A characterisation of the boundary displacements which induce cavitation in an elastic body

Pablo V. Negrón–Marrero
Department of Mathematics
University of Puerto Rico
Humacao, PR 00791-4300
pnm@mate.uprh.edu

Jeyabal Sivaloganathan
Department of Mathematical Sciences
University of Bath, Bath
BA2 7AY, UK
masjs@bath.ac.uk

December 6, 2011

Abstract

In this paper we present numerical and theoretical results for characterising the onset of cavitation-type material instabilities in solids. To model this phenomenon we use nonlinear elasticity to allow for the large, potentially infinite, stresses and strains involved in such deformations. We give a characterisation of the set of linear displacement boundary conditions for which energy minimising deformations produce a *single isolated* hole inside an originally perfect elastic body, based on a notion of the derivative of the stored energy functional with respect to hole-producing deformations. We conjecture that, for many stored energy functions, the critical linear boundary conditions which cause an isolated cavity to form correspond to the zero set of this derivative. We use this characterisation to propose a numerical procedure for computing these critical boundary displacements for general stored energy functions and give numerical examples for specific materials. For a degenerate stored energy function (with spherically symmetric boundary deformations) and for an elastic fluid, we show that the vanishing of the volume derivative gives exactly the critical boundary conditions for the onset of this type of cavitation.

Key words: nonlinear elasticity, onset of cavitation, volume derivative, singular minimisers, quasiconvexity, numerical methods.

Mathematics Subject Classification (2000): 74B20, 35J50, 49K20, 74G65, 74G15, 74G55, 74S05, 74S30, 74G70

1 Introduction

When certain materials, such as rubber, are subjected to sufficiently large triaxial loading, holes or bubbles begin to appear inside of the stressed specimen (see, e.g., Gent and

Lindley [11], Gent [10]). These holes appear initially spherical but may loose their symmetry as the loading is increased. The first variational model, based on the equations of nonlinear elasticity, that predicts this phenomenon of void formation was given by Ball in [3]. In this paper, Ball modeled a spherical body composed of an isotropic "soft" material and showed that, in the class of radial deformations, any minimiser of the stored energy functional must open a hole at the center of the deformed ball for sufficiently large boundary displacements (the phenomenon of cavitation). Following this seminal paper, many others appeared on different aspects of radial cavitation, e.g., Antman and Negrón-Marrero [1], Sivaloganathan [42] and Stuart [52] (see the review article by Horgan and Polignone [19] for further references).

In the multidimensional setting, work of Ball and Murat [7] introduced the notion of $W^{1,p}$–quasiconvexity, extending a concept stemming from work of Morrey (see, e.g., [33]), and highlighted the difficulty in extending the existence theory in [2] for minimisers (in nonsymmetric situations) to spaces that allow cavitation, the difficulty stemming from a lack of sequential weak lower semicontinuity of the energy functional in these spaces. James and Spector [21] subsequently showed that $W^{1,p}$–quasiconvexity is also a necessary condition for a strong local minimiser at any point of smoothness of the minimiser, generalising a classical result of Meyers [32]. They use this approach in [22] to give conditions under which the energy of a radial cavitation solution (obtained in previous works on the symmetric problem) can be further lowered through the introduction of one or more filamentary voids, oriented in a radial direction and situated near the cavity surface.

The first breakthrough in the nonsymmetric situation was a general existence theory for energy minimisers in spaces allowing for cavitation in the work of Müller and Spector [34]. Key ideas in this work, in a Sobolev space setting, included a restriction on admissible deformations which they call condition INV, and the addition of a surface energy term to the total energy functional penalising new surfaces created by a deformation. Innovative recent work of Henao and Mora-Corral [13], building on the work in [34], gives an existence theory for minimisers which allows for the formation of both cavities and (higher dimensional) fractures within the one model. Their various existence results apply in Sobolev spaces and in the space of special functions of bounded variation, SBV. Key ingredients include the addition of one or more 'surface energy' terms to the energy functional to obtain sequential weak lower semicontinuity and the use of a finer characterisation of the new surface created by a deformation, differing from that used in [34]. In particular, the approach in [13] does not require the condition INV on the admissible deformations that was introduced in [34].

Work in [44] utilises the approach of [34] to prove existence of cavitation solutions in a nonsymmetric setting, without the need for a surface energy term, by viewing cavities as initiating from specified flaw points in the material. (Further results relating to this approach are contained in [45], [46], [12].) It is this latter model, utilising flaw points, that we adopt in the current paper.

The numerical aspects of computing cavitated solutions are challenging due to the singular nature of such deformations. The work of Negrón–Marrero [36] generalised to the multidimensional case of elasticity a method introduced by Ball and Knowles [5] for one dimensional problems, which is based on a decoupling technique that detects singular minimisers and avoids the Lavrentiev phenomena [24]. The convergence result in [36], however, involved a very strong condition on the finite element approximations which, in particular, excluded cavitated solutions. The element removal method introduced by Li ([25], [26]) improves upon this by penalising or excluding the elements of the finite element grid where the deformation gradient becomes very large. None of these methods, however, have been tested on higher dimensional problems. To our knowledge, the work of Negrón-Marrero and Betancourt [37] was the first attempt to compute nonsymmetric cavitated solutions in two-dimensional nonlinear elasticity. Their approach is based on the use of a spectral collocation method that can predict the formation of holes in a (circular) domain, but the method cannot be generalised to more complex geometries. At present, the best numerical schemes known to us which can compute cavitated solutions for general domains, even with multiple flaws, are those of Henao and Xu [16] and Lian and Li ([27], [28]).

To introduce the results in this paper, consider a nonlinear hyperelastic body occupying the bounded region $\tilde{\Omega} \subset \mathbb{R}^n$ in its reference state. A deformation of the body is a mapping $\tilde{\mathbf{u}} : \tilde{\Omega} \to \mathbb{R}^n$ satisfying the local invertibility condition

$$\det \nabla \tilde{\mathbf{u}}(\mathbf{x}) > 0 \quad \text{a.e. } \mathbf{x} \in \tilde{\Omega}. \tag{1.1}$$

The energy stored in the deformed body under a deformation $\tilde{\mathbf{u}}$ is given by

$$\int_{\tilde{\Omega}} W(\nabla \tilde{\mathbf{u}}(\mathbf{x}))\, \mathrm{d}\mathbf{x}, \tag{1.2}$$

where $W : M_+^{n\times n} \to \mathbb{R}$ is the stored energy function of the material and $M_+^{n\times n}$ denotes the set of $n \times n$ matrices with positive determinant. In this paper we consider the *displacement boundary value problem* in which we fix a matrix $\mathbf{A} \in M_+^{n\times n}$ and consider deformations satisfying

$$\tilde{\mathbf{u}}(\mathbf{x}) = \mathbf{A}\mathbf{x} \text{ for } \mathbf{x} \in \partial\tilde{\Omega}.$$

For technical reasons[1] we require to extend our deformations to a slightly larger domain. To this end, we next suppose that $\tilde{\Omega} \subset\subset \Omega$, where $\Omega \subset \mathbb{R}^n$ is a bounded domain with strongly Lipschitz boundary and we define the homogeneous extension of $\tilde{\mathbf{u}}$ to Ω, denoted $\mathbf{u}^e$, by

$$\mathbf{u}^e(\mathbf{x}) = \begin{cases} \tilde{\mathbf{u}}(\mathbf{x}) \text{ for } \mathbf{x} \in \tilde{\Omega} \\ \mathbf{A}\mathbf{x} \text{ for } \mathbf{x} \in \Omega\backslash\tilde{\Omega}. \end{cases} \tag{1.3}$$

We henceforth assume that all deformations have been extended in this way and we write $\mathbf{u}$ instead of $\mathbf{u}^e$ when referring to such extended deformations. We next fix a "flaw" point

[1]To prevent cavitation at the boundary (see [44]).

$\mathbf{x}_0 \in \Omega$, and look for minimisers of the energy functional

$$E(\mathbf{u}) = \int_\Omega W(\nabla \mathbf{u}(\mathbf{x}))\, \mathrm{d}\mathbf{x}, \tag{1.4}$$

over the *admissible set* of deformations given by

$$\begin{aligned} \mathcal{A}_{\mathbf{A}} \;\; = \;\; & \big\{ \mathbf{u} \in W^{1,p}(\Omega) \mid \mathrm{Det}\nabla\mathbf{u} = \det\nabla\mathbf{u}\; \mathcal{L}^n + \alpha\delta_{\mathbf{x_0}},\;\; \alpha \geq 0, \\ & \qquad \det \nabla\mathbf{u} > 0 \text{ a.e.},\;\; \mathbf{u}(\mathbf{x}) = \mathbf{A}\mathbf{x} \text{ on } \partial\Omega,\;\; \mathbf{u} \text{ satisfies INV on } \Omega \big\}. \end{aligned} \tag{1.5}$$

Here $\mathrm{Det}\nabla\mathbf{u}$ denotes the distributional determinant of $\mathbf{u}$, defined by

$$< \mathrm{Det}\nabla\mathbf{u}, \phi >= -\frac{1}{n}\int_\Omega \nabla\phi \cdot (\mathrm{Adj}\,\nabla\mathbf{u})\mathbf{u}\,\mathrm{d}\mathbf{x}, \quad \forall\;\; \phi \in C_0^\infty(\Omega), \tag{1.6}$$

$\mathcal{L}^n$ denotes n-dimensional Lebesgue measure, $p > n-1$, $\delta_{\mathbf{x_0}}$ denotes the Dirac measure supported at $\mathbf{x_0} \in \Omega$, and (INV) denotes the condition, relating to invertibility, introduced in Definition 3.2 of [34].

Results in [44] give conditions on the stored energy function W under which a minimiser for (1.4) exists on the set $\mathcal{A}_{\mathbf{A}}$. The results of Henao and Mora-Corral [13] give conditions under which a minimiser also exists in the case $p = n-1$ and their work in [14] includes justification of the interpretation of α in (1.5) as the volume of the hole formed by the deformation. Hence, if $\mathbf{u} \in \mathcal{A}_{\mathbf{A}}$ with $\alpha > 0$, then the deformation $\mathbf{u}$ produces a hole of volume α in the deformed body.

The next definition adapts the terminology of Ball and Murat [7], which extended previous work of Morrey on quasiconvexity (see, e.g., [33]), together with an adapted notion of uniform strict quasiconvexity originating in work of Evans (see, e.g., [9]).

Definition 1.1. Let $p > n-1$. We say that the stored energy function W is *$W^{1,p}$–quasiconvex (relative to the formation of a cavity) at the matrix* $\mathbf{A}$ if the homogeneous deformation $\mathbf{u}^{\mathrm{h}}_{\mathbf{A}}(\mathbf{x}) \equiv \mathbf{A}\mathbf{x}$ is a minimiser of (1.4) on $\mathcal{A}_{\mathbf{A}}$.

We say that W is *uniformly strictly $W^{1,p}$–quasiconvex (relative to the formation of a cavity) at the matrix at* $\mathbf{A}$ if there exists a constant $\gamma = \gamma(\mathbf{A}) > 0$ such that

$$\int_\Omega W(\mathbf{A}) + \gamma|\nabla\mathbf{u} - \mathbf{A}|^p \;\mathrm{d}\mathbf{x} \leq \int_\Omega W(\nabla\mathbf{u})\;\mathrm{d}\mathbf{x},\; \text{ for all } \mathbf{u} \in \mathcal{A}_{\mathbf{A}}.$$

We say that W is *uniformly strictly $W^{1,p}$–quasiconvex (relative to the formation of a cavity) on the set $\mathcal{B} \subseteq M^{n\times n}_+$* if the above condition holds with a $\gamma > 0$ which is independent of the choice of $\mathbf{A} \in \mathcal{B}$.

A standard rescaling argument (see Remark 2.5) can be adapted to show that our notion of $W^{1,p}$–quasiconvexity in Definition 1.1 is independent of the choice of the domain Ω and of the point $\mathbf{x_0} \in \Omega$ which appear in the definition of $\mathcal{A}_{\mathbf{A}}$ in (1.5).

If an energy minimising deformation $\mathbf{u}$ corresponding to the boundary displacement $\mathbf{Ax}$, opens a hole inside the deformed body, then W is not $W^{1,p}$–quasiconvex at $\mathbf{A}$ and we correspondingly define the set of unstable boundary strains by

$$\mathcal{U} = \{\mathbf{A} \in M^{n\times n}_+ \mid E(\mathbf{u}) < E(\mathbf{u}^{\mathrm{h}}_{\mathbf{A}}) \text{ for some } \mathbf{u} \in \mathcal{A}_{\mathbf{A}}\}. \tag{1.7}$$

Thus the set of all matrices $\mathbf{A}$ following which cavitation "first" occurs, is equal to the boundary of the set of matrices $\mathbf{A}$ for which W is not $W^{1,p}$–quasiconvex (relative to the formation of a cavity) at $\mathbf{A}$. However, characterising this boundary directly from the definition of quasiconvexity is a difficult task due to the "non local" nature of this notion (see [23]).

In this paper we propose an alternative characterisation of the set of unstable boundary strains $\mathcal{U}$ which we then use as the basis for a numerical method to evaluate $\partial\mathcal{U}$ for a number of energy functions. To introduce the method, we first define the set of deformations

$$\mathcal{A}_{\mathbf{A},V} = \{\mathbf{u} \in \mathcal{A}_{\mathbf{A}} \mid \alpha = V\}, \tag{1.8}$$

which produce a hole of a fixed volume $V > 0$. For any matrix $\mathbf{A} \in M^{n\times n}_+$, we define

$$F(\mathbf{A}, V) = \inf\nolimits_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},V}} \frac{E(\mathbf{u}) - E(\mathbf{u}^h_{\mathbf{A}})}{V}. \tag{1.9}$$

A straightforward scaling argument then shows that $F(\mathbf{A}, V)$ is a monotone increasing function of V and thus that the following limit

$$G(\mathbf{A}) = \inf\nolimits_{V>0} F(\mathbf{A}, V) = \lim_{V\searrow 0} F(\mathbf{A}, V), \tag{1.10}$$

exists, and we call $G(\mathbf{A})$ the *volume derivative*[2] of W at $\mathbf{A}$. This expression first appears in work of Varvaruca [54] in a study of degenerate cavitation (see Example 3.6 in the current paper), where it is calculated for $n = 3$ in the class of deformations of a ball for $W(\mathbf{F}) = |\mathbf{F}|^q,\ q \in [2, 3)$, and in the case when $\mathbf{A} = \lambda\mathbf{I}$.

Remark 1.2. The hypotheses and results of [45] are easily adapted to prove that a (not necessarily unique) minimiser of E on $\mathcal{A}_{\mathbf{A},V}$ exists for each $V > 0$ and we denote such a minimiser by $\mathbf{u}_V$. In this case, the volume derivative (1.10) is then given by

$$G(\mathbf{A}) = \lim_{V\searrow 0} \frac{E(\mathbf{u}_V) - E(\mathbf{u}^h_{\mathbf{A}})}{V}, \tag{1.11}$$

which further motivates our choice of the terminology "derivative".

[2]We note that this notion of derivative differs from the notion of the topological derivative used in shape-optimisation (see, e.g., [49, 50]) in which, for example, a small ball $B_\varepsilon(\mathbf{x}_0)$ is excised around a point $\mathbf{x}_0$ in the reference configuration and a limit is taken as $\varepsilon \to 0$ of the quotient of the energy drop and the volume of the excised region.

We define the set of stable boundary strains by

$$\mathcal{S} = \{\mathbf{A} \in M_+^{n\times n} \mid G(\mathbf{A}) > 0\}.$$

Thus

(i) $G(\mathbf{A}) > 0$ for all $\mathbf{A}$ in the stable set $\mathcal{S}$,

(ii) $G(\mathbf{A}) < 0$ for all $\mathbf{A}$ in the unstable set $\mathcal{U}$ (see Lemma 2.7),

and we conjecture that, for many stored energy functions W which satisfy a uniform strict quasiconvexity condition (in the sense of Definition 1.1) on the set $\mathcal{S}$, we have

(iii) $\partial\mathcal{S} = \partial\mathcal{U}$ and $G(\mathbf{A}) = 0$ for all $\mathbf{A}$ on this common boundary.

