$ are two supporting lines of $C(\mathcal{U}) \supset \bigcup_{i=1}^n L^e(\mathcal{U}_i)$. Equivalently, there exist two linear functionals $\ell, \tilde{\ell} : \Pi_Q \to \mathbb{R}$, see Eq. (3.15) and Eq. (3.16), such that $\ell(P_1) \leq \ell(U)$ and $\tilde{\ell}(U) \leq \tilde{\ell}(P_n)$ for every $U \in C(\mathcal{U})$.

By contradiction, if $U \in \bigcap_{i=1}^{n} \mathcal{B}_{i} \neq \emptyset$, then $U = U_{0}^{i} + (\gamma_{i}, \delta_{i})$ for some $\gamma_{i}\delta_{i} \geq 0$, and $U \notin L^{e}(\mathcal{U}_{i})$ for every $i = 1, 2, \cdots, n$. Now, we have two options: (a) $U \notin L^{e}(\mathcal{U}_{n})$ and $U = U_{0}^{n} + (\gamma_{n}, \delta_{n})$ for some $\gamma_{n} \geq 0$ and $\delta_{n} \geq 0$ or (b) $U \notin L^{e}(\mathcal{U}_{1})$ and $U = U_{0}^{1} + (\gamma_{1}, \delta_{1})$ for some $\gamma_{1} \leq 0$ and $\delta_{1} \leq 0$. Since $\mathcal{A}_{1} \cap \mathcal{B}_{1} = \emptyset$, $\mathcal{A}_{n} \cap \mathcal{B}_{n} = \emptyset$, and \mathcal{U} is a basic configuration, we conclude that $\ell(U) < \ell(P_{1})$ and $\tilde{\ell}(U) > \tilde{\ell}(P_{n})$ in cases (a) and (b), respectively. So we get a contradict to $U \in C(\mathcal{U})$ and the claim is proved.

3.3 Explicit Examples

Four Wells Example

Let $\mathcal{U} = \{U_1, U_2, U_3, U_4\}$ where

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}, \quad U_3 = \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix}, \text{ and } U_4 = \begin{pmatrix} -2 & 0 \\ 0 & 1 \end{pmatrix}.$$
 (3.19)

By a direct computation, we have that $\langle Q, U_i \rangle = 0$ for every $i = 1, 2, \dots, 4$ where

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sqrt{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \odot \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$



Figure 3.9 The wells U_1, \dots, U_4 , are represented with green dots, solid blue lines are compatible segments and dashed lines represent rank-one compatible segments. The auxiliary wells U_0 and U'_0 are represented with red dots.

Hence, $Q = \nu n \odot a$, with $n = (1, 0)^T$ and $a = (0, 1)^T$, and the set Π_Q contains the origin. The rank-one directions that determine this set are given by,

$$n^{\perp} \odot n^{\perp} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
, and $a^{\perp} \odot a^{\perp} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$.

Since $\langle n^{\perp} \odot n^{\perp}, a^{\perp} \odot a^{\perp} \rangle = 0$, the rank-one lines spanned by each of these matrices make an angle of $\pi/2$. By Lemma 2.5, $V \in \Pi_Q$ and U_i are compatible if and only if $V = U_i + \text{diag}(a, b)$, with $ab \leq 0$, see Fig. 3.9a. It follows that U_2 is compatible with U_1 and U_4 , also U_4 and U_3 are also compatible, see Fig. 3.9b. Now, let

$$\mathcal{F} = \{\{U_1, U_2, U_3\}, \{U_1, U_3, U_4\}, \{U_1, U_2, U_4\}, \{U_2, U_3, U_4\}\}$$

Since inside the first and second sets, only a pair of wells are compatible, from Proposition 2.13, it follows that

$$L^{e}(\{U_{1}, U_{2}, U_{3}\}) = \{U_{3}\} \cup C(\{U_{1}, U_{2}\}), \text{ and } L^{e}(\{U_{1}, U_{3}, U_{4}\}) = \{U_{1}\} \cup C(\{U_{3}, U_{4}\}).$$

For the two remaining sets in \mathcal{F} , we have two compatibility relations inside each three-well set. Hence, by Proposition 2.13, it follows that

$$L^{e}(\{U_{1}, U_{2}, U_{4}\}) = C(\{U_{0}, U_{2}, U_{4}\}) \cup C(\{U_{1}, U_{2}, U_{0}\}),$$

$$L^{e}(\{U_{2}, U_{3}, U_{4}\}) = C(\{U_{0}', U_{2}, U_{4}\}) \cup C(\{U_{4}, U_{3}, U_{0}'\}),$$

where $U_0 = \text{Id} \in C(\{U_1, U_2, U_4\})$ and $U'_0 = -\text{Id} \in C(\{U_2, U_3, U_4\})$ are the solutions of

$$\det(U_1 - U_0) = \det(U_4 - U_0) = 0, \text{ and } \det(U_3 - U_0') = \det(U_2 - U_0') = 0.$$

Now, we notice that there are only one compatible pair in $\{U_1, U_2, U_3\}$ and $\{U_1, U_3, U_4\}$ within each set, but $\{U_1, U_2, U_4\}$ and $\{U_2, U_3, U_4\}$, have two compatible pairs within each set. Therefore, $L^{e,1}(\{U_1, U_2, U_3\}) \cup L^{e,1}(\{U_1, U_3, U_4\}) \subset L^{e,1}(\{U_1, U_2, U_4\}) \cup L^{e,1}(\{U_2, U_3, U_4\})$ and in turns, $L^e(\{U_1, U_2, U_3\}) \cup L^e(\{U_1, U_3, U_4\}) \subset L^e(\{U_1, U_2, U_4\}) \cup L^e(\{U_2, U_3, U_4\})$. Hence, by Theorem 3.7, the symmetric lamination convex hull of the set \mathcal{U} , see Fig. 3.9b, is

$$L^{e}(\mathcal{U}) = C(\{U'_{0}, U_{2}, U_{4}\}) \cup C(\{U_{4}, U_{3}, U'_{0}\}) \cup C(\{U'_{0}, U_{2}, U_{4}\}) \cup C(\{U_{4}, U_{3}, U'_{0}\}).$$
(3.20)

A Degenerated Four-Well Example

We consider a *degenerate* case of the previous four-well problem. Let $\mathcal{U} = \{U_1, U'_2, U_3, U'_4\}$ such that U_1 and U_3 are as in Eq. (3.19) and

$$U_2' = \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}$$
, and $U_4' = \begin{pmatrix} -1 & 0\\ 0 & 1 \end{pmatrix}$.

