

**GEOMETRIC PARAMETERS AND THE RELAXATION OF
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GEOMETRIC PARAMETERS AND THE RELAXATION OF MULTIWELL ENERGIES

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Abstract. This paper discusses the relaxation of a multiwell energy of the special form $W = \min_i \{|\nabla u - a^i|^2\}$. We explain how the relaxation QW can be expressed in terms of certain “tensors of geometric parameters.” The exact set \mathcal{F}_θ of attainable geometric parameters is not known, but we show that it must lie inside an explicitly given convex set \mathcal{F}_θ^U . This leads to a new Geometric Parameters Lower Bound for QW . For the special case of three wells in two space dimensions we give a complete characterization of the extreme points of \mathcal{F}_θ^U . The final section addresses the “three gradient problem,” which asks whether three pairwise incompatible gradients can nevertheless be mutually compatible. We do not solve this problem, but we show that it is linked to the attainability of the type 3 extreme points of \mathcal{F}_θ^U .

1. Introduction. A basic problem in the variational modeling of coherent phase transitions is the identification of energy-minimizing microstructures, see e.g. [4,5,14,15,17,25]. Mathematically speaking, this is equivalent to the relaxation of a multiwell energy $W(\nabla u)$ of the form

$$(1.1) \quad W(\nabla u) = \min_{i=1,\dots,N} \{W_i(\nabla u)\},$$

see e.g. [17]. The individual “wells” $\{W_i(\nabla u)\}$ are the energies of the N component phases. The relaxed or “macroscopic” energy is QW , the quasiconvexification of W , defined by

$$(1.2) \quad QW(\xi) = \inf_{u|_{\partial\Omega}=\xi \cdot x} \frac{1}{|\Omega|} \int_{\Omega} W(\nabla u) dx.$$

It represents the average energy of the system when the average gradient is ξ , assuming that both the phase geometry and the locally varying deformation gradient are governed by energy minimization. The process of relaxation is discussed, for example, in [1,7,9,18,19].

To calculate the relaxed energy, one must find a formula that is at once an upper bound and a lower bound for $QW(\xi)$. Upper bounds are obtained by considering specific microstructures, obtained for example by “sequential lamination.” (The best such upper bound is the “rank-one convexification,” see [8,18,23].) Lower bounds are usually established by some version of the “translation method,” which is based on the use of weakly

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lower semicontinuous functions and convexification [12]. (The best such bound using only weakly continuous translations is the “polyconvexification,” see [8,18,23].) These methods have the advantage of being quite general. However, it can be difficult to apply them optimally in specific cases. Moreover, we do not know whether the optimal translation bound agrees in general with the rank-one convexification. Therefore it is natural to seek new approaches to computing relaxed energies.

This paper explores a new method for bounding QW from below, when W has the specific form

$$(1.3) \quad W(\nabla u) = \min_{i=1,\dots,N} \{|\nabla u - a^i|^2\}$$

for some matrices a^i , $1 \leq i \leq N$. The basic idea is as follows. To any microstructure we shall associate a “tensor of geometric parameters” $F = (F_{ij\alpha\beta})$. The effective energy of the microstructure is explicitly representable as a linear function of F . If we knew the exact set \mathcal{F}_θ of geometric parameters attained by microstructures with volume fraction θ , then we could compute $QW(\xi)$ exactly by minimizing this linear function over \mathcal{F}_θ . We do not know \mathcal{F}_θ explicitly, but we do know a set \mathcal{F}_θ^U which contains it; minimization over \mathcal{F}_θ^U gives a lower bound for QW .

The set \mathcal{F}_θ^U is convex; hence for the purpose of minimizing a linear function one need only consider its extreme points. For the specific case of three phases and two space dimensions we shall give a complete classification of these extreme points in Section 4.

One would like to know whether our lower bound on QW is optimal, i.e. whether it is equal to QW . This amounts to asking whether $\mathcal{F}_\theta = \mathcal{F}_\theta^U$. We shall show that \mathcal{F}_θ , too, is convex, so it is equivalent to ask whether each extreme point of \mathcal{F}_θ^U lies in \mathcal{F}_θ . For three phases in two space dimensions the extreme points come in three types. The first two types are attained by sequentially laminated microstructures of rank 2; in particular, they are in \mathcal{F}_θ . We have been unable to find any microstructure corresponding to an extreme point of type 3. The question whether $\mathcal{F}_\theta = \mathcal{F}_\theta^U$ is equivalent to whether the type 3 extreme points are attained by microstructures; this question, however, remains open.

The final section of this paper addresses the “three gradient problem.” It asks whether three pairwise incompatible gradients can nevertheless be mutually compatible. In other words, given matrices a^1 , a^2 , and a^3 such that $\text{rank}(a^i - a^j) > 1$ for $i \neq j$, and defining W by (1.3), does $QW(\xi)$ vanish for some $\xi \notin \{a^1, a^2, a^3\}$? (We refer to Section 5 for a discussion motivating this question, and for a summary of related results.) Our analysis is restricted to two space dimensions; for maximum simplicity it is focused primarily on the case when $\{a^i\}$ are simultaneously diagonal. Our main result is an equivalence between the three gradient problem and the attainability of our type 3 extreme points (see Theorem 5.4). It should be emphasized, however, that the three gradient problem has not been settled, since the attainability of type 3 extreme points remains open.

Our attention is focused throughout on $N \geq 3$ phases, because the situation for two

phases is much simpler. That case is analyzed in [17,20,24]. When $N = 2$ it turns out that $\mathcal{F}_\theta = \mathcal{F}_\theta^U$, so the ‘‘Geometric Parameters Lower Bound’’ is actually a formula for QW .

It is natural to ask how our ‘‘Geometric Parameters Lower Bound’’ compares with the polyconvexification of W or the optimal translation bound. For two phases the Geometric Parameters bound can also be proved using the translation method [17,24]. For $N \geq 3$ phases we know no direct relation between geometric parameters and the translation method. Section 5 offers one indication of a possible connection: whenever we can prove that $QW(\xi) > 0$ for $\xi \notin \{a^1, a^2, a^3\}$ using polyconvexification, the same conclusion can also be deduced independently using geometric parameters (see Remark 5.6).

Acknowledgement. The tensor of geometric parameters that we study here was first considered a few years ago by G. Milton, in an attempt to improve upon the Haskin-Shtrikman bounds for the effective conductivity of a multicomponent composite. His analysis included the basic properties (3.2)-(3.6) and the layering formula (3.13)-(3.14), though it did not extend to a classification of the extreme points. We are grateful to Milton for sharing with us his insight and his unpublished notes on this subject.

2. Relaxation and the Tensor of Geometric Parameters. This section defines the tensor of geometric parameters associated to a microstructure, and explains its relationship to the relaxed energy. We assume that W has the form (1.3) for some $\{a^i\}_{i=1}^N$. Each a^i is an $m \times n$ matrix; in other words we are considering $u : \mathbb{R}^n \rightarrow \mathbb{R}^m$.

The relaxed energy QW has already been defined by (1.2). However we plan to use Fourier analysis, so it is more convenient to use a characterization based on periodic functions. We choose $C = [0, 2\pi]^n$ as the period cell in \mathbb{R}^n , and we write $\int f$ for the average value of a C -periodic function f . Then QW has the alternative characterization

$$(2.1) \quad QW(\xi) = \inf_{\varphi \text{ per}} \int W(\xi + \nabla\varphi),$$

where φ ranges over C -periodic H^1 functions from \mathbb{R}^n to \mathbb{R}^m [17].

Because of the special form of W , (2.1) can also be written another way:

$$(2.2) \quad QW(\xi) = \inf_{\varphi} \inf_{\chi_i} \int \sum \chi_i |\xi + \nabla\varphi - a^i|^2,$$

where φ ranges over periodic functions as before, and $\{\chi_i\}_{i=1}^N$ range over C -periodic characteristic functions:

$$\begin{aligned} \chi_i(x) &= 0 \text{ or } 1 \text{ for every } x \\ \chi_i(x)\chi_j(x) &= 0 \text{ for } i \neq j \\ \sum_{i=1}^N \chi_i(x) &= 1 \text{ for every } x. \end{aligned}$$

The equivalence of (2.1) and (2.2) is elementary: if φ is fixed then an optimal choice of $\{\chi_i\}$ for (2.2) has

$$\chi_i(x) = 1 \implies |\xi + \nabla\varphi - a^i|^2 = \min_{1 \leq j \leq N} |\xi + \nabla\varphi - a^j|^2,$$

and substitution yields (2.1). We think of $\{\chi_i\}$ as a (spatially periodic) phase arrangement or *microstructure*. One sees from (2.2) that QW is obtained by minimizing the energy of the N -phase system over all possible microstructures, while holding the average gradient equal to ξ .

