MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:1–28
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.545
MOS subject classification: 35 A 05; 76 N 10

Global existence of the radially symmetric solutions of the Navier–Stokes equations for the isentropic compressible fluids

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Communicated by M. Mitrea

SUMMARY

We study the isentropic compressible Navier–Stokes equations with radially symmetric data in an annular domain. We first prove the global existence and regularity results on the radially symmetric *weak solutions* with non-negative bounded densities. Then we prove the global existence of radially symmetric *strong solutions* when the initial data ρ_0, $\mathbf{u}_0$ satisfy the compatibility condition

$$-\mu\Delta\mathbf{u}_0-(\lambda+\mu)\nabla\operatorname{div}\mathbf{u}_0+\nabla(A\rho_0^\gamma)=\rho_0^{1/2}\mathbf{g}$$

for some radially symmetric $\mathbf{g}\in L^2$. The initial density ρ_0 needs not be positive. We also prove some uniqueness results on the strong solutions. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: Navier–Stokes equations; isentropic compressible fluids; radially symmetric solutions; vacuum

1. INTRODUCTION

We consider the initial boundary value problem for the isentropic compressible Navier–Stokes equations in $(0,\infty)\times\Omega$,

$$(\rho\mathbf{u})_t+\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u})-\mu\Delta\mathbf{u}-(\lambda+\mu)\nabla\operatorname{div}\mathbf{u}+\nabla p=\rho\mathbf{f} \tag{1}$$

$$\rho_t+\operatorname{div}(\rho\mathbf{u})=0, \quad p=A\rho^\gamma \quad (A>0,\ \gamma>1) \tag{2}$$

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Contract/grant sponsor: Korea Research Foundation; contract/grant number: KRF C-00005
Contract/grant sponsor: Japan Society for the Promotion of Science

Received 7 May 2003

where Ω is a bounded or unbounded annulus in $\mathbb{R}^n$ ($n\geqslant 2$) and the given data are radially symmetric. More precisely, the domain Ω and the external force f are given by

$$\Omega=\{\mathbf{x}\in\mathbb{R}^n : a<|\mathbf{x}|<b\},\quad \mathbf{f}(t,\mathbf{x})=f(t,|\mathbf{x}|)\,\frac{\mathbf{x}}{|\mathbf{x}|}$$

for some constants a, b with $0<a<b\leqslant\infty$, and the initial and boundary conditions are imposed as follows:

$$(\rho,\rho\mathbf{u})|_{t=0}=(\rho_0,\rho_0\mathbf{u}_0)\text{ in }\Omega,\quad \mathbf{u}(t,\mathbf{x})\to 0\text{ as }|\mathbf{x}|\to a\text{ or }b,\ t>0 \tag{3}$$

where

$$\rho_0(\mathbf{x})=\rho_0(|\mathbf{x}|)\geqslant 0\quad\text{and}\quad \mathbf{u}_0(\mathbf{x})=u_0(|\mathbf{x}|)\,\frac{\mathbf{x}}{|\mathbf{x}|}\quad\text{for }\mathbf{x}\in\Omega \tag{4}$$

Here ρ, $\mathbf{u}$ and p denote the unknown density, velocity and pressure, respectively. The viscosity constants μ and λ are assumed to satisfy the usual physical requirements $\mu>0$, $2\mu+n\lambda\geqslant 0$.

The main goals of the present paper are to prove global existence and regularity of radially symmetric solutions to the initial boundary value problem (1)–(3) with non-negative initial densities. The first existence result was proved by Hoff [1]; he proved the global existence of radially symmetric weak solutions to problem (1)–(3) with strictly positive initial densities in annular domains. Then it was extended by Jiang and Zhang [2] to the Cauchy problem with general non-negative initial densities. Roughly speaking, they proved the global existence of radially symmetric weak solutions under the regularity assumption that $0\leqslant\rho_0\in L^\gamma(\mathbb{R}^n)$, $\sqrt{\rho_0}\mathbf{u}_0\in L^2(\mathbb{R}^n)$ and $\mathbf{f}=0$, where $n=2$ or 3.

One of the results of Hoff [1] is that the density remains bounded for all time when it is initially bounded away from zero and infinity. The first main result in this paper shows that the same result holds for general non-negative initial densities. See Lemma 3.2 and Theorem 4.1. These results have been proved only for annular domains and cannot be extended to a ball $\Omega=B_R=\{\mathbf{x}\in\mathbb{R}^n : |\mathbf{x}|<b<\infty\}$ because of a counter-example of Weigant [3]. For the case that $1<\gamma<1+1/n-1$, he constructed a radially symmetric strong solution $(\rho,\mathbf{u})$ to problem (1)–(3) in $[0,1)\times B_R$ such that $|\rho(t)|_{L^\infty(B_R)}\to\infty$ as $t\to 1$.

Using the boundedness of the density, we then prove Theorem 4.2, a global regularity result on radially symmetric weak solutions. In particular, assuming that $0\leqslant\rho_0\in L^1\cap H^1$ and $\mathbf{u}_0\in D_0^1$ (the notations will be explained below), we prove the strong continuity of the density and momentum:

$$\rho\in C([0,\infty);L^1\cap H^1)\quad\text{and}\quad \rho\mathbf{u}\in C([0,\infty);L^2) \tag{5}$$

But since the density ρ may vanish in Ω, the continuity of the velocity $\mathbf{u}$ cannot be deduced from (5). In fact, the continuity of $\mathbf{u}$ in a very weak sense is an open problem until now. Moreover, the uniqueness of solutions is also open unless the initial density has a positive lower bound. For a relevant uniqueness result, see Theorem 4.4.

To guarantee the continuity of $\mathbf{u}$ as well as the uniqueness of solutions, it is necessary that the initial data $(\rho_0,\mathbf{u}_0)$ satisfy a compatibility condition. We prove in Theorem 5.1 that for any initial data $(\rho_0,\mathbf{u}_0)$ with $0\leqslant\rho_0\in L^1\cap H^1$ and $\mathbf{u}_0\in D_0^1\cap D^2$, there exists a radially symmetric strong solution $(\rho,\mathbf{u})$ to the initial boundary value problem (1)–(3) satisfying the regularity

$$\rho\in C([0,\infty);L^1\cap H^1),\ \ \mathbf{u}\in C([0,\infty);D_0^1\cap D^2),\ \ \sqrt{\rho}\mathbf{u}_t\in L^\infty_{\text{loc}}(0,\infty;L^2)$$

if and only if there exists a radially symmetric $\mathbf{g} \in L^2$ such that

$$-\mu\Delta\mathbf{u}_0 - (\lambda+\mu)\nabla \operatorname{div}\mathbf{u}_0 + \nabla(A\rho_0^\gamma) = \rho_0^{1/2}\mathbf{g} \tag{6}$$

The uniqueness of solutions of Theorem 5.1 can be proved by a rather standard method, if the initial density has an additional regularity. See Theorem 5.5. The compatibility condition (6) has been considered by Salvi and Straškraba [4], Choe and Kim [5] and Cho *et al.* [6] to prove the local existence of unique strong solutions with non-negative densities. Hence our result on the global existence of strong solutions is an extension of the previous local ones in case of radially symmetric data.

Finally, we remark that for the Navier–Stokes equations of compressible heat-conducting gases, the local existence of strong solutions with non-negative densities was recently proved by Cho and Kim [7]. In case of positive initial densities, the existence of strong solutions has been well-known and in particular, Jiang [8] and Nikolaev [9] proved the global existence of radially symmetric strong solutions in annular domains. Hence it is an interesting problem to extend their results to the case of general non-negative densities.

The paper is organized as follows. Sections 4 and 5 are devoted to proving all the main results. The essential parts of the proofs are to derive some *a priori* estimates for radially symmetric strong solutions. In Sections 2 and 3, we prove a local existence result on the radially symmetric strong solutions and derive the necessary *a priori* estimates.

Notations

Throughout this paper, we will use the following simplified notations for the standard Sobolev spaces:

$$L^q = L^q(\Omega),\ H^k = W^{k,2}(\Omega),\ D_0^1 = D_0^{1,2}(\Omega),\ D^k = D^{k,2}(\Omega)$$

$$L^r_{\text{loc}}(0,\infty;X) = \bigcap_{T>0} L^r(0,T;X) \quad \text{for } X = L^q,\ H^k,\ \text{etc.}$$

For a detailed study of *homogeneous* Sobolev spaces $D_0^{1,2}(\Omega)$ and $D^{k,2}(\Omega)$, please refer to Reference [10].

2. A LOCAL EXISTENCE RESULT

To construct radially symmetric solutions to problem (1)–(3), we first solve the following initial boundary value problem in $(0,\infty)\times(a,b)$:

$$\rho_t + (\rho u)_r + m\frac{\rho u}{r} = 0 \tag{7}$$

$$(\rho u)_t + (\rho u^2)_r + m\frac{\rho u^2}{r} - v\left(u_r + m\frac{u}{r}\right)_r + p_r = \rho f \tag{8}$$

$$\rho(0,r) = \rho_0(r), \quad u(0,r) = u_0(r), \quad u(t,a) = u(t,b) = 0 \tag{9}$$

where $p = A\rho^\gamma$, $v = \lambda + 2\mu > 0$, $m = n-1 \geqslant 1$ and $0 < a < b < \infty$. The global weak solutions were constructed by Hoff [1] via a finite difference method. For the case of $m=0$, the global existence of strong solutions has been well-known and was proved, for instance, by Straškraba and Valli [11]. In this section, we prove the following local existence result for any $m \geqslant 1$.

Proposition 2.1
Assume that

$$\rho_0 \in H^2(a,b),\ u_0 \in H_0^1(a,b) \cap H^2(a,b),\ f, f_r, f_t \in L^2_{\rm loc}(0,\infty; L^2(a,b))$$

and

$$\rho_0 \geqslant \varepsilon \text{ on } [a,b] \quad \text{for some constant } \varepsilon > 0$$

Then there exist a small time $T>0$ and a unique strong solution (ρ, u) to the initial boundary value problem (7)–(9) such that

$$\begin{aligned} &\rho \in C([0,T]; H^2(a,b)), \quad \rho_t \in C([0,T]; H^1(a,b)) \\ &u \in C([0,T]; H_0^1(a,b) \cap H^2(a,b)) \cap L^2(0,T; H^3(a,b)) \\ &u_t \in C([0,T]; L^2(a,b)) \cap L^2(0,T; H_0^1(a,b)) \\ &\rho > 0 \text{ on } [0,T] \times [a,b] \end{aligned} \tag{10}$$

Remark 2.2
In fact, the strong solution exists globally in time, as is proved in the next section.

Proof
Introducing a new variable $\sigma = \rho r^m$, we can rewrite problem (7)–(9) as an equivalent one

$$\sigma_t + (\sigma u)_r = 0 \tag{11}$$

$$(\sigma u)_t + (\sigma u^2)_r - \nu \left(u_r + m\frac{u}{r}\right)_r r^m + p_r r^m = \sigma f \tag{12}$$

$$\sigma(0,r) = \rho_0(r) r^m, \quad u(0,r) = u_0(r), \quad u(t,a) = u(t,b) = 0 \tag{13}$$

where $p = A(\sigma r^{-m})^\gamma$. We prove the local existence of a unique strong solution to problem (11)–(13) by using a standard fixed point argument. For this purpose, consider the following linearized problem:

$$\sigma_t + (\sigma v)_r = 0 \tag{14}$$

$$(\sigma u)_t + (\sigma v u)_r - \nu \left(u_r + m\frac{u}{r}\right)_r r^m + p_r r^m = \sigma f \tag{15}$$

$$\sigma(0,r) = \rho_0(r) r^m, \quad u(0,r) = u_0(r), \quad u(t,a) = u(t,b) = 0 \tag{16}$$

where v is a known smooth function which satisfies the boundary condition $v(t,a) = v(t,b) = 0$ for $t \geqslant 0$. Since $\sigma(0) \geqslant \varepsilon a^m > 0$ on $[a,b]$, it follows from classical arguments that the above linear problem has a unique global strong solution. The following result for the linearized problem is sufficient to prove the local existence of a strong solution to (11)–(13). □

Lemma 2.3
Let T be a fixed time with $0<T<1$, and assume that

$$\sup_{0\leqslant t\leqslant T}(|v(t)|^2_{H^1_0\cap H^2}+|v_t(t)|^2_{L^2})+\int_0^T(|v(t)|^2_{H^3}+|v_t(t)|^2_{H^1_0})\,\mathrm{d}t\leqslant K \tag{17}$$

for some constant $K>1$. Then there exists a unique strong solution (σ,u) to problem (14)–(16) such that

$$\sup_{0\leqslant t\leqslant T}(|\sigma(t)|^2_{H^2}+K^{-1}|\sigma_t(t)|^2_{H^1}+|u(t)|^2_{H^1_0\cap H^2}+|u_t(t)|^2_{L^2})$$
$$+\int_0^T(|u(t)|^2_{H^3}+|u_t(t)|^2_{H^1_0})\,\mathrm{d}t\leqslant C\exp[CK^2T^{1/2}\exp(CKT^{1/2})] \tag{18}$$

Throughout this section, we use the simplified notations $L^2=L^2(a,b)$, etc. Moreover, we denote by C a generic positive constant which depends only on v, a, b, ε and the norms of the data (ρ_0,u_0,f).

Assuming the validity of Lemma 2.3, we continue to prove the proposition. First, choose K, $T>0$ such that

$$K>2C \quad \text{and} \quad \exp[CK^2T^{1/2}\exp(CKT^{1/2})]<2$$

where C is the constant in (18). Let X be the set of all functions v satisfying condition (17). Finally, for each $v\in X$, let $u=\mathcal{L}v$ be the solution to the linearized problem (14)–(16). Then Lemma 2.3 shows that $\mathcal{L}$ maps X into itself. The set X is convex, and moreover in view of a standard embedding result, X is a compact subset of $C([0,T];H^1)$. The continuity of $\mathcal{L}$ can be easily proved by an energy method. See Reference [12] for a detailed proof. Therefore, it follows from Schauder's fixed point theorem that $\mathcal{L}$ has a fixed point. This proves the existence of a strong solution to problem (11)–(13). A simple energy argument shows the uniqueness. Finally, the continuity property of the strong solution follows from standard arguments (see Reference [12] also). This completes the proof of Proposition 2.1. □

Now we turn to the proof of Lemma 2.3.

Proof of Lemma 2.3
The existence of the unique strong solution of the hyperbolic equation (14) has been well-known. Moreover, the solution σ satisfies the following estimate:

$$\sup_{0\leqslant t\leqslant T}(|\sigma(t)|_{H^2}+K^{-1/2}|\sigma_t(t)|_{H^1}+|\sigma(t)^{-1}|_{L^\infty})\leqslant C\exp(CKT^{1/2}) \tag{19}$$

For a proof, see Reference [12]. Then (15) can be written as a linear parabolic equation $u_t+vu_r-v\sigma^{-1}r^m(u_r+(m/r)u)_r=F$ with the force term $F=f-\sigma^{-1}r^m p_r$ satisfying F, F_r, $F_t\in L^2(0,T;L^2)$. The existence of the unique strong solution u has been also well-known. Hence it remains to prove the desired estimates for u.

To begin with, we rewrite (15) as

$$\sigma u_t+\sigma v u_r-v\left(u_r+m\frac{u}{r}\right)_r r^m=\sigma F \tag{20}$$

multiply this by u_t and then integrate over (a,b). Then using the boundary condition (16), we deduce that

$$\int_a^b \sigma u_t^2\,\mathrm{d}r + \frac{\nu}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b \left(u_r^2 + m\,\frac{u^2}{r^2}\right) r^m\,\mathrm{d}r = \int_a^b \sigma(F - vu_r)u_t\,\mathrm{d}r$$

Integrating over $(0,t)$ and using Young's inequality, we obtain

$$\int_0^t |\sqrt{\sigma}u_t|_{L^2}^2\,\mathrm{d}s + C^{-1}|u(t)|_{H_0^1}^2 \leqslant C + C\int_0^t |\sigma|_{L^\infty}(|F|_{L^2}^2 + |v|_{L^\infty}^2|u_r|_{L^2}^2)\,\mathrm{d}s$$

On the other hand, it follows from Sobolev inequality and (19) that for $0\leqslant t\leqslant T$

$$|\sigma(t)|_{L^\infty} + |F(t)|_{L^2}^2 \leqslant C\exp(CKT^{1/2}) \quad \text{and} \quad |v(t)|_{L^\infty}^2 \leqslant CK \tag{21}$$

Therefore, applying Gronwall's inequality, we deduce that

$$\int_0^T |u_t(t)|_{L^2}^2\,\mathrm{d}t + \sup_{0\leqslant t\leqslant T}|u(t)|_{H_0^1}^2 \leqslant C\exp[CKT^{1/2}\exp(CKT^{1/2})] \tag{22}$$

Next, if we differentiate (20) with respect to t, then we obtain

$$\sigma u_{tt} + \sigma v u_{tr} - \nu\left(u_{tr} + m\,\frac{u_t}{r}\right)_r r^m = \sigma_t(F - u_t - vu_r) + \sigma(F_t - v_t u_r)$$

Multiplying this by u_t, integrating over (a,b) and using (14), we derive

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b \frac{1}{2}\,\sigma u_t^2\,\mathrm{d}r + \nu\int_a^b\left(u_{tr}^2 + m\,\frac{u_t^2}{r^2}\right) r^m\,\mathrm{d}r\\ &\quad= \int_a^b (\sigma_t(F - vu_r) + 2\sigma v u_{tr} + \sigma(F_t - v_t u_r))u_t\,\mathrm{d}r\end{aligned} \tag{23}$$

Recall from (16) and (20) that

$$|\sqrt{\sigma}u_t(0)|_{L^2} \leqslant |\sigma(0)|_{L^\infty}^{1/2}|v(0)(u_0)_r - F(0)|_{L^2} + C\varepsilon^{-1}|u_0|_{H^2} \leqslant C$$

Hence integrating (23) over $(0,t)\subset(0,T)$ and using (19), (21) and (22), we have

$$\begin{aligned}&|\sqrt{\sigma}u_t(t)|_{L^2}^2 + C^{-1}\int_0^t |u_t|_{H_0^1}^2\,\mathrm{d}s\\
&\quad\leqslant C + C\int_0^t |\sigma_t|_{L^2}^2(|F|_{L^2}^2 + |v|_{H^1}^2|u_r|_{L^2}^2)\,\mathrm{d}s + C\int_0^t |\sigma|_{H^1}|v|_{H^1}^2|\sqrt{\sigma}u_t|_{L^2}^2\,\mathrm{d}s\\
&\qquad + C\int_0^t |\sigma|_{H^1}^{1/2}(|F_t|_{L^2} + |v_t|_{H^1}|u_r|_{L^2})|\sqrt{\sigma}u_t|_{L^2}\,\mathrm{d}s\\
&\quad\leqslant C\exp[CK^2T^{1/2}\exp(CKT^{1/2})] + CK\exp(CKT^{1/2})\int_0^t |\sqrt{\sigma}u_t|_{L^2}^2\,\mathrm{d}s\\
&\qquad + C\exp(CKT^{1/2})\int_0^t (|F_t|_{L^2} + |v_t|_{H^1}|u_r|_{L^2})|\sqrt{\sigma}u_t|_{L^2}\,\mathrm{d}s\end{aligned}$$

An easy variant of Gronwall's inequality shows that

$$\sup_{0\leqslant t\leqslant T} |\sqrt{\sigma}u_t|_{L^2}^2 + \int_0^T |u_t|_{H_0^1}^2 \,\mathrm{d}t$$

$$\leqslant C\left[1+\int_0^T (|F_t|_{L^2} + |v_t|_{H^1}|u_r|_{L^2})\,\mathrm{d}s\right]^2 \exp[CK^2T^{1/2}\exp(CKT^{1/2})]$$

Therefore, we conclude from (19) and (22) that

$$\sup_{0\leqslant t\leqslant T} |u_t(t)|_{L^2}^2 + \int_0^T |u_t(t)|_{H_0^1}^2 \,\mathrm{d}t \leqslant C\exp[CK^2T^{1/2}\exp(CKT^{1/2})] \tag{24}$$

Since Equation (20) is parabolic, the remaining regularity estimates for u can be easily derived from estimates (19), (22) and (24). This completes the proof of Lemma 2.3. □

3. *A PRIORI* ESTIMATES AND GLOBAL EXISTENCE

In this section, we derive various *a priori* estimates for radially symmetric solutions of the Navier–Stokes equations (1) and (2), which are independent of b and lower bounds of the initial density. As a corollary, we also prove a global existence result for problem (7)–(9).

Let (ρ, u) be a strong solution to problem (7)–(9) satisfying regularity (10), and let us define

$$\rho(t,\mathbf{x}) = \rho(t,|\mathbf{x}|) \quad \text{and} \quad \mathbf{u}(t,\mathbf{x}) = u(t,|\mathbf{x}|)\,\frac{\mathbf{x}}{|\mathbf{x}|}$$

Then a direct calculation shows that

$$\Delta\mathbf{u} = \nabla\,\mathrm{div}\,\mathbf{u} = \left(u_r + m\,\frac{u}{r}\right)_r \frac{\mathbf{x}}{r} \quad \text{with } r = |\mathbf{x}| \tag{25}$$

Thanks to this identity, we can easily show that $(\rho,\mathbf{u})$ is a radially symmetric strong solution to the original problem (1)–(3). From now on, we will derive some *a priori* estimates for $(\rho,\mathbf{u})$, independent of b and $\varepsilon = \inf \rho_0 > 0$.

To begin with, we recall the following elementary result (the conservation of mass and energy inequality).

Lemma 3.1

$$\sup_{0\leqslant t\leqslant T} \left(|\sqrt{\rho}\mathbf{u}(t)|_{L^2}^2 + |\rho(t)|_{L^1} + |p(t)|_{L^1}\right) + \int_0^T |\nabla\mathbf{u}|_{L^2}^2 \,\mathrm{d}t \leqslant C_0 \tag{26}$$

for some C_0 depending only on v, $|\rho_0|_{L^1\cap L^\gamma}$, $|\sqrt{\rho_0}\mathbf{u}_0|_{L^2}$ and $|\mathbf{f}|_{L^1(0,T;L^{2\gamma/\gamma-1})}$.

Throughout this paper, we denote by C_0, C_1, C_2 and C_3 generic positive constants depending only on v, a, T and the norms of the data, but independent of b and $\varepsilon = \inf \rho_0$.

Next, we prove the boundedness of the density, which is one of the most important estimates in this paper. Our proof is based on the *Lagrangian formulation* for problem

(2)–(3). This idea of Lagrangian approach originated from Kazhikhov and Shelukhin [13], and was adapted by Hoff [1] to obtain a upper bound on the radially symmetric density which is initially bounded away from zero and infinity.

Lemma 3.2

$$\sup_{0\leqslant t\leqslant T} |\rho(t)|_{L^\infty} \leqslant C_1 \tag{27}$$

for some C_1 depending only on a, n, T, $|\rho_0|_{L^\infty}$ and the parameters of C_0.

Proof
We introduce the *Lagrangian mass co-ordinates* (t, y), defined by

$$t = t \quad \text{and} \quad y = \int_a^r \rho(t, r) r^m \, \mathrm{d}r$$

Then since

$$\frac{\partial(t,y)}{\partial(t,r)} = \begin{pmatrix} 1 & 0 \\ -\rho u r^m & \rho r^m \end{pmatrix} \quad \text{and} \quad \frac{\partial(t,r)}{\partial(t,y)} = \begin{pmatrix} 1 & 0 \\ u & (\rho r^m)^{-1} \end{pmatrix}$$

problem (7)–(9) can be rewritten in Lagrangian co-ordinates as

$$\begin{cases} \rho_t + \rho^2 (r^m u)_y = 0 \\ r^{-m} u_t - v(\rho(r^m u)_y)_y + p_y = r^{-m} f(t,r) \\ r^n = a^n + n \displaystyle\int_0^y \frac{1}{\rho(t,z)} \, \mathrm{d}z \\ \rho(0,y) = \rho_0(y), \ u(0,y) = u_0(y), \ u(t,0) = u(t,Y) = 0 \end{cases} \tag{28}$$

where $0 \leqslant t \leqslant T$, $0 \leqslant y \leqslant Y = \int_a^b \rho_0(r) r^m \, \mathrm{d}r$ and $p = p(t,y) = A\rho(t,y)^\gamma$. Note also that $Y = \int_a^b \rho(t,r) r^m \, \mathrm{d}r$ for all $t \in [0,T]$ (conservation of mass).

Now we have only to show that $\rho(t,y) \leqslant C_1$ for $0 \leqslant t \leqslant T$ and $0 \leqslant y \leqslant Y$. To begin with, we observe from (28) that

$$v(\log \rho)_{ty} = v\left(\frac{\rho_t}{\rho}\right)_y = -v(\rho(r^m u)_y)_y = -r^{-m} u_t - p_y + r^{-m} f$$

$$= -(r^{-m} u)_t - p_y + r^{-m}\left(f - m\frac{u^2}{r}\right)$$

Thus, integrating over $(0,t) \times (0,y)$, we deduce that

$$v \log \frac{\rho(t,y)}{\rho(t,0)} = v \log \frac{\rho_0(y)}{\rho_0(0)} + \int_0^y ((r^{-m}u)(0,z) - (r^{-m}u)(t,z)) \, \mathrm{d}z$$

$$+ \int_0^t (p(s,0) - p(s,y)) \, \mathrm{d}s + \int_0^t \int_0^y r^{-m}\left(f - m\frac{u^2}{r}\right) \mathrm{d}z \, \mathrm{d}s$$

and

$$\frac{\rho(t,y)}{\rho(t,0)} = \frac{\rho_0(y)}{\rho_0(0)} \exp\left(\frac{1}{v}\int_0^y ((r^{-m}u)(0,z) - (r^{-m}u)(t,z))\,\mathrm{d}z\right)$$
$$\times \exp\left(\frac{1}{v}\int_0^t (p(s,0) - p(s,y))\,\mathrm{d}s\right) \exp\left(\frac{1}{v}\int_0^t\int_0^y r^{-m}\left(f - m\,\frac{u^2}{r}\right)\mathrm{d}z\,\mathrm{d}s\right)$$

From this identity, we derive a representation formula for ρ:

$$\rho(t,y) = P(t)Q(t,y)\exp\left(-\frac{1}{v}\int_0^t p(s,y)\,\mathrm{d}s\right) \tag{29}$$

where

$$P(t) = \frac{\rho(t,0)}{\rho_0(0)}\exp\left(\frac{1}{v}\int_0^t p(s,0)\,\mathrm{d}s\right)$$

and

$$Q(t,y) = \rho_0(y)\exp\left(\frac{1}{v}\int_0^y ((r^{-m}u)(0,z) - (r^{-m}u)(t,z))\,\mathrm{d}z\right)$$
$$\times \exp\left(\frac{1}{v}\int_0^t\int_0^y r^{-m}\left(f - m\,\frac{u^2}{r}\right)\mathrm{d}z\,\mathrm{d}s\right)$$

Moreover, ρ can be represented only in terms of $P(t)$ and $Q(t,y)$. Since $p = A\rho^\gamma$, it follows from (29) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(\frac{\gamma}{v}\int_0^t p(s,y)\,\mathrm{d}s\right) = \frac{A\gamma}{v}\,\rho(t,y)^\gamma \exp\left(\frac{\gamma}{v}\int_0^t p(s,y)\,\mathrm{d}s\right)$$
$$= \frac{A\gamma}{v}\,\{P(t)Q(t,y)\}^\gamma$$

and thus

$$\exp\left(\frac{1}{v}\int_0^t p(s,y)\,\mathrm{d}s\right) = \left[1 + \frac{A\gamma}{v}\int_0^t \{P(s)Q(s,y)\}^\gamma\,\mathrm{d}s\right]^{1/\gamma}$$

Therefore, substituting this into (29), we obtain

$$\rho(t,y) = \frac{P(t)Q(t,y)}{[1 + (A\gamma/v)\int_0^t \{P(s)Q(s,y)\}^\gamma\,\mathrm{d}s]^{1/\gamma}} \tag{30}$$

To prove the boundedness of ρ, it thus remains to estimate $P(t)$ and $Q(t,y)$. First, converting back into the Eulerian co-ordinates and using the previous lemma, we have

$$\int_0^Y r^{-m}|u|\,\mathrm{d}y = \int_a^b \rho|u|\,\mathrm{d}r \leqslant \frac{1}{a^m}\int_a^b \rho|u|r^m\,\mathrm{d}r$$
$$\leqslant \frac{C_0}{a^m}\int \rho|\mathbf{u}|\,\mathrm{d}x \leqslant C_1 \quad \text{for } 0\leqslant t\leqslant T$$

and

$$\int_0^T\int_0^Y r^{-m}\left(|f| + m\,\frac{|u|^2}{r}\right)\mathrm{d}y\,\mathrm{d}t = \int_0^T\int_a^b\left(\rho|f| + m\,\frac{\rho|u|^2}{r}\right)\mathrm{d}r\,\mathrm{d}t$$
$$\leqslant \frac{C_0}{a^m}\int_0^T\int\left(\rho|\mathbf{f}| + \frac{m}{a}\,\rho|\mathbf{u}|^2\right)\mathrm{d}x\,\mathrm{d}t \leqslant C_1$$

Hence it follows from the definition of $Q(t,y)$ that

$$\left|\log\frac{Q(t,y)}{\rho_0(y)}\right| \leqslant C_1$$

or equivalently

$$C_1^{-1}\rho_0(y)\leqslant Q(t,y)\leqslant C_1\rho_0(y) \tag{31}$$

Next, to estimate $P(t)$, observe that

$$\int_0^Y \frac{1}{\rho(t,y)}\,\mathrm{d}y = \int_a^b r^m\,\mathrm{d}r = \frac{b^n-a^n}{n}$$

Then we deduce from (30) and (31) that

$$\frac{b^n-a^n}{n}\,P(t) = \int_0^Y \frac{P(t)}{\rho(t,y)}\,\mathrm{d}y = \int_0^Y \frac{[1+(A\gamma/v)\int_0^t\{P(s)Q(s,y)\}^\gamma\,\mathrm{d}s]^{1/\gamma}}{Q(t,y)}\,\mathrm{d}y$$
$$\leqslant \int_0^Y \frac{1}{Q(t,y)}\,\mathrm{d}y + \left(\frac{A\gamma}{v}\right)^{1/\gamma}\int_0^Y\left[\int_0^t\left(P(s)\,\frac{Q(s,y)}{Q(t,y)}\right)^\gamma\mathrm{d}s\right]^{1/\gamma}\mathrm{d}y$$
$$\leqslant C_1\,\frac{b^n-a^n}{n} + C_1\left(\int_0^t P(s)^\gamma\,\mathrm{d}s\right)^{1/\gamma}$$

Therefore, dividing both sides by $(b^n-a^n)/n$, taking the γth power and then using Grownall's inequality, we deduce that

$$P(t)\leqslant C_1\exp\left(\frac{C_1}{(b^n-a^n)^\gamma}\right) \quad \text{for } 0\leqslant t\leqslant T \tag{32}$$

We may assume, without loss of generality, that $b \geqslant a+1$. Hence the estimate (32) is independent of b. Combining (30)–(32), we complete the proof of Lemma 3.2. □

To obtain further estimates, we make use of the following Sobolev inequalities for radially symmetric functions:

$$|\rho|_{L^\infty} \leqslant C_1 |\rho|_{H^1}, \quad |\mathbf{f}|_{L^\infty} \leqslant C_1 |\mathbf{f}|_{H^1} \quad \text{and} \quad |\mathbf{u}|_{L^\infty} \leqslant C_1 |\nabla \mathbf{u}|_{L^2} \tag{33}$$

The first and second inequalities follow immediately from the one-dimensional Sobolev inequality

$$\sup_{a \leqslant r \leqslant b} |\varphi(r)| \leqslant C_1 |\varphi|_{H^1(a,b)}$$

by taking $\varphi(r) = \rho(t,r)$ or $f(t,r)$. To prove the third one, assume that $a < r = |\mathbf{x}| < b$. Then since u satisfies the boundary condition $u(t,a) = 0$, we have

$$\begin{aligned}
|\mathbf{u}(t,\mathbf{x})||\mathbf{x}|^m = |u(t,r)|r^m &= \left| \int_a^r (u(t,s)s^m)_s \, \mathrm{d}s \right| \\
&= \left| \int_a^r \left(u_s + m \frac{u}{s} \right) s^m \, \mathrm{d}s \right| \\
&\leqslant \left[\int_a^r \left(u_s + m \frac{u}{s} \right)^2 s^m \, \mathrm{d}s \right]^{1/2} \left(\frac{r^{m+1}}{m+1} \right)^{1/2} \\
&= C_1 |\mathbf{x}|^{(m+1)/2} |\operatorname{div} \mathbf{u}(t)|_{L^2}
\end{aligned}$$

Thus it follows from identity (25) that

$$|\mathbf{u}(t,\mathbf{x})| \leqslant C_1 |\operatorname{div} \mathbf{u}(t)|_{L^2} = C_1 |\nabla \mathbf{u}(t)|_{L^2}$$ □

To prove the following lemma, we also need to use the regularizing property of the *effective viscous flux* $G = v \operatorname{div} \mathbf{u} - p$.

Lemma 3.3

$$\sup_{0 \leqslant t \leqslant T} (|\mathbf{u}(t)|_{L^\infty} + |\mathbf{u}(t)|_{D_0^1}) + \int_0^T \left(|\sqrt{\rho} \mathbf{u}_t(t)|_{L^2}^2 + |G(t)|_{H^1}^2 \right) \mathrm{d}t \leqslant C_2 \tag{34}$$

for some C_2 depending only on $|\rho_0|_{H^1}$, $|\mathbf{u}_0|_{D_0^1}$ and the parameters of C_1.

Proof

In view of the continuity equation (2) and identity (25), the momentum equation (1) can be rewritten as

$$\rho \mathbf{u}_t + \rho \mathbf{u} \cdot \nabla \mathbf{u} - v \nabla \operatorname{div} \mathbf{u} + \nabla p = \rho \mathbf{f}$$

Multiplying this by $\mathbf{u}_t$, integrating (by parts) over Ω and using Young's inequality, we have

$$\frac{1}{2}\int \rho|\mathbf{u}_t|^2\,\mathrm{d}x + \frac{\mathrm{d}}{\mathrm{d}t}\int \frac{\nu}{2}(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x \leqslant \int \rho|\mathbf{f}|^2\,\mathrm{d}x + \int \rho|\mathbf{u}|^2|\nabla\mathbf{u}|^2\,\mathrm{d}x + \int p\operatorname{div}\mathbf{u}_t\,\mathrm{d}x \tag{35}$$

Using the continuity equation (2), we obtain,

$$\begin{aligned}\int p\operatorname{div}\mathbf{u}_t\,\mathrm{d}x &= \frac{\mathrm{d}}{\mathrm{d}t}\int p\operatorname{div}\mathbf{u}\,\mathrm{d}x + \int(\operatorname{div}(p\mathbf{u}) + (\gamma-1)p\operatorname{div}\mathbf{u})\operatorname{div}\mathbf{u}\,\mathrm{d}x\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int p\operatorname{div}\mathbf{u}\,\mathrm{d}x - \int p\,\mathbf{u}\cdot\nabla\operatorname{div}\mathbf{u}\,\mathrm{d}x + (\gamma-1)\int p(\operatorname{div}\mathbf{u})^2\mathrm{d}x\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int p\operatorname{div}\mathbf{u}\,\mathrm{d}x + \frac{4\gamma-3}{2\nu}\int p^2\operatorname{div}\mathbf{u}\,\mathrm{d}x\\ &\quad + \frac{\gamma-1}{\nu^2}\int p(G^2-p^2)\,\mathrm{d}x - \frac{1}{\nu}\int p\,\mathbf{u}\cdot\nabla G\,\mathrm{d}x\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int p\operatorname{div}\mathbf{u}\,\mathrm{d}x - \frac{\mathrm{d}}{\mathrm{d}t}\int \frac{4\gamma-3}{2\nu(2\gamma-1)}\,p^2\,\mathrm{d}x\\ &\quad + \frac{\gamma-1}{\nu^2}\int p(G^2-p^2)\,\mathrm{d}x - \frac{1}{\nu}\int p\mathbf{u}\cdot\nabla G\,\mathrm{d}x\end{aligned}$$

Substituting this identity into (35), integrating over $(0,t)$ and using the obvious inequality

$$\nu\,\frac{2\gamma-2}{4\gamma-3}(\operatorname{div}\mathbf{u})^2 \leqslant \nu(\operatorname{div}\mathbf{u})^2 - 2p(\operatorname{div}\mathbf{u}) + \frac{4\gamma-3}{\nu(2\gamma-1)}\,p^2$$

we derive

$$\int_0^t\int \rho|\mathbf{u}_t|^2\,\mathrm{d}x\,\mathrm{d}s + \int|\operatorname{div}\mathbf{u}(t)|^2\,\mathrm{d}x \leqslant C_2 + C_2\int_0^t\int(\rho|\mathbf{u}|^2|\nabla\mathbf{u}|^2 + pG^2 + p|\mathbf{u}||\nabla G|)\,\mathrm{d}x\,\mathrm{d}s \tag{36}$$

We estimate each term of the right-hand side of (36). By virtue of the estimates (26), (27) and (33), we have

$$\int_0^t\int \rho|\mathbf{u}|^2|\nabla\mathbf{u}|^2\,\mathrm{d}x\,\mathrm{d}s \leqslant \int_0^t |\rho|_{L^\infty}|\mathbf{u}|_{L^\infty}^2|\nabla\mathbf{u}|_{L^2}^2\,\mathrm{d}s \leqslant C_1\int_0^t|\nabla\mathbf{u}|_{L^2}^4\,\mathrm{d}s$$

and

$$\int_0^t\int pG^2\,\mathrm{d}x\,\mathrm{d}s \leqslant C_1\int_0^t\int p(|\nabla\mathbf{u}|^2 + p^2)\,\mathrm{d}x\,\mathrm{d}s \leqslant C_1$$

Using the identity

$$\nabla G = \rho \mathbf{u}_t + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \rho \mathbf{f} \tag{37}$$

together with (26) and (27), we also have

$$\begin{aligned} C_2 \int_0^t \int p|\mathbf{u}||\nabla G| \, dx \, ds &\leqslant C_2 \int_0^t |\rho|_{L^\infty}^{\gamma-1/2} |\sqrt{\rho}\mathbf{u}|_{L^2} |\nabla G|_{L^2} \, ds \\ &\leqslant C_2 \int_0^t (|\rho \mathbf{u}_t|_{L^2} + |\rho \mathbf{u} \cdot \nabla \mathbf{u}|_{L^2} + |\rho \mathbf{f}|_{L^2}) \, ds \\ &\leqslant C_2 + \frac{1}{2} \int_0^t |\sqrt{\rho}\mathbf{u}_t|_{L^2}^2 \, ds \end{aligned}$$

Substituting these estimates into (36) and recalling that $|\mathrm{div}\, \mathbf{u}|_{L^2} = |\nabla \mathbf{u}|_{L^2}$, we finally obtain,

$$\int_0^t |\sqrt{\rho}\mathbf{u}_t|_{L^2}^2 \, ds + |\nabla \mathbf{u}(t)|_{L^2}^2 \leqslant C_2 + C_2 \int_0^t |\nabla \mathbf{u}|_{L^2}^4 \, ds$$

Since $\int_0^T |\nabla \mathbf{u}|_{L^2}^2 \, ds \leqslant C_0$, it follows from Gronwall's lemma that

$$\int_0^T |\sqrt{\rho}\mathbf{u}_t|_{L^2}^2 \, ds + \sup_{0 \leqslant t \leqslant T} |\nabla \mathbf{u}|_{L^2}^2 \leqslant C_2$$

Then utilizing (33) and (37), we complete the proof of Lemma 3.3. □

We are now ready to prove

Lemma 3.4

$$\sup_{0 \leqslant t \leqslant T} |\nabla \rho(t)|_{L^2} + \int_0^T (|\nabla \mathbf{u}(t)|_{L^\infty}^2 + |\mathbf{u}(t)|_{D^2}^2) \, dt \leqslant C_2 \tag{38}$$

Proof
First, since G is a radially symmetric scalar function, we can use Sobolev inequality (33) and the estimate (34) to obtain

$$\int_0^T |G|_{L^\infty}^2 \, dt \leqslant C_1 \int_0^T |G|_{H^1}^2 \, dt \leqslant C_2 \tag{39}$$

A simple calculation shows that

$$\begin{aligned} |\nabla \mathbf{u}|^2 = u_r^2 + m \frac{u^2}{r^2} &\leqslant 2 \left(u_r + m \frac{u}{r} \right)^2 + m(2m+1) \frac{u^2}{r^2} \\ &\leqslant 2(\mathrm{div}\, \mathbf{u})^2 + m(2m+1) \frac{u^2}{a^2} \leqslant C_1 (G^2 + p^2 + |\mathbf{u}|^2) \end{aligned}$$

Hence it follows from estimates (27), (34) and (39) that

$$\int_0^T |\nabla \mathbf{u}|_{L^\infty}^2 \,\mathrm{d}t \leqslant C_1 \int_0^T (|G|_{L^\infty}^2 + |p|_{L^\infty}^2 + |\mathbf{u}|_{L^\infty}^2)\,\mathrm{d}t \leqslant C_2 \tag{40}$$

To obtain the estimate for $\nabla\rho$, we differentiate the continuity equation

$$\rho_t + \mathbf{u}\cdot\nabla\rho + \rho\,\mathrm{div}\,\mathbf{u} = 0 \tag{41}$$

with respect to x_j and obtain

$$(\rho_{x_j})_t + \mathbf{u}_{x_j}\cdot\nabla\rho + \mathbf{u}\cdot\nabla\rho_{x_j} + \rho_{x_j}\,\mathrm{div}\,\mathbf{u} + \rho\,\mathrm{div}\,\mathbf{u}_{x_j} = 0$$

Then multiplying this equation by ρ_{x_j}, integrating over Ω and summing over j, we deduce that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int |\nabla\rho|^2\,\mathrm{d}x &\leqslant C_2\int |\nabla\mathbf{u}||\nabla\rho|^2 + \rho|\nabla\rho||\nabla\,\mathrm{div}\,\mathbf{u}|\,\mathrm{d}x\\ &\leqslant C_2\int |\nabla G|^2\,\mathrm{d}x + C_2(|\nabla\mathbf{u}|_{L^\infty}+1)\int|\nabla\rho|^2\,\mathrm{d}x\end{aligned}$$

Thanks to estimates (34) and (40), we thus obtain,

$$\sup_{0\leqslant t\leqslant T} |\nabla\rho|_{L^2} \leqslant C_2$$

Finally, in view of the well-known elliptic regularity estimate (see Reference [6] for instance) and identity (25), we obtain,

$$\begin{aligned}\int_0^T |\nabla^2\mathbf{u}|_{L^2}^2\,\mathrm{d}t &\leqslant C_0\int_0^T (|\Delta\mathbf{u}|_{L^2}^2 + |\nabla\mathbf{u}|_{L^2}^2)\,\mathrm{d}t \leqslant C_2\int_0^T (|\nabla\,\mathrm{div}\,\mathbf{u}|_{L^2}^2 + 1)\,\mathrm{d}t\\ &\leqslant C_2\int_0^T (|\nabla G|_{L^2}^2 + |\nabla p|_{L^2}^2 + 1)\,\mathrm{d}t \leqslant C_2\end{aligned}$$

This completes the proof of Lemma 3.4. □

The following result is the key estimate to prove the existence of the radially symmetric strong solutions to problem (1)–(3).