In this case Q, a, n, U_0 and U'_0 are as in the previous example. Thus, $L^e(\mathcal{U})$ is as



Figure 3.10 A four-well configuration where two pairs of wells are rank-one compatible. Here $Q^e(\mathcal{U}) = L^e(\mathcal{U})$ and both sets are strictly contained in $C(\mathcal{U})$

in Eq. (3.20) with U_2 and U_4 replaced by U'_2 and U'_4 , respectively. This four-well set satisfies the conditions of Item 1 in Theorem 3.10 and $Q^e(\mathcal{U}) = L^e(\mathcal{U})$. Notice that this configuration is the union of two flag configurations, see Fig. 3.10.

Five Wells Example

Now we consider a five-well problem. Let $\mathcal{U} = \{U_1, \dots, U_5\}$ where

$$U_{1} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}, \quad U_{2} = \begin{pmatrix} 1 & 1 \\ 1 & 5 \end{pmatrix}, \quad U_{3} = \begin{pmatrix} 2 & 2 \\ 2 & 6 \end{pmatrix},$$

$$U_{4} = \begin{pmatrix} 3 & 3 \\ 3 & 3 \end{pmatrix}, \quad \text{and} \quad U_{5} = \begin{pmatrix} 2 & 2 \\ 2 & 0 \end{pmatrix}$$
(3.21)

By direct computation, we have that $\langle Q, U_i \rangle = 0$ for every i = 1, 2, 3, 4, where

$$Q = \frac{1}{\sqrt{6}} \begin{pmatrix} 2 & -1 \\ -1 & 0 \end{pmatrix}.$$

Hence, \mathcal{U} is coplanar and the plane Π_Q is well defined. Due to Lemma 2.3 and det Q < 0, we have that $Q = \nu a \odot n$, where ν is a real number and $a, n \in S^1$. Notice that these vectors are linear combinations of the eigenvectors of Q, thus

$$a = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}, \quad n = \begin{pmatrix} 1\\0 \end{pmatrix} \quad \text{and} \quad a^{\perp} \otimes a^{\perp} = \frac{1}{2} \begin{pmatrix} 1&1\\1&1 \end{pmatrix}, \quad n^{\perp} \otimes n^{\perp} = \begin{pmatrix} 0&0\\0&1 \end{pmatrix}. \quad (3.22)$$





(a) The planar compatible cone $\mathscr{C}_Q(U_i)$.

(b) A five-well configuration. The set $L^e(\{U_1, \dots, U_4\})$ is the yellow region.

Figure 3.11 The five-well example. The wells U_1, \dots, U_5 , are represented with green dots, solid blue lines are compatible segments and dashed lines represent rank-one compatible segments. The auxiliary wells U_0 and U'_0 are represented with red dots.

In this case $\langle a^{\perp} \otimes a^{\perp}, n^{\perp} \otimes n^{\perp} \rangle = 1/2$, and the angle between the rank-one lines generated by those matrices is $\pi/3$, see Fig. 3.11a. Arguing as in the previous example, we conclude that

$$L^{e}(\mathcal{U}) = L^{e}(\{U_{1}, U_{2}, U_{5}\}) \cup L^{e}(\{U_{2}, U_{3}, U_{4}\}) \cup L^{e}(\{U_{2}, U_{4}, U_{5}\}).$$

Moreover, by the compatibility relations among the wells, see Fig. 3.11b, we get

$$L^{e}(\{U_{1}, U_{2}, U_{5}\}) = C(\{U_{0}, U_{1}, U_{5}\}) \cup C(\{U_{0}, U_{5}, U_{2}\}),$$

$$L^{e}(\{U_{2}, U_{4}, U_{5}\}) = C(\{U_{2}, U_{4}, U_{0}'\}) \cup C(\{U_{2}, U_{0}', U_{5}\}),$$

$$L^{e}(\{U_{2}, U_{3}, U_{4}\}) = C(\{U_{2}, U_{3}, U_{4}\}),$$

where $U_0 \in C(\{U_1, U_2, U_5\})$ and $U'_0 \in C(\{U_2, U_4, U_5\})$ are the solutions of (see Fig. 3.11b),

det
$$(U_1 - U_0) = \det (U_2 - U_0) = 0$$
, and det $(U_4 - U_0') = \det (U_5 - U_0') = 0$.

Chapter 4 Rigidity in Flag Configurations

In this chapter we study rigidity of configurations in the three-well problem. We present two main results. First, we show that the existence of triple junctions is conditioned to a very restrictive statement, namely, the set $\mathcal{U} = \{U_0, U_1, U_2\}$, such that $\operatorname{Aff}(\mathcal{U})$ has codimension is one, admits a triple junction if and only if $\operatorname{Aff}(\mathcal{U})$ is tangent to the cone \mathcal{C}_{U_0} . Second, we prove that if \mathcal{U} has a flag configuration (see Theorem 2.24), and there exists $u \in W^{1,\infty}(\Omega, \mathbb{R}^2)$ such that the level sets of $e(Du) \in \mathcal{U}$ are union of finitely many polygons, then u locally is a simple lamination with deviations near the boundary.

