Computational stability of phase-tip splitting in the presence of small interfacial energy in a simple two-phase solid

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We report on further results for the problem studied in [1], concerning stable equilibria for a two-phase model of an elastic solid in anti-plane shear in the presence of small interfacial energy. The existence and computation of global solution branches of equilibria for arbitrarily small interfacial energy is presented in [1], and the computational stability (local energy minimization) is used as the selection criterion. However, the stability of important solutions associated with so-called phase-tip splitting (the formation of fine “needles” at the tips of phase stripes) was missed in [1]. This is due to a delicate inaccuracy involved in the numerical diagnostics of the second variation of the energy, which is uncovered and resolved in this work.

keywords: phase-tip splitting; solid-solid phase transitions; two-phase equilibria; interfacial energy; meta-stability; finite differences

1 Introduction

Here we report on further results for the problem posed and analyzed in our earlier work [1], viz., the anti-plane shear of a two-phase elastic solid in the presence of small interfacial energy. In the first part of [1], the existence of solutions characterized by arbitrarily small interfacial effects is rigorously obtained via global bifurcation methods and a-priori bounds. Then locally stable equilibria comprising “striped” phases are computed via a finite-difference discretization combined with numerical bifurcation/continuation methods. A key idea in [1] is the choice of bifurcation/continuation parameter: For both
existence theorems and constructive numerics, the use of the reciprocal of the 
small parameter characterizing interfacial energy avoids an analysis associated 
with the singularly perturbed state. Remarkably the solutions obtained 
in [1] exhibit many features seen in 2-dimensional planar experiments on 
shape-memory alloys [2, 3]. For example, three different length scales are 
oberved in solutions found in [1], corresponding to – in descending order of 
fineness – the size of the striped phases, the transition layers at frustrated 
boundaries, and the transition layers between the two phases.

In this work we compute locally stable equilibria exhibiting phase-tip 
splitting, i.e., the formation of fine “needles” at the tips of phase stripes, 
which is another characteristic seen in shape-memory alloys [2, 3, 4, 5]. Such 
solutions were overlooked in [1], due to a delicate inaccuracy involved in the 
numerical determination of stability (local energy minimization), which is 
uncovered in this work.

The outline of the paper is as follows: In Section 2 we summarize the 
problem formulation and the existence results from [1]. In Section 3 we 
pinpoint the loss of accuracy in the stability analysis employed in [1] and 
present an accurate method that resolves the problem. In Section 4 we 
provide a sampling of our numerical results exhibiting locally stable equilibria 
characterized by phase-tip splitting.

2 Formulation

We consider an infinite, cylindrical, elastic body of square cross-section, \( \Omega = (0, \pi) \times (0, \pi) \), undergoing anti-plane shear displacement, \( u : \Omega \rightarrow \mathbb{R} \), in 
response to hard loading at the boundary. Specifically, the total potential 
energy functional for our model is the following:

\[
V(u) := \int_{\Omega} \left[ \frac{\varepsilon}{2} \nabla^2 u \cdot \nabla^2 u + W(\lambda + u_x, u_y) \right] dx, \quad u|_{\partial \Omega} = 0, \tag{1}
\]

where \( \varepsilon > 0 \) is a “small” parameter (interfacial), \( \lambda \geq 0 \) is the loading param-
eter, \( \nabla^2(\cdot) := \nabla \circ \nabla(\cdot) \) denotes the second gradient, and \( W : \mathbb{R}^2 \rightarrow \mathbb{R} \) is the 
two-well potential (c.f. Figure 1 for \( \gamma_2 = 0 \))

\[
W(\gamma_1, \gamma_2) = \frac{1}{2} [\gamma_1^2 (\gamma_1 - 1)^2 + \gamma_2^2]. \tag{2}
\]

The Euler-Lagrange equilibrium equation for (1) is

\[
\Delta^2 u - \kappa \Delta u + \kappa f(\lambda + u_x) u_{xx} = 0 \quad \text{in} \quad \Omega; \quad \Delta u = u = 0 \quad \text{on} \quad \partial \Omega, \tag{3}
\]
where $\kappa := 1/\varepsilon$; $f(t) := 6t(1 - t)$; $\Delta(\cdot)$ denotes the Laplace operator, $\Delta u = u_{xx} + u_{yy}$, and $\Delta^2(\cdot) := \Delta \circ \Delta(\cdot)$ denotes the biharmonic operator.