In [39] a radial version of the above conjecture is shown to be true in the case of radial cavitation, where detailed analytical properties of a corresponding radial volume derivative are derived and presented together with numerical results.

Remark 1.3. We prove in Proposition 2.4 that the volume derivative (1.10) is independent of the domain Ω and of the location of the flaw point $\mathbf{x}_0$ within the domain. It therefore follows that our definitions of the stable and unstable sets $\mathcal{S}$ and $\mathcal{U}$ are also independent of these choices.

When considering the formation of individual cavities, the boundary of $\mathcal{U}$ can be interpreted as a *fracture surface* or an *onset of cavitation surface* in the set of strains. To describe this interpretation, we first recall the following theorem of James and Spector [21].

Theorem 1.4 (James and Spector [21])**.** *If $\mathbf{u}_0 \in W^{1,p}(\Omega)$ is a strong local minimiser of the energy functional in $L^\infty(\Omega)\cap W^{1,p}(\Omega)$, $p \geq 1$, and $\mathbf{u}_0$ is C^1 in a neighbourhood of the point $\mathbf{x}_0 \in \Omega$, then the stored energy function W must be $W^{1,p}$–quasiconvex at the matrix $\mathbf{A}_0 = \nabla\mathbf{u}_0(\mathbf{x}_0)$.*

Hence, if $\mathbf{A}_0 = \nabla\mathbf{u}_0(\mathbf{x}_0)$ lies in $\mathcal{U}$, then forming a suitable small hole at $\mathbf{x}_0$ will lower the energy below that of $\mathbf{u}_0$ and so the smooth equilibrium solution $\mathbf{u}_0$ is locally unstable to the formation of a void. In particular, if the local strain $\nabla\mathbf{u}_0(\mathbf{x})$ produced by a general smooth equilibrium solution $\mathbf{u}_0$ crosses the boundary $\partial\mathcal{U}$ of the unstable set from inside $\mathcal{S}$ and into $\mathcal{U}$ as $\mathbf{x}$ varies in Ω, then this represents a transition from a stable into an unstable region of strain space in which local cavitation is energetically favoured.

A fundamental problem in studies of cavitation is to mathematically or computationally predict the onset of cavitation. Many of the previous studies to date on cavitation have focussed on the case of radial deformations with $\mathbf{A} = \lambda\mathbf{I}$. In this case, the problem is to characterise the value of λ_{crit} such that for $\lambda > \lambda_{crit}$ one has cavitation, but for $\lambda < \lambda_{crit}$ the minimiser of the stored energy functional is given by $\lambda\mathbf{x}$. In [52], Stuart uses a shooting argument for the radial equilibrium equation to give an implicit characterisation of λ_{crit} and this approach is further applied in [53] to give bounds for λ_{crit} for a class of stored energy functions. Connections of Stuart's approach with a radial version of the volume derivative considered in the current paper are contained in [39]. Other results on determining for λ_{crit} fall under the category of exact formulae for specific materials (see, e.g., [18], [17], [41] and the references in [19]).

A general numerical scheme for computing λ_{crit} was proposed by Negrón–Marrero and Sivaloganathan [38]. In this method, after specifying a cavity size $c > 0$, the corresponding boundary displacement λ_c producing this hole is computed. As the cavity size c tends to zero, one can show that the corresponding computed boundary displacements λ_c converge to λ_{crit}.

For the general non–symmetric case, the results for the critical boundary displacements characterising the onset of cavitation are mostly in the form of bounds, some of which are sharp for certain specific materials. We mention the work of López–Pamies et al [29, 30, 31] via homogenisation methods, Hou and Abeyaratne [20] for incompressible materials and for a particular class of deformations, and Müller, Sivaloganathan and Spector [35] and Varvaruca [54] using isoperimetric estimates. The current paper suggests a new approach to this problem in nonsymmetric situations based on computing or finding the zero set of the volume derivative.

The structure of the paper is as follows. In Section 2 we define the volume derivative and derive some of its general properties. In particular, it can be shown that the volume derivative is independent of the domain Ω and the location of the flaw point $\mathbf{x}_0$ (Proposition 2.4), and that it is a function of the singular values of the matrix $\mathbf{A}$ appearing in the linear boundary condition in the definition of the admissible set of deformations $\mathcal{A}_{\mathbf{A}}$ (see Theorem 2.10). In Sections 3 and 4 we present results on the volume derivative for the energy functions $W(\mathbf{F}) = |\mathbf{F}|^q$ and $W(\mathbf{F}) = h(\det \mathbf{F})$ respectively, which comprise our model polyconvex energy function in (2.3). In Section 5 we show, for certain families of sufficiently regular minimisers parametrised by the volume V in (1.10), that the volume derivative of a general stored energy function represents the negative of the work done per unit volume in opening a hole in the deformed configuration around the deformed flaw point $\mathbf{x}_0$. Finally, in Section 6 we show how the volume derivative can be used as the basis for a numerical scheme for computing the onset for cavitation as given by the solutions of $G(\mathbf{A}) = 0$. We discuss various of the numerical aspects of such a procedure, in particular, regularisation, a gradient flow iteration, and penalisation. We give examples of approximate fracture surfaces in strain space for the onset of cavitation (in the sense of this paper) for both two and three dimensional problems.

2 The volume derivative

In this section we define the volume derivative of a stored energy function and derive some of its general properties. We assume that the stored energy function W in (1.4) satisfies that

$$W(\mathbf{F}) \to \infty \text{ as either } \det \mathbf{F} \to 0^+ \text{ or } \|\mathbf{F}\| \to \infty. \tag{2.1}$$

If W is frame indifferent and isotropic, then it is well known that there is a symmetric function Φ such that

$$W(\mathbf{F}) = \Phi(v_1, \ldots, v_n), \tag{2.2}$$

where $v_1, \ldots, v_n$ are the singular values of the matrix $\mathbf{F}$.

A simple class of polyconvex isotropic stored energy functions to which the results in this paper can be applied is given by

$$\begin{aligned} W(\mathbf{F}) &= \frac{\mu}{q}|\mathbf{F}|^q + h(\det \mathbf{F}), \\ &= \frac{\mu}{q}(v_1^2 + \cdots + v_n^2)^{q/2} + h(v_1 \cdots v_n) \quad \text{for } \mathbf{F} \in M_+^{n\times n}, \end{aligned} \tag{2.3}$$

where $\kappa > 0$, $q \in [n-1, n)$ and $h : (0, \infty) \to (0, \infty)$ is such that

$$h \text{ is a } C^2, \text{ convex function and} \tag{2.4a}$$

$$h(\delta) \to \infty \text{ and } \tfrac{h(\delta)}{\delta} \to \infty \text{ as } \delta \to 0, \infty \text{ respectively.} \tag{2.4b}$$

However, we note that that the results of this paper apply to more general polyconvex stored energy functions under varied hypotheses.

We recall that for $\mathbf{u} \in \mathcal{A}_{\mathbf{A}}$ (given by (1.5)), the α in the distributional jacobian measures the volume of the hole produced by $\mathbf{u}$ at the flaw point. For each $V > 0$ and $\mathbf{A} \in M_+^{n\times n}$, we consider the subset of $\mathcal{A}_{\mathbf{A}}$ given by:

$$\mathcal{A}_{\mathbf{A},V} = \{\mathbf{u} \in \mathcal{A}_{\mathbf{A}} \,:\, \alpha = V\}, \tag{2.5}$$

and we define

$$F(\mathbf{A}, V) = \inf_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},V}} \frac{E(\mathbf{u}) - E(\mathbf{u}^h_{\mathbf{A}})}{V}, \tag{2.6}$$

where $\mathbf{u}^h_{\mathbf{A}}(\mathbf{x}) \equiv \mathbf{A}\mathbf{x}$ is the homogeneous deformation corresponding to the given linear boundary data. We note that, under the assumptions given in [44], one can show that (1.4) has a minimiser on $\mathcal{A}_{\mathbf{A},V}$. However, our definition of $F(\mathbf{A}, V)$ does not require that a minimiser exist. The next result yields an interesting property of the function F (see also [45, Lemma 1.2], [54]).

Proposition 2.1. *For each $\mathbf{A} \in M_+^{n\times n}$, $F(\mathbf{A}, V)$ is monotone increasing in V.*

Proof: Let $\mathbf{u}_V \in \mathcal{A}_{\mathbf{A},V}$ with the location of the flaw point at $\mathbf{x}_0 \in \Omega$. Let $V_1 < V$ and $\varepsilon > 0$ be such that $V_1 = \varepsilon^n V$. Define $\mathbf{u}_\varepsilon$ by

$$\mathbf{u}_\varepsilon(\mathbf{x}) = \begin{cases} \varepsilon \mathbf{u}_V\left(\dfrac{\mathbf{x}-\mathbf{x}_0}{\varepsilon} + \mathbf{x}_0\right) + \mathbf{A}\mathbf{x}_0 - \varepsilon\mathbf{A}\mathbf{x}_0, & \mathbf{x} \in \varepsilon(\Omega - \mathbf{x}_0) + \mathbf{x}_0, \\ \mathbf{A}\mathbf{x}, & \text{otherwise.} \end{cases}$$

Clearly for ε sufficiently small $\mathbf{u}_\varepsilon \in \mathcal{A}_{\mathbf{A},V_1}$ and since

$$\begin{aligned} E(\mathbf{u}_\varepsilon) - E(\mathbf{u}^h_{\mathbf{A}}) &= \int_{\varepsilon(\Omega-\mathbf{x}_0)+\mathbf{x}_0} \left[W\left(\nabla \mathbf{u}_V \left(\frac{\mathbf{x}-\mathbf{x}_0}{\varepsilon} + \mathbf{x}_0 \right) \right) - W(\mathbf{A}) \right] \mathrm{d}\mathbf{x} \\ &= \varepsilon^n \int_\Omega (W(\nabla \mathbf{u}_V(\mathbf{y})) - W(\mathbf{A}))\, \mathrm{d}\mathbf{y}, \end{aligned}$$

it follows that

$$\frac{E(\mathbf{u}_\varepsilon) - E(\mathbf{u}^h_{\mathbf{A}})}{V_1} = \frac{E(\mathbf{u}_V) - E(\mathbf{A}\mathbf{x})}{V}.$$

Hence

$$F(\mathbf{A}, V_1) \le \frac{E(\mathbf{u}_\varepsilon) - E(\mathbf{u}^h_{\mathbf{A}})}{V_1} = \frac{E(\mathbf{u}_V) - E(\mathbf{u}^h_{\mathbf{A}})}{V}$$

and taking the infimum of the right hand side over $\mathbf{u}_V \in \mathcal{A}_V$ now yields

$$F(\mathbf{A}, V_1) \le F(\mathbf{A}, V)$$

as required. □

Definition 2.2. With the notation of Proposition 2.1, we define the *volume derivative of the energy functional* (1.4) *at* $\mathbf{A}$ by:

$$G(\mathbf{A}) = \inf_{V>0} F(\mathbf{A}, V) = \lim_{V \searrow 0} F(\mathbf{A}, V). \tag{2.7}$$

(The monotonicity of $F(\mathbf{A}, \cdot)$ ensures that the above limit exists.)

Remark 2.3. It follows from the definition of the volume derivative that

$$G(\mathbf{A}) \le F(\mathbf{A}, V) \le \frac{E(\mathbf{u}) - E(\mathbf{u}^h_{\mathbf{A}})}{V} \quad \text{for all } \mathbf{u} \in \mathcal{A}_{\mathbf{A},V}, \text{ for any } V > 0,$$

and so

$$E(\mathbf{u}^h_{\mathbf{A}}) + G(\mathbf{A})V \le E(\mathbf{u}) \quad \text{for all } \mathbf{u} \in \mathcal{A}_{\mathbf{A},V}, \text{ for any } V > 0.$$

Hence, in particular, if $G(\mathbf{A}) \ge 0$, then the stored energy function W is $W^{1,p}$–quasiconvex at $\mathbf{A}$ in the sense of Definition 1.1.

The next result shows that the volume derivative is independent of the domain and of the choice of flaw point.

Proposition 2.4. *Let* $\mathbf{A} \in M^{n\times n}_+$ *and let the domains* Ω_1, Ω_2 *contain the flaw points* $\mathbf{x}_1$ *and* $\mathbf{x}_2$ *respectively. Let* $G_{\Omega_1}(\mathbf{A})$ *and* $G_{\Omega_2}(\mathbf{A})$ *denote the volume derivatives on the respective domains. Then* $G_{\Omega_1}(\mathbf{A}) = G_{\Omega_2}(\mathbf{A})$.

Proof: Fix $V > 0$ and let $\mathbf{u} : \Omega_1 \to \mathbb{R}^n$, $\mathbf{u} \in \mathcal{A}_{\mathbf{A},V,\mathbf{x_1}}$ (we add the subscript $\mathbf{x}_i$ to the admissible set of deformations to emphasise the location of the flaw). Correspondingly, for $\varepsilon > 0$ we define

$$\tilde{\mathbf{u}}(\mathbf{x}) = \begin{cases} \varepsilon \mathbf{u}\left(\frac{\mathbf{x}-\mathbf{x_2}}{\varepsilon} + \mathbf{x_1}\right) - \varepsilon \mathbf{A}\mathbf{x}_1 + \mathbf{A}\mathbf{x}_2 & \text{for } \mathbf{x} \in \varepsilon(\Omega_1 - \mathbf{x}_1) + \mathbf{x}_2, \\ \mathbf{A}\mathbf{x} & \text{otherwise.} \end{cases} \tag{2.8}$$

Then it is straightforward to verify that, for sufficiently small ε, we have that $\tilde{\mathbf{u}} : \Omega_2 \to \mathbb{R}^n$, $\tilde{\mathbf{u}} \in \mathcal{A}_{\mathbf{A},\varepsilon^n V,\mathbf{x_2}}$ and

$$\frac{E_{\Omega_1}(\mathbf{u}) - E_{\Omega_1}(\mathbf{u}^h_{\mathbf{A}})}{V} = \frac{E_{\Omega_2}(\tilde{\mathbf{u}}) - E_{\Omega_2}(\mathbf{u}^h_{\mathbf{A}})}{\varepsilon^n V}. \tag{2.9}$$

Hence

$$\frac{E_{\Omega_1}(\mathbf{u}) - E_{\Omega_1}(\mathbf{u}^h_{\mathbf{A}})}{V} \geq F_{\Omega_2}(\mathbf{A}, \varepsilon^n V) \geq G_{\Omega_2}(\mathbf{A}),$$

and so

$$F_{\Omega_1}(\mathbf{A}, V) \geq G_{\Omega_2}(\mathbf{A}),$$

and thus

$$G_{\Omega_1}(\mathbf{A}) \geq G_{\Omega_2}(\mathbf{A}).$$

Interchanging the roles of Ω_1 and Ω_2 we also obtain the reverse inequality and so $G_{\Omega_1}(\mathbf{A}) = G_{\Omega_2}(\mathbf{A})$. □

Remark 2.5. The construction and argument used in the last proposition (see (2.8), (2.9)) show that our notion of $W^{1,p}$–quasiconvexity (relative to the formation of a cavity) of the stored energy function W in Definition 1.1, is independent of the choice of domain Ω and of the location of the flaw point $\mathbf{x_0} \in \Omega$. However, the proof fails in general if we work with an admissible set of deformations which contains more than one flaw point.

Henceforth, when computing volume derivatives in this paper, we will always assume that $\Omega = B$ the unit ball in $\mathbb{R}^n$ and that the flaw point is at the centre of B so that $\mathbf{x}_0 = \mathbf{0}$. We next obtain some general properties of the volume derivative.

Definition 2.6. We define the set of stable boundary strains $\mathcal{S}$ and the set of unstable boundary strains $\mathcal{U}$ by

$$\mathcal{S} = \{\mathbf{A} \in M^{n\times n}_+ \mid G(\mathbf{A}) > 0\}, \tag{2.10}$$

$$\mathcal{U} = \{\mathbf{A} \in M^{n\times n}_+ \mid E(\mathbf{u}) < E(\mathbf{u}^{\mathrm{h}}_{\mathbf{A}}) \text{ for some } \mathbf{u} \in \mathcal{A}_{\mathbf{A}}\}. \tag{2.11}$$

Lemma 2.7. *An alternative characterisation of the unstable set $\mathcal{U}$ is given by*

$$\mathcal{U} = \{\mathbf{A} \in M^{n\times n}_+ \mid G(\mathbf{A}) < 0\}. \tag{2.12}$$

In addition, $G(\mathbf{A}) \geq 0$ if and only if the homogeneous deformation $\mathbf{u}^h_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ is a minimiser of the energy on the set $\mathcal{A}_{\mathbf{A}}$.