4.1 Triple Junctions and the Invertibility of Q

From now on, we assume that the set of wells \mathcal{U} consists of three linearly independent wells. The simplest non-trivial (namely constant or simple laminate) case corresponds to triple junctions, more precisely:

Definition 4.1. Let $\{M_0, M_1, M_2\} \subset \mathbb{R}^{2 \times 2}$ be such that the their symmetric parts $e(M_0), e(M_1)$ and $e(M_2)$ are linearly independent and assume they are pairwise compatible matrices, that is,

$$M_i - M_{i+1} + \mu_{i+2}R = a^{i+2} \otimes (n^{i+2})^{\perp} \quad i \in \mathbb{N} \cup \{0\} \text{ mod } 3$$

$$(4.1)$$

for some $n^0, n^1, n^2 \in S^1$ and $a^0, a^1, a^2 \in \mathbb{R}^2$. We say that $\{M_0, M_1, M_2\}$ admits a *triple junction* if and only if

$$a^{0} \otimes (n^{0})^{\perp} + a^{1} \otimes (n^{1})^{\perp} + a^{2} \otimes (n^{2})^{\perp} = 0.$$
(4.2)

It is well-known [21] that in the case of three pairwise compatible wells, triple junctions do not exist under the assumption that $Tr(M_1) = Tr(M_2) = Tr(M_3)$. Despite being a natural condition corresponding to the incompressibility assumption in linear elasticity, there are cases where this condition does not necessarily hold. For instance, we may obtain a two-dimensional linear elasticity model by taking a thin-film limit in nonlinear elasticity as in [6] and then consider the small deformation regime. In this procedure, the limiting energy-wells depend on the film's normal direction and, in general, do not satisfy the incompressibility assumption. For some particular normal directions, we can show the existence of triple junctions.

We begin by giving an account of some properties of triple junctions.

Lemma 4.2. Let $\{M_0, M_1, M_2\} \subset \mathbb{R}^{2 \times 2}_{sym}$ be linearly independent and pairwise compatible matrices such that (4.1) hold. The set of matrices $\{M_0, M_1, M_2\}$ admits a triple junction if and only if all $\{a_0, a_1, a_2\}$ are parallel vectors and $\{n^0, n^1, n^2\}$ are pairwise linearly independent.

From Lemma 4.2, any triple junctions with two parallel normal vectors, say n^1 and n^2 , must satisfy that the three symmetric matrices involved, M_0 , M_1 and M_2 , must be linearly dependent (see Fig. 4.1(b)), and the matrix Q is not uniquely defined, see Section 1.2 and Definition 2.2. In the case of symmetric matrices, we have that the coefficient of the non-symmetric part of equations (4.1) satisfy $\mu_0 + \mu_1 + \mu_2 = 0$. Finally, notice that by Lemma 4.2 there is not any angle between two different interphases equal to 180°, see figure 4.1.b.



Figure 4.1 (a) Admissible triple junction, vectors a^1 , a^2 and a^3 are parallel but the normal vectors are pairwise linearly independent. (b) Non-admissible triple junction where two out of the three normal vectors are parallel.

Proof of Lemma 4.2. We assume first that the there exist $a \in \mathbb{R}^2$ and $\alpha^i \in \mathbb{R}$ such that $a^i = \alpha^i a$ for $i \in \{0, 1, 2\}$ and without loss of generality the vectors n^0 and n^2 are linearly independent. From equation (4.1) we have that

$$M_0 - M_1 + \mu_2 R = \alpha^2 a \otimes (n^2)^{\perp}$$
 and $M_1 - M_2 + \mu_0 R = \alpha^0 a \otimes (n^0)^{\perp}$. (4.3)

Adding the last two equations we find

$$M_0 - M_2 + (\mu_2 + \mu_0)R = a \otimes (\alpha^2 n^2 + \alpha^0 n^0))^{\perp}.$$

Now, we let $\tilde{\alpha}^1 = -|\alpha^2 n^2 + \alpha^0 n^0|$, $\tilde{n}^1 = (\alpha^2 n^2 + \alpha^0 n^0)/\tilde{\alpha}^1$ and $\mu_1 = -\mu_2 - \mu_0$. Hence,

$$M_2 - M_0 + \mu_1 R = \tilde{\alpha}^1 a \otimes (\tilde{n}^1)^{\perp}.$$
 (4.4)

Finally by adding equation (4.3) and (4.4) we find out

$$\alpha^0 a \otimes (n^0)^{\perp} + \tilde{\alpha}_1 a \otimes (\tilde{n}^1)^{\perp} + \alpha^2 a \otimes (n^2)^{\perp} = (\mu_0 + \mu_1 + \mu_2)R = 0,$$

and $\{M_0, M_1, M_2\}$ admits a triple junction.

For the reverse implication we assume that there exist n^0 , n^1 , $n^2 \in S^1$ and $a^0, a^1, a^2 \in \mathbb{R}^2$ such that

$$a^{0} \otimes (n^{0})^{\perp} + a^{1} \otimes (n^{1})^{\perp} + a^{2} \otimes (n^{2})^{\perp} = 0.$$
 (4.5)

First, we notice that due to the symmetric role of the vectors n^i and a^i in equation (4.1), if all $n^0, n^1, n^2 \in S^1$ are parallel, we interchange the role of the *n*'s and *a*'s vectors into equation (4.1). Hence, we only need to show that n^0, n^1 and n^2 are pairwise linearly independent. We argue by contradiction and without loss of generality, we assume n^1 and n^2 are parallel vectors in \mathbb{R}^2 . So, there exists a number $\alpha_1 \in \mathbb{R}$ such that

$$\alpha_1(M_2 - M_0) + \alpha_1 \mu_1 R = \alpha_1 a^1 \otimes (n^1)^{\perp} = a^2 \otimes (n^2)^{\perp} = M_0 - M_1 + \mu_2 R,$$

and we obtain that $\{M_0, M_1, M_2\}$ are linearly dependent matrices, a contradiction.