Lemma 3.5

$$\sup_{0\leqslant t\leqslant T} (|\sqrt{\rho}\,\mathbf{u}_t(t)|_{L^2} + |\mathbf{u}(t)|_{D^2}) + \int_0^T (|\mathbf{u}_t(t)|_{D_0^1}^2 + |G(t)|_{H^2}^2)\,\mathrm{d}t \leqslant C_3 \tag{42}$$

for some C_3 depending only on $\mathcal{C}(\rho_0, \mathbf{u}_0)$ as well as the parameters of C_2. Here the functional $\mathcal{C}$ is defined by

$$\mathcal{C}(\rho_0,\mathbf{u}_0) = \int \rho_0^{-1}|\mu\Delta\mathbf{u}_0 + (\lambda+\mu)\nabla\,\mathrm{div}\,\mathbf{u}_0 - \nabla(A\rho_0^\gamma)|^2\,\mathrm{d}x \tag{43}$$

Proof
To begin with, rewrite the momentum equation (1) as

$$\rho \mathbf{u}_t + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = \rho \mathbf{f} \tag{44}$$

If we differentiate this with respect to time, then

$$\rho \mathbf{u}_{tt} + \rho \mathbf{u} \cdot \nabla \mathbf{u}_t - \nu \Delta \mathbf{u}_t + \nabla p_t = (\rho \mathbf{f})_t - \rho_t(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) - \rho \mathbf{u}_t \cdot \nabla \mathbf{u}$$

and thus by virtue of the continuity equation, we obtain

$$\begin{aligned} &\tfrac{1}{2}(\rho|\mathbf{u}_t|^2)_t + \tfrac{1}{2}\operatorname{div}(\rho \mathbf{u}|\mathbf{u}_t|^2) - \nu \Delta \mathbf{u}_t \cdot \mathbf{u}_t + \nabla p_t \cdot \mathbf{u}_t \\ &\quad = \operatorname{div}(\rho \mathbf{u})(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} - \mathbf{f}) \cdot \mathbf{u}_t - \rho(\mathbf{u}_t \cdot \nabla \mathbf{u}) \cdot \mathbf{u}_t + \rho \mathbf{f}_t \cdot \mathbf{u}_t \end{aligned}$$

Hence integrating over Ω, we obtain

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\int \frac{1}{2}\rho|\mathbf{u}_t|^2\,\mathrm{d}x + \nu\int |\nabla \mathbf{u}_t|^2\,\mathrm{d}x - \int p_t \operatorname{div}\mathbf{u}_t\,\mathrm{d}x \\ &\quad = \int \rho \mathbf{u} \cdot \nabla((\mathbf{f} - \mathbf{u}_t - \mathbf{u} \cdot \nabla \mathbf{u}) \cdot \mathbf{u}_t) - \rho(\mathbf{u}_t \cdot \nabla \mathbf{u}) \cdot \mathbf{u}_t + \rho \mathbf{f}_t \cdot \mathbf{u}_t\,\mathrm{d}x \end{aligned} \tag{45}$$

This identity can be proved rigorously by means of a standard regularization technique. For a simple proof, see Reference [6]. Using the continuity equation again, we have,

$$\begin{aligned} -\int p_t \operatorname{div}\mathbf{u}_t\,\mathrm{d}x &= \int (\nabla p \cdot \mathbf{u} + \gamma p \operatorname{div}\mathbf{u}) \operatorname{div}\mathbf{u}_t\,\mathrm{d}x \\ &= \int \nabla p \cdot (\mathbf{u} \operatorname{div}\mathbf{u}_t)\,\mathrm{d}x + \frac{\mathrm{d}}{\mathrm{d}t}\int \frac{\gamma}{2} p(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x - \frac{\gamma}{2}\int p_t(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\int \frac{\gamma}{2} p(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x + \int \nabla p \cdot (\mathbf{u} \operatorname{div}\mathbf{u}_t)\,\mathrm{d}x \\ &\quad + \frac{\gamma}{2}\int -p\mathbf{u} \cdot \nabla(\operatorname{div}\mathbf{u})^2 + (\gamma - 1)p(\operatorname{div}\mathbf{u})^3\,\mathrm{d}x \end{aligned}$$

Substituting this identity into (45), we deduce that

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\int \frac{1}{2}\rho|\mathbf{u}_t|^2 + \frac{\gamma}{2}p(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x + \nu\int |\nabla \mathbf{u}_t|^2\,\mathrm{d}x \\ &\quad \leqslant \int 2\rho|\mathbf{u}||\mathbf{u}_t||\nabla \mathbf{u}_t| + \rho|\mathbf{u}||\mathbf{u}_t||\nabla \mathbf{u}|^2 + \rho|\mathbf{u}|^2|\mathbf{u}_t||\nabla^2 \mathbf{u}| + \rho|\mathbf{u}|^2|\nabla \mathbf{u}||\nabla \mathbf{u}_t| \\ &\qquad + \rho|\mathbf{u}_t|^2|\nabla \mathbf{u}| + |\nabla p||\mathbf{u}||\nabla \mathbf{u}_t| + \gamma p|\mathbf{u}||\nabla \mathbf{u}||\nabla^2 \mathbf{u}| + \gamma^2 p|\nabla \mathbf{u}|^3 \\ &\qquad + \rho|\mathbf{u}||\mathbf{u}_t||\nabla \mathbf{f}| + \rho|\mathbf{u}||\mathbf{f}||\nabla \mathbf{u}_t| + \rho|\mathbf{u}_t||\mathbf{f}_t|\,\mathrm{d}x \end{aligned}$$

Using the previous lemmas and Young's inequality, we can easily show that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \rho|\mathbf{u}_t|^2 + \gamma p(\operatorname{div}\mathbf{u})^2\,\mathrm{d}x + \int |\nabla \mathbf{u}_t|^2\,\mathrm{d}x$$
$$\leqslant C_2(1 + |\nabla \mathbf{u}|_{L^\infty}^2 + |\nabla^2 \mathbf{u}|_{L^2}^2 + |\mathbf{f}_t|_{L^2}^2 + |\nabla \mathbf{f}|_{L^2}^2) + C_2|\nabla \mathbf{u}|_{L^\infty}\int \frac{1}{2}\rho|\mathbf{u}_t|^2\,\mathrm{d}x$$

Then integrating over $(\tau, t)\subset\subset(0,T)$ and using the lemmas again, we obtain

$$|\sqrt{\rho}\mathbf{u}_t(t)|_{L^2}^2 + \int_\tau^t |\nabla \mathbf{u}_t|_{L^2}^2\,\mathrm{d}s \leqslant C_2 + |\sqrt{\rho}\mathbf{u}_t(\tau)|_{L^2}^2 + C_2\int_0^t |\nabla \mathbf{u}|_{L^\infty}|\sqrt{\rho}\mathbf{u}_t|_{L^2}^2\,\mathrm{d}s \tag{46}$$

On the other hand, we can deduce from the momentum equation (44) that

$$|\sqrt{\rho}\mathbf{u}_t(\tau)|_{L^2}^2 \leqslant |\sqrt{\rho}(\mathbf{u}\cdot\nabla\mathbf{u} - \mathbf{f})(\tau)|_{L^2}^2 + |(\sqrt{\rho})^{-1}(\nu\Delta\mathbf{u} - \nabla p)(\tau)|_{L^2}^2$$
$$\rightarrow |\sqrt{\rho_0}(\mathbf{u}_0\cdot\nabla\mathbf{u}_0 - \mathbf{f}(0))|_{L^2}^2 + \mathcal{C}(\rho_0,\mathbf{u}_0) \leqslant C_3 \quad \text{as } \tau\rightarrow 0$$

where $\mathcal{C}(\rho_0,\mathbf{u}_0)$ was defined in (43). Therefore, letting $\tau\rightarrow +0$ in (46), we conclude that

$$|\sqrt{\rho}\mathbf{u}_t(t)|_{L^2}^2 + \int_0^t |\nabla \mathbf{u}_t|_{L^2}^2\,\mathrm{d}s \leqslant C_3 + C_3\int_0^t |\nabla \mathbf{u}|_{L^\infty}|\sqrt{\rho}\mathbf{u}_t|_{L^2}^2\,\mathrm{d}s$$

Now since $\int_0^T |\nabla \mathbf{u}|_{L^\infty}^2\,\mathrm{d}t \leqslant C_2$, we can apply Gronwall's lemma to obtain

$$\sup_{0\leqslant t\leqslant T}|\sqrt{\rho}\mathbf{u}_t(t)|_{L^2}^2 + \int_0^T |\mathbf{u}_t(t)|_{D_0^1}^2\,\mathrm{d}s \leqslant C_3$$

The remaining estimates for $|\mathbf{u}|_{D^2}$ and $|\nabla^2 G|_{L^2}$ can be easily derived from this estimate and the previous lemmas by using elliptic regularity estimates on the momentum equation. This completes the proof of the lemma. □

Now we can prove the final lemma.

Lemma 3.6

$$\sup_{0\leqslant t\leqslant T}(|\rho(t)|_{H^2} + |\rho_t(t)|_{H^1}) + \int_0^T |\mathbf{u}(t)|_{D^3}^2\,\mathrm{d}t \leqslant C_4(\varepsilon) \tag{47}$$

for some $C_4(\varepsilon)$ depending only on ε and $|\rho_0|_{H^2}$ as well as the parameters of C_3. If $\gamma\geqslant 2$, then $C_4(\varepsilon)$ is independent of ε.

Proof

If we take the differential operator ∇^2 to the continuity equation (41), multiply by $\nabla^2\rho$ and then integrate over Ω, we get,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int |\nabla^2\rho|^2\,\mathrm{d}x \leqslant C_0\int |\nabla\mathbf{u}||\nabla^2\rho|^2 + |\nabla^2\mathbf{u}||\nabla\rho||\nabla^2\rho| + \rho|\nabla^2\operatorname{div}\mathbf{u}||\nabla^2\rho|\,\mathrm{d}x$$

Using the previous lemmas and Sobolev inequality (33), we have,

$$\frac{\mathrm{d}}{\mathrm{d}t}|\nabla^2\rho|_{L^2}^2 \leqslant C_1[|\nabla\mathbf{u}|_{H^1}|\nabla\rho|_{H^1}^2 + (|\nabla^2 G|_{L^2} + |\nabla^2 p|_{L^2})|\nabla^2\rho|_{L^2}]$$

$$\leqslant C_3(|\rho^{\gamma-2}|_{L^\infty}+1)|\nabla\rho|_{H^1}^2 + C_3|G|_{H^2}^2$$

and thus

$$|\rho(t)|_{H^2}^2 \leqslant C_3(1+|\nabla^2\rho_0|_{L^2}^2) + C_3\int_0^t (|\rho^{\gamma-2}|_{L^\infty}+1)|\rho|_{H^2}^2\,\mathrm{d}s$$

Note that the continuity equation (41) yields

$$\inf\rho(t) \geqslant (\inf\rho_0)\exp\left(-\int_0^t |\mathrm{div}\,\mathbf{u}|_{L^\infty}\,\mathrm{d}s\right) \geqslant \varepsilon\mathrm{e}^{-C_3 t}$$

Then we can easily show that $|\rho^{\gamma-2}|_{L^\infty} \leqslant C_4(\varepsilon)$. Therefore, in view of Gronwall's inequality, we get the desired estimate for ρ. The estimate for ρ_t follows from this estimate by using the continuity equation. Finally, using an elliptic regularity estimate, we can obtain the estimate for $\mathbf{u}$. This completes the proof of the lemma. □

Combining Proposition 2.1 and all the lemmas in this section, we conclude that the solutions obtained in Proposition 2.1 exist globally in time.

Theorem 3.7
If the data (ρ_0, u_0, f) satisfy the hypotheses of Proposition 2.1, then there exists a unique global strong solution (ρ, u) to the initial boundary value problem (7)–(9), which satisfies (10) for each $T>0$.

4. GLOBAL EXISTENCE AND REGULARITY OF WEAK SOLUTIONS

Thanks to Lemmas 3.1 and 3.2, we can adapt the arguments of Jiang and Zhang [2] to prove the global existence of radially symmetric weak solutions. Hence we may state the following theorem without a proof.

Theorem 4.1
Let $(\rho_0, \mathbf{u}_0, \mathbf{f})$ be a given radially symmetric data satisfying the regularity

$$0 \leqslant \rho_0 \in L^1\cap L^\infty, \quad \mathbf{u}_0 \in L^2 + L^\infty \quad \text{and} \quad \mathbf{f} \in L^1_{\mathrm{loc}}(0,\infty; L^{2\gamma/\gamma-1}) \tag{48}$$

Then there exists a radially symmetric weak solution $(\rho, \mathbf{u})$ to problem (1)–(3) satisfying the regularity

$$\rho \in L^\infty_{\mathrm{loc}}(0,\infty; L^1\cap L^\infty),\ \ \sqrt{\rho}\mathbf{u} \in L^\infty_{\mathrm{loc}}(0,\infty; L^2),\ \ \mathbf{u}\in L^2_{\mathrm{loc}}(0,\infty; D_0^1)$$

Using Lemmas 3.1–3.4, we can prove the following regularity result on radially symmetric weak solutions.

Theorem 4.2
Let $(\rho_0, \mathbf{u}_0, \mathbf{f})$ be a given radially symmetric data satisfying the regularity

$$0 \leqslant \rho_0 \in L^1 \cap H^1, \quad \mathbf{u}_0 \in D_0^1 \quad \text{and} \quad \mathbf{f} \in L^2_{\text{loc}}(0,\infty; L^{2\gamma/\gamma-1}) \tag{49}$$

Then there exists a radially symmetric weak solution $(\rho, \mathbf{u})$ to the initial boundary value problem (1)–(3) such that

$$\begin{aligned} &\rho \in C([0,\infty); L^1 \cap H^1), \quad \rho_t \in L^\infty_{\text{loc}}(0,\infty; L^2) \\ &\mathbf{u} \in L^\infty_{\text{loc}}(0,\infty; D_0^1) \cap L^2_{\text{loc}}(0,\infty; D^2), \quad (\rho\mathbf{u})_t \in L^2_{\text{loc}}(0,\infty; L^2) \end{aligned} \tag{50}$$

Proof
We may consider only the finite case $b<\infty$, since the estimates derived below are independent of b. The results for the remaining case can be obtained by passing to the limit $b \to \infty$.

Regularizing the data, we construct a sequence $(\rho_0^\varepsilon, u_0^\varepsilon, f^\varepsilon)$ of smooth radial functions such that for each $T>0$,

$$0 < \varepsilon \leqslant \rho_0^\varepsilon, \quad \rho_0^\varepsilon \in H^2(a,b)$$
$$u_0^\varepsilon \in H_0^1 \cap H^2(a,b), \quad (\rho_0^\varepsilon, u_0^\varepsilon) \to (\rho_0, u_0) \text{ in } H^1(a,b)$$
$$f^\varepsilon \in H^1((0,T)\times(a,b)), \quad f^\varepsilon \to f \text{ in } L^2(0,T; L^{2\gamma/\gamma-1}(a,b))$$
$$\text{and} \quad |\rho_0^\varepsilon|_{L^1(\Omega)\cap H^1(\Omega)} + |\mathbf{u}_0^\varepsilon|_{D_0^1(\Omega)} + \int_0^T |\mathbf{f}^\varepsilon|^2_{L^{2\gamma/\gamma-1}(\Omega)}\, \mathrm{d}t \leqslant C_2(T)$$

where

$$\rho_0^\varepsilon(\mathbf{x}) = \rho_0^\varepsilon(|\mathbf{x}|), \; \mathbf{u}_0^\varepsilon(\mathbf{x}) = u_0(|\mathbf{x}|)\frac{\mathbf{x}}{|\mathbf{x}|} \quad \text{and} \quad \mathbf{f}^\varepsilon(t,\mathbf{x}) = f^\varepsilon(t,|\mathbf{x}|)\frac{\mathbf{x}}{|\mathbf{x}|}$$

for $\mathbf{x} \in \Omega$. Throughout the proof, we denote by C_2 (and $C_2(T)$) a generic positive constant depending only on a and the norms of the data (also on T), but independent of b and ε.

Next, let $(\rho^\varepsilon, u^\varepsilon)$ be a global strong solution in $(0,\infty)\times(a,b)$ to the initial boundary value problem (7)–(9) with the data $(\rho_0^\varepsilon, u_0^\varepsilon, f^\varepsilon)$. Define

$$\rho^\varepsilon(t,\mathbf{x}) = \rho^\varepsilon(t,|\mathbf{x}|) \quad \text{and} \quad \mathbf{u}^\varepsilon(t,\mathbf{x}) = u^\varepsilon(t,|\mathbf{x}|)\frac{\mathbf{x}}{|\mathbf{x}|}$$

Then $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ is a global strong solution to the initial boundary value problem (1)–(3) with the data $(\rho_0^\varepsilon, \mathbf{u}_0^\varepsilon, \mathbf{f}^\varepsilon)$. Moreover, in view of Lemmas 3.1–3.4, we find that the solution satisfies the following uniform estimate: for each $0<T<\infty$,

$$\sup_{0\leqslant t\leqslant T}(|\rho^\varepsilon|_{L^1\cap H^1} + |\rho_t^\varepsilon|_{L^2} + |\mathbf{u}^\varepsilon|_{D_0^1}) + \int_0^T (|\mathbf{u}^\varepsilon|^2_{D^2} + |(\rho^\varepsilon\mathbf{u}^\varepsilon)_t|^2_{L^2})\, \mathrm{d}t \leqslant C_2(T) \tag{51}$$

Therefore, we may conclude that a subsequence of approximate solutions $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ converges, in a weak or weak-* sense, to a radially symmetric weak solution $(\rho, \mathbf{u})$ satisfying regularity (50) except the continuity of ρ. Hence the proof of the theorem will be completed if we prove the following regularity result.

Lemma 4.3
Let $\mathbf{u}$ be a radially symmetric vector field with the regularity

$$\mathbf{u} \in L^{\infty}_{\text{loc}}(0,\infty; D^1_0) \cap L^2_{\text{loc}}(0,\infty; D^2)$$

If $\rho \in L^{\infty}_{\text{loc}}(0,\infty; L^1 \cap H^1)$ is a weak solution of the linear transport equation

$$\rho_t + \operatorname{div}(\rho\mathbf{u}) = 0 \quad \text{in } (0,\infty) \times \Omega \tag{52}$$

then

$$\rho \in C([0,\infty); L^1 \cap H^1) \quad \text{and} \quad \rho_t \in L^{\infty}_{\text{loc}}(0,\infty; L^2)$$

Proof
The second assertion follows easily from Equation (52), since $\rho \in L^{\infty}_{\text{loc}}(0,\infty; L^{\infty})$ and $\mathbf{u} \in L^{\infty}_{\text{loc}}(0, \infty; L^{\infty})$ thanks to Sobolev inequality (33). Hence the well-known embedding result shows that $\rho \in C([0,\infty); L^2)$. Then we deduce that $\rho \in C([0,\infty); H^1 - \textit{weak})$, that is, ρ is weakly continuous with values in H^1. For a proof, we refer to Chapter 3 in Reference [14]. Moreover, it follows from a result of Diperna and Lions [15] that $\rho \in C([0,\infty); L^1)$.

It thus remains to show that $\nabla\rho \in C([0,\infty); L^2)$. Note that the linear transport equation (52) is invariant under the translation and reflection in time. Hence it suffice to show that

$$\lim_{t\to+0} |\nabla\rho(t) - \nabla\rho(0)|_{L^2} = 0 \tag{53}$$

To show this, we differentiate (52) with respect to x_j, multiply by ρ_{x_j} and integrate over Ω. Then summing over j, we obtain

$$\frac{d}{dt}\int |\nabla\rho|^2 \, dx \leqslant C_2 \int |\nabla\mathbf{u}||\nabla\rho|^2 + \rho|\nabla\rho||\nabla \operatorname{div} \mathbf{u}| \, dx$$

In view of Sobolev inequality (33) and the regularity of ρ, we deduce

$$\frac{d}{dt}\int |\nabla\rho|^2 \, dx \leqslant C_2 |\nabla\mathbf{u}|_{H^1} |\rho|^2_{H^1} \leqslant C_2 |\nabla\mathbf{u}|_{H^1}$$

and thus

$$|\nabla\rho(t)|^2_{L^2} \leqslant |\nabla\rho(0)|_{L^2} + C_2 \int_0^t |\nabla\mathbf{u}(s)|_{H^1} \, ds \tag{54}$$

This inequality can be proved rigorously by using a standard regularization technique. Now letting $t \to +0$ in inequality (54), we deduce that

$$\limsup_{t\to+0} |\nabla\rho(t)|^2_{L^2} \leqslant |\nabla\rho(0)|_{L^2} \tag{55}$$

The strong convergence (53) follows from (55) and the weak continuity of ρ in H^1. This completes the proof of Lemma 4.3 (and thus Theorem 4.2). □

The continuity of the momentum $\rho\mathbf{u}$ follows immediately from regularity (50). But the continuity of $\mathbf{u}$ requires some additional assumption. For instance, assume that in addition to (49), $\rho_0 \geqslant \varepsilon$ in Ω for some constant $\varepsilon > 0$. Then it follows from the continuity equation and Sobolev inequality (33) that

$$\inf \rho(t) \geqslant (\inf \rho_0) \exp\left(-\int_0^t |\operatorname{div} \mathbf{u}|_{L^\infty} \, \mathrm{d}s\right) \geqslant \varepsilon \mathrm{e}^{-C_2\sqrt{t}}$$

Hence we can easily show that $\mathbf{u}_t \in L^2_{\text{loc}}(0,\infty; L^2)$ and thus $\mathbf{u} \in C([0,\infty); L^2)$. Moreover, we can prove the following uniqueness result.

Theorem 4.4
Let $(\rho, \mathbf{u})$ and $(\bar{\rho}, \bar{\mathbf{u}})$ be radially symmetric solutions to problem (1)–(3) satisfying regularity (50). If, in addition, $\rho_0 \geqslant \varepsilon$ in Ω for some constant $\varepsilon > 0$ and $f \in L^2_{\text{loc}}(0,\infty; L^2)$, then

$$\rho = \bar{\rho} \quad \text{and} \quad \mathbf{u} = \bar{\mathbf{u}}$$

Proof
Using the momentum equations, we first obtain,

$$\begin{aligned} &\bar{\rho}(\bar{\mathbf{u}} - \mathbf{u})_t + \bar{\rho}\,\bar{\mathbf{u}} \cdot \nabla(\bar{\mathbf{u}} - \mathbf{u}) - \mu\Delta(\bar{\mathbf{u}} - \mathbf{u}) - (\lambda + \mu)\nabla \operatorname{div}(\bar{\mathbf{u}} - \mathbf{u}) \\ &\quad = (\bar{\rho} - \rho)(\mathbf{f} - \mathbf{u}_t - \mathbf{u} \cdot \nabla \mathbf{u}) - \bar{\rho}(\bar{\mathbf{u}} - \mathbf{u}) \cdot \nabla \mathbf{u} - \nabla(\bar{p} - p) \\ &\quad = (\bar{\rho} - \rho)\mathbf{h} - \bar{\rho}(\bar{\mathbf{u}} - \mathbf{u}) \cdot \nabla \mathbf{u} - \nabla(\bar{p} - p) \end{aligned}$$

where $\mathbf{h} = \mathbf{f} - \mathbf{u}_t - \mathbf{u} \cdot \nabla \mathbf{u} \in L^2_{\text{loc}}(0,\infty; L^2)$. Then multiplying this identity by $(\bar{\mathbf{u}} - \mathbf{u})$ and integrating over Ω, we obtain

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t}\int \frac{1}{2}\bar{\rho}|\bar{\mathbf{u}} - \mathbf{u}|^2 \, \mathrm{d}x + \int \mu|\nabla(\bar{\mathbf{u}} - \mathbf{u})|^2 + (\lambda + \mu)|\operatorname{div}(\bar{\mathbf{u}} - \mathbf{u})|^2 \, \mathrm{d}x \\ &\quad \leqslant \int |\bar{\rho} - \rho||\mathbf{h}||\bar{\mathbf{u}} - \mathbf{u}| + \bar{\rho}|\bar{\mathbf{u}} - \mathbf{u}|^2|\nabla \mathbf{u}| + (\bar{p} - p)\operatorname{div}(\bar{\mathbf{u}} - \mathbf{u}) \, \mathrm{d}x \end{aligned}$$

From Sobolev inequality (33), it follows that,

$$\begin{aligned} &\mu|\nabla(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\bar{\rho}^{1/2}(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} \\ &\quad \leqslant (|\bar{\rho} - \rho|_{L^2}|\mathbf{h}|_{L^2} + |\bar{p} - p|_{L^2})|\nabla(\bar{\mathbf{u}} - \mathbf{u})|_{L^2} + |\nabla \mathbf{u}|_{L^\infty}|\bar{\rho}^{1/2}(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} \end{aligned}$$

and thus

$$\mu|\nabla(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} + \frac{\mathrm{d}}{\mathrm{d}t}|\bar{\rho}^{1/2}(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} \leqslant A(t)(|\bar{\rho}^{1/2}(\bar{\mathbf{u}} - \mathbf{u})|^2_{L^2} + |\bar{\rho} - \rho|^2_{L^2}) \tag{56}$$

for some non-negative function $A(t) \in L^1_{\text{loc}}(0,\infty)$.

On the other hand, using the identity

$$(\bar{\rho} - \rho)_t + \nabla(\bar{\rho} - \rho) \cdot \bar{\mathbf{u}} + \nabla\rho \cdot (\bar{\mathbf{u}} - \mathbf{u}) + (\bar{\rho} - \rho)\operatorname{div} \mathbf{u} + \bar{\rho}\operatorname{div}(\bar{\mathbf{u}} - \mathbf{u}) = 0$$

we deduce that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int|\bar{\rho}-\rho|^2\,\mathrm{d}x &\leqslant 2\int(|\mathrm{div}\,\mathbf{u}|+|\mathrm{div}\,\bar{\mathbf{u}}|)|\bar{\rho}-\rho|^2+|\nabla\rho||\bar{\rho}-\rho||\bar{\mathbf{u}}-\mathbf{u}|\\ &\quad+\bar{\rho}|\bar{\rho}-\rho||\mathrm{div}(\bar{\mathbf{u}}-\mathbf{u})|\,\mathrm{d}x\\ &\leqslant C_2(|\nabla\mathbf{u}|_{L^\infty}+|\nabla\bar{\mathbf{u}}|_{L^\infty})|\bar{\rho}-\rho|_{L^2}^2\\ &\quad+C_2(|\nabla\rho|_{L^2}+|\bar{\rho}|_{L^\infty})|\bar{\rho}-\rho|_{L^2}|\nabla(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}\end{aligned}$$

and thus

$$\frac{\mathrm{d}}{\mathrm{d}t}|\bar{\rho}-\rho|_{L^2}^2\leqslant\frac{\mu}{2}|\nabla(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}^2+B(t)|\bar{\rho}-\rho|_{L^2}^2 \tag{57}$$

for some non-negative $B(t)\in L^1_{\mathrm{loc}}(0,\infty)$.

Therefore, combining estimates (56) and (57), we conclude that

$$\begin{aligned}&\frac{\mu}{2}|\nabla(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}^2+\frac{\mathrm{d}}{\mathrm{d}t}(|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}^2+|\bar{\rho}-\rho|_{L^2}^2)\\ &\quad\leqslant(A(t)+B(t))(|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}^2+|\bar{\rho}-\rho|_{L^2}^2)\end{aligned}$$

In view of Gronwall's inequality, we complete the proof. □

5. GLOBAL EXISTENCE AND REGULARITY OF STRONG SOLUTIONS

In this section, we prove the existence and uniqueness results on the radially symmetric strong solutions to problem (1)–(3).

Theorem 5.1

Assume that the radially symmetric data $\rho_0,\mathbf{u}_0,\mathbf{f}$ satisfy the regularity condition

$$0\leqslant\rho_0\in L^1\cap H^1,\quad \mathbf{u}_0\in D_0^1\cap D^2,\quad \mathbf{f},\nabla\mathbf{f},\mathbf{f}_t\in L^2_{\mathrm{loc}}(0,\infty;L^2) \tag{58}$$

Then there exists a radially symmetric strong solution $(\rho,\mathbf{u})$ to the initial boundary value problem (1)–(3) satisfying the regularity,

$$\begin{aligned}&\rho\in C([0,\infty);L^1\cap H^1),\quad \mathbf{u}\in C([0,\infty);D_0^1\cap D^2)\\ &\rho_t\in C([0,\infty);L^2),\quad \mathbf{u}_t\in L^2_{\mathrm{loc}}(0,\infty;D_0^1),\quad \sqrt{\rho}\mathbf{u}_t\in L^\infty_{\mathrm{loc}}(0,\infty;L^2)\end{aligned} \tag{59}$$

if and only if the initial data $(\rho_0,\mathbf{u}_0)$ satisfy the compatibility condition

$$-\mu\Delta\mathbf{u}_0-(\lambda+\mu)\nabla\,\mathrm{div}\,\mathbf{u}_0+\nabla(A\rho_0^\gamma)=\rho_0^{1/2}\mathbf{g} \tag{60}$$

for some radially symmetric $\mathbf{g}\in L^2$. In this case, the initial condition is satisfied in the following sense:

$$|\rho(t)-\rho_0|_{L^1\cap H^1}+|\mathbf{u}(t)-\mathbf{u}_0|_{D_0^1\cap D^2}\to 0\quad\text{as } t\to 0 \tag{61}$$

Proof
We first prove the necessity of the compatibility condition (60), an easy part of the theorem. Let (ρ, u) be a strong solution to problem (1)–(3) satisfying (59) and (61). Since $\sqrt{\rho}\mathbf{u}_t \in L^\infty_{\rm loc}(0,\infty; L^2)$, we can find a sequence $\{t_k\}$, $t_k \to 0$, such that $\{\sqrt{\rho}\mathbf{u}_t(t_k)\}$ converges weakly in L^2. Therefore, letting $t_k \to 0$ in the momentum equation (1), we obtain

$$-\mu\Delta\mathbf{u}(0) - (\lambda+\mu)\nabla\,\mathrm{div}\,\mathbf{u}(0) + \nabla(A\rho(0)^\gamma) = \rho(0)^{1/2}\tilde{\mathbf{g}} \tag{62}$$

for some $\tilde{\mathbf{g}} \in L^2$. Since $\rho(0) = \rho_0$ and $\mathbf{u}(0) = \mathbf{u}_0$, this proves the necessity of condition (60).

To prove the converse, let $(\rho_0, \mathbf{u}_0, \mathbf{f})$ be a given data satisfying conditions (58) and (60). We consider only the case that $b < \infty$, since the results for the remaining case can be proved by passing to the limit $b \to \infty$. For a detailed argument, one may also refer to Reference [6].

Throughout the proof, we denote by C_3 (and $C_3(T)$) a generic positive constant depending only on a, $|\mathbf{g}|_{L^2}$ and the norms of the data (also on T), but independent of b and ε. To begin with, we construct a sequence $\rho_0^\varepsilon \in H^2(a,b)$ of smooth radial functions such that

$$0 < \varepsilon \leqslant \rho_0^\varepsilon, \quad \rho_0^\varepsilon \to \rho_0 \text{ in } H^1(a,b) \quad \text{and} \quad |\rho_0^\varepsilon|_{L^1(\Omega)\cap H^1(\Omega)} \leqslant C_3$$

where $\rho_0^\varepsilon(\mathbf{x}) = \rho_0^\varepsilon(|\mathbf{x}|)$ for $\mathbf{x} \in \Omega$, and let $u_0^\varepsilon \in H_0^1(a,b) \cap H^2(a,b)$ be the solution to the boundary value problem

$$-v\left((u_0^\varepsilon)_r + m\,\frac{u_0^\varepsilon}{r}\right)_r + (A\rho_0^\varepsilon)_r = (\rho_0^\varepsilon)^{1/2} g, \quad a < r < b$$

Then, let $(\rho^\varepsilon, u^\varepsilon)$ be the strong solution in $(0,\infty)\times(a,b)$ to the radial problem (7)–(9) with the initial data $(\rho_0^\varepsilon, u_0^\varepsilon)$. As shown in the previous sections, if we define

$$\rho^\varepsilon(t,\mathbf{x}) = \rho^\varepsilon(t,|\mathbf{x}|) \quad \text{and} \quad \mathbf{u}^\varepsilon(t,\mathbf{x}) = u^\varepsilon(t,|\mathbf{x}|)\,\frac{\mathbf{x}}{|\mathbf{x}|}$$

then $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ is a global radially symmetric strong solution to problem (1)–(3) with the initial data $(\rho_0^\varepsilon, \mathbf{u}_0^\varepsilon)$, where $\mathbf{u}_0^\varepsilon(\mathbf{x}) = u_0^\varepsilon(|\mathbf{x}|)(\mathbf{x}/|\mathbf{x}|)$.

Note that the regularized initial data $(\rho_0^\varepsilon, \mathbf{u}_0^\varepsilon)$ satisfy the same compatibility condition as (60) of $(\rho_0, \mathbf{u}_0)$:

$$-\mu\Delta\mathbf{u}_0^\varepsilon - (\lambda+\mu)\nabla\,\mathrm{div}\,\mathbf{u}_0^\varepsilon + \nabla(A(\rho_0^\varepsilon)^\gamma) = (\rho_0^\varepsilon)^{1/2}\mathbf{g}$$

In particular, it follows from the elliptic regularity estimate that $\mathbf{u}_0^\varepsilon \to \mathbf{u}_0$ in H^2 as $\varepsilon \to 0$ since $\rho_0^\varepsilon \to \rho_0$ in $L^\infty \cap H^1$ as $\varepsilon \to 0$. Therefore, using Lemmas 3.1–3.5, we conclude that $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ satisfies the following uniform estimate: for each $0 < T < \infty$,

$$\sup_{0\leqslant t\leqslant T}(|\rho^\varepsilon|_{L^1\cap H^1} + |\mathbf{u}^\varepsilon|_{D_0^1\cap D^2} + |\sqrt{\rho^\varepsilon}\mathbf{u}^\varepsilon|_{L^2}) + \int_0^T |\mathbf{u}_t^\varepsilon|^2_{D_0^1}\,\mathrm{d}t \leqslant C_3(T)$$

Now it can be easily shown that a subsequence of approximate solutions $(\rho^\varepsilon, \mathbf{u}^\varepsilon)$ converges, in a weak or weak-* sense, to a radially symmetric strong solution $(\rho, \mathbf{u})$ satisfying regularity (59) except the continuity of $\mathbf{u}$.

The weak-type continuity of $\mathbf{u}$ follows from the standard embedding results: $\mathbf{u} \in C([0,\infty); D_0^1) \cap C([0,\infty); D^2\text{-}weak)$. Hence it remains to prove the strong continuity of $\mathbf{u}$ in D^2. We first prove the continuity of $\rho\mathbf{u}_t$ in L^2. From the momentum equation (44), we easily deduce that

$(\rho\mathbf{u}_t)_t \in L^2_{\text{loc}}(0,\infty;H^{-1})$, where H^{-1} is the dual space of H^1_0. Then since $\rho\mathbf{u}_t \in L^2_{\text{loc}}(0,\infty;H^1_0)$, it follows from a standard embedding result that $\rho\mathbf{u}_t \in C([0,\infty);L^2)$. Therefore, we can conclude that for each $t\in[0,\infty)$, $\mathbf{u}=\mathbf{u}(t)\in D^1_0\cap D^2$ is a solution of the elliptic system

$$\nu\Delta\mathbf{u} = \rho\mathbf{u}_t + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla(A\rho^\gamma) - \rho\mathbf{f}$$

Now it is not difficult to show that $\mathbf{u}\in C([0,\infty);D^2)$. Recall from the elliptic estimate in Reference [6] that for $s,t\geqslant 0$,

$$\begin{aligned}|\mathbf{u}(t)-\mathbf{u}(s)|_{D^2} &\leqslant C_0|\rho\mathbf{u}\cdot\nabla\mathbf{u}(t)-\rho\mathbf{u}\cdot\nabla\mathbf{u}(s)|_{L^2} + C_0|\nabla(A\rho^\gamma)(t)-\nabla(A\rho^\gamma)(s)|_{L^2}\\ &\quad + C_0(|\rho\mathbf{u}_t(t)-\rho\mathbf{u}_t(s)|_{L^2} + |\rho\mathbf{f}(t)-\rho\mathbf{f}(s)|_{L^2} + |\mathbf{u}(t)-\mathbf{u}(s)|_{D^1_0}) \qquad (63)\end{aligned}$$

Using Sobolev inequality together with the regularity of $(\rho,\mathbf{u})$, we obtain,

$$\begin{aligned}&|\rho\mathbf{u}\cdot\nabla\mathbf{u}(t)-\rho\mathbf{u}\cdot\nabla\mathbf{u}(s)|_{L^2}\\ &\quad\leqslant C_0|(\rho(t)-\rho(s))\mathbf{u}(t)\cdot\nabla\mathbf{u}(t)|_{L^2} + C_0|\rho(s)(\mathbf{u}(t)-\mathbf{u}(s))\cdot\nabla\mathbf{u}(t)|_{L^2}\\ &\qquad + C_0|\rho(s)\mathbf{u}(s)\cdot(\nabla\mathbf{u}(t)-\nabla\mathbf{u}(s))|_{L^2}\\ &\quad\leqslant C_0|\rho(t)-\rho(s)|_{L^\infty}|\nabla\mathbf{u}(t)|^2_{L^2} + C_0|\rho(s)|_{L^\infty}|\nabla(\mathbf{u}(t)-\mathbf{u}(s))|_{L^2}|\nabla\mathbf{u}(t)|_{L^2}\\ &\qquad + C_0|\rho(s)|_{L^\infty}|\nabla\mathbf{u}(s)|_{L^2}|\nabla(\mathbf{u}(t)-\mathbf{u}(s))|_{L^2}\\ &\quad\leqslant C_3(|\rho(t)-\rho(s)|_{L^\infty} + |\mathbf{u}(t)-\mathbf{u}(s)|_{D^1_0})\end{aligned}$$

and

$$\begin{aligned}|\nabla(\rho^\gamma)(t)-\nabla(\rho^\gamma)(s)|_{L^2} &\leqslant C_0|(\rho^{\gamma-1}(t)-\rho^{\gamma-1}(s))\nabla\rho(t)|_{L^2} + C_0|\rho^{\gamma-1}(\nabla\rho(t)-\nabla\rho(s))|_{L^2}\\ &\leqslant C_3(|\rho^{\gamma-1}(t)-\rho^{\gamma-1}(s)|_{L^\infty} + |\nabla\rho(t)-\nabla\rho(s)|_{L^2})\end{aligned}$$

Substituting these results into (63), we conclude that $|\mathbf{u}(t)-\mathbf{u}(s)|_{D^2}\leqslant\Theta(t,s)$ for some function $\Theta(t,s)$ such that $\lim_{t\to s}\Theta(t,s)=0$.

We have proved the existence of a radially symmetric strong solution $(\rho,\mathbf{u})$ satisfying regularity (59). Hence to complete the proof of the sufficiency, it remains to prove the convergence property (61) of $(\rho,\mathbf{u})$ as $t\to 0$. Now we show that

$$\rho(0)=\rho_0 \quad\text{and}\quad \mathbf{u}(0)=\mathbf{u}_0 \text{ in } \Omega \qquad (64)$$

which is equivalent to (61) because of the continuity of $(\rho,\mathbf{u})$. The first identity in (64) follows easily from the weak formulation of the continuity equation (2). But from the momentum equation (1), we deduce only that $(\rho\mathbf{u})(0)=\rho_0\mathbf{u}_0$ in Ω. Hence we have to show that $\mathbf{u}(0)=\mathbf{u}_0$ in the set $\Omega_0=\{\mathbf{x}\in\Omega:\rho_0(\mathbf{x})=0\}$. Define $\mathbf{w}=\mathbf{u}(0)-\mathbf{u}_0$. Then since $(\rho(0),\mathbf{u}(0))$ also satisfies condition (62) for some $\tilde{\mathbf{g}} \in L^2$, we find that the radial part w of $\mathbf{w}$ satisfies

$$-v\left(w_r + m\,\frac{w}{r}\right)_r = 0 \quad \text{in } V \tag{65}$$

where $V = \operatorname{int}\{r \in (a,b) : \rho_0(r) = 0\}$. It is clear that $w \in D_0^1(V) \cap D^2(V)$. Moreover, since V is a countable union of open intervals, we easily prove that $w = 0$ in V, that is, $\mathbf{u}(0) = \mathbf{u}_0$ in the set Ω_0. Therefore, the proof of Theorem 5.1 has been completed. □

In view of Lemma 3.6, the regularity of solutions of Theorem 5.1 can be improved, provided that $\gamma \geqslant 2$ and $\rho_0 \in H^2$. This can be achieved by following exactly the same arguments as in the proof of Theorem 5.1. Hence we may state the following result without a proof.

Theorem 5.2
Let $\gamma \geqslant 2$, and let $(\rho_0, \mathbf{u}_0, \mathbf{f})$ be a radially symmetric data satisfying conditions (58) and (60). Assume further that $\rho_0 \in H^2$. Then there exists a radially symmetric strong solution $(\rho, \mathbf{u})$ to the initial boundary value problem (1)–(3) satisfying the regularity,

$$\rho \in C([0,\infty); L^1 \cap H^2), \quad \mathbf{u} \in C([0,\infty); D_0^1 \cap D^2) \cap L^2_{\text{loc}}(0,\infty; D^3)$$

$$\rho_t \in C([0,\infty); H^1), \quad \mathbf{u}_t \in L^2_{\text{loc}}(0,\infty; D_0^1), \quad \sqrt{\rho}\,\mathbf{u}_t \in L^\infty_{\text{loc}}(0,\infty; L^2)$$

Moreover, the initial condition is satisfied in the following sense:

$$|\rho(t) - \rho_0|_{L^1 \cap H^2} + |\mathbf{u}(t) - \mathbf{u}_0|_{D_0^1 \cap D^2} \to 0 \quad \text{as } t \to 0$$

To obtain a uniqueness result on strong solutions, we first prove the following weak–strong uniqueness result for $n \geqslant 4$.

Proposition 5.3
Assume that $n \geqslant 4$, and let $(\rho, \mathbf{u})$ and $(\overline{\rho}, \overline{\mathbf{u}})$ be global weak solutions (in the sense of Lions [16]) to problem (1)–(3) with the same initial data $(\rho_0, \mathbf{u}_0)$. If $\mathbf{f} \in L^2_{\text{loc}}(0,\infty; L^\infty)$, and if the solutions satisfy the additional regularity

$$\rho, \overline{\rho} \in L^\infty_{\text{loc}}(0,\infty; L^{2n/n+2} \cap L^\infty), \quad \nabla\rho \in L^2_{\text{loc}}(0,\infty; L^2 \cap L^n)$$

$$\mathbf{u} \in L^\infty_{\text{loc}}(0,\infty; L^\infty) \quad \text{and} \quad \nabla\mathbf{u},\, \mathbf{u}_t \in L^2_{\text{loc}}(0,\infty; L^\infty)$$

then $\rho = \overline{\rho}$ and $\mathbf{u} = \overline{\mathbf{u}}$.

Proof
To explain ideas more clearly, we present a formal argument. From the momentum equations, it follows easily that,

$$\overline{\rho}(\overline{\mathbf{u}} - \mathbf{u})_t + \overline{\rho}\,\overline{\mathbf{u}} \cdot \nabla(\overline{\mathbf{u}} - \mathbf{u}) - \mu\Delta(\overline{\mathbf{u}} - \mathbf{u}) - (\lambda + \mu)\nabla \operatorname{div}(\overline{\mathbf{u}} - \mathbf{u})$$

$$= (\overline{\rho} - \rho)\mathbf{h} - \overline{\rho}(\overline{\mathbf{u}} - \mathbf{u}) \cdot \nabla\mathbf{u} - \nabla(\overline{p})$$

where $\mathbf{h}=\mathbf{f}-\mathbf{u}_t-\mathbf{u}\cdot\nabla\mathbf{u}\in L^2_{\text{loc}}(0,\infty;L^\infty)$. Then multiplying this identity by $(\bar{\mathbf{u}}-\mathbf{u})$ and integrating over Ω, we obtain,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\frac{1}{2}\bar{\rho}|\bar{\mathbf{u}}-\mathbf{u}|^2\,\mathrm{d}x+\int\mu|\nabla(\bar{\mathbf{u}}-\mathbf{u})|^2+(\lambda+\mu)|\mathrm{div}(\bar{\mathbf{u}}-\mathbf{u})|^2\,\mathrm{d}x$$
$$\leqslant\int|\bar{\rho}-\rho||\mathbf{h}||\bar{\mathbf{u}}-\mathbf{u}|+\bar{\rho}|\bar{\mathbf{u}}-\mathbf{u}|^2|\nabla\mathbf{u}|+(\bar{p}-p)\,\mathrm{div}(\bar{\mathbf{u}}-\mathbf{u})\,\mathrm{d}x$$

In view of the usual Sobolev inequality in $\mathbb{R}^n$ $(n\geqslant 4)$, we obtain

$$\mu|\nabla(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}$$
$$\leqslant(|\bar{\rho}-\rho|_{L^{2n/n+2}}|\mathbf{h}|_{L^\infty}+|\bar{p}-p|_{L^2})|\nabla(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}+|\nabla\mathbf{u}|_{L^\infty}|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}$$

and thus

$$\mu|\nabla(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}+\frac{\mathrm{d}}{\mathrm{d}t}|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}$$
$$\leqslant A(t)(|\bar{\rho}^{1/2}(\bar{\mathbf{u}}-\mathbf{u})|^2_{L^2}+|\bar{\rho}-\rho|^2_{L^{2n/n+2}}+|\bar{p}-p|^2_{L^2})\tag{66}$$

for some non-negative function $A(t)\in L^1_{\text{loc}}(0,\infty)$.