Proof: The first part of the Lemma follows from Proposition 2.1. The second part of the Lemma follows since $F(\mathbf{A}, V) \geq 0$ for all $V > 0$ if and only if $G(\mathbf{A}) \geq 0$. $\square$

We next show that, under a mild hypothesis on the stored energy function, the unstable set $\mathcal{U}$ is open. We refer to [4] for further details and background relating to our hypothesis (2.13)[3].

Proposition 2.8. *Suppose that there exist constants $k, \varepsilon_0 > 0$ such that the stored energy function satisfies:*

$$|W(\mathbf{CF})| \leq k\,[W(\mathbf{F}) + 1] \quad \text{for all } \mathbf{F} \in \mathrm{M}^{n\times n}_{+}, \tag{2.13}$$

whenever $|\mathbf{C} - \mathbf{I}| < \varepsilon_0$. Then the set of unstable boundary strains $\mathcal{U}$ is open.

Proof: Suppose for a contradiction that the result is false. Then there exist $\mathbf{A} \in \mathcal{U}$ and a sequence of matrices $(\mathbf{A}_k)$ converging to $\mathbf{A}$ and satisfying $G(\mathbf{A}_k) \geq 0$ for all k. Since $\mathbf{A} \in \mathcal{U}$, for some $V_0 > 0$ there exists a deformation $\mathbf{u}_0 \in \mathcal{A}_{\mathbf{A},V_0}$, such that

$$E(\mathbf{u}_0) < E(\mathbf{u}^h_{\mathbf{A}}).$$

Now define $\mathbf{u}_k \in \mathcal{A}_{\mathbf{A}_k,V_k}$ by $\mathbf{u}_k = \mathbf{A}_k\mathbf{A}^{-1}\mathbf{u}_0$, where $V_k = \frac{\det \mathbf{A}_k}{\det \mathbf{A}} V_0$. Then

$$E(\mathbf{u}_k) - E(\mathbf{u}^h_{\mathbf{A}_k}) = \int_B W(\mathbf{A}_k\mathbf{A}^{-1}\nabla\mathbf{u}_0(\mathbf{x}))\,\mathrm{d}\mathbf{x} - \int_B W(\mathbf{A}_k)\,\mathrm{d}\mathbf{x} \quad \text{for all } k.$$

Now passing to the limit $k \to \infty$ in the above expression, using $\mathbf{A}_k\mathbf{A}^{-1} \to \mathbf{I}$, (2.13) and the dominated convergence theorem, we obtain that

$$\int_B W(\mathbf{A}_k\mathbf{A}^{-1}\nabla\mathbf{u}_0(\mathbf{x}))\,\mathrm{d}\mathbf{x} - \int_B W(\mathbf{A}_k)\,\mathrm{d}\mathbf{x} < 0 \quad \text{for all sufficiently large } k.$$

Finally, it follows by Lemma 2.7 and (2.11) that $G(\mathbf{A}_k) < 0$ for all sufficiently large k, which is a contradiction. $\square$

Remark 2.9. It follows from Proposition 2.8 that the boundaries of the unstable and stable sets satisfy $\partial\mathcal{U}, \partial\mathcal{S} \subseteq \{\mathbf{A} \mid G(\mathbf{A}) \geq 0\}$ and we seek conditions under which $\partial\mathcal{U} = \partial\mathcal{S} = \{\mathbf{A} \mid G(\mathbf{A}) = 0\}$.

The next result shows that the volume derivative of a frame indifferent, isotropic, stored energy function at a given matrix $\mathbf{A} \in M^{n\times n}_{+}$ depends only on the singular values of $\mathbf{A}$ (see also [54, Proposition 1.50]).

[3] See, in particular, expression (2.24) in the proof of Lemma 2.4 in [4]

Theorem 2.10. *Let $\mathbf{A} \in M_+^{n\times n}$ and suppose that the stored energy function W is frame indifferent and isotropic. Then the volume derivative of W at $\mathbf{A}$ satisfies $G(\mathbf{A}) = G(\mathbf{d})$ where $\mathbf{d} = \operatorname{diag}(\lambda_1, ..., \lambda_n)$ is the diagonal matrix of singular values of $\mathbf{A}$. Hence, $\mathbf{A}$ belongs to the stable set of strains $\mathcal{S}$ given by (2.10) (respectively to the unstable set of strains $\mathcal{U}$ given by (2.11)) if and only if $\mathbf{d}$ belongs to $\mathcal{S}$ (respectively to $\mathcal{U}$).*

Proof: By Proposition 2.4 we may assume without loss of generality that $\Omega = B$ the unit ball in $\mathbb{R}^n$ and that the flaw point is located at the centre of B. Let $\mathbf{A} \in M_+^{n\times n}$, then by the polar decomposition theorem, $\mathbf{A} = \mathbf{RU}$ for some orthogonal matrix $\mathbf{R}$ and positive definite, symmetric matrix $\mathbf{U}$ with eigenvalues $\lambda_1, ..., \lambda_n$. For each $\mathbf{u} \in \mathcal{A}_{V,\mathbf{A}}$, define $\tilde{\mathbf{u}}(\mathbf{x}) = \mathbf{Qu}(\tilde{\mathbf{R}}\mathbf{x})$, where the orthogonal matrix $\mathbf{Q} = \tilde{\mathbf{R}}^{\mathbf{T}}\mathbf{R}^{\mathbf{T}}$ and the orthogonal matrix $\tilde{\mathbf{R}}$ is chosen so that $\tilde{\mathbf{R}}^{\mathbf{T}}\mathbf{U}\tilde{\mathbf{R}} = \mathbf{d} = \operatorname{diag}(\lambda_1, ..., \lambda_n)$. Then $\tilde{\mathbf{u}}(\mathbf{x}) = \mathbf{QA}\tilde{\mathbf{R}}\mathbf{x} = \mathbf{dx}$ for $\mathbf{x} \in \partial B$ and $\tilde{\mathbf{u}} \in \mathcal{A}_{V,\mathbf{d}}$ (note that the volume of the hole formed by $\tilde{\mathbf{u}}$ and the location of the flaw point are unchanged, even though the hole formed may be rotated). This yields a one-to-one correspondence between deformations $\mathbf{u} \in \mathcal{A}_{V,\mathbf{A}}$ and $\tilde{\mathbf{u}} \in \mathcal{A}_{V,\mathbf{d}}$. Moreover,

$$E(\tilde{\mathbf{u}}) = \int_B W(\mathbf{Q}\nabla\mathbf{u}(\tilde{\mathbf{R}}\mathbf{x})\tilde{\mathbf{R}})\mathrm{d}\mathbf{x} = \int_{\tilde{\mathbf{R}}B} W(\mathbf{Q}\nabla\mathbf{u}(\mathbf{y})\tilde{\mathbf{R}})\mathrm{d}\mathbf{y} = \int_B W(\nabla\mathbf{u}(\mathbf{y}))\mathrm{d}\mathbf{y} = E(\mathbf{u}),$$

by the isotropy and frame indifference of W. The claim of the first part of the Theorem now follows from the definition of the volume derivative (see (2.6), (2.7)). □

It is an elementary consequence of the definition of the volume derivative that it has the following superadditivity property.

Proposition 2.11. *If the energy functions $W^{(1)}(\mathbf{F}), W^{(2)}(\mathbf{F})$ have volume derivatives $G^{(1)}(\mathbf{A}), G^{(2)}(\mathbf{A})$ respectively at the matrix $\mathbf{A}$, then the volume derivative of the energy function $W^{(3)}(\mathbf{F}) = W^{(1)}(\mathbf{F}) + W^{(2)}(\mathbf{F})$ satisfies $G^{(3)}(\mathbf{A}) \geq G^{(1)}(\mathbf{A}) + G^{(2)}(\mathbf{A})$.*

As consequence of this observation, we have the following two results. The first of these relates to a result that first appears in [51].

Lemma 2.12. *Let $\mathbf{A} \in M_+^{n\times n}$, $p \in (n-1, n)$ and let $\tilde{W}$ be $W^{1,p}$–quasiconvex (in the sense of Definition 1.1) at $\mathbf{A}$ so that the volume derivative for $\tilde{W}$ satisfies $\tilde{G}(\mathbf{A}) \geq 0$. Suppose further that the W in (1.4) is given by $W(\mathbf{F}) = \tilde{W}(\mathbf{F}) + h(\det \mathbf{F})$. Then the volume derivative for W satisfies*

$$G(\mathbf{A}) \geq -h'(\det \mathbf{A}).$$

In particular, if $h'(\det \mathbf{A}) < 0$ then $\mathbf{A} \in \mathcal{S}$.

Proof: This result follows from Propositions 2.11 and 4.1. □

Lemma 2.13. *Let $\mathbf{A} \in M_+^{n\times n}$, $p \in (n-1, n)$ and let $\tilde{W}$ be $W^{1,p}$–quasiconvex (in the sense of Definition 1.1) at $\mathbf{A}$ (so that the volume derivative for $\tilde{W}$ satisfies $\tilde{G}(\mathbf{A}) \geq 0$) and let the W in (1.4) be given by $W(\mathbf{F}) = \tilde{W}(\mathbf{F}) + \eta\,|\mathbf{F}|^q$ for some $\eta > 0$, $n-1 \leq q \leq p$. Then the volume derivative for the stored energy function W satisfies $G(\mathbf{A}) > 0$ and hence $\mathbf{A}$ belongs to the stable set $\mathcal{S}$ for W.*

Proof: This result follows from Proposition 2.11 and Theorem 3.3. $\square$

3 The Case $W(\mathbf{F}) = |\mathbf{F}|^q$

In this section we consider the particular case of the stored energy function $W(\mathbf{F}) = |\mathbf{F}|^q$, $q \in [n-1, n)$. We give an explicit expression for $G(\lambda \mathbf{I})$ for any $\lambda > 0$, and obtain upper and lower bounds for $G(\mathbf{A})$ for any matrix $\mathbf{A} = \mathrm{diag}(\lambda_1, ..., \lambda_n)$. (Note that by the Sobolev Embedding Theorem, the volume derivative of $W(\mathbf{F}) = |\mathbf{F}|^q$ is infinite for $q > n$.) Throughout this section, though we allow the possibility that $q = n-1$, we still require that $p > n-1$ in the definition of the admissible set of deformations (1.5) (so that, in particular, condition (INV) still makes sense).

3.1 A lower bound for $G(\mathbf{A})$ for general matrices $\mathbf{A}$

In this subsection we prove, in particular, that the volume derivative (1.10) for the above stored energy function is strictly positive for all matrices $\mathbf{A} \in M_+^{n\times n}$. We first recall some results from [35].

Lemma 3.1. *[35, Section 3] Let $n \geq 2$, $n-1 < p < n$, and $n-1 \leq q \leq p$. Then there exists a constant $\alpha = \alpha(n;q) > 0$, which is independent of the domain, such that*

$$V = \int_\Omega [\det \mathbf{A} - \det \nabla \mathbf{u}(\mathbf{x})] \mathrm{d}\mathbf{x} \leq \alpha |\mathbf{A}|^{n-q} \int_\Omega |\mathbf{A} - \nabla \mathbf{u}(\mathbf{x})|^q \, \mathrm{d}\mathbf{x}, \text{ for all } \mathbf{u} \in \mathcal{A}_{\mathbf{A},V}.$$

We will also require the following lemma.

Lemma 3.2. *[35, Proposition A.1] Let $q \in [2, \infty)$. Then there exists a constant $\kappa = \kappa(q) > 0$, such that*

$$|\mathbf{a}|^q \geq |\mathbf{b}|^q + q|\mathbf{b}|^{q-2}\mathbf{b} \cdot (\mathbf{a} - \mathbf{b}) + \kappa |\mathbf{a} - \mathbf{b}|^q, \quad \text{for all } \mathbf{a}, \mathbf{b} \in \mathbb{R}^n.$$

The constant κ is independent of the dimension and the largest such κ satisfies $2^{2-q} \leq \kappa \leq q\, 2^{1-q}$.

We now derive a lower bound for $G(\mathbf{A})$ in this case.

Theorem 3.3. *Let $n \geq 2$ and $n-1 < p < n$. Let the stored energy function be given by $W(\mathbf{F}) = |\mathbf{F}|^q$, where $n-1 \leq q \leq p$, and let $G(\mathbf{A})$ be its volume derivative at $\mathbf{A} \in M_+^{n\times n}$. Then there exists a constant $c > 0$ such that $G(\mathbf{A}) \geq c|\mathbf{A}|^{q-n}$ for all $\mathbf{A} \in M_+^{n\times n}$.*

Proof: It follows from Lemma 3.2 and the definition of $\mathcal{A}_{\mathbf{A},V}$ that for each $V > 0$ and for any $\mathbf{u} \in \mathcal{A}_{\mathbf{A},V}$ we have

$$\begin{aligned} \int_B |\nabla \mathbf{u}|^q - |\mathbf{A}|^q \quad &\geq \quad \int_B q|\mathbf{A}|^{q-2}\mathbf{A} \cdot (\nabla \mathbf{u} - \mathbf{A}) + \kappa \int_B |\nabla \mathbf{u} - \mathbf{A}|^q \\ &= \quad \kappa \int_B |\nabla \mathbf{u} - \mathbf{A}|^q, \end{aligned} \tag{3.1}$$

and hence by Lemma 3.1, it follows that

$$\frac{\int_B |\nabla \mathbf{u}|^q - |\mathbf{A}|^q}{V} \geq \frac{\kappa}{\alpha |\mathbf{A}|^{n-q}}.$$

The claim of the theorem now follows, from the definition of the volume derivative, on setting $c = \frac{\kappa}{\alpha}$. □

3.2 Evaluation of $G(\lambda\mathbf{I})$ for $\lambda > 0$ and $n = 3$

In the case $\mathbf{A} = \lambda\mathbf{I}$ and $n = 3$ it is possible to calculate $G(\lambda\mathbf{I})$ explicitly for the stored energy function $W(\mathbf{F}) = |\mathbf{F}|^q$ using the results of [43] (in the case $q = 2$) and the generalisation of [54] (for $q \in (2, 3)$). For simplicity, we present the results in the case[4] $q = 2$.