We now rewrite (2.2) by computing the minimum over φ explicitly, for given $\{\chi_i\}$. Writing

$$(2.4) \quad \theta_i = \int \chi_i$$

for the volume fraction of the i th phase, one easily sees that the integral in (2.2) is equal to

$$(2.5) \quad \sum_{i=1}^N \theta_i |\xi - a^i|^2 + \int \left(|\nabla\varphi|^2 - 2\langle \nabla\varphi, \sum \chi_i a^i \rangle \right).$$

(Here and henceforth we write $\langle A, B \rangle = \text{tr}(AB^T)$ for the inner product of $m \times n$ matrices, and $\nabla\varphi$ represents the $m \times n$ matrix $(\nabla\varphi)_{\alpha\beta} = \partial\varphi_\alpha/\partial x_\beta$.) We are fixing $\{\chi_i\}$, so the first term in (2.5) is determined. Hence the optimal φ solves

$$(2.6) \quad \inf_{\varphi \text{ per}} \int |\nabla\varphi|^2 - 2\langle \nabla\varphi, \sum \chi_i a^i \rangle,$$

or equivalently

$$(2.7) \quad \Delta\varphi_\alpha - \sum_{\beta=1}^n \frac{\partial}{\partial x_\beta} \left(\sum_{i=1}^N \chi_i a_{\alpha\beta}^i \right) = 0.$$

It is a straightforward matter to solve (2.7) by means of Fourier analysis. Writing

$$(2.8) \quad \chi_j(x) = \sum_{k \in \mathbf{Z}^n} \widehat{\chi}_j(k) e^{ik \cdot x},$$

one finds after some calculation that

$$(2.9) \quad |\widehat{\nabla\varphi}|^2(k) = \sum \frac{k_\alpha k_\beta \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)} a_{\gamma\alpha}^i a_{\gamma\beta}^j}{|k|^2}$$

for any $k \in \mathbb{Z}^n$, $k \neq 0$. (The sum in (2.9) is over all repeated indices: α and β range from 1 to n , i and j range from 1 to N , and γ runs from 1 to m .) Now, an integration by parts based on (2.7) gives

$$\int |\nabla \varphi|^2 - 2 \langle \nabla \varphi, \sum \chi_i a^i \rangle = - \int |\nabla \varphi|^2.$$

Using this along with (2.9) and Plancherel's Theorem, we deduce that

$$\inf(2.7) = - \sum_{k \neq 0} \sum_{\alpha, \beta, \gamma, i, j} \frac{k_\alpha k_\beta}{|k|^2} \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)} a_{\gamma\alpha}^i a_{\gamma\beta}^j.$$

We have thus derived the following alternative representation of (2.2):

$$(2.10) \quad QW(\xi) = \inf_{\chi_i} \left\{ \sum \theta_i |\xi - a^i|^2 - \sum \frac{k_\alpha k_\beta}{|k|^2} \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)} a_{\gamma\alpha}^i a_{\gamma\beta}^j \right\}.$$

The right hand side of (2.10) depends only on certain features of the microstructure $\{\chi_i\}$. To clarify this dependence, we define the *tensor of geometric parameters* associated to $\{\chi_i\}$ by

$$(2.11) \quad F_{ij\alpha\beta} = \sum_{k \neq 0} \frac{k_\alpha k_\beta}{|k|^2} \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)}.$$

(It is not a true tensor, since i and j refer to phases rather than spatial dimensions.) Let V be the simplex of all possible volume fractions:

$$(2.12) \quad V = \left\{ \theta = (\theta_1, \dots, \theta_N) : \theta_i \geq 0, \sum_{i=1}^N \theta_i = 1 \right\}.$$

For any $\theta \in V$, let \mathcal{F}_θ be the set of all geometric parameters attainable with volume fraction θ :

$$(2.13) \quad \begin{aligned} \mathcal{F}_\theta = & \text{The closure of the set of all } F_{ij\alpha\beta} \\ & \text{defined by (2.11), as } \{\chi_i\} \text{ ranges over} \\ & \text{C-periodic characteristic functions with} \\ & \int \chi_i = \theta_i. \end{aligned}$$

Then (2.10) may be expressed as

$$(2.14) \quad QW(\xi) = \inf_{\theta \in V} \inf_{F \in \mathcal{F}_\theta} \left\{ \sum \theta_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j \right\}.$$

We emphasize that (2.14) is an exact “formula” for $QW(\xi)$. It is better than the other representations (1.2) or (2.1) or (2.2), because it involves only a finite dimensional minimization. It is not a computable representation, however, because we do not know the exact form of the set \mathcal{F}_θ . Our “Geometric Parameters Lower Bound” will be obtained in Section 3 by replacing \mathcal{F}_θ with a (possibly) larger set \mathcal{F}_θ^U which is known explicitly.

To place the tensor of geometric parameters in its proper mathematical context, we now explain its relationship to the H -measure of the microstructure [29], also called its microlocal defect measure [13]. Given a (spatially periodic) microstructure $\{\chi_i\}$, the associated H -measure is the symmetric matrix-valued measure on S^{n-1} defined by

$$(2.15) \quad \mu_{ij} = \operatorname{Re} \sum_{k \neq 0} \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)} \delta_{\frac{k}{|k|}},$$

where $\delta_{\frac{k}{|k|}}$ is the Dirac measure concentrated at $\frac{k}{|k|}$. The tensor of geometric parameters keeps track precisely of the second moments of the H -measure. Indeed, it is an easy consequence of the definitions (2.11) and (2.15) that

$$(2.16) \quad F_{ij\alpha\beta} = \int_{S^{n-1}} \eta_\alpha \eta_\beta d\mu_{ij}(\eta).$$

A discussion of multiwell energies based on H -measures rather than geometric parameters will be found in [17].

3. Properties of the Geometric Parameters. This section presents the known algebraic properties of the tensor of geometric parameters. It also discusses the geometric parameters associated with sequentially laminated microstructures. Its main result is the “Geometric Parameters Lower Bound” for QW , (3.8).

We introduce some notation for use in the following proposition: given any $\theta \in V$, let

$$(3.1) \quad \Gamma_{ij} = \begin{cases} \theta_i(1 - \theta_i) & \text{if } i = j \\ -\theta_i\theta_j & \text{if } i \neq j. \end{cases}$$

PROPOSITION 3.1. *If $F \in \mathcal{F}_\theta$, then*

$$(3.2) \quad F_{ij\alpha\beta} = F_{ji\alpha\beta} = F_{ij\beta\alpha},$$

$$(3.3) \quad \sum_{i=1}^N F_{ij\alpha\beta} = \sum_{j=1}^N F_{ij\alpha\beta} = 0,$$

$$(3.4) \quad \sum_{\alpha=1}^n F_{ij\alpha\alpha} = \Gamma_{ij},$$

$$(3.5) \quad \sum F_{ij\alpha\beta} q_{i\alpha} q_{j\beta} \geq 0 \text{ for any real } N \times n \text{ matrix } q_{i\alpha},$$

$$(3.6) \quad \sum (\delta_{\alpha\beta} \Gamma_{ij} - F_{ij\alpha\beta}) q_{i\alpha} q_{j\beta} \geq 0 \text{ for any real } N \times n \text{ matrix } q_{i\alpha}.$$

Proof. The symmetries (3.2) are immediate from the definition (2.11), using the fact that $\{\chi_i\}$ are real. Property (3.3) follows from the fact that $\sum_{i=1}^N \chi_i = 1$. To prove (3.4) we use Plancherel's Theorem:

$$\begin{aligned} \sum_{\alpha=1}^n F_{ij\alpha\alpha} &= \sum_{k \neq 0} \widehat{\chi}_i(k) \overline{\widehat{\chi}_j(k)} \\ &= \int (\chi_i - \theta_i)(\chi_j - \theta_j) = \Gamma_{ij}. \end{aligned}$$

For (3.5) we observe that

$$\sum F_{ij\alpha\beta} q_{i\alpha} q_{j\beta} = \sum_{k \neq 0} \sum \widehat{\chi}_i(k) \frac{k_\alpha}{|k|} q_{i\alpha} \overline{\widehat{\chi}_j(k) \frac{k_\beta}{|k|} q_{j\beta}},$$

which is a sum of squares. Property (3.6) follows similarly from the observation that

$$\sum_{k \neq 0} \sum \widehat{\chi}_i(k) \left(\delta_{\alpha\gamma} - \frac{k_\alpha k_\gamma}{|k|^2} \right) q_{i\alpha} \overline{\widehat{\chi}_j(k) \left(\delta_{\beta\gamma} - \frac{k_\beta k_\gamma}{|k|^2} \right) q_{j\beta}}$$

is a sum of squares. \square

In view of Proposition 3.1, \mathcal{F}_θ is contained in the set

$$(3.7) \quad \mathcal{F}_\theta^U = \{F = (F_{ij\alpha\beta}) : F \text{ satisfies (3.2)-(3.6)}\}.$$

We therefore deduce

COROLLARY 3.2. (*The ‘‘Geometric Parameters Lower Bound.’’*) For W of the form (1.3),

$$(3.8) \quad QW(\xi) \geq \inf_{\theta \in V} \inf_{F \in \mathcal{F}_\theta^U} \left\{ \sum \theta_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j \right\}.$$

The advantage of (3.8) is that it involves minimization over a set which is known explicitly. Thus (3.8) is a computable lower bound, at least in principle. It is not easy to evaluate, however, because \mathcal{F}_θ^U is defined by inequalities (3.5)-(3.6) as well as linear relations (3.2)-(3.4). We shall make it easier to evaluate in Section 4, for the special case of 3 wells in two space dimensions.