On the other hand, using the identity

$$(\bar{\rho}-\rho)_t+\nabla(\bar{\rho}-\rho)\cdot\bar{\mathbf{u}}+\nabla\rho\cdot(\bar{\mathbf{u}}-\mathbf{u})+(\bar{\rho}-\rho)\,\mathrm{div}\,\mathbf{u}+\bar{\rho}\,\mathrm{div}(\bar{\mathbf{u}}-\mathbf{u})=0$$

we deduce formally that

$$(|\bar{\rho}-\rho|)_t+\nabla(|\bar{\rho}-\rho|)\cdot(\bar{\mathbf{u}}-\mathbf{u})+\nabla(|\bar{\rho}-\rho|)\cdot\mathbf{u}$$
$$\leqslant|\nabla\rho||\mathbf{u}-\bar{\mathbf{u}}|+|\bar{\rho}-\rho||\mathrm{div}\,\mathbf{u}|+\rho|\mathrm{div}(\bar{\mathbf{u}}-\mathbf{u})|$$

Multiplying this by $|\bar{\rho}-\rho|^{(n-2)/(n+2)}$ and integrating over Ω, we obtain,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int|\bar{\rho}-\rho|^{2n/n+2}\,\mathrm{d}x$$
$$\leqslant C_0\int(|\bar{\rho}-\rho|+\rho)|\bar{\rho}-\rho|^{(n-2)/(n+2)}|\mathrm{div}\,(\bar{\mathbf{u}}-\mathbf{u})|$$
$$+|\bar{\rho}-\rho|^{2n/n+2}|\mathrm{div}\,\mathbf{u}|+|\nabla\rho\,||\bar{\rho}-\rho|^{(n-2)/(n+2)}|\bar{\mathbf{u}}-\mathbf{u}|\,\mathrm{d}x$$
$$\leqslant C_0(|\bar{\rho}-\rho|_{L^n}+|\rho|_{L^n}+|\nabla\rho|_{L^{n/2}})|\bar{\rho}-\rho|^{(n-2)/(n+2)}_{L^{2n/n+2}}|\nabla(\bar{\mathbf{u}}-\mathbf{u})|_{L^2}$$
$$+C_0|\nabla\mathbf{u}|_{L^\infty}|\bar{\rho}-\rho|^{2n/n+2}_{L^{2n/n+2}}$$

and hence

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\overline{\rho}-\rho|^2_{L^{2n/n+2}} &= \frac{n+2}{n}|\overline{\rho}-\rho|^{4/n+2}_{L^{2n/n+2}}\frac{\mathrm{d}}{\mathrm{d}t}|\overline{\rho}-\rho|^{2n/n+2}_{L^{2n/n+2}}\\ &\leqslant C_1(|\overline{\rho}-\rho|^2_{L^n}+|\rho|^2_{L^n}+|\nabla\rho|^2_{L^{n/2}})|\overline{\rho}-\rho|^2_{L^{2n/n+2}}\\ &\quad+\frac{\mu}{4}|\nabla(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+C_1|\nabla u|_{L^\infty}|\overline{\rho}-\rho|^2_{L^{2n/n+2}}\\ &\leqslant \frac{\mu}{4}|\nabla(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+B(t)|\overline{\rho}-\rho|^2_{L^{2n/n+2}} \end{aligned} \tag{67}$$

for some non-negative $B(t)\in L^1_{\mathrm{loc}}(0,\infty)$.

Finally, using the identity

$$(\overline{p}-p)_t+\nabla(\overline{p}-p)\cdot\overline{\mathbf{u}}+\nabla p\cdot(\overline{\mathbf{u}}-\mathbf{u})+\gamma(\overline{p}-p)\operatorname{div}\mathbf{u}+\gamma\overline{p}\operatorname{div}(\overline{\mathbf{u}}-\mathbf{u})=0$$

we deduce in a similar way that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int|\overline{p}-p|^2\,\mathrm{d}x &\leqslant C_0(|\overline{p}-p|_{L^\infty}+|\overline{p}|_{L^\infty}+|\nabla p|_{L^n})|\overline{p}-p|_{L^2}|\nabla(\overline{\mathbf{u}}-\mathbf{u})|_{L^2}\\ &\quad+C_0|\nabla\mathbf{u}|_{L^\infty}|\overline{p}-p|^2_{L^2}\\ &\leqslant\frac{\mu}{4}|\nabla(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+C(t)|\overline{p}-p|^2_{L^2}\end{aligned} \tag{68}$$

for some non-negative $C(t)\in L^1_{\mathrm{loc}}(0,\infty)$.

Therefore, combining all estimates (66)–(68), we conclude that,

$$\begin{aligned}&\frac{\mu}{2}|\nabla(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+\frac{\mathrm{d}}{\mathrm{d}t}(|\overline{\rho}^{1/2}(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+|\overline{\rho}-\rho|^2_{L^{2n/n+2}}+|\overline{p}-p|^2_{L^2})\\ &\quad\leqslant(A(t)+B(t)+C(t))(|\overline{\rho}^{1/2}(\overline{\mathbf{u}}-\mathbf{u})|^2_{L^2}+|\overline{\rho}-\rho|^2_{L^{2n/n+2}}+|\overline{p}-p|^2_{L^2})\end{aligned}$$

Applying Gronwall's inequality, we complete the proof of Proposition 5.3. □

Remark 5.4

The integral form of the differential inequality (66) can be proved rigorously by using the weak formulation and energy inequality. For details, please refer to the proof of a weak–strong uniqueness result by Lions [17]. Moreover, (67) and (68) may be verified by means of a regularization technique developed in paper [15] for the linear transport equations. A similar uniqueness result by Desjardins [18] is also applicable to the case of bounded domains.

Combining Proposition 5.3 and a uniqueness result of the authors in Reference [5], we can prove the following uniqueness result.

Theorem 5.5
Assume that $n \geqslant 3$ or $b < \infty$, and let $(\rho, \mathbf{u})$ be a radially symmetric solution to the initial boundary value problem (1)–(3), which satisfies regularity (59). If $(\bar{\rho}, \bar{\mathbf{u}})$ is any weak solution to (1)–(3) with $\bar{\rho} \in L^{\infty}_{\text{loc}}(0, \infty; L^1 \cap L^{\infty})$, then

$$\rho = \bar{\rho} \quad \text{and} \quad \mathbf{u} = \bar{\mathbf{u}}$$

provided that ρ_0 has the additional regularity $\nabla \rho_0 \in L^n$.

Proof
We first show that $\nabla \rho \in L^2_{\text{loc}}(0, \infty; L^n)$. For this purpose, we differentiate the continuity equation (2) with respect to x_j and multiply by $\rho_{x_j} |\rho_{x_j}|^{n-2}$. Then integrating over Ω and using Lemmas 3.1, 3.2 and 3.5, we deduce that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \int |\nabla \rho|^n \, \mathrm{d}x &\leqslant C_0 \int |\nabla \mathbf{u}| |\nabla \rho|^n + \rho |\nabla \rho|^{n-1} |\nabla \operatorname{div} \mathbf{u}| \, \mathrm{d}x \\
&\leqslant C_3 \int |\nabla \rho|^n \, \mathrm{d}x + C_3 \int \rho |\nabla \rho|^{n-1} |\nabla G| \, \mathrm{d}x \\
&\leqslant C_3 (|\nabla G|_{L^{\infty}} + 1)(|\nabla \rho|^n_{L^n} + 1)
\end{aligned}$$

Using Lemma 3.5 together with Sobolev inequality (33), we thus obtain

$$\sup_{0 \leqslant t \leqslant T} |\nabla \rho(t)|_{L^n} \leqslant C_3(T) \quad \text{for any } T < \infty \tag{69}$$

Therefore, the solution $(\rho, \mathbf{u})$ satisfies the hypotheses of Proposition 5.3 and thus the uniqueness is guaranteed at least for $n \geqslant 4$. The uniqueness for the finite case $b < \infty$ can be proved in a similar and even simpler way, because the embedding $D^1_0 \hookrightarrow L^2$ is then available. But, for the (most important) case that $n = 3$, Proposition 5.3 may not be helpful because an estimate for $|\rho(t) - \bar{\rho}(t)|_{L^{6/5}}$ requires that $\nabla \rho \in L^{\infty}_{\text{loc}}(0, \infty; L^{3/2})$ (see the proof of (67)). Nevertheless, we can show that the uniqueness also hold for $n = 3$ by using a similar argument based on the fact that $\rho - \bar{\rho} \in L^{\infty}_{\text{loc}}(0, \infty; L^{3/2})$. For a detailed argument, please refer to the proof of the weak–strong uniqueness result in Reference [5]. This completes the proof of Theorem 5.5. □

ACKNOWLEDGEMENTS

The authors would like to thank the referees for their helpful comments on the proofs of uniqueness results. The first author was supported by KRF C-00005 of Korea Research Foundation. The second author was supported by Japan Society for the Promotion of Science.

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MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:29–41
Published online in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.547
MOS subject classification: 42 A 16; 35 J 25; 35 D 10

On solution of Lamé equations in axisymmetric domains with conical points

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Communicated by H.-D. Alber

SUMMARY

Partial Fourier series expansion is applied to the Dirichlet problem for the Lamé equations in axisymmetric domains $\hat{\Omega} \subset \mathbb{R}^3$ with conical points on the rotation axis. This leads to dimension reduction of the three-dimensional boundary value problem resulting to an infinite sequence of two-dimensional boundary value problems on the plane meridian domain $\Omega_a \subset \mathbb{R}^2_+$ of $\hat{\Omega}$ with solutions $\mathbf{u}_n$ $(n = 0, 1, 2, \ldots)$ being the Fourier coefficients of the solution $\hat{\mathbf{u}}$ of the 3D BVP. The asymptotic behaviour of the Fourier coefficients $\mathbf{u}_n$ $(n = 0, 1, 2, \ldots)$ near the angular points of the meridian domain Ω_a is fully described by singular vector-functions which are related to the zeros α_n of some transcendental equations involving Legendre functions of the first kind. Equations which determine the values of α_n are given and a numerical algorithm for the computation of α_n is proposed with some plots of values obtained presented. The singular vector functions for the solution of the 3D BVP is obtained by Fourier synthesis. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: Fourier series; boundary value problems; singularities

1. INTRODUCTION

Many problems in physics and engineering belong to the class of boundary value problems for the elliptic partial differential equations with solutions having singularities due to boundary irregularities. The construction of suitable finite element (boundary element) methods for treating BVPs with singularities (e.g. adaptive mesh refinement, singular function augmentation, etc.) requires *a priori* knowledge of the form of the singular functions. Moreover, some physical useful parameters such as stress intensity factors can be computed if the singular

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Contract/grant sponsor: Swedish International Development Cooperation Agency (SIDA)

Received 9 December 2003

forms are known. Thus, the need to analyse and characterize singular forms and regularity results for BVPs is crucial and much work has been done in this area (cf. References [1–17]).

In this paper we consider the homogeneous Dirichlet problem for the Lamé system in axisymmetric domains $\hat{\Omega} \subset \mathbb{R}^3$ with conical points on the rotation axis, i.e.

$$-\mu \triangle \hat{\mathbf{u}}(\mathbf{x}) - (\lambda + \mu)\text{grad div}\, \hat{\mathbf{u}}(\mathbf{x}) = \hat{\mathbf{f}}(\mathbf{x}) \quad \text{for } \mathbf{x} \in \hat{\Omega} \tag{1}$$

$$\hat{\mathbf{u}}(\mathbf{x}) = \mathbf{0} \quad \text{for } \mathbf{x} \in \hat{\Gamma} := \partial\hat{\Omega} \tag{2}$$

where $\hat{\mathbf{u}}$ denotes the displacement vector field, $\hat{\mathbf{f}} \in (L_2(\hat{\Omega}))^3$ is the vector of the volume forces and $\mu > 0$, $\lambda > 0$ are the Lamé coefficients. Analysis of solutions of BVPs for the Lamé equations in domains with conical points and re-entrant vertices has been quite intensive (cf. References [1,7,10,12–17]). More precisely, suppose for convenience that the domain $\hat{\Omega} \subset \mathbb{R}^3$ has only one conical point which coincides with the origin O, then according to the general theory (cf. References [1,2,7,12,14,16,17]), in the vicinity of the conical point O the solution $\hat{\mathbf{u}}$ of (1), (2) behaves like a linear combination of terms of the form,

$$|\mathbf{x}|^{\alpha} \sum_{s=0}^{k} (\ln |\mathbf{x}|)^s \mathbf{u}^{k-s}(\mathbf{x}/|\mathbf{x}|) \tag{3}$$

The exponents α (in general complex) are eigenvalues of a certain operator pencil which arises from the Mellin transformation of the principal parts of the differential and boundary operators in (1), (2) on the tangent cone, and the functions $\mathbf{u}^s$ $(0 \leqslant s \leqslant k)$ are the generalized eigenvectors corresponding to α.

In view of the fact that boundary value problems in axisymmetric domains $\hat{\Omega} \subset \mathbb{R}^3$ with non-axisymmetric data, are treated numerically, preferably by the Fourier-finite-element method (FFEM) (cf. References [18–23]), the characterization of singular forms and regularity results for the Fourier coefficients of the solution of the 3D BVP is crucial for an efficient application of this method. In this paper we give a precise description of the singular vector-functions that describe the asymptotic behaviour of the Fourier coefficients of the solution of the 3D BVP near the angular points of the plane meridian domain Ω_a. The singular vector-functions depend on a parameter α which is related to the roots of some transcendental equations involving Legendre functions. We present equations which determine the values of α and give a numerical procedure for computing α. Some graphs of the computed values of α are presented. The analysis shows that Fourier coefficients $\mathbf{u}_n$ for $n \geqslant 2$ of the solution $\hat{\mathbf{u}}$ of (1), (2) have the required regularity for any conical points, whenever the right-hand side $\hat{\mathbf{f}}$ belong to $(L_2(\hat{\Omega}))^3$. The singular forms for the solution of the 3D BVP is obtained by means of Fourier synthesis.

2. ANALYTICAL PRELIMINARIES

Let $\hat{\Omega} \subset \mathbb{R}^3$ be an open bounded and simply connected set with Lipschitz boundary $\hat{\Gamma}$ and let (x_1, x_2, x_3) denote the Cartesian co-ordinates of the point $\mathbf{x} \in \mathbb{R}^3$. Suppose that $\hat{\Omega}$ is axisymmetric with respect to the x_3-axis and that the set $\hat{\Omega} \backslash \Gamma_0$ (Γ_0 is part of the x_3-axis contained in $\hat{\Omega}$) is obtain by rotation of a bounded plane meridian domain Ω_a about the x_3-axis. Let

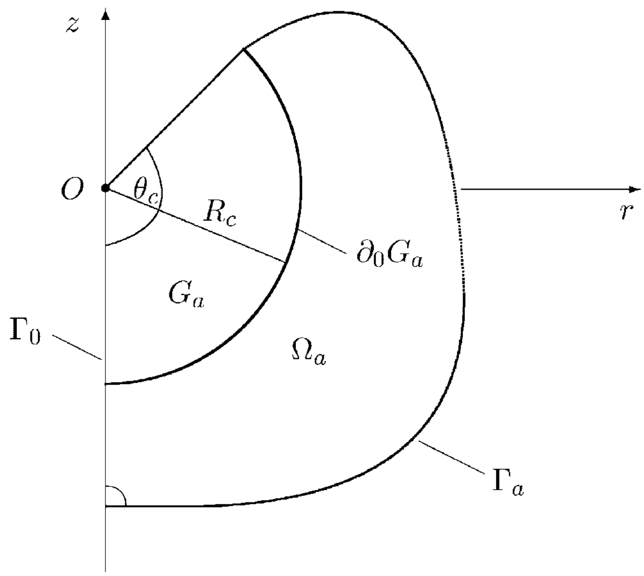

Figure 1. Meridian plane of $\hat{\Omega}$.

$\Gamma_a := \partial\Omega_a \backslash \bar{\Gamma}_0$ and suppose that $\Gamma_a \in C^2$ and that Γ_a is straight line in some neighbourhood of the points of intersection of $\bar{\Gamma}_a$ and $\bar{\Gamma}_0$ (see Figure 1). With this assumption we exclude axisymmetric edges on the boundary of $\hat{\Omega}$, this case has been handled in Reference [24]. We assume for convenience that the axisymmetric domain $\hat{\Omega}$ has only one conical point on its boundary which coincides with the origin O and let the interior opening angle be equal θ_c.

Subsequently we employ cylindrical co-ordinates r, φ, z ($\varphi \in (-\pi, \pi]$) which are related to the Cartesian co-ordinates by $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$, $x_3 = z$. Thus the sets $\hat{\Omega}\backslash\Gamma_0$ and $\hat{\Gamma}\backslash\Gamma_0$ are mapped into the sets $\Omega := \Omega_a \times (-\pi, \pi]$ and $\Gamma := \Gamma_a \times (-\pi, \pi]$, respectively, in cylindrical co-ordinates. For any vector function $\hat{\mathbf{u}}(\mathbf{x}) = (\hat{u}_1(\mathbf{x}), \hat{u}_2(\mathbf{x}), \hat{u}_3(\mathbf{x}))^{\mathrm{T}}$, $\mathbf{x} \in \hat{\Omega}\backslash\Gamma_0$, some vector function $\mathbf{u} = (u_r(r,\varphi,z), u_\varphi(r,\varphi,z), u_z(r,\varphi,z))^{\mathrm{T}}$, $(r,\varphi,z) \in \Omega$ is uniquely defined by

$$u_r := \hat{u}_1 \cos\varphi + \hat{u}_2 \sin\varphi, \quad u_\varphi := -\hat{u}_1 \sin\varphi + \hat{u}_2 \cos\varphi, \quad u_z := \hat{u}_3 \tag{4}$$

Let us introduce with respect to the origin O local polar co-ordinates R, θ viz. $r = R\sin\theta$ $z = -R\cos\theta$ and define a circular sector G_a in Ω_a with radius R_c and angle θ_c by (see Figure 1)

$$\bar{G}_a := \{(r,z) \in \bar{\Omega}_a\colon\ 0 \leqslant R \leqslant R_c,\ 0 \leqslant \theta \leqslant \theta_c\}, \quad G_a := \bar{G}_a \backslash \partial G_a \tag{5}$$

where ∂G_a denotes the boundary of G_a. Let $\hat{G}$ denote the domain generated by rotation of G_a about the x_3-axis and $\partial\hat{G}$ its boundary. Then the images of the sets $\hat{G}\backslash\Gamma_0$ and $\hat{\partial}G\backslash\Gamma_0$ in cylindrical co-ordinates are $G := G_a \times (-\pi, \pi]$ and $\partial G := \partial_0 G_a \times (-\pi, \pi]$, respectively, where $\partial_0 G_a := \partial G_a \backslash \bar{\Gamma}_0$.

For the analysis of the behaviour of the solution $\hat{\mathbf{u}}$ of (1), (2) and its Fourier coefficients $\mathbf{u}_n$, $n \in \mathbf{N}_0 := \{0, 1, 2, \ldots\}$, near the conical point O, we consider in cylindrical co-ordinates the homogeneous Lamé system in the neighbourhood G of O with homogeneous boundary conditions.

$$\begin{aligned}
\triangle_{r\varphi z}u_r - \frac{1}{r^2}u_r - \frac{2}{r^2}\frac{\partial u_\varphi}{\partial\varphi} + \frac{1}{1-2v}\frac{\partial e}{\partial r} &= 0 \quad \text{in } G\\
\triangle_{r\varphi z}u_\varphi - \frac{1}{r^2}u_\varphi + \frac{2}{r^2}\frac{\partial u_r}{\partial\varphi} + \frac{1}{1-2v}\frac{\partial e}{\partial\varphi} &= 0 \quad \text{in } G\\
\triangle_{r\varphi z}u_z + \frac{1}{1-2v}\frac{\partial e}{\partial z} &= 0 \quad \text{in } G\\
u_r = u_\varphi = u_z &= 0 \quad \text{on } \partial G\backslash\{0\}
\end{aligned} \tag{6}$$

Here

$$\triangle_{r\varphi z} := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}, \quad e := \frac{\partial u_r}{\partial r} + \frac{1}{r}u_r + \frac{1}{r}\frac{\partial u_\varphi}{\partial\varphi} + \frac{\partial u_z}{\partial z}$$

and the Poisson's ratio $0<v<0.5$ is related to the Lamé coefficients by $v=\lambda/2(\lambda+\mu)$.

Using the orthogonal and complete system $\{1, \sin\varphi, \cos\varphi, \ldots, \sin n\varphi, \cos n\varphi, \ldots\}$ in $L_2(-\pi,\pi)$ we can represent the solution $\mathbf{u}$ of (6) in partial Fourier series in the form (cf. References [18,25]):

$$\begin{aligned}
u_r(r,\varphi,z) &= \sum_{n=0}^{\infty}(u_{rn}^s(r,z)\cos n\varphi + u_{rn}^a(r,z)\sin n\varphi)\\
u_\varphi(r,\varphi,z) &= \sum_{n=0}^{\infty}(u_{\varphi n}^s(r,z)(-\sin n\varphi) + u_{\varphi n}^a(r,z)\cos n\varphi)\\
u_z(r,\varphi,z) &= \sum_{n=0}^{\infty}(u_{zn}^s(r,z)\cos n\varphi + u_{zn}^a(r,z)\sin n\varphi)
\end{aligned} \tag{7}$$

where the Fourier coefficients are defined the usual way (cf. Reference [25]). Substituting (7) into (6) we obtain in G_a the following sequence of decoupled two-dimensional boundary value problems (we omit the superscript s and a):

$$\begin{aligned}
\triangle_{rz}u_{rn} - \frac{n^2+1}{r^2}u_{rn} + \frac{2n}{r^2}u_{\varphi n} + \frac{1}{1-2v}\frac{\partial e_{rzn}}{\partial r} &= 0 \quad \text{in } G_a\\
\triangle_{rz}u_{\varphi n} - \frac{n^2+1}{r^2}u_{\varphi n} + \frac{2n}{r^2}u_{rn} + \frac{n}{1-2v}e_{rzn} &= 0 \quad \text{in } G_a\\
\triangle_{rz}u_{zn} - \frac{n^2}{r^2}u_{zn} + \frac{1}{1-2v}\frac{\partial e_{rzn}}{\partial z} &= 0 \quad \text{in } G_a\\
u_{rn} = u_{\varphi n} = u_{zn} &= 0 \quad \text{on } \partial_0 G_a
\end{aligned} \tag{8}$$

where

$$\triangle_{rz} := \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}, \quad e_{rzn} := \frac{\partial u_{rn}}{\partial r} + \frac{1}{r}u_{rn} + \frac{\partial u_{zn}}{\partial z} - \frac{n}{r}u_{\varphi n}$$

For the analysis of the generalized solutions $\mathbf{u}_n$, $n \in \mathbf{N}_0$, of (8) we introduce the following spaces (see also References [21,25]):

$$\begin{aligned}
L_2(G_a) &:= \left\{ w = w(r,z):\ \int_{G_a} |w|^2 \,\mathrm{d}r\,\mathrm{d}z < \infty \right\} \\
L_{2,1/2}(G_a) &:= \{ w = w(r,z):\ r^{1/2} w \in L_2(G_a) \} \\
W^{1,2}_{1/2}(G_a) &:= \left\{ w \in L_{2,1/2}(G_a):\ \frac{\partial w}{\partial r}, \frac{\partial w}{\partial z} \in L_{2,1/2}(G_a) \right\} \\
W^{2,2}_{1/2}(G_a) &:= \left\{ w \in W^{1,2}_{1/2}(G_a):\ \frac{\partial^2 w}{\partial r^2}, \frac{\partial^2 w}{\partial z^2}, \frac{\partial^2 w}{\partial r \partial z} \in X(G_a) \right\}
\end{aligned} \tag{9}$$

These spaces are endowed with the norms:

$$\begin{aligned}
\|w\|_{L_{2,1/2}(G_a)} &:= \left\{ \int_{G_a} \|w\|^2 r \,\mathrm{d}r\,\mathrm{d}z \right\}^{1/2} \\
\|w\|_{W^{1,2}_{1/2}(G_a)} &:= \left\{ \|w\|^2_{L_{2,1/2}(G_a)} + \left\| \frac{\partial w}{\partial r} \right\|^2_{L_{2,1/2}(G_a)} + \left\| \frac{\partial w}{\partial z} \right\|^2_{L_{2,1/2}(G_a)} \right\}^{1/2} \\
\|w\|_{W^{2,2}_{1/2}(G_a)} &:= \left\{ \left\| \frac{\partial^2 w}{\partial r^2} \right\|^2_{L_{2,1/2}(G_a)} + \left\| \frac{\partial^2 w}{\partial z^2} \right\|^2_{L_{2,1/2}(G_a)} + 2 \left\| \frac{\partial^2 w}{\partial r \partial z} \right\|^2_{L_{2,1/2}(G_a)} \right\}^{1/2} \\
\|w\|_{W^{2,2}_{1/2}(G_a)} &:= \{ \|w\|^2_{W^{2,2}_{1/2}(G_a)} + \|w\|^2_{W^{1,2}_{1/2}(G_a)} \}^{1/2}
\end{aligned} \tag{10}$$

Remark 2.1

We note here that if the function $\hat{\mathbf{u}}$ belong to the Sobolev space $(W_2^2(\hat{\Omega}))^3$, then its Fourier coefficients $\mathbf{u}_n$, $n \in \mathbf{N}_0$ belong naturally in the space $(W^{2,2}_{1/2}(\Omega_a))^3$ (cf. References [22,24]).

Our main concern in the next sections is to determine the maximum value of the angle θ_c at the conical point which is permissible if the Fourier coefficients $\mathbf{u}_n$, $n \in \mathbf{N}_0$ of the solution $\hat{\mathbf{u}}$ of the BVP (1), (2) to belong to $(W^{2,2}_{1/2}(\Omega_a))^3$. We also determine the singular forms for the Fourier coefficients.

3. THE SINGULARITY FUNCTIONS

We are interested on the solutions of (8) which have the form,

$$\mathbf{u}_n = R^{\alpha_n} \mathbf{U}_n(\alpha_n, \theta) \tag{11}$$

where R, θ are the local polar co-ordinates (cf. (5)). To determine expressions involving the parameter α_n, we use the Boussinesq–Papkovich–Neuber representation of the general solution of homogeneous Lamé equations in three-dimensional domains in terms of three harmonic functions Ψ, Φ, Λ (cf. References [1,7,26]). Thus in $\hat{G}$ the solution $\hat{\mathbf{u}}$ of the homogeneous Lamé system in Cartesian co-ordinates has the form,

$$\hat{\mathbf{u}} = a\nabla\Psi + 2b\nabla \times (\Phi \mathbf{e}_3) + c(\nabla(x_3\Lambda) - 4(1-\nu)\Lambda \mathbf{e}_3) \tag{12}$$

where ∇ denotes the gradient operator in Cartesian co-ordinates, $\mathbf{e_3}$ is the unit vector in x_3 direction and a, b, c are arbitrary constants. We now seek to find the specific harmonic functions which have the required property. In cylindrical co-ordinates (12) has the form,

$$\begin{pmatrix} u_r \\ u_\varphi \\ u_z \end{pmatrix} = a \begin{pmatrix} \dfrac{\partial \Psi}{\partial r} \\ \dfrac{1}{r}\dfrac{\partial \Psi}{\partial \varphi} \\ \dfrac{\partial \Psi}{\partial z} \end{pmatrix} + 2b \begin{pmatrix} \dfrac{1}{r}\dfrac{\partial \Phi}{\partial \varphi} \\ -\dfrac{\partial \Phi}{\partial r} \\ 0 \end{pmatrix} + c \begin{pmatrix} z\dfrac{\partial \Lambda}{\partial r} \\ z\dfrac{1}{r}\dfrac{\partial \Lambda}{\partial \varphi} \\ z\dfrac{\partial \Lambda}{\partial z} - (3-4v)\Lambda \end{pmatrix} \tag{13}$$

We expand the functions Ψ, Φ, Λ in partial Fourier series with respect to the co-ordinate variable φ in the form,

$$\Psi = \sum_{n=0}^{\infty} (\Psi_n^s(r,z)\cos n\varphi + \Psi_n^a(r,z)\sin n\varphi)$$

By comparing coefficients with the representation of $\mathbf{u}$ according to (7) we obtain the following relation for the solutions $\mathbf{u}_n$ $(n \in \mathbf{N}_0)$ of (8):

$$\begin{pmatrix} u_{rn} \\ u_{\varphi n} \\ u_{zn} \end{pmatrix} = a \begin{pmatrix} \dfrac{\partial \Psi_n}{\partial r} \\ \dfrac{n}{r}\Psi_n \\ \dfrac{\partial \Psi_n}{\partial z} \end{pmatrix} + 2b \begin{pmatrix} -\dfrac{n}{r}\Phi_n \\ -\dfrac{\partial \Phi_n}{\partial r} \\ 0 \end{pmatrix} + c \begin{pmatrix} z\dfrac{\partial \Lambda_n}{\partial r} \\ z\dfrac{n}{r}\Lambda_n \\ z\dfrac{\partial \Lambda_n}{\partial z} - (3-4v)\Lambda_n \end{pmatrix} \tag{14}$$

We introduce for simplicity the 3×3 matrix $\mathbf{B}(R, \theta)$ with columns,

$$\begin{pmatrix} \sin\theta \dfrac{\partial \Psi_n}{\partial R} + \dfrac{\cos\theta}{R}\dfrac{\partial \Psi_n}{\partial \theta} \\ \dfrac{n}{R\sin\theta}\Psi_n \\ -\cos\theta\dfrac{\partial \Psi_n}{\partial R} + \dfrac{\sin\theta}{R}\dfrac{\partial \Psi_n}{\partial \theta} \end{pmatrix}; \quad \begin{pmatrix} -\dfrac{2n}{R\sin\theta}\Phi_n \\ -2\sin\theta\dfrac{\partial \Phi_n}{\partial R} - 2\dfrac{\cos\theta}{R}\dfrac{\partial \Phi_n}{\partial \theta} \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} -R\cos\theta\left(\sin\theta\dfrac{\partial \Lambda_n}{\partial R} + \dfrac{\cos\theta}{R}\dfrac{\partial \Lambda_n}{\partial \theta}\right) \\ -n\cot\theta\Lambda_n \\ -R\cos\theta\left(-\cos\theta\dfrac{\partial \Lambda_n}{\partial R} + \dfrac{\sin\theta}{R}\dfrac{\partial \Lambda_n}{\partial \theta}\right) - (3-4v)\Lambda_n \end{pmatrix}$$

Relation (14) expressed in terms of local polar co-ordinates R, θ has the form,

$$\begin{pmatrix} u_{rn} \\ u_{\varphi n} \\ u_{zn} \end{pmatrix} = \mathbf{B}(R,\theta) \begin{pmatrix} a \\ b \\ c \end{pmatrix} \tag{15}$$

Now, let $T(r,\varphi,z)$, $(r,\varphi,z)\in G$ be a harmonic function in G, i.e. $\triangle_{r\varphi z}T=0$ in G. Suppose the Fourier coefficients $T_n(r,z)$, $(r,z)\in G_a$, $n\in\mathbf{N}_0$, of T have the form $R^{\alpha_n}\Upsilon_{\alpha_n}^{(n)}(\theta)$ with respect to the local co-ordinates R,θ, then the functions $\Upsilon_{\alpha_n}^{(n)}(\theta)$ must satisfy the homogeneous differential equation

$$\frac{\mathrm{d}^2\Upsilon_{\alpha_n}^{(n)}}{\mathrm{d}\theta^2} + \cot\theta\,\frac{\mathrm{d}\Upsilon_{\alpha_n}^{(n)}}{\mathrm{d}\theta} + \left(\alpha_n(\alpha_n+1) - \frac{n^2}{\sin^2\theta}\right)\Upsilon_{\alpha_n}^{(n)} = 0 \tag{16}$$

Equation (16) is the associated Legendre equation and the general solution is given by (cf. References [27,28])

$$\Upsilon_{\alpha_n}^{(n)} = c_1 P_{\alpha_n}^{-n}(\cos\theta) + c_2 Q_{\alpha_n}^{n}(\cos\theta) \tag{17}$$

where $P_{\alpha_n}^{-n}(\cos\theta)$ and $Q_{\alpha_n}^{n}(\cos\theta)$ are the associated Legendre functions of the first and second kind, respectively. But, since the functions T_n are expected to be bounded, we must choose $c_2=0$ in (17) as $Q_{\alpha_n}^{n}(\cos\theta)$ is unbounded at $\cos\theta=\pm 1$. Thus,

$$T_n(r,z) = R^{\alpha_n} P_{\alpha_n}^{-n}(\cos\theta) \tag{18}$$

This suggests that we must choose the functions Ψ, Φ, Λ in (12) such that their Fourier coefficients on G_a have form (18) and such that the solutions $\mathbf{u}_n$ $(n\in\mathbf{N}_0)$ of (8) having form (11) satisfy (15). Thus,

$$\begin{aligned} \Psi_n(r,z) &= R^{\alpha_n+1} P_{\alpha_n+1}^{-n}(\cos\theta) \\ \Phi_n(r,z) &= R^{\alpha_n+1} P_{\alpha_n+1}^{-n}(\cos\theta) \\ \Lambda_n(r,z) &= R^{\alpha_n} P_{\alpha_n}^{-n}(\cos\theta) \end{aligned} \tag{19}$$

We introduce for simplicity the 3×3 matrix $\mathbf{M}_n(\alpha_n,\theta)$ with columns,

$$\begin{pmatrix} (\alpha_n+1)\sin^{-1}\theta P_{\alpha_n+1}^{-n} - (\alpha_n+1-n)\cot\theta P_{\alpha_n}^{-n} \\ n\sin^{-1}\theta P_{\alpha_n+1}^{n} \\ -(\alpha_n+1-n)P_{\alpha_n}^{-n} \end{pmatrix}$$

$$\begin{pmatrix} -2n\sin^{-1}\theta P_{\alpha_n+1}^{-n} \\ -2(\alpha_n+1)\sin^{-1}\theta P_{\alpha_n+1}^{-n} + 2(\alpha_n+1-n)\cot\theta P_{\alpha_n}^{-n} \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} ((\alpha_n+1)-(2\alpha_n+1)\sin^2\theta)\cot\theta P_{\alpha_n}^{-n}-(\alpha_n+n+1)\cos\theta\cot\theta P_{\alpha_n+1}^{-n} \\ -n\cot\theta P_{\alpha_n}^{-n} \\ ((2\alpha_n+1)\cos^2\theta-(3-4v))P_{\alpha_n}^{-n}-(\alpha_n+n+1)\cos\theta P_{\alpha_n+1}^{-n} \end{pmatrix}$$

Substitution of (19) into (15) gives the proof of the following lemma.

Lemma 3.1
Let $\{\alpha_n\}_{n\in\mathbf{N}_0}$ be a sequence of real numbers. Then the Fourier coefficients given by (19) define uniquely harmonic functions Ψ, Φ and Λ in G and the functions

$$\mathbf{u}_n = R^{\alpha_n}\mathbf{U}_n(\alpha_n,\theta) \quad \text{with } \mathbf{U}_n(\alpha_n,\theta) = \mathbf{M}_n(\alpha_n,\theta)\begin{pmatrix} a \\ b \\ c \end{pmatrix} \tag{20}$$

are solutions of the differential equations (8) for any constant vector $(a,b,c)^{\mathrm{T}}$.

Now we determine a non-trivial vector $(a,b,c)^{\mathrm{T}}$ in (20) such that the homogeneous boundary condition at $\theta=\theta_c$ is satisfied, that is

$$\mathbf{M}_n(\alpha_n,\theta_c)\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \mathbf{0} \tag{21}$$

Equation (21) has a non-trivial solution only if

$$\det \mathbf{M}_n(\alpha_n,\theta_c) = 0 \tag{22}$$

The solutions α_n of the transcendental equation (22) are the eigenvalues of the operator pencil in G_a that determines the asymptotic behaviour of the coefficients $\mathbf{u}_n^{s/a}$ $(n\in\mathbf{N}_0)$ near the vertex O. The vector functions $\mathbf{U}_n(\alpha_n,\theta)$ from (20), where the vector $(a,b,c)^{\mathrm{T}}$ is the non-trivial solution of the algebraic equation (21), are the corresponding eigenvector functions to α_n. For $\theta_c\in(0,\pi)$ given, we have,

$$\begin{aligned} \det\mathbf{M}_n = {} & 2(n^2(P_{\alpha_n+1}^{-n})^2-((\alpha_n+1)P_{\alpha_n+1}^{-n}-(\alpha_n-n+1)P_{\alpha_n}^{-n}\cos\theta_c)^2) \\ & \times(-(\alpha_n+n+1)P_{\alpha_n+1}^{-n}\cos\theta_c+P_{\alpha_n}^{-n}(-3+4v+(2\alpha_n+1)\cos^2\theta_c))\sin^{-2}\theta_c \\ & +(-\alpha_n+n-1)P_{\alpha_n}^{-n}\cot\theta_c(2n^2P_{\alpha_n}^{-n}P_{\alpha_n+1}^{-n}\sin^{-1}\theta_c-(-(\alpha_n+n+1)P_{\alpha_n+1}^{-n}\cos\theta_c \\ & +\frac{1}{2}P_{\alpha_n}^{-n}(1+(2\alpha_n+1)\cos 2\theta_c))(2(\alpha_n-n+1)P_{\alpha_n}^{-n}\cot\theta_c \\ & -2(\alpha_n+1)P_{\alpha_n+1}^{-n}\sin^{-1}\theta_c))=0 \end{aligned} \tag{23}$$

For each $n\in\mathbf{N}_0$ and $\theta_c\in(0,\pi)$, the roots of Equation (23) consist of an infinite set $\{\alpha_{n_l}\}_{l\in\mathbf{Z}}$ of isolated real numbers with no accumulation point. At each point (α_{n_l},θ_c) where Equation (23) is satisfied, we seek for a non-trivial vector $(a,b,c)^{\mathrm{T}}$ that satisfies (21), and verify via (20) if $\mathbf{U}_n(\alpha_{n_l},\theta)$ is a non-trivial eigenvector function. We notice, for example, that for any $\theta_c\in(0,\pi)$ and $n\in\mathbf{N}_0$, the number $\alpha_n=n-1$ satisfies Equation (22), but for this eigenvalue there is no corresponding non-trivial eigenvector function. Also, for $\alpha_n=0$, Equation (23) is satisfied for any $\theta_c\in(0,\pi)$, but for this value there is no non-trivial eigenvector function. We also note that the geometric multiplicity of each eigenvalue α_{n_l} is one, that is to each eigenvalue there is only one linearly independent eigenvector function. This is easy to justify, since for there to be two linearly independent eigenvector functions corresponding to the same eigenvalue α_{n_l}, the determinant of the matrix $\mathbf{M}_n$ must vanish at all points (α_{n_l},θ) for $\theta\in(0,\pi)$. This is only possible if $\mathbf{M}_n$ is a null matrix.

We are interested in positive solutions of Equation (23). We assume that for each $n\in\mathbf{N}_0$ the roots $\{\alpha_{n_l}\}_{l\in\mathbf{N}}$ are arranged in ascending order. Firstly, we are interested in the range of values of α_n for which the Fourier coefficients $\mathbf{u}_n^{s/a}$ would exhibit singularities near the vertex O, and secondly to determine which solutions of Equation (23) lie in that range. Of course, Equation (23) cannot be solved by analytical means and we must use numerical means to approximate the solutions. This will be done in the next section. Now by Remark 2.1, we expect regular solutions $\mathbf{u}_n^{s/a}$ of the 2D problem (8) to belong to the space $(W_{1/2}^{2,2}(G_a))^3$. The following lemma gives us a useful criterion for deciding if a function of the form $v(r,z)=R^\alpha T(\theta)$ belongs to the space $W_{1/2}^{2,2}(G_a)$ or not.

Lemma 3.2

Let $v\in W_{1/2}^{1,2}(G_a)$ be a function defined on the circular sector G_a with vertex O, and whose expression in terms of the local polar co-ordinates R,θ is of the form $v(r,z)=R^\alpha T(\theta)$ for some real number $\alpha>0$ and with $T(\theta)\in\mathbf{C}^\infty([0,\pi])$. Then $v\in W_{1/2}^{2,2}(G_a)$ if and only if $\alpha>\frac{1}{2}$.

Proof

The norm $\|v\|_{W_{1/2}^{2,2}(G_a)}$ of functions $v\in W_{1/2}^{2,2}(G_a)$ in local polar co-ordinates R,θ is given by

$$\|v\|_{W_{1/2}^{2,2}(G_a)}=\int_{G_a}\left\{|v|^2+\left|\frac{\partial v}{\partial R}\right|^2+\frac{1}{R^2}\left|\frac{\partial v}{\partial\theta}\right|^2+\left|\frac{\partial^2 v}{\partial R^2}\right|^2\right.$$
$$\left.+2\left|\frac{1}{R}\frac{\partial^2 v}{\partial R\partial\theta}-\frac{1}{R^2}\frac{\partial v}{\partial\theta}\right|^2+\left|\frac{1}{R^2}\frac{\partial^2 v}{\partial\theta^2}+\frac{1}{R}\frac{\partial v}{\partial R}\right|^2\right\}R^2\sin\theta\,\mathrm{d}R\theta \tag{24}$$

We need to show that each term on the right-hand side of (24) is bounded for $v=R^\alpha T(\theta)$ if and only if $\alpha>1/2$. Let us consider the term

$$\int_{G_a}\left|\frac{1}{R}\frac{\partial^2 v}{\partial R\partial\theta}-\frac{1}{R^2}\frac{\partial v}{\partial\theta}\right|^2 R^2\sin\theta\,\mathrm{d}R\theta \tag{25}$$

Substituting $v=R^\alpha T(\theta)$ into (25) and taking into account that $\int_0^\pi|T'(\theta)|^2\sin\theta\,\mathrm{d}\theta<C<\infty$, we get the identity,

$$\int_{G_a}\left|\frac{1}{R}\frac{\partial^2 v}{\partial R\partial\theta}-\frac{1}{R^2}\frac{\partial v}{\partial\theta}\right|^2 R^2\sin\theta\,\mathrm{d}R\theta=(\alpha-1)^2\int_0^\pi|T'(\theta)|^2\sin\theta\,\mathrm{d}\theta\int_0^{R_c}R^{2\alpha-2}\,\mathrm{d}R \tag{26}$$

We see that the integral on the right-hand side of (26) is bounded only if $2\alpha - 2 > -1$, i.e. $\alpha > 1/2$. The same argument holds for the other terms. □

Lemma 3.3
Let $\hat{\mathbf{u}} \in (W_2^1(\hat{\Omega}))^3$ be the generalized solution of the boundary value problem (1), (2) for the right-hand side $\hat{\mathbf{f}} \in (L_2(\hat{\Omega}))^3$. Let $\mathbf{u}_n^s$, $\mathbf{u}_n^a$ and $\mathbf{f}_n^s$, $\mathbf{f}_n^a$ $(n \in \mathbf{N}_0)$ denote the Fourier coefficients of $\hat{\mathbf{u}}$ and $\hat{\mathbf{f}}$, respectively, defined almost everywhere on Ω_a. For each $n \in \mathbf{N}_0$, let α_{n_l} $(l = 1, 2, \ldots)$ denote the positive roots of Equation (23) associated with non-trivial eigenvector functions $\mathbf{U}_n(\alpha_{n_l}, \theta)$. Then

(i) if $\alpha_{n_l} > 1/2$, $l = 1, 2, \ldots$, for all $n \in \mathbf{N}_0$ and $l \in \mathbf{N}$, then the coefficients $\mathbf{u}_n^s$ and $\mathbf{u}_n^a$ satisfy the relations,

$$\mathbf{u}_n^{s/a} \in (W_{1/2}^{2,2}(\Omega))^3, \quad \|\mathbf{u}_n^{s/a}\|_{(W_{1/2}^{2,2}(\Omega_a))^3} \leqslant M_0 \|\mathbf{f}_n^{s/a}\|_{(L_{2,1/2}(\Omega_a))^3} \tag{27}$$

(ii) if $\alpha_{n_l} \leqslant 1/2$, $l = 1, \ldots, L_n$ holds for some coefficients $\mathbf{u}_n^s$ and $\mathbf{u}_n^a$, then there exist real constants $\gamma_{n_l}^s$ and $\gamma_{n_l}^a$ so that these coefficients can be represented in the form,

$$\mathbf{u}_n^{s/a} = \mathbf{s}_n^{s/a} + \mathbf{w}_n^{s/a}, \quad \mathbf{s}_n^{s/a} = \eta(R) \sum_{l=1}^{L_n} \gamma_{n_l}^{s/a} R^{\alpha_{n_l}} \mathbf{U}_n(\alpha_{n_l}, \theta), \quad \mathbf{w}_n^{s/a} \in (W_{1/2}^{2,2}(\Omega_a))^3 \tag{28}$$

$$\sum_{l=1}^{L_n} |\gamma_{n_l}^{s/a}| + \|\mathbf{w}_n^{s/a}\|_{(W_{1/2}^{2,2}(\Omega_a))^3} \leqslant M_1 \|\mathbf{f}_n^{s/a}\|_{(L_{2,1/2}(\Omega_a))^3} \tag{29}$$

In (28) η denotes a smooth cut-off function.

Proof
Lemma 3.3 follows from the preceding analysis and Lemma 3.2 together with classical results regarding the regularity of solutions of elliptic boundary value problems (cf. References [10,12]). Formulas for computing the coefficients $\gamma_{n_l}^{s/a}$ are given, for example, in References [16,17]. □

Remark 3.1
A regularity result for the solution $\hat{\mathbf{u}}$ of the three-dimensional boundary value problem (1), (2) can be obtained from representation (28) of the Fourier coefficients by means of Fourier synthesis. However $\hat{\mathbf{u}} \in (W_2^2(\hat{\Omega}))^3$ cannot be proved by assuming that the Fourier coefficients satisfy the relation $\mathbf{u}_n^{s/a} \in (W_{1/2}^{2,2}(\Omega_a))^3$, $n \in \mathbf{N}_0$. That is if $\alpha_{n_l} \leqslant 1/2$, $n = 0, \ldots, K$, $l = 1, \ldots, L_n$, then the solution $\hat{\mathbf{u}}$ can be represented in the form,

$$\hat{\mathbf{u}} = \hat{\mathbf{u}}_s + \hat{\mathbf{w}}, \quad \hat{\mathbf{u}}_s := \eta(R) \sum_{n=0}^{K} \sum_{l=1}^{L_n} (\gamma_{n_l}^s \mathbb{R}_n^s(\varphi) + \gamma_{n_l}^a \mathbb{R}_n^a(\varphi)) R^{\alpha_{n_l}} \mathbf{U}_n(\alpha_{n_l}, \theta)$$

where the diagonal matrices $\mathbb{R}_n^s(\varphi)$ and $\mathbb{R}_n^a(\varphi)$ $(n \in \mathbf{N}_0, \varphi \in (-\pi, \pi])$ are defined by

$$\mathbb{R}_n^s(\varphi) := \mathrm{diag}[\cos n\varphi, -\sin n\varphi, \cos n\varphi], \quad \mathbb{R}_n^a(\varphi) := \mathrm{diag}[\sin n\varphi, \cos n\varphi, \sin n\varphi]$$

4. NUMERICAL EXPERIMENT

Now we introduce a numerical algorithm with which one can compute the roots of Equation (23). From the computation we are going to answer principally the following three questions:

(a) What is the minimum value of the opening angle θ_c at the conical point of $\hat{\Omega}$ which can affect the regularity of the Fourier coefficients?