Theorem 3.4. *Let the stored energy function be given by* $W(\mathbf{F}) = |\mathbf{F}|^2$ *with* $n = 3$. *Then the volume derivative of* W *at* $\lambda\mathbf{I}$ *is given by*

$$G(\lambda\mathbf{I}) = \frac{8}{3\lambda}, \quad \lambda > 0. \tag{3.2}$$

Proof: It follows from the work of ([43], [54]) that the value of the infimum:

$$F(\lambda\mathbf{I}, V) = \inf_{\mathbf{u} \in \mathcal{A}_{\lambda\mathbf{I},V}} \left[\frac{\int_B (|\nabla \mathbf{u}|^2 - |\lambda\mathbf{I}|^2)\, \mathrm{d}\mathbf{x}}{V} \right] \tag{3.3}$$

can be obtained by evaluating the expression in square brackets in (3.3) with $\mathbf{u} = \mathbf{u}^{\mathrm{rad}}$, where $\mathbf{u}^{\mathrm{rad}}(\mathbf{x}) = (r(R)/R)\mathbf{x}$, $R = \|\mathbf{x}\|$, is the degenerate radial deformation with $r : [0, 1] \to \mathbb{R}$ given by:

$$r(R) = \begin{cases} c & , \quad 0 \leq R \leq R_0, \\ aR + \dfrac{\lambda - a}{R^2} & , \quad R_0 \leq R \leq 1. \end{cases} \tag{3.4}$$

(Note that the corresponding deformation $\mathbf{u}^{\mathrm{rad}}$ is not a minimiser because $\det \nabla \mathbf{u}^{\mathrm{rad}}(\mathbf{x}) = 0$ on a ball of radius R_0 around the origin and thus $\mathbf{u}^{\mathrm{rad}}$ does not belong to $\mathcal{A}_{\lambda\mathbf{I},V}$.) The constants a, R_0 can be determined from the conditions that $r(R_0) = c$ and $r'(R_0) = 0$, where $\frac{4}{3}\pi c^3 = V$. Hence the relations between R_0, c and a are given by:

$$aR_0 + \frac{(\lambda - a)}{R_0^2} = c, \quad a - \frac{2(\lambda - a)}{R_0^3} = 0,$$

[4]However, recall that for technical reasons when calculating the volume derivative, we work with the admissible set of deformations (1.5) with $p > n - 1 = 2$.

and from these equations it follows that

$$c = \frac{3}{2} a R_0, \quad c^3 = \frac{27}{4} a^2 (\lambda - a). \tag{3.5}$$

It now follows from elementary calculations using the above relations that

$$\begin{aligned} F(\lambda \mathbf{I}, V) &= \frac{4\pi \left[\int_0^1 R^2 \left((r')^2 + 2 \left(\frac{r}{R} \right)^2 - 3\lambda^2 \right) \, dR \right]}{4\pi c^3/3} \\ &= \frac{3a\lambda - 3\lambda^2 + \frac{4c^3}{3a}}{c^3/3}. \end{aligned}$$

A straightforward application of L'Hopital's Rule, using the implicit relation between a and c^3 given in $(3.5)_2$, and noting that $a \to \lambda$ as $c^3 \to 0$, yields that

$$G(\lambda \mathbf{I}) = \lim_{c^3 \to 0} F\left(\lambda \mathbf{I}, \frac{4\pi c^3}{3} \right) = \frac{8}{3\lambda}.$$

□

Remark 3.5. The last result can be generalised to include the cases $q \in (2, 3)$ using the results of Varvaruca [54]. From these it can be shown that that the volume derivative, in this case, at the matrix $\mathbf{A} = \lambda \mathbf{I}$ is given by

$$G(\lambda \mathbf{I}) = \frac{\Upsilon_q}{\lambda^{3-q}}, \quad \lambda > 0,$$

where a closed form expression for

$$\Upsilon_q = \inf_{V>0} \inf_{\mathbf{u} \in \mathcal{A}_{V,\mathbf{I}}} \frac{\int_B (|\nabla \mathbf{u}|^q - |\mathbf{I}|^q) \, \mathrm{d}\mathbf{x}}{V} > 0 \tag{3.6}$$

is given for $q \in [2, 3)$ in [54, chapter 3].

Example 3.6. An example in which the criterion $G(\mathbf{A}) = 0$ gives exactly the critical boundary displacements $\mathbf{A} = \lambda \mathbf{I}$ for cavitation, is furnished by the example of degenerate cavitation considered in [43], [54]. In this case we consider

$$\tilde{W}(\mathbf{F}) = \mu \, |\mathbf{F}|^q + \kappa \det \mathbf{F} = \mu (v_1^2 + v_2^2 + v_3^2)^{q/2} + \kappa v_1 v_2 v_3, \tag{3.7}$$

where $q \in [2, 3)$ and $\kappa > 0$ is a constant. It follows that for $\mathbf{u} \in \mathcal{A}_{\lambda \mathbf{I}, V}$:

$$\begin{aligned} \tilde{E}(\mathbf{u}) &= \mu \int_B |\nabla \mathbf{u}|^q \, \mathrm{d}\mathbf{x} + \left(\frac{4\pi}{3} \lambda^3 - V \right) \kappa, \\ \tilde{E}(\mathbf{A}\mathbf{x}) &= \mu \int_B |\lambda \mathbf{I}|^q \, \mathrm{d}\mathbf{x} + \frac{4\pi}{3} \kappa \lambda^3. \end{aligned}$$

For ease of exposition we consider the case $q = 2$. In this case,

$$\begin{aligned}\tilde{F}(\lambda\mathbf{I}, V) &= \inf_{\mathbf{u}\in\mathcal{A}_{\lambda\mathbf{I},V}} \frac{\int_B \mu(|\nabla\mathbf{u}|^2 - |\lambda\mathbf{I}|^2)\,\mathrm{d}\mathbf{x} - \kappa V}{V} \\ &= \inf_{\mathbf{u}\in\mathcal{A}_{\lambda\mathbf{I},V}} \left[\frac{\int_B \mu(|\nabla\mathbf{u}|^2 - |\lambda\mathbf{I}|^2)\,\mathrm{d}\mathbf{x}}{V}\right] - \kappa\end{aligned}$$

and by the earlier calculations of this section, this infimum can be calculated by evaluating the expression in square brackets at the degenerate radial deformation $\mathbf{u}^{\mathrm{rad}}(\mathbf{x}) = (r(R)/R)\mathbf{x}$, $R = \|\mathbf{x}\|$, where the function $r : [0,1] \to \mathbb{R}$ is given by (3.4) and (3.5). (As noted earlier, the corresponding deformation $\mathbf{u}^{\mathrm{rad}}$ is not a minimiser because $\det \nabla\mathbf{u}^{\mathrm{rad}}(\mathbf{x}) = 0$ on a ball of radius R_0 around the origin and so $\mathbf{u}^{\mathrm{rad}}$ does not belong to $\mathcal{A}_{\lambda\mathbf{I},V}$.) Hence by (3.2), the volume derivative of (3.7) at $\lambda\mathbf{I}$ is given by

$$\tilde{G}(\lambda\mathbf{I}) = \frac{8\mu}{3\lambda} - \kappa. \tag{3.9}$$

The criterion $\tilde{G}(\lambda\mathbf{I}) = 0$ then yields $\lambda = \frac{8\mu}{3\kappa}$ which agrees with the critical value λ_{crit} obtained in [43] after which degenerate cavitation occurs. Hence, for this example, the unstable and stable sets (within the class of matrices of the form $\lambda\mathbf{I}$) are given by

$$\tilde{\mathcal{U}} = \left\{\lambda\mathbf{I} \mid \lambda > \frac{8\mu}{3\kappa}\right\} = \left\{\lambda\mathbf{I} \mid \tilde{G}(\lambda\mathbf{I}) < 0\right\},$$

$$\tilde{\mathcal{S}} = \{\lambda\mathbf{I} \mid \lambda < \frac{8\mu}{3\kappa}\} = \{\lambda\mathbf{I} \mid \tilde{G}(\lambda\mathbf{I}) > 0\},$$

respectively and the relative boundaries of these sets, in the class of diagonal matrices, are given by

$$\partial\tilde{\mathcal{U}} = \partial\tilde{\mathcal{S}} = \{\lambda\mathbf{I} \mid \tilde{G}(\lambda\mathbf{I}) = 0\}.$$

Remark 3.7. The results in the above example can be extended, by using a similar reasoning, to $q \in (2,3)$ using the results of [54]. From these (see also Remark 3.5) it follows that $\tilde{G}(\lambda\mathbf{I}) = 0$ if and only if

$$\lambda^{3-q} = \frac{\mu}{\kappa}\Upsilon_q, \tag{3.10}$$

where an explicit, though somewhat lengthy expression for Υ_q, for all $q \in (2,3)$, can be found in [54, Remark 3.2].

3.3 An upper bound on $G(\mathbf{A})$ for $q = 2$ and $n = 3$

In this subsection we derive an upper bound for the volume derivative of $W(\mathbf{F}) = |\mathbf{F}|^2$ at a general matrix $\mathbf{A}$ for $n = 3$. (Recall, however, that the volume derivative is calculated using deformations in the set (1.5), with $p > n - 1 = 2$.)

Theorem 3.8. *Let the stored energy function be given by $W(\mathbf{F}) = |\mathbf{F}|^2$ with $n = 3$. Then the volume derivative of W at $\mathbf{A} \in M_+^{n\times n}$ satisfies*

$$G(\mathbf{A}) \leq \frac{8}{9} \frac{(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)}{\lambda_1\lambda_2\lambda_3}, \tag{3.11}$$

where $(\lambda_1, \lambda_2, \lambda_3)$ are the singular values of $\mathbf{A}$.

Proof: By Theorem 2.10, is enough to consider the case $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$, $\lambda_i > 0$, $i = 1, 2, 3$. We now consider the case of the infima (3.3) when $\lambda = 1$. In this case, this infimum is attained at the degenerate radial deformation $\mathbf{u}^{\mathrm{rad}}(\mathbf{x}) = (r(R)/R)\mathbf{x}$ with r given by (3.4) with $\lambda = 1$. Then, for each $\varepsilon > 0$ (and V sufficiently small), we can choose this radial map so that

$$\frac{\int_B (|\nabla \mathbf{u}^{\mathrm{rad}}|^2 - |\mathbf{I}|^2)\,\mathrm{d}\mathbf{x}}{V} \leq \Upsilon_2 + \varepsilon,$$

where $\Upsilon_2 = \frac{8}{3}$ (by (3.2), (3.6)). By the symmetry of $\mathbf{u}^{\mathrm{rad}}$, it follows that each component of this deformation satisfies:

$$\frac{\int_B (|\nabla \mathrm{u}_i^{\mathrm{rad}}|^2 - |\mathbf{e}_i|^2)\,\mathrm{d}\mathbf{x}}{V} \leq \frac{1}{3}(\Upsilon_2 + \varepsilon) \quad \text{for } i = 1, 2, 3,$$

where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ is the standard basis for $\mathbb{R}^3$. Hence, for each such radial deformation, it follows that for each $\lambda_1, \lambda_2, \lambda_3 > 0$,

$$\frac{1}{V}\int_B \sum_{i=1}^{3} \lambda_i^2 \left(|\nabla \mathrm{u}_i^{\mathrm{rad}}|^2 - |\mathbf{e}_i|^2\right)\,\mathrm{d}\mathbf{x} \leq \frac{1}{3}(\Upsilon_2 + \varepsilon)\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2\right). \tag{3.12}$$

Thus, setting $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$, it follows from (3.12) that $\tilde{\mathbf{u}} = \mathbf{A}\mathbf{u}^{\mathrm{rad}}$ satisfies

$$\tilde{\mathbf{u}} \in \mathcal{A}_{\mathbf{A},\tilde{V}}, \;\; \tilde{V} = \lambda_1\lambda_2\lambda_3 V,$$

and

$$\int_B \frac{|\nabla \tilde{\mathbf{u}}|^2 - |\mathbf{A}|^2}{\tilde{V}}\,\mathrm{d}\mathbf{x} \leq \frac{(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)}{\lambda_1\lambda_2\lambda_3}\frac{1}{3}(\Upsilon_2 + \varepsilon). \tag{3.13}$$

Thus

$$\inf{}_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\tilde{\mathrm{V}}}} \int_B \frac{|\nabla \mathbf{u}|^2 - |\mathbf{A}|^2}{\tilde{V}}\,\mathrm{d}\mathbf{x} \leq \frac{(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)}{\lambda_1\lambda_2\lambda_3}\frac{1}{3}(\Upsilon_2 + \varepsilon).$$

By the arbitrariness of ε it follows from (3.13) that

$$G(\mathbf{A}) = \inf_{\tilde{V}>0} \inf{}_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\tilde{\mathrm{V}}}} \int_B \frac{|\nabla \mathbf{u}|^2 - |\mathbf{A}|^2}{\tilde{V}}\,\mathrm{d}\mathbf{x} \leq \frac{(\lambda_1^2 + \lambda_2^2 + \lambda_3^2)}{\lambda_1\lambda_2\lambda_3}\frac{1}{3}\Upsilon_2.$$

The result now follows since $\Upsilon_2 = 8/3$. □

It follows now for the stored energy function (3.7) (with $q = 2$) that:

$$G(\mathbf{A}) \leq \frac{8}{9}\,\mu\,\frac{(\lambda_1^2+\lambda_2^2+\lambda_3^2)}{\lambda_1\lambda_2\lambda_3} - \kappa.$$

This gives an approximate bifurcation criterion

$$\frac{\lambda_1\lambda_2\lambda_3}{\lambda_1^2+\lambda_2^2+\lambda_3^2} = \frac{8}{9}\,\frac{\mu}{\kappa}. \tag{3.14}$$

From the results of Section 3.2, we have that for the case $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$, the bound (3.11) holds with equality and (3.14) reduces to $\tilde{G}(\lambda\mathbf{I}) = 0$ where $\tilde{G}$ is given by (3.9).

4 An elastic fluid: the case $W(\mathbf{F}) = h(\det \mathbf{F})$

In this section we evaluate the volume derivative for the stored energy function $W(\mathbf{F}) = h(\det \mathbf{F})$. The results in this case are sharp, yielding an exact characterisation of the unstable and stable sets.

Proposition 4.1. *Let $n-1 < p < n$ and let*

$$W(\mathbf{F}) = h(\det \mathbf{F}), \tag{4.1}$$

where h satisfies (2.4). *Then the volume derivative is given by*

$$G(\mathbf{A}) = -h'(\det \mathbf{A}).$$

and hence the unstable and stable sets are given by

$$\begin{aligned} \mathcal{U} &= \{\mathbf{A} \in M_+^{n\times n} \mid h'(\det \mathbf{A}) > 0\}, \\ \mathcal{S} &= \{\mathbf{A} \in M_+^{n\times n} \mid h'(\det \mathbf{A}) < 0\}. \end{aligned}$$

Suppose further that $h'' > 0$, then it follows that

$$\partial\mathcal{S} = \{\mathbf{A} \in M_+^{n\times n} \mid h'(\det \mathbf{A}) = 0\} = \partial\mathcal{U}.$$

Proof: For any $\mathbf{A} \in M_+^{n\times n}$ and $d \in (0,1)$, we define the map:

$$\mathbf{u}_d(\mathbf{x}) = [dR^n + (1-d)]^{1/n}\,\frac{\mathbf{A}\mathbf{x}}{R}, \quad R = \|\mathbf{x}\|\,. \tag{4.2}$$

An easy computation shows that $\det \nabla\mathbf{u}_d = d \det \mathbf{A}$. For $V > 0$ sufficiently small, we set

$$d = 1 - \frac{nV}{\omega_n \det \mathbf{A}} > 0. \tag{4.3}$$

It follows that $\mathbf{u}_d \in \mathcal{A}_{\mathbf{A},V}$, and for any $\mathbf{u} \in \mathcal{A}_{\mathbf{A},V}$, using the convexity of h, we have

$$\begin{aligned} E(\mathbf{u}) &= \int_B h(\det \nabla \mathbf{u})\,\mathrm{d}\mathbf{x}, \\ &\geq \int_B [h(\det \nabla \mathbf{u}_d) + h'(\det \nabla \mathbf{u}_d)(\det \nabla \mathbf{u} - \det \nabla \mathbf{u}_d)]\ \mathrm{d}\mathbf{x}, \\ &= E(\mathbf{u}_d) + h'(d \det \mathbf{A}) \int_B (\det \nabla \mathbf{u} - \det \nabla \mathbf{u}_d)\ \mathrm{d}\mathbf{x} = E(\mathbf{u}_d), \end{aligned}$$

and so $\mathbf{u}_d$ is a minimiser of E on $\mathcal{A}_{\mathbf{A},V}$. Thus

$$F(\mathbf{A}, V) = \frac{h(d \det \mathbf{A}) - h(\det \mathbf{A})}{(1-d)\det \mathbf{A}},$$

and hence

$$\begin{aligned} G(\mathbf{A}) &= \lim_{V \searrow 0} F(\mathbf{A}, V) \\ &= \lim_{d \nearrow 1} \frac{h(d \det \mathbf{A}) - h(\det \mathbf{A})}{(1-d)\det \mathbf{A}} = -h'(\det \mathbf{A}). \end{aligned}$$

□

Remark 4.2. Using the arguments of the last proposition, we can construct an example of a polyconvex energy function for which $\partial\mathcal{U} \neq \partial\mathcal{S}$. Replace the hypothesis $h'' > 0$ by $h'' \geq 0$ and suppose that $h'(d) = 0$ for all $d \in [a, b]$ (and only for these values of d), where $0 < a < b < +\infty$. Then $W(\mathbf{F}) = h(\det \mathbf{F})$ is still polyconvex but $\partial\mathcal{U} = \{\mathbf{A} \in M_+^{n\times n} \mid \det \mathbf{A} = b\} \neq \{\mathbf{A} \in M_+^{n\times n} \mid \det \mathbf{A} = a\} = \partial\mathcal{S}$. (Note that in this case the stored energy function is not uniformly strictly $W^{1,p}$-quasiconvex in the sense of Definition 1.1.)