It is interesting to observe that in two space dimensions properties (3.5) and (3.6) are equivalent. This is analogous to the fact that for 2×2 symmetric matrices A , $A \geq 0 \iff (\text{tr} A)I - A \geq 0$ in the sense of quadratic forms.

LEMMA 3.3. *In space dimension $n = 2$, suppose that F satisfies (3.2) and (3.4). Then it satisfies (3.5) iff it satisfies (3.6).*

Proof. Consider the $2N \times 2N$ matrix

$$G = \begin{pmatrix} F_{11} & \dots & F_{1N} \\ \vdots & \ddots & \vdots \\ F_{N1} & \dots & F_{NN} \end{pmatrix},$$

in which F_{ij} represents the 2×2 block $(F_{ij\alpha\beta})_{\alpha,\beta=1,2}$. By (3.2), G is symmetric. Property (3.5) is equivalent to the statement that $G \geq 0$. This holds for G iff it holds for any matrix similar to G . Let $R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, and consider the $2N \times 2N$ rotation

$$M = \begin{pmatrix} R & & 0 \\ & \ddots & \\ 0 & & R \end{pmatrix}.$$

Noting that $R^T A R = (\text{tr} A)I - A$ for any symmetric 2×2 matrix, and making use of (3.4), we find that

$$M^T G M = \begin{pmatrix} \Gamma_{11}I - F_{11} & \dots & \Gamma_{1N}I - F_{1N} \\ \vdots & \ddots & \vdots \\ \Gamma_{N1}I - F_{N1} & \dots & \Gamma_{NN}I - F_{NN} \end{pmatrix}.$$

The positivity of $M^T G M$ is equivalent to (3.6). \square

We deduce as a consequence

COROLLARY 3.4. *In space dimension two, the set \mathfrak{F}_θ^U is invariant under the map*

$$F_{ij\alpha\beta} \rightarrow \Gamma_{ij}\delta_{\alpha\beta} - F_{ij\alpha\beta}.$$

It is well-known that the convexification of W always provides a lower bound for QW . As a partial confirmation that (3.8) is a good bound, we now verify that it always lies above the convexification.

LEMMA 3.5. *Let CW denote the convexification of W . Then*

$$(3.9) \quad \sum \theta_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j \geq CW(\xi)$$

for any $\theta \in V$ and any $F \in \mathfrak{F}_\theta^U$. In particular, the ‘‘geometric parameters lower bound’’ is greater than or equal to CW .

Proof. First let us show that

$$(3.10) \quad CW(\xi) = \inf_{\theta \in V} |\xi - \sum \theta_i a^i|^2.$$

Indeed, for any W one has

$$CW(\xi) = \inf_{\int \lambda d\mu(\lambda) = \xi} \int W(\lambda) d\mu(\lambda),$$

in which μ ranges over probability measures on the space of $m \times n$ matrices, see e.g. [9]. Since each “well” $|\xi - a^i|^2$ is convex, an easy application of Jensen’s inequality shows that the optimal μ will be a sum of N point masses. It follows that

$$CW(\xi) = \inf_{\sum \theta_i \xi_i = \xi} \sum \theta_i |\xi_i - a^i|^2,$$

where $\theta = (\theta_1, \dots, \theta_N)$ ranges over V and ξ_i over $m \times n$ matrices. Optimization over ξ_i (with θ held fixed) yields (3.10).

Now let us rearrange the expression in (3.10):

$$\begin{aligned} |\xi - \sum \theta_i a^i|^2 &= |\xi|^2 - 2\langle \xi, \sum_i \theta_i a^i \rangle + \sum_{i,j} \theta_i \theta_j \langle a^i, a^j \rangle \\ (3.11) \quad &= \sum_i \theta_i |\xi - a^i|^2 - \sum_i \theta_i |a^i|^2 + \sum_{i,j} \theta_i \theta_j \langle a^i, a^j \rangle \\ &= \sum \theta_i |\xi - a^i|^2 - \sum \Gamma_{ij} \delta_{\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j. \end{aligned}$$

We use (3.6) and (3.11) to bound the left hand side of (3.9):

$$\begin{aligned} (3.12) \quad \sum \theta_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j &\geq \sum \theta_i |\xi - a^i|^2 - \sum \Gamma_{ij} \delta_{\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j \\ &= |\xi - \sum \theta_i a^i|^2 \\ &\geq CW(\xi), \end{aligned}$$

as asserted. \square

A crucial question is whether or not $\mathcal{F}_\theta = \mathcal{F}_\theta^U$. This remains open. An affirmative answer would provide, for each $F \in \mathcal{F}_\theta^U$, a microstructure whose tensor of geometric parameters is equal to F . To make progress in this direction, it is important to look for microstructures whose tensors of geometric parameters are explicitly computable. One such class are the microstructures obtained by *sequential lamination*. That construction has played a central role in recent work on the effective moduli of composites, see e.g. [2,22,28]. In the present context the construction is as follows: consider any pair of microstructures, with possibly different volume fractions $\theta', \theta'' \in V$, and with tensors of geometric parameters $F' \in \mathcal{F}_{\theta'}$, $F'' \in \mathcal{F}_{\theta''}$. We construct a new microstructure by layering the two with one another, using volume fractions ρ and $1 - \rho$ respectively, in layers orthogonal to some unit vector k . If the length scale of the microstructure is small compared to the length scale of the layering, then the geometric parameters of the new microstructure depend only on $F', F'', \theta', \theta'', \rho$, and k :

PROPOSITION 3.6. Suppose that $F' \in \mathcal{F}_\theta$, $F'' \in \mathcal{F}_{\theta''}$. For any ρ , $0 < \rho < 1$, and any unit vector k , consider the microstructure associated with “layering F' and F'' in volume fractions ρ , $1 - \rho$ with layers orthogonal to k ,” as described in more detail above. It has volume fractions

$$(3.13) \quad \theta_i = \rho\theta'_i + (1 - \rho)\theta''_i$$

and its tensor of geometric parameters is

$$(3.14) \quad F_{ij\alpha\beta} = \rho F'_{ij\alpha\beta} + (1 - \rho)F''_{ij\alpha\beta} + \rho(1 - \rho)(\theta'_i - \theta''_i)(\theta'_j - \theta''_j)k_\alpha k_\beta.$$

Proof. Assertion (3.13) is elementary. Assertion (3.14) follows by (2.16) from the analogous layering formula for H -measures, see formula (8.16) of [17]. \square

An important corollary of the layering formula is the convexity of \mathcal{F}_θ :

COROLLARY 3.7. For any $\theta \in V$, \mathcal{F}_θ is convex.

Proof. Let $F', F'' \in \mathcal{F}_\theta$. Then (since both have the *same* volume fractions) (3.13)-(3.14) give

$$F = \rho F' + (1 - \rho)F'' \in \mathcal{F}_\theta$$

for any ρ , $0 < \rho < 1$. Notice that in this case the result of layering is independent of the direction of the layers. \square

The term “sequential lamination” arises from the observation that the layering process can be repeated any numbers of times. We begin with the N “pure” phases, described by $F \equiv 0$ and $\theta = (0, \dots, 1, \dots, 0)$. (The 1 is in the i th place for the i th phase.) One says a microstructure is “sequentially laminated of rank r ” if it is obtained from these by r applications of the layering construction. We denote by \mathcal{F}_θ^L the set of all geometric parameters attainable by sequential lamination. Since the layering formula generally mixes microstructures with different volume fractions, \mathcal{F}_θ^L is best described as the slice at $\theta \in V$ of a set in the product space of { volume fractions } \times { geometric parameters }:

$$(3.15) \quad \mathcal{F}_\theta^L = \text{slice at } \theta \in V \text{ of the smallest closed set of pairs } (\theta, F) \text{ that contains the } N \text{ pure phases and is preserved under application of the layering procedure (3.13) - (3.14).}$$

We do not have an explicit representation of \mathcal{F}_θ^L .

Since $\mathcal{F}_\theta^L \subset \mathcal{F}_\theta$, we could formulate an associated upper bound for QW :

$$(3.16) \quad QW(\xi) \leq \inf_{\theta \in V} \inf_{F \in \mathcal{F}_\theta^L} \left\{ \sum \theta_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j \right\}.$$

This is not a new bound, however: the right side of (3.16) is precisely the rank-one convexification of W . Indeed, for any W the rank-one convexification can be characterized as the best upper bound achievable by a sequentially laminated microstructure [8,18,23]. The right hand side of (3.16) is the same thing, specialized to W of the form (1.3) and phrased in terms of geometric parameters.

To recapitulate, the main goal is to find \mathcal{F}_θ . We have described sets \mathcal{F}_θ^L and \mathcal{F}_θ^U such that

$$\mathcal{F}_\theta^L \subseteq \mathcal{F}_\theta \subseteq \mathcal{F}_\theta^U.$$

We shall show in Section 5 that the inclusion $\mathcal{F}_\theta^L \subset \mathcal{F}_\theta^U$ is strict, for some choices of $\theta \in V$, in the context of three wells and two space dimensions. It remains a possibility that $\mathcal{F}_\theta^L = \mathcal{F}_\theta$; in this case the list of properties (3.2) - (3.6) is incomplete. It is also a possibility that $\mathcal{F}_\theta = \mathcal{F}_\theta^U$; in that case the class of sequentially laminated microstructures is not rich enough to include an energetically optimal configuration. Finally, it might be the case that both inequalities are strict. The question whether $\mathcal{F}_\theta^L = \mathcal{F}_\theta$ corresponds to asking whether, for W of the form (1.3), the quasiconvexification equals the rank-one convexification. The question whether $\mathcal{F}_\theta^U = \mathcal{F}_\theta$ is analogous to (but apparently different from) asking whether, for such W , the quasiconvexification equals the polyconvexification.