(b) How many Fourier coefficients can possibly be affected by the presence of a conical point on $\hat{\Omega}$?

(c) In each case, what is the value of L_n for which $\alpha_{n_l} \leqslant 1/2, \ l = 1, \ldots, L_n$?

We use the Mehler–Dirichlet formula (cf. Reference [28]),

$$P_{\alpha}^{-n}(\cos\theta) = \sqrt{\frac{2}{\pi}} \frac{\sin^{-n}\theta}{\Gamma(n+\frac{1}{2})} \int_0^{\theta} \frac{\cos(\alpha+\frac{1}{2})t}{(\cos t - \cos\theta)^{(1/2)-n}} \, \mathrm{d}t, \quad n \geqslant 0 \tag{30}$$

We notice that the integrand in (30) is singular at $t = \theta$. By trigonometric identity, we can write the integrand in the form,

$$\frac{\cos(\alpha+\frac{1}{2})t}{[-\sin((t+\theta)/2)]^{(1/2)-n}[2\sin((t-\theta)/2)]^{(1/2)-n}} \tag{31}$$

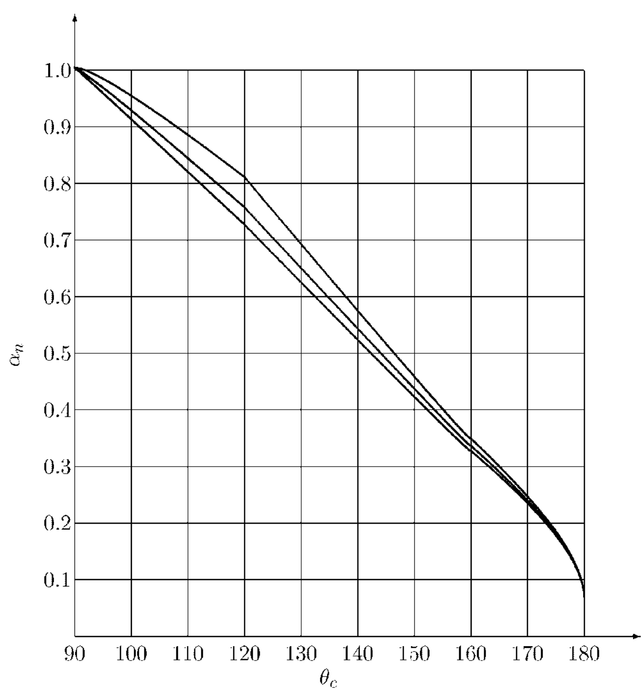

Figure 2. Solutions of (23) for $n = 0$, $v = 0.2$, $v = 0.3$, $v = 0.4$.

Table I. Solutions of (23) for $n = 1$ and selected values for v and θ.

θ	$v = 0.2$	$v = 0.3$	$v = 0.4$
60	0.994145	0.993887	0.993500
100	0.812927	0.806797	0.797492
120	0.553730	0.544059	0.529804
150	0.3234873	0.315972	0.304933
160	0.277894	0.271532	0.262139

and use

$$\frac{\cos(\alpha+\frac{1}{2})t}{[-\sin((t+\theta)/2)]^{(1/2)-n}}(t-\theta)^{n-1/2} \tag{32}$$

to approximate (31) for t close to θ. Using Gauss–Legendre quadrature formula with 45 partition points, integral (30) is approximated by a sum containing the parameter α. The expression is then used in (23) and with a root finding procedure values for α are computed. The softwares MATLAB 6 and MATHEMATCA were used for the computation. From the computation it was established that the Fourier coefficients $\mathbf{u}_n$ for $n \geqslant 2$ of the solution $\hat{\mathbf{u}} \in (W_2^1(\hat{\Omega}))^3$ of (1), (2) belong to $(W_{1/2}^{2,2}(\Omega_a))^3$, for any conical point, whenever the right-hand side $\hat{\mathbf{f}}$ belong to $(L_2(\hat{\Omega}))^3$. Moreover, the effect of the conical points on $\mathbf{u}_1^{s/a}$ is more than on $\mathbf{u}_0^{s/a}$. In both cases the sum in (28) has only one term, i.e. $L_n = 1$ for $n = 0, 1$. The critical angle depends on the Poisson's ratio. Figure 2 shows the dependence of the eigenvalues $0 < \alpha_0 \leqslant 1$ for $n = 0$ on $\theta \in (\pi/2, \pi)$ for different Poisson's ratios. For fixed θ the eigenvalues increase monotonically with respect to the Poisson's ratio v. In Table I the roots α of Equation (23) for a few selected values of θ and for $n = 1$, $v = 0.2, 0.3, 0.4$ are presented. We note that the eigenvalues in this case are lower than the corresponding eigenvalues for $n = 0$ and are monotonically decreasing for increasing v and fixed θ.

ACKNOWLEDGEMENTS

This work was done while the author was visiting the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, under the Junior Associateship Scheme. The visit was sponsored by the Swedish International Development Cooperation Agency (SIDA). The author gratefully acknowledges this support.

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MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:43–57
Published online 23 July 2004 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.548
MOS subject classification: 35 L 35; 74 F 05; 74 G 50

Spatial behaviour of solutions of the dual-phase-lag heat equation

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Communicated by B. Straughan

SUMMARY

In this paper we study the spatial behaviour of solutions of some problems for the dual-phase-lag heat equation on a semi-infinite cylinder. The theory of dual-phase-lag heat conduction leads to a hyperbolic partial differential equation with a third derivative with respect to time. First, we investigate the spatial evolution of solutions of an initial boundary-value problem with zero boundary conditions on the lateral surface of the cylinder. Under a boundedness restriction on the initial data, an energy estimate is obtained. An upper bound for the amplitude term in this estimate in terms of the initial and boundary data is also established. For the case of zero initial conditions, a more explicit estimate is obtained which shows that solutions decay exponentially along certain spatial-time lines. A class of non-standard problems is also considered for which the temperature and its first two time derivatives at a fixed time T are assumed proportional to their initial values. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: dual-phase-lag heat equation; spatial evolution on a semi-infinite cylinder; hyperbolic partial differential equation; third derivative with respect to time

1. INTRODUCTION

It is well known that the usual theory of heat conduction based on Fourier's law predicts infinite heat propagation speed. It is also known that heat transmission at low temperature propagates by means of waves. These aspects have caused intense activity in the field of heat propagation. Extensive reviews on the second sound theories (hyperbolic heat conduction) are given in Reference [1] and in the books of Müller and Ruggeri [2] and Jou *et al.* [3]. A theory of heat conduction in which the evolution equation contains a third-order derivative

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Contract/grant sponsor: U.S. National Science Foundation; contract/grant number: DMS 0202834
Contract/grant sponsor: Spanish Ministry of Science and Technology; contract/grant number: BFM 2003-00309

Received 18 November 2003

with respect to time was proposed in Reference [4]. Several instability results have been obtained for the theory [5,6], as well as proof of the nonexistence of global solutions in the non-linear theory [7].

In 1995, Tzou [8] proposed a theory of heat conduction in which the Fourier law is replaced by an approximation of the equation

$$\mathbf{q}(\mathbf{x}, t+\tau_q) = -k\nabla\theta(\mathbf{x}, t+\tau_\theta), \quad \tau_q > 0, \; \tau_\theta > 0 \tag{1}$$

where τ_q is the phase-lag of the heat flux and τ_θ is the phase-lag of the gradient of temperature. Relation (1) states that the gradient of temperature at a point in the material at time $t+\tau_\theta$ corresponds to the heat flux vector at the same point at time $t+\tau_q$. The delay time τ_θ is caused by microstructural interactions such as phonon scattering or phonon–electron interactions. The delay τ_q is interpreted as the relaxation time due to fast-transient effects of thermal inertia. In this paper, we consider the theory developed by taking a Taylor series expansion on both sides of (1) and retaining terms up to the second-order in τ_q, but only to the first-order in τ_θ. One then obtains Equation (3) or equivalently (5) below.

The model that we consider here (see (5)) involves a partial differential equation with a third-order derivative with respect to time. Such equations have not received much attention in the literature. It is known that, when $\tau_\theta = 0$, solutions of (5) are not determined by means of a semigroup [9] (see p. 125). However in Reference [10], it was established that whenever $\tau_\theta > 0$, one can obtain solutions by means of a semigroup. Thus, the term $\tau_\theta \triangle \dot{\theta}$ plays a role in stabilization for the equation.

A natural question is the determination of the time parameters τ_q and τ_θ (see Reference [11]) and our work is motivated by this question. One might expect that mathematical analysis of existence, uniqueness and stability issues, for example, would furnish certain restrictions on the parameters. One condition to be satisfied by solutions of a heat equation should be exponential stability (or at least stability). In Reference [10], exponential stability was established whenever

$$\tau_\theta > \tau_q/2 \tag{2}$$

Thus, under this condition, one has a theory with a third-order derivative in time that predicts exponential stability. This is of interest in the light of the results obtained in the theory proposed in Reference [4]. By means of several exact solutions instability of solutions was also established in Reference [10] whenever condition (2) is violated. Thus, one may assume that condition (2) must be satisfied in order to use this model to describe heat transmission.

In this paper we study the spatial behaviour of solutions of some problems concerning the dual-phase-lag heat equation on a three-dimensional semi-infinite cylinder R with cross-section D. The finite end face of the cylinder is in the plane $x_3 = 0$. The boundary ∂D is supposed regular enough to allow the use of the divergence theorem. We denote by $R(z)$ the set of points of the cylinder R such that x_3 is greater than z and by $D(z)$ the cross-section of the points such that $x_3 = z$. The spatial evolution with distance from the end for solutions of elliptic equations is relevant to the study of Saint–Venant's principle in continuum mechanics (see, e.g. References [12–15] for reviews of this work). Such results for parabolic equations have also been obtained (see References [12–16]) and more recently for hyperbolic equations (see Reference [17] and the references cited therein).

2. PRELIMINARIES

We consider solutions $\theta(\mathbf{x},t)$ of the heat equation in the theory of dual-phase-lag heat conduction defined by

$$\triangle\hat{\theta} = \dot{\tilde{\theta}} \tag{3}$$

where Δ is the three-dimensional Laplace operator and the superposed dot denotes the derivative with respect to time t. The variables $\mathbf{x}$ and t have been suitably non-dimensionalized. We have used the notation

$$\hat{\theta} = \theta + \tau_\theta\dot{\theta}, \quad \tilde{\theta} = \theta + \tau_q\dot{\theta} + \frac{\tau_q^2}{2}\ddot{\theta} \tag{4}$$

where $\tau_\theta > 0, \tau_q > 0$ are the dimensionless time lag parameters. Equation (3) for the dimensionless temperature $\theta(\mathbf{x},t)$ can be written explicitly as

$$\frac{\tau_q^2}{2}\dddot{\theta} + \tau_q\ddot{\theta} + \dot{\theta} - \tau_\theta\triangle\dot{\theta} - \triangle\theta = 0 \tag{5}$$

We study the qualitative behaviour of classical solutions $\theta(\mathbf{x},t)$ of (5) subject to the initial conditions

$$\theta(\mathbf{x},0) = \theta^0(\mathbf{x}),\ \dot{\theta}(\mathbf{x},0) = \vartheta^0(\mathbf{x}),\ \ddot{\theta}(\mathbf{x},0) = \phi^0(\mathbf{x}) \tag{6}$$

and the boundary conditions

$$\theta(\mathbf{x},t) = 0, \quad \mathbf{x} \in \partial D \times [0,\infty) \tag{7}$$

$$\theta(x_1,x_2,0,t) = f(x_\alpha,t) \text{ on } D(0)\times[0,\infty) \tag{8}$$

where the prescribed boundary data f on the end $x_3 = 0$ is assumed compatible with the initial conditions (6) and f is assumed to vanish on $\partial D(0)\times[0,\infty)$. We will not make any *a priori* assumption regarding the behaviour of solutions as $x_3 \to \infty$. Indeed the analysis to follow will give rise to appropriate hypotheses ensuring that solutions either grow or decay asymptotically.

Observe that in the limit as τ_θ and $\tau_q \to 0$, we recover from (3) or (5) the usual heat equation where, in this limiting case, only the first of (6) is assumed to hold. In this limit, where (5) is *parabolic*, the spatial evolution of solutions has been studied in a variety of contexts (see, e.g. Reference [16] and the references cited therein). When τ_q and τ_θ are positive, it can be shown that (5) is *hyperbolic* and the results to be described in the sequel will be seen to be similar to those obtained previously for such equations (see, e.g. Reference [17] and the references cited therein).

In the course of our calculations, we will use the fact that the eigenvalues of the real symmetric positive definite matrix

$$\begin{pmatrix} a & b \\ b & c \end{pmatrix} \tag{9}$$

are

$$\lambda^{\pm} = \frac{1}{2}\left(a + c \pm \sqrt{(a-c)^2 + 4b^2}\right) \tag{10}$$

so that the smallest eigenvalue is:

$$\lambda^{-} = \frac{1}{2}\left(a + c - \sqrt{(a-c)^2 + 4b^2}\right) \tag{11}$$

We will use (9) in two particular cases. When

$$a = \tau_q + \tau_\theta,\ \ b = \frac{\tau_q^2}{2},\ \ c = \frac{\tau_q^2 \tau_\theta}{2} \tag{12}$$

it can be easily verified on using (2) that the matrix (9) is indeed positive definite and so its smallest positive eigenvalue, denoted by λ_0, is given by

$$\lambda_0 = \frac{1}{2}\left(\tau_q + \tau_\theta + \frac{1}{2}\tau_q^2\tau_\theta - \sqrt{\tau_q^4 + \tau_q^2 + \tau_\theta^2 + \frac{1}{4}\tau_q^4\tau_\theta^2 + 2\tau_q\tau_\theta - \tau_\theta^2\tau_q^2 - \tau_q^3\tau_\theta}\right) \tag{13}$$

When

$$a = 2 + \gamma(\tau_q + \tau_\theta), \quad b = \frac{\gamma}{2}\tau_q^2, \quad c = \frac{\gamma}{2}\tau_q^2\tau_\theta + 2\left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right), \gamma > 0 \tag{14}$$

the matrix (9) is again positive definite with the smallest eigenvalue, denoted by μ_γ, given by

$$\mu_\gamma = \frac{1}{2}\left(2 + \gamma(\tau_q + \tau_\theta) + \frac{\gamma}{2}\tau_q^2\tau_\theta + 2\left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)\right.$$
$$\left. - \sqrt{\left[2 + \gamma(\tau_q + \tau_\theta) - \frac{\gamma}{2}\tau_q^2\tau_\theta - 2\left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)\right]^2 + \gamma^2\tau_q^4}\right) \tag{15}$$

3. NON-ZERO INITIAL CONDITIONS

In this section, we establish results on the spatial evolution of solutions of (5)–(8), provided that the initial data (6) is assumed to be bounded in a certain energy norm.

We begin by considering the measure

$$F(z,t) = -\int_0^t \int_{D(z)} \hat{\theta}_{,3}\tilde{\theta}\,\mathrm{d}A\,\mathrm{d}s \tag{16}$$

From (16) we find that

$$\frac{\partial F(z,t)}{\partial t} = -\int_{D(z)} \hat{\theta}_{,3}\tilde{\theta}\,\mathrm{d}A \tag{17}$$

and, on using (3), the divergence theorem on $D(z)$ and (6), (7), we obtain,

$$\frac{\partial F(z,t)}{\partial z} = -\frac{1}{2}\int_{D(z)}\left((\tilde{\theta})^2 + (\tau_q+\tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}A$$

$$-\int_0^t\int_{D(z)}\left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\mathrm{d}A\,\mathrm{d}s + E_1(z) \tag{18}$$

where

$$E_1(z) = \frac{1}{2}\int_{D(z)}\left((\tilde{\theta}^0)^2 + (\tau_q+\tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right)\,\mathrm{d}A \tag{19}$$

Note that $E_1(z)$ depends on the initial data (6). On re-writing (18) with z replaced by the variable η and on integration with respect to η from 0 to z, we get

$$F(z,t) - F(0,t) = -\frac{1}{2}\int_0^z\int_{D(\eta)}\left((\tilde{\theta})^2 + (\tau_q+\tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}V$$

$$-\int_0^t\int_0^z\int_{D(\eta)}\left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\mathrm{d}V\,\mathrm{d}s$$

$$+\frac{1}{2}\int_0^z\int_{D(\eta)}\left((\tilde{\theta}^0)^2 + (\tau_q+\tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right)\,\mathrm{d}V \tag{20}$$

Our next step is to establish an inequality between the time and spatial derivatives of $F(z,t)$. By virtue of (2), the second integral on the right in (18) is non-negative. The last three terms in the integrand in the first integral on the right in (18) are a quadratic form and may be bounded below on using the smallest positive eigenvalue λ_0 of (9), (12) given in (13). Thus we find that,

$$\frac{\partial F(z,t)}{\partial z} \leqslant -\frac{1}{2}\int_{D(z)}\left((\tilde{\theta})^2 + \lambda_0(|\nabla\theta|^2 + |\nabla\dot{\theta}|^2)\right)\mathrm{d}A + E_1(z) \tag{21}$$

On applying Schwarz's inequality in (17) and on using (4), we get

$$\left|\frac{\partial F}{\partial t}\right| \leqslant \left(\int_{D(z)}(\tilde{\theta})^2\,\mathrm{d}A\right)^{1/2}\left(\int_{D(z)}(\theta_{,3}^2 + \tau_\theta^2\dot{\theta}_{,3}^2 + 2\tau_\theta\theta_{,3}\dot{\theta}_{,3})\,\mathrm{d}A\right)^{1/2}$$

$$\leqslant \sqrt{1+\tau_\theta^2}\left(\int_{D(z)}(\tilde{\theta})^2\,\mathrm{d}A\right)^{1/2}\left(\int_{D(z)}(|\nabla\theta|^2 + |\nabla\dot{\theta}|^2)\,\mathrm{d}A\right)^{1/2}$$

$$\leqslant \frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\lambda_0}}\left(\int_{D(z)}\left((\tilde{\theta})^2 + \lambda_0(|\nabla\theta|^2 + |\nabla\dot{\theta}|^2)\right)\mathrm{d}A\right) \tag{22}$$

where the weighted arithmetic-geometric mean inequality has been employed to obtain each of the last two steps of (22).

In view of (21) we can write (22) as

$$\left|\frac{\partial F}{\partial t}\right| + \beta\frac{\partial F}{\partial z} \leqslant \beta E_1(z) \tag{23}$$

where

$$\beta = \sqrt{\frac{1+\tau_\theta^2}{\lambda_0}} \tag{24}$$

and λ_0 is given explicitly in terms of τ_θ and τ_q in (13).

Inequality (23) implies that

$$\frac{\partial F}{\partial t} + \beta\frac{\partial F}{\partial z} \leqslant \beta E_1(z) \tag{25}$$

and

$$\frac{\partial F}{\partial t} - \beta\frac{\partial F}{\partial z} \geqslant -\beta E_1(z) \tag{26}$$

On integrating (25) and recalling the definition of $E_1(z)$ in (19) we obtain

$$F(z,\beta^{-1}(z-z^*)) \leqslant \frac{1}{2}\int_{z^*}^{z}\int_{D(\eta)}\left((\tilde{\theta}^0)^2 + (\tau_q+\tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right)\,\mathrm{d}V \tag{27}$$

where $z \geqslant z^*$. Similarly on integrating (26) we obtain

$$F(z,\beta^{-1}(z^{**}-z)) \geqslant -\frac{1}{2}\int_{z}^{z^{**}}\int_{D(\eta)}\left((\tilde{\theta}^0)^2 + (\tau_q+\tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right)\,\mathrm{d}V \tag{28}$$

where $z^{**} \geqslant z$.

If we now assume that the initial data (6) is such that

$$\mathscr{E}(0,0) = \frac{1}{2}\int_R\left((\tilde{\theta}^0)^2 + (\tau_q+\tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right)\,\mathrm{d}V < \infty \tag{29}$$

where, by virtue of (4) and (6), we have

$$\tilde{\theta}^0 = \theta^0 + \tau_q\vartheta^0 + \frac{\tau_q^2}{2}\phi^0 \tag{30}$$

then inequalities (27), (28) imply that, for each finite time t,

$$\lim_{z\to\infty} F(z,t) = 0 \tag{31}$$

Thus, we may rewrite

$$F(z,t) = \frac{1}{2}\int_{R(z)} \left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right) \mathrm{d}V$$

$$+ \int_0^t \int_{R(z)} \left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right) \mathrm{d}V\,\mathrm{d}s$$

$$-\frac{1}{2}\int_{R(z)} \left((\tilde{\theta}^0)^2 + (\tau_q + \tau_\theta)|\nabla\theta^0|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\vartheta^0|^2 + \tau_q^2\nabla\theta^0\nabla\vartheta^0\right) \mathrm{d}V \tag{32}$$

Now inequality (25) implies that

$$\mathscr{E}(z,t) \leqslant \mathscr{E}(z^*,0) \tag{33}$$

where

$$\mathscr{E}(z,t) = \frac{1}{2}\int_z^\infty \int_{D(\eta)} \left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right) \mathrm{d}V$$

$$+ \int_0^t \int_z^\infty \int_{D(\eta)} \left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right) \mathrm{d}V\,\mathrm{d}s \tag{34}$$

and z, z^* and t are related by $t = \beta^{-1}(z - z^*)$. In a similar way, we get,

$$\mathscr{E}(z,t) \geqslant \mathscr{E}(z^{**},0) \tag{35}$$

for $t = \beta^{-1}(z^{**} - z)$. From inequalities (33) and (35), we conclude that

$$\mathscr{E}(z,t) \leqslant \mathscr{E}(z^*,t^*) \tag{36}$$

for $|t - t^*| \leqslant \beta^{-1}(z - z^*)$. Thus, we have proved:

Theorem 3.1
Let θ be a solution of the initial-boundary-value problem (5)–(8). Then the energy function $\mathscr{E}(z,t)$ defined in (34) satisfies inequality (36) whenever $|t - t^*| \leqslant \beta^{-1}(z - z^*)$, provided that the initial data satisfy (29).

If one defines the measure

$$\mathscr{E}^*(z,t) = \int_0^t \mathscr{E}(z,s)\,\mathrm{d}s \tag{37}$$

the following inequalities can be obtained as in Reference [17]:

$$\mathscr{E}^*(z,t) \leqslant \beta^{-1}\int_{z-\beta t}^z \mathscr{E}(\eta,0)\,\mathrm{d}\eta, \quad \beta t \leqslant z \tag{38}$$

$$\mathscr{E}^*(z,t) \leqslant \beta^{-1}\int_0^z \mathscr{E}(\eta,0)\,\mathrm{d}\eta + \left(1 - \frac{z}{\beta t}\right)\mathscr{E}^*(0,t), \quad \beta t \geqslant z \tag{39}$$

4. AN UPPER BOUND FOR THE TOTAL ENERGY

To complete the previous estimates it is natural to seek an upper bound for the energy $\mathscr{E}^*(0,t)$ in terms of the initial and boundary data.

From the equality

$$\int_0^t \int_R \tilde{\theta}((\dot{\hat{\theta}}) - \hat{\theta}_{,ii})\, \mathrm{d}V\, \mathrm{d}s = 0 \tag{40}$$

we deduce that

$$\mathscr{E}(0,t) = \mathscr{E}(0,0) - k\int_0^t \int_{D(0)} \hat{\theta}_{,3}\tilde{\theta}\, \mathrm{d}A\, \mathrm{d}s \tag{41}$$

We also consider the identity

$$\int_0^t \int_R \hat{\theta}_{,3}((\dot{\hat{\theta}}) - \hat{\theta}_{,ii})\, \mathrm{d}V\, \mathrm{d}s = 0 \tag{42}$$

We have

$$\begin{aligned}\hat{\theta}_{,3}\dot{\hat{\theta}} &= (\theta_{,3} + \tau_\theta\dot{\theta}_{,3})(\dot{\theta} + \tau_q\ddot{\theta} + \frac{\tau_q^2}{2}\dddot{\theta})\\ &= \frac{\tau_q^2}{2}\frac{\mathrm{d}}{\mathrm{d}s}(\hat{\theta}_{,3}\ddot{\theta}) - \frac{\tau_q^2}{2}\left(\dot{\theta}_{,3}\ddot{\theta} + \frac{\tau_\theta}{2}\frac{\mathrm{d}}{\mathrm{d}x_3}(\ddot{\theta})^2\right) + \tau_q\frac{\mathrm{d}}{\mathrm{d}s}(\theta_{,3}\dot{\theta}) - \frac{\tau_q}{2}\frac{\mathrm{d}}{\mathrm{d}x_3}(\dot{\theta})^2 + \tau_q\tau_\theta\dot{\theta}_{,3}\ddot{\theta}\\ &\quad + \theta_{,3}\dot{\theta} + \frac{\tau_\theta}{2}\frac{\mathrm{d}}{\mathrm{d}x_3}(\dot{\theta})^2\end{aligned} \tag{43}$$

By virtue of (8), we have

$$\theta(x_\alpha,t) = f(x_\alpha,t),\ \ \dot{\theta}(x_\alpha,t) = \dot{f}(x_\alpha,t),\ \ \ddot{\theta}(x_\alpha,t) = \ddot{f}(x_\alpha,t) \quad \text{on } D(0)\times[0,\infty) \tag{44}$$

For convenience of notation, we write

$$f(x_\alpha,t) = l,\ \ \dot{f}(x_\alpha,t) = m,\ \ \ddot{f}(x_\alpha,t) = n \tag{45}$$

where l, m, n are prescribed functions. We have

$$\begin{aligned}\int_0^t \int_R \hat{\theta}_{,3}\dot{\hat{\theta}}\, \mathrm{d}V\, \mathrm{d}s &= \frac{\tau_q^2}{2}\left(\int_R \hat{\theta}_{,3}\ddot{\theta}\, \mathrm{d}V\, \mathrm{d}s - \int_R (\theta^0_{,3} + \tau_\theta\vartheta^0_{,3})\phi^0\, \mathrm{d}V\right) + \left(\tau_q\tau_\theta - \frac{\tau_q^2}{2}\right)\int_0^t \int_R \dot{\theta}_{,3}\ddot{\theta}\, \mathrm{d}V\, \mathrm{d}s\\ &\quad + \int_0^t \int_{D(0)} \left(\frac{\tau_q^2\tau_\theta}{4}n^2 + \frac{\tau_q - \tau_\theta}{2}m^2\right) \mathrm{d}A\, \mathrm{d}s + \tau_q\int_R \theta_{,3}\dot{\theta}\, \mathrm{d}V\\ &\quad - \tau_q\int_R \theta^0_{,3}\vartheta^0\, \mathrm{d}V + \int_0^t \int_R \theta_{,3}\dot{\theta}\, \mathrm{d}V\, \mathrm{d}s\end{aligned} \tag{46}$$

From (42) and (46), it follows that,

$$
\begin{aligned}
\int_0^t \int_{D(0)} \hat{\theta}_{,3}^2 \,\mathrm{d}A\,\mathrm{d}s = & \int_0^t \int_{D(0)} (l_{,\alpha} + \tau_\theta n_{,\alpha})(l_{,\alpha} + \tau_\theta n_{,\alpha})\,\mathrm{d}A\,\mathrm{d}s \\
& -\tau_q^2 \left(\int_R \hat{\theta}_{,3}\ddot{\theta}\,\mathrm{d}V\,\mathrm{d}s - \int_R (\theta_{,3}^0 + \tau_\theta \vartheta_{,3}^0)\phi^0\,\mathrm{d}V \right) \\
& -(2\tau_q\tau_\theta - \tau_q^2) \int_0^t \int_R \dot{\theta}_{,3}\ddot{\theta}\,\mathrm{d}V\,\mathrm{d}s \\
& - \int_0^t \int_{D(0)} \left(\frac{\tau_q^2 \tau_\theta}{2} n^2 + (\tau_q - \tau_\theta) m^2 \right) \mathrm{d}A\,\mathrm{d}s - 2\tau_q \int_R \theta_{,3}\dot{\theta}\,\mathrm{d}V \\
& +2\tau_q \int_R \theta_{,3}^0 \vartheta^0\,\mathrm{d}V - 2\int_0^t \int_R \theta_{,3}\dot{\theta}\,\mathrm{d}V\,\mathrm{d}s
\end{aligned}
\tag{47}
$$

From (47) one can obtain constants $c_i, i = 1, ..4$ such that

$$
\begin{aligned}
\int_0^t \int_{D(0)} \hat{\theta}_{,3}^2 \,\mathrm{d}A\,\mathrm{d}s = & \int_0^t \int_{D(0)} (l_{,\alpha} + \tau_\theta n_{,\alpha})(l_{,\alpha} + \tau_\theta n_{,\alpha})\,\mathrm{d}A\,\mathrm{d}s \\
& +c_1\mathscr{E}(0,t) + \tau_q^2 \int_R (\theta_{,3}^0 + \tau_\theta \vartheta_{,3}^0)\phi^0\,\mathrm{d}V + c_2 \int_0^t \mathscr{E}(0,s)\,\mathrm{d}s \\
& - \int_0^t \int_{D(0)} \left(\frac{\tau_q^2 \tau_\theta}{2} n^2 + (\tau_q - \tau_\theta) m^2 \right) \mathrm{d}A\,\mathrm{d}s + c_3\mathscr{E}(0,t) \\
& +2\tau_q \int_R \theta_{,3}^0 \vartheta^0\,\mathrm{d}V + c_4\mathscr{E}(0,t)
\end{aligned}
\tag{48}
$$

In view of (41), (48) and on using the arithmetic-geometric mean inequality with weight ε (for $\varepsilon > 0$) we obtain the inequality

$$
\begin{aligned}
\mathscr{E}(0,t) \leqslant \mathscr{E}(0,0) & + \frac{1}{2\varepsilon} \int_0^t \int_{D(0)} \left(l + \tau_q m + \frac{\tau_q^2}{2} n \right)^2 \mathrm{d}A\,\mathrm{d}s \\
& + \frac{\varepsilon}{2} \left(\int_0^t \int_{D(0)} (l_{,\alpha} + \tau_\theta n_{,\alpha})(l_{,\alpha} + \tau_\theta n_{,\alpha})\,\mathrm{d}A\,\mathrm{d}s + \tau_q^2 \int_R (\theta_{,3}^0 + \tau_\theta \vartheta_{,3}^0)\phi^0\,\mathrm{d}V \right. \\
& - \int_0^t \int_{D(0)} \left(\frac{\tau_q^2 \tau_\theta}{2} n^2 + (\tau_q - \tau_\theta) m^2 \right) \mathrm{d}A\,\mathrm{d}s \\
& \left. +2\tau_q \int_R \theta_{,3}^0 \vartheta^0\,\mathrm{d}V + d\mathscr{E}(0,t) + c_2 \int_0^t \mathscr{E}(0,s)\,\mathrm{d}s \right)
\end{aligned}
\tag{49}
$$

where $d = c_1 + c_3 + c_4$. After a quadrature, we obtain

$$\begin{aligned}\mathscr{E}^*(0,t) \leqslant tP_\varepsilon + \frac{1}{2\varepsilon}\int_0^t\int_0^s\int_{D(0)}\left(l+\tau_q m+\frac{\tau_q^2}{2}n\right)^2 \mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\\ +\frac{\varepsilon}{2}\left(\int_0^t\int_0^s\int_{D(0)}(l_{,\alpha}+\tau_\theta n_{,\alpha})(l_{,\alpha}+\tau_\theta n_{,\alpha})\,\mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\right.\\ \left.-\int_0^t\int_0^s\int_{D(0)}\left(\frac{\tau_q^2\tau_\theta}{2}n^2+(\tau_q-\tau_\theta)m^2\right)\mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\right)\\ +\frac{\varepsilon}{2}(c_2 t+d)\mathscr{E}^*(0,t)\end{aligned} \tag{50}$$

where

$$P_\varepsilon = \mathscr{E}(0,0) + \frac{\varepsilon}{2}\left(\tau_q^2\int_R(\theta_{,3}^0+\tau_\theta\vartheta_{,3}^0)\phi^0\,\mathrm{d}V + 2\tau_q\int_R\theta_{,3}^0\vartheta^0\,\mathrm{d}V\right) \tag{51}$$

If we take $\varepsilon = (c_2 t + d)^{-1}$, it follows that

$$\begin{aligned}\mathscr{E}^*(0,t) \leqslant 2tP_{(c_2t+d)^{-1}} + (c_2t+d)\int_0^t\int_0^s\int_{D(0)}\left(l+\tau_q m+\frac{\tau_q^2}{2}n\right)^2\mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\\ +(c_2t+d)^{-1}\left(\int_0^t\int_0^s\int_{D(0)}(l_{,\alpha}+\tau_\theta n_{,\alpha})(l_{,\alpha}+\tau_\theta n_{,\alpha})\,\mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\right.\\ \left.-\int_0^t\int_0^s\int_{D(0)}\left(\frac{\tau_q^2\tau_\theta}{2}n^2+(\tau_q-\tau_\theta)m^2\right)\mathrm{d}A\,\mathrm{d}\tau\,\mathrm{d}s\right)\end{aligned} \tag{52}$$

which gives the desired upper bound for the amplitude term $\mathscr{E}^*(0,t)$ appearing in (39) in terms of the initial and boundary data.

5. ZERO INITIAL CONDITIONS

In this section, we study the spatial behaviour of solutions of (5) subject to the boundary conditions (7), (8) and *homogeneous* initial conditions.

In this situation we define the function

$$F_\gamma(z,t) = -\int_0^t\int_{D(z)}\exp(-\gamma s)\hat{\theta}_{,3}\tilde{\theta}\,\mathrm{d}A\,\mathrm{d}s \tag{53}$$

where $\gamma > 0$ is an arbitrary positive constant. We have

$$F_\gamma(z,t) = F_\gamma(0,t) - \frac{1}{2}\int_0^z \int_{D(\eta)} \exp(-\gamma t)\left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}V$$
$$-\frac{\gamma}{2}\int_0^t\int_0^z\int_{D(\eta)} \exp(-\gamma s)\left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}V\,\mathrm{d}s$$
$$-\int_0^t\int_0^z\int_{D(\eta)} \exp(-\gamma s)\left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\,\mathrm{d}V\,\mathrm{d}s \tag{54}$$

On using arguments similar of those of Section 3, we obtain,

$$\left|\frac{\partial F_\gamma}{\partial t}\right| + \beta\frac{\partial F_\gamma}{\partial z} \leqslant 0 \tag{55}$$

where β is given in (24). Inequality (55) is the counterpart of (23) for the case of zero initial data.

Inequality (55) implies that

$$\frac{\partial F_\gamma}{\partial t} + \beta\frac{\partial F_\gamma}{\partial z} \leqslant 0, \quad \frac{\partial F_\gamma}{\partial t} - \beta\frac{\partial F_\gamma}{\partial z} \geqslant 0 \tag{56}$$

As in Section 3, we can establish the analog of (31) for F_γ. Thus, we can write

$$F_\gamma(z,t) = \frac{1}{2}\int_{R(z)} \exp(-\gamma t)\left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}V$$
$$+\frac{\gamma}{2}\int_0^t\int_{R(z)} \exp(-\gamma s)\left((\tilde{\theta})^2 + (\tau_q + \tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\,\mathrm{d}V\,\mathrm{d}s$$
$$+\int_0^t\int_{R(z)} \exp(-\gamma s)\left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\,\mathrm{d}V\,\mathrm{d}s \tag{57}$$

We also obtain the analog of (33), that is,

$$F_\gamma(z,t) \leqslant F_\gamma(z^*,0) \tag{58}$$

for $t = \beta^{-1}(z - z^*)$. Since the initial conditions are homogeneous, we see that $F_\gamma(z,t) = 0$ whenever $t \leqslant \beta^{-1}z$.

Next, we obtain the main spatial estimate of this section. To this end we estimate the absolute value of F_γ in terms of its derivative with respect to a space–time direction. On using Schwarz's inequality in (53), and recalling the notation (4), we get

$$|F_\gamma| \leqslant \left(\int_0^t\int_{D(z)} \exp(-\gamma s)(\tilde{\theta})^2\,\mathrm{d}A\,\mathrm{d}s\right)^{1/2}$$
$$\times\left(\int_0^t\int_{D(z)} \exp(-\gamma s)(|\nabla\theta|^2 + \tau_\theta^2|\nabla\dot{\theta}|^2 + 2\tau_\theta\nabla\theta\nabla\dot{\theta})\,\mathrm{d}A\,\mathrm{d}s\right)^{1/2} \tag{59}$$

On twice using the weighted arithmetic-geometric mean inequality we find from (59) that

$$|F_\gamma| \leqslant \sqrt{1+\tau_\theta^2}\left(\int_0^t \int_{D(z)} \exp(-\gamma s)(\tilde{\theta})^2\, \mathrm{d}A\, \mathrm{d}s\right)^{1/2}\left(\int_0^t \int_{D(z)} \exp(-\gamma s)(|\nabla\theta|^2+|\nabla\dot{\theta}|^2)\, \mathrm{d}A\, \mathrm{d}s\right)^{1/2}$$

$$\leqslant \frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\gamma\mu_\gamma}}\left(\int_0^t \int_{D(z)} \exp(-\gamma s)\left(\gamma(\tilde{\theta})^2+\mu_\gamma(|\nabla\theta|^2+|\nabla\dot{\theta}|^2)\right)\, \mathrm{d}A\, \mathrm{d}s\right)$$

We now employ the inequality

$$\left(\gamma(\tilde{\theta})^2+\mu_\gamma(|\nabla\theta|^2+|\nabla\dot{\theta}|^2)\right)$$
$$\leqslant \gamma\left((\tilde{\theta})^2+(\tau_q+\tau_\theta)|\nabla\theta|^2+\frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2+\tau_q^2\nabla\theta\nabla\dot{\theta}\right)+2\left(|\nabla\theta|^2+\left(\tau_\theta\tau_q-\frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)$$

which is a consequence of the positiveness definiteness of matrix (9) with the choice (14), with smallest eigenvalue given by (15). Thus we find that

$$|F_\gamma| \leqslant \frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\gamma\mu_\gamma}}\left(\left|\frac{\partial F_\gamma}{\partial t}\right| - \beta\frac{\partial F_\gamma}{\partial z}\right) \tag{60}$$

where the constant μ_γ is given explicitly in (15), and β is given in (24). On letting τ measure distance along a line

$$\beta(t-t^*)=z \tag{61}$$

inequality (60) implies that

$$\frac{\partial F_\gamma}{\partial \tau}+2\sqrt{\frac{\gamma\mu_\gamma}{(1+\tau_\theta^2)(1+\beta^2)}}F_\gamma \leqslant 0 \tag{62}$$

An integration from the point $(0,t^*)$ to the point (z,t) along the line (61) leads to

$$F_\gamma(z,t) \leqslant F_\gamma(0,t^*)\exp\left(-2\sqrt{\frac{\gamma\mu_\gamma}{1+\tau_\theta^2}}z\right) \tag{63}$$

On recalling the definition of $\mathscr{E}$ in (34), we may write

$$\mathscr{E}(z,t) \leqslant \exp(\gamma t)F_\gamma(z,t) \leqslant \exp(\gamma t)F_\gamma(0,t^*)\exp\left(-2\sqrt{\frac{\gamma\mu_\gamma}{1+\tau_\theta^2}}z\right) \tag{64}$$

On using (61), we thus obtain

$$\mathscr{E}(z,t) \leqslant \exp(\gamma t^*)F(0,t^*)\exp\left(\left(\beta^{-1}\gamma-2\sqrt{\frac{\gamma\mu_\gamma}{1+\tau_\theta^2}}\right)z\right) \tag{65}$$

The constant $\gamma>0$ is an arbitrary constant. We may now choose γ small enough so that the quantity

$$\beta^{-1}\gamma-2\sqrt{\frac{\gamma\mu_\gamma}{(1+\tau_\theta^2)}} \tag{66}$$

is negative. This implies that the energy decays exponentially along the line (61). A similar estimate was obtained by Song [18] for the hyperbolic heat equation with dissipation where the lines intersect the region where it is known that the solution vanishes, but this is not required in our analysis.

We note that the foregoing analysis may be readily modified to obtain results for the backward in time problem.

6. A NON-STANDARD PROBLEM FOR (5)

In this section, we briefly discuss the behaviour of solutions of (5) subject to the boundary conditions (7), (8) and the non-standard conditions

$$\theta(\mathbf{x},T)=\alpha_1\theta(\mathbf{x},0),\ \ \dot{\theta}(\mathbf{x},T)=\alpha_2\dot{\theta}(\mathbf{x},0),\ \ \ddot{\theta}(\mathbf{x},T)=\alpha_3\ddot{\theta}(\mathbf{x},0) \tag{67}$$

where α_i, $i=1,2,3$ are positive constants such that $\alpha_i>1$. Such non-standard conditions have been the subject of much recent attention (see, e.g. References [18–20] in the context of the heat equation, [21] for generalized heat conduction and [22] for viscous flows). For simplicity here, we consider the special case of (67) where

$$\alpha_1=\alpha_2=\alpha_3=\alpha \tag{68}$$

A more elaborate analysis would be required in the general case. The boundary data in (8) is assumed compatible with (67), (68).

The analysis begins by considering the function

$$F_\gamma(z)=-\int_0^T\int_{D(z)}\exp(-\gamma s)\hat{\theta}_{,3}\tilde{\theta}\,\mathrm{d}A\,\mathrm{d}s \tag{69}$$

where, guided by results established in References [18–20], the positive constant γ is given by

$$\gamma=\frac{2}{T}\ln\alpha \tag{70}$$

We have

$$\begin{aligned}F_\gamma(z)=F_\gamma(0)&+\frac{\gamma}{2}\int_0^T\int_0^z\int_{D(\eta)}\exp(-\gamma s)\left((\tilde{\theta})^2+(\tau_q+\tau_\theta)|\nabla\theta|^2+\frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2+\tau_q^2\nabla\theta\nabla\dot{\theta}\right)\mathrm{d}V\,\mathrm{d}s\\&+\int_0^T\int_0^z\int_{D(\eta)}\exp(-\gamma s)\left(|\nabla\theta|^2+\left(\tau_\theta\tau_q-\frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\mathrm{d}V\,\mathrm{d}s\end{aligned} \tag{71}$$

An argument similar to the one used in the previous section leads to the estimate

$$|F_\gamma|\leqslant\frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\gamma\mu_\gamma}\frac{\partial F_\gamma}{\partial z}} \tag{72}$$

This inequality is well-known in the study of spatial decay estimates. It implies that

$$F_\gamma \leqslant \frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\gamma\mu_\gamma}}\,\frac{\partial F_\gamma}{\partial z} \quad \text{and} \quad -F_\gamma \leqslant \frac{1}{2}\sqrt{\frac{(1+\tau_\theta^2)}{\gamma\mu_\gamma}}\,\frac{\partial F_\gamma}{\partial z} \tag{73}$$

From (73), we can obtain an alternative of Phragmen–Lindelof type which states (see Reference [23]) that the solutions either grow exponentially for z sufficiently large or solutions decay exponentially in the form,

$$\mathscr{E}_\gamma(z) \leqslant \mathscr{E}_\gamma(0)\exp\left(-2\sqrt{\frac{\gamma\mu_\gamma}{(1+\tau_\theta^2)}}z\right) \tag{74}$$

for all $z \geqslant 0$, where

$$\begin{aligned}\mathscr{E}_\gamma(z) = {} & \frac{\gamma}{2}\int_0^T \int_{R(z)} \exp(-\gamma s)\left((\tilde{\theta})^2 + (\tau_q+\tau_\theta)|\nabla\theta|^2 + \frac{1}{2}\tau_q^2\tau_\theta|\nabla\dot{\theta}|^2 + \tau_q^2\nabla\theta\nabla\dot{\theta}\right)\mathrm{d}V\,\mathrm{d}s \\ & + \int_0^T \int_{R(z)} \exp(-\gamma s)\left(|\nabla\theta|^2 + \left(\tau_\theta\tau_q - \frac{1}{2}\tau_q^2\right)|\nabla\dot{\theta}|^2\right)\mathrm{d}V\,\mathrm{d}s\end{aligned} \tag{75}$$

The decay rate in (74) depends explicitly on γ given in (70) and on τ_q, τ_θ.