As shown in [1], problem (3) has solutions in periodic Hölder spaces defined on the infinite strip $S := (-\infty, \infty) \times (0, \pi)$:

$$X^n_{k,\alpha} = \{ u \in C^{k,\alpha}(S) : x \to u \text{ is } \frac{2\pi}{n} \text{-periodic and odd} \}$$

$$Y^n_{0,\alpha} = \{ v \in C^{0,\alpha}(S) : x \to v \text{ is } \frac{2\pi}{n} \text{-periodic and odd} \}$$

for each $n = 1, 2, \ldots$, where $C^{k,\alpha}(S)$, $k = 1, 2, \ldots$, denotes the usual space of $k$-times (locally) Hölder continuously differentiable functions ($0 < \alpha < 1$).

We endow these spaces with the usual appropriate uniform Hölder norm over the closure of the subdomain $\Omega_n = (0, \pi/n) \times (0, \pi)$, so that each is a Banach space.

We may now represent (3) abstractly via

$$F(\kappa, \lambda, u) = 0,$$

where $F : [0, \infty) \times \mathbb{R} \times X^{4,\alpha}_n \rightarrow Y^{0,\alpha}_n$, observing that $F(\kappa, \lambda, 0) \equiv 0$. The rigorous linearization of (5) about the trivial solution is then given by

$$\Delta^2 u - \kappa \Delta u + \kappa f(\lambda)u_{xx} = 0, \quad u \in X^{4,\alpha}_n,$$
which admits the nontrivial solution \( u = \sin nx \sin y \), provided that
\[
(1 + n^2)^2 + \kappa[(1 - 6\lambda + 6\lambda^2)n^2 + 1] = 0, \quad n \in \mathbb{N}.
\] (7)

Of particular interest here is for \( \lambda = 1/2 \) (the peak of the “spinodal” region, cf. Figure 1), in which case (7) yields potential bifurcations at
\[
\kappa_n = \frac{(n^2 + 1)^2}{n^2/2 - 1}, \quad n = 2, 3, ...
\] (8)

Also, for \( \kappa > 0 \) sufficiently large and fixed, we have the pairs
\[
\lambda^\pm_n = \frac{1}{2} \pm \frac{1}{6} \sqrt{3 - \frac{6}{n^2} - \frac{6(n^2 + 1)^2}{\kappa n^2}}.
\] (9)

We now summarize from [1]:

**Proposition 1** Each \((\kappa_n, 0) \in (0, \infty) \times X_n^{4,\alpha} \) with \( \kappa_n \) given by (8), is a bifurcation point of a global continuum of non-trivial solution pairs of (5) (with \( \lambda = 1/2 \)), denoted by \( \Sigma_{\kappa_n} \subset \mathbb{R}^+ \times X_n^{4,\alpha} \). Each solution branch, \( \Sigma_{\kappa_n} \), \( n = 2, 3, ... \), is either unbounded in \( \mathbb{R}^+ \times X_n^{4,\alpha} \) and/or meets the trivial line of solutions at some other bifurcation point \((\kappa_m, 0), m \neq n \). When (9) admits real solutions (for some \( n \in \mathbb{N} \) at a fixed value \( \kappa_o > 0 \)), each of the pairs \((\lambda^\pm_n, 0) \in \mathbb{R}^+ \times X_n^{4,\alpha} \) is a bifurcation point of a global continuum of solutions, denoted by \( \Lambda_{\lambda^\pm_n} \subset \mathbb{R}^+ \times X_n^{4,\alpha} \). Each \( \Lambda_{\lambda^\pm_n} \) is bounded in \( \mathbb{R}^+ \times X_n^{4,\alpha} \) and thus meets the trivial line at another such bifurcation point.