Second, we assume that n^0 and n^2 are linearly independent and consider $\bar{n}^2 := (Id - n^0 \otimes n^0)n^2$. Thus, n^0 and \bar{n}^2 are perpendicular, hence $n^1 = \alpha_0 n^0 + \alpha_2 \bar{n}^2$ and $n^2 = \lambda_0 n^0 + \lambda_2 \bar{n}^2$ for some $\alpha_0, \alpha_2, \lambda_0, \lambda_2 \in \mathbb{R}$. We use the last expressions into (4.5) to get

$$(a^{0} + \alpha_{1}a^{1} + \lambda_{0}a^{2}) \otimes (n^{0})^{\perp} + (\alpha_{2}a^{1} + \lambda_{2}a^{2}) \otimes (\bar{n}^{2})^{\perp} = 0,$$

and multiplying by \bar{n}^2 and n^0 we obtain $(a^0 + \alpha_1 a^1 + \lambda_0 a^2) = 0$ and $(\alpha_2 a^1 + \lambda_2 a^2) = 0$. Hence, a^0 , a^1 and a^2 are parallel as claimed. Finally, by the above argument, n^1 is pairwise linearly independent from n^0 and n^2 , as claimed.

The next lemma shows that for each $U \in \mathbb{R}^{2 \times 2}_{sym}$ and every non-invertible symmetric Q, there exists an affine space $\Pi_Q(U)$ that contains U and for every $N, M \in \Pi_Q(U)$, the set $\{U, N, M\}$ admits a triple junctions. This affine space Π_Q has been used in previous chapters without emphasizing any well contained in it but from now on we will use the notation $\Pi_Q(U)$ to avoid confusion.

Lemma 4.3. Assume $Q, U \in \mathbb{R}^{2 \times 2}_{sym}$ and let $\Pi_Q(U)$ be the plane normal to Q that contains U. The matrix Q is non-invertible if and only if $\Pi_Q(U)$ is tangent to ∂C_U . Moreover, ∂C_U is the envelope of the family

$$\{\Pi_Q(U) \text{ such that } \det Q = 0, \ Q \in \mathbb{R}^{2 \times 2}_{sum}\}.$$
(4.6)

Proof. Without loss of generality, we assume U = 0. A nonzero symmetric matrix $Q \in \mathbb{R}^{2\times 2}$ has null determinant if and only if there exists a vector $e \in S^1$ such that

 $Q = \alpha n \otimes n$ for some $\alpha \in \mathbb{R}$. Since $\mathcal{B} = \{n \odot n, n^{\perp} \odot n^{\perp}, n \odot n^{\perp}\}$ defines an orthonormal basis for $\mathbb{R}^{2 \times 2}_{sym}$, it follows that $\Pi_Q(0) = \text{Span}(\{n^{\perp} \odot n^{\perp}, n \odot n^{\perp}\})$. Also notice that $n \odot n$ and $n^{\perp} \odot n^{\perp}$ both have null determinant thus, they belong to the boundary of \mathcal{C}_0 . Moreover, since the cone \mathcal{C}_0 has a 90° aperture angle (see Section 2.1), we conclude that $\Pi_Q(0)$ is tangent to $\partial \mathcal{C}_0$.

Conversely, if $\Pi_Q(0)$ is tangent to $\partial \mathcal{C}_0$, both meet on a generatrix line, and there exists $n \in S^1$ such that $n \odot n$ spans $\Pi_Q(0) \cap \mathcal{C}_0$. As before, we construct the orthonormal basis $\{n \odot n, n^{\perp} \odot n^{\perp}, n \odot n^{\perp}\}$ for $\mathbb{R}^{2 \times 2}_{sym}$. The direction $n^{\perp} \odot n^{\perp}$ is perpendicular to $n \odot n$, has null determinant –i.e. belongs the boundary of \mathcal{C}_0 – and does not belong to $\Pi_Q(0)$. Therefore, since the aperture angle of the cone is 90°, the normal to $\Pi_Q(0)$ is given by $n^{\perp} \odot n^{\perp}$ and det Q = 0 as claimed.

Finally, we show that ∂C_0 is given by the envelope of the planes given in (4.6). With the parametrization $n_{\theta} := (\cos \theta, \sin \theta)$ for $\theta \in [0, 2\pi)$, the envelope (4.6) is represented in terms of of the following system

$$V \in \mathbb{R}^{2 \times 2}_{sym}, \quad \langle n_{\theta} \otimes n_{\theta}, V \rangle = 0, \quad \text{and} \quad 2 \left\langle n_{\theta}^{\perp} \odot n_{\theta}, V \right\rangle = \frac{\partial}{\partial \theta} \left\langle n_{\theta} \otimes n_{\theta}, V \right\rangle = 0$$

Now, for every fixed θ , the set $\{\alpha n_{\theta}^{\perp} \otimes n_{\theta}^{\perp} \mid \alpha \in \mathbb{R}\}$ satisfies the previous system and its envelope is given $\{V \in \mathbb{R}^{2 \times 2}_{sym} \mid \det V = 0\}$. By Lemma 2.6, this envelope coincides with $\partial \mathcal{C}_0$, and the proof is completed.

Next, we present the first main result of this chapter. Here, we characterize the existence of triple junctions, its relationship with the matrix Q, and the incompatible cone.

Proposition 4.4. Let $\mathcal{U} = \{U_0, U_1, U_2\} \subset \mathbb{R}^{2 \times 2}_{sym}$ be as in the assumptions of Definition 4.1, and $Q \in \mathbb{R}^{2 \times 2}_{sym}$ such that $\langle Q, U \rangle = \alpha$ for some $\alpha \in \mathbb{R}$ fixed and every $U \in \mathcal{U}$. The following statements are equivalent:

- (i) The set $\{U_0, U_1, U_2\}$ admits a triple junction.
- (ii) The normal matrix Q is not invertible.