ACKNOWLEDGEMENTS

The research of C.O.H. was supported by the U.S. National Science Foundation under Grant DMS 0202834. The work was initiated during a visit of C.O.H. to the Universidad Politécnica de Catalunya in March 2003. The hospitality of the Departmento Matemática Aplicada 2 at U.P.C. is gratefully acknowledged. The research of R.Q. was supported by the Spanish Ministry of Science and Technology under project 'Aspects of Stability in Thermomechanics' (BFM 2003-00309). We are grateful to P.W. Schaefer for supplying preprints prior to publication.

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MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:59–76
Published online 13 July 2004 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.549
MOS subject classification: 35 K 20; 35 K 60; 80 A 22

A sharp interface model for phase transitions in crystals with linear elasticity

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Communicated by W. Sprößig

SUMMARY

A model describing phase transitions coupled with diffusion and linear elasticity in crystals under isothermal conditions is introduced. The elastic deformation as well as the phase parameter are obtained directly by the minimization of the free energy. After stating the model, the existence of strong solutions is proved. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: phase change problems; free boundary problems; non-linear PDE of parabolic type

1. INTRODUCTION

The model introduced here represents a crystal for fixed temperature where n different species of molecules diffuse and where two phases may coexist. The elastic behaviour is described by a linear approximation. The model is related to the Stefan model but allows for deformation and considers an isothermal setting without diffusion of latent heat. For a survey of results on the Stefan problem see References [1,2]. The present article is part of a larger program to bring forward the understanding of mechanics of multi-phase structures in solids. In Reference [3] the case of non-linear deformations is analysed imposing suitable growth conditions on the gradient of the deformation. The techniques in Reference [3] are fully non-linear and exclude the case of linear elasticity treated here. In Reference [4] the model of this article is studied numerically in two space dimensions making use of a level set method to find the local minimum of the free energy w.r.t. the phase parameter.

The existence result shown in Section 9 will, in particular, imply that even though the density function may jump across a phase transition the chemical potential remains a smooth function. This allows to set up jump conditions and is crucial for the numerical treatment

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 Received 24 October 2003

of the model. The structure of the existence proof pursued in this paper follows Reference [5]. The main modifications arise from the additional formulation as a minimum in the phase parameter, see Equation (10) below, and from the fact that no regularizing gradient term of the concentration vector occurs. The general outline of the approach is related to the earlier work [6]. The idea of approximation by a discrete scheme and showing compactness in time is classical and goes back to Leray [7].

This work is organized in the following way. In Section 2, the model is derived and the physical assumptions for the validity of the model are listed. Section 3 provides the necessary notations and function spaces.

Starting from the time-discrete solution, uniform bounds are derived and the discrete solution is extended by linear interpolation. This is first done for polynomial free energies f_l and the existence of global solutions in Section 9 is only valid for polynomial f_l. Using these results, in Sections 10–12 the existence proof is extended to logarithmic free energies that become singular as the density of one component approaches 0 or 1.

2. DERIVATION OF THE MODEL

Let $\Omega \subset \mathbb{R}^D$, $1 \leqslant D \leqslant 3$ be the bounded domain of reference, $\Phi : \mathbb{R}^D \times \mathbb{R}_{\geqslant 0} \longrightarrow \mathbb{R}^D$ a deformation. $\Phi(\Omega, t)$ defines the crystal at time t, $x \in \Omega$ are the Lagrange co-ordinates.

Instead of Φ we will use the displacement vector u, where

$$\Phi(t) = \mathrm{Id} + u(t)$$

$\Omega = \Phi(\Omega, 0)$ is the unstrained body, which goes along with $u(t=0)=0$.

The particle densities of the n different species of molecules are determined by $\varrho_i = \varrho_i(x,t)$. Let $\varrho := (\varrho_1, \dots, \varrho_n)$. The densities fulfil for $1 \leqslant i \leqslant n$

$$\varrho_i \geqslant 0, \varrho_i \in H^{1,2}(\Omega), \quad \int_\Omega \varrho_i(x,t)\,\mathrm{d}x = \int_\Omega \varrho_{i_0}(x)\,\mathrm{d}x$$

with given initial values ϱ_{i_0} and, due to the possible presence of vacancies,

$$\sum_{i=1}^n \varrho_i \leqslant 1$$

This reflects the possibility that some positions in the lattice crystal are not occupied by particles.

By $H^{m,2}(\Omega)$ we denote the Sobolev space of m-times weakly differentiable functions in the Hilbert space $L^2(\Omega)$, by $H_0^{m,2}(\Omega)$ the closure of $C_0^\infty(\Omega)$ w.r.t. $\|\cdot\|_{H^{1,2}(\Omega)}$ and by $\mathrm{BV}(\Omega)$ the space of functions with bounded variation, see for instance Reference [8]. By $\|\cdot\|_{H^1}$ and $\|\cdot\|_{\mathrm{BV}}$ we always mean $\|\cdot\|_{H^{1,2}(\Omega)}$ and $\|\cdot\|_{\mathrm{BV}(\Omega)}$. $C_0^\infty(\Omega) := \bigcap_{m=0}^\infty C_0^m(\Omega)$ where $C_0^m(\Omega)$ is the space of m-times continuously differentiable functions over Ω with compact support.

Since we are concerned with two-phase structures we introduce $\chi = \chi(\cdot, t) \in X_2$, where

$$X_2 := \{\chi' \in \mathrm{BV}(\Omega) \,|\, \chi'(1-\chi') = 0 \text{ almost everywhere in } \Omega\}$$

$f_j = f_j(\varrho, u)$ denotes the free energy density of phase j, $j = 1, 2$. f_j are smooth functions and convex in ϱ; possible examples are

$$f_j(\varrho, u) := \tfrac{1}{2}(\varrho - \bar{\varrho}_j)^2 + W^{\mathrm{el}}(\varrho, u) \tag{1}$$

$$f_j(\varrho, u) := \alpha_j \sum_{i=1}^{n} \varrho_i \ln \varrho_i + W^{\mathrm{el}}(\varrho, u) \tag{2}$$

The coefficients α_j will in general depend on temperature T which is kept constant here. W^{el} in (1), (2) is the elastic energy density, i.e. the contribution of the deformation to the free energy. It was first studied by Eshelby [9].

W^{el} can by Hooke's law be computed to

$$W^{\mathrm{el}}(\varrho, u) := \tfrac{1}{2}(\mathscr{E}(u) - \bar{\varepsilon}(\varrho)) : C(\varrho)(\mathscr{E}(u) - \bar{\varepsilon}(\varrho)) \tag{3}$$

where

$$\mathscr{E} = \mathscr{E}(u) = \mathscr{E}_{ij}(u) := \tfrac{1}{2}(\partial_i u_j + \partial_j u_i)$$

is the elasticity tensor. If e denotes the lattice misfit we assume the linear relationship (*Vegard's law*)

$$\bar{\varepsilon}(\varrho) := e\varrho \, \mathrm{Id} \tag{4}$$

$C(\varrho)$ is the elasticity tensor that maps symmetric tensors in $\mathbb{R}^{D \times D}$ onto itself. We assume that C is symmetric, positive definite and does not depend on χ. $\bar{\varepsilon}(\varrho)$ is the eigenstrain at density ϱ. Under the assumptions that lead to Equation (4) the eigenstrain $\bar{\varepsilon}$ is uniquely defined.

Since the system free energy density f is the convex hull of f_1, f_2, we define f as the convex combination

$$f = \chi f_1 + (1 - \chi) f_2$$

The interfacial surface energy for given surface tension $\sigma > 0$ is

$$F_{\mathrm{S}}(\chi(t)) = \sigma \int_\Omega |\nabla \chi(x, t)| \, \mathrm{d}x$$

Thus, if the surface energy is bounded the total variation of χ in Ω is bounded, too. The term

$$F^{\mathrm{out}}(u) := \int_\Omega \overline{W}(\mathscr{E}(u))$$

represents energy effects due to applied outer forces. We assume that there are no body forces and that the tractions applied to $\partial\Omega$ are dead loads and equal $\overline{S}\mathbf{n}$, where $\mathbf{n}$ is the unit outer normal to $\partial\Omega$. We assume that the symmetric tensor $\overline{S}$ defined by this property is constant, i.e. independent of time. The work necessary to transform $\Omega = \Phi(\Omega, 0)$ to $\Phi(\Omega, t)$ with corresponding displacement vector $u(t)$ is therefore

$$-\int_{\partial\Omega} u \cdot \overline{S}\mathbf{n} = -\int_\Omega \nabla u : \overline{S} = -\int_\Omega \mathscr{E}(u) : \overline{S}$$

and we find that $\overline{W}(\mathscr{E}(u)) := -\mathscr{E}(u) : \overline{S}$ describes the energy density of the applied outer forces.

The deformation in the non-linear model [3] is computed by taking the infimum of f over all allowed deformations. In the case of linear elasticity we can simplify this. The displacement u is obtained by solving the elliptic equation

$$\operatorname{div}(S) = 0 \quad \text{in } \Omega$$

with the stress tensor

$$S := \partial_\varepsilon W^{\text{el}}(\varrho, \mathscr{E}(u))$$

So the system free energy obeys the formula

$$F(\varrho(t), \chi(t), u(t)) = F_S(\chi(t)) + F^{\text{out}}(u(t)) + \int_\Omega \chi(t) f_1(\varrho(t), u(t)) + (1-\chi(t)) f_2(\varrho(t), u(t))\,\mathrm{d}x \tag{5}$$

The diffusive flow is caused by the gradient of the chemical potentials. By Onsager's law, the flux J is given by

$$J(t) = L\nabla\mu(t)$$

where $\nabla\mu := (\nabla\mu_1, \ldots, \nabla\mu_n)$ and L is the $n \times n$ mobility tensor. L is positive semi-definite, but in order to avoid degenerate cases we will assume in the sequel that L is positive definite.

Hence, for a given stop time $T_0 > 0$ we end up with the following model:

Find for $t \geqslant 0$ the vector (ϱ, χ, μ, u) such that in $\Omega_{T_0} := \Omega \times (0, T_0)$

$$\partial_t \varrho = \operatorname{div}(L\nabla\mu) \tag{6}$$

$$\mu = \frac{\partial f}{\partial \varrho} \tag{7}$$

$$\operatorname{div}(S) = 0 \tag{8}$$

$$S = \partial_\varepsilon W^{\text{el}}(\varrho, \mathscr{E}(u)) \tag{9}$$

$$F(\varrho(t), \chi(t), u(t)) = \min_{\tilde{\chi} \in X_2} F(\varrho(t), \tilde{\chi}, u(t)) \tag{10}$$

with the initial data for $t = 0$ in Ω

$$\varrho(\cdot, 0) = \varrho_0(\cdot) \tag{11}$$

and for $t > 0$ in $\partial\Omega$

$$\varrho = \varrho_d, \quad \mu = \mu_d, \quad S\mathbf{n} = \overline{S}\mathbf{n} \tag{12}$$

Remarks

- Instead of the Dirichlet boundary condition on ϱ and μ, other conditions as Neumann conditions or periodic conditions are as well possible in (12).
- Equation (10) does not control the variation of χ in time.
- In other models an evolution equation like

$$\tau \partial_t \chi = -\frac{\partial F}{\partial \chi}(\varrho, \chi, u)$$

  for a given constant governs χ. Here, χ may get stuck in a local minimum whereas Equation (10) means that the phase parameter is a global minimizer.
- Simple examples show that the solutions of (6)–(12) are in general not unique due to an ambiguity in χ.
- The existence of a minimum in Equation (10) w.r.t. χ is guaranteed by the Poincaré inequality and the term $\sigma|\nabla\chi|$.

3. PRELIMINARIES TO THE EXISTENCE PROOF

In the remaining sections, we discuss the existence theory to the sharp interface model (6)–(12). We will show that under suitable growth conditions on the free energy density, collected in Section 6 and for logarithmic energies in Section 10, discrete solutions to the implicit time discretization exist. *A priori* estimates allow to pass to the limit and show the existence of solutions to the model with polynomial free energy. This result is then used to generalize to the sharp interface model with logarithmic free energy.

We will carry out the proof for classical Dirichlet boundary data, i.e. set w.l.o.g. $\varrho_d = \mu_d = 0$ in (12). If the general Dirichlet condition $\varrho = \varrho_d$ on $\partial\Omega$ is imposed, one can formally set $\tilde{\varrho} := \varrho - \varrho_d$ and gain from the results for $\tilde{\varrho}$ provided in Theorem 2 directly the corresponding statements for ϱ. Other boundary conditions will be shortly discussed in the remark at the end of this section.

We begin by collecting general properties of the model and necessary tools that will be needed in the sequel. The concentration vector ϱ lies inside the simplex Σ,

$$\varrho \in \Sigma := \left\{ \varrho' = (\varrho'_1, \dots, \varrho'_n) \in \mathbb{R}^n \;\middle|\; \sum_{i=1}^{n} \varrho'_i = 1 \right\}$$

Notice that the condition $0 \leqslant \varrho_i \leqslant 1$ in Ω may be violated for polynomial free energies considered in the first part of this article. Let

$$X_1 := \{\varrho' \in L^2(\Omega; \mathbb{R}^n) \mid \varrho' \in \Sigma \text{ almost everywhere in } \Omega\}$$

$$X_3 := \{u' \in H^1(\Omega, \mathbb{R}^D) \mid (u', v)_{H^1} = 0 \text{ for all } v \in X_{\text{ird}}\}$$

where $X_{\text{ird}} = \{u \in H^1(\Omega, \mathbb{R}^D) \mid \text{there exist } b \in \mathbb{R}^D,\ A \in \mathbb{R}^{D\times D} \text{such that } u(x) = Ax + b\}$ is the space of all infinitesimal rigid displacements.

Since we have (classical) Dirichlet boundary conditions for the equations of conservation of mass, we consider the space of test functions

$$Y := H_0^{1,2}(\Omega; \mathbb{R}^n)$$

and its dual

$$\mathscr{D} := (H_0^{1,2}(\Omega; \mathbb{R}^n))' = H^{-1,2}(\Omega; \mathbb{R}^n)$$

Let us now consider the mapping $\mathscr{L}(\mu) : Y \to \mathscr{D}$ corresponding to $\mu \mapsto -\mathrm{div}(L\nabla\mu)$ with Dirichlet boundary conditions, defined by

$$\mathscr{L}(\mu)(\zeta) := \int_\Omega L\nabla\mu : \nabla\zeta$$

To simplify the further argumentation we will introduce the inverse $\mathscr{G}$ of $\mathscr{L}$. The existence of $\mathscr{G}$ is derived from the Poincaré inequality and the Lax–Milgram theorem, since L is positive definite. From this we find that $\mathscr{G}$ is positive definite, self-adjoint, injective and compact.

Hence, we have

$$(L\nabla\mathscr{G}v, \nabla\zeta)_{L^2} = (\zeta, v) \quad \text{for all } \zeta \in Y \text{ and } v \in \mathscr{D}$$

Since L is positive definite, we define for $v_1, v_2 \in \mathscr{D}$ the L scalar product

$$(v_1, v_2)_L := (L\nabla\mathscr{G}v_1, \nabla\mathscr{G}v_2)_{L^2}$$

and the corresponding norm

$$\|v\|_L := \sqrt{(v,v)_L}$$

Functions $v \in Y$ canonically define an element in $\mathscr{D}$ and consequently, $(\cdot,\cdot)_L$ and $\|\cdot\|_L$ are also well-defined for elements in Y.

The Green's function $\mathscr{G}$ allows to rewrite the conservation of mass equation (6) as

$$\mathscr{G}\partial_t\varrho = \mu = \left(\frac{\partial f}{\partial\varrho_j}\right)_{1\leqslant j\leqslant n} \tag{13}$$

Remark

If we replace the Dirichlet conditions for ϱ and μ by a Neumann boundary condition or periodic boundary conditions, a (generalized) Poincaré inequality holds in $H^{1,2}(\Omega)$. For instance in case of periodic boundary conditions the inverse $\mathscr{G}$ of $\mathscr{L}$ (now defined with periodicity condition) exists and the above construction as well as all the results found below continue to hold.

4. THE WEAK FORMULATION

The vector $(\varrho, \chi, \mu, u) \in L^2(\Omega_{T_0};\ \mathbb{R}^n) \times \mathrm{BV}(\Omega_{T_0}) \times L^2(0, T_0;\ H_0^{1,2}(\Omega; \mathbb{R}^n)) \times L^2(0, T_0;\ X_3)$ is called a *weak solution of* (6)–(12) if

$$-\int_{\Omega_{T_0}} \partial_t\xi \cdot (\varrho - \varrho_0) + \int_{\Omega_{T_0}} L\nabla\mu : \nabla\xi = 0 \tag{14}$$

for all $\xi \in L^2(0,T_0;\, H_0^1(\Omega;\mathbb{R}^n))$ with $\partial_t \xi \in L^2(\Omega_{T_0})$, $\xi(T_0)=0$, and

$$\int_{\Omega_{T_0}} \mu \cdot \zeta = \int_{\Omega_{T_0}} \frac{\partial f}{\partial \varrho}(\varrho,\chi,u)\cdot\zeta \tag{15}$$

for all $\zeta \in L^2(\Omega_{T_0};\, \mathbb{R}^n)$, and

$$\int_{\Omega_{T_0}} W^{\mathrm{el}}(\varrho,\mathscr{E}(u)) : \nabla\eta = \int_{\Omega_{T_0}} \overline{S} : \nabla\eta \tag{16}$$

for all $\eta \in L^2(0,T_0;\, H^1(\Omega;\mathbb{R}^n))$ and if for all $t\in[0,T_0]$

$$F(\varrho(t),\chi(t),u(t)) = \min_{\tilde\chi\in X_2} F(\varrho(t),\tilde\chi,u(t)) \tag{17}$$

5. THE IMPLICIT TIME DISCRETIZATION

We fix an $M\in\mathbb{N}$ and set $h:=T_0/M$. For $m\geqslant 1$ and given ϱ^{m-1} consider

$$\frac{\varrho^m-\varrho^{m-1}}{h} = \operatorname{div}(L\nabla\mu^m) \tag{18}$$

$$\mu^m = \frac{\partial f}{\partial\varrho}(\varrho^m,\chi^m,u^m) \tag{19}$$

$$\operatorname{div}(S^m)=0 \tag{20}$$

$$S^m = \partial_\varepsilon W^{\mathrm{el}}(\varrho^m,\mathscr{E}^m) \tag{21}$$

$$F(\varrho^m,\chi^m,u^m) = \min_{\tilde\chi\in X_2} F(\varrho^m,\tilde\chi,u^m) \tag{22}$$

6. STRUCTURAL ASSUMPTIONS

In order to be able to establish the existence of weak solutions in the sense of Section 4, the following assumptions are made:

(A1) $\Omega\subset\mathbb{R}^D$ is a bounded domain with Lipschitz boundary.
(A2) The free energy density f can be written as

$$f(\varrho,\chi,u) = \bar f(\varrho,\chi) + W^{\mathrm{el}}(\varrho,\mathscr{E}(u)) \quad \text{for all } \varrho\in\mathbb{R}^n,\ \chi\in\mathbb{R},\ u\in\mathbb{R}^D$$

with $\bar f \in C^1(\mathbb{R}^n\times\mathbb{R};\mathbb{R})$ for every $\chi\in[0,1]$ and $\bar f(\cdot,\chi)$ is convex for every $\chi\in[0,1]$. Additionally we postulate

(A2.1) $\bar f\geqslant 0$.

(A2.2) There exist constants $C_1 > 0$, $C_2 \geqslant 0$ such that

$$C_1|\varrho|^2 - C_2 \leqslant \bar{f}(\varrho,\chi) \quad \text{for all } \varrho \in \Sigma,\ \chi \in [0,1]$$

(A2.3) For all $\delta > 0$ there exists a constant $C_\delta > 0$ such that

$$|\partial_\varrho \bar{f}(\varrho,\chi)| \leqslant \delta \bar{f}(\varrho,\chi) + C_\delta \quad \text{for all } \varrho \in \Sigma,\ \chi \in [0,1]$$

(A3) The initial datum ϱ_0 fulfils

$$f(\varrho_0, \chi_0, u_0) < \infty$$

where u_0 is the solution of (16) and $\chi_0 \in X_2$ the minimum in Equation (17).

(A4.1) The diffusion tensor L is assumed to be symmetric and positive definite.
(A4.2) The surface tension $\sigma > 0$ is a constant.
(A5) The elastic energy density $W^{\text{el}} \in C^1(\mathbb{R}^n \times \mathbb{R}^{D\times D}; \mathbb{R})$ satisfies
(A5.1) $W^{\text{el}}(\varrho', \mathscr{E}')$ only depends on the symmetric part of $\mathscr{E}' \in \mathbb{R}^{D\times D}$, i.e. $W^{\text{el}}(\varrho', \mathscr{E}') = W^{\text{el}}(\varrho', (\mathscr{E}')^t)$ for all $\varrho' \in \mathbb{R}^n$ and $\mathscr{E}' \in \mathbb{R}^{D\times D}$.
(A5.2) $\partial_\varepsilon W^{\text{el}}(\varrho', \cdot)$ is strongly monotone uniformly in ϱ', i.e. there exists a $c_1 > 0$ such that for all symmetric $\mathscr{E}_1', \mathscr{E}_2' \in \mathbb{R}^{D\times D}$

$$\partial_\varepsilon W^{\text{el}}(\varrho', \mathscr{E}_2') - \partial_\varepsilon W^{\text{el}}(\varrho', \mathscr{E}_1') : (\mathscr{E}_2' - \mathscr{E}_1') \geq c_1 |\mathscr{E}_2' - \mathscr{E}_1'|^2$$

(A5.3) There exists a constant $C_3 > 0$ such that for all $\varrho' \in \Sigma$ and all symmetric $\mathscr{E}' \in \mathbb{R}^{D\times D}$

$$|W^{\text{el}}(\varrho', \mathscr{E}')| \leqslant C_3(|\mathscr{E}'|^2 + |\varrho'|^2 + 1)$$

$$|\partial_\varrho W^{\text{el}}(\varrho', \mathscr{E}')| \leqslant C_3(|\mathscr{E}'|^2 + |\varrho'|^2 + 1)$$

$$|\partial_\varepsilon W^{\text{el}}(\varrho', \mathscr{E}')| \leqslant C_3(|\mathscr{E}'| + |\varrho'| + 1)$$

(A6) The energy density of the applied outer forces is of the form $\overline{W}(\mathscr{E}') = -\mathscr{E}' : \overline{S}$ with a constant symmetric tensor $\overline{S}$.

The decomposition of f in (A2) exploits the fact that the elastic energy is the same in both phases and hence does not depend on χ.

The assumptions on f are in particular valid for the case that is most interesting to us, namely

$$\bar{f}(\varrho,\chi) := \chi \tilde{f}_1(\varrho) + (1-\chi)\tilde{f}_2(\varrho)$$

where $\tilde{f}_j$ is the free energy density of phase j without the elastic and interaction terms, i.e. for the polynomial choice (1)

$$\tilde{f}_j(\varrho) := \tfrac{1}{2}(\varrho - \overline{\varrho}_j)^2, \quad j = 1, 2$$

From now on we assume that Assumptions (A1)–(A6) hold.

7. EXISTENCE OF SOLUTIONS TO THE TIME DISCRETE SCHEME

For each time step $m\geqslant 1$ in the implicit time discretization (18)–(22), given time step size $h>0$, and given ϱ^{m-1} we define the discrete energy functional

$$F^{m,h}(\varrho,\chi,u):=F(\varrho,\chi,u)+\frac{1}{2h}\|\varrho-\varrho^{m-1}\|_L^2$$

Lemma 1 (*Existence of a minimizer*)
For $\varrho^{m-1}\in X_1$ given and any $h>0$, the functional $F^{m,h}$ possesses a minimizer (ϱ^m,χ^m,u^m) in $X_1\times X_2\times X_3$.

Proof
The proof is an application of the direct method in the calculus of variations. The term $\int_\Omega \sigma|\nabla\chi|$ in the definition of F guarantees the coercivity of F for $\chi\in X_2$ and similarly $\int_\Omega W^{\mathrm{el}}$ the coercivity of F for $u\in X_3$. Using Estimate (A2.2), we find that the functional $F^{m,h}$ is weakly lower semicontinuous and coercive in $X_1\times X_2\times X_3$ and hence possesses a minimizer. By construction, the minimizer χ^m of $F^{m,h}$ w.r.t. χ is at the same time a solution to (17) for $t=mh$. □

The following lemma shows that the energy functional $F^{m,h}$ is the correct one and corresponds to the implicit time discretization (18)–(22).

Lemma 2 (*Euler–Lagrange equations*)
The minimizer (ϱ^m,χ^m,u^m) of $F^{m,h}$ fulfils

$$\int_\Omega \frac{\varrho^m-\varrho^{m-1}}{h}\cdot\xi+\int_\Omega L\nabla\mu^m:\nabla\xi=0 \quad \text{for all } \xi\in Y \tag{23}$$

$$\int_\Omega \partial_\varrho f(\varrho^m,\chi^m)\cdot\zeta=\int_\Omega \mu^m\cdot\zeta \quad \text{for all } \zeta\in Y\cap L^\infty(\Omega;\mathbb{R}^n) \tag{24}$$

$$\int_\Omega \partial_\varepsilon W^{\mathrm{el}}(\varrho^m,\mathscr{E}(u^m)):\nabla\eta=\int_\Omega \overline{S}:\nabla\eta \quad \text{for all } \eta\in H^1(\Omega,\mathbb{R}^D) \tag{25}$$

Here, $\mu^m=\mathscr{G}((\varrho^m-\varrho^{m-1}/h))$.

Proof
We choose directions $\xi\in Y\cap L^\infty(\Omega;\mathbb{R}^n)$, $\zeta\in X_3\cap L^\infty(\Omega;\mathbb{R})$ and determine the variations of $F^{m,h}(\varrho,\chi,u)$ with respect to ϱ and u for ξ, ζ. The variation w.r.t. ϱ is

$$\lim_{s\to 0}\Big((F^{m,h}(\varrho^m+s\xi,\chi^m,u^m)-F^{m,h}(\varrho^m,\chi^m,u^m))s^{-1}\Big) \tag{26}$$

Since $\varrho\mapsto\bar{f}(\varrho,\chi)$ is convex for arbitrary χ, we have

$$\bar{f}(\varrho^m,\chi^m)\geqslant\bar{f}(\varrho^m+s\xi,\chi^m)-s\partial_\varrho\bar{f}(\varrho^m+s\zeta,\chi^m)\cdot\xi$$

This implies

$$\bar{f}(\varrho^m + s\xi, \chi^m) \leqslant \bar{f}(\varrho^m, \chi^m) + |s\partial_\varrho \bar{f}(\varrho^m + s\xi, \chi^m)| \, \|\xi\|_{L^\infty}$$
$$\leqslant \bar{f}(\varrho^m, \chi^m) + |s| \, \bar{f}(\varrho^m + s\xi, \chi^m) \, \|\xi\|_{L^\infty} + C|s|$$

The last is by Assumption (A2.3) with $\delta = 1$. Hence, for s small enough, we find

$$\left| \frac{\bar{f}(\varrho^m + s\xi, \chi^m) - \bar{f}(\varrho^m, \chi^m)}{s} \right| \leqslant C(\bar{f}(\varrho^m, \chi^m) + 1)$$

Lebesgue's dominated convergence theorem implies

$$\lim_{s\to 0} \frac{1}{s} \Big(\int_\Omega f(\varrho^m + s\xi, \chi^m) - f(\varrho^m, \chi^m) \Big) = \int_\Omega \partial_\varrho f(\varrho^m, \chi^m) \cdot \xi$$

The variation of the quadratic form $\varrho \mapsto 1/2h\|\varrho^m - \varrho^{m-1}\|_L^2$ yields

$$\lim_{s\to 0} \Big(s^{-1}(2h)^{-1} \left(\|\varrho^m + s\xi - \varrho^{m-1}\|_L^2 - \|\varrho^m - \varrho^{m-1}\|_L^2 \right) \Big)$$
$$= \Big(\frac{\varrho^m - \varrho^{m-1}}{h}, \xi \Big)_L = \Big(\mathscr{G}\Big(\frac{\varrho^m - \varrho^{m-1}}{h} \Big), \xi \Big)_{L^2} = \Big(\mu^m, \xi \Big)_{L^2}$$

Equality (24) follows because (ϱ^m, χ^m, u^m) is a minimizer and thus the limit in (26) is 0. Equation (23) follows from the definition of μ^m. To derive (25), we vary $F^{m,h}$ w.r.t. u. From the symmetry of $\partial_\varepsilon W^{\mathrm{el}}$ and $\overline{S}$ we find (25). □

8. UNIFORM ESTIMATES

In the preceding section, we proved the existence of a discrete solution $(\varrho^m, \mu^m, \chi^m, u^m)$ for $1 \leqslant m \leqslant M$ and arbitrary $M \in \mathbb{N}$. We define the piecewise constant extension $(\varrho_M, \mu_M, \chi_M, u_M)$ of $(\varrho^m, \mu^m, \chi^m, u^m)_{1 \leqslant m \leqslant M}$ by

$$(\varrho_M(t), \mu_M(t), \chi_M(t), u_M(t)) := (\varrho_M^m, \mu_M^m, \chi_M^m, u_M^m) := (\varrho^m, \mu^m, \chi^m, u^m) \quad \text{for } t \in ((m-1)h, mh]$$

and $\varrho_M(0) = \varrho_0, \chi_M(0)$ given by Equation (22), $\mu_M(0)$ given by Equation (19) and $u_M(0)$ given by Equation (20).

The piecewise linear extension $(\overline{\varrho}_M, \overline{\mu}_M, \overline{\chi}_M, u_M)$ for $t = (\beta m + (1-\beta)(m-1))h$ with appropriate $\beta \in [0,1]$ is given by the interpolation

$$(\overline{\varrho}_M, \overline{\mu}_M, \overline{\chi}_M, u_M)(t) := \beta(\varrho_M^m, \mu_M^m, \chi_M^m, u_M^m) + (1-\beta)(\varrho_M^{m-1}, \mu_M^{m-1}, \chi_M^{m-1}, u_M^{m-1})$$

Lemma 3 (*A priori estimates*)
The following *a priori* estimates are valid.

(a) For all $M \in \mathbb{N}$ and all $t \in [0, T_0]$ we have the dissipation inequality

$$F(\varrho_M, \chi_M, u_M)(t) + \frac{1}{2} \int_{\Omega_t} L\nabla\mu_M : \nabla\mu_M \leqslant F(\varrho_0, \chi_0, u_0)$$

(b) There exists a constant $C>0$ such that

$$\sup_{0\leqslant t\leqslant T_0}\left\{\|\varrho_M(t)\|_{L^2}+\|\chi_M(t)\|_{\mathrm{BV}}+\|u_M(t)\|_{H^1}\right\}\leqslant C \tag{27}$$

$$\sup_{0\leqslant t\leqslant T_0}\int_\Omega \bar{f}(\varrho_M(t),\chi_M(t))+\|\nabla\mu_M\|_{L^2(\Omega_{T_0})}\leqslant C \tag{28}$$

Proof
Since (ϱ^m,χ^m,u^m) is a minimizer of $F^{m,h}$, we have for every $m\geqslant 1$

$$F(\varrho^m,\chi^m,u^m)+\frac{1}{2h}\|\varrho^m-\varrho^{m-1}\|_L^2\leqslant F(\varrho^{m-1},\chi^{m-1},u^{m-1}) \tag{29}$$

and by a direct calculation

$$\frac{1}{2h}\|\varrho^m-\varrho^{m-1}\|_L^2=\frac{h}{2}(\nabla\mu^m,L\nabla\mu^m)_{L^2} \tag{30}$$

When iterating (29), Equation (30) yields

$$F(\varrho_M^m,\chi_M^m,u_M^m)+\frac{1}{2}\int_0^{mh}(\nabla\mu_M^m,L\nabla\mu_M^m)_{L^2}\,\mathrm{d}t\leqslant F(\varrho_0,\chi_0,u_0)$$

Using the assumptions, in particular (A2.2) to get an L^2-bound on ϱ_M, and with the help of Korn's inequality this proves the lemma. □

For the linear interpolation $\overline{\varrho}_M$ of ϱ_M^m, the Euler–Lagrange equation (23) can be rewritten as

$$\int_\Omega \partial_t\overline{\varrho}_M(t)\cdot\xi+\int_\Omega L\nabla\mu_M(t):\nabla\xi=0\quad\text{for all }\ \xi\in Y \tag{31}$$

which holds for almost all $t\in(0,T_0)$. Equation (31) controls the variation of $\overline{\varrho}_M$ in time and, together with the uniform estimates of Lemma 3, allows to show compactness in time. □

The following theorem is the first main result and states the convergence of the solution of the time-discretized problem. In the next part, we will show that the limit is in fact a solution to (6)–(12).

Theorem 1 (*Compactness for* $(\varrho_M,\mu_M,\chi_M,u_M)$)
There exists a constant $C>0$ such that for all $t_1,t_2\in[0,T_0]$

$$\|\overline{\varrho}_M(t_2)-\overline{\varrho}_M(t_1)\|_{L^2}\leqslant C|t_2-t_1|^{1/4}$$

Furthermore, there are subsequences $(\varrho_M)_{M\in\mathcal{N}}$, $(\mu_M)_{M\in\mathcal{N}}$, $(\chi_M)_{M\in\mathcal{N}}$ and $(u_M)_{M\in\mathcal{N}}$, with $\mathcal{N}\subset\mathbb{N}$ and there are $\varrho\in L^\infty(0,T_0;L^2(\Omega))$, $\mu\in L^2(0,T_0;Y)$, $\chi\in L^\infty(0,T_0;\mathrm{BV}(\Omega))$ and

$u \in L^\infty(0, T_0; H^1(\Omega))$ such that

$$
\begin{array}{rll}
\text{(i)} & \overline{\varrho}_M & \to \varrho \text{ in } C^{0,\alpha}([0,T_0]; L^2(\Omega;\mathbb{R}^n)) \text{ for all } \alpha \in (0,1/4),\\
\text{(ii)} & \varrho_M & \to \varrho \text{ in } L^\infty(0,T_0; L^2(\Omega;\mathbb{R}^n)),\\
\text{(iii)} & \varrho_M & \to \varrho \text{ almost everywhere in } \Omega_{T_0},\\
\text{(iv)} & \varrho_M & \overset{*}{\rightharpoonup} \varrho \text{ in } L^\infty(0,T_0; L^2(\Omega;\mathbb{R}^n)),\\
\text{(v)} & \mu_M & \rightharpoonup \mu \text{ in } L^2(0,T_0; H^1_0(\Omega;\mathbb{R}^n)),\\
\text{(vi)} & u_M & \to u \text{ in } L^2(0,T_0; H^1(\Omega)),\\
\text{(vii)} & \chi_M & \to \chi \text{ almost everywhere in } \Omega_{T_0},\\
\text{(viii)} & \chi_M & \to \chi \text{ in } L^\infty(0,T_0; BV(\Omega)), \text{ with } \chi(1-\chi)=0 \text{ a.e. in } \Omega,\\
\text{(ix)} & \partial_\varrho \bar{f}(\varrho_M,\chi_M) & \to \partial_\varrho \bar{f}(\varrho,\chi) \text{ in } L^1(\Omega_{T_0})
\end{array}
$$

as $M \in \mathcal{N}$ tends to infinity.

Proof

We test Equation (31) with $\xi := \overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)$, where $t_1, t_2 \in [0, T_0]$ with $t_1 < t_2$. After integration in time from t_1 to t_2, we obtain

$$\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|^2_{L^2} + \int_{t_1}^{t_2} \int_\Omega L\nabla \mu_M(t) : \nabla(\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1))\,\mathrm{d}t = 0$$

The ϱ_M^m are uniformly bounded in $L^2(\Omega; \mathbb{R}^n)$, therefore the linear interpolants $\overline{\varrho}_M$ are uniformly bounded in $L^\infty(0, T_0; L^2(\Omega))$. Thus, we obtain

$$
\begin{aligned}
\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|^2_{L^2} &\leqslant C\|\overline{\varrho}_M\|_{L^\infty(L^2)} \int_{t_1}^{t_2} \|\nabla \mu_M(t)\|_{L^2}\,\mathrm{d}t\\
&\leqslant C\|\overline{\varrho}_M\|_{L^\infty(L^2)} (t_2 - t_1)^{\frac{1}{2}} \|\nabla \mu\|_{L^2(\Omega_{T_0})}
\end{aligned}
$$

Employing the *a priori* estimates (27) and (28) we have proved

$$\|\overline{\varrho}_M(t_2) - \overline{\varrho}_M(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/4} \quad \text{for all } t_1, t_2 \in [0, T_0]$$

for a positive constant C. This is the equicontinuity of $(\overline{\varrho}_M)_{M\in\mathbb{N}}$.

The boundedness of $(\overline{\varrho}_M)$ in $L^\infty(0, T_0; L^2(\Omega))$ yields as a consequence of the Arzelà–Ascoli theorem statement (i).

Claims (ii),(iii) and (iv) are shown as follows. Choose for $t \in [0, T_0]$ values $m \in \{1, \ldots, M\}$ and $\beta \in [0, 1]$ such that $t = (\beta m + (1 - \beta)(m - 1))h$. From the definition of $\overline{\varrho}$ we get at once

$$
\begin{aligned}
\|\overline{\varrho}_M(t) - \varrho_M(t)\|_{L^2} &= \|\beta \varrho_M^m + (1-\beta)\varrho_M^{m-1} - \varrho_M^m\|_{L^2}\\
&= (1-\beta)\|\varrho_M^m - \varrho_M^{m-1}\|_{L^2}\\
&\leqslant Ch^{1/4}
\end{aligned}
$$

This tends to zero as M becomes infinite. With the help of (i), this proves (ii). Since for a sub-sequence we have convergence almost everywhere, (iii) is proved, too. Claim (iv) is a direct consequence of Estimate (27) which gives the boundedness of ϱ_M in $L^\infty(0, T_0; L^2(\Omega; \mathbb{R}^n))$.

For the proof of (v) we notice that due to Estimate (28), the $(\nabla \mu_M)$ are uniformly bounded in $L^2(\Omega_{T_0})$. By the Poincaré inequality (μ_M) are in fact uniformly bounded in $L^2(0, T_0;\ H_0^1(\Omega))$. With the Banach–Alaoglu theorem (v) follows.

The proof of (vi) is contained in Reference [5, Lemma 3.5] (no $H^{1,2}$-regularity of $\varrho(\cdot, t)$ is needed).

To prove (vii), fix $t \in [0, T_0]$. The sequence $\chi_M(\cdot, t) \subset \mathrm{BV}(\Omega)$ is uniformly bounded in $\mathrm{BV}(\Omega)$ and from the compact imbedding $\mathrm{BV}(\Omega) \hookrightarrow L^1(\Omega)$ we infer the existence of a subsequence $\mathscr{N}$ with $\chi_{\mathscr{N}}(\cdot, t) \to \chi(\cdot, t)$ in $L^1(\Omega)$. If $\varphi \in C_0^\infty(\Omega)$, then for $1 \leqslant i \leqslant n$

$$\lim_{\mathscr{N}\to\infty} \int_\Omega \varphi D_i \chi_{\mathscr{N}}(\cdot, t) = -\lim_{\mathscr{N}\to\infty} \int_\Omega \chi_{\mathscr{N}}(\cdot, t) D_i \varphi = \int_\Omega \chi(\cdot, t) D_i \varphi$$

and furthermore

$$\left| \int_\Omega \chi(\cdot, t) D_i \varphi \right| \leqslant \sup_{x\in\Omega} |\varphi(x)| \liminf_{\mathscr{N}\to\infty} \int_\Omega |\nabla \chi_{\mathscr{N}}(\cdot, t)| < \infty$$

Hence, $\chi(\cdot, t) \in \mathrm{BV}(\Omega)$ and $\chi_{\mathscr{N}} \to \chi$ in $L^\infty(0, T_0;\ \mathrm{BV}(\Omega))$. Since in particular $\chi_{\mathscr{N}} \to \chi$ in $L^1(\Omega_{T_0})$, we conclude $\chi_{\mathscr{N}} \to \chi$ almost everywhere in Ω_{T_0} for a subsequence $\mathscr{N}$. This proves (vii). From the pointwise limit we get $\chi \geqslant 0$ and $\chi(1-\chi) = 0$ almost everywhere in Ω, hence (viii).

In order to prove (ix), we first notice that by Assumption (A2), $\partial_\varrho \bar{f}$ is a continuous function. Hence, by (iii) and (vii),

$$\partial_\varrho \bar{f}(\varrho_M, \chi_M) \to \partial_\varrho \bar{f}(\varrho, \chi) \quad \text{almost everywhere in } \Omega_{T_0}$$

The growth condition of Assumption (A2.3) on $\bar{f}$ now yields that for arbitrary $\delta > 0$ and all measurable $E \subset \Omega$

$$\int_E |\partial_\varrho \bar{f}(\varrho_M, \chi_M)| \leqslant \delta \int_E \bar{f}(\varrho_M, \chi_M) + C_\delta |E| \leqslant \delta C + C_\delta |E|$$

Therefore, $\int_E |\partial_\varrho \bar{f}(\varrho_M, \chi_M)| \to 0$ as $|E| \to 0$ uniformly in M and by Vitali's theorem we find $\bar{f}(\varrho_M, \chi_M) \to \bar{f}(\varrho, \chi)$ in $L^1(\Omega_{T_0})$ as $M \in \mathscr{N}$ tends to infinity. □

9. GLOBAL EXISTENCE OF SOLUTIONS TO THE SHARP INTERFACE MODEL

We are now in the position to state the existence result.

Theorem 2 (*Global existence for the sharp interface model with polynomial free energy*)
Let the assumptions of Section 6 hold. Then, there exists a weak solution (ϱ, μ, χ, u) of (6)–(12) in the sense of Section 4 such that

(i) $\varrho \in C^{0,1/4}([0, T_0];\ L^2(\Omega; \mathbb{R}^n))$,
(ii) $\partial_t \varrho \in L^2(0, T_0;\ (H_0^1(\Omega; \mathbb{R}^n))')$,
(iii) $\chi \in L^\infty(0, T_0;\ \mathrm{BV}(\Omega))$ with $\chi(1-\chi) = 0$ almost everywhere in Ω,
(iv) $u \in L^2(0, T_0;\ H^1(\Omega))$.

Remark
In general, the global solution (ϱ, μ, χ, u) in Theorem 2 will not be unique because the minimum in χ may not be uniquely defined.

Proof
We are going to prove that (ϱ, μ, χ, u) introduced in Theorem 1 is the desired weak solution in the sense of Section 4. From Equation (31) we learn

$$-\int_{\Omega_{T_0}} \partial_t \xi(\bar{\varrho}_M - \varrho_0) + \int_{\Omega_{T_0}} L\nabla\mu_M : \nabla\xi = 0$$

for all $\xi \in L^2(0, T_0; Y)$ with $\partial_t \xi \in L^2(\Omega_{T_0})$ and $\xi(T_0) = 0$. Passing to the limit $M \to \infty$ together with Theorem 1 this implies (14). Now we show (15). From (31) we see

$$\int_\Omega \partial_\varrho f(\varrho_M, \chi_M) \cdot \eta = \int_\Omega \mu_M \cdot \eta \quad \text{for all } \eta \in Y \cap L^\infty(\Omega; \mathbb{R}^n)$$

The convergence of

$$\int_\Omega \partial_\varrho f(\varrho_M, \chi_M) \cdot \eta \to \int_\Omega \partial_\varrho f(\varrho, \chi) \cdot \eta$$

is evident by Vitali's theorem similar to the proof of Theorem 1 by using the almost everywhere convergence of ϱ_M and χ_M, the growth condition (A2.3), Estimate (28) on $\bar{f}$ and the boundedness of η. The dominated convergence theorem of Lebesgue, the strong convergence of ϱ_M and ∇u_M in L^2 and the growth condition (A5.3) guarantee that we can perform the limit

$$\lim_{M\to\infty} \int_\Omega \partial_\varepsilon W^{\mathrm{el}}(\varrho_M, \mathscr{E}(u_M)) \cdot \zeta$$

Similarly, we can pass to the limit in Equation (25). χ is easily seen to fulfill (10). □

10. LOGARITHMIC FREE ENERGY

In the following three sections, we are going to extend Theorem 2 to logarithmic free energies. The results will be valid for the particular free energy functional that is most interesting to us,

$$f(\varrho, \chi, u) = \chi\alpha_1 \sum_{j=1}^n \varrho_j \ln \varrho_j + (1-\chi)\alpha_2 \sum_j \varrho_j \ln \varrho_j + W^{\mathrm{el}}(\varrho, \mathscr{E}(u)) \qquad (32)$$

and we will exploit the particular structure of f in the following.

As is well known the mathematical discussion is much more subtle, f becomes singular as one ϱ_j approaches 0. To show that $0 < \varrho_j < 1$ for every j, we approximate f for $\delta > 0$ by some f^δ that fulfils the requirements of Section 6 and find suitable *a priori* estimates that allow to pass to the limit $\delta \to 0$.

Despite the mathematical difficulties, the logarithmic free energy guarantees that the concentration vector ϱ lies in the transformed Gibbs simplex

$$G := \Sigma \cap \{\varrho \in \mathbb{R}^n \mid \varrho_j \geqslant 0 \text{ for } 1 \leqslant j \leqslant n\}$$

and is therefore physically meaningful.