### 3 Computational stability analysis

As in [1] we begin by computing the branches \( \Sigma_{\kappa_n} \subset \mathbb{R}^+ \times X_n^{4,\alpha}, n = 2, 3, ... \). We employ the usual method of finite differences, applied directly to (3), on the sub-domain \( \Omega_n = (0, \pi/n) \times (0, \pi) \), exploiting the inherent symmetry properties on \( X_n^{4,\alpha} \), cf. (4). We then obtain solution branches of equilibria via standard path-following – with \( \kappa \) as the free (bifurcation) parameter. As in [1], accuracy of solutions is inferred via consistency under increased mesh size. Once an accurate equilibrium solution belonging to \( \Sigma_{\kappa_n} \) is known, we are interested in its stability: an equilibrium solution that renders the potential energy a local minimum is said to be stable; otherwise, it is unstable. Of course the solution on the entire domain \( \Omega \) is required for this, which is
easily generated from that on \( \Omega_n \) by inversion-reflection and periodicity, cf. (4).

From (1) we find that the second variation of the energy (evaluated at a given equilibrium \( u \in X_4^{4, \alpha} \), for fixed values of \( \lambda, \kappa \)) is given by

\[
D^2V_{\lambda,\kappa}(u)[\eta, \eta] = \int_\Omega \left[ \frac{1}{\kappa} |\nabla^2 \eta|^2 + |\nabla \eta|^2 - f(\lambda + u_x) \eta_x^2 \right] \, dx,
\]

for all admissible test functions \( \eta \in C^2(\Omega) \) satisfying \( \eta = \Delta \eta = 0 \) on \( \partial\Omega \), where \( f(t) \) is defined as in (3). Our determination of stability amounts to testing the positive-definiteness of (10) in a numerically consistent manner.

The numerical representation \( u_d \) of an equilibrium comprises the values of \( u \) at the \( M \cdot N \) grid points \( (M, N \in \mathbb{N}) \) of the finite difference scheme; there are \( M \cdot N \) internal points, uniformly spaced, in direction \( x \) (\( y \)), respectively. The numerical approximation of the second variation (10) can be formulated directly as the sum of three quadratic terms:

\[
\frac{(M + 1)(N + 1)}{\pi^2} D^2V_{\lambda,\kappa} \cong \frac{1}{\kappa} \eta_d^T (B_x + B_y) (B_x + B_y) \eta_d + \eta_d^T (A_x^T A_x + A_y^T A_y) \eta_d - \eta_d^T A_x^T F A_x \eta_d,
\]

where \( A_x, A_y, B_x \) and \( B_y \) are the coefficient matrices associated with the first and second central difference quotients in the directions \( x \) and \( y \), respectively, on a uniform rectangular grid. The vectors \( u_d \) and \( \eta_d \) each have \( M \cdot N \) elements, and the size of each of the matrices in (11) is \( (MN) \times (MN) \). The value of \( u_d \) corresponding to grid point \( (i, j) \) is stored at component \( (u_d)_i N + j \), where \( 0 \leq i < M \) and \( 0 < j \leq N \). (Due to the zero boundary conditions (3), values of \( u \) along the boundaries are not stored in \( u_d \).) In the last term in (11), \( F \) denotes a diagonal matrix, constructed as follows. We first approximate \( u_x \) via the \( M \cdot N \) vector \( A_x u_d := (u_{1x}^1, u_{2x}^1, \ldots, u_{MNx}^1) \). Then \( F := \text{diag}[f(\lambda + u_{1x}^1), f(\lambda + u_{2x}^1), \ldots, f(\lambda + u_{MNx}^1)] \).

The Hessian (11) was employed to test the stability of equilibria found in [1]. Unfortunately (11) can give a poor approximation of (10). This is typical for finite difference schemes. We give a one-dimensional problem to illustrate the origin of the inaccuracy. Specifically, suppose we want to determine the second derivative of a sufficiently smooth function \( f(x) \) on the domain \( \Omega = (0, 1) \), with \( f(0) = f(1) = 0 \). We use a uniform grid for the discrete representation of \( f(x) \) with \( N \) internal points and step size
\[ h = 1/(N + 1). \] The \( i \)th grid point is denoted by \( x_i \). By the second-order accurate central difference scheme, the first and second derivatives at the \( i \)th grid point can be approximated as

\[
\frac{df(x)}{dx} = f_1(x_i) + O(h^2) := \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \quad (12)
\]

\[
\frac{df^2(x)}{dx^2} = f_2(x_i) + O(h^2) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2), \quad i = 1, \ldots, N.
\]