Remark 4.3. Assume h satisfies (2.4a) and the first condition of (2.4b). Suppose further that $h' \leq 0$. It follows then (e.g., from the last proposition) that $\tilde{W}(\mathbf{F}) = h(\det \mathbf{F})$ is $W^{1,p}$–quasiconvex at all matrices $\mathbf{A}$, and by Lemma 2.13, that $W(\mathbf{F}) = \eta|\mathbf{F}|^p + h(\det \mathbf{F})$ is uniformly strictly $W^{1,p}$–quasiconvex in the sense of Definition 1.1. (The uniformity can also be proved directly by using Lemma 3.2.)

5 Characterisation of the volume derivative for general stored energies

In this section we adapt an approach in [45] to obtain an alternative expresssion for the volume derivative at a general matrix $\mathbf{A}$. We *assume* the existence of a parametrised family of sufficiently regular energy minimisers and use this to evaluate the volume derivative.

We begin by deriving an expression for the energy of a, sufficiently regular but discontinuous, minimiser.

Proposition 5.1. *Suppose that* $\mathbf{u} \in C^2(B \setminus \{\mathbf{x}_0\}) \cap C^1(\bar{B} \setminus \{\mathbf{x}_0\})$ *is a minimiser of the energy functional* E *on* $\mathcal{A}_{\mathbf{A},V}$ *(given by (1.5)) for some* $V > 0$*, and assume that there exist constants* $k, \varepsilon_0 > 0$ *such that the stored energy function* W *satisfies:*

$$\left|\mathbf{F}^T \frac{\mathrm{d}W}{\mathrm{d}\mathbf{F}}(\mathbf{FC})\right| \leq k\,[W(\mathbf{F}) + 1] \quad \text{for all } \mathbf{F} \in \mathrm{M}^{n\times n}_+, \tag{5.1}$$

whenever $|\mathbf{C} - \mathbf{I}| < \varepsilon_0$*. Then*

$$\begin{aligned} nE(\mathbf{u}) &= \int_{\partial B} \left[\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)W(\nabla\mathbf{u}) + (\mathbf{u} - (\nabla\mathbf{u})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\right]\mathrm{d}s \\ &\quad - \lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} \mathbf{u}\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\,\mathrm{d}s, \qquad (5.2) \\ &= \int_{\partial B} \left[\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)W(\nabla\mathbf{u}) + (\mathbf{u} - (\nabla\mathbf{u})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\right]\mathrm{d}s \\ &\quad - \lim_{\delta\to 0}\int_{\mathbf{u}(\partial B_\delta(\mathbf{x}_0))} \mathbf{y}\cdot\mathbf{T}(\mathbf{y})\tilde{\mathbf{N}}(\mathbf{y})\,\mathrm{d}s(\mathbf{y}), \qquad (5.3) \end{aligned}$$

where $\mathbf{T}(\mathbf{u}(\mathbf{x}))$ *is the Cauchy stress tensor given by*

$$\mathbf{T}(\mathbf{u}(\mathbf{x})) = (\det\nabla\mathbf{u}(\mathbf{x}))^{-1}\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\nabla\mathbf{u}(\mathbf{x})^T. \tag{5.4}$$

Proof: The proof follows from modifying an argument (based on a well-known divergence identity for smooth solutions due originally to A.E. Green) which is used in [45, section 3]. From [45, expression (3.3)], it follows that for $\delta > 0$ sufficiently small, taking the normal $\mathbf{N}$ to $\partial B_\delta(\mathbf{x}_0)$ to point in the outward direction, that

$$\begin{aligned} n\int_{B\setminus B_\delta(\mathbf{x}_0)} W(\nabla\mathbf{u}(\mathbf{x}))\,\mathrm{d}\mathbf{x} &= \int_{\partial B}\Big[\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)W(\nabla\mathbf{u}) \\ &\quad + (\mathbf{u} - (\nabla\mathbf{u})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\Big]\,\mathrm{d}s \\ &\quad - \int_{\partial B_\delta(\mathbf{x}_0)}\Big[\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)W(\nabla\mathbf{u}) \\ &\quad + (\mathbf{u} - (\nabla\mathbf{u})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\Big]\,\mathrm{d}s. \qquad (5.5) \end{aligned}$$

As in [45, section 3] (using hypothesis (5.1) for the second limit), the assumption that $E(\mathbf{u})$ is finite implies that

$$\int_{\partial B_\delta(\mathbf{x}_0)} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)W(\nabla\mathbf{u})\,\mathrm{d}s,\ \int_{\partial B_\delta(\mathbf{x}_0)} ((\nabla\mathbf{u})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\,\mathrm{d}s \to 0,$$

as $\delta \to 0$. Using this in (5.5) we obtain (5.2). Moreover,

$$\int_{\partial B_\delta(\mathbf{x}_0)} \mathbf{u} \cdot \frac{\partial W}{\partial \mathbf{F}}(\nabla \mathbf{u})\mathbf{N}\, \mathrm{d}s = \int_{\partial B_\delta(\mathbf{x}_0)} \mathbf{u} \cdot \mathbf{T}(\mathbf{u})\nabla \mathbf{u}(\mathbf{x})^{-T}\mathbf{N} \det \nabla \mathbf{u}\, \mathrm{d}s,$$

and since the normal $\mathbf{N}$ to $\partial B_\delta(\mathbf{x}_0)$ is mapped by $\mathbf{u}$ to

$$\tilde{\mathbf{N}}(\mathbf{u}) = (\det \nabla \mathbf{u})\nabla \mathbf{u}(\mathbf{x})^{-T}\mathbf{N},$$

it now follows, upon setting $\mathbf{y} = \mathbf{u}(\mathbf{x})$, that

$$\int_{\partial B_\delta(\mathbf{x}_0)} \mathbf{u} \cdot \frac{\partial W}{\partial \mathbf{F}}(\nabla \mathbf{u})\mathbf{N}\, \mathrm{d}s = \int_{\mathbf{u}(\partial B_\delta(\mathbf{x}_0))} \mathbf{y} \cdot \mathbf{T}(\mathbf{y})\tilde{\mathbf{N}}(\mathbf{y})\, \mathrm{d}s(\mathbf{y}),$$

for $\delta > 0$ sufficiently small, which completes the proof. □

Corollary 5.2. *Under the assumptions of Proposition 5.1,*

$$\begin{aligned} nE(\mathbf{u}) \;\; = \;\; & \int_{\partial B} \mathbf{N} \cdot (\mathbf{x} - \mathbf{x}_0) W(\nabla \mathbf{u})\, \mathrm{d}s \\ & + \int_{\partial B} (\mathbf{u} + \mathbf{c} - (\nabla \mathbf{u})(\mathbf{x} - \mathbf{x}_0)) \cdot \frac{\partial W}{\partial \mathbf{F}}(\nabla \mathbf{u})\mathbf{N}\, \mathrm{d}s \\ & - \lim_{\delta \to 0} \int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u} + \mathbf{c}) \cdot \frac{\partial W}{\partial \mathbf{F}}(\nabla \mathbf{u})\mathbf{N}\, \mathrm{d}s, \end{aligned}$$

for any vector $\mathbf{c} \in \mathbb{R}^n$.

Proof: This follows from the fact that $E(\mathbf{u} + \mathbf{c}) = E(\mathbf{u})$, since the stored energy is translation invariant. □

Families of minimisers Let $\mathbf{A} \in M^{n\times n}_{+}$. For each $V \in (0, V_0)$, $V_0 > 0$ and $\mathbf{x}_0 \in B$, we denote by $\mathbf{u}(\mathbf{x}, \mathbf{x}_0, V)$ a minimiser of (1.4) over $\mathcal{A}_{\mathbf{A},V}$ given by (1.8). (Throughout this section, the operator ∇ will denote differentiation with respect to $\mathbf{x}$.) Following the approach of [45], we assume that the following hypotheses hold.

(M1) For each $\mathbf{x}_0 \in B$ and $V \in (0, V_0)$, the deformation $\mathbf{u}(\cdot, \mathbf{x}_0, V)$ is a minimiser of the energy (1.4) on $\mathcal{A}_{\mathbf{A},V}$ and satisfies:

a)

$$\mathbf{u}(\cdot, \mathbf{x}_0, V) \in C^2(B \setminus \{\mathbf{x}_0\}) \cap C^1(\overline{B} \setminus \{\mathbf{x}_0\}),$$

$$\mathbf{u}(\mathbf{x}, \mathbf{x}_0, V) = \mathbf{A}\mathbf{x}, \quad \mathbf{x} \in \partial B.$$

b) For each $\mathbf{x}_0 \in B$,

$$\mathbf{u}(\cdot, \mathbf{x}_0, \cdot) \in C^3\left((\overline{B} \setminus \{\mathbf{x}_0\}) \times (0, V_0)\right).$$

(M2) For each $\mathbf{x}_0 \in B$ and $\delta > 0$ sufficiently small:

$$\mathbf{u}(\cdot, \mathbf{x}_0, V) \to \mathbf{u}^h_{\mathbf{A}}(\cdot) \text{ in } C^2(\overline{B} \setminus B_\delta(\mathbf{x}_0)) \text{ as } V \searrow 0,$$

where $\mathbf{u}^h_{\mathbf{A}}(\mathbf{x}) \equiv \mathbf{A}\mathbf{x}$ for $\mathbf{x} \in \overline{B}$.

The above assumptions differ from those used in [45] in that we use the hole volume V and not the boundary displacement matrix $\mathbf{A}$ to parametrise the minimisers. To motivate the convergence assumption (M2), the next proposition proves an analogous convergence result but in a weaker norm.

Proposition 5.3. *Let $p \in (n-1, n)$ and let $q \in [n-1, n)$, $q \leq p$. Suppose that the stored energy function W is of the form*

$$W(\mathbf{F}) = \tilde{W}(\mathbf{F}) + \mu|\mathbf{F}|^q + h(\det \mathbf{F}),$$

where $\tilde{W}$ is $W^{1,p}$–quasiconvex (in the sense of Definition 1.1) at $\mathbf{A}$ and that h satisfies the hypotheses in (2.4). Then $\mathbf{u}(\cdot, \mathbf{x}_0, V) \to \mathbf{u}^h_{\mathbf{A}}(\cdot)$ in $W^{1,q}(B)$ as $V \searrow 0$.

Proof: The proof is divided into two cases.

Case 1. Assume that $G(\mathbf{A}) < 0$ (so that $\mathbf{A} \in \mathcal{U}$). Then there exist a sequence $V_k \to 0$ as $k \to \infty$, and a corresponding sequence $(\mathbf{u}_k) \subset \mathcal{A}_{\mathbf{A},V_k}$, $\mathbf{u}_k = \mathbf{u}(\cdot, \mathbf{x}_0, V_k)$, satisfying $E(\mathbf{u}_k) < E(\mathbf{u}^h_{\mathbf{A}})$ for all k. Then it follows, on using the assumed quasiconvexity of $\tilde{W}$ and expression (3.1) in the proof of Theorem 3.3, that

$$\begin{aligned}
0 &\leq E(\mathbf{u}^h_{\mathbf{A}}) - E(\mathbf{u}_k) \\
&= \int_B \tilde{W}(\mathbf{A}) + \mu|\mathbf{A}|^q + h(\det \mathbf{A}) - \tilde{W}(\nabla \mathbf{u}_k) - \mu|\nabla \mathbf{u}_k|^q - h(\det \nabla \mathbf{u}_k) \\
&\leq \int_B \mu(|\mathbf{A}|^q - |\nabla \mathbf{u}_k|^q) + h(\det \mathbf{A}) - h(\det \nabla \mathbf{u}_k) \\
&\leq \int_B -\mu\kappa|\mathbf{A} - \nabla \mathbf{u}_k|^q + \int_B h'(\det \mathbf{A})(\det \mathbf{A} - \det \nabla \mathbf{u}_k) \\
&= \int_B -\mu\kappa|\mathbf{A} - \nabla \mathbf{u}_k|^q + h'(\det \mathbf{A})V_k,
\end{aligned}$$

where we have used the convexity of h. Since[5] $h'(\det \mathbf{A}) > 0$ and since $V_k \to 0$ as $k \to \infty$, it follows that $\nabla \mathbf{u}_k \to \nabla \mathbf{u}^h_{\mathbf{A}}$ in $L^q(B)$. As both $\mathbf{u}_k$ and $\mathbf{u}^h_{\mathbf{A}}$ satisfy the same boundary condition on ∂B, it follows that $\mathbf{u}_k \to \mathbf{u}^h_{\mathbf{A}}$ in $W^{1,q}(B)$.

[5] Note that by the results of [35], there exists a constant $c > 0$ such that $h'(\det \mathbf{A}) < c$ implies that $E(\mathbf{u}) \geq E(\mathbf{u}^h_{\mathbf{A}})$ for all $\mathbf{u} \in \mathcal{A}_{\mathbf{A},V}$, for any $V > 0$.

Case 2. Let $G(\mathbf{A}) \geq 0$. In this case the convergence result can be obtained by applying the reasoning in Case 1 to $W_\alpha(\mathbf{F}) = W(\mathbf{F}) + \alpha \det \mathbf{F}$, where $\alpha > 0$ is a constant. Note that the integral of the additional term is constant on $\mathcal{A}_{\mathbf{A},V}$. However, given any $\mathbf{u}_V \in \mathcal{A}_{\mathbf{A},V}$, for large enough α, $E_\alpha(\cdot)$ will satisfy $E_\alpha(\mathbf{u}_V) < E_\alpha(\mathbf{u}^h_{\mathbf{A}})$. Hence, the argument used in Case 1 can be applied to any sequence $(\mathbf{u}_{V_k})$ satisfying $E_\alpha(\mathbf{u}_{V_k}) < E_\alpha(\mathbf{u}^h_{\mathbf{A}})$, with $V_k \to 0$ as $k \to \infty$, to show that $\mathbf{u}_{V_k} \to \mathbf{u}^h_{\mathbf{A}}$ in $W^{1,q}(B)$ as $k \to \infty$.