Assumptions (A2) and (A3) of Section 6 are replaced by the following ones:

(A2′) f is of form (32) with $\alpha_1 > 0$, $\alpha_2 > 0$.
(A3′) The initial value $\varrho_0 = (\varrho_{01}, \dots, \varrho_{0n}) \in X_1$ fulfils $\varrho_0 \in G$ almost everywhere and

$$\int_\Omega \varrho_{0j} > 0 \quad \text{for } 1 \leqslant j \leqslant n$$

The other assumptions are unchanged and continue to hold.

To proceed, we define for $d \in \mathbb{R}$ and given $\delta > 0$ the regularized free energy functional

$$\psi^\delta(d) := \begin{cases} d \ln d & \text{for } d \geqslant \delta \\ d \ln \delta - \frac{\delta}{2} + \frac{d^2}{2\delta} & \text{for } d < \delta \end{cases}$$

The regularized free energy functional is defined in such a way that $\psi^\delta \in C^2$ and the derivative $(\psi^\delta)'$ is monotone. This definition goes back to the work by Elliott and Luckhaus [10].

Due to Assumption (A2’) this leads to

$$f^\delta = \bar{f}^\delta + W^{\mathrm{el}}(\mathscr{E}(u)) \tag{33}$$

$$\bar{f}^\delta(\varrho, \chi) := \chi \alpha_1 \sum_{j=1}^n \psi^\delta(\varrho_j) + (1 - \chi)\alpha_2 \sum_{j=1}^n \psi^\delta(\varrho_j) \tag{34}$$

As can be easily checked, $\bar{f}^\delta$ fulfils the assumptions of Section 6.

11. UNIFORM ESTIMATES

The following lemma was first stated and proved in Reference [10] for logarithmic free energies typical for the Cahn–Hilliard system. The proof of Elliott and Luckhaus can be directly transferred to the situation considered here with the regularized free energy defined by (33), (34).

Lemma 4 (*Uniform bound from below on* f^δ)
There exists a $\delta_0 > 0$ and a $K > 0$ such that for all $\delta \in (0, \delta_0)$

$$f^\delta(\varrho, \chi, u) \geqslant -K \quad \text{for all } \varrho \in \Sigma, \quad \chi \in [0,1], \quad u \in \mathbb{R}^D$$

Now we summarize the results for the regularized problem proved in Lemma 3 and Theorem 1. Lemma 5 also states the boundedness and convergence of the numerical solutions as $\delta \searrow 0$.

Lemma 5 (*A priori and compactness results for the regularized problem*)

(a) For all $\delta \in (0, \delta_0)$ there exists a weak solution $(\varrho^\delta, \mu^\delta, \chi^\delta)$ of (6)–(12) with a logarithmic free energy that satisfies (A2'), (A3'), (A4)–(A6) in the sense of Section 4.
(b) There exists a constant $C > 0$ independent of δ such that for all $\delta \in (0, \delta_0)$

$$\sup_{t\in[0,T_0]} \left\{ \|\varrho^\delta(t)\|_{L^2} + \|\chi^\delta(t)\|_{\mathrm{BV}} + \|u^\delta(t)\|_{H^1} \right\} \leqslant C$$

$$\sup_{t\in[0,T_0]} \int_\Omega \bar{f}^\delta(\varrho^\delta(t), \chi^\delta(t)) + \|\nabla\mu^\delta\|_{L^2(\Omega_{T_0})} \leqslant C$$

and

$$\|\varrho^\delta(t_2) - \varrho^\delta(t_1)\|_{L^2} \leqslant C|t_2 - t_1|^{1/4}$$

for all $t_1, t_2 \in [0, T_0]$.

(c) One can extract a subsequence $(\varrho^\delta)_{\delta\in\mathscr{R}}$, where $\mathscr{R} \subset (0, \delta_0)$ is a countable set with zero as the only accumulation point such that

(i)	ϱ^δ	$\to$	ϱ in $C^{0,\alpha}([0,T_0]; L^2(\Omega;\mathbb{R}^n))$ for all $\alpha \in (0, 1/4)$,
(ii)	ϱ^δ	$\to$	ϱ in $L^\infty(0,T_0; L^2(\Omega;\mathbb{R}^n))$,
(iii)	ϱ^δ	$\to$	ϱ almost everywhere in Ω_{T_0},
(iv)	ϱ^δ	$\overset{*}{\rightharpoonup}$	ϱ in $L^\infty(0,T_0; L^2(\Omega;\mathbb{R}^n))$,
(v)	μ^δ	$\rightharpoonup$	μ in $L^2(0,T_0; H^1_0(\Omega;\mathbb{R}^n))$,
(vi)	u^δ	$\to$	u in $L^2(0,T_0; H^1(\Omega))$,
(vii)	χ^δ	$\to$	χ almost everywhere in Ω_{T_0},
(viii)	χ^δ	$\to$	χ in $L^\infty(0,T_0; BV(\Omega))$ with $\chi(1-\chi) = 0$ a.e. in Ω,
(ix)	$\partial_\varrho \bar{f}(\varrho^\delta, \chi^\delta)$	$\to$	$\partial_\varrho \bar{f}(\varrho, \chi)$ in $L^1(\Omega_{T_0})$

as $\delta \in \mathscr{R}$ tends to zero.

Proof
Using Lemma 4, the regularized problem satisfies the assumptions of Section 6 and by Theorem 2, a weak solution for fixed $\delta \in (0, \delta_0)$ exists. This proves (a). Lemma 3 and Theorem 1 imply directly (b). From Lemma 3 it follows that $F^\delta(\varrho_0, \chi_0, u_0)$ does not depend on δ, hence the constant on the right-hand side does not depend on δ.

Theorem 1 leads to Assertion (c). □

12. GLOBAL EXISTENCE OF SOLUTIONS FOR LOGARITHMIC FREE ENERGIES

Theorem 3 (*Global existence for the sharp interface model with logarithmic free energy*)
Let the assumptions of Section 10 hold. Then, there exists a weak solution (ϱ, μ, χ, u) in the sense of Section 4 of the sharp interface equations (6)–(12) with logarithmic free energy

such that

(i) $\varrho \in C^{0,1/4}([0,T_0]; L^2(\Omega;\mathbb{R}^n))$,
(ii) $\partial_t\varrho \in L^2(0,T_0; (H_0^1(\Omega;\mathbb{R}^n))')$,
(iii) $\chi \in L^\infty(0,T_0; BV(\Omega))$,
(iv) $u \in L^\infty(0,T_0; H^1(\Omega,\mathbb{R}^D))$,
(v) $\ln \varrho_j \in L^1(\Omega_{T_0})for1\leqslant j\leqslant n$ and in particular $0 < \varrho_j < 1$ almost everywhere.

Proof
We pass to the limit $\delta \searrow 0$ in the weak formulation (14)–(17) with f defined by (32) and have to show that (ϱ,μ,χ,u) found in Lemma 5 is a solution. The limit for (14) and (16) can be justified in the same way as in the proof of Theorem 2. It remains to control the limit $\delta \searrow 0$ in (15). We have

$$\chi^\delta\alpha_1 \sum_{k=1}^n \varphi^\delta(\varrho_k^\delta) + (1-\chi^\delta)\alpha_2 \sum_{k=1}^n \varphi^\delta(\varrho_k^\delta) = \mu^\delta - \partial_\varrho W^{\mathrm{el}}(\varrho^\delta, \mathscr{E}(u^\delta))$$

As $\nabla u^\delta \in L^2(\Omega_{T_0})$, we have $\partial_\varrho W^{\mathrm{el}}(\varrho^\delta,\mathscr{E}(u^\delta)) \in L^2(0,T_0; L^1(\Omega))$ and from Lemma 5 $\mu^\delta \in L^2(0,T_0; H^{1,2}(\Omega))$. Since additionally $\alpha_1>0$, $\alpha_2>0$ and $\mu^\delta(1-\mu^\delta)\equiv 0$ in Ω_{T_0}, we find

$$\|\varphi^\delta(\varrho_k^\delta)\|_{L^1(\Omega_{T_0})} \leqslant C \tag{35}$$

Now, we will show that $\varphi^\delta(\varrho_k^\delta)$ converges to $\varphi(\varrho_k)$ almost everywhere in Ω_{T_0}. From the almost everywhere convergence of ϱ_k^δ to ϱ_k, (35) and the lemma of Fatou we find

$$\int_{\Omega_{T_0}} \liminf_{\delta\searrow 0} |\varphi^\delta(\varrho_k^\delta)| \leqslant \liminf_{\delta\searrow 0} \int_{\Omega_{T_0}} |\varphi^\delta(\varrho_k^\delta)| \leqslant C$$

Next, we will show that

$$\lim_{\delta\searrow 0} \varphi^\delta(\varrho_k^\delta) = \begin{cases} \varphi(\varrho_k) & \text{if } \lim_{\delta\searrow 0} \varrho_k^\delta = \varrho_k \in (0,1) \\ \infty & \text{if } \lim_{\delta\searrow 0} \varrho_k^\delta = \varrho_k \notin (0,1) \end{cases} \tag{36}$$

almost everywhere in Ω_{T_0}. For a point $(x,t)\in\Omega_{T_0}$ with $\lim_{\delta\searrow 0} \varrho_k^\delta(x,t) = \varrho_k(x,t)$, we obtain from $\varphi^\delta(d)=\varphi(d)$ for $d\geqslant\delta$ that $\varphi^\delta(\varrho^\delta(x,t)) \to \varphi(\varrho(x,t))$ as $\delta\searrow 0$. In the second case of a point $(x,t)\in\Omega_{T_0}$ with $\lim_{\delta\searrow 0}\varrho_k^\delta(x,t)=\varrho_k(x,t)\leqslant 0$, we have for δ small enough

$$|\varphi^\delta(\varrho_k^\delta(x,t))| \geqslant \varphi(\max\{\delta,\varrho_k^\delta(x,t)\}) \to \infty \quad \text{for } \delta\searrow 0.$$

This proves (36).

From (36) and (35) we deduce $0<\varrho_k<1$ almost everywhere, $\int_{\Omega_{T_0}} |\varphi(\varrho_k)| \leqslant C$ and $\varphi^\delta(\varrho_k^\delta) \to \varphi(\varrho_k)$ almost everywhere. With the higher regularity result of Reference [5] and Vitali's theorem we find

$$\varphi^\delta(\varrho_k^\delta) \to \varphi(\varrho_k) \quad \text{in } L^1(\Omega_{T_0})$$

Since $\chi^\delta \to \chi$ almost everywhere in Ω_{T_0}, we can pass to the limit in (15). □

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MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:77–100
Published online 15 July 2004 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.550
MOS subject classification: 86 A 17; 86 A 15; 47 J 10; 65 N 25; 74 L 05

Interaction of faults under slip-dependent friction. Non-linear eigenvalue analysis

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Communicated by W. Allegretto

SUMMARY

We analyse the evolution of a system of finite faults by considering the non-linear eigenvalue problems associated to static and dynamic solutions on unbounded domains. We restrict our investigation to the first eigenvalue (Rayleigh quotient). We point out its physical significance through a stability analysis and we give an efficient numerical algorithm able to compute it together with the corresponding eigenfunction.

We consider the anti-plane shearing on a system of finite faults under a slip-dependent friction in a linear elastic domain, not necessarily bounded. The static problem is formulated in terms of local minima of the energy functional. We introduce the non-linear (static) eigenvalue problem and we prove the existence of a first eigenvalue/eigenfunction characterizing the isolated local minima. For the dynamic problem, we discuss the existence of solutions with an exponential growth, to deduce a (dynamic) non-linear eigenvalue problem. We prove the existence of a first dynamic eigenvalue and we analyse its behaviour with respect to the friction parameter. We deduce a mixed finite element discretization of the non-linear spectral problem and we give a numerical algorithm to approach the first eigenvalue/eigenfunction. Finally we give some numerical results which include convergence tests, on a single fault and a two-faults system, and a comparison between the non-linear spectral results and the time evolution results. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: domains with cracks; slip–dependent friction; wave equation; earthquake initiation; non-linear eigenvalue problem; Rayleigh quotient; unilateral conditions; mixed finite element method

1. INTRODUCTION

The earthquake nucleation (or initiation) phase, preceding the dynamic rupture, has been pointed out by detailed seismological observations (e.g. References [1,2]) and it has been

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 Received 10 November 2003

recognized in laboratory experiments (e.g. References [3,4]) to be related to slip-weakening friction (i.e. the decrease of the friction force with the slip). This physical model was thereafter used in the qualitative description of the initiation phase in unbounded (e.g. References [5,6]) and bounded (e.g. References [7,8]) fault models.

Important physical properties of the nucleation phase (characteristic time, critical fault length, etc.) were obtained in References [5,7] through simple mathematical properties of the unstable evolution. In the description of the instabilities, the spectral analysis played a key role. Moreover, the shape of the eigenfunctions was shown to determine the signature of the initiation phase (see Reference [9]), and the spectral equivalence was the main principle in the renormalization of a heterogeneous fault in Reference [10].

Many of the above papers concern the anti-plane case (see Reference [11] for a complete description). Even if only a limited number of geophysical faults (e.g. 'normal' faults) are satisfactorily described by the anti-plane geometry, this case reveals to capture the main features of the physical phenomenon. The relative mathematical simplicity of its governing equations and its relevance in almost all applications imposed the anti-plane case as the basis of the analysis. Moreover, in the description of the friction phenomenon, it allows a very important simplification: the normal stress can be considered constant. This simplification, which is reasonable in earthquake mechanics (contact between two elastic bodies), is very restrictive in contact mechanics (contact between an elastic and a rigid body).

For the anti-plane shear of an elastic plane containing a system of coplanar faults, the (linear) eigenvalue problem was solved in Reference [12] through a semi-analytical integral equation technique to compute the set of eigenvalues and the shape of the eigenfunctions. For bounded domains, it was also proved that the spectrum consists of a decreasing and unbounded sequence of eigenvalues. To ensure the physical significance of the (linear) eigenvalue problem, the first eigenfunction must have a constant sign all along the fault. For a system of coplanar faults, it was found from numerical computations (see References [7,12]) that this property holds. Hence, in this case, the linear approach was sufficient to give a satisfactory model for the initiation of instabilities.

If the faults are not coplanar, then the unilateral condition is no longer satisfied, that is the first eigenfunction of the tangent (linear) problem has no physical significance. Hence, in modelling initiation of friction instabilities, a non-linear (unilateral) eigenvalue problem has to be considered. This difficulty arises with the effect of stress shadowing which does not exist for coplanar fault segments. From the mathematical point of view, the main novelty in this particular non-linear eigenvalue problem is the presence of the convex cone of functions with non-negative jump across an internal boundary (a finite number of bounded connected arcs called faults).

This non-linear eigenvalue variational inequality was considered in Reference [13] by Ionescu and Radulescu. In the dynamic case they established, for a bounded domain, the existence of infinitely many solutions. They also proved that the number of solutions of the perturbed problem becomes greater and greater if the perturbation tends to zero with respect to an appropriate topology. Their proofs rely on algebraic topology methods developed by Krasnoselski, combined with adequate tools in the sense of the Degiovanni non-smooth critical point theory.

Our goal here is to analyse the case of a finite fault system by considering the non-linear eigenvalue problems associated to static and dynamic solutions on unbounded domains. We restrict our investigation to the first eigenvalue (Rayleigh quotient). We aim to point out its physical significance through a stability analysis and to find an efficient numerical algorithm able to compute it together with the corresponding eigenfunction. The non-linear eigenvalue method presented in this paper is used in Reference [14] for some geophysical applications, in particular the slip patterns of normal faults in Afar (East Africa).

Let us sketch here the contents of the paper. In Section 2, we consider the anti-plane shearing on a system of finite faults under a slip-dependent friction in a linear elastic domain, not necessarily bounded. We first formulate the static problem (Section 3) and give its variational formulation in terms of local minima of the energy functional. We introduce the non-linear eigenvalue problem and we prove the existence of a first eigenvalue/eigenfunction. We also prove that, if the non-dimensional friction parameter β is less than the first eigenvalue β_0, then we deal with an isolated local minimum.

For the dynamic problem, we discuss (in Section 4) the existence of solutions with an exponential growth to deduce a non-linear eigenvalue problem depending on the parameter β. We prove the existence of a first eigenvalue λ_0^2 and we analyse its behaviour with respect to β. In Section 5, we consider a mixed finite element discretization of the non-linear spectral problem and we give a numerical algorithm to approach the first eigenvalue/eigenfunction. In all our tests and applications, we found that the algorithm is convergent. The proof of the convergence is beyond the scope of the present paper. These numerical results are detailed in Section 6: they include convergence tests, on a single fault and on a two-faults system, and a comparison between the solution of the non-linear spectral analysis and the time evolution results.

2. PROBLEM STATEMENT

Consider, as in References [7,8,12,14], the anti-plane shearing on a system of finite faults under a slip-dependent friction in a linear elastic domain (see Figure 1). Let $\Omega \subset \mathbb{R}^2$ be a domain, not necessarily bounded, containing a finite number of cuts. Its boundary $\partial\Omega$ is supposed to be smooth and divided into two disjoint parts: the exterior boundary $\Gamma_d = \partial\bar{\Omega}$ and

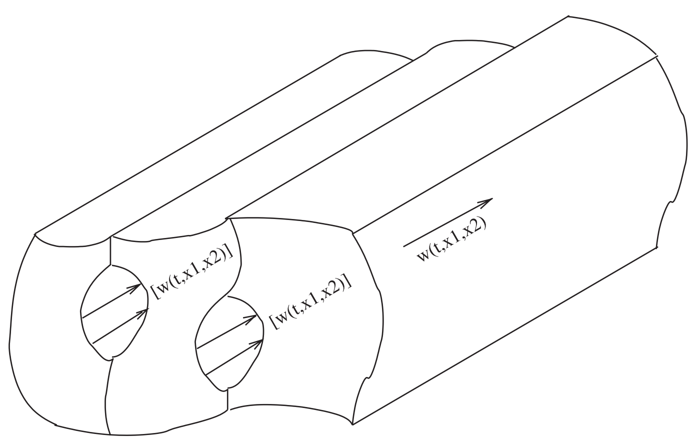

Figure 1. The anti-plane shearing of a system of two parallel faults.

the internal one Γ composed of N_f bounded connected arcs Γ_f^i, $i=1,\ldots,N_f$, called cracks or faults. We suppose that the displacement field $u=(u_1,u_2,u_3)$ is 0 in directions Ox_1 and Ox_2 and that u_3 does not depend on x_3. The displacement is therefore denoted simply by $w=w(t,x_1,x_2)$. The elastic medium has the shear rigidity G, the density ρ and the shear velocity $c=\sqrt{G/\rho}$ with the following regularity:

$$\rho, G\in L^\infty(\Omega), \quad \rho(x)\geqslant\rho_0>0, \quad G(x)\geqslant G_0>0, \quad \text{a.e. } x\in\Omega$$

The non-vanishing shear stress components are $\sigma_{31}=\tau_1^\infty+G\partial_1 w$, $\sigma_{32}=\tau_2^\infty+G\partial_2 w$, and $\sigma_{11}=\sigma_{22}=-S$, where τ^∞ is the pre-stress and $S>0$ is the normal stress on the faults, such that

$$S, \tau_1^\infty, \tau_2^\infty \in C^0(\bar{\Omega})$$

We denote by [ ] the jump across Γ (i.e. $[w]=w^+-w^-$), and by $\partial_n=\nabla\cdot n$ the corresponding normal derivative, with the unit normal n outwards the positive side. On the contact zone Γ, we have

$$[G\partial_n w]=0$$

On the interface Γ, we consider a constitutive law of friction type. The friction force depends on the slip $[w]$ through a friction coefficient $\mu=\mu([w])$ which is multiplied by the normal stress S. Concerning the regularity of $\mu:\Gamma\times\mathbb{R}_+\to\mathbb{R}_+$ we suppose that the friction coefficient is a Lipschitz function, with respect to the slip, and let H be the antiderivative

$$H(x,u):=S(x)\int_0^u \mu(x,s)\,\mathrm{d}s$$

We suppose that there exist L, $a\geqslant 0$, $\gamma\in L^\infty(\Gamma)$, and $\beta\geqslant 0$ a nondimensional and nonnegative number such that

$$|\mu(x,s_1)-\mu(x,s_2)|\leqslant L|s_1-s_2|, \quad H(x,s)-S(x)\mu(x,0)s+\beta\gamma(x)s^2/2+as^3\geqslant 0 \tag{1}$$

a.e. $x\in\Gamma$, and for all $s,s_1,s_2\in\mathbb{R}_+$.

A quite often used friction law (see Reference [15]) is piecewise linear and has the following form:

$$\begin{cases} \mu(x,u)=\mu_s(x)-\dfrac{\mu_s(x)-\mu_d(x)}{2D_c(x)}u & \text{if } u\leqslant 2D_c(x) \\ \mu(x,u)=\mu_d(x) & \text{if } u>2D_c(x) \end{cases} \tag{2}$$

where u is the relative slip, μ_s and μ_d ($\mu_s>\mu_d$) are the static and dynamic friction coefficients, and D_c is the critical slip (see Figure 2). This piecewise linear function is a reasonable approximation of the experimental observations reported in Reference [4], and will be used in Sections 5 and 6. If we put

$$\beta:=\frac{1}{G_0}\int_\Gamma \frac{(\mu_s(x)-\mu_d(x))S(x)}{2D_c(x)}\,\mathrm{d}\sigma, \quad \gamma:=\frac{1}{\beta}\,\frac{(\mu_s-\mu_d)S}{2D_c}\in L^\infty(\Gamma) \tag{3}$$

then (1) holds.

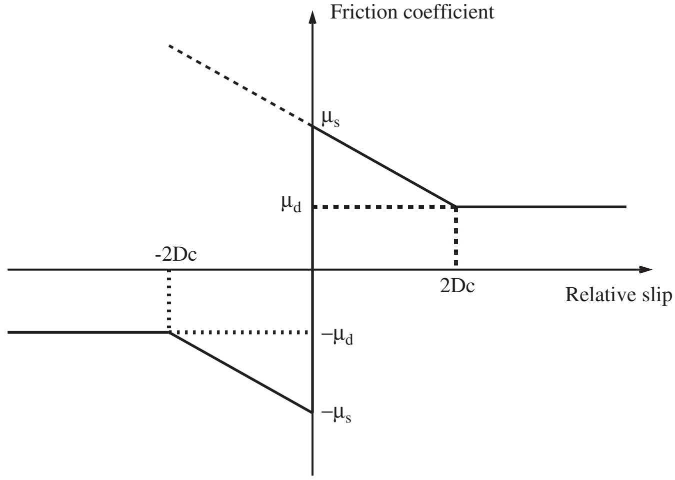

Figure 2. The piecewise linear slip weakening friction law (solid line). Without constraints on the sign of the slip and shear stress, the linearization can lead to solutions lying on the dashed line.

We suppose that we can choose the orientation of the unit normal of each connected fault (cut) of Γ such that

$$q(x) := \tau_1^\infty(x) n_1(x) + \tau_2^\infty(x) n_2(x) \leqslant q_0 < 0, \quad \text{a.e. } x \in \Gamma \tag{4}$$

This holds in many concrete applications, where the pre-stress τ^∞ gives a dominant direction of slip.

3. STATIC ANALYSIS

The slip dependent friction law on Γ in the static case is described by

$$G\partial_n w + q = -\mu(|[w(t)]|) S \operatorname{sign}([w]) \quad \text{if } [w] \neq 0 \tag{5}$$

$$|G\partial_n w + q| \leqslant \mu(|[w]|) S \quad \text{if } [w] = 0 \tag{6}$$

The above equations assert that the tangential (frictional) stress is bounded by the normal stress S multiplied by the value of the friction coefficient μ. If such a limit is not attained, sliding does not occur. Otherwise the frictional stress is opposed to the slip $[w]$ and its absolute value depends on the slip through μ.

Since we are looking for equilibrium positions in the neighborhood of $w \equiv 0$, and since the direction of slip is given by τ^∞ (see (4)), we get that we can restrict the above friction law to the case of nonnegative slip ($[w] \geqslant 0$). This is a usual assumption in earthquake source geophysics. From the equilibrium equation and the boundary conditions, we get the following static problem (SP): find $w:\Omega\to\mathbb{R}$ such that

$$\operatorname{div}(G\nabla w)=0 \quad \text{in } \Omega \tag{7}$$

$$w=0 \quad \text{on } \Gamma_d,\ [\partial_n w]=0 \quad \text{on } \Gamma \tag{8}$$

$$[w]\geqslant 0,\ G\partial_n w+q+S\mu([w])\geqslant 0, \quad [w](G\partial_n w+q+S\mu([w]))=0 \quad \text{on } \Gamma \tag{9}$$

We introduce, as in Reference [16], the functional space of finite elastic energy V. Let $\mathscr{V}$ be the following subspace of $H^1(\Omega)$:

$$\mathscr{V}=\{v\in H^1(\Omega);\ v=0 \text{ on } \Gamma_d, \text{ there exists } R>0 \text{ such that } v(x)=0 \text{ if } |x|>R\}$$

endowed with the norm $\|\ \|_V$ generated by the following scalar product:

$$(u,v)_V=\int_\Omega G\nabla u\cdot\nabla v\,\mathrm{d}x,\ \|u\|_V^2=(u,u)_V, \quad \forall u,v\in\mathscr{V} \tag{10}$$

We define V as the closure of $\mathscr{V}$ in the norm $\|u\|_V$, and by $\int_\Omega G\nabla u\cdot\nabla v\,\mathrm{d}x$ we mean $(u,v)_V$. The space V is continuously embedded in $H^1(\Omega_R)$ for all $R>0$, with $\Omega_R:=\{x\in\Omega/|x|<R\}$. If Ω is not bounded, V is not a subspace of $H^1(\Omega)$. Indeed, if $v\in V$ then $v(x)$ is not vanishing for $|x|\to+\infty$.

If we denote

$$V_+:=\{v\in V/[v]\geqslant 0 \text{ on } \Gamma\}$$

then the following quasi-variational inequality represents the variational approach of (SP): find $w\in V_+$ such that

$$\int_\Omega G\nabla w\cdot\nabla(v-w)\,\mathrm{d}x+\int_\Gamma S\mu([w])([v]-[w])\,\mathrm{d}\sigma+\int_\Gamma q([v]-[w])\,\mathrm{d}\sigma\geqslant 0 \tag{11}$$

for all $v\in V_+$.

We consider $\mathscr{W}:V\to\mathbb{R}$ the energy function:

$$\mathscr{W}(v)=\frac{1}{2}\int_\Omega G|\nabla v|^2\,\mathrm{d}x+\int_\Gamma H([v])+q[v]\,\mathrm{d}\sigma \tag{12}$$

Then we have the following result:

Theorem 3.1
If $w\in V$ is a local extremum for $\mathscr{W}$, then w is a solution of (11). Moreover, there exists at least a global minimum for $\mathscr{W}$.

Proof
Let w be a local minimum, i.e. there exists δ such that $\mathscr{W}(w)\leqslant\mathscr{W}(u)$ for all $u\in V_+$ with $\|w-u\|_V\leqslant\delta$. For all $v\in V_+$ we put $u=w+t(v-w)$, with $t>0$ small enough, in the last inequality and we pass to the limit with $t\to 0$ to deduce (11).

In order to prove that $\mathscr{W}$ has a global minimum, we remark that $[\ ]:V\to L^2(\Gamma)$ is compact. Hence $v\to\int_\Gamma H([v])+q[v]\,\mathrm{d}\sigma$ is weakly continuous on V, which implies that $\mathscr{W}$ is weakly lower semicontinuous. Bearing in mind that $\liminf\mathscr{W}(v)=\infty$ for $\|v\|_V\to\infty$, from a Weierstrass type theorem we deduce that $\mathscr{W}$ has at least a global minimum. □

Let us consider the following non-linear eigenvalue problem:

$$\begin{cases} \text{find } \varphi \in V_+, \ \varphi \neq 0 \text{ and } \beta \in \mathbb{R}_+ \text{ such that} \\ \int_\Omega G\nabla\varphi \cdot \nabla(v-\varphi)\,\mathrm{d}x \geqslant \beta \int_\Gamma \gamma[\varphi][v-\varphi]\,\mathrm{d}\sigma, \quad \forall v \in V_+ \end{cases} \tag{13}$$

The non-linear eigenvalue problem (13) can be written as an eigenproblem involving the Laplace operator and Signorini-type boundary conditions:

$$\text{find } \varphi : \Omega \to \mathbb{R} \text{ and } \beta \in \mathbb{R} \text{ such that}$$

$$\mathrm{div}(G\nabla u) = 0 \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \Gamma_d \tag{14}$$

$$[G\partial_n u] = 0, \quad [u] \geqslant 0, \ G\partial_n u \geqslant \beta\gamma[u], \quad [u](G\partial_n u - \beta\gamma[u]) = 0 \quad \text{on } \Gamma \tag{15}$$

The linear case, that is Equation (14) with the boundary condition

$$[G\partial_n u] = 0, \quad G\partial_n u = \beta\gamma[u] \quad \text{on } \Gamma \tag{16}$$

was analysed in Reference [17]. For bounded domains, they proved that the spectrum of (14), (16) consists of a nondecreasing and unbounded positive sequence of eigenvalues β. Let us remark that, if φ is a solution of (14), (16) and $[\varphi] \geqslant 0$ on Γ, then φ is a solution for (14), (15), too. For colinear faults, the first eigenfunction φ_0 corresponding to λ_0^2 was found in numerical computations to have a positive slip on Γ (see References [7,12]), hence the linear case was sufficient to give a satisfactory model for the initiation of instabilities. If the faults are not colinear, then this condition is no longer satisfied, that is the first eigenfunction of the linear problem has no physical significance. The explanation lies in the linearization of the friction law around the equilibrium position $w \equiv 0$ (see Figure 2): an unconstrained linearization can lead to solutions lying on the dashed line of the friction law, whereas the constrained formulation ensures that the solutions lie on the solid line, so that the corresponding slip is necessarily of constant sign.

If $\gamma(x) \geqslant \gamma_0 > 0$ then we can associate to the eigenvalue variational inequality (13) the Rayleigh quotient β_0,

$$\beta_0 = \inf_{v \in V_+} \frac{\int_\Omega G|\nabla v|^2\,\mathrm{d}x}{\int_\Gamma \gamma[v]^2 \mathrm{d}\sigma} \tag{17}$$

which is the smallest eigenvalue β. More precisely we have the following result, which holds for a rather general $\gamma \in L^\infty(\Gamma)$.

Theorem 3.2
Suppose that γ is such that $S_+ = \{v \in V_+; \int_\Gamma \gamma[v]^2\,\mathrm{d}\sigma = 1\} \neq \emptyset$. Then there exists (φ_0, β_0) a solution of the non-linear eigenvalue problem (13) such that

$$\beta_0 = \int_\Omega G|\nabla\varphi_0|^2\,\mathrm{d}x = \beta_0 \int_\Gamma \gamma[\varphi_0]^2\,\mathrm{d}\sigma \tag{18}$$

$$\int_\Omega G|\nabla v|^2\,\mathrm{d}x \geqslant \beta_0 \int_\Gamma \gamma[v]^2\,\mathrm{d}\sigma, \quad \forall v \in V_+ \tag{19}$$

and if (φ, β) is another solution of (13) then $\beta \geqslant \beta_0$.

Proof
Let $\beta_0 := \inf_{v\in S_+} \|v\|_V$, and let (v_n) be a sequence of S_+ such that $\|v_n\|_V \to \beta_0$. Since (v_n) is a bounded sequence in V, we get that there exist $\varphi_0 \in V$ and a subsequence, denoted again by (v_n), with $v_n \to \varphi_0$ weakly in V. Let R be such that $\Gamma \subset \Omega_R$, where $\Omega_R = \Omega \cap B_R(0)$. Bearing in mind that (v_n) is bounded in $H^1(\Omega_R)$, from the compact embedding of $H^1(\Omega_R)$ in $L^2(\Gamma)$ we deduce that $\varphi_0 \in S_+$. On the other hand, $\|\varphi_0\|_V \leqslant \liminf \|v_n\|_V = \beta_0$, hence $\|\varphi_0\|_V = \beta_0 = \min_{v\in S_+} \|v\|_V$ and we obtain (18).

We prove now that (19) holds. Let $v \in V_+$ and $d := \int_\Gamma \gamma[v]^2\, \mathrm{d}\sigma$. If $d>0$ then we put $w = v/\sqrt{d} \in S_+$, and from $\|w\|_V \geqslant \beta_0$ inequality (19) yields. If $d \leqslant 0$ then the inequality is obvious.

In order to prove that (φ_0, β_0) is a solution of (13), we replace v by $\varphi_0 + t(v - \varphi_0) \in V_+$ in (19) and we pass to the limit with $t \to 0+$.

We prove now that β_0 is the smallest eigenvalue. Let (φ, β) be another solution of (13). If we put $v=0$ and then $v = 2\varphi$ in (13), we get $\beta \int_\Gamma \gamma[\varphi]^2\, \mathrm{d}\sigma = \int_\Omega G|\nabla\varphi|^2\, \mathrm{d}x$, hence $\int_\Gamma \gamma[\varphi]^2\, \mathrm{d}\sigma > 0$, and from (19) we get $\beta \geqslant \beta_0$. □

Let us suppose in the following that $w \equiv 0$ is a solution of (11). An equivalent condition is

$$q(x) + S(x)\mu(x,0) \geqslant 0, \quad \text{a.e. } x \in \Gamma \tag{20}$$

Theorem 3.3
Suppose that (20) holds, let β be as in (1) and let β_0 be given by the previous theorem. If $\beta < \beta_0$ then $w \equiv 0$ is an isolated local minimum for $\mathscr{W}$, i.e. there exists $\delta > 0$ such that

$$\mathscr{W}(0) < \mathscr{W}(v), \quad \forall v \in V_+, \ v \neq 0, \ \|v\|_V < \delta$$

Proof
Let us suppose that $w=0$ is not a local minimum for $\mathscr{W}$, i.e. there exists $v_n \to 0$ strongly in V such that $\mathscr{W}(v_n) \leqslant \mathscr{W}(0) = 0$. From (1) and (20) we get $\mathscr{W}(v_n) \geqslant 1/2\|v_n\|_V^2 - \int_\Gamma (\gamma\beta/2[v_n]^2 + a[v_n]^3)\, \mathrm{d}\sigma$. If we make use of (19) then we deduce

$$0 \geqslant \mathscr{W}(v_n) \geqslant \frac{\beta_0 - \beta}{2\beta_0} \|v_n\|_V^2 - a \int_\Gamma [v_n]^3\, \mathrm{d}\sigma$$

Since V is continuously embedded in $L^3(\Gamma)$, from the above inequality we get that $(\beta_0 - \beta)/(2\beta_0) \leqslant aC\|v_n\|_V$, a contradiction. □

4. DYNAMIC ANALYSIS

The slip dependent friction law on Γ_f in the dynamic case is described by

$$G\partial_n w(t) + q = -\mu(|[w(t)]|)S\,\mathrm{sign}([\partial_t w(t)]) \quad \text{if } [\partial_t w(t)] \neq 0 \tag{21}$$

$$|G\partial_n w(t) + q| \leqslant \mu(|[w(t)]|)S \quad \text{if } \partial_t[w(t)] = 0 \tag{22}$$

Unlike the static case, in dynamics the frictional stress is opposed to the slip rate $[\partial_t w]$. As in statics, the direction of slip is given by τ^∞ (see (4)) and we can restrict the above friction law to the case of nonnegative slip rate ($[\partial_t w(t)] \geqslant 0$). Since the initial slip can also be supposed nonnegative, in addition we have $[w(t)] \geqslant 0$. Using the above assumptions, the momentum balance law $\operatorname{div} \sigma = \rho \partial_{tt} u$ and the boundary conditions, we obtain the following dynamic problem (DP): find $w : \mathbb{R}_+ \times \Omega \to \mathbb{R}$ solution of the wave equation

$$\rho \partial_{tt} w(t) = \operatorname{div}(G \nabla w(t)) \quad \text{in } \Omega \tag{23}$$

with boundary conditions of Signorini type:

$$w(t) = 0 \quad \text{on } \Gamma_d, \quad [G \partial_n w(t)] = 0, \quad [\partial_t w(t)] \geqslant 0 \quad \text{on } \Gamma \tag{24}$$

$$G \partial_n w(t) + q + \mu([w(t)]) S \geqslant 0, \quad [\partial_t w(t)](G \partial_n w(t) + q + \mu([w(t)]) S) = 0 \quad \text{on } \Gamma \tag{25}$$

The initial conditions are

$$w(0) = w_0, \quad \partial_t w(0) = w_1 \quad \text{in } \Omega \tag{26}$$

Any solution of the above problem satisfies the following variational problem (VP): find $w : [0, T] \to V$ such that

$$\begin{aligned} \partial_t w(t) \in W_+, \quad & \int_\Omega \rho \partial_{tt} w(t)(v - \partial_t w(t)) \, \mathrm{d}x + \int_\Omega G \nabla w(t) \cdot \nabla(v - \partial_t w(t)) \, \mathrm{d}x \\ & + \int_\Gamma S \mu([w(t)])([v] - [\partial_t w(t)]) \, \mathrm{d}\sigma \\ & \geqslant - \int_\Gamma q([v] - [\partial_t w(t)]) \, \mathrm{d}\sigma, \quad \forall v \in W_+ \end{aligned} \tag{27}$$

where

$$W := \{ v \in H^1(\Omega) / v = 0 \text{ on } \Gamma_d \}, \quad W_+ := \{ v \in W / [v] \geqslant 0 \text{ on } \Gamma \} \tag{28}$$

The main difficulty in the study of the above evolution variational inequality is the non-monotone dependence of μ with respect to the slip $[w]$. The existence of a solution w of the following regularity:

$$w \in W^{1,\infty}(0, T, W) \cap W^{2,\infty}(0, T, L^2(\Omega)) \tag{29}$$

can be deduced for two-dimensional bounded domains using the method developed in Reference [18].

Since our intention is to study the evolution of the elastic system near an unstable equilibrium position, we shall suppose that $q = -\mu(0) S$. We remark that $w \equiv 0$ is an equilibrium solution of (27), and w_0, w_1 may be considered as small perturbations of this equilibrium.

For simplicity, let us assume in the following that the friction law is given by (2). Since the initial perturbation (w_0, w_1) of the equilibrium ($w \equiv 0$) is small, we have $[w(t, x)] \leqslant 2D_c$ for $t \in [0, T_c]$ and $x \in \Gamma$, where T_c is a critical time for which the slip on the fault reaches the critical value $2D_c$ at least at one point. Hence for a first period $[0, T_c]$, called the initiation phase, we deal with a linear function μ.

Our purpose is to analyse the evolution of the perturbation during this nucleation phase. That is why we are interested in the existence of solutions of the type

$$w(t,x) = \sinh(|\lambda| t) u(x), \quad w(t,x) = \sin(|\lambda| t) u(x) \quad \text{for } t \in [0, T_c] \tag{30}$$

If we put the above expression in (27) and we have in mind that from (2) we get $S\mu(s) + q = -\beta\gamma s$, with γ and β given by (3), then we deduce that (u, λ^2) is the solution of the following nonlinear eigenvalue problem:

$$\begin{cases} \text{find } u \in W_+ \text{ and } \lambda^2 \in \mathbb{R} \text{ such that} \\ \displaystyle\int_\Omega G\nabla u \cdot \nabla(v-u)\,\mathrm{d}x - \beta \int_\Gamma \gamma[u][v-u]\,\mathrm{d}\sigma + \lambda^2 \int_\Omega \rho u(v-u)\,\mathrm{d}x \geqslant 0 \end{cases} \tag{31}$$

for all $v \in W_+$. Solutions of the first type in (30) have an exponential growth in time and correspond to $\lambda^2 > 0$. Solutions of the second type have a constant amplitude during the initiation phase and correspond to $\lambda^2 < 0$.

The nonlinear eigenvalue problem (31) can be written as a classical eigenproblem for the Laplace operator with Signorini-type boundary conditions:

$$\text{find } u : \Omega \to \mathbb{R} \text{ and } \lambda^2 \in \mathbb{R} \text{ such that}$$

$$\operatorname{div}(G\nabla u) = \lambda^2 \rho u \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \Gamma_d \tag{32}$$

$$[G\partial_n u] = 0, \quad [u] \geqslant 0, \quad G\partial_n u \geqslant \beta\gamma[u], \quad [u](G\partial_n u - \beta\gamma[u]) = 0 \quad \text{on } \Gamma \tag{33}$$

The linear case, that is Equation (32) with the boundary condition

$$[G\partial_n u] = 0, \quad G\partial_n u = \beta\gamma[u] \quad \text{on } \Gamma \tag{34}$$

was analysed in Reference [12]. For bounded domains, they proved that the spectrum of (32), (34) consists of a decreasing and unbounded sequence of eigenvalues. The largest one, λ_0^2, which may be positive, is shown to be an increasing function of the friction parameter β. Let us remark that, if u is a solution of (32), (34) and $[u] \geqslant 0$ on Γ, then u is a solution for (32), (33), too. For colinear faults, as in the static analysis, the first eigenfunction u_0 corresponding to λ_0^2 was found in numerical computations to have a positive slip on Γ (see References [7,12]), hence the linear analysis was sufficient to give a satisfactory model for the initiation of instabilities. If the faults are not colinear, then this condition is no longer satisfied, that is the first eigenfunction of the linear problem has no physical significance. Hence, in modelling the initiation of friction instabilities, the nonlinear eigenvalue problem has to be considered. As reported in Reference [14], where fault systems of realistic geometries were analysed, there is an important gap between the first eigenvalues of the linear and non-linear problems.

The non-linear eigenvalue variational inequality (31) was considered in Reference [13], where the existence of infinitely many solutions was established for bounded domains. The proof relies on algebraic topology methods developed by Krasnoselski, combined with adequate tools in the sense of the Degiovanni non-smooth critical point theory.

We restrict here our investigation to the first eigenvalue (Rayleigh quotient) and to the case of positive eigenvalues λ^2, which have important physical significance. Indeed, the unstable evolution of a perturbation during the initiation phase can be described by the solutions of type

(30) which exhibit an exponential growth with time, i.e. by the eigenfunctions corresponding to positive eigenvalues λ^2.

We have the following result:

Theorem 4.1
Suppose that γ is such that $T_+ := \{v \in W_+; \int_\Gamma \gamma[v]^2 \,d\sigma = 1\} \neq \emptyset$ and let β_0 be given by Theorem 3.2. Then we have

(i) For all $\beta > \beta_0$, there exists $(\Phi_0(\beta), \lambda_0^2(\beta))$ a solution of the non-linear eigenvalue problem (31) with $\lambda_0^2(\beta) > 0$ being the Rayleigh quotient

$$\lambda_0^2(\beta) = -\min_{v \in W_+} \frac{\int_\Omega G|\nabla v|^2 - \beta \int_\Gamma \gamma[v]^2 \,d\sigma}{\int_\Omega \rho v^2 \,dx} \tag{35}$$

If (Φ, λ^2) is another solution of (31) then $\lambda^2 \leqslant \lambda_0^2(\beta)$. Moreover, $\beta \mapsto \lambda_0^2(\beta)$ is a positive convex function and

$$\limsup_{\beta \to +\infty} \frac{\lambda_0(\beta)}{\beta} < +\infty, \quad \lim_{\beta \to \beta_0 +} \lambda_0^2(\beta) = 0$$

(ii) If $\beta \leqslant \beta_0$, then there exists no solution of (31) with $\lambda^2 > 0$.

Proof
Let $s > 0$ be fixed and let us consider the minimization problem

$$\inf_{v \in T_+} J_s(v), \quad J_s(v) := \int_\Omega G|\nabla v|^2 \,dx + s \int_\Omega \rho |v|^2 \,dx$$

We can use now the same arguments as in the proof of Theorem 3.2 to deduce that there exist $\Psi_0(s) \in T_+$ and $b(s) > 0$ such that

$$b(s) = J_s(\Psi_0(s)) = \min_{v \in T_+} J_s(v) \tag{36}$$

Let us prove now that

$$\int_\Omega G|\nabla v|^2 \,dx + s \int_\Omega \rho v^2 \,dx - b(s) \int_\Gamma \gamma[v]^2 \,d\sigma \geqslant 0, \quad \forall v \in W_+ \tag{37}$$

For $v \in W_+$ we put $d := \int_\Gamma \gamma[v]^2 \,d\sigma$. If $d > 0$ then $v/\sqrt{d} \in T_+$ and from (36) we obtain (37). If $d \leqslant 0$ then (37) is obvious.

Let us prove now that $\liminf_{s \to +\infty} b(s)/\sqrt{s} > 0$. From (36) we obtain the following inequality for $s > 1$:

$$\|\Psi_0(s)\|^2_{H^1(\Omega)} + (s-1)\|\Psi_0(s)\|^2_{L^2(\Omega)} \leqslant Cb(s)\|\gamma\|_{L^\infty(\Gamma)}\|\Psi_0(s)\|^2_{L^2(\Gamma)} \tag{38}$$

We use now the following inequality (see Reference [19, Lemma 5.1], for a simple proof)

$$\|v\|^2_{L^2(\Gamma)} \leqslant C\|v\|_{L^2(\Omega)}\|v\|_{H^1(\Omega)}, \quad \forall v \in V \tag{39}$$

to get $Cb(s)\|\gamma\|_{L^\infty(\Gamma)} \geqslant 1/B(s) + (s-1)B(s) \geqslant 2\sqrt{s-1}$ with

$$B(s) := \|\Psi_0(s)\|_{L^2(\Omega)}/\|\Psi_0(s)\|_{H^1(\Omega)}$$

By passing to the limit in the above inequality, we deduce $\liminf_{s\to+\infty} b(s)/\sqrt{s} > 0$.