We may also employ \( f_1 \) from (12) to compute an approximation of the second derivative of \( f(x) \), namely

\[
\frac{df^2(x)}{dx^2} = \frac{df(x)}{dx} \approx \frac{f_1(x_{i+1}) - f_1(x_{i-1})}{2h} = \frac{f(x_{i+2}) - f(x_{i}) - f(x_{i-2}) + f(x_{i})}{(2h)^2} = (13)
\]

The method (13) clearly yields \( O(4h^2) \) accuracy. In other words, this approach leads to an approximation of the second derivative that belongs to a half dense grid at each grid point. In order to express (12) in matrix form, we write their coefficient matrices as \( A_x \) and \( B_x \), respectively. Then the last inequality in (13) reads

\[
A_x A_x \neq B_x.
\]

Our simple example also reveals that \( A_x A_x \) is less accurate than \( B_x \).

The approximation (11) for the second variation contains three terms, each one requiring distinct considerations in order to avoid the loss of accuracy mentioned above. The coefficient matrix of the first term is \((B_x + B_y)^T (B_x + B_y)\), but according to (12), the coefficient matrices for the second derivatives are symmetric, i.e., the transpose plays no role here. Also, by a calculation similar to (13), we see that this is the “exceptional” case: There is no loss of accuracy and

\[
(B_x + B_y)^T (B_x + B_y) = (B_x + B_y)^2 = L, \quad (15)
\]

where \( L \) denotes the coefficient matrix for the biharmonic operator, i.e.,

\[
L := D_{xx} + 2D_{xy} + D_{yy}, \quad (16)
\]
where $D_{xx}u_d$ approximates $u_{xxxx}$, $D_{xy}u_d$ approximates $u_{xyy}$ and $D_{yy}u_d$ approximates $u_{yyyy}$ from the appropriate $O(h^2)$-accurate central finite difference scheme for any vector $u_d$. It is worth mentioning here that (15) does not hold for finite difference schemes with accuracy higher than order $O(h^2)$.

The second term in (11) contains $(A_x^TA_x + A_y^TA_y)$, which leads to an inaccurate approximation according to our simple example discussed above. Since both $A_x$ and $A_y$ are skew-symmetric, we have

$$A_x^TA_x = -(A_x)^2 \quad \text{and} \quad A_y^TA_y = -(A_y)^2.$$  \hspace{1cm} (17)

Based on our discussion involving (12 – 14), we now substitute $B_x$ for $(A_x)^2$ and $B_y$ for $(A_y)^2$ in (11) in order to have $O(h^2)$ accuracy.

With hindsight we now observe that

$$\frac{1}{\kappa} \eta_d^T (B_x + B_y)^T (B_x + B_y) \eta_d - \eta_d^T (B_x + B_y) \eta_d = \frac{1}{\kappa} \eta_d^T L \eta_d - \eta_d^T (B_x + B_y) \eta_d,$$  \hspace{1cm} (18)

(multiplied by $\pi^2 / [(M + 1) (N + 1)]$) is nothing more than the approximation of the left side of

$$\int \Omega \left[ \frac{1}{\kappa} \Delta^2 \eta - \Delta \eta \right] \eta d\chi = \int \Omega \left[ \frac{1}{\kappa} |\nabla^2 \eta|^2 + |\nabla \eta|^2 \right] d\chi,$$  \hspace{1cm} (19)

the last equality being a consequence of integration by parts for any admissible test function.