Proof. We show that (i) implies (ii). We assume that $\{U_0, U_1, U_2\} \subset \mathbb{R}^{2 \times 2}_{sym}$ admits a triple junction, that is,

$$U_i - U_{i+1} + \mu_{i+2}R = \nu_{i+2}a^{i+2} \otimes (n^{i+2})^{\perp} \quad i \in \mathbb{N} \cup \{0\} \text{ mod } 3, \tag{4.7}$$

for some vectors n^i , $a^i \in S^1$, and scalars $\nu_i \neq 0$ for i = 0, 1, 2. By letting $V_i = (a^i)^{\perp} \odot (n^i)^{\perp}$, the symmetric part of (4.7) is given by

$$U_i - U_{i+1} = \nu_{i+2}V_{i+2}$$
 $i \in \mathbb{N} \cup \{0\} \mod 3$

Since Q is perpendicular to the differences $U_i - U_{i+1}$ for i = 1, 2, 3, it is also perpendicular to V_1, V_2 and V_3 . Therefore, in terms of the isomorphism (1.24) between $\mathbb{R}^{2\times 2}_{sym}$ and \mathbb{R}^3 ,

the vector \tilde{Q} is parallel to all three vectors $\tilde{V}_0 \times \tilde{V}_1$, $\tilde{V}_1 \times \tilde{V}_2$ and $\tilde{V}_2 \times \tilde{V}_0$, where \times denotes the usual wedge product in \mathbb{R}^3 . Hence, $\tilde{Q} = \beta \tilde{V}_0 \times \tilde{V}_2$ for some $\beta \in \mathbb{R}$, or in terms of the components of n^i and a^i ,

$$\tilde{Q} = \beta \left(\left| n^0 | n^2 \right| \begin{pmatrix} a_1^2 a_1^0 \\ a_2^2 a_2^0 \\ \sqrt{2} a_1^2 a_2^0 \end{pmatrix} + \left| a^0 | a^2 \right| \begin{pmatrix} n_1^2 n_1^0 \\ n_2^2 n_2^0 \\ \sqrt{2} n_2^2 n_1^0 \end{pmatrix} \right),$$

where |a|b| denotes the 2-by-2 determinant of a matrix whose first and second columns are given by vectors a and b, respectively. We readily find that \tilde{Q} 's last expression can be mapped back to $\mathbb{R}^{2\times 2}_{sym}$ and becomes

$$Q = \beta \left(\left| n^0 | n^2 \right| a^0 \otimes a^2 + \left| a^0 | a^2 \right| n^0 \otimes n^2 \right).$$

$$(4.8)$$

Notice that the right-hand side of equation (4.8) is symmetric, although it is given in terms of the tensor product instead of the symmetric tensor product. Now, since $\{U_0, U_1, U_2\}$ admits a triple junction, the vectors a^0 and a^2 are parallel and $|a^0|a^2| = 0$, see Lemma 4.2. Hence, Q is a rank-one matrix and det Q = 0 as claimed.

Finally, we show that *(ii)* implies *(i)*. We assume det Q = 0, compute the determinant on both sides of equation (4.8), and use the multi-linearity of the determinant to obtain

$$\left| n^{0}|n^{2} \right| \left| a^{0}|a^{2} \right| \left(a_{1}^{2}a_{2}^{0} \left| n^{0}|n^{2} \right| - n_{1}^{0}a_{2}^{0} \left| a^{2}|n^{2} \right| + a_{1}^{2}n_{2}^{2} \left| a^{0}|n^{0} \right| - n_{1}^{0}n_{2}^{2} \left| a^{0}|a^{2} \right| \right) = 0.$$

Rearranging terms, the last equation becomes

$$\left| n^{0}|n^{2} \right| \left| a^{0}|a^{2} \right| \left| a^{0}|n^{2} \right| \left| a^{2}|n^{0} \right| = 0.$$

Thus, one of the pairs contains at least two parallel vectors. Depending on the pair of parallel vectors, we define a new set of vectors \hat{n}^i, \hat{a}^i

$$\begin{array}{lll} \text{if} & n^0 \parallel n^2, & \text{then} & (\hat{n}^0, \hat{a}^0, \hat{n}^2, \hat{a}^2) = (a^0, n^0, a^2, n^2), \\ \text{if} & a^0 \parallel a^2, & \text{then} & (\hat{n}^0, \hat{a}^0, \hat{n}^2, \hat{a}^2) = (n^0, a^0, n^2, a^2), \\ \text{if} & a^0 \parallel n^2, & \text{then} & (\hat{n}^0, \hat{a}^0, \hat{n}^2, \hat{a}^2) = (n^0, a^0, a^2, n^2), \\ \text{if} & a^2 \parallel n^0, & \text{then} & (\hat{n}^0, \hat{a}^0, \hat{n}^2, \hat{a}^2) = (a^0, n^0, n^2, a^2), \end{array}$$

and scalars $\hat{\mu}_i = (\chi_{\{\hat{n}^i = n^i\}} - \chi_{\{\hat{n}^i = a^i\}})\mu_i$ for $i \in \{0, 2\}$. In all cases \hat{a}^0 and \hat{a}^2 are parallel vectors. Now, on the one hand, due to the symmetric role of n^i and a^i (namely a^i) in equation (4.7), we have that

$$U_0 - U_1 + \hat{\mu}_2 R = \nu_2(\hat{a}^2)^{\perp} \otimes (\hat{n}^2)^{\perp}$$
 and $U_1 - U_2 + \hat{\mu}_0 R = \nu_0(\hat{a}^0)^{\perp} \otimes (\hat{n}^0)^{\perp}$.