Since $s \to J_s(v)$ is an affine function for all $v \in T_+$, we get from (36) that $s \to b(s)$ is concave. This property and the fact that $\liminf_{s\to+\infty} b(s) = +\infty$ imply that b is increasing. Let us denote $b_0 = \lim_{s\to 0+} b(s)$. Since b is one-to-one from $(0, +\infty)$ to $(b_0, +\infty)$, we can define $\lambda_0^2 : (b_0, +\infty) \to (0, +\infty)$ by $\lambda_0^2(\beta) := b^{-1}(\beta)$. From the above properties of b we get that $\beta \mapsto \lambda_0^2(\beta)$ is a positive convex function with $\limsup_{\beta\to+\infty} \lambda_0(\beta)/\beta < +\infty$.

We replace now v by $\Psi_0(s) + t(v - \Psi_0(s)) \in W_+$ in (36) and pass to the limit with $t \to 0+$ to get that

$$\int_\Omega G\nabla\Psi_0(s)\cdot\nabla(v - \Psi_0(s))\,\mathrm{d}x + s\int_\Omega \rho\Psi_0(s)(v - \Psi_0(s))\,\mathrm{d}x$$

$$\geqslant b(s)\int_\Gamma \gamma[\Psi_0(s)][v - \Psi_0(s)]\,\mathrm{d}\sigma$$

If we put now $\beta = b(s)$, $s = \lambda^2(\beta)$ and $\Phi_0(\beta) = \Psi_0(s)$, we deduce that $(\Phi_0(\beta), \lambda_0^2(\beta))$ is a solution of (31) for all $\beta > b_0$. Moreover, inequality (35) yields from (37).

Let us prove now that $\beta_0 = b_0$. Bearing in mind that $T_+ \subset S_+$, from (36) we have $b(s) \geqslant \inf_{v\in T_+} J_0(v) \geqslant \inf_{v\in S_+} J_0(v) = \beta_0$. Passing to the limit with s we get $b_0 \geqslant \beta_0$. Let φ_0 be as in Theorem 3.2 and let $(v_n) \subset \mathscr{V}$ be such that $[v_n] \geqslant 0$ on Γ and $v_n \to \varphi_0$ in V. Since $\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma \to 1$ we have $\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma > 0$ and $b(s)\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma \geqslant b_0\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma$ for all $s > 0$, and from (37) we deduce

$$\int_\Omega G|\nabla v_n|^2\,\mathrm{d}x + s\int_\Omega \rho v_n^2\,\mathrm{d}x \geqslant b_0\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma$$

We pass to the limit with $s \to 0$ to get $\int_\Omega G|\nabla v_n|^2 \geqslant b_0\int_\Gamma \gamma[v_n]^2\,\mathrm{d}\sigma$, then we take the limit with respect to n to deduce that $\beta_0 = \|\varphi_0\|_V^2 \geqslant b_0\int_\Gamma \gamma[\varphi_0]^2\,\mathrm{d}\sigma = b_0$, i.e. $\beta_0 \geqslant b_0$.

Let (Φ, λ^2) be another solution of (31). If we put $v = 0$ and then $v = 2\Phi$ in (31), we get

$$\int_\Omega G|\nabla\Phi|^2\,\mathrm{d}x + \lambda^2\int_\Omega \rho\Phi^2\,\mathrm{d}x = \beta\int_\Gamma \gamma[\Phi]^2\,\mathrm{d}\sigma \tag{40}$$

and $\lambda^2 \leqslant \lambda_0^2(\beta)$ follows from (35). If $\lambda^2 > 0$ then (40) implies that $\int_\Gamma \gamma[\Phi]^2\,\mathrm{d}\sigma > 0$, and from (37) we have $\beta\int_\Gamma \gamma[\Phi]^2\,\mathrm{d}\sigma \geqslant b(\lambda^2)\int_\Gamma \gamma[\Phi]^2\,\mathrm{d}\sigma$. Hence, $\beta \geqslant b(s) > \beta_0$, i.e. there exists no solution of (31) with $\lambda^2 > 0$ for $\beta \leqslant \beta_0$. □

5. MIXED FINITE ELEMENT APPROXIMATION

In this section, we consider a mixed finite element discretization of the non-linear spectral problem and we give a numerical algorithm to approach the first eigenvalue/eigenfunction.

For the sake of simplicity, we shall suppose in this section that Ω is bounded. We explain, at the beginning of the next section, how to handle unbounded domains using the infinite elements technique.

The body Ω is discretized by using a family of triangulations $(\mathcal{T}_h)_h$ made of finite elements of degree $k \geqslant 1$. The discretization parameter, defined as the largest edge of the triangulation $\mathcal{T}_h$, is denoted by $h > 0$. The set W_h approximating W becomes

$$W_h := \{v_h; v_h \in C(\bar{\Omega} \setminus \Gamma),\ v_h|_T \in P_k(T)\ \forall T \in \mathcal{T}_h,\ v_h = 0 \text{ on } \Gamma_d\}, \quad W_h^+ = W_h \cap W_+$$

where $P_k(T)$ is the space of polynomial functions of degree k on T. Let us mention that we focus on the discrete problem and that any discussion concerning the convergence of the finite element problem towards the continuous model is out of the scope of this paper.

We suppose that we deal with a conforming mesh of Ω, i.e. the two families of mono-dimensional meshes inherited by $(\mathcal{T}_h)_h$ on each side of Γ coincide (and are denoted by $(\mathcal{T}_h)_h$). Set

$$F_h := \{\tau; \tau = [v_h],\ v_h \in W_h\}, \quad F_h^+ := \{\tau \in F_h; \tau \geqslant 0 \text{ on } \Gamma\}$$

which are included in the space of continuous functions on Γ being piecewise of degree k on $(T_h)_h$. We denote by p the dimension of F_h and by ψ_i, $1 \leqslant i \leqslant p$, the corresponding canonical finite element basis functions of degree k.

The discrete problem derived from (31) is

For a given β, find $(u_h, \tau_h) \in W_h^+ \times F_h$ and $\lambda^2 > 0$ such that

$$\int_\Omega G\nabla u_h \cdot \nabla v_h \, \mathrm{d}x + \lambda^2 \int_\Omega \rho u_h v_h \, \mathrm{d}x = \int_\Gamma \tau_h [v_h] \, \mathrm{d}\sigma, \quad \forall v_h \in W_h \tag{41}$$

$$\int_\Gamma (\tau_h - \beta\gamma[u_h])(\sigma_h - [u_h]) \geqslant 0, \quad \forall \sigma_h \in F_h^+ \tag{42}$$

Since $\beta \to \lambda_0^2(\beta)$ is one-to-one from $(\beta_0, +\infty)$ to $(0, +\infty)$, we can choose to compute $(\Phi_{0h}, \tau_h, b(s))$ for each $s = \lambda_0^2$, rather than $(\Phi_{0h}, \tau_h, \lambda_0^2(\beta))$ for each β. In this case the above problem becomes:

For a given $\lambda^2 \geqslant 0$, find $(u_h, \tau_h) \in W_h^+ \times F_h$ and $\beta = \beta(\lambda^2) > 0$ such that (41)–(42) holds

Note that in this way we can formulate both static and dynamic problems in one non-linear eigenvalue problem (you just have to put $\lambda^2 = 0$ for the static case).

Let us give here the formulation of (41)–(42) as an eigenvalue problem for a nonlinear operator. For this, let us denote by $Q: W_h \to F_h$ the operator which associates to $u_h \in W_h$ the stress $\tau_h \in F_h$ through (41), and by $R: F_h \to W_h$ the operator which associates to $\tau_h \in F_h$ the unique solution $u_h \in W_h$ of Equation (41). If we put now $\sigma_h = [v_h]$ in (42) then we deduce

$$\int_\Omega G\nabla(u_h - \beta R(\gamma[u_h])) \cdot \nabla(v_h - u_h) \, \mathrm{d}x + \lambda^2 \int_\Omega \rho(u_h - \beta R(\gamma[u_h]))(v_h - u_h) \, \mathrm{d}x \geqslant 0 \tag{43}$$

for all $v_h \in W_h^+$. Let also denote by $P: W_h \to W_h^+$ the projector map on W_h^+, with respect to the scalar product $\langle v, w \rangle_W =: \int_\Omega G\nabla v \cdot \nabla w \, dx + \lambda^2 \int_\Omega \rho v w \, dx$. From (43) we have $\langle u_h - \beta R(\gamma[u_h]), v_h - u_h \rangle_W \geqslant 0$, for all $v_h \in W_h$ which is equivalent with $u_h = P(\beta R(\gamma[u_h]))$. For convenience, we define $q_h := \gamma[u_h]$. If we denote by $\mathscr{P}_h: F_h \to F_h$ the operator $\mathscr{P}_h(\sigma_h) = \gamma[P(R(\sigma_h))]$ and we have in mind that P is positively homogeneous (W_+ is a convex cone), then we get that (41)–(42) can be written as

$$q_h = \beta \mathscr{P}_h(q_h), \quad u_h = \beta P(R(q_h)), \quad \tau_h = Q(u_h) \tag{44}$$

Let $\mathscr{L}: W_h \times F_h \to \mathbb{R}$ be the Lagrangian

$$\mathscr{L}(v, p) := \frac{1}{2} \int_\Omega G|\nabla v|^2 \, dx + \frac{1}{2} \lambda^2 \int_\Omega \rho v^2 \, dx - \int_\Gamma p[v] \, d\sigma \tag{45}$$

The following algorithm will be used to obtain an approximation $b_h = b_h(\lambda^2)$ of the smallest eigenvalue $\beta(\lambda^2)$ of (41)–(42), and the corresponding approximate eigenfunction Φ_{0h}.

Algorithm 5.1
The algorithm starts with an arbitrary $p_h^0 \in F_h^+$. At iteration $n+1$, having $p_h^n \in F_h^+$, we compute $\psi_h^n \in W_h^+$ solution of

$$\mathscr{L}(\psi_h^n, p_h^n) \leqslant \mathscr{L}(v_h, p_h^n) \quad \text{for all } v_h \in W_h^+ \tag{46}$$

Then we update:

$$p_h^{n+1} = \gamma[\psi_h^n], \quad b_h^{n+1} = \frac{\|p_h^n\|_{L^2(\Gamma)}}{\|p_h^{n+1}\|_{L^2(\Gamma)}}, \quad \Phi_{0h}^{n+1} = \frac{\psi_h^n}{\|p_h^{n+1}\|_{L^2(\Gamma)}}$$

The algorithm stops when $|b_h^{n+1} - b_h^n| + \|\Phi_{0h}^{n+1} - \Phi_{0h}^n\|$ is small enough. If we put $\tau_h^n \in F_h$ such that

$$\int_\Omega G\nabla \Phi_{0h}^n \cdot \nabla v_h \, dx + \lambda^2 \int_\Omega \rho \Phi_{0h}^n v_h \, dx = \int_\Gamma \tau_h^n [v_h] \, d\sigma, \quad \forall v_h \in W_h$$

then from (46) we get

$$\int_\Gamma (\tau_h^{n+1} - b_h^{n+1} \gamma[\Phi_{0h}^n])(\sigma_h - [\Phi_{0h}^{n+1}]) \geqslant 0, \quad \forall \sigma_h \in F_h^+$$

Hence, if the convergence of the algorithm is assured, i.e. $b_h^n \to b_h, \Phi_{0h}^n \to \Phi_{0h}$, then $\tau_h^n \to \tau_h$ and Φ_{0h}, τ_h, b_h is a solution of (41)–(42).

Let us relate here the Algorithm 5.1 to formulation (44) of the non-linear eigenvalue problem. For this, let us remark that (46) is equivalent with $\psi_h^n = P(R(p_h^n))$, which means that

$$p_h^{n+1} = \mathscr{P}_h(p_h^n), \quad b_h^{n+1} = \frac{\|p_h^n\|_{L^2(\Gamma)}}{\|p_h^{n+1}\|_{L^2(\Gamma)}} \tag{47}$$

We see now that Algorithm 5.1 makes use of the successive iterates of the non-linear operator $\mathscr{P}_h$: the ratio of the moduli of two consecutive iterates should converge towards the largest eigenvalue $\frac{1}{b_h}$ of $\mathscr{P}_h$. Moreover, if we denote $q_h^n = p_h^n / \| p_h^n \|_{L^2(\Gamma)}$, then from the update of the algorithm we get the following formulation related to (44):

$$q_h^{n+1} = b_h^{n+1} \mathscr{P}_h(q_h^n), \quad \Phi_{0h}^{n+1} = b_h^{n+1} P(R(q_h^n)), \quad \tau_h^{n+1} = Q(\Phi_{0h}^{n+1}) \tag{48}$$

To minimize $\mathscr{L}(\cdot, p_h^n)$ in (46), we use the Usawa algorithm. We start with an arbitrary $s_h^0 \in F_H^+$. At iteration $k+1$, having $s_h^k \in F_h^+$, we compute $\psi_h^{n,k+1} \in W_h$ the solution of

$$\mathscr{L}(\psi_h^{n,k+1}, p_h^n + s_h^k) \leqslant \mathscr{L}(v_h, p_h^n + s_h^k) \quad \text{for all } v_h \in W_h \tag{49}$$

without any difficulty since we minimize here a quadratic functional. Then we update

$$s_h^{k+1} = (s_h^k - r\psi_h^{n,k+1})_+$$

with some $r > 0$ (here w_+ denotes the positive part of w). The algorithm stops when $\|s_h^{k+1} - s_h^k\| + \|\psi_h^{k+1} - \psi_h^k\|$ is small enough. The process can be accelerated using the augmented Lagrangian, i.e. we put $\bar{\mathscr{L}}(v, p) = \mathscr{L}(v, p) + q \int_\Gamma [v]_-^2$ instead of $\mathscr{L}$ in (49) (here w_- denotes the negative part of w). It saves up to 20% of computation time in one step of Algorithm 5.1.

In our case, Lagrange multipliers p_h^n are not stress components, as it is frequently in mixed formulations, but the displacement jump on the fault. Nevertheless, the tangential (shear) stress can be retrieved, for k large enough, as

$$\tau_h^{n+1} = b_h^{n+1} \gamma[\Phi_{0h}^n] + \frac{s_h^k}{\|\gamma[\psi_h^{n,k}]\|_{L^2(\Gamma)}} = \frac{p_h^n + s_h^k}{\| p_h^{n+1} \|_{L^2(\Gamma)}} \tag{50}$$

The non-linear eigenvalue method presented in this paper and the above algorithm were used in Reference [14] for some geophysical applications, in particular to explain the slip patterns of normal faults in Afar (East Africa). In all our tests and applications, we found that the algorithm is convergent; but the proof of the convergence is beyond the scope of the present paper.

6. NUMERICAL RESULTS

Numerical simulations were performed with Γ being a set of parallel planar faults. Examples of curved faults were investigated in Reference [14]. The friction coefficient is piecewise linear, as suggested in (2), with D_c, S, μ_s and μ_d constant. The stability of the system is characterized by the comparison of the friction parameter $\beta = S(\mu_s - \mu_d)/2aD_c$ (here a is a characteristic length) with the first eigenvalue β_0, as discussed in Sections 3 and 4.

The first eigenvalue/eigenfunction was found numerically using Algorithm 5.1. In the stopping criterion (i.e. $|b_h^{n+1} - b_h^n| + \|\Phi_{0h}^{n+1} - \Phi_{0h}^n\| < \varepsilon$), we chose $\varepsilon = 10^{-6}$ for a single fault and $\varepsilon = 10^{-4}$ for two-faults systems.

We used finite elements of degree $k = 1$. To handle unbounded domains, $\Omega = \mathbb{R}^2 \backslash \Gamma$ was splitted in two parts Ω^0 and Ω^∞ (see Figure 3). The first one (Ω^0) is a square containing Γ, and is covered by a classical triangulation. The second part (Ω^∞) is covered by *infinite*

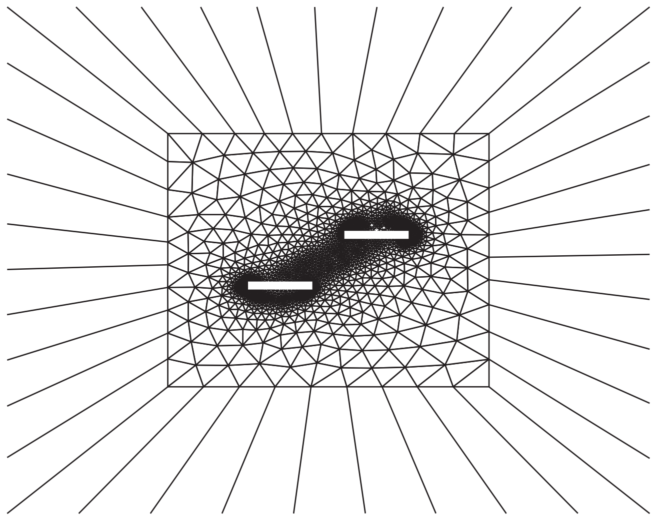

Figure 3. Example of finite/infinite element mesh. Remark the density of the refined mesh around fault tips and in the zones of interaction.

elements (see Reference [20] for a precise description). Infinite elements have two nodes on the exterior boundary of Ω^0 and a third one at infinity. Without them, we would have to clamp the boundary of Ω^0, so that it would have to be far away from Γ and the resulting number of nodes would be very large. Note that infinite elements do not require any additional degree of freedom, since the points added at infinity necessarily have zero displacements. The solution is computed only on the nodes that lie along the boundary of Ω^0, i.e. on two nodes per infinite element. This requires one single additional information, that is the overall behavior at infinity. For this, we assume that the shape of the solution at infinity is r^{-p}, r being the distance to the centre of Ω^0. In the static case, we must take $p>0$ to obtain solutions of finite potential energy ($\nabla u \in L^2(\mathbb{R}^2)$). In the dynamic case, the kinetic energy also must be finite ($u \in L^2(\mathbb{R}^2)$), so that we must have $p>1$. In the following, we have taken $p=1$ for $\lambda^2=0$, and $p=2$ for $\lambda^2>0$. An example of finite/infinite element mesh is presented in Figure 3.

In this case as well as in the case Ω bounded (with its exterior boundary clamped), the assumptions we have to make on the shape of the solution outside the finite element mesh are reasonable only if the boundary of Ω (or Ω^0) is far away from the fault. However, numerical examples showed that infinite elements are helpful.

The overall accuracy of any finite element model is deteriorated by local singularities. In our model, such singularities exist at the fault tips. To include them in the computed solution, and to reduce the size of computations without any loss of accuracy, we need to refine the mesh by increasing the number of nodes in the critical zones. The remeshing principle is an iterative process: from the computation of the local error of the solution on each element, we deduce the local size of the mesh required to achieve a prescribed maximum error. At each step, a new mesh is built on the basis of these size requirements. The error estimator, given by Reference [21], is based on an averaging of the gradient, which is a piecewise constant vector-field. The local error is estimated as the modulus of the difference between the gradient

Table I. Description of the six meshes considered in the convergence analysis. The first four are regular meshes, whereas meshes 5 and 6 are optimized.

Mesh	Mesh size	Nb. of nodes	Nb. of edges on the fault	Nb. of iterations
1	0.4	2969	5	10
2	0.2	11625	10	10
3	0.1	46130	20	10
4	0.05	183818	40	11
5	—	24483	131	11
6	—	21522	281	11

and its projection on the finite element space (which is piecewise of degree 1). We first build an initial homogeneous mesh then, using the above remeshing method, after a few iterations, we obtain an optimised mesh such as the example presented in Figure 3.

Several kinds of numerical tests are reported in the following. First of all, the convergence of Algorithm 5.1 is investigated on a single planar fault, where (46) reduces to a simple linear system. Then the resolution of (46) is tested on a system of two parallel overlapping faults, where the existence of stress shadow zones induces, on the 'shadowed' fault segment, an asymmetric slip profile with a single singularity and a locked zone at the other tip. The computed eigenfunction being the most unstable mode of deformation, it is also compared with dynamic simulations.

6.1. Convergence tests on a single fault

Computations were performed on four regular and two optimized meshes, described in Table I, with $\Gamma = [-1,1] \times \{0\}$, $\Omega = \mathbb{R}^2 \backslash \Gamma$, $\Omega^0 = [-10,10]^2 \backslash \Gamma$, $\Gamma_d = \partial\bar{\Omega} = \emptyset$ and $\lambda^2 = 0$. The mesh size given by Table I is defined as the length of the largest edge. Note that Γ is made up of one single planar fault.

In the case of a single planar fault, the first eigenvalue is the universal constant $\beta_0 = 1.157777\ldots$ which has been accurately computed in Reference [7]. Slip profiles resulting from the eigenfunctions computed on meshes 1, 2, 3, 6 can be compared in Figure 4: the optimized mesh, having more nodes in the fault vicinity, allows a more accurate approximation of the fault-tip singularities. Note that the number of iterations in Algorithm 5.1 is independent of the mesh size.

The corresponding computed eigenvalues b_h are plotted with respect to the number of edges on the fault in Figure 5. The reference value β_0, represented by the dashed line, requires a large number of fault nodes to be approached. This remark justifies the use of mesh refinement.

Note that, in the above computations, the unbounded domain is represented by infinite elements. The corresponding eigenvalue on mesh 5 is $b_h = 1.15712$. The same calculus performed without infinite elements, with $\bar{\Omega} = \Omega^0$ and $\tilde{\Gamma}_d = \partial\bar{\Omega}^0$, leads to $\tilde{b}_h = 1.16565$. Hence, the use of infinite elements does not allow to reduce strongly the number of nodes or the size of Ω, but it significantly increases accuracy.

6.2. Interaction of two parallel faults

The non-linear nature of our slip–dependent friction law expresses through fault interaction. Indeed, as reported in Reference [14], for systems of two overlapping parallel faults, a fully

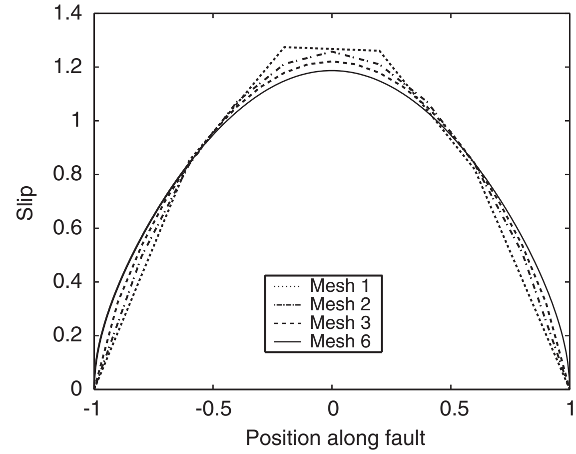

Figure 4. Slip profiles $[\Phi_{0h}]$ on the fault (corresponding to the first eigenfunction Φ_{0h}) for regular meshes 1, 2, 3 and optimized mesh 6 of Table I.

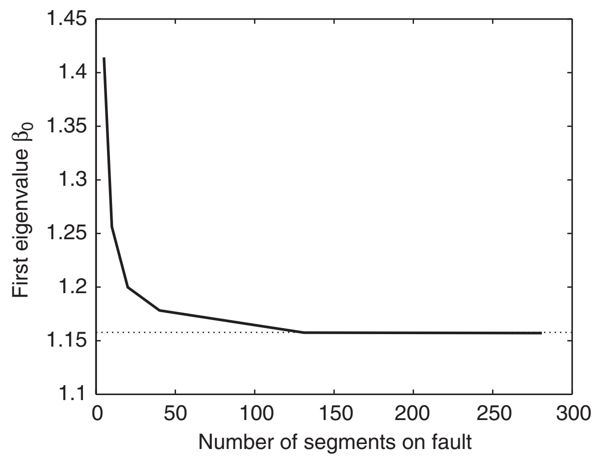

Figure 5. Dependence of the computed eigenvalue b_h on the fault discretization. The dashed line corresponds to the universal constant $\beta_0 = 1.15777\ldots$.

linear numerical model leads to modes of deformation which do not fulfill the condition on the sign of the slip, with both faults sliding in opposite senses. A non-linear approach must be used to handle the configurations where one of the fault segments lies in a stress shadow zone and has an asymmetric slip profile, with a single tip-singularity, and a large zone where slip is inhibited. These profiles are found on systems of overlapping faults.

Two parallel fault segments $\Gamma_1 = [-1.5, 0.5] \times \{-0.1\}$ and $\Gamma_2 = [-0.5, 1.5] \times \{0.1\}$ are considered (see Figure 6). Here, $\Gamma = \Gamma_1 \cup \Gamma_2$, $\Omega = \mathbb{R}^2 \backslash \Gamma$, $\Omega^0 = [-7, 7]^2 \backslash \Gamma$, $\Gamma_d = \partial\bar{\Omega} = \emptyset$ and $\lambda^2 = 1.0$. The optimized mesh has 8781 nodes, and 154 edges on Γ. The two faults overlap each

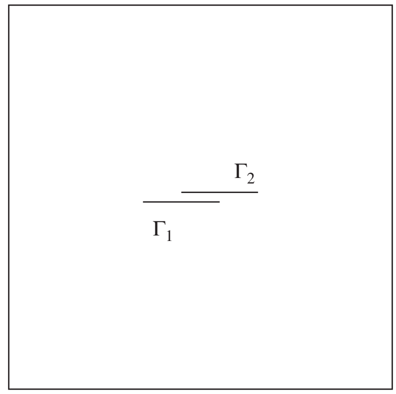

Figure 6. Geometry of the two-faults system.

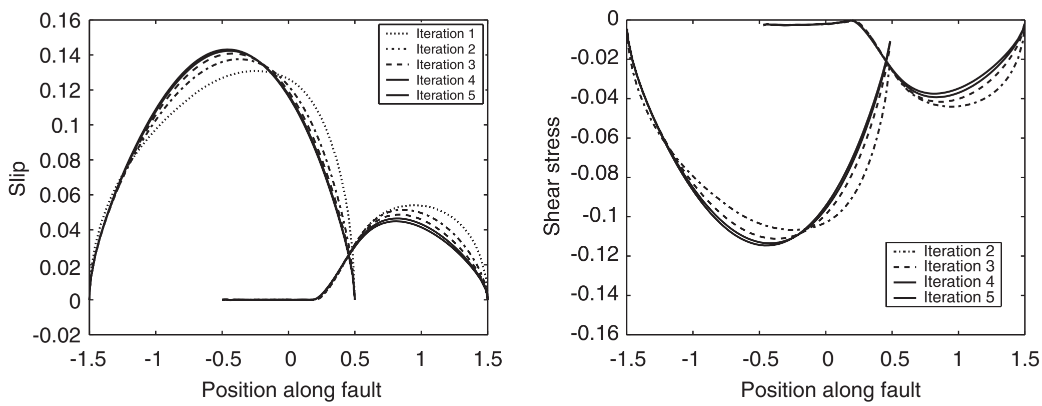

Figure 7. The slip ($[\Phi^n_{0h}]$: left) and stress profiles ($-\tau^n_h$: right) at the first five steps n of Algorithm 5.1.

other, so that a constrained optimization problem must be solved at each iteration. Here, the augmented Lagrangian is used in the Usawa algorithm.

Figure 7 depicts the convergence of Algorithm 5.1. The displacement jump $[\Phi^n_{0h}]$ and the shear stress $-\tau^n_h$ are plotted after each of the first five iterations n, 21 iterations are required to reach the desired precision. Note that the length of the locked zone of the shadowed fault is found after a very short number of iterations. Computing the shape of the slip profile on the rest of the fault takes a few iterations more. As expected, the slip and stress profiles only differ by a multiplicative constant on the sliding zone, and the shear stress is negative on the locked zone. The corresponding values of b^n_h are plotted in Figure 8.

6.3. Spectral analysis vs time evolution on two parallel faults

Dynamic simulations were performed on the above configuration, using a Newmark finite difference scheme and a domain decomposition method (see Reference [22] for a detailed

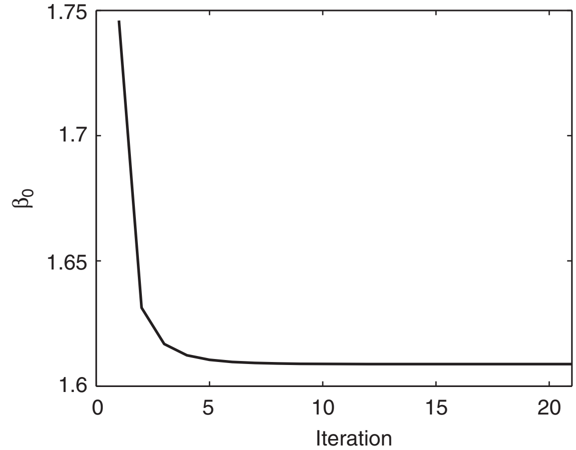

Figure 8. The approximate value of the first eigenvalue b_h^n computed at each step n of Algorithm 5.1.

description). Such simulations can be used to check the validity of the computed value of β_0 (found with $\lambda^2 = 0$). As suggested by Theorem 4.1, the system is supposed to be stable if $\beta < \beta_0$, and unstable with an exponentially growing slip of the shape of the first dynamic eigenfunction if $\beta > \beta_0$. The spectral analysis detailed in the previous subsection gives $\beta_0 \simeq 1.1$. The evolution of the velocity field is presented in Figure 9 for $\beta = 1.0$ (left) and $\beta = 1.2$ (right).

At $t = 0$ s, a small gaussian velocity perturbation is applied at an arbitrary point, here $(0, -0.5)$. At $t = 0.05$ and -2.5 s, the shear waves propagate in a similar way, except that the slip grows faster for $\beta = 1.2$. Then, between $t = 2.5$ and 5 s, the initiation phase begins in the unstable case ($\beta = 1.2 > 1.1 = \beta_0$), i.e. slip rate has the shape of Φ_{0h} and grows exponentially, as shown in details on Figure 12. Note that part of Γ_1 remains locked, since the static friction level has not been exceeded. Meanwhile, the slip on the first configuration is rapidly stabilized ($\beta = 1.0 < \beta_0$). Hence, this dynamic computation illustrates the physical meaning of the first eigenvalue, as a critical value of the friction parameter regarding the stability of the system.

Figure 10 shows the corresponding stress fields at $t = 10$s. The unstable configuration (right) exhibits three stress concentrations only: due to the effects of stress shadowing, the left tip of Γ_1 is inhibited. On the stable configuration (right), the stress concentrations have all vanished.

Figure 11 displays the evolution of the velocity jump on the fault system, for $0\,\text{s} \leqslant t \leqslant 4\,\text{s}$ in the unstable case ($\beta > \beta_0$). The perturbation first reaches Γ_2, where it propagates and is finally reflected by both tips of Γ_2. On Γ_1, once the perturbation has propagated from the right tip to the left one, we can see another wave coming from the left tip of Γ_2. Then, one can see the beginning of the initiation phase, i.e. the slip rate grows exponentially. Note that a part of Γ_1 remains locked, since the static friction level has not been exceeded.

Figure 12 compares the slip profile on the fault system during the initiation phase, at $t = 4$ and 5 s, and the first eigenfunction Φ_{0h}, computed both for $\beta = 1.6$, on the same mesh. As the effects of the propagation of the initial perturbation vanish, the slip profile resulting from the dynamic simulation becomes more and more similar to the profile predicted by the spectral analysis. Indeed, since the slip rate is growing exponentially, the characteristic pattern of the initiation phase dominates and the remaining waves cannot be seen any longer. Small

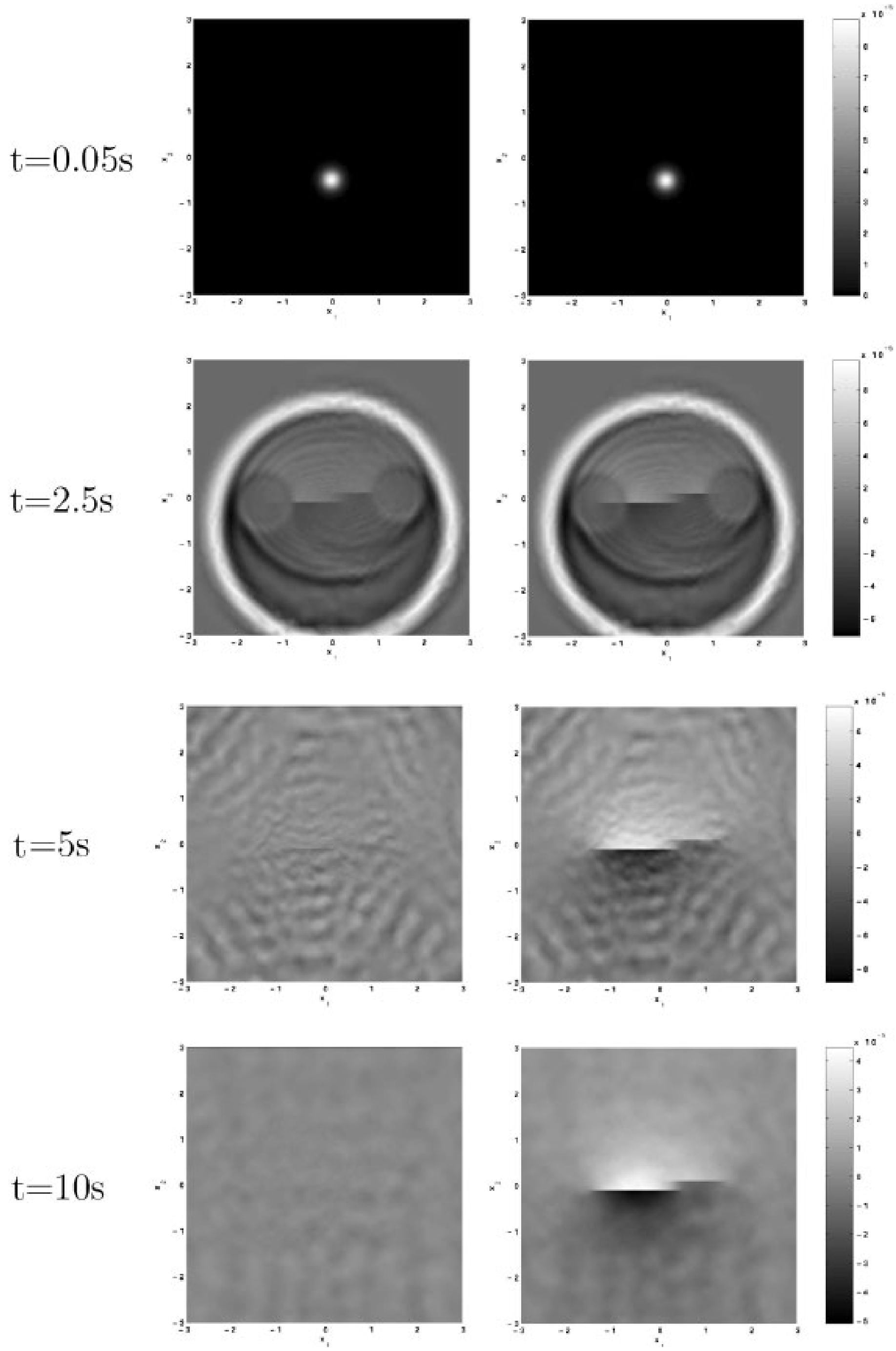

Figure 9. Dynamic evolution of the velocity distribution, $(x_1, x_2) \to \partial_t w(t, x_1, x_2)$, in the stable case $\beta = 1.0 < 1.1 = \beta_0$ (left) and in the unstable case $\beta = 1.2 > 1.1 = \beta_0$ (right).

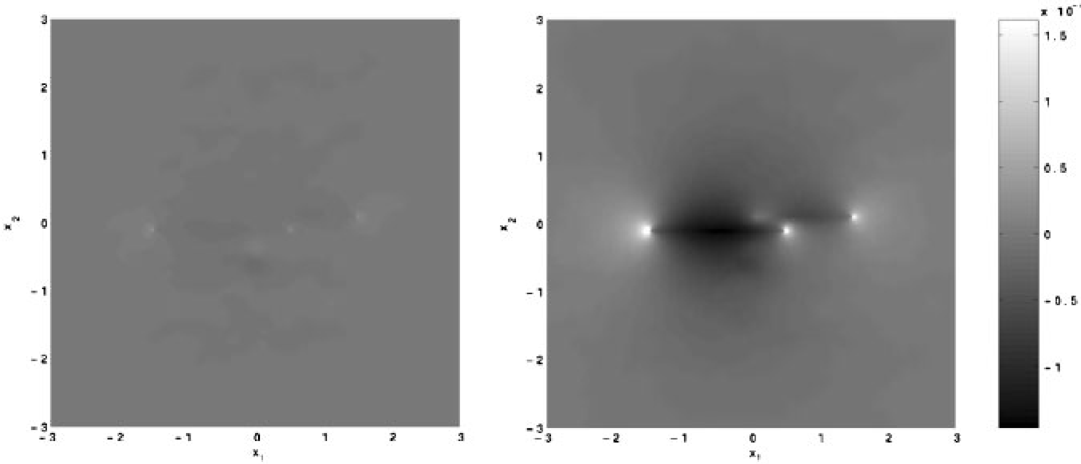

Figure 10. Shear stress distribution, $(x_1,x_2)\rightarrow G\partial_y w(t,x_1,x_2)$ at the final stage ($t=10\,\mathrm{s}$) of the dynamic process, for the stable case $\beta=1.0<1.1=\beta_0$ (left) and for the unstable case $\beta=1.2>1.1=\beta_0$ (right).

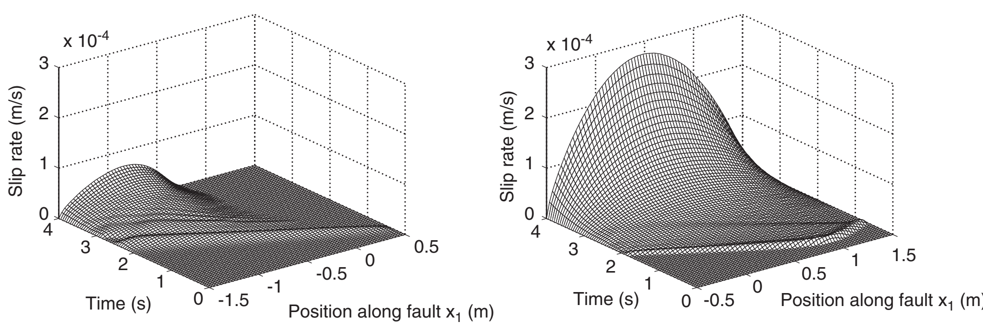

Figure 11. The time evolution of the slip rate $[\partial_t w]$ on two interacting parallel faults (left: Γ_1, right: Γ_2).

scale differences may persist, because of the mesh size away from the fault. A coarse mesh is reasonable for spectral analysis, but it can increase local error when wave propagation is involved. However, the first eigenfunction gives a sharp description of the pattern of the initiation phase.

7. CONCLUSIONS

The anti-plane shearing on a system of finite faults under a slip-dependent friction in a linear elastic domain (not necessarily bounded) was considered. The static problem is formulated in terms of local minima of the energy functional. For non coplanar faults, the first eigenfunction of the tangent (linear) problem has no physical significance. This difficulty arises with the effect of stress shadowing which does not exist for coplanar fault segments.

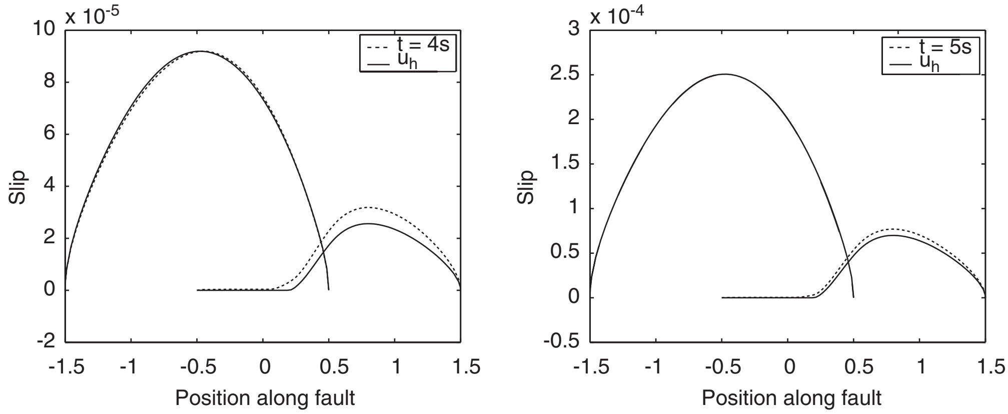

Figure 12. Comparison of the slip rate profiles resulting from the spectral analysis ($[\Phi_0]$: solid line) and from a dynamic simulation ($[w(t)]$: dashed line) at $t = 4$ s (left) and $t = 5$ s (right). Note that the first eigenfunction gives a sharp description of the pattern of the initiation phase.

In modelling initiation of friction instabilities, we introduce a non-linear (unilateral) eigenvalue problem. The main novelty in this particular non-linear eigenvalue problem is the presence of the convex cone of functions with non-negative jump across an internal boundary. We prove the existence of a first eigenvalue/eigenfunction characterizing the isolated local minima.

For the dynamic problem, the existence of solutions with an exponential growth is pointed out through a (dynamic) non-linear eigenvalue problem. The investigation is restricted to the first eigenvalue (Rayleigh quotient). The existence of a first dynamic eigenvalue is proved and the behaviour with respect to the friction parameter is analysed.

A mixed finite element discretization of the non-linear spectral problem is used and a numerical algorithm is proposed to approach the first eigenvalue/eigenfunction. Even if the convergence is not proved, in all tests and applications, the algorithm was found to be convergent. The numerical results include convergence tests, on a single fault and on a two-faults system, and a comparison between the solution of the non-linear spectral analysis and the time evolution results. This non-linear eigenvalue method and the numerical scheme were used in Reference [14] to get the slip patterns of normal faults in Afar (East Africa).

ACKNOWLEDGEMENTS

We would like to thank Michel Campillo for interesting discussions on the interacting faults which generated the present mathematical development.

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MATHEMATICAL METHODS IN THE APPLIED SCIENCES
Math. Meth. Appl. Sci. 2005; **28**:101–126
Published online 5 November 2004 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/mma.560
MOS subject classification: 15 A 66; 51 M 15; 58 D 15; 44 A 12

A concise quaternion geometry of rotations

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Communicated by W. Sprößig

SUMMARY

This communication compiles propositions concerning the spherical geometry of rotations when represented by unit quaternions. The propositions are thought to establish a two-way correspondence between geometrical objects in the space of real unit quaternions representing rotations and geometrical objects constituted by directions in the three-dimensional space subjected to these rotations. In this way a purely geometrical proof of the spherical Ásgeirsson's mean value theorem and a geometrical interpretation of integrals related to the spherical Radon transform of a probability density functions of unit quaternions are accomplished. Copyright © 2004 John Wiley & Sons, Ltd.

1. INTRODUCTION

The background of this communication is in crystallography, in particular in patterns of preferred crystallographic orientations of crystals within a polycrystalline specimen. Neglecting crystal symmetry for the sake of simplicity, a crystallographic orientation is a rotation. Thus the focus is on even probability density functions f defined on the sphere[‡] $\mathbb{S}^3 \subset \mathbb{R}^4$ in four-dimensional space $\mathbb{R}^4$ when rotations are represented by unit quaternions. A useful spherical distribution for this purpose is the Bingham distribution and its special cases which provide a characterization of distinct patterns of preferred crystallographic orientation [1,2]. Since a distribution on $\mathbb{S}^3$ is hard to visualize and grasp, it proved helpful to look at the distribution of unit vectors $\mathbf{h} \in \mathbb{S}^2 \subset \mathbb{R}^3$ which have been subjected to random rotations $q \in \mathbb{S}^3$ with a given—say Bingham—distribution f ([3,4]). The distribution of these unit vectors is actually given in terms of the spherical $\mathscr{R}$ Radon transform $\mathscr{R}f$ of the probability density function f.

Let SO(3) denote the special orthogonal group of proper rotations $\boldsymbol{g}$ in $\mathbb{R}^3$. Since in the context of crystallography normal unit vectors of lattice planes are subjected to rota-

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‡Incompatible conventions for the meaning of ‘*n*-sphere’ are used in geometry and topology. We use the topological definition.

 Received 7 January 2004

tions, considerations are confined to the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ in three-dimensional space $\mathbb{R}^3$.

Let $f : \mathrm{SO}(3) \mapsto [0, \infty)$ be a probability density function of a random rotation $\boldsymbol{g} \in \mathrm{SO}(3)$. For any given direction $\mathbf{h} \in \mathbb{S}^2$ the probability density function of coincidence of the random direction $\boldsymbol{g}\mathbf{h} \in \mathbb{S}^2$ with a given direction $\mathbf{r} \in \mathbb{S}^2$ is provided by

$$(\mathscr{R} f)(\mathbf{h}, \mathbf{r}) = \frac{1}{2\pi} \int_{G(\mathbf{h},\mathbf{r})} f(\boldsymbol{g})\, \mathrm{d}\boldsymbol{g}$$

with fibres

$$G(\mathbf{h}, \mathbf{r}) = \{\boldsymbol{g} \in \mathrm{SO}(3) \mid \boldsymbol{g}\,\mathbf{h} = \mathbf{r}\}$$

inducing a double fibration of SO(3).