Carrying on with this idea, we now integrate the last term in (10) by parts for any admissible test function, which together with (19) yields

$$D^2V_{\lambda,\eta}(u)[\eta, \eta] = \int \Omega \left[ \frac{1}{\kappa} \Delta^2 \eta - \Delta \eta + [f(\lambda + u_x)]_x \eta_x + f(\lambda + u_x) \eta_{xx} \right] \eta d\chi.$$  \hspace{1cm} (20)

We then obtain the Hessian approximation

$$\frac{1}{\pi^2} \frac{(M + 1)(N + 1)}{\eta_d^T L \eta_d} D^2V_{\lambda,\eta} \approx \frac{1}{\kappa} \eta_d^T L \eta_d - \eta_d^T (B_x + B_y) \eta_d + \eta_d^T [f(\lambda + u_x)]_x A_x \eta_d + \eta_d^T f(\lambda + u_x) B_x \eta_d := \eta_d^T H_1 \eta_d.$$  \hspace{1cm} (21)

In fact $H_1$ is formally identical to the full Jacobian derived from the discretized Euler-Lagrange equations, which exhibits fast convergence in the
Newton method underlying the numerical continuation procedure for computing equilibria. Due to the fact that the last two terms in (21) are not purely quadratic, we find that $H_1$ is slightly asymmetrical in practice, rendering Cholesky factorization unreliable for the purposes of testing the positive-definiteness of $H_1$. Instead we seek an alternative approach to represent the last term in (11).

That latter contains $A_f^T F A_{f,x}$, but due to the presence of the diagonal matrix $F$, a simple substitution of $B_x$ here is not possible. Instead we seek a matrix $\tilde{A}_x$ that approximates the first derivative of $u$. Since in some special cases $F$ reduces to the identity matrix $I$, and in view of (14), we require $\tilde{A}_x$ to satisfy

$$\tilde{A}_x^T I \tilde{A}_x = \tilde{A}_x^T \tilde{A}_x = B_x. \quad (22)$$

A suitable candidate for $\tilde{A}_x$ can be the derived from the coefficient matrix $A_{f,x}$ of the $O(h)$-accurate forward difference scheme approximating the first derivative. By direct calculation, $A_{f,x}$ does not fulfill (22). However we can correct the deficiency by adding $N$ rows to it in a strategic way, thus rendering $\tilde{A}_x$ an $(NM + N) \times (NM)$ matrix. For example, for $N = 2$ and $M = 3$, we choose

$$\tilde{A}_x = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
\end{bmatrix} A_{f,x} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
-1 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 & 1 & 0 \\
0 & 0 & 0 & -1 & 0 & 1 \\
0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 \\
\end{bmatrix}, \quad (23)$$

which satisfies condition (22). In general, we choose the new rows to correspond to the first $N$ consecutive unit basis vectors of length $MN$. But due to the $(MN + N)$ rows of $\tilde{A}_x$, $F$ must now be inflated to an $(MN + N) \times (MN + N)$ matrix, denoted by $\tilde{F}$. The way we extend $A_{f,x}$ to $\tilde{A}_x$ makes it clear that $\tilde{F}$ should be a diagonal matrix the form

$$\tilde{F} = \begin{bmatrix}
F_o & 0 \\
0 & F \\
\end{bmatrix}, \quad (24)$$

where $F_o$ is an $N \times N$ diagonal matrix, with each entry evaluating $f(\lambda + u_x)$ at different grid points along the boundary $x = 0$. 8
From the symmetry conditions inherent in (4), \( x \mapsto u_x(x, y) \) is even, and hence, along the boundary, \( u_x \) can be approximated as

\[
|u_x|_{x=0} \approx \frac{-u(-h, y) + u(h, y)}{2h} = \frac{u(h, y)}{h},
\]

where \( h := \pi/(M + 1) \). Writing \( (u_{d,1}^{o1}, u_{d,2}^{o2}, \ldots, u_{d,N}^{oN}) := \frac{M+1}{\pi}(u_1^d, u_2^d, \ldots, u_d^N) \), we then set

\[
F_o := \text{diag}[f(\lambda + u^{o1}_d), f(\lambda + u^{o2}_d), \ldots, f(\lambda + u^{oN}_d)].
\]

In this way we obtain another discrete approximation of the second variation:

\[
\frac{(M + 1)(N + 1)}{\pi^2} D^2 V_{\lambda, \kappa} \approx \frac{1}{\kappa} \eta_d^T L \eta_d - \eta_d^T (B_x + B_y) \eta_d - \eta_d^T \tilde{A}_x \eta_d := \eta_d^T H_2 \eta_d.
\]