Adding the last two equations, we obtain

$$U_0 - U_2 + (\hat{\mu}_0 + \hat{\mu}_2) R = \nu(\hat{a}^0)^{\perp} \otimes (n)^{\perp}, \qquad (4.9)$$

where $n \in S^1$ and $\nu n = \nu_0 \hat{n}^0 + \nu_2 (\chi_{\{\hat{a}^0 = \hat{a}^2\}} - \chi_{\{\hat{a}^0 = -\hat{a}^2\}}) \hat{n}^2$. On the other hand, by hypothesis, we have that

$$U_2 - U_0 + \mu_1 R = \nu_1 (a^1)^{\perp} \otimes (n^1)^{\perp}.$$

Thus, $\hat{a}^0 \parallel a^1$ or $\hat{a}^0 \parallel n^1$. In either case, we may interchange a^1 and n^1 to get that vectors \hat{a}^0 , a^1 and \hat{a}^2 in (4.7) are parallel. By Lemma 4.2 this implies the existence of a triple junction, and this finishes the proof.

4.2 Rigidity for Polygonal Strains on Flag Configurations

In this section we study three-well basic blocks $\mathcal{U} = \{U_0, U_1, U_2\}$ and deformations $u \in W^{1,p}(\Omega, \mathbb{R}^2)$ such that $e(Du) \in \mathcal{U}$ where the level sets of e(Du) is the union of finitely many polygons. Since we are interested in general deformations, besides the triple junctions introduced in the last section, we also need to consider more general cases. We say that $\{V_0, V_1, V_2, \cdots, V_{k-1}\} \subset \mathbb{R}^{2\times 2}_{sym}$ admits a k-tuple junction if and only if there exist $\mu_i \in \mathbb{R}$, $a^i \in \mathbb{R}^2$ and $n^i \in S^1$ for $i \in \{0, 1, \cdots, k-1\}$ such that

$$V_i - V_{i+1} + \mu_{i+2}R = a^{i+2} \otimes n^{i+2}, \text{ and } \sum_{i=0}^{k-1} a^i \otimes n^i = 0,$$
 (4.10)

where *i* is *k*-mod cyclic. The last relation in Eq. (4.10) and Theorem 1.1 imply the existence of a deformation $u \in W^{1,\infty}(\mathbb{R}^2, \mathbb{R}^2)$ such that $e(Du) \in \{V_0, V_1, V_2, \cdots, V_{k-1}\}$ a.e. $x \in \Omega$, see [22] for the proof of this statement.

We recall two-dimensional version of a very well-known result in linear elasticity.

Lemma 4.5. Let $\Omega \subset \mathbb{R}^2$ be simply connected and e be a tensor field on Ω . The tensor field e satisfies e = e(Du) for some deformation $u : \Omega \to \mathbb{R}^2$ if and only if e satisfies $\partial_{11}^2 e_{22} + \partial_{22}^2 e_{11} - 2\partial_{12}^2 e_{12} = 0$ in distributional sense.

Proof. Necessity follows from a straight forward calculation. For sufficiency, we notice that

$$0 = \partial_{11}^2 e_{22} + \partial_{22}^2 e_{11} - 2\partial_{12}^2 e_{12} = \partial_2 \left(\partial_2 e_{11} - \partial_1 e_{12} \right) - \partial_1 \left(\partial_2 e_{12} - \partial_1 e_{22} \right),$$

and since Ω is simply connected, due to Poincaré's lemma, we get

$$\begin{array}{l} \partial_2 e_{11} - \partial_1 e_{12} = \partial_1 v\\ \partial_2 e_{12} - \partial_1 e_{22} = \partial_2 v \end{array}, \quad \text{for some } v: \Omega \to \mathbb{R}. \end{array}$$

Last two equations can be rearranged to apply Poincaré's lemma again. We get that there exists $u = (u_1, u_2) : \Omega \to \mathbb{R}$ such that

$$e_{11} = \partial_1 u_1$$
, and $e_{12} - v = \partial_1 u_2$.
 $e_{12} + v = \partial_2 u_1$, $e_{22} = \partial_2 u_2$.

It readily follows that $e_{12} = \frac{1}{2}(\partial_2 u_1 + \partial_1 u_2)$ and the proof is complete.

Following Rüland [23], we make the next

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Definition 4.6. Let $e : \mathbb{R}^2 \to \mathbb{R}^{2 \times 2}$ be a tensor field. we say that *e* is a *zero homogeneous tensor field* if and only if

$$e(\lambda x) = e(x)$$
 for all $\lambda > 0$

Moreover, if e = e(Du) for some $u : \mathbb{R}^2 \to \mathbb{R}^2$, we say e is a zero-homogeneous strain.

Notice that zero-homogeneous tensor fields do not depend on the radial component of the argument x. We will use this property later on.

Lemma 4.7. Let $e \in L^{\infty}(\mathbb{R}^2, \mathbb{R}^2)$ be a zero-homogeneous strain with $e \in \mathcal{U}$. Then e can only be discontinuous along a line through the origin determined by a compatibility relation among the wells \mathcal{U} .

Proof. First, since e is a zero-homogeneous strain, it does not depend on the radial component of the argument and in terms of polar coordinates, we let $\hat{e} := e \cdot (\rho \cos \theta, \rho \sin \theta) \in L^{1,\infty}((0,\infty) \times [0,2\pi), \mathbb{R}^2)$. By Lemma 4.5, e satisfies $\partial_{11}^2 e_{22} + \partial_{22}^2 e_{11} - 2\partial_{12}^2 e_{12} = 0$ in a distributional sense. Since \hat{e} does not depend on the radial component, we get that

$$\frac{\partial^2 \hat{e}_{11}}{\partial x_2^2} = -\frac{1}{r^2} \sin \theta \cos \theta \frac{\partial \hat{e}_{11}}{\partial \theta} + \frac{1}{r^2} \cos \theta \frac{\partial}{\partial \theta} \left(\cos \theta \frac{\partial \hat{e}_{11}}{\partial \theta} \right) = -\frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\cos^2 \theta \frac{\partial \hat{e}_{11}}{\partial \theta} \right),$$
$$\frac{\partial^2 \hat{e}_{22}}{\partial x_1^2} = -\frac{1}{r^2} \sin \theta \cos \theta \frac{\partial \hat{e}_{22}}{\partial \theta} + \frac{1}{r^2} \sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \hat{e}_{22}}{\partial \theta} \right) = -\frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\sin^2 \theta \frac{\partial \hat{e}_{22}}{\partial \theta} \right),$$