4. Extreme Points for Three Wells in Two Dimensions. This section determines the extreme points of the convex set \mathcal{F}_θ^U in the special case of three wells and two space dimensions. The restriction $N = 3$, $n = 2$ applies through the section.

We have already observed in Lemma 3.3 that it is useful to view a tensor of geometric parameters as a block matrix:

$$(4.1) \quad F = \begin{pmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{pmatrix}$$

where F_{ij} represents the 2×2 block $F_{ij\alpha\beta}$. By (3.2)-(3.3) each block is symmetric, and there are only three independent blocks:

$$(4.2) \quad F = \begin{pmatrix} A & B & -A - B \\ B & C & -B - C \\ -A - B & -B - C & A + 2B + C \end{pmatrix}$$

with $A = F_{11}$, $B = F_{12}$, $C = F_{22}$. Condition (3.4) is equivalent to

$$(4.3) \quad \text{tr} A = \theta_1(1 - \theta_1), \quad \text{tr} B = -\theta_1\theta_2, \quad \text{tr} C = \theta_2(1 - \theta_2).$$

The following proposition gives conditions on A, B , and C which are equivalent to F satisfying (3.2) - (3.6).

PROPOSITION 4.1. For $N = 3$, $n = 2$, the set \mathcal{F}_θ^U is in 1 – 1 correspondence with the triplets of symmetric, 2×2 matrices (A, B, C) that satisfy the trace relations (4.3) and the following positivity condition:

$$(4.4) \quad \langle Ax, x \rangle + 2\langle Bx, y \rangle + \langle Cy, y \rangle \geq 0 \quad \text{for all } x, y \in \mathbb{R}^2.$$

Proof. We have only to prove that (4.4) is equivalent to (3.5) - (3.6). By Lemma 3.3, (3.5) and (3.6) are equivalent, so it suffices to consider (3.5). Written in terms of A, B , and C , this condition asserts that

$$(4.5) \quad \begin{aligned} &\langle Ax, x \rangle + \langle By, y \rangle + \langle (A + 2B + C)z, z \rangle \\ &+ 2\langle Bx, y \rangle - 2\langle (A + B)x, z \rangle - 2\langle (B + C)y, z \rangle \geq 0 \end{aligned}$$

for every $x, y, z \in \mathbb{R}^2$. Clearly (4.5) implies (4.4) by taking $z = 0$. On the other hand, (4.5) can also be written as

$$\langle A(x - z), x - z \rangle + 2\langle B(x - z), y - z \rangle + \langle C(y - z), y - z \rangle \geq 0.$$

This condition is implied by (4.4). \square

Let us examine the positivity condition (4.4) more closely. If A is invertible then (4.4) holds if and only if

$$(4.6) \quad A \geq 0, C \geq 0, \text{ and } C - BA^{-1}B \geq 0$$

in the sense of quadratic forms. (Actually, the condition $C \geq 0$ in (4.6) is redundant, since $BA^{-1}B \geq 0$.) Indeed, it is obvious that (4.4) implies $A \geq 0$ and $C \geq 0$. If we rewrite (4.4) as

$$(4.7) \quad |A^{1/2}x + A^{-1/2}By|^2 + \langle (C - BA^{-1}B)y, y \rangle \geq 0,$$

then the positivity of the Schur complement $C - BA^{-1}B$ becomes clear as well. Conversely, (4.6) clearly implies (4.7) and hence also (4.4).

When A is not invertible, we can retain the equivalence of (4.4) and (4.6) by interpreting the latter properly. Specifically, we interpret “ $C - BA^{-1}B \geq 0$ ” as the assertion that

$$(4.8) \quad \lim_{\varepsilon \downarrow 0} C - B(A + \varepsilon I)^{-1}B \geq 0.$$

Since (4.4) is a closed condition, one easily checks that (4.6) (with the convention (4.8)) is equivalent to (4.4) even when A is not invertible.

Condition (4.8) really amounts to two separate assertions:

(4.9) The range of B is contained in the range of A ; and

$$(4.10) \quad C - BA^+B \geq 0,$$

where A^+ is the Moore-Penrose inverse of A , i.e. the inverse of the operator obtained by restricting A to the orthogonal complement of its kernel (which is also its range, since A is symmetric). In our 2×2 setting A fails to be invertible only if $A = 0$ or if A has rank 1: $A = \alpha k \otimes k$, $\alpha > 0$, $|k| = 1$. In the former case (4.9) forces $B = 0$; in the latter case it forces $B = \beta k \otimes k$, and (4.10) becomes $C - (\beta^2/\alpha)k \otimes k \geq 0$. We note that when A is not invertible, the quadratic form (4.4) can still be written in the form (4.7) provided that (4.8) holds; here “ $A^{-1/2}$ ” must be interpreted as the nonnegative, symmetric square root of A^+ .

All the above remarks apply just as well when the roles of A and C are interchanged. In particular, (4.4) is also equivalent to

$$(4.11) \quad A \geq 0, \quad C \geq 0, \quad A - BC^{-1}B \geq 0,$$

with the convention analogous to (4.8) when C is not invertible.

Our classification of the extreme points will make use of the following well-known fact.

LEMMA 4.2. *Let \mathbf{M}_+ denote the set of nonnegative, symmetric, $n \times n$ matrices with trace 1. Then the extreme points of \mathbf{M}_+ are precisely the rank-one matrices $k \otimes k$ with $|k| = 1$.*

Proof. To see that $k \otimes k$ is extreme, suppose $k \otimes k = \rho M_1 + (1-\rho)M_2$ with $M_1, M_2 \in \mathbf{M}_+$. Then $\langle M_1 v, v \rangle = \langle M_2 v, v \rangle = 0$ for any $v \perp k$, and it follows that $M_1 = M_2 = k \otimes k$. There can be no other extreme points, because the spectral decomposition of any $M \in \mathbf{M}_+$ expresses it as a convex combination of rank-one matrices. \square

We are now ready to classify the extreme points of \mathfrak{F}_θ^U .

THEOREM 4.3. *Let (A, B, C) be a triplet of matrices corresponding to a point of \mathfrak{F}_θ^U . They correspond to an extreme point precisely if they fall in one of the following three classes.*

- *Extreme points of type 1:*

$$(4.12) \quad A = \theta_1(1 - \theta_1)k \otimes k, \quad B = -\theta_1\theta_2k \otimes k, \quad C = \theta_2(1 - \theta_2)k \otimes k$$

for some unit vector k .

- *Extreme points of type 2: either*

$$(4.13) \quad \begin{aligned} A &= \theta_1(1 - \theta_1)k \otimes k, & B &= -\theta_1\theta_2k \otimes k \\ C &= \frac{\theta_1^2\theta_2^2}{\theta_1(1 - \theta_1)}k \otimes k + \left[\theta_2(1 - \theta_2) - \frac{\theta_1^2\theta_2^2}{\theta_1(1 - \theta_1)} \right] l \otimes l \end{aligned}$$

or else

$$(4.14) \quad \begin{aligned} C &= \theta_2(1 - \theta_2)k \otimes k, & B &= -\theta_1\theta_2k \otimes k \\ A &= \frac{\theta_1^2\theta_2^2}{\theta_2(1 - \theta_2)}k \otimes k + \left[\theta_1(1 - \theta_1) - \frac{\theta_1^2\theta_2^2}{\theta_2(1 - \theta_2)} \right] l \otimes l \end{aligned}$$

for some unit vectors k and l .

- *Extreme points of type 3:* A and B are both invertible, $A^{-1}B \neq \lambda I$ for $\lambda \in \mathbb{R}$, and $C = BA^{-1}B$.

Proof. Suppose first that $A = 0$. Then the trace relations (4.3) force $\theta_1 = 0$ or 1 and $B = 0$. The trace relations (4.3) and the positivity condition (4.6) permit any C with $C \geq 0$ and $\text{tr}C = \theta_2(1 - \theta_2)$. By Lemma 4.2, the only such extreme point is

$$A = 0, \quad B = 0, \quad C = \theta_2(1 - \theta_2)k \otimes k$$

for some $|k| = 1$. (It is simultaneously of types 1 and 2 due to the degeneracy $\theta_1 = 0$ or $\theta_1 = 1$.)