The Hessians \( H_1 \) and \( H_2 \) each correspond to a discrete representation of the second variation. The matrix \( H_2 \) is symmetric, since it comprises only quadratic terms. As a consequence, it is ideal for Cholesky factorization to test for positive definiteness, i.e., for stability. More specifically, recall that any square, symmetric matrix like \( H_2 \) has a Cholesky decomposition if and only if it is positive definite. Thus, failure of the decomposition implies that \( H_2 \) has one or more negative eigenvalues. The problem here is that it is difficult to directly judge the accuracy of \( H_2 \). On the other hand, \( H_1 \) is slightly asymmetrical but, as mentioned before, exhibits a faster convergence in the Newton continuation. Observe that \( H_1 = H_2 \) for an arbitrarily fine grid. Hence, a comparison of the two Hessians \( H_1 \) and \( H_2 \) provides an ideal tool to describe whether the applied finite-difference scheme is fine enough for a given solution. In particular, it is suitable to judge the accuracy of the stability of a given equilibrium solution via the positivity of \( H_2 \).

For a given grid, we define the distance ”\( d \)” between \( H_1^* \) and \( H_2^* \), at a given equilibrium, say, at \((\lambda_*, \kappa_*, u_*)\), from their ”\( m \)” smallest eigenvalues as follows:

\[
d = \frac{1}{m} \sum_{i=1}^{m} |\sigma_{1,i} - \sigma_{2,i}|,
\]

where the \( \sigma_{1,i} \) and \( \sigma_{2,j} \) denote the eigenvalues of \( H_1^* \) and \( H_2^* \), respectively, ordered as \( \sigma_{j,1} \leq \sigma_{j,2} \leq \sigma_{j,3} \leq \ldots \), where \( j = 1, 2 \). The eigenvalues in (28) are computed by Matlab routine \texttt{eigs}, which provides exactly the \( m \) smallest eigenvalues. The number \( d \) characterizes the grid and the accuracy of the
finite difference scheme at the given equilibrium. If for a given small number $\delta > 0$, we have
\[ d|_{(\lambda^*, \kappa^*, u^*)} \leq \delta, \]  
then the applied grid is deemed sufficiently fine for the accuracy of the equilibrium and also to employ $H^2_\ast$ in the test for stability (via Cholesky factorization).

Throughout we use $m = 30$ in (28) to check (29) with $\delta = 0.01$. For example, in Figure 2 we present results for continuation in $\kappa$ for $n = 4$ with $\lambda = 0.5$ fixed; $d_{100}$ and $d_{200}$ denote the values of $d$ along the equilibrium path with a $100 \times 403$ grid and a $200 \times 803$ grid, respectively. (Details about the continuation and the application of the involved symmetries can be found in [1].) On the vertical axis we plot $\|u^2\| = \|u^2\|_{L^1(\Omega)}$. Based on the requirement of (29) with $m = 30$ and $\delta = 0.01$, among the three chosen equilibria marked along the equilibrium paths, only the stability of the left-most one can be decided from the results of the $100 \times 403$ grid. For the middle one, the $200 \times 803$ resolution is needed, while the right one requires an even finer discretization.

Figure 2: Continuation in $\kappa = 1/\varepsilon$ with two finite difference schemes.
4 Numerical Results

The strategy here is to first compute the primary branches $\Sigma_{\kappa_n} \subset \mathbb{R}^+ \times X^4_{n,\alpha}$, $n = 2, 3, \ldots$, (cf. Proposition 1) for large values of $\kappa = 1/\varepsilon$ such that the solution points are stable. Recall that for these solution branches, the hard-loading parameter is fixed at $\lambda = 0.5$, corresponding to the “peak” of the so-called spinodal region, cf. Figure 1. Next we fix such large values of $\kappa_o = 1/\varepsilon_o$ at stable equilibria on $\Sigma_{\kappa_n}$ and compute branches $\Lambda_{\kappa^o \lambda \pm n} \subset \mathbb{R}^+ \times X^4_{n,\alpha}$, generated via continuation of the hard-loading parameter $\lambda \geq 0.5$. In illustrating a given solution below, we color the 2 phases and transition layers, “dark”, “grey” and “white”, respectively, according to the value of the total shear strain $\gamma(x, y) := \lambda + u_x(x, y)$, as defined in Figure 1. The results of this section are obtained as presented in Section 3: equilibrium paths are computed on $M \times N$ grids over the reduced domain $\Omega_n$. The sparse, symmetric Hessian $H_2$ (for the entire domain $\Omega$), calibrated by $H_1$ as precisely described at the end of Section 3, is employed to diagnose stability. In particular, we efficiently track the smallest eigenvalues to deduce the positive definiteness of $H_2$.