$$\frac{\partial^2 \hat{e}_{12}}{\partial x_1 \partial x_2} = -\frac{1}{r^2} \cos^2 \theta \frac{\partial \hat{e}_{12}}{\partial \theta} - \frac{1}{r^2} \sin \theta \frac{\partial}{\partial \theta} \left(\cos \theta \frac{\partial \hat{e}_{12}}{\partial \theta} \right) = \frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\cos \theta \sin \theta \frac{\partial \hat{e}_{12}}{\partial \theta} \right).$$

Therefore, the equation $\partial_{11}^2 e_{22} + \partial_{22}^2 e_{11} - 2\partial_{12}^2 e_{12} = 0$ is equivalent to

$$\partial_{\theta} \left(\cos^2 \theta \, \partial_{\theta} \hat{e}_{11} + \sin^2 \theta \, \partial_{\theta} \hat{e}_{22} + 2 \cos \theta \sin \theta \, \partial_{\theta} \hat{e}_{12} \right) = 0, \quad \text{in distributional sense.}$$

By integration, the last equation becomes

$$\cos^2\theta\,\partial_\theta \hat{e}_{11} + \sin^2\theta\,\partial_\theta \hat{e}_{22} + 2\cos\theta\sin\theta\,\partial_\theta \hat{e}_{12} = C, \quad \text{a.e. } x \in \Omega.$$

Hence, we have that

$$\partial_{\theta} \left(\cos^2 \theta \, \hat{e}_{11} + \sin^2 \theta \, \hat{e}_{22} + 2 \cos \theta \sin \theta \, \hat{e}_{12} \right) = C + \left[\hat{e}_{11} \partial_{\theta} \cos^2 \theta + \hat{e}_{22} \partial_{\theta} \sin^2 \theta + 2 \hat{e}_{12} \partial_{\theta} (\cos \theta \sin \theta) \right].$$
(4.11)

Now, since $\hat{e} \in L^{\infty}((0,\infty) \times [0,2\pi), \mathbb{R}^2)$, the second term on the right hand side of (4.11) belongs $L^{\infty}(\Omega, \mathbb{R}^2)$ and we conclude that

$$\cos^2\theta \,\hat{e}_{11} + \sin^2\theta \,\hat{e}_{22} + 2\cos\theta\sin\theta \,\hat{e}_{12} \in W^{1,\infty}((0,\infty)\times[0,2\pi),\mathbb{R}^2).$$

Hence, by Sobolev embeddings, $\cos^2 \theta \,\hat{e}_{11} + \sin^2 \theta \,\hat{e}_{22} + 2\cos\theta\sin\theta \,\hat{e}_{12}$ is continuous, and by letting $r_{\theta} = (\cos\theta, \sin\theta)^T$, it can be written as $\langle \hat{e}, r_{\theta} \otimes r_{\theta} \rangle$. By continuity, the tensor \hat{e} changes from U_i to U_j along the line $\ell = \{tr_{\theta} | t \in \mathbb{R}\}$ if and only if $\langle U_i, r_{\theta} \otimes r_{\theta} \rangle - \langle U_j, r_{\theta} \otimes r_{\theta} \rangle = 0$. Thus, from Proposition 2.1 Item (c), U_i and U_j are compatible and r_{θ} satisfies

$$U_i - U_i + \mu R = a \otimes r_{\theta}^{\perp}$$
 for some $a \in \mathbb{R}^2$ and $\mu \in \mathbb{R}$.

Since a and r_{θ} are determined by U_j and U_i , and r_{θ}^{\perp} is normal to the transition line ℓ , the proof is completed.

Now we define a family of three-well sets that contains any other set with a flag configuration. We say that a three-well set \mathcal{U} has a *P*-configuration if up to a relabeling there exists a cyclic index $i \in \{0, 1, 2\}$ such that $\mathcal{U} = \{U_{i-1}, U_i, U_{i+1}\}$ is a pairwise linearly independent set where $\det(U_j - U_{j+1}) = 0$ and $\det(U_j - U_{j-1}) > 0$. The following lemma displays the rigidity in the microstructures when $e \in \mathcal{U}$ and \mathcal{U} has a P-configuration.

Proposition 4.8. Let e be a zero-homogeneous strain that takes values in a set $\mathcal{U} = \{U_0, U_1, U_2\}$ with a P-configuration, then e is either a constant state or a lamination of degree one.

Proof. We split the proof into two cases:

1. Assume that there is only one pair of compatible matrices in \mathcal{U} , so these matrices are rank-one compatible, and without lost of generality we assume $\det(U_1 - U_0) = 0$ and $\det(U_2 - U_i) > 0$ for i = 0 or 1.

Since U_2 is incompatible with the remaining wells, if $e = U_2$ in a subset of positive measure, then it is constant $a.e \ x \in \mathbb{R}^2$. Also if $e \in \{U_0, U_1\}$, then only laminations of degree one between U_1 and U_0 are allowed in the direction n due to Theorem 1.1 and $U_1 - U_0 = \nu n \otimes n$ for a fixed $n \in S^1$.

2. We assume that there is only one pair of incompatible matrices in \mathcal{U} or equivalently, it has a flag configuration, see Chapter 3. Without lost of generality, let $\det(U_1 - U_0) = 0$, $\det(U_2 - U_1) \leq 0$ and $\det(U_2 - U_0) > 0$. Hence

$$U_1 - U_0 = kn^2 \otimes n^2$$
, and $U_2 - U_1 + \mu_0 R = a^0 \otimes n^0$, (4.12)

for some n^2 and $n^0 \in S^1$, $a^0 \in \mathbb{R} \setminus \{0\}$, and $\mu_0 \in \mathbb{R}$. Then, transition layers between U_0 and U_1 exist only through the line with normal n^2 passing through the origin. Meanwhile, for U_1 and U_2 , transitions layers may exist along the lines with normal n^0 or $a^0/|a^0|$, and no more single layer transitions are allowed.