Next, suppose that A has rank one: $A = \theta_1(1 - \theta_1)k \otimes k$ with $|k| = 1$. By (4.3) and (4.6), B and C must satisfy $B = -\theta_1\theta_2k \otimes k$ and

$$(4.15) \quad C - \frac{\theta_1^2\theta_2^2}{\theta_1(1 - \theta_1)}k \otimes k \geq 0.$$

If the left side of (4.15) is strictly positive definite then C can be expressed as a convex combination of matrices satisfying both (4.15) and the trace condition. So if (A, B, C) is extreme then the left side of (4.15) equals zero or has rank one. These two alternatives correspond to (4.12) and (4.13) respectively. Let us check that such points are indeed extreme. If (A, B, C) are as in (4.12), consider a convex combination

$$(A, B, C) = \rho(A_1, B_1, C_1) + (1 - \rho)(A_2, B_2, C_2).$$

Since the volume fraction θ is fixed, Lemma 4.2 yields $A_1 = A_2 = A$ and $C_1 = C_2 = C$. Since A has rank one, we also have $B_1 = B_2 = B$. Thus points of the form (4.12) are extreme. Similarly, suppose that (A, B, C) are as in (4.13) and consider a convex combination as above. Lemma 4.2 still yields $A_1 = A_2 = A$, and it still follows that $B_1 = B_2 = B$. So C_1 and C_2 must satisfy the analogue of (4.15). An application of Lemma 4.2 shows that $C_1 = C_2 = C$, since the left hand side of (4.15) has rank one. Thus points of the form (4.13) are extreme.

If A is nonsingular but C is singular then we can repeat the preceding arguments with A replaced by C . This leads to either (4.12) or (4.14).

Now suppose that A and C are both nonsingular. If in addition $C - BA^{-1}B > 0$ then (A, B, C) lies in the interior of the region determined by the positivity condition (4.6); it is easy to see that such (A, B, C) are not extreme points. If $C - BA^{-1}B$ has rank one, then we see that (A, B, C) is not an extreme point as follows. Let $y_0 \neq 0$ satisfy $(C - BA^{-1}B)y_0 = 0$ and set $x_0 = -A^{-1}By_0$. Next, choose symmetric matrices A_0, B_0 , and C_0 such that

$$(4.16) \quad \begin{aligned} \langle A_0 x_0, x_0 \rangle &= 0, & \langle B_0 x_0, y_0 \rangle &= 0, & \langle C_0 y_0, y_0 \rangle &= 0 \\ \text{tr} A_0 &= \text{tr} B_0 = \text{tr} C_0 &= 0. \end{aligned}$$

Let $Q(x, y)$ denote the quadratic form in (4.4):

$$(4.17) \quad Q(x, y) = \langle Ax, x \rangle + 2\langle Bx, y \rangle + \langle Cy, y \rangle.$$

Our special choice of A_0, B_0, C_0 assures that

$$(4.18) \quad Q(x, y) \geq c \{ |\langle A_0 x, x \rangle| + |\langle B_0 x, y \rangle| + |\langle C_0 y, y \rangle| \}$$

for all $x, y \in \mathbf{R}^2$ if the constant $c > 0$ is chosen sufficiently small. Indeed, if (4.18) were to fail for every $c > 0$ then there would exist $x_1, y_1 \in \mathbf{R}^2$ such that $Q(x_1, y_1) = 0$ and

$$(4.19) \quad |\langle A_0 x_1, x_1 \rangle| + |\langle B_0 x_1, y_1 \rangle| + |\langle C_0 y_1, y_1 \rangle| = 1.$$

From (4.7) we see that $Q(x_1, y_1) = 0$ implies $x_1 = \lambda x_0$ and $y_1 = \lambda y_0$ for some $\lambda \in \mathbf{R}$, so (4.19) contradicts (4.16). Thus (4.18) holds for some $c > 0$. It follows that $(A \pm \varepsilon A_0, B \pm \varepsilon B_0, C \pm \varepsilon C_0)$ satisfies (4.6) when ε is sufficiently small. So

$$(A, B, C) = \frac{1}{2}(A + \varepsilon A_0, B + \varepsilon B_0, C + \varepsilon C_0) + \frac{1}{2}(A - \varepsilon A_0, B - \varepsilon B_0, C - \varepsilon C_0)$$

is not an extreme point.

We have shown that for A and C invertible, the only possibility of an extreme point is when $C = BA^{-1}B$. If it should happen that $A^{-1}B = \lambda I$, then this is not an extreme point. Indeed, if $B = \lambda A$ and $C = BA^{-1}B = \lambda^2 A$, then the positivity condition (4.4) becomes

$$\langle A(x + \lambda y), x + \lambda y \rangle \geq 0,$$

which holds whenever A is positive definite. Choosing any matrix δA such that $\text{tr} \delta A = 0$ and $A + \delta A \geq 0$, we have

$$\begin{aligned} (A, \lambda A, \lambda^2 A) &= \frac{1}{2}(A + \delta A, \lambda(A + \delta A), \lambda^2(A + \delta A)) \\ &\quad + \frac{1}{2}(A - \delta A, \lambda(A - \delta A), \lambda^2(A - \delta A)), \end{aligned}$$

so $(A, \lambda A, \lambda^2 A)$ is not an extreme point. We note that this exceptional case can occur only for certain θ : the trace relations (4.3) force $\lambda = -\theta_2/(1 - \theta_1)$ and $\theta_1\theta_2 = (1 - \theta_1)(1 - \theta_2)$.

The only remaining task is to show that our “extreme points of type 3” are indeed extreme. Consider a convex combination

$$(A, B, C) = \rho(A_1, B_1, C_1) + (1 - \rho)(A_2, B_2, C_2).$$

Since A, B , and C are nonsingular, we may suppose without loss of generality that A_i, B_i , and C_i are also nonsingular. As a first step we shall show that $C_i = B_i A_i^{-1} B_i$ and $A_i^{-1} B_i = A^{-1} B$ for $i = 1, 2$. Indeed, consider the quadratic form $Q(x, y)$ associated to (A, B, C) , defined by (4.17), and the analogous forms $Q_i(x, y)$ associated to (A_i, B_i, C_i) . Since $C = BA^{-1}B$,

$$Q(x, y) = |A^{1/2}x + A^{-1/2}By|^2,$$

which vanishes on the subspace $x = -A^{-1}By$. Since each Q_i is nonnegative, Q_1 and Q_2 must vanish on this subspace. We have

$$Q_1(x, y) = |A_1^{1/2}x + A_1^{-1/2}By|^2 + \langle (C_1 - B_1 A_1^{-1} B_1)y, y \rangle.$$

As y varies over R^2 with $x = -A^{-1}By$ this forces $C_1 = B_1 A_1^{-1} B_1$ and $A_1^{-1} B_1 = A^{-1} B$. The same argument shows that $C_2 = B_2 A_2^{-1} B_2$ and $A_2^{-1} B_2 = A^{-1} B$.

Let $e_i, i = 1, 2$, be the generalized eigenvectors

$$\begin{aligned} B e_1 &= -\lambda_1 A e_1 \\ B e_2 &= -\lambda_2 A e_2 \end{aligned}$$

with $\langle A e_1, e_1 \rangle = \langle A e_2, e_2 \rangle = 1$ and $\langle A e_1, e_2 \rangle = 0$. Notice that $\lambda_1 \neq \lambda_2$, since otherwise we would have $A^{-1}B = -\lambda I$. From the preceding paragraph we deduce that

$$\begin{aligned} B_i e_1 &= -\lambda_1 A_i e_1 \\ B_i e_2 &= -\lambda_2 A_i e_2 \end{aligned}$$

for $i = 1, 2$. Since the eigenvalues are distinct, this forces

$$\langle B_i e_1, e_2 \rangle = 0, \quad \langle A_i e_1, e_2 \rangle = 0,$$

using the symmetry of A_i and B_i .

We return now to the quadratic forms $Q(x, y)$, $Q_1(x, y)$, and $Q_2(x, y)$. Consider the associated forms on R^2 defined by

$$\tilde{Q}(s, t) = Q(se_1, te_1) = \begin{pmatrix} s \\ t \end{pmatrix}^T \begin{pmatrix} \langle A e_1, e_1 \rangle & \langle B e_1, e_1 \rangle \\ \langle B e_1, e_1 \rangle & \langle B A^{-1} B e_1, e_1 \rangle \end{pmatrix} \begin{pmatrix} s \\ t \end{pmatrix},$$

and similarly for \tilde{Q}_1, \tilde{Q}_2 . By the preceding paragraph, all three forms vanish on the one-dimensional subspace $s = \lambda_1 t$. By hypothesis they are all nonnegative, and

$$\tilde{Q} = \rho \tilde{Q}_1 + (1 - \rho) \tilde{Q}_2.$$

It follows that the matrices associated to \tilde{Q}_1 and \tilde{Q}_2 are multiples of that associated to \tilde{Q} . Thus

$$\begin{aligned} \begin{pmatrix} \langle A_1 e_1, e_1 \rangle & \langle B_1 e_1, e_1 \rangle \\ \langle B_1 e_1, e_1 \rangle & \langle B_1 A_1^{-1} B_1 e_1, e_1 \rangle \end{pmatrix} &= \mu_1 \begin{pmatrix} \langle A e_1, e_1 \rangle & \langle B e_1, e_1 \rangle \\ \langle B e_1, e_1 \rangle & \langle B A^{-1} B e_1, e_1 \rangle \end{pmatrix} \\ &= \mu_1 \begin{pmatrix} 1 & -\lambda_1 \\ -\lambda_1 & \lambda_1^2 \end{pmatrix}. \end{aligned}$$

A similar relation holds for A_2 and B_2 , with a different constant μ_2 . Summarizing this information, we have:

$$\begin{aligned} \langle A_1 e_1, e_1 \rangle &= \mu_1, & \langle B_1 e_1, e_1 \rangle &= -\mu_1 \lambda_1, \\ \langle A_2 e_1, e_1 \rangle &= \mu_2, & \langle B_2 e_1, e_1 \rangle &= -\mu_2 \lambda_1, \end{aligned}$$

A parallel argument using e_2 in place of e_1 gives

$$\begin{aligned} \langle A_1 e_2, e_2 \rangle &= \nu_1, & \langle B_1 e_2, e_2 \rangle &= -\nu_1 \lambda_2 \\ \langle A_2 e_2, e_2 \rangle &= \nu_2, & \langle B_2 e_2, e_2 \rangle &= -\nu_2 \lambda_2, \end{aligned}$$

for two new constants ν_1, ν_2 .