We first describe our results for the branch $\Sigma_{\kappa_8}$, emanating from the trivial solution at $\kappa_8 = 4200/31$ (cf. (8) and Proposition 1), which we illustrate in Figure 3. At first, on the ascending part emanating from the bifurcation point, the branch is highly unstable, with the Hessian matrix of the second variation having 6 negative eigenvalues. Here the Hessians $H_1$ (21) and $H_2$ (27) are very “close” according to (29). Thus a coarse grid ($M = N = 100$) is enough for the investigation. After undergoing a series of pitchfork bifurcations (not shown in Figure 3), the ascending part of the branch becomes stable and remains stable for large values of $\kappa$ on the flattened part of the branch. Along this region a finer grid ($M = N = 150$) is needed for the computation. After that it loses stability at a subcritical pitchfork bifurcation at around $\kappa = 54,000$. Along that stable part from the maximum in $\|u^2\|$ to the bifurcation point, the solutions exhibit phase-tip splitting at the top and bottom boundaries of the domain, as illustrated in Figure 3.

Next we fix $\kappa_o = 30,000$ and compute $\Lambda_{\kappa^o \lambda 8 \pm}$ via continuation from the stable equilibrium on $\Sigma_{\kappa_8}$ (at $\kappa_o = 30,000$) for $\lambda \geq 0.5$. We illustrate our results in Figure 4 below. Observe that phase-tip splitting is most profound on the first descending part, in the neighborhood of $\lambda = 0.5$. After going
through 2 turning points the branch is stable again and we observe the trend to stripes (e.g. at $\lambda = 0.872$) which were already found to be stable in [1].

We also make the following observation here concerning the branches $\Lambda_{\kappa_0 \lambda_\pm}^n$, viz., there is a simple mapping of $\Lambda_{\kappa_0 \lambda_+}^n$ into $\Lambda_{\kappa_0 \lambda_-}^n$. To see this, as in [6] we note the material reflection symmetry inherent in the double-well potential (2), leading to (3), with $f(t) = 6t(1-t)$. In particular, if $(\lambda_*, u_*) \in \Lambda_{\kappa_0 \lambda_+}^n$, note that $f(1 - \lambda_* - u_* x) \equiv f(\lambda_* + u_* x)$. We then readily verify that $(\lambda, u) = (1 - \lambda_*, -u_*)$ is also a solution point of (3) (for $\kappa_0$ fixed). We conclude that $(1 - \lambda_*, -u_*) \in \Lambda_{\kappa_0 \lambda_-}^n$ from the observation that (at the trivial solution) the roots (9) satisfy $\lambda_n = 1 - \lambda_n^+$. Hence, the hard-loading branch $\Lambda_{\kappa_0 \lambda_-}^n$ is always the “mirror image” of $\Lambda_{\kappa_0 \lambda_+}^n$, with the dark and the grey phases interchanged.

We also investigated the cases $n = 2, 3, 4, 5, 6, 7, 9, 12, 16$ and found that the description above is qualitatively the same for each. In particular, we now summarize the results for the cases $n = 9, 12, 16$. Figures 5-7 depict the primary bifurcating branches $\Sigma_{\kappa_9}$, $\Sigma_{\kappa_{12}}$, $\Sigma_{\kappa_{16}}$, respectively. Observe that the bifurcation point where the flat part of the branch finally loses stability
occurs at increasingly greater values of $\kappa = 1/\varepsilon$ as $n$ increases: $\kappa = 54,000$ for $n = 8$, $\kappa = 63,000$ for $n = 9$, $\kappa = 98,000$ for $n = 12$ and $\kappa = 142,000$ for $n = 16$.