In flag configuration, there exists at least one incompatible pair of matrices in \mathcal{U} , and the plane $\Pi_Q(U_0)$ intersects the incompatible cone \mathcal{C}_{U_0} . Thus, det Q < 0 and by Proposition 4.4, \mathcal{U} does not admit triple junctions, so we look for k-tuple junctions. Since we only have three normal directions for the transition lines, it is straight forward that at most only quadruple junctions could be admissible. Now we claim that no quadruple junction is admissible. Indeed, there is only one generic quadruple junction that we need to consider, namely U_0, U_1, U_2, U_1 , see Fig. 4.2(b). In this case, by the second relation in the system 4.10, we have that $kn^2 \odot n^2 + a^0 \odot n^0 = 0$. Thus, by (4.12) we get that the wells in \mathcal{U} are not linearly independent, hence a contradiction.



Figure 4.2 Fig. (a) illustrates a possible configuration of vectors n^0 , n^2 and a/|a| and their associated transition lines. We denote by T_{ij} the transition lines between phases U_i and U_j . Fig. (b) shows one of the only two possible quadruple junctions.

Now, we assume that only two wells are present. If e takes the value U_0 in a set of positive measure, by (4.12) either e is constant $a.e. \ x \in \mathbb{R}^2$, or by Theorem 1.1, only laminations of degree one between U_1 and U_0 are allowed in the direction n^2 . Next, we consider the case where $e \in \{U_1, U_2\}$, and since $e \in L^{\infty}(\mathbb{R}^2, \mathbb{R}^2)$ there

exists $\chi : \mathbb{R}^2 \to \{0, 1\}$ a indicator function of the phase U_2 such that

$$e(x) = (1 - \chi(x))U_1 + \chi(x)U_2$$
 a.e. $x \in \mathbb{R}^2$.

By translation, we may assume $U_1 = 0$, $U_2 = a^0 \odot n^0$, and $e = a^0 \odot n^0 \chi$. In view of Lemma 4.5, the characteristic function χ satisfies

$$0 = a_2^0 n_2^0 \partial_{11}^2 \chi + a_1^0 n_1^0 \partial_{22}^2 \chi - (a_1^0 n_2^0 + a_2^0 n_1^0) \partial_{12}^2 \chi.$$

Since last equation's discriminant is negative, it can be written as the following wave equation

$$\left(n_2^0\partial_1 - n_1^0\partial_2\right)\left(a_2^0\partial_1 - a_1^0\partial_2\right)\chi = 0.$$

Hence, χ is the solution of a one-dimensional wave equation and can be written as the sum of two plane waves

$$\chi(x_1, x_2) = f(n_1^0 x_1 + n_2^0 x_2) + g(a_1^0 x_1 + a_2^0 x_2).$$

But, since χ takes only two values, it follows either that f = 0 or g = 0, so laminations of degree one occur, and the claim follows.

Finally, by all the above arguments, we conclude that the only possible configurations for e are constant states or laminations of degree one between U_1 and U_2 in the direction n are allowed.

Definition 4.9. We say that a strain e(Du) is a piecewise polygonal provided it takes values in a finite number of level sets, where each level set is the union finitely many polygons.

Now we are ready to state the main result of this chapter concerning the rigidity of *piecewise polygonal* strains.

Theorem 4.10. Let \mathcal{U} have a *P*-configuration, and let Ω be a simply-connected bounded domain in \mathbb{R}^2 . Assume that $e(Du) \in L^{\infty}(\Omega, \mathcal{U})$ is a piecewise polygonal strain. Then, u locally is a lamination of degree in Ω .

This result shows that piecewise polygonal strains are locally simple laminates inside any bounded domain and deviations may exist near the edges of the domain due to boundary conditions.

Proof. Since e(Du) is a piecewise polygonal strain, at any point $x_0 \in \Omega$ there exists a ball $B(x_0, r_0)$ where e(Du) is either a simple laminate or a k-tuple junction, whenever x_0 is a vertex of the polygonal level sets. In the latter case, relation in (4.10) holds for some $V_j \in \mathcal{U}$. Without loss of generality we assume $x_0 = 0, 0 < t < 1$, and let

$$v(x,t) = \frac{1}{t}u(tx)$$
 for every $x \in B(0, x_0/t).$

A straightforward computation yields

$$e(Dv)(x,t) = e(Du)(tx) \in \mathcal{U}$$
 for every $x \in B(0, r_0/t)$.

Now, we define the blow-up $e_0(x)$ of e(Du) as the limit

$$e_0(x) := \lim_{t \to 0} e(Dv)(x, t).$$

By construction, e_0 is defined in all of \mathbb{R}^2 , and it is a zero-homogeneous strain. Indeed, as t tends to zero, the ball $B(0, r_0/t)$ tends to \mathbb{R}^2 , and on each of these balls, e(Dv)(x,t)is a constant k-tuple or a simple laminate. Notice $e_0(x)$ is a zero-homogeneous strain since it is constant along rays. Moreover, by Theorem 1.1 it follows the existence of $v_0 : \mathbb{R}^2 \to \mathbb{R}^{2\times 2}$ such that $e_0(x) = e(Dv_0)(x)$ a.e. $x \in \mathbb{R}^2$, and $e(Dv_0)$ is either a constant state or a single transition layer between two wells due to Proposition 4.8. Hence, the continuity in the limit as $t \to \infty$ yields that e(Du) is also a constant state or a single transition layer inside $B(0, r_0)$ and the result follows.

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