We claim that the trace relations force $\mu_1 = \mu_2 = \nu_1 = \nu_2 = 1$. Indeed, since e_1 and e_2 span \mathbf{R}^2 , $e_1 \otimes e_1, e_2 \otimes e_2$, and $(e_1 \otimes e_2 + e_2 \otimes e_1)/2$ span the space of symmetric 2×2 matrices. So there are constants α, β , and γ such that

$$I = \alpha e_1 \otimes e_1 + \beta e_2 \otimes e_2 + \frac{\gamma}{2}(e_1 \otimes e_2 + e_2 \otimes e_1).$$

The above relations give

$$\begin{aligned} \operatorname{tr} A &= \alpha + \beta & \operatorname{tr} B &= -(\lambda_1 \alpha + \lambda_2 \beta) \\ \operatorname{tr} A_1 &= \alpha \mu_1 + \beta \nu_1 & \operatorname{tr} B_1 &= -(\lambda_1 \alpha \mu_1 + \lambda_2 \beta \nu_1) \\ \operatorname{tr} A_2 &= \alpha \mu_2 + \beta \nu_2 & \operatorname{tr} B_2 &= -(\lambda_1 \alpha \mu_2 + \lambda_2 \beta \nu_2). \end{aligned}$$

Setting the traces equal gives

$$\begin{aligned} \alpha(\mu_1 - 1) + \beta(\nu_1 - 1) &= 0, & \alpha(\mu_2 - 1) + \beta(\nu_2 - 1) &= 0, \\ \lambda_1 \alpha(\mu_1 - 1) + \lambda_2 \beta(\nu_1 - 1) &= 0, & \lambda_1 \alpha(\mu_2 - 1) + \lambda_2 \beta(\nu_2 - 1) &= 0. \end{aligned}$$

Since $\lambda_1 \neq \lambda_2$, the only solution is $\mu_1 = \mu_2 = \nu_1 = \nu_2 = 1$.

We have thus shown that $\langle A_i e_1, e_1 \rangle = \langle A_i e_2, e_2 \rangle = 1$ and $\langle A_i e_1, e_2 \rangle = 0$ for $i = 1, 2$. It follows that $A_1 = A_2 = A$ and $B_1 = B_2 = B$. Therefore the point (A, B, C) under consideration is an extreme point. \square

We have been unable to find a microstructure corresponding to any extreme point of type 3. However, the extreme points of types 1 and 2 are easily realized using sequential lamination. To achieve (4.12), we first layer pure phases 1 and 2 in volume fractions $\rho = \theta_1/(\theta_1 + \theta_2)$ and $1 - \rho = \theta_2/(\theta_1 + \theta_2)$ using layers normal to k . Representing F as a block matrix as in (4.1), the layering formula (3.14) gives

$$F = \rho(1 - \rho) \begin{pmatrix} k \otimes k & -k \otimes k & 0 \\ -k \otimes k & k \otimes k & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

for the result. Its volume fractions are of course $(\rho, 1 - \rho, 0)$. Now we layer pure phase 3 with this, using volume fractions θ_3 and $1 - \theta_3$ respectively, and still using layers normal to k . The result has volume fractions

$$\theta_3(0, 0, 1) + (1 - \theta_3)(\rho, 1 - \rho, 0) = (\theta_1, \theta_2, \theta_3).$$

Its geometric parameters are seen, after some calculation, to be in agreement with (4.12).

The construction leading to a type 2 extreme point is similar. To achieve (4.13) we first layer pure phases 2 and 3 in volume fractions $\rho = \theta_2/(\theta_2 + \theta_3)$ and $(1 - \rho) = \theta_3/(\theta_2 + \theta_3)$ respectively, using layers normal to l . The result has volume fractions $(0, \rho, 1 - \rho)$ and geometric parameters

$$F = \rho(1 - \rho) \begin{pmatrix} 0 & 0 & 0 \\ 0 & l \otimes l & -l \otimes l \\ 0 & -l \otimes l & l \otimes l \end{pmatrix}.$$

Now we layer pure phase 1 with this, using volume fractions θ_1 and $1 - \theta_1$ respectively, and using layers normal to k . The result has volume fractions

$$\theta_1(1, 0, 0) + (1 - \theta_1)(0, \rho, 1 - \rho) = (\theta_1, \theta_2, \theta_3).$$

Its geometric parameters are seen, after some calculation, to be in agreement with (4.13). An analogous construction can be used to achieve (4.14).

To understand the nature of the type 3 extreme points better, it is interesting to consider those for which A, B , and C are simultaneously diagonal. This class will play a special role in Section 5. They have the form

$$(4.20) \quad \begin{pmatrix} A & B \\ B & C \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix} & \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix} \\ \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix} & \begin{pmatrix} b_1^2/a_1 & 0 \\ 0 & b_2^2/a_2 \end{pmatrix} \end{pmatrix}$$

with $a_1 > 0$, $a_2 > 0$, $b_1 \neq 0$, $b_2 \neq 0$, and $b_1/a_1 \neq b_2/a_2$. The trace relations require

$$(4.21) \quad \begin{aligned} a_1 + a_2 &= \theta_1(1 - \theta_1), & b_1 + b_2 &= -\theta_1\theta_2, \\ b_1^2/a_1 + b_2^2/a_2 &= \theta_2(1 - \theta_2). \end{aligned}$$

A convenient way to classify the solutions of (4.21) is to seek them in the form $a_1 = \lambda b_1$, $a_2 = \mu b_2$, for some $\lambda \neq \mu \in \mathbf{R}$. Then (4.21) becomes

$$\begin{aligned} b_1 + b_2 &= -\theta_1\theta_2, & \lambda b_1 + \mu b_2 &= \theta_1(1 - \theta_1), \\ \lambda^{-1}b_1 + \mu^{-1}b_2 &= \theta_2(1 - \theta_2). \end{aligned}$$

These are three independent equations in two unknowns b_1 , b_2 . They are consistent precisely if

$$(4.22) \quad (\lambda + 1)(\mu + 1)\theta_1\theta_2 + \theta_1\theta_3 + \lambda\mu\theta_2\theta_3 = 0,$$

and in that case they imply

$$(4.23) \quad \begin{aligned} a_1 &= \frac{\lambda}{\lambda - \mu} [\theta_1\theta_3 + (\mu + 1)\theta_1\theta_2] \\ a_2 &= \frac{-\mu}{\lambda - \mu} [\theta_1\theta_3 + (\lambda + 1)\theta_1\theta_2]. \end{aligned}$$

We want $a_1 \neq 0$ and $a_2 \neq 0$, so λ and μ should be non-zero. We also want $\lambda \neq \mu$. If

$$(4.24) \quad (\lambda + 1)(\mu + 1) \geq 0 \text{ and } \lambda\mu > 0$$

then each term in (4.22) must vanish separately; it is easy to see that this cannot yield an extreme point of type 3. If however

$$(4.25) \quad (\lambda + 1)(\mu + 1) < 0 \quad \text{or} \quad \lambda\mu < 0$$

then (4.22) has a one-parameter family of solutions $\theta \in V$. A tedious but straightforward calculation shows that the resulting values of a_1 and a_2 , given by (4.23), are always positive. We have thus proved:

PROPOSITION 4.4. *Let λ and μ be given, with $\lambda \neq 0$, $\mu \neq 0$, and $\lambda \neq \mu$. If (4.24) holds then there is no type 3 extreme point of the form (4.20) with $a_1 = \lambda b_1$ and $a_2 = \mu b_2$. If on the other hand (4.25) holds, then there are type 3 extreme points of the form (4.20) with $a_1 = \lambda b_1$ and $a_2 = \mu b_2$. In fact there is one such extreme point in \mathcal{F}_θ^U whenever $\theta \in V$ satisfies (4.22).*

We chose this section with an observation that will be useful in Section 5.