□

We next define $\mathbf{w}(\mathbf{x}, \mathbf{x}_0, V)$ by

$$\mathbf{u}(\mathbf{x}, \mathbf{x}_0, V) = \mathbf{u}^h_{\mathbf{A}}(\mathbf{x}) + \mathbf{w}(\mathbf{x}, \mathbf{x}_0, V). \tag{5.6}$$

It then follows from this definition and hypotheses (M1) and (M2) that

$$\mathbf{w}(\mathbf{x}, \mathbf{x}_0, V) = \mathbf{0}, \quad \forall \mathbf{x} \in \partial B, \tag{5.7a}$$

$$\mathbf{w}(\mathbf{x}, \mathbf{x}_0, 0) = \mathbf{0}, \quad \forall \mathbf{x} \in \overline{B} \setminus \{\mathbf{x}_0\}, \tag{5.7b}$$

$$\nabla \mathbf{w}(\mathbf{x}, \mathbf{x}_0, V) = \frac{\partial \mathbf{w}}{\partial \mathbf{N}} \otimes \mathbf{N}, \quad \forall \mathbf{x} \in \partial B. \tag{5.7c}$$

Proposition 5.4. *Under the hypotheses (M1), (M2), the energy difference*

$$\Delta E := E(\mathbf{u}(\cdot, \mathbf{x}_0, V)) - E(\mathbf{u}^h_{\mathbf{A}}) \tag{5.8}$$

is given by

$$\begin{aligned} n\Delta E &= -\frac{1}{2}V^2 \int_{\partial B} \mathbf{N} \cdot (\mathbf{x} - \mathbf{x}_0) \nabla \dot{\mathbf{w}} : \mathbf{C}[\nabla \dot{\mathbf{w}}] \,\mathrm{d}s + o(V^2) \\ &\quad - \lim_{\delta \to 0} \int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u} - \mathbf{A}\mathbf{x}_\mathbf{0}) \cdot \frac{\partial W}{\partial \mathbf{F}} (\mathbf{A} + \nabla \mathbf{w}) \mathbf{N} \,\mathrm{d}s, \end{aligned} \tag{5.9}$$

where $\mathbf{C}$ *is the second derivative of* W *evaluated at* $\mathbf{A}$*. Hence the volume derivative of* W *at* $\mathbf{A}$ *is given by*

$$\begin{aligned} G(\mathbf{A}) &= -\frac{1}{n} \lim_{V \to 0} V^{-1} \left[\lim_{\delta \to 0} \int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u} - \mathbf{A}\mathbf{x}_\mathbf{0}) \cdot \frac{\partial W}{\partial \mathbf{F}} (\nabla \mathbf{u}) \mathbf{N} \,\mathrm{d}s \right], \\ &= -\frac{1}{n} \lim_{V \to 0} V^{-1} \left[\lim_{\delta \to 0} \int_{\mathbf{u}(\partial B_\delta(\mathbf{x}_0))} (\mathbf{y} - \mathbf{A}\mathbf{x}_\mathbf{0}) \cdot \mathbf{T}(\mathbf{y}) \tilde{\mathbf{N}}(\mathbf{y}) \,\mathrm{d}s(\mathbf{y}) \right], \end{aligned} \tag{5.10}$$

where $\mathbf{T}$ *is the Cauchy stress tensor given by (5.4).*

Proof: It follows from Corollary 5.2 and (5.8) that

$$
\begin{aligned}
n\Delta E &= \int_{\partial B} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)(W(\nabla\mathbf{u})-W(\mathbf{A}))\,\mathrm{d}s \\
&\quad + \int_{\partial B} (\mathbf{w}-(\nabla\mathbf{w})(\mathbf{x}-\mathbf{x}_0))\cdot\frac{\partial W}{\partial\mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\,\mathrm{d}s \\
&\quad + \int_{\partial B} (\mathbf{c}+\mathbf{A}\mathbf{x}_0)\cdot\left[\frac{\partial W}{\partial\mathbf{F}}(\nabla\mathbf{u})-\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A})\right]\mathbf{N}\,\mathrm{d}s \\
&\quad - \lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u}+\mathbf{c})\cdot\frac{\partial W}{\partial\mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\,\mathrm{d}s,
\end{aligned}
$$

where we have used that

$$\lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{A}\mathbf{x}+\mathbf{c})\cdot\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A})\mathbf{N}\,\mathrm{d}s = 0.$$

Choosing $\mathbf{c}=-\mathbf{A}\mathbf{x}_0$ and using (5.6), (5.7a)-(5.7c), the above expression becomes

$$
\begin{aligned}
n\Delta E &= \int_{\partial B} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)(W(\mathbf{A}+\nabla\mathbf{w})-W(\mathbf{A}))\,\mathrm{d}s \\
&\quad - \int_{\partial B} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)\left[\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A}+\nabla\mathbf{w}):\left(\frac{\partial\mathbf{w}}{\partial\mathbf{N}}\otimes\mathbf{N}\right)\right]\mathrm{d}s \\
&\quad - \lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u}-\mathbf{A}\mathbf{x}_\mathbf{0})\cdot\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A}+\nabla\mathbf{w})\mathbf{N}\,\mathrm{d}s.
\end{aligned}
$$

Let

$$\Phi(V) = W(\mathbf{A}+\nabla\mathbf{w})-W(\mathbf{A})-\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A}+\nabla\mathbf{w}):\left(\frac{\partial\mathbf{w}}{\partial\mathbf{N}}\otimes\mathbf{N}\right).$$

Using (5.7) one can check that

$$\Phi(0)=0,\quad \Phi'(0)=0,\quad \Phi''(0)=-\nabla\dot{\mathbf{w}}:\mathbf{C}[\nabla\dot{\mathbf{w}}]\quad \text{on } \partial\mathrm{B},$$

where the dot in $\dot{\mathbf{w}}$ denotes the right-sided derivative with respect to V at $V=0$. Thus

$$\Phi(V) = -\frac{1}{2}V^2\nabla\dot{\mathbf{w}}:\mathbf{C}[\nabla\dot{\mathbf{w}}]+o(V^2)\quad \text{on } \partial\mathrm{B}.$$

By hypothesis M2 restricted to ∂B, we obtain

$$
\begin{aligned}
n\Delta E &= -\frac{1}{2}V^2\int_{\partial B} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)\nabla\dot{\mathbf{w}}:\mathbf{C}[\nabla\dot{\mathbf{w}}]\,\mathrm{d}s+o(V^2) \\
&\quad - \lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u}-\mathbf{A}\mathbf{x}_\mathbf{0})\cdot\frac{\partial W}{\partial\mathbf{F}}(\mathbf{A}+\nabla\mathbf{w})\mathbf{N}\,\mathrm{d}s,
\end{aligned}
$$

which gives (5.9). Thus

$$\begin{aligned} G(\mathbf{A}) &= -\frac{1}{n}\lim_{V\to 0} V^{-1}\left[\lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{x}_0)} (\mathbf{u}-\mathbf{A}\mathbf{x_0})\cdot\frac{\partial W}{\partial \mathbf{F}}(\nabla\mathbf{u})\mathbf{N}\,\mathrm{d}s\right], \\ &= -\frac{1}{n}\lim_{V\to 0} V^{-1}\left[\lim_{\delta\to 0}\int_{\mathbf{u}(\partial B_\delta(\mathbf{x}_0))} (\mathbf{y}-\mathbf{A}\mathbf{x_0})\cdot\mathbf{T}(\mathbf{y})\tilde{\mathbf{N}}(\mathbf{y})\,\mathrm{d}s(\mathbf{y})\right], \end{aligned}$$

where $\mathbf{T}$ is the Cauchy stress tensor given by (5.4). □

Remark 5.5. Intuitively, for each $V > 0$, the term in square brackets divided by V in the expression (5.10) for the volume derivative represents the work done per unit volume in opening a hole of volume V in the deformed configuration around the point $\mathbf{A}\mathbf{x}_0$.

Remark 5.6. The Cauchy stress tensor $\mathbf{T}$ is defined on the deformed configuration $\mathbf{u}(B)$ which corresponds to $\mathbf{u}^h_{\mathbf{A}}(B)\backslash H$, where H is the region occupied by the cavity that is formed and the volume of H is V. Suppose now that, for each sufficiently small $V > 0$, $\mathbf{T}$ can be extended into the cavity region H as a constant tensor $\mathbf{T}_0(H)$, say, in such a way that the normal component of stress is continuous across ∂H (as occurs in the case of radial cavitation considered in [39]), i.e.,

$$\mathbf{T}(\mathbf{y})\tilde{\mathbf{N}}(\mathbf{y}) = \mathbf{T}_0(H)\tilde{\mathbf{N}}(\mathbf{y}) \quad \text{for } \mathbf{y}\in\partial H,$$

where $\tilde{\mathbf{N}}(\mathbf{y})$ is the outward pointing unit normal to H at $\mathbf{y}\in\partial H$. Then, using (5.10), the volume derivative can be expressed as

$$\begin{aligned} G(\mathbf{A}) &= -\frac{1}{n}\lim_{V\to 0} V^{-1}\left[\lim_{\delta\to 0}\int_{\mathbf{u}(\partial B_\delta(\mathbf{x}_0))} (\mathbf{y}-\mathbf{A}\mathbf{x_0})\cdot\mathbf{T}(\mathbf{y})\tilde{\mathbf{N}}(\mathbf{y})\,\mathrm{d}s(\mathbf{y})\right] \\ &= -\frac{1}{n}\lim_{V\to 0} V^{-1}\left[\int_{\partial H} (\mathbf{y}-\mathbf{A}\mathbf{x_0})\cdot\mathbf{T}_0(H)\tilde{\mathbf{N}}(\mathbf{y})\,\mathrm{d}s(\mathbf{y})\right] \\ &= -\frac{1}{n}\lim_{V\to 0} V^{-1}\left[\int_{H} \operatorname{trace}\mathbf{T}_0(H)\ \mathrm{d}\mathbf{y}\right] = -\frac{1}{n}\lim_{V\to 0}\operatorname{trace}\mathbf{T}_0(H). \end{aligned}$$

This result relating the volume derivative to the limiting value of the trace of the Cauchy stress tensor as $V\to 0$, is analogous to a result derived in [39] for the radial problem. In [39] it is shown that the vanishing of the volume derivative for the radial problem exactly coincides with an equation for determining the onset of radial cavitation obtained by Stuart in [52] using a shooting argument.

Remark 5.7. We note that the coefficient multiplying $-\frac{1}{2}V^2$ in (5.9) is given by

$$\int_{\partial B}\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)\nabla\dot{\mathbf{w}} : \mathbf{C}[\nabla\dot{\mathbf{w}}]\,\mathrm{d}s,$$

which by (5.7c) is given by

$$\int_{\partial B} \mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)\left(\frac{\partial \dot{\mathbf{w}}}{\partial \mathbf{N}}\otimes\mathbf{N} : \mathbf{C}\left[\frac{\partial \dot{\mathbf{w}}}{\partial \mathbf{N}}\otimes\mathbf{N}\right]\right)\,\mathrm{d}s,$$

where $\dot{\mathbf{w}}$ denotes the right-sided derivative of $\mathbf{w}$ with respect to V at $V=0$. Since B is convex, it is star-shaped with respect to any point $\mathbf{x}_0$ within it. Hence $\mathbf{N}\cdot(\mathbf{x}-\mathbf{x}_0)>0$ on ∂B and if W is strongly elliptic, then

$$\lambda_i\mu_\alpha C^{ij}_{\alpha\beta}\lambda_j\mu_\beta > 0 \ \text{ for all } \boldsymbol{\lambda},\boldsymbol{\mu}\in\mathbb{R}^n,\quad \boldsymbol{\lambda},\boldsymbol{\mu}\neq\mathbf{0}.$$

It now follows that the coefficient of V^2 in (5.9) is strictly negative unless $\frac{\partial\dot{\mathbf{w}}}{\partial\mathbf{N}}=\mathbf{0}$ on ∂B.

It would be tempting, though false in general, to conclude from (5.9) and (5.10) that the coefficient of V^2 in (5.9) yields the second derivative of ΔE with respect to V at $V=0$. The following example illustrates this point.

Example 5.8. Consider the case of the stored energy function $W(\mathbf{F})=h(\det\mathbf{F})$ where h satisfies (2.4). It follows from the proof of Proposition 4.1 that the function (4.2) with d given by (4.3) is a minimiser of the energy over $\mathcal{A}_{\mathbf{A},V}$. For the case $\mathbf{A}=\lambda\mathbf{I}$, this minimum energy is given by

$$E(\mathbf{u}_d)=\frac{\omega_n}{n}\,h\left(\lambda^n-\frac{nV}{\omega_n}\right).$$

An easy calculation now yields that

$$\Delta E=-h'(\lambda^n)V+\frac{n}{2\omega_n}\,h''(\lambda^n)V^2+o(V^2), \tag{5.11}$$

from which it follows that the second derivative of ΔE with respect to V at $V=0$ is given by $\frac{n}{\omega_n}\,h''(\lambda^n)$.

We now compute the terms in the expansion (5.9). For $W(\mathbf{F})=h(\det\mathbf{H})$ we have that

$$\begin{aligned}\frac{\mathrm{d}W}{\mathrm{d}\mathbf{F}}(\mathbf{F}) &= (\det\mathbf{F})h'(\det\mathbf{F})\mathbf{F}^{-T},\\ \frac{\mathrm{d}^2W}{\mathrm{d}\mathbf{F}^2}(\mathbf{F})[\mathbf{H}] &= (\det\mathbf{F})h'(\det\mathbf{F})((\mathbf{F}^{-T}\cdot\mathbf{H})\mathbf{I}-\mathbf{F}^{-T}\mathbf{H}^{-T})\mathbf{F}^{-T}\\ &\quad +(\det\mathbf{F})^2h''(\det\mathbf{F})(\mathbf{F}^{-T}\cdot\mathbf{H})\mathbf{F}^{-T}.\end{aligned}$$

Also, since $\mathbf{w}(\mathbf{x})=\mathbf{u}_d(\mathbf{x})-\lambda\mathbf{x}$, it follows from a straightforward calculation, that

$$\nabla\dot{\mathbf{w}}=-\frac{n}{\omega_n\lambda^{n-1}}\,\mathbf{x}\otimes\mathbf{x},\quad \mathbf{x}\in\partial B.$$

Using these calculations and taking $\mathbf{x}_0=\mathbf{0}$, it follows that

$$-\frac{1}{n}\int_{\partial B}(\mathbf{N}\cdot\mathbf{x})\nabla\dot{\mathbf{w}} : \mathbf{C}[\nabla\dot{\mathbf{w}}]\,\mathrm{d}s=-\frac{n}{\omega_n}\,h''(\lambda^n), \tag{5.12}$$

which is not equal to the second derivative of ΔE with respect to V at $V = 0$. On the other hand

$$
\begin{aligned}
-\frac{1}{n}\lim_{\delta\to 0}\int_{\partial B_\delta(\mathbf{0})} \mathbf{u}_d \cdot \frac{\partial W}{\partial \mathbf{F}}(\nabla \mathbf{u}_d)\mathbf{N}\,\mathrm{d}s &= -Vh'\left(\lambda^n - \frac{nV}{\omega_n}\right) \\
&= -h'(\lambda^n)V + \frac{n}{\omega_n}\,h''(\lambda^n)V^2 + o(V^2).
\end{aligned}
$$

Combining this with expression (5.12) (multiplied by $\frac{1}{2}V^2$) gives that the right-hand side of (5.9) yields the same expression for ΔE as in (5.11). Thus, the second derivative of ΔE with respect to V at $V = 0$ is, in general, a combination of terms arising from both the outer and inner boundary integral terms in (5.9).

6 Numerical Considerations

In this section we show how the volume derivative can be used as the basis for a numerical scheme for computing the 'onset of cavitation' as given by the solutions of $G(\mathbf{A}) = 0$. The bulk of the computational work in computing this set is on the evaluation of $G(\mathbf{A})$ for many values of $\mathbf{A}$. To approximate $G(\mathbf{A})$, one first must compute for given $V > 0$, a function $\mathbf{u}_V$ such that

$$
E(\mathbf{u}_V) = \min_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},V}} \int_B W(\nabla \mathbf{u}(\mathbf{x}))\,\mathrm{d}\mathbf{x}. \tag{6.1}
$$

Next one needs to compute the difference quotient

$$
\frac{E(\mathbf{u}_V) - E(\mathbf{u}^h_{\mathbf{A}})}{V},
$$

where $\mathbf{u}^h_{\mathbf{A}}(\mathbf{x}) \equiv \mathbf{A}\mathbf{x}$. This two-step process is then repeated for successively smaller values of V until some convergence criteria is satisfied. In actual computations, we do not make the volume V extremely small to prevent loss of significant digits in the computation of this quotient. Another source of error in the above computation comes from the discretisations required to compute the minima in the first step, namely from the use of finite elements and quadrature rules. (This error can be reduced by using finer meshes and high order quadrature rules, but this increases the number of unknowns to be computed.) In general, the corresponding approximate problem for (6.1) is a large-scale constrained optimization problem.

To implement the two-step process described above, we use a numerical scheme which combines three different numerical techniques, namely, regularization, penalization and a gradient flow iteration. We now discuss each of these techniques in the context of our problem. For ease of exposition, we present the discussion of the numerical methods for the case $n = 3$. However, the particular numerical examples presented are for both $n = 2$ and $n = 3$.