We also illustrate the hard-loading branches $\Lambda^{30,000}_{\lambda_8}$, $\Lambda^{30,000}_{\lambda_{12}}$ and $\Lambda^{100,000}_{\lambda_{16}}$. 

13
in Figures 8, 9 and 10, respectively. As before for $\lambda_{30,000}$, each of these contains two turning points connected by a small path of unstable solutions that separates two larger stable solution paths. Again phase-tip splitting is most profound on the first descending part, in the neighborhood of $\lambda = 0.5$, with stable striped phases occurring on the lower stable part of the branch.

We end this section with Table 1, summarizing the data associated with the computations for the accurate determination of stability for each of the
Figure 8: Hard-loading branch $\Lambda_{1}^{30000}$.  

Figure 9: Hard-loading branch $\Lambda_{2}^{30000}$.  

presented solution branches.

5 Concluding Remarks

Stable solutions exhibiting phase-tip splitting along the primary bifurcating branches were missed in [1] due to inaccuracies associated with the straightforward discretization (11) of the second variation (10). Although integration by parts (20) offers an improvement via $H_1$ (21), the slight asymmetry of the latter causes inaccuracies as well in the delicate diagnostics of determining
Figure 10: Hard-loading branch $\Lambda^{100000}_{16}$.

<table>
<thead>
<tr>
<th>Solution branch</th>
<th>Grid size for continuation $M \times N$</th>
<th>Size of $H_2$ for stability $(nM + n - 1)N \times (nM + n - 1)N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_{n8}$</td>
<td>100 $\times$ 100</td>
<td>87000 $\times$ 87000</td>
</tr>
<tr>
<td></td>
<td>150 $\times$ 150</td>
<td>181050 $\times$ 181050</td>
</tr>
<tr>
<td>$\Lambda^{30000}_{16}$</td>
<td>150 $\times$ 150</td>
<td>181050 $\times$ 181050</td>
</tr>
<tr>
<td>$\Sigma_{n9}$</td>
<td>120 $\times$ 120</td>
<td>130560 $\times$ 130560</td>
</tr>
<tr>
<td>$\Lambda^{30000}_{16}$</td>
<td>120 $\times$ 120</td>
<td>130560 $\times$ 130560</td>
</tr>
<tr>
<td>$\Sigma_{n12}$</td>
<td>100 $\times$ 100</td>
<td>121100 $\times$ 121100</td>
</tr>
<tr>
<td>$\Lambda^{30000}_{16}$</td>
<td>100 $\times$ 100</td>
<td>121100 $\times$ 121100</td>
</tr>
<tr>
<td>$\Sigma_{n16}$</td>
<td>135 $\times$ 135</td>
<td>293625 $\times$ 293625</td>
</tr>
<tr>
<td>$\Lambda^{100000}_{16}$</td>
<td>135 $\times$ 135</td>
<td>293625 $\times$ 293625</td>
</tr>
</tbody>
</table>

Table 1: Computational data

positive definiteness. Our approach employs the symmetrization $H_2$ (27), as calibrated by $H_1$ for accuracy. Fortunately we find that the accurate methods employed here do not obviate the claims of stable striped-phase solutions in [1].

The results of Section 4 demonstrate what is often referred to as metastability, i.e., the simultaneous existence of several local minima of the energy under the same data. For example, Figures 4, 8 and 9 demonstrate a multi-
tude of such solutions exhibiting phase-tip splitting at $\kappa = 1/\varepsilon = 30,000$ for each fixed value of $\lambda$ in a neighborhood of 0.5. Our results also suggest that as the “mode number” $n$ increases, each associated branch is stable for smaller and smaller values of the interfacial-energy coefficient $\varepsilon > 0$. This is in keeping with the “infinite refinement” of phases associated with sharp-interface models in the absence of a length scale ($\varepsilon = 0$), e.g., cf. [2].

Finally we mention that the ideas of Section 3 are potentially applicable to many other conservative problems where the computation of local energy minima via the second variation is sought for the determination of stability. Whenever an integration by parts affords two distinct discretizations of the second variation (i.e. the tangent stiffness matrix), their distance (either defined via (28) or by some other measure) can be employed to judge the accuracy of stability results without an exact error analysis of the numerical scheme.

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References