LEMMA 4.5. *The map $F_{ij\alpha\beta} \mapsto \Gamma_{ij}\delta_{\alpha\beta} - F_{ij\alpha\beta}$ takes type k extreme points to type k extreme points for each $k = 1, 2, 3$.*

Proof. We know from Corollary 3.4 that this map preserves \mathcal{F}_θ^U . It is also affine and invertible, so it takes extreme points to extreme points. One verifies readily that $F_{11\alpha\beta}$ has rank 2 exactly if $\Gamma_{11}\delta_{\alpha\beta} - F_{11\alpha\beta}$ has rank 2, and similarly for $F_{22\alpha\beta}$. The desired conclusion follows easily from the character of the extreme points, c.f. (4.12) - (4.14). \square

5. The Three Gradient Problem. In this section we consider W of the form (1.3), with three wells in two space dimensions, under the further hypothesis that $a^i - a^j$ has rank 2 for each $i \neq j$. Our attention is focused on the question: is QW strictly positive for $\xi \notin \{a^i\}$? This question remains open, despite recent progress by Pedregal [23] and Šverák [27]. We do not solve it. Rather, we show a direct link between this problem and the attainability of our type 3 extreme points.

We begin with a digression, to set this discussion in its proper mathematical context. One reason for studying this “three gradient problem” is its analogy to the variational theory of phase transitions. In that setting it is an important task to identify all “macroscopically stress-free states.” In other words, suppose that W has the form (1.1), and that each W_i has minimum value zero. Then one wants to know the exact set where $QW(\xi) = 0$. This is among the principal goals of [4,5]; there each W_i is assumed to be frame-invariant, as is appropriate for geometrically nonlinear elasticity. The analogous question in a geometrically linear setting is addressed for example in [6] and [17]. Our attention here is on the corresponding question for “gradients,” i.e. for energies of the form (1.3).

The “three gradient problem” is also of interest because it promises to shed light on the relationship between polyconvexity, rank-one convexity, and quasiconvexity. It is well-known that $PW \leq QW \leq RW$, where PW is the polyconvexification of W and RW is the rank-one convexification of W [9]. For a three-well energy with appropriately chosen “wells” $\{a^i\}$, it can happen that PW vanishes on a one-dimensional curve in the space of all matrices, while $RW(\xi) > 0$ for $\xi \notin \{a^i\}$ [23,27]. Knowing where QW vanishes could give some indication of whether $QW = PW$ or $QW = RW$ in this case.

Some of the relevant mathematical literature avoids discussing a relaxed energy, focussing instead on other concepts such as Young measures. To clarify the relation between such work and ours, we note some consequences of the assertion that $QW(\xi) = 0$. First, from the definition (1.1), if $QW(\xi) = 0$ then for every $\varepsilon, \delta > 0$ there exists $u : \Omega \rightarrow \mathbf{R}^m$ with affine boundary values $u|_{\partial\Omega} = \xi \cdot x$ such that

$$(5.1) \quad \text{meas}\{x : |\nabla u - a^i|^2 \geq \varepsilon \text{ for all } i\} \leq \delta.$$

Thus, loosely speaking, if $QW(\xi) = 0$ then a gradient field can have average value ξ and yet “approximately take only the values $a^i, 1 \leq i \leq N$.” A second conclusion amounts to the same thing in different language: if $QW(\xi) = 0$ then there is a Young-measure limit of

gradients with mean value ξ , whose support is contained in $\{a_i\}_{1 \leq i \leq N}$. This is immediate from (1.2), by taking the Young-measure limit of a minimizing sequence. (See [3] and the references there for basic facts about Young measures, and [16] for more about the relation between quasiconvexity and Young measures.) The statement that $QW(\xi) = 0$ actually carries somewhat more information than (5.1). Among energies with super- or sub-quadratic growth

$$W(\nabla u) = \min_{1 \leq i \leq N} \{|\nabla u - a^i|^p\},$$

one might expect the set where $QW(\xi) = 0$ to depend on the value of p . Actually, it does not: motivated by a result of Šverák [26], Zhang [30] has shown, (under the hypothesis that the set where $W(\xi) = 0$ has compact support, which certainly applies in the case we are considering), that the set where $QW(\xi) = 0$ is independent of $1 \leq p < \infty$. In any case, we focus here on $p = 2$ because that is the case in which Fourier transform-based methods apply.

In any spatial dimension, and for any number of wells, we say that a^i and a^j are *compatible* if their difference has rank one. It is easy to see that if a^i and a^j are compatible for some $i \neq j$, then QW vanishes along the line segment joining a^i to a^j . The associated microstructure is a layered mixture of phases i and j with layer normal ν , where $a^i - a^j = w \otimes \nu$. It is natural to ask whether the converse holds.

Question 5.1: If $\{a^i\}_{1 \leq i \leq N}$ are pairwise incompatible, does it follow that $QW(\xi) > 0$ except when $\xi \in \{a^i\}$?

The answer is yes for $N = 2$ [17,20,24]. Surprisingly, it is no for $N = 4$ [6]. The case $N = 3$, which is the focus of our attention here, remains open in general.

In view of the discussion above concerning Young measures, etc., we think of the assertion that $QW(\xi) = 0$ for some $\xi \notin \{a^i\}$ as a statement that $\{a^i\}$ are *mutually compatible* (as gradients). Thus Question 5.1 asks whether a set of pairwise incompatible gradients is automatically mutually incompatible. See Section 8 of [17] for a related discussion in terms of microstructures.

Since the study of multiwell energies is motivated in part by the theory of coherent phase transitions, it seems appropriate to mention that the situation for strains is different from that for gradients. For geometrically linear elasticity, (1.3) should be replaced by

$$W(e) = \min_{1 \leq i \leq N} \{|e - a^i|^2\}$$

where $e(u) = (\nabla u + \nabla u^T)/2$ is a linear strain and $\{a^i\}$ are now symmetric $n \times n$ matrices. In this setting a^i and a^j are compatible if $a^i - a^j = v \otimes w + w \otimes v$ for some $v, w \in \mathbb{R}^n$. In space dimension 2, analogue of Question 5.1 has an affirmative answer for *any* number of wells. A similar result even holds in the geometrically nonlinear setting [6,10,21]. The situation in space dimension three is open, except for some special cases.

We return now to energies of the form (1.3). For the remainder of this section W is a three-well energy, involving incompatible, 2×2 matrices $\{a^i\}$. The following result gives an affirmative answer to Question 5.1 under certain conditions on $\{a^i\}$. The proof uses only the weak continuity of the determinant. Essentially the same result figures in the recent work of Pedregal and Šverák [23,27].

PROPOSITION 5.2. *Let a^1, a^2 , and a^3 be pairwise incompatible 2×2 matrices. Assume that $\det(a^1 - a^2)$, $\det(a^2 - a^3)$, and $\det(a^1 - a^3)$ all have the same sign. Then $QW(\xi) > 0$ except when $\xi \in \{a^i\}$.*

Proof. We use Dacorogna's formula for the polyconvexification [8]:

$$(5.2) \quad PW(\xi) = \inf_{\nu \in \mathcal{A}_\xi} \int W(\lambda) d\nu(\lambda),$$

where ν ranges over the set \mathcal{A}_ξ of probability measures on 2×2 matrices that satisfy the "minors relations":

$$\mathcal{A}_\xi = \left\{ \nu : \int \lambda d\nu(\lambda) = \xi, \quad \int \det \lambda d\nu(\lambda) = \det \xi \right\}.$$

It is easy to see that the infimum in (5.2) is achieved, since W has quadratic growth at infinity.

Suppose that $QW(\xi) = 0$. It follows that $PW(\xi) = 0$, and therefore any extremal for (5.2) must be supported on the set where $W = 0$. We thus conclude the existence of

$$\nu = \sum_{i=1}^3 \theta_i \delta_{a^i}, \quad \theta_i \geq 0, \quad \sum \theta_i = 1,$$

such that

$$\begin{aligned} \int \lambda d\nu(\lambda) &= \sum \theta_i a^i = \xi \\ \int \det \lambda d\nu(\lambda) &= \sum \theta_i \det(a^i) = \det \xi. \end{aligned}$$

Combining these relations gives

$$(5.3) \quad \sum \theta_i \det(a^i) = \det\left(\sum \theta_i a^i\right).$$

Since we are in two dimensions, $\det(a)$ is a quadratic form and

$$\det\left(\sum \theta_i a^i\right) = \sum_i \theta_i^2 \det a^i + \sum_{i < j} \theta_i \theta_j \langle a^i, \text{cof } a^j \rangle.$$

Using this in (5.3), we obtain after some manipulation that

$$(5.4) \quad \theta_1 \theta_2 \det(a^1 - a^2) + \theta_1 \theta_3 \det(a^1 - a^3) + \theta_2 \theta_3 \det(a^2 - a^3) = 0.$$

By hypothesis the terms $\det(a^i - a^j)$ are either all positive or all negative. So it follows that $\theta_1 \theta_2 = \theta_1 \theta_3 = \theta_2 \theta_3 = 0$, whence $\xi = a^i$ for some i . \square

What happens when $\{\det(a^i - a^j)\}$ are not all of the same sign? The answer is not known, however Pedregal and Šverák have proved the following [23,27]:

PROPOSITION 5.3. *Let a^1, a^2 , and a^3 be incompatible 2×2 matrices. If $QW(\xi) = 0$ for some $\xi \notin \{a^i\}$, then the associated microstructure cannot be sequentially laminated. Equivalently, the rank-one convexification RW satisfies $RW(\xi) > 0$ whenever $\xi \notin \{a^i\}$.*

We turn now to the relationships between these issues and the calculus of geometric parameters. To keep matters as simple as possible, we shall consider only the case of *diagonal* matrices a^i . By a translation and a linear change of variables, there is no further loss of generality in taking $a^3 = 0$ and $a^1 = I$. So we shall henceforth concentrate on the case

$$(5.5) \quad a^1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad a^2 = \begin{pmatrix} -\lambda & 0 \\ 0 & -\mu \end{pmatrix}, \quad a^3 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

The real numbers λ and μ should satisfy

$$(5.6) \quad (\lambda + 1)(\mu + 1) < 0 \quad \text{or} \quad \lambda\mu < 0,$$

since otherwise Proposition 5.2 applies. (Our notation is chosen for later convenience in making contact with Proposition 4.4.)