The regularised constrained problem: The volume constraint in (6.1) is given by

$$\int_B \det \nabla \mathbf{u} \, \mathrm{d}\mathbf{x} = \frac{4\pi}{3} \det \mathbf{A} - V. \tag{6.2}$$

In actual computations and to avoid the Lavrentiev phenomena ([24], [6]), we work on a ball with a pre–existing hole of size $\varepsilon > 0$ (as in [48], [12]). Thus, we replace the minimisation problem (6.1) with the problem of determining $\mathbf{u}_{V,\varepsilon}$ such that

$$E_\varepsilon(\mathbf{u}_{V,\varepsilon}) = \begin{cases} \min_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\varepsilon}} & \int_{B\setminus B_\varepsilon} W(\nabla \mathbf{u}(\mathbf{x}))\, \mathrm{d}\mathbf{x}, \\ \text{subject to} & \int_{B\setminus B_\varepsilon} \det \nabla \mathbf{u} \, \mathrm{d}\mathbf{x} = \frac{4\pi}{3} \det \mathbf{A} - V, \end{cases} \tag{6.3}$$

where B_ε is the ball of radius $\varepsilon > 0$ with center at the origin, and

$$\begin{aligned} \mathcal{A}_{\mathbf{A},\varepsilon} \;\; = \;\; & \{\mathbf{u} \in W^{1,p}(B \setminus B_\varepsilon) \,|\, \mathrm{Det}\nabla\mathbf{u} = \det\nabla\mathbf{u}\, \mathcal{L}^n, \\ & \det \nabla\mathbf{u} > 0 \;\, a.e.,\;\; \mathbf{u}(\mathbf{x}) = \mathbf{A}\mathbf{x} \text{ on } \partial B,\;\; \mathbf{u}^e \text{ satisfies INV}\}, \end{aligned}$$

where, for this mixed problem (analogously to (1.3) for the pure displacement problem) $\mathbf{u}^e$ denotes the homogeneous extension of $\mathbf{u}$ outside B to a (slightly) larger domain. For the radial case, one can prove (see [39]) that the computed volume derivatives[6] for the shell problems (with the pre–existing hole) converge to the exact volume derivative provided that $\varepsilon = o(V^{1/3})$.

A penalty method: To compute approximations of the constrained problem (6.3), we use a penalty method in which the functional in (6.3) is replaced by:

$$E_{\varepsilon,\eta}(\mathbf{u}) = \int_{B\setminus B_\varepsilon} W(\nabla \mathbf{u}(\mathbf{x}))\, \mathrm{d}\mathbf{x} + \eta \left(\int_{B\setminus B_\varepsilon} \det \nabla \mathbf{u} \, \mathrm{d}\mathbf{x} - K \right)^2, \tag{6.4}$$

where η is a "large" parameter and

$$K = \frac{4\pi}{3} \det \mathbf{A} - V.$$

Thus, we replace (6.3) with the unconstrained variational problem of determining $\mathbf{u}_{V,\varepsilon,\eta}$ such that

$$E_{\varepsilon,\eta}(\mathbf{u}_{V,\varepsilon,\eta}) = \min_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\varepsilon}} E_{\varepsilon,\eta}(\mathbf{u}). \tag{6.5}$$

By the structure of the penalty term which is non-negative and equal to zero when the constraint is exactly satisfied, for any $\eta > 0$, we have

$$\min_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\varepsilon}} E_{\varepsilon,\eta}(\mathbf{u}) \le \begin{cases} \min_{\mathbf{u}\in\mathcal{A}_{\mathbf{A},\varepsilon}} \int_{B\setminus B_\varepsilon} W(\nabla \mathbf{u}(\mathbf{x}))\, \mathrm{d}\mathbf{x}, \\ \text{subject to } \int_{B\setminus B_\varepsilon} \det \nabla \mathbf{u} \, \mathrm{d}\mathbf{x} = \frac{4\pi}{3} \det \mathbf{A} - V. \end{cases} \tag{6.6}$$

[6]The volume derivative in the radial case is the restricted version of the one introduced in this paper, all deformations being constrained to lie in the class of radially symmetric maps.

The following result shows that, as the penalisation parameter η tends to infinity, a subsequence of corresponding minimisers and minimum energies in (6.5) converge, respectively, to those corresponding to the problem (6.3).

Proposition 6.1. *Let the stored energy function $W(\mathbf{F})$ satisfy*

(i) (Polyconvexity) $W(\mathbf{F}) = G(\mathbf{F}, \mathrm{Adj}\mathbf{F}, \det \mathbf{F})$, with $G(\cdot,\cdot,\cdot) = M_+^{3\times 3}\times M_+^{3\times 3}\times(0,\infty) \to \mathbb{R}$ continuous and convex.

(ii) (Growth) $W(\mathbf{F}) \geq K + c_1|\mathbf{F}|^p + h(\det \mathbf{F})$ for $\mathbf{F} \in M_+^{n\times n}$, where $p \in (2,3)$, $c_1 > 0$, and h satisfies (2.4).

Then for each $\varepsilon, \eta, V > 0$, there exists a minimiser $\mathbf{u}_{V,\varepsilon,\eta}$ of $E_{\varepsilon,\eta}$ on $\mathcal{A}_{\mathbf{A},\varepsilon}$. Moreover, for any sequence $\eta_j \to \infty$, there exist a subsequence (η_{j_k}) such that $\left(\mathbf{u}_{V,\varepsilon,\eta_{j_k}}\right)$ converges weakly to $\mathbf{u}_{V,\varepsilon}$ in $W^{1,p}(B \setminus B_\varepsilon)$, $E_{\varepsilon,\eta_{j_k}}(\mathbf{u}_{V,\varepsilon,\eta_{j_k}}) \to E_\varepsilon(\mathbf{u}_{V,\varepsilon})$ as $k \to \infty$, and $\mathbf{u}_{V,\varepsilon}$ is a solution of (6.3).

Proof: Under the growth hypotheses in [48, Section 3], and adapting the lower semicontinuity arguments used therein, it can be shown that, for each $\eta > 0$, $E_{\varepsilon,\eta}$ is sequentially weakly lower semicontinuous and hence that a minimiser $\mathbf{u}_{V,\varepsilon,\eta}$ exists for the unconstrained variational problem (6.5). Without loss of generality, we may assume that (η_j) is monotone increasing. It follows that

$$\eta_j \left(\int_{B\setminus B_\varepsilon} \det \nabla \mathbf{u}_{V,\varepsilon,\eta_j} \,\mathrm{d}\mathbf{x} - K \right)^2 \leq E_{\varepsilon,\eta_j}(\mathbf{u}_{V,\varepsilon,\eta_j}) \leq \text{const.}, \tag{6.7}$$

and thus that

$$\lim_{j\to\infty} \int_{B\setminus B_\varepsilon} \det \nabla \mathbf{u}_{V,\varepsilon,\eta_j} \,\mathrm{d}\mathbf{x} = K. \tag{6.8}$$

From the growth hypotheses (ii), it can then be shown that there exists a subsequence $\left(\mathbf{u}_{V,\varepsilon,\eta_{j_k}}\right)$ which converges weakly in $W^{1,p}(B\setminus B_\varepsilon)$ to a function $\mathbf{u}_{V,\varepsilon}$, and that $\left(\det \nabla \mathbf{u}_{V,\varepsilon,\eta_{j_k}}\right)$ converges weakly in $L^1(B \setminus B_\varepsilon)$ to a function θ. Since $p \in (2,3)$, it follows from [34, Theorem 4.2], that $\mathbf{u}_{V,\varepsilon}$ satisfies condition INV, $\theta = \det \nabla \mathbf{u}_{V,\varepsilon}$, and $\det \nabla \mathbf{u}_{V,\varepsilon} > 0$ almost everywhere. It now follows from (6.8) that $\mathbf{u}_{V,\varepsilon}$ satisfies the volume constraint. Moreover,

$$\int_{B\setminus B_\varepsilon} W(\nabla \mathbf{u}_{V,\varepsilon}) \,\mathrm{d}\mathbf{x} = E_{\varepsilon,\eta_1}(\mathbf{u}_{V,\varepsilon}) \leq \liminf_{k\to\infty} E_{\varepsilon,\eta_1}(\mathbf{u}_{V,\varepsilon,\eta_{j_k}}) \leq \liminf_{k\to\infty} E_{\varepsilon,\eta_{j_k}}(\mathbf{u}_{V,\varepsilon,\eta_{j_k}}),$$

which together with (6.6) implies that $\mathbf{u}_{V,\varepsilon}$ solves (6.3), and gives the corresponding convergence of the energies. □

Remark 6.2. We note that the convergence result in the last proposition is only for a subsequence since the limit problem may not have a unique minimiser in general. We also anticipate that a similar convergence result to that obtained in the last proposition with $\epsilon_k \to 0$ and $\eta_j \to \infty$ simultaneously, should follow on adapting the arguments of [48] (see also the generalisation in [12]).

The flow equation: To compute minimisers of (6.5) we use the gradient flow equation

$$\Delta\mathbf{u}_t = -\mathrm{div}\,\left[\frac{\mathrm{d}W}{\mathrm{d}\mathbf{F}}(\nabla\mathbf{u}) + 2\eta\left(\int_{B\setminus B_\varepsilon}\det\nabla\mathbf{u}\,\mathrm{d}\mathbf{x} - K\right)(\mathrm{adj}\,\nabla\mathbf{u})^T\right] \ \text{in} \ \ B\setminus B_\varepsilon,$$

where for all $t \geq 0$, $\mathbf{u}(\mathbf{x},t) = \mathbf{A}\mathbf{x}$ on ∂B and

$$\left[\nabla\mathbf{u}_t + \frac{\mathrm{d}W}{\mathrm{d}\mathbf{F}}(\nabla\mathbf{u}) + 2\eta\left(\int_{B\setminus B_\varepsilon}\det\nabla\mathbf{u}\,\mathrm{d}\mathbf{x} - K\right)(\mathrm{adj}\,\nabla\mathbf{u})^T\right]\mathbf{N} = \mathbf{0},\ \text{over}\ \partial B_\varepsilon.$$

It is easy to check that the gradient flow equation leads to a descent method for the solution of (6.5). After discretising the partial derivative with respect to "t", one uses a non–conforming finite element method to solve the resulting flow equation. This process is repeated up to a maximum value of t or until some convergence criteria is satisfied. For more details about the gradient flow method and its properties we refer to [40], and for its use in problems leading to cavitation see [16]. For the implementation of the gradient flow method we used the freely available finite element package FreeFem++ (www.freefem.org).

Numerical results: For the actual numerical computations we consider the special case of (2.3) in which:

$$W(\mathbf{F}) = \frac{\mu}{p}\,|\mathbf{F}|^p + b(\det\mathbf{F})^\beta + c(\det\mathbf{F})^{-\gamma}, \tag{6.9}$$

where $p \in (1,n)$, $\beta,\gamma > 0$, and $b,c \geq 0$. The reference configuration is stress free provided:

$$c = \frac{\mu(\sqrt{n})^{p-2} + b\beta}{\gamma}.$$

For the calculations we used the values $\mu = 1$, $p = 1.5$, $\beta = 2$, $\gamma = 1$, $b = 1$ and $\eta = 100$ for the penalisation parameter.

For the case $n = 2$, we begin by showing in Figure 1, a section of $G(\mathrm{diag}(\lambda_1,\lambda_2))$. To generate this figure, the values of (λ_1,λ_2) were parameterised as $\lambda_1 = \sqrt{d/k}$ and $\lambda_2 = \sqrt{kd}$ so that $\lambda_1\lambda_2 = d$ and $\lambda_2 = k\lambda_1$. We used a pre–existing hole of radius $\varepsilon = 0.025$ and the constraint (6.2) with a value of V equivalent to a disk of radius 0.1. In Figure 2 we show the zero level curve of this surface. For this example this curve gives an approximation of the critical boundary for the onset of cavitation.

For the case $n = 3$, we used a domain with a pre–existing hole of radius $\varepsilon = 0.1$, and the constraint (6.2) with a value of V equivalent to a spherical hole of radius 0.2. The mesh used has approximately 17,000 nodes. We iterated 400 times in the gradient flow method leading to a step size increment $O(10^{-3})$ with the same order of error on the volume constraint. We show in Figure 3 a volumetric sketch of $G(\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3))$. The colors in this sketch represent the values of the volume derivative from positive (reddish)

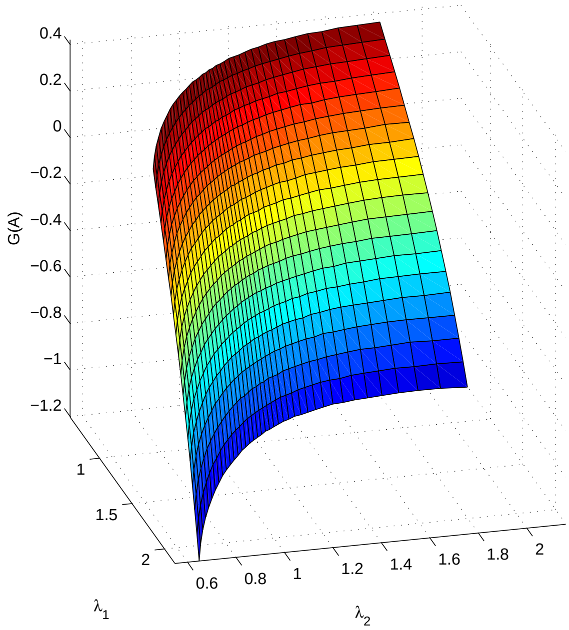

Figure 1: Sketch of the graph of the approximate volume derivative at $\mathbf{A} = \operatorname{diag}(\lambda_1, \lambda_2)$ for the stored energy function (6.9) for $n = 2$, $\mu = 1$, $p = 1.5$, $\beta = 2$, $\gamma = 1$, and $b = 1$.

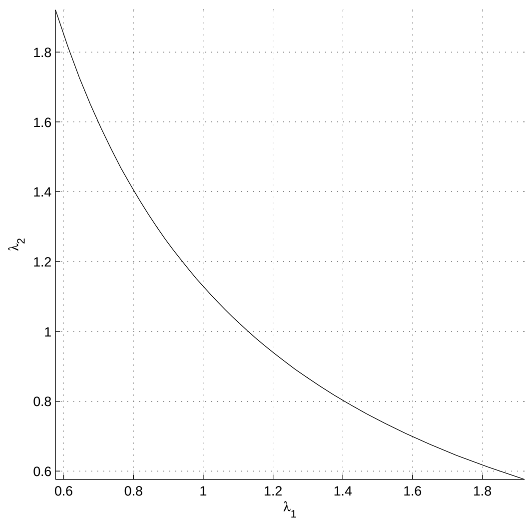

Figure 2: Approximate zero level curve for the volume derivative corresponding to the stored energy function (6.9) for $n = 2$, $\mu = 1$, $p = 1.5$, $\beta = 2$, $\gamma = 1$, and $b = 1$.

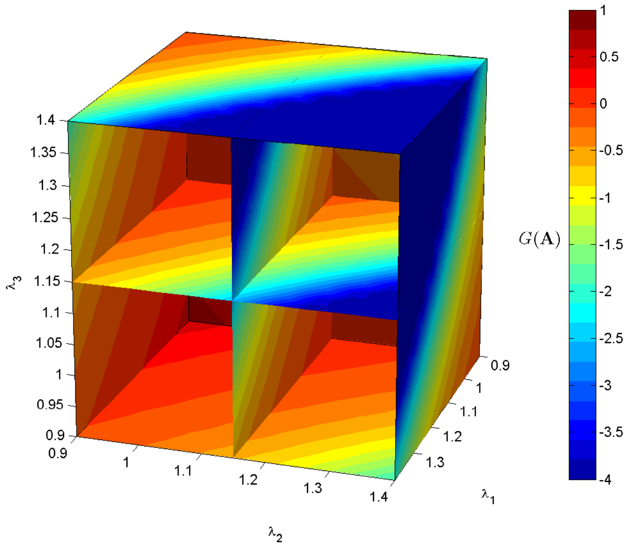

Figure 3: Sketch of the approximate volume derivative for the stored energy function (6.9) for $n = 3$, $\mu = 1$, $p = 1.5$, $\beta = 2$, $\gamma = 1$, and $b = 1$. (The colour coding shows the value of $G(\mathbf{A})$ at $\mathbf{A} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$.)

values to negative (blue) values. This hyper–surface is composed of 1728 data points and it took approximately 50 hours to generate it using two dual core 2.5 GHz computers, using all four cores. Finally, in Figure 4 we show a section of the zero level surface of this hyper–surface which gives an approximation to the critical boundary (in the space of strains $(\lambda_1, \lambda_2, \lambda_3)$) for the onset of cavitation in this case.

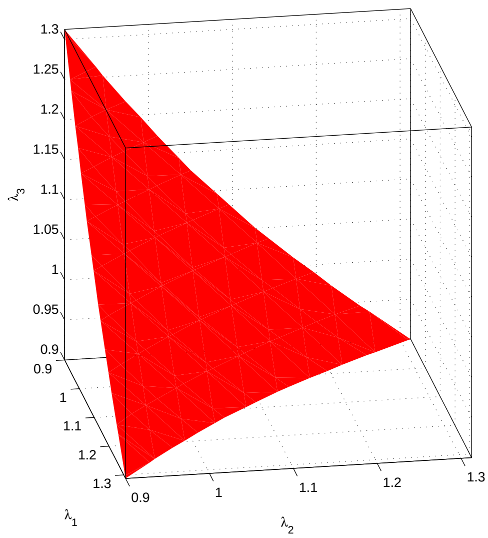

Figure 4: Approximate zero level surface for the volume derivative corresponding to the stored energy function (6.9) for $n = 3$, $\mu = 1$, $p = 1.5$, $\beta = 2$, $\gamma = 1$, and $b = 1$.

7 Concluding remarks

In this paper we have defined a derivative $G(\mathbf{A})$ (given by (2.7)) of the energy functional (1.4) at a given matrix $\mathbf{A} \in M_+^{n\times n}$ with respect to hole–producing deformations. We also proposed a criterion to compute the boundary of the set of matrices $\mathcal{U}$ on which the stored energy is not $W^{1,p}$–quasiconvex relative to formation of a cavity, by computing the zero set of G. The boundary $\partial\mathcal{U}$ of this unstable set corresponds to the onset of cavitation. One could, alternatively, try to compute $\partial\mathcal{U}$ by determining the matrices $\mathbf{A}$ at which the minimum energy jump $\Delta E(\mathbf{A}) = \inf_{\mathbf{u}\in\mathcal{A}_{\mathbf{A}}} [E(\mathbf{u}) - E(\mathbf{Ax})]$ equals zero. A difficulty with this approach is that the minimum energy jump is zero for all $\mathbf{A} \in \mathcal{S}$ (the stable set on which the stored energy function is $W^{1,p}$–quasiconvex relative to the formation of a cavity) thus making it difficult to measure, from within $\mathcal{S}$, how close $\mathbf{A}$ is to $\partial\mathcal{S}$. In contrast to the above, we expect in general that the graph of the volume derivative $G(\mathbf{A})$, considered as a function of the singular values of $\mathbf{A}$, crosses its zero-level set transversally (as in the example in Figure 1), thus making computation of the 'onset of cavitation surface' a more stable task (see [39]).

The method employed in this paper to compute the zero level set of G, is based on computing $G(\mathbf{A})$ for many different matrices $\mathbf{A}$, and then approximating the zero level set of the resulting graph using a contour finding routine. As pointed out in section 6, this is a very time consuming process, especially in the case $n = 3$, since one has to compute $G(\mathbf{A})$ for many matrices $\mathbf{A}$ and each of these calculations requires solving a large-scale constrained nonlinear optimisation problem. We are currently experimenting with a continuation scheme to speed up the calculation of the zero set of G.

Since the units of the volume derivative are energy per unit volume, if $G(\mathbf{A})$ is positive it measures the amount of energy required to open a hole of unit volume in the given material. If negative, the volume derivative measures the corresponding amount of energy liberated by opening up such a hole. (See also Remark 5.5 for an interpretation in terms of the work done by the Cauchy stress in opening the hole.)

In our study of the volume derivative and for ease of exposition, we have chosen to work within the framework developed by Muller and Spector in [34] and as subsequently applied in [44], [45]. Hence, in particular, we have used condition (INV) from [34] and worked in the set of admissible deformations given by (1.5), considering the formation of a single cavity in the case $p > n-1$. However, the interesting work of [8], [13], [14], [12] would be relevant in generalising our results, in particular to include the case $p = n-1$.

The approach in this paper gives a criterion for local formation of a single cavity in a deforming elastic body. In particular, our proofs of Proposition 2.4 and Theorem 2.10 do not extend to the case of two or more flaw points. Hence, we anticipate that our results would be most applicable to the case in which the cavities formed are well-separated relative to their dimensions, as occurs in the initial stages of certain types of fracture. We refer to interesting recent work of Henao and Serfaty [15] on the interaction between cavities that are not well-separated in this sense.

We have focussed in the current paper on the changes in bulk energy due to the formation of cavities and have not included surface energy effects or a cavity initiation energy to mitigate cavity formation. It is known that the inclusion of such effects may dramatically affect the predictions of models for cavitation in an elastic body (see, e.g., [10]). However, it is clear that the addition to the energy functional (1.4) of a term proportional to the surface area of the cavity formed would result in the corresponding volume derivative being infinite (this is a consequence of the isoperimetric inequality since the surface area of a cavity of volume V is bounded from below by a positive constant times $V^{\frac{2}{3}}$). One might anticipate in this case taking alternative forms of derivative, e.g. in three dimensions, replacing V in the denominator of (2.6) by $V^{\frac{2}{3}}$. Indeed, one might in general envisage utilising a hierarchy of such derivatives using V^{α} as a way of obtaining further information on the nature of an isolated singularity in a minimiser. (Related calculations are contained in [47].)

In this regard, it is interesting to note that the argument used in Proposition 2.1 to prove monotonicity in V of the intermediate functional (2.6), which led to the definition of the volume derivative (2.7), can clearly be extended to prove monotonicity in the case of intermediate functionals of the form

$$\tilde{F}(\mathbf{A}, V) = \inf_{\mathbf{u} \in \mathcal{A}_{\mathbf{A},V}} \left(\frac{\int_\Omega W^{(1)}(\nabla \mathbf{u}) - W^{(1)}(\mathbf{A})}{\int_\Omega W^{(2)}(\nabla \mathbf{u}) - W^{(2)}(\mathbf{A})} \right),$$

where $W^{(1)}, W^{(2)}$ are general functions. Thus, one could define a relative derivative $\tilde{G}(\mathbf{A}) = \lim_{V \searrow 0} \tilde{F}(\mathbf{A}, V)$, where the choice of (2.6) considered in the current paper would correspond to the case $W^{(2)}(\mathbf{F}) = -\det \mathbf{F}$. This might lead to a more general notion of a relative energy drop due to the formation of a cavity and provide a corresponding partial-ordering of energy functionals.

Acknowledgements: This research was supported by an International Joint Project Grant from the Royal Society of London. The work of Negrón–Marrero was also supported in part by the University of Puerto Rico at Humacao (UPRH) during sabbatical leave, and by the NSF–PREM Program of the UPRH (Grant No. DMR–0934195). JS would like to thank J.G. Lloyd for helpful discussions relating to this work.

References

[1] Antman, S.S. and Negrón-Marrero, P.V., *The Remarkable Nature of Radially Symmetric Equilibrium States of Aelotropic Nonlinearly Elastic Bodies*, J. Elasticity, 18, 131-164, 1987.

[2] Ball, J.M., *Convexity conditions and existence theorems in nonlinear elasticity*, Arch. Rational Mech. Anal., 63, 337–403, 1977.

[3] Ball, J.M., *Discontinuous Equilibrium Solutions and Cavitation in Nonlinear Elasticity*, Phil. Trans. Royal Soc. London **A 306**, 557-611, 1982.

[4] Ball, J.M., *Some open problems in elasticity*, in "Geometry, Mechanics, and Dynamics", pages 3–59, Springer, New York, 2002.

[5] Ball, J.M. and Knowles, G., *A Numerical Method for Detecting Singular Minimisers*, Numer. Math., 51, 181–197, 1987.

[6] Ball, J.M. and Mizel, V.J., *One-dimensional variational problems whose minimisers do not satisfy the Euler-Lagrange equation*, Arch. Rational Mech. Anal. 90, 325–388, 1985.

[7] Ball, J.M. and Murat, F., $W^{1,p}$-quasiconvexity and variational problems for multiple integrals. *J. Funct. Anal.*, **58**, 225-253, (1984).

[8] Conti, S. and De Lellis, C., *Some remarks on the theory of elasticity for compressible Neohookean materials*, Ann. Sc. Norm. Super. Pisa Cl. Sci. **5**, 521549, (2003).

[9] Evans, L.C., Quasiconvexity and partial regularity in the Calculus of Variations, *Proceeedings of the International Congress of Mathematicians, Berkeley, California, U.S.A.*, 1986.

[10] Gent, A.N., *Cavitation in Rubber: A Cautionary Tale*, Rubber Chemistry and Technology, G49-G53, 1990.

[11] Gent, A. N. and Lindley, P. B., *Internal Rupture of Bonded Rubber Cylinders in Tension*, Proc. R. Soc. Lond. A 249, 195-205, 1958.

[12] Henao, D., *Cavitation, invertibility, and convergence of regularized minimisers in nonlinear elasticity*, J. Elasticity, 94, 55–68, 2009.

[13] Henao, D. and Mora-Corral C., *Invertibility and weak continuity of the determinant for the modelling of cavitation and fracture in nonlinear elasticity*, Arch. Rational Mech. Anal., 197, 619–655, 2010.

[14] Henao, D. and Mora-Corral C., *Lusins condition and the distributional determinant for deformations with finite energy*, preprint 2009. Advances in Calculus of Variations. Page -, ISSN (Online) 1864-8266, ISSN (Print) 1864-8258, DOI: 10.1515/ACV.2011.016

[15] Henao, D. and Serfaty, S., *Energy estimates and cavity interaction for a critical-exponent cavitation model*, preprint 2011.

[16] Henao, D. and Xu, .X., *An efficient numerical method for cavitation in nonlinear elasticity* , Mathematical Models and Methods in Applied Sciences, in press, 2010.

[17] Horgan, C.O., *Void nucleation and growth for compressible non–linearly elastic materials: an example*, Int. J. Solids Structures, Vol. 29, No. 3, 279–291, 1992.

[18] Horgan, C.O. and Abeyaratne, R., *A bifurcation problem for a compressible nonlinearly elastic medium: growth of a microvoid*, Journal of Elasticity, 16, 189-200 (1986).

[19] Horgan, C.O. and Polignone, D.A., *Cavitation in Nonlinearly Elastic Solids: A Review*, Appl. Mech. Rev., Vol. 48, No. 8, 1995.

[20] Hou, H.-S. and Abeyaratne, R., *Cavitation in elastic and elastic-plastic solids*, J. Mech. Phys. Solids 40, 571–592, 1992.

[21] James, R. and Spector, S.J., *Remarks on $W^{1,p}$–quasiconvexity, interpenetration of matter, and function spaces for elasticity,*, J. Mech. Phys. Solids 39, Pages 783–813, 1991

[22] James, R. and Spector, S.J., *The formation of filamentary voids in solids*, Anal. Non-Lineaire 9, 263–280, 1992.

[23] Kristensen, J., *On the non locality of Quasiconvexity*, Analyse Non-Lineaire, 16, 1-13, 1999.

[24] Lavrentiev, M., *Sur quelques problemes du calcul des variations*, Ann. Mat. Pura Appl. 4, 107–124, 1926.

[25] Li, Z., *Element Removal Method for Singular Minimizers in Variational Problems Involving Lavrentiev Phenomenon*, Proc. Roy. Soc. Lond., A, 439, 131–137, 1992.

[26] Li, Z., *Element Removal Method for Singular Minimizers in Problems of Hyperelasticity*, Math. Models and Methods in Applied Sciences, Vol. 5, No. 3, 387–399, 1995.

[27] Lian, Y. and Li, Z., *A dual–parametric finite element method for cavitation in nonlinear elasticity*, Journal of Computational and Applied Mathematics, doi: 10.1016/j.cam.2011.05.020, 2011.

[28] Lian, Y. and Li, Z., *A numerical study on cavitations in nonlinear elasticity – defects and configurational forces*, Mathematical Models and Methods in Applied Sciences, doi:10.1142/S0218202511005830, 2011.

[29] Lopez-Pamies, O., Idiart, M.I. and Nakamura, T., *Cavitation in elastomeric solids: I A defect-growth theory*, Journal of the Mechanics and Physics of Solids, in press, 2011.

[30] Lopez-Pamies, O., Idiart, M.I. and Nakamura, T.. *Cavitation in elastomeric solids: II Onset-of-cavitation surfaces for Neo-Hookean materials*, Journal of the Mechanics and Physics of Solids, in press, 2011.

[31] Lopez-Pamies, O.. *Onset of cavitation in compressible, isotropic, hyperelastic solids*, Journal of Elasticity 94, 115–145, 2009.

[32] Meyers, N.G., *Quasiconvexity and lower semicontinuity of multiple integrals of any order*, Trans. Am. Math. Soc., 119, 225-249, 1965.

[33] Morrey, C.B., *Quasi-convexity and the lower semicontinuity of multiple integrals*, Pacific J. Math. 2, 25-53, 1952.

[34] Müller, S. and Spector, S.J., *An existence theory for nonlinear elasticity that allows for cavitation*, Arch. Rational Mech. Anal., 131, 1–66, 1995.

[35] Müller, S. and Sivaloganathan, J. and Spector, S.J., *An isoperimetric estimate and* $W^{1,p}$*–quasiconvexity in nonlinear elasticity*, Calc. Var., 8, 159–176, 1999.

[36] Negrón-Marrero, P. V., *A Numerical Method for Detecting Singular Minimizers of Multidimensional Problems in Nonlinear Elasticity*, Numerische Mathematik, 58, 135–144, 1990.

[37] Negrón-Marrero, P. V. and Betancourt O., *The Numerical Computation of Singular Minimizers in Two Dimensional Elasticity*, Journal of Computational Physics, Vol. 113, No. 2, pp. 291–303, 1994.

[38] Negrón-Marrero, P. V. and Sivaloganathan, J., *The Numerical Computation of the Critical Boundary Displacement for Radial Cavitation*, Mathematics and Mechanics of Solids, 14: 696726, 2009.

[39] Negrón-Marrero, P. V. and Sivaloganathan, J., *The volume derivative and its approximation in the case of radial cavitation*, SIAM J. Appl. Math., in press, 2011.

[40] Neuberger, J. W., Sobolev Gradients and Differential Equations, *Lecture Notes in Math.* 1670, Springer, Berlin, 1997.

[41] Polignone, D.A. and Horgan, C.O., *Cavitation for Incompressible Anisotropic Nonlinearly Elastic Spheres*, Journal of Elasticity, 33, 27–65, 1993.

[42] Sivaloganathan, J., *Uniqueness of regular and singular equilibria for spherically symmetric problems of nonlinear elasticity*, Arch. Rat. Mech. Anal., 96, 97–136, 1986.

[43] Sivaloganathan, J., *Singular minimisers in the Calculus of Variations: a degenerate form of cavitation*, Analyse Non-Lineaire, 9, 657–681, 1992.

[44] Sivaloganathan, J. and Spector, S. J., *On the existence of minimisers with prescribed singular points in nonlinear elasticity*, J. Elasticity, 59, 83–113, 2000.

[45] Sivaloganathan, J. and Spector, S. J., *On the optimal location of singularities arising in variational problems in nonlinear elasticity*, Journal of Elasticity, 58: 191–224, 2000.

[46] Sivaloganathan, J. and Spector, S. J., *On cavitation, configurational forces and implications for fracture in a nonlinearly elastic matrial*, Journal of Elasticity, 67: 25–49, 2002.

[47] Sivaloganathan, J. and Spector, S. J., *Necessary conditions for a minimum at a radial cavitating singularity in nonlinear elasticity*, Analyse Non-Lineaire, 25, 201-213, 2008.

[48] Sivaloganathan, J., Spector, S. J. and Tilakraj, V., *The convergence of regularised minimisers for cavitation problems in nonlinear elasticity*, SIAM Journal of Applied Mathematics, 66, 736–757, 2006.

[49] Sokolowski, J., and Zochowski, A., *On topological derivative in shape optimization.* SIAM J. Control Optim. 37, 1251–1272, 1999.

[50] Sokolowski, J., and Zochowski, A., *Energy change due to the appearance of cavities in elastic solids.* Int. J. Solids and Structures. 40:1765–1803, 2003.

[51] Spector, S. J., *Linear deformations as global minimizers in nonlinear elasticity*, Q. Appl. Math., 32, 59–64, 1994.

[52] Stuart, C. A., *Radially symmetric cavitation for hyperelastic materials*, Ann. Inst. H. Poincaré 2, 33–66, 1985.

[53] Stuart, C.A., *Estimating the Critical Radius for Radially Symmetric Cavitation*, Quarterly of Applied Mathematics, Vol. 13, No. 2, 251-263, 1993.

[54] Varvaruca, L., Singular minimizers in the calculus of variations and nonlinear elasticity, doctoral dissertation, University of Bath, Department of Mathematical Sciences, April 2007.