THEOREM 5.4. *Let $\{a^i\}$ be as above. Then $QW(\xi) = 0$ with $\xi \notin \{a^i\}$ if and only if a certain associated type 3 extreme point of \mathcal{F}_θ^U is achievable. The specific extreme point is given by (5.16)-(5.17) below.*

Proof. Suppose that $QW(\xi) = 0$. Then obviously $CW(\xi) = 0$, so ξ lies in the convex hull of $\{a^i\}$:

$$(5.7) \quad \xi = \sum \theta_i a^i, \quad \theta_i \geq 0, \quad \sum \theta_i = 1.$$

Therefore ξ is necessarily diagonal. The ‘‘volume fractions’’ $\theta = (\theta_1, \theta_2, \theta_3)$ are uniquely determined by (5.7) since we have only three wells. The possible values of θ are restricted by (5.4), which becomes

$$(5.8) \quad \theta_1 \theta_3 + \lambda \mu \theta_2 \theta_3 + (\lambda + 1)(\mu + 1) \theta_1 \theta_2 = 0$$

in this case. In view of (5.6), the possible values of ξ lie on a one-dimensional curve. (An explicit representation of this curve is easy enough to obtain, but we omit it.)

We assert that in this situation there exists a tensor of geometric parameters $F_{ij\alpha\beta} \in \mathcal{F}_\theta$ satisfying

$$(5.9) \quad \sum (\Gamma_{ij} \delta_{\alpha\beta} - F_{ij\alpha\beta}) a_{\gamma\alpha}^i a_{\gamma\beta}^j = 0.$$

More specifically, we assert (5.9) whenever F represents the limiting behavior of a minimizing sequence in the definition of $QW(\xi)$. Indeed, for such F (2.10) - (2.11) yield

$$(5.10) \quad QW(\xi) = \sum \rho_i |\xi - a^i|^2 - \sum F_{ij\alpha\beta} a_{\gamma\alpha}^i a_{\gamma\beta}^j,$$

where $\rho = (\rho_1, \rho_2, \rho_3) \in V$ gives the volume fraction of the microstructure. Since $QW(\xi) = 0$, (5.10) and (3.11) yield

$$(5.11) \quad |\xi - \sum \rho_i a^i|^2 + \sum (\Gamma_{ij} \delta_{\alpha\beta} - F_{ij\alpha\beta}) a_{\gamma\alpha}^i a_{\gamma\beta}^j = 0.$$

The first term is a perfect square, and the second one is nonnegative as well, by (3.6). We therefore conclude that $\xi = \sum \rho_i a^i$, whence $\rho_i = \theta_i$. We furthermore conclude that F satisfies (5.9).

Next, we assert that any F satisfying (5.9) must be a type 3 extreme point of \mathcal{F}_θ^U . Indeed, if (5.9) holds then

$$(5.12) \quad \inf_{F \in \mathcal{F}_\theta^U} \sum (\Gamma_{ij} \delta_{\alpha\beta} - F_{ij\alpha\beta}) a_{\gamma\alpha}^i a_{\gamma\beta}^j = 0,$$

using the fact that $\mathcal{F}_\theta \subset \mathcal{F}_\theta^U$ along with (3.6). The extremal value of any affine function on a compact, convex set is achieved at an extreme point; therefore F is either an extreme point of \mathcal{F}_θ^U or else a convex combination of extreme points all of which achieve 0 in (5.12). Now, there is no extreme point of type 1 or 2 that achieves 0 in (5.12). This can be proved by direct calculation using the formulae (4.12) - (4.14). Alternatively, it suffices to recall that these extreme points correspond to rank-two laminates, whereas it is impossible to achieve $QW(\xi) = 0$ by means of a rank-two lamination construction. We shall show presently that (5.12) vanishes (for given ξ) at a *unique* type 3 extreme point of \mathcal{F}_θ^U . So F can satisfy (5.9) only by being equal to this type 3 extreme point.

Consider a type 3 extreme point $G \in \mathcal{F}_\theta^U$ which achieves 0 in (5.12). By Lemma 4.5,

$$(5.13) \quad H_{ij\alpha\beta} = \Gamma_{ij} \delta_{\alpha\beta} - G_{ij\alpha\beta}$$

is also an extreme point of type 3. Writing it as a block matrix

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{12} & H_{22} \end{pmatrix} = \begin{pmatrix} A & B \\ B & C \end{pmatrix}$$

as in Section 4, we have $C = BA^{-1}B$, and AB^{-1} is not a multiple of the identity. The hypothesis that G achieves 0 in (5.12) can be written as

$$(5.14) \quad \langle Aa^1, a^1 \rangle + 2\langle Ba^1, a^2 \rangle + \langle Ca^2, a^2 \rangle = 0.$$

Because $C = BA^{-1}B$, (5.14) is a perfect square, i.e. (5.14) is equivalent to

$$|A^{1/2}a^1 + A^{-1/2}Ba^2|^2 = 0.$$

So $B^{-1}Aa^1 = -a^2$, i.e.

$$(5.15) \quad B^{-1}A = \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix}.$$

Since A and B are symmetric, (5.15) implies that they are diagonal. To see this, we observe that $B^{-1}A = -a^2$ implies $A = -Ba^2$, so

$$A = A^T \implies Ba^2 = a^2B,$$

using the symmetry of a^2 as well as that of A and B . Thus B and a^2 commute, whence either $\lambda = \mu$ or else B is simultaneously diagonal with a^2 . The case $\lambda = \mu$ does not arise, since $B^{-1}A$ cannot be a multiple of the identity at a type 3 extreme point. Thus B and $A = -Ba^2$ are both diagonal, and H has the form (4.20) with $a_1 = \lambda b_1$, $a_2 = \mu b_2$. By Proposition 4.4 there is exactly one such extreme point in \mathcal{F}_θ^U whenever θ satisfies (5.8), and it is given by (4.23). An easy calculation shows that if H is given by (4.23), then $G_{ij\alpha\beta} = \Gamma_{ij}\delta_{\alpha\beta} - H_{ij\alpha\beta}$ is given by

$$(5.16) \quad G = \begin{pmatrix} \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix} & \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} \\ \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} & \begin{pmatrix} d_1^2/c_1 & 0 \\ 0 & d_2^2/c_2 \end{pmatrix} \end{pmatrix}$$

with

$$(5.17) \quad \begin{aligned} c_1 &= \frac{\mu}{\mu - \lambda} [\theta_1 \theta_3 + (\lambda + 1) \theta_1 \theta_2] \\ c_2 &= \frac{-\lambda}{\mu - \lambda} [\theta_1 \theta_3 + (\mu + 1) \theta_1 \theta_2] \\ d_1 &= \mu^{-1} c_1, \quad d_2 = \lambda^{-1} c_2. \end{aligned}$$

(Notice that (5.16) - (5.17) are simply (4.20) - (4.23) with the roles of λ and μ reversed.) Recapitulating, we have shown that if $QW(\xi) = 0$ then $\xi = \sum \theta_i a^i$ with $\theta \in V$ satisfying (5.8), and the associated microstructure achieves the tensor of geometric parameters determined by (5.16) - (5.17), which is an extreme point of type 3. The argument is entirely reversible: if $\theta \in V$ satisfies (5.8) and if the tensor of geometric parameters (5.16) - (5.17) is achievable by a microstructure, then retracing the argument leads to $QW(\xi) = 0$ with $\xi = \sum \theta_i a^i$. \square

COROLLARY 5.5. *Type-3 extreme points with A, B , and C simultaneously diagonal cannot be achieved by laminated microstructures.*

Proof. Suppose that such a type 3 extreme point were achievable. Then by Theorem 5.4 we could obtain an example of a^1, a^2 , and a^3 which are pairwise incompatible but mutually compatible. According to Proposition 5.3 the associated microstructure could not be sequentially laminated. \square

Remark 5.6. The proof of Theorem 5.4 actually includes a new proof of Proposition 5.2, based on the “Geometric Parameters Lower Bound” instead of polyconvexification, when a^1, a^2 , and a^3 are simultaneously diagonal. Indeed, the general case is easily reduced that of $\tilde{a}^3 = 0$, $\tilde{a}^1 = I$, $\tilde{a}^2 = (a^2 - a^3)(a^1 - a^3)^{-1}$. Condition (5.8) for $\tilde{a}^1, \tilde{a}^2, \tilde{a}^3$ is the same as (5.4) for a^1, a^2 , and a^3 .

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