In practice, the inverse problem arises and may be specified as to which extent and for which assumptions is it possible to determine a reasonable approximation of f globally on SO(3) or locally in a neighbourhood $\mathscr{U}(\boldsymbol{g}_0) \subset \mathrm{SO}(3)$ numerically from data sampled from $(\mathscr{R} f)(\mathbf{h}, \mathbf{r})$.

It is well-known that a rotation $\boldsymbol{g}$ mapping the unit vector $\mathbf{h} \in \mathbb{S}^2$ onto the unit vector $\mathbf{r} \in \mathbb{S}^2$ according to $\boldsymbol{g}\,\mathbf{h} = \mathbf{r}$ may be represented by its corresponding (3×3) orthogonal matrix $M(\boldsymbol{g})$ or by its corresponding real quaternion $q(\boldsymbol{g})$. The quaternion representation has some clear advantages which have been discussed by many authors.

In the present communication we pursue geometry in quaternion space $\mathbb{H}$, in particular we consider geometrical objects in the space of real unit quaternions representing rotations with respect to geometrical objects in three-dimensional space of unit vectors being subjected to these rotations. We show, for instance, that the set of quaternions mapping a unit vector onto another one is a circle, and that the set of quaternions mapping a unit vector onto a small circle is a torus, and more generally that there is a correspondence between objects like circle, sphere, and torus of unit quaternions in $\mathbb{S}^3$ representing rotations and objects like point and circle of unit vectors in $\mathbb{S}^2$.

Our geometrical approach leads to an alternative proof of a spherical variant of Ásgeirsson's mean value theorem [5], and to clarifications of the interpretation of some integrals related to the spherical Radon transform [6] of probability density functions of unit quaternions.

We use the symbol $\square$ to mark the end of proofs.

2. NOTATION

The algebra of real quaternions $\mathbb{H}$ is the tuple of $\mathbb{R}^4$ endowed with the operation of quaternion multiplication; furtheron, $\mathbb{H}$ is referred to as skew-field of real quaternions. Its exposition follows References [7–9].

2.1. Skew-field of real quaternions

An arbitrary quaternion $q \in \mathbb{H}$ is composed of its scalar and vector part

$$q = q_0 + \mathbf{q} = \mathrm{Sc}q + \mathrm{Vec}q$$

with $\mathbf{q} = \sum_{i=1}^{3} q^i e_i = \mathrm{Vec}q$ and $q_0 = \mathrm{Sc}q$, where Vec$q$ denotes the vector part of q, and Scq denotes the scalar part of q. The basis elements $e_i,\ i = 1,2,3$, fulfil the relations

(i) $e_i^2 = -1,\ i = 1,2,3;$
(ii) $e_1 e_2 = e_3,\ e_2 e_3 = e_1,\ e_3 e_1 = e_2;$
(iii) $e_i e_j + e_j e_i = 0,\ i,j = 1,2,3;\ i \neq j.$

If $\mathrm{Sc}q = 0$, then q is called a pure quaternion, the subset of all pure quaternions is denoted $\mathrm{Vec}\mathbb{H}$. For $q \in \mathrm{Vec}\mathbb{H}$, q and $\mathbf{q}$ are identified, i.e. $q = \mathbf{q}$. The subset of all scalars may be denoted $\mathrm{Sc}\mathbb{H}$. In this way $\mathbb{R}$ and $\mathbb{R}^3$ are embedded in $\mathbb{H}$.

Given two quaternions, $p, q \in \mathbb{H}$, their product according to the algebraic rules of multiplications given above is

$$pq = p_0 q_0 - \mathbf{p}\cdot\mathbf{q} + p_0\mathbf{q} + q_0\mathbf{p} + \mathbf{p}\times\mathbf{q}$$

where $\mathbf{p}\cdot\mathbf{q}$ and $\mathbf{p}\times\mathbf{q}$ represent the standard inner and cross product in $\mathbb{R}^3$; thus

$$\begin{aligned} \mathrm{Sc}(pq) &= p_0 q_0 - \mathbf{p}\cdot\mathbf{q} \\ \mathrm{Vec}(pq) &= p_0\mathbf{q} + q_0\mathbf{p} + \mathbf{p}\times\mathbf{q} \end{aligned} \tag{1}$$

Quaternion multiplication reduces for pure quaternions $p, q \in \mathrm{Vec}\mathbb{H}$ to

$$pq = \mathbf{pq} = -\mathbf{p}\cdot\mathbf{q} + \mathbf{p}\times\mathbf{q} \tag{2}$$

and thus

$$\mathrm{Sc}(pq) = \mathrm{Sc}(\mathbf{pq}) = -\mathbf{p}\cdot\mathbf{q}$$

$$\mathrm{Vec}(pq) = \mathrm{Vec}(\mathbf{pq}) = \mathbf{p}\times\mathbf{q}$$

2.2. Conjugation of a real quaternion

The quaternion $q^* = \mathrm{Sc}q - \mathrm{Vec}q$ is called the conjugate of q. With conjugated quaternions it is possible to represent the scalar and vector part in an algebraic fashion as

$$q_0 = \mathrm{Sc}q = \tfrac{1}{2}(q + q^*) \tag{3}$$

$$\mathbf{q} = \mathrm{Vec}q = \tfrac{1}{2}(q - q^*) \tag{4}$$

Since

$$\mathrm{Vec}q^* = -\mathrm{Vec}q$$

conjugation of pure quaternions $q \in \mathrm{Vec}\mathbb{H}$ means change of sign, i.e. $q^* = \mathbf{q}^* = -\mathbf{q} = -q$. Therefore, for arbitrary pure quaternions we have

$$\mathrm{Sc}(pq^*) = \mathbf{p}\cdot\mathbf{q} = -\frac{1}{2}(pq + qp)$$

$$\mathrm{Vec}(pq^*) = -\mathbf{p}\times\mathbf{q} = -\frac{1}{2}(pq - qp)$$

2.3. *Norm of a real quaternion*

It holds that

$$qq^* = q^*q = \|q\|^2 = q_0^2 + (q^1)^2 + (q^2)^2 + (q^3)^2$$

and the number $\|q\|$ is called the norm of q. The norm of quaternions coincides with the Euclidean norm of q regarded as an element of the vector space $\mathbb{R}^4$. The usual Euclidean inner product in the space $\mathbb{R}^4$ corresponds to the scalar part of pq^*, i.e. considering quaternions as vectors in $\mathbb{R}^4$, one gets

$$p \cdot q = \mathrm{Sc}(pq^*)$$

It holds that $(pq)^* = q^* p^*$, and therefore $\|pq\| = \|p\|\,\|q\|$.

A quaternion q with $\|q\| = 1$ is called a unit quaternion. Furthermore, let $\mathbb{S}^2$ denote the unit sphere in $\mathrm{Vec}\mathbb{H} \simeq \mathbb{R}^3$ of all unit vectors, and $\mathbb{S}^3$ the sphere in $\mathbb{H} \simeq \mathbb{R}^4$ of all unit quaternions.

In complete analogy to $\mathbb{S}^3 \subset \mathbb{R}^4$, $\mathrm{Sc}(pq^*)$ provides a canonical measure for the spherical distance of unit quaternions $p, q \in \mathbb{S}^3$ in terms of their enclosed angle.

2.4. *Inverse of a real quaternion*

Moreover, each non-zero quaternion q has a unique inverse $q^{-1} = q^*/\|q\|^2$ with $\|q^{-1}\| = \|q\|^{-1}$. For unit quaternions it is $q^{-1} = q^*$; for pure unit quaternions it is $q^{-1} = -q$, implying $qq = -1$.

2.5. *Orthogonality of real quaternions*

Since orthogonality of unit quaternions will provide essential arguments throughout the paper, we shall give its formal definition.

Definition 1
Two quaternions $p, q \in \mathbb{H}$ are said to be orthogonal if pq^* is a pure quaternion. If p, q are orthogonal unit quaternions, they are called orthonormal quaternions.

The condition of orthogonality means that $pq^* \in \mathrm{Vec}\mathbb{H}$, or due to Equation (3)

$$\mathrm{Sc}(pq^*) = \tfrac{1}{2}(pq^* + qp^*) = 0$$

It is emphasized that pure quaternions with orthogonal vector parts are orthogonal, but that the inverse is not generally true. Orthogonality of two quaternions does not imply orthogonality of their vector parts unless they are pure quaternions.

If the pure quaternions p, q are orthogonal, then their multiplication simplifies further to

$$pq = \mathbf{p} \times \mathbf{q}$$

Proposition 1
Two unit quaternions $p, q \in \mathbb{S}^3$ are orthogonal, if and only if $p = vq$, where v is a pure unit quaternion.

Proof
If p and q are orthogonal, then pq^* is a pure quaternion, say v, for some $\mathbf{v} \in \mathbb{S}^2$. Hence, $p = vq \in \mathbb{S}^2 q$. The inverse is evident. □

2.6. *Representation of real quaternions*

An arbitrary quaternion $q \neq 0$ permits the representation

$$q = \|q\| \left(\frac{q_0}{\|q\|} + \frac{\mathbf{q}}{\|\mathbf{q}\|} \frac{\|\mathbf{q}\|}{\|q\|} \right) = \|q\| \left(\cos \frac{\omega}{2} + \frac{\mathbf{q}}{\|\mathbf{q}\|} \sin \frac{\omega}{2} \right)$$

with $\omega = 2 \arccos(q_0/\|q\|)$, and $\|\mathbf{q}\|^2 = \mathbf{q}\mathbf{q}^*$ considering $\mathbf{q}$ as a pure quaternion. For an arbitrary unit quaternion the representation

$$q = \cos \frac{\omega}{2} + \mathbf{n} \sin \frac{\omega}{2} \tag{5}$$

with the normalized vector part $\mathbf{n} = \mathbf{q}/\|\mathbf{q}\| \in \mathbb{S}^2$ will often be applied in the context of rotations, where $\mathbf{n} \in \mathbb{S}^2$ denotes the axis and ω the angle of a counter-clockwise rotation about $\mathbf{n}$.

2.7. *Quaternion representation of rotations in* $\mathbb{R}^3$

Any active rotation $\boldsymbol{g} \in \mathrm{SO}(3)$ mapping the unit vector $\mathbf{h} \in \mathbb{S}^2$ onto the unit vector $\mathbf{r} \in \mathbb{S}^2$ according to

$$\boldsymbol{g}\,\mathbf{h} = \mathbf{r}$$

can be written in terms of its quaternion representation $q \in \mathbb{H}$ as

$$q(\boldsymbol{g})\mathbf{h}\, q^{-1}(\boldsymbol{g}) = \mathbf{r} \tag{6}$$

equivalent to $q(\boldsymbol{g})\,\mathbf{h} - \mathbf{r}q(\boldsymbol{g}) = 0$, where quaternion multiplication applies. To perform quaternion multiplication, $\mathbf{h}$ and $\mathbf{r}$ must be read as pure quaternions, i.e. they must be augmented with a zero scalar quaternion part; then Equation (6) reads

$$qhq^{-1} = r \tag{7}$$

Moreover, for $q \in \mathbb{S}^3$ the previous expression becomes

$$qhq^* = r$$

which explicitly reads then [7]

$$\mathbf{r} = \mathbf{h} \cos \omega + (\mathbf{n} \times \mathbf{h}) \sin \omega + (\mathbf{n} \cdot \mathbf{h})\mathbf{n}(1 - \cos \omega) \tag{8}$$

where the representation of Equation (5) has been applied.[§]

The unit quaternion $q \in \mathbb{S}^3$ represents the rotation about the unit axis $\mathbf{q}/\|\mathbf{q}\|, \mathbf{q} \neq 0$, by the angle $\omega = 2 \arccos(q_0)$. Therefore, each unit quaternion $q \in \mathbb{S}^3$ can be seen as a representation of a rotation in $\mathbb{R}^3$, i.e. $\mathbb{S}^3$ stands for a double covering of the group SO(3). It is emphasized that $\mathbb{S}^2 \subset \mathrm{Vec}\mathbb{H}$ consists of all quaternions representing rotations by the angle π about arbitrary axes, as every unit vector $\mathbf{q}$ can be considered as the pure quaternion $q = \cos(\pi/2) + \mathbf{q} \sin(\pi/2)$.

[§]Nice proofs that Equation (7) actually represents a rotation can be found, for instance, at http://www.cs.berkeley.edu/ laura/cs184/quat/quatproof.html.

The unit quaternion q^* represents the inverse rotation $\boldsymbol{g}^{-1}\mathbf{r}=\mathbf{h}$, either by the angle $2\pi-\omega$ or by the angle $-\omega$, respectively, and the axis $\mathbf{n}$, or by the angle ω and the axis $-\mathbf{n}$.

Proposition 2
Let $p,q\in\mathbb{S}^3$ be arbitrary unit quaternions, where q represents the rotation about the axis $\mathbf{n}$ by the angle ω according to Equation (5). Then the quaternion $pqp^*\in\mathbb{S}^3$ represents the rotation about the rotated axes $p\,\mathbf{n}\,p^*\in\mathbb{S}^2$ by the same angle ω.

Proof
It simply holds that

$$pqp^*=p\left(\cos\frac{\omega}{2}+\mathbf{n}\sin\frac{\omega}{2}\right)p^*=\cos\frac{\omega}{2}+p\mathbf{n}p^*\sin\frac{\omega}{2} \tag{9}$$

□

The left-hand side of Equation (9) is referred to as representing the conjugation of rotations.

In terms of passive rotations, $q\mathbf{h}q^{-1}$ provides the coordinate transformation of a unique vector $\mathbf{h}_{K_\mathscr{C}}$ with respect to the (crystal) co-ordinate system $K_\mathscr{C}$ and $\mathbf{r}=\mathbf{h}_{K_\mathscr{S}}$ with respect to the (specimen) coordinate system $K_\mathscr{S}$ if the coordinate systems are related to each other by $\boldsymbol{g}:K_\mathscr{S}\mapsto K_\mathscr{C}$.

Henceforward, no distinction will be made between the rotation $\boldsymbol{g}$ and its (up to the sign) unique quaternion representation q. In the same way, a unit vector $\mathbf{x}\in\mathbb{S}^2\subset\mathrm{Vec}\mathbb{H}$ is identified with its corresponding pure unit quaternion $x\in\mathbb{S}^3\subset\mathbb{H}$, for which the rules of quaternion multiplication apply.

3. CORRESPONDENCE OF GEOMETRICAL OBJECTS OF $\mathbb{S}^3\subset\mathbb{H}$ AND GEOMETRICAL OBJECTS OF $\mathbb{S}^2\subset\mathbb{R}^3$ IN TERMS OF ROTATIONS

3.1. Mapping a given vector onto another one

We shall start with the geometric interpretation of the well-known problem to find all rotations which map a given unit vector onto another one. This problem arises in different areas of applied sciences like crystallography, robotic, photogrammetry, navigation, calibration of measurement equipment, image recognition, computer games, etc. Many authors tackled the problem using features of their application. A review of three methods of solution: an algebraic method, a geometric method, and the method of conditional extrema is given, for instance, in Reference [10]. Here, we pursue the geometric approach to the problem based on the orthogonality of quaternions.

We begin with the following definition.

Definition 2
Let q_1 and q_2 be two orthogonal unit quaternions. The set of quaternions

$$q(t)=q_1\cos t+q_2\sin t,\quad t\in[0,2\pi) \tag{10}$$

is called a circle in the space of quaternions and is denoted $C(q_1,q_2)$.

Obviously, the circle $C(q_1,q_2)$ is the intersection of the plane $E(q_1,q_2)=\langle q_1,q_2\rangle \subset \mathbb{H}$ spanned by q_1,q_2 and passing through the origin $\mathcal{O}$ with the unit sphere $\mathbb{S}^3 \subset \mathbb{H}$, i.e. $C(q_1,q_2)=E(q_1,q_2)\cap\mathbb{S}^3$.

Proposition 3
Given a pair of unit vectors $(\mathbf{h},\mathbf{r})\in\mathbb{S}^2\times\mathbb{S}^2$ with $\mathbf{h}\times\mathbf{r}\neq 0$, the set $G(\mathbf{h},\mathbf{r})\subset \mathrm{SO}(3)$ of all rotations with $\boldsymbol{g}\,\mathbf{h}=\mathbf{r}$ may be represented as a circle $C(q_1,q_2)$ of unit quaternions such that

$$q\mathbf{h}q^* = \mathbf{r},\ \ \forall\ q\in C(q_1,q_2) \tag{11}$$

with orthogonal quaternions

$$q_1 := \frac{1}{\|1-rh\|}(1-rh) = \cos\frac{\eta}{2} + \frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|}\sin\frac{\eta}{2} \tag{12}$$

$$q_2 := \frac{1}{\|h+r\|}(h+r) = 0 + \frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|} \tag{13}$$

where η denotes the angle between $\mathbf{h}$ and $\mathbf{r}$, and

$$\|1-rh\| = \sqrt{2(1+\cos\eta)} = 2\cos\frac{\eta}{2} \tag{14}$$

$$\|h+r\| = 2\cos\frac{\eta}{2} \tag{15}$$

Proof
By geometrical reasoning (see Figure 1) it can be seen that the axis of any rotation $\boldsymbol{g}\mathbf{h}=\mathbf{r}$ is in the plane spanned by

$$\mathbf{n}_1 := \frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|} = \frac{1}{\sin\eta}(\mathbf{h}\times\mathbf{r}) \tag{16}$$

$$\mathbf{n}_2 := \frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|} = \frac{1}{2\cos(\eta/2)}(\mathbf{h}+\mathbf{r}) \tag{17}$$

The plane $E(\mathbf{n}_1,\mathbf{n}_2)=\langle\mathbf{n}_1,\mathbf{n}_2\rangle\subset\mathbb{R}^3$ of rotation axes is uniquely given by its unit normal

$$\mathbf{n}_1\times\mathbf{n}_2 = \frac{1}{2\sin(\eta/2)}(\mathbf{r}-\mathbf{h}) \tag{18}$$

The angles of rotations about the axes $\mathbf{n}_1$ and $\mathbf{n}_2$ are η and π, respectively. The quaternions representing these rotations are

$$\begin{aligned} q_1 &= \cos\frac{\eta}{2} + \mathbf{n}_1\sin\frac{\eta}{2} \\ q_2 &= \mathbf{n}_2 \end{aligned} \tag{19}$$

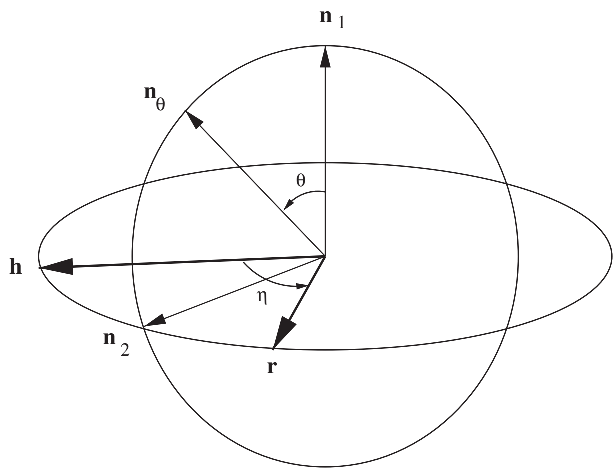

Figure 1. Axes of rotations $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_\theta$.

respectively. Clearly, q_1 and q_2 are orthogonal quaternions, as their vector parts are orthogonal and the scalar part of q_2 is zero.

The normalized axis $\mathbf{n}_\theta$ of any rotation $\boldsymbol{g}\mathbf{h} = \mathbf{r}$, i.e. the normalized vector part of a unit quaternion q with $q\mathbf{h}q^* = \mathbf{r}$, is an element of the circle $C(\mathbf{n}_1, \mathbf{n}_2) = E(\mathbf{n}_1, \mathbf{n}_2) \cap \mathbb{S}^2$. The corresponding angle ω_θ of rotation varies between η and $2\pi - \eta$. Thus

$$G(\mathbf{h}, \mathbf{r}) = \{\boldsymbol{g}_\theta \in \mathrm{SO}(3); \boldsymbol{g}_\theta = \boldsymbol{g}(\omega_\theta, \mathbf{n}_\theta)\} \tag{20}$$

where the axis of rotation $\mathbf{n}_\theta$ is

$$\mathbf{n}_\theta = \mathbf{n}_1 \cos\theta + \mathbf{n}_2 \sin\theta, \quad \theta \in [0, 2\pi) \tag{21}$$

and θ is the angle between the axis $\mathbf{n}_\theta$ and $\mathbf{n}_1$, i.e. $\cos\theta = \mathbf{n}_\theta \cdot \mathbf{n}_1$, see Figure 1.

The angle of rotation ω_θ is related to $\mathbf{n}_\theta$ [11] by

$$\tan\frac{\omega_\theta}{2} = \frac{\sin(\eta/2)}{\cos\theta\,\cos(\eta/2)} \tag{22}$$

Then the set of unit quaternions $q(\theta)$ defined as

$$q(\theta) = \cos\frac{\omega_\theta}{2} + \mathbf{n}_\theta \sin\frac{\omega_\theta}{2} \tag{23}$$

represents the set of all required rotations.

Let us show now that $q(\theta) \in C(q_1, q_2)$. Indeed, based on the trigonometric relations for an arbitrary φ

$$\tan\varphi = \frac{a}{b}; \quad \sin\varphi = \frac{a}{\sqrt{a^2 + b^2}}; \quad \cos\varphi = \frac{b}{\sqrt{a^2 + b^2}}$$

with signs of sin φ and cos φ depending on φ, due to (22) we can write

$$\begin{aligned}\sin\frac{\omega_\theta}{2} &= \frac{\sin(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ \cos\frac{\omega_\theta}{2} &= \frac{\cos\theta\cos(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\end{aligned} \tag{24}$$

Substituting (21) and (24) in (23) and rearrangement gives

$$\begin{aligned}q(\theta) &= \left(\cos\frac{\eta}{2}+\mathbf{n}_1\sin\frac{\eta}{2}\right)\frac{\cos\theta}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ &\quad+\mathbf{n}_2\frac{\sin\theta\sin(\eta/2)}{(\sin^2(\eta/2)+\cos^2(\eta/2)\cos^2\theta)^{1/2}}\\ &= q_1a_1(\theta)+q_2a_2(\theta)\end{aligned} \tag{25}$$

Direct calculations give $a_1^2(\theta)+a_2^2(\theta)=1$ for every θ, hence we can introduce a new parameter $t\in[0,2\pi)$ such that $\cos t=a_1(\theta)$ and $\sin t=a_2(\theta)$ and rewrite Equation (25) as follows

$$q(t)=q_1\cos t+q_2\sin t,\quad t\in[0,2\pi). \tag{26}$$

Thus we conclude that the circle $C(q_1,q_2)$ corresponding to Equation (26) represents all rotations mapping $\mathbf{h}$ on $\mathbf{r}$, and obviously $q(0)=q_1$ and $q(\pi/2)=q_2$.

The case $\mathbf{r}=-\mathbf{h}$ must be considered separately. All rotations q with $q\mathbf{h}q^*=-\mathbf{h}$ are provided by rotations with their axes in the orthogonal complement $\mathbf{h}^\perp\cap\mathbb{S}^2$ of $\mathbf{h}$, which again represents a circle, and their angles constantly equal to π. □

Some useful equalities follow. Since r and h are pure unit quaternions, we get

$$r(1-rh)=(1-rh)h=h+r,$$

and obviously, $\|1-rh\|=\|h+r\|$. Then with Equation (12) and Equation (13)

$$rq_1=q_1h=q_2, \tag{27}$$

i.e. rq_1 and q_1h also represent rotations mapping $\mathbf{h}$ onto $\mathbf{r}$. Moreover, it should be noted that Equation (27) implies

$$q_2^*rq_1=1 \tag{28}$$

$$q_1hq_2^*=1 \tag{29}$$

which may be interpreted as a remarkable 'factorization' of 1. It follows also from Equation (27) that

$$h = q_1^* q_2 \tag{30}$$

$$r = q_2 q_1^* \tag{31}$$

It can be easily proved by straightforward quaternion calculations that if an arbitrary quaternion $q \in C(q_1, q_2)$ is given, then rq and qh also represent rotations mapping $\mathbf{h}$ onto $\mathbf{r}$, and so does rqh, too. Moreover, with the unit quaternions

$$h(t) := \cos\frac{t}{2} + \mathbf{h}\sin\frac{t}{2}, \quad t \in [0, 2\pi) \tag{32}$$

$$r(t) := \cos\frac{t}{2} + \mathbf{r}\sin\frac{t}{2}, \quad t \in [0, 2\pi) \tag{33}$$

the elements of circle $C(q_1, q_2)$ can obviously be factorized by virtue of

$$C(q_1, q_2) = \{qh(t); q \in C(q_1, q_2), t \in [0, 2\pi)\} \tag{34}$$

$$C(q_1, q_2) = \{r(t)q; q \in C(q_1, q_2), t \in [0, 2\pi)\} \tag{35}$$

This factorization will prove useful for a unique specification of a rotation mapping $\mathbf{h}$ onto $\mathbf{r}$ as required in an advanced visualization approach suggested in References [3,4].

More generally, a quaternion $q(t) \in C(q_1, q_2)$ can be represented by

$$q(t) = p_2 v(t) p_1, \quad t \in [0, 2\pi) \tag{36}$$

where (i) $p_1 \in \mathbb{S}^3$ is any fixed quaternion such that $p_1 \mathbf{h} p_1^* = \mathbf{v}$ with an arbitrarily given unit vector $\mathbf{v} \in \mathbb{S}^2$, (ii) $v(t) := \cos t/2 + \mathbf{v} \sin t/2 \in \mathbb{S}^3$ such that $v(t)\mathbf{v}v^*(t) = \mathbf{v}$, and (iii) $p_2 \in \mathbb{S}^3$ is any fixed quaternion such that $p_2 \mathbf{v} p_2^* = \mathbf{r}$.

The inverse assertion to Proposition 3 is also true.

Proposition 4

Let $C(q_1, q_2)$ denote the circle with centre $\mathcal{O}$ in the plane $E(q_1, q_2) \subset \mathbb{H}$ spanned by the orthonormal quaternions $q_1, q_2 \in \mathbb{S}^3$. Then there exists a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r} \;\; \forall \; q \in C(q_1, q_2) \tag{37}$$

and $C(q_1, q_2)$ is the set of all rotations mapping $\mathbf{h}$ to $\mathbf{r}$. The pair of unit vectors is unique up to the common sign of $\mathbf{h}$ and $\mathbf{r}$, because $q(-\mathbf{h})q^* = -\mathbf{r}$ if and only if $q\mathbf{h}q^* = \mathbf{r}$.

Proof

The circle $C(q_1, q_2)$ with the centre $\mathcal{O}$ is given by Equation (26). Since q_1 and q_2 are orthogonal quaternions, $\mathrm{Sc}(q_1 q_2^*) = \mathrm{Sc}(q_2 q_1^*) = 0$. Then, the circle $C(q_1, q_2)$ represents the set of all rotations mapping the vector $\mathbf{h} = q_1^* q_2$ on the vector $\mathbf{r} = q_2 q_1^*$. In fact, for every $q(t) \in C(q_1, q_2)$ it holds $\|q(t)\|^2 = q^*(t)q(t) = 1$ and

$$\begin{aligned} q(t)hq^*(t) &= (q_1 \cos t + q_2 \sin t) q_1^* q_2 (q_1^* \cos t + q_2^* \sin t) \\ &= q_2 q_1^* \cos^2 t + q_2 q_1^* q_2 q_1^* \sin t \cos t + \sin t \cos t + q_2 q_1^* \sin^2 t \\ &= q_2 q_1^* = r \end{aligned}$$

Here we used that for orthogonal quaternions $q_2 q_1^* = -q_1 q_2^*$ holds, hence $q_2 q_1^* q_2 q_1^* = -1$. □

It should be noted that a one-to-one relationship exists between a circle $C = E \cap \mathbb{S}^3$ and a pair $\mathbf{h}, \mathbf{r}$ of unit vectors. However, since the circle may be represented as being spanned by a different pair of unit quaternions in the plane E, different pairs of spanning quaternions may be related to the same pair of unit vectors $\mathbf{h}, \mathbf{r}$.

Even though the sets $G(\mathbf{h}, \mathbf{r})$ and $G(\mathbf{r}, \mathbf{h})$ have the same set of rotation axes and the same interval of rotation angles in common, they are not equal because the association of axes and angles is reversed. Therefore, $C(q_1, q_2)$ representing $G(\mathbf{h}, \mathbf{r})$ is not equal to $C(q_1^*, q_2^*) = C^*(q_1, q_2)$ representing $G(\mathbf{r}, \mathbf{h})$.

Proposition 5
The two circles $C(q_1, q_2)$ and $C(q_3, q_4)$ representing the sets of rotations $G(\mathbf{h}, \mathbf{r})$ and $G(-\mathbf{h}, \mathbf{r})$, respectively, are orthonormal to one another.

Proof
It was shown above in Proposition 3 that q_1 and q_2 are defined by Equation (19), and the circle $C(q_3, q_4)$ represents all rotations mapping $-\mathbf{h}$ into $\mathbf{r}$ with

$$\begin{aligned} q_3 &:= \frac{1 + rh}{\|1 + rh\|} = \cos \frac{\pi - \eta}{2} + \mathbf{n}_3 \sin \frac{\pi - \eta}{2} \\ q_4 &:= \frac{-h + r}{\| - h + r\|} = \mathbf{n}_4 \end{aligned} \tag{38}$$

From geometrical reasons, it is clear that

$$\begin{aligned} \mathbf{n}_3 &:= \frac{-\mathbf{h} \times \mathbf{r}}{\| - \mathbf{h} \times \mathbf{r}\|} = -\mathbf{n}_1 \\ \mathbf{n}_4 &:= \frac{\mathbf{r} - \mathbf{h}}{\|\mathbf{r} - \mathbf{h}\|} = \frac{1}{2 \sin(\eta/2)} (\mathbf{r} - \mathbf{h}) = \mathbf{n}_1 \times \mathbf{n}_2 \end{aligned} \tag{39}$$

The two circles $C(\mathbf{n}_1, \mathbf{n}_2) \subset \mathbb{S}^2$ and $C(\mathbf{n}_3, \mathbf{n}_4) \subset \mathbb{S}^2$ are orthogonal to one another.

Now, let $q \in C(q_1, q_2)$ and $p \in C(q_3, q_4)$ be arbitrary unit quaternions

$$\begin{aligned} q &= q_1 \cos t + q_2 \sin t \\ p &= q_3 \cos t + q_4 \sin t \end{aligned} \tag{40}$$

Substituting expressions for q_1, q_2, q_3, q_4, i.e. Equations (19), (38), and (39) in Equation (40) we get

$$\begin{aligned} q &= \cos \frac{\eta}{2} \cos t + \mathbf{n}_1 \sin \frac{\eta}{2} \cos t + \mathbf{n}_2 \sin t \\ p &= \cos \frac{\pi - \eta}{2} \cos t + \mathbf{n}_3 \sin \frac{\pi - \eta}{2} \cos t + \mathbf{n}_4 \sin t \\ &= \sin \frac{\eta}{2} \cos t - \mathbf{n}_1 \cos \frac{\eta}{2} \cos t + (\mathbf{n}_1 \times \mathbf{n}_2) \sin t \end{aligned}$$

Now, ordinary quaternion multiplication yields

$$\begin{aligned} \mathrm{Sc}(q p^*) &= \cos \frac{\eta}{2} \cos t \sin \frac{\eta}{2} \cos t \\ &\quad + \left(\mathbf{n}_1 \sin \frac{\eta}{2} \cos t + \mathbf{n}_2 \sin t\right) \cdot \left(-\mathbf{n}_1 \cos \frac{\eta}{2} \cos t + \mathbf{n}_1 \times \mathbf{n}_2 \sin t\right) = 0 \end{aligned}$$

Thus, the two circles $C(q_1, q_2) \subset \mathbb{S}^3$ and $C(q_3, q_4) \subset \mathbb{S}^3$ are orthonormal to one another. □

Remark
Obviously, $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_4$ provide a right-handed orthonormal basis of $\mathrm{Vec}\mathbb{H} \simeq \mathbb{R}^3$, and $q_i, i = 1, \ldots, 4$, provide a right-handed orthonormal basis of $\mathbb{H}$.

Corollary 1
Eventually, it holds that

(i) given $\mathbf{h}_0$, it holds that $G(\mathbf{h}_0, \mathbf{r}_1) \cap G(\mathbf{h}_0, \mathbf{r}_2) = \emptyset$ if $\mathbf{r}_1 \neq \mathbf{r}_2$, and, analogously, given $\mathbf{r}_0$, it holds that $G(\mathbf{h}_1, \mathbf{r}_0) \cap G(\mathbf{h}_2, \mathbf{r}_0) = \emptyset$ if $\mathbf{h}_1 \neq \mathbf{h}_2$;

(ii) $$\bigcup_{\mathbf{r} \in \mathbb{S}^2} G(\mathbf{h}_0, \mathbf{r}) = \bigcup_{\mathbf{h} \in \mathbb{S}^2} G(\mathbf{h}, \mathbf{r}_0) = \mathrm{SO}(3)$$

(iii) given $\boldsymbol{g} \in \mathrm{SO}(3)$ and $\mathbf{h}_0$, there exists a vector $\mathbf{r}$ such that $\boldsymbol{g} \in G(\mathbf{h}_0, \mathbf{r})$, and, analogously, given $\boldsymbol{g} \in \mathrm{SO}(3)$ and $\mathbf{r}_0$, there exists a vector $\mathbf{h}$ such that $\boldsymbol{g} \in G(\mathbf{h}, \mathbf{r}_0)$.

The major property of the circle $C(q_1, q_2)$ is that it consists of all quaternions $q(t), t \in [0, 2\pi)$, with $q(t)\mathbf{h}q^*(t) = \mathbf{r}$ for all $t \in [0, 2\pi)$, and that it is uniquely characterized by the pair $\mathbf{h}, \mathbf{r} \in \mathbb{S}^2$. For any other $\mathbf{h}' \in \mathbb{S}^2$ with $\mathbf{h} \cdot \mathbf{h}' = \cos \rho$ the vector $q(t)\mathbf{h}'q^*(t) =: \mathbf{r}'(t) \in \mathbb{S}^2$ is not a constant unit vector, but it encloses the same angle ρ with $\mathbf{r}$ for every t

$$\mathbf{r} \cdot \mathbf{r}'(t) = (q(t)\mathbf{h}q^*(t)) \cdot (q(t)\mathbf{h}'q^*(t)) = \mathbf{h} \cdot \mathbf{h}' = \cos \rho \tag{41}$$

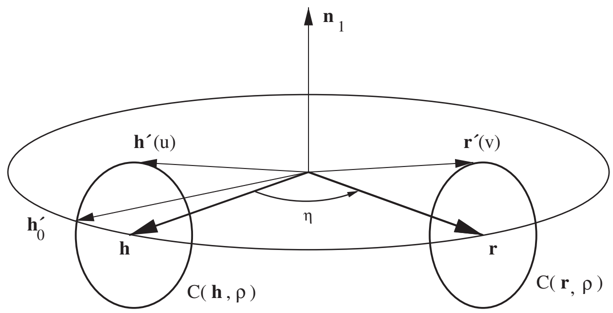

Figure 2. Circles $C(\mathbf{h},\rho)$ and $C(\mathbf{r},\rho)$.

Next, it is shown that $\mathbf{r}'(t)$ actually represents the small circle with centre $\mathbf{r}$ and angle ρ of $\mathbb{S}^2$. To this end we define the small circle $C(\mathbf{r},\rho)\subset\mathbb{S}^2$ properly by

$$C(\mathbf{r},\rho)=\{\mathbf{r}'\in\mathbb{S}^2|\mathbf{r}\cdot\mathbf{r}'=\cos\rho\} \tag{42}$$

and observe that it can be parametrized by virtue of Equation (33) and represented as

$$\mathbf{r}'(t)=r(t)\mathbf{r}'_0r^*(t) \tag{43}$$

with $\mathbf{r}'_0\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h}\cdot\mathbf{r}'_0=\cos(\eta-\rho)$. In this way the small circle $C(\mathbf{r},\rho)$ is seen as the result of all rotations of the vector $\mathbf{r}'_0$ about the axis $\mathbf{r}$, see Figure 2. Analogously, the small circle $C(\mathbf{h},\rho)$ can be represented as

$$\mathbf{h}'(t)=h(t)\mathbf{h}'_0h^*(t) \tag{44}$$

with $\mathbf{h}'_0\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h}'_0\cdot\mathbf{r}=\cos(\eta+\rho)$.

Proposition 6
The circle $C(q_1,q_2)$ represents rotations mapping the small circle $C(\mathbf{h},\rho)$ onto the small circle $C(\mathbf{r},\rho)$; i.e. for every $\mathbf{h}'(u)\in C(\mathbf{h},\rho)$ and $q(t)\in C(q_1,q_2)$

$$q(t)\mathbf{h}'(u)q^*(t)=\mathbf{r}'(u+2t),\quad t,u\in[0,2\pi) \tag{45}$$

holds.

Proof
Let us consider the vector $\mathbf{r}'_0=q_1\mathbf{h}'_0q_1^*$. Since rotations preserve angles, the angle between $\mathbf{r}'_0$ and $\mathbf{r}$ is ρ as the angle between $\mathbf{h}'_0$ and $\mathbf{h}$. Then

$$\begin{aligned}q(t)\mathbf{h}'(u)q^*(t)&=q(t)h(u)\mathbf{h}'_0h^*(u)q^*(t)\\&=(q(t)h(u)q_1^*)(q_1\mathbf{h}'_0q_1^*)(q_1h^*(u)q^*(t))\\&=(q(t)h(u)q_1^*)\mathbf{r}'_0(q_1h^*(u)q^*(t))\end{aligned} \tag{46}$$

Substituting Equations (32) and (26) yields

$$q(t)h(u)q_1^* = (q_1 \cos t + q_2 \sin t)\left(\cos\frac{u}{2} + \mathbf{h}\sin\frac{u}{2}\right)q_1^*$$
$$= \cos t\cos\frac{u}{2} + q_2 q_1^* \sin t\cos\frac{u}{2}$$
$$+ q_1\mathbf{h}q_1^* \cos t\sin\frac{u}{2} + q_2\mathbf{h}q_1^*\sin t\sin\frac{u}{2} \qquad (47)$$

It follows from Equation (29) that $q_2\mathbf{h}q_1^* = -1$. With this substitution in Equation (47) and with Equation (31) in mind, we accomplish

$$q(t)h(u)q_1^* = \cos t\cos\frac{u}{2} - \sin t\sin\frac{u}{2} + \mathbf{r}\left(\sin t\cos\frac{u}{2} + \cos t\sin\frac{u}{2}\right)$$
$$= \cos\frac{u+2t}{2} + \mathbf{r}\sin\frac{u+2t}{2} \qquad (48)$$

Thus, for every t the vector $q(t)\mathbf{h}'(u)q^*(t)$ is the result of the rotation of $\mathbf{r}_0'$ about $\mathbf{r}$ by the angle $u+2t$. This completes the proof. □

Corollary 2
Let $p(u)$ be a quaternion mapping $\mathbf{h}$ onto $\mathbf{h}'(u) \in C(\mathbf{h},\rho)$, then for every $q(t) \in C(q_1,q_2)$ the quaternion $q(t)p(u)q^*(t)$ is mapping $\mathbf{r}$ onto $\mathbf{r}'(v) \in C(\mathbf{r},\rho), v = u+2t$.

It should be noted that $C(q_1,q_2)$ does not represent all rotations mapping an element of $C(\mathbf{h},\rho)$ onto an element of $C(\mathbf{r},\rho)$. In fact, the rotation about $(\mathbf{h}_0'+\mathbf{r}_0')/\|\mathbf{h}_0'+\mathbf{r}_0'\|$ by π mapping $\mathbf{h}_0' \in C(\mathbf{h},\rho)$ on $\mathbf{r}_0' \in C(\mathbf{r},\rho)$ cannot be represented by any element of $C(q_1,q_2)$ as the pure unit quaternion $(\mathbf{h}_0'+\mathbf{r}_0')/\|\mathbf{h}_0'+\mathbf{r}_0'\| \notin C(q_1,q_2)$.

Slightly generalizing the notation of Proposition 3, the set $\bigcup_{u\in[0,2\pi)}\bigcup_{v\in[0,2\pi)} G(\mathbf{h}'(u),\mathbf{r}'(v))$ of all rotations mapping $C(\mathbf{h},\rho)$ onto $C(\mathbf{r},\rho)$ is represented by the union of all circles $\bigcup_{u\in[0,2\pi)}\bigcup_{v\in[0,2\pi)} C(q_1(\mathbf{h}'(u),\mathbf{r}'(v)), q_2(\mathbf{h}'(u),\mathbf{r}'(v))$ representing rotations $\boldsymbol{g}\mathbf{h}'(u) = \mathbf{r}'(v)$. Rewriting Equation (45) as

$$q\left(\frac{v-u}{2}\right)\mathbf{h}'(u)q^*\left(\frac{v-u}{2}\right) = \mathbf{r}'(v) \text{ for all } u,v \in [0,2\pi)$$

leads to

$$\bigcap_{v-u=2t} C(q_1(\mathbf{h}'(u),\mathbf{r}'(v)), q_2(\mathbf{h}'(u),\mathbf{r}'(v)) = \{q(t;\mathbf{h},\mathbf{r})\}$$

and furthermore to

$$\bigcup_{t\in[0,2\pi)}\bigcap_{v-u=2t} C(q_1(\mathbf{h}'(u),\mathbf{r}'(v)), q_2(\mathbf{h}'(u),\mathbf{r}'(v)) = \bigcup_{t\in[0,2\pi)}\{q(t;\mathbf{h},\mathbf{r})\}$$
$$= C(q_1(\mathbf{h},\mathbf{r}), q_2(\mathbf{h},\mathbf{r}))$$

With respect to small circles another proposition holds.

Proposition 7
The set of all rotations mapping $\mathbf{h}$ on $C(\mathbf{r},\rho)$ is equal to the set of all rotations mapping $C(\mathbf{h},\rho)$ onto $\mathbf{r}$, i.e.

$$\bigcup_{\mathbf{r}'\in C(\mathbf{r},\rho)} G(\mathbf{h},\mathbf{r}') = \bigcup_{\mathbf{h}'\in C(\mathbf{h},\rho)} G(\mathbf{h}',\mathbf{r})$$

or equivalently

$$\bigcup_{v\in[0,2\pi)} G(\mathbf{h},\mathbf{r}'(v)) = \bigcup_{u\in[0,2\pi)} G(\mathbf{h}'(u),\mathbf{r})$$

employing the parametric representation, Equations (43) and (44), respectively.

Proof
The set of rotations $G(\mathbf{h},\mathbf{r}'(v))$, $v\in[0,2\pi)$, is represented by the circle

$$C(q_1(\mathbf{h},\mathbf{r}'(v)),q_2(\mathbf{h},\mathbf{r}'(v))) = \{q(t;\mathbf{h},\mathbf{r}'(v)),\ \ t,v\in[0,2\pi)\} \tag{49}$$

such that

$$q(t;\mathbf{h},\mathbf{r}'(v))\mathbf{h}q^*(t;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}'(v),\ \ \forall\ \ t,v\in[0,2\pi),$$

Applying Proposition 6 implies that $q(t;\mathbf{h},\mathbf{r}'(v))$ of Equation (49) maps $\mathbf{h}'(u)$ for arbitrary $t,u\in[0,2\pi)$ onto the circle $C(\mathbf{r}'(v),\rho)$, i.e.

$$q(t;\mathbf{h},\mathbf{r}'(v))\mathbf{h}'(u)q^*(t;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}''(u+2t)\in C(\mathbf{r}'(v),\rho)$$

where

$$\mathbf{r}''(v) = r'(v)\mathbf{r}_0''r'^*(v)$$

with $\mathbf{r}_0''\in\mathbb{S}^2$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}'(v)$ with $\mathbf{h}\cdot\mathbf{r}_0'' = \cos(\eta'(v)-\rho)$ with $\cos\eta'(v) = \mathbf{h}\cdot\mathbf{r}'(v)$. Since $\mathbf{r}\in C(\mathbf{r}'(v),\rho)$, it holds that $t_0\in[0,2\pi)$ exists such that $q(t_0;\mathbf{h},\mathbf{r}'(v))\mathbf{h}'(u)$ $q^*(t_0;\mathbf{h},\mathbf{r}'(v)) = \mathbf{r}$. Thus, $q(t_0;\mathbf{h},\mathbf{r}'(v))$ represents a rotation g_0 such that $g_0\mathbf{h} = \mathbf{r}'(v)$ and also $g_0\mathbf{h}'(u) = \mathbf{r}$.

The same argument applies analogously in the other direction.

Let us find an explicit form of these rotations. Considering the sequence of rotations

$$\mathbf{h}'(u)\xrightarrow{p^*(u)}\mathbf{h}\xrightarrow{q(t)}\mathbf{r} \tag{50}$$

where $p(u)$ is a rotation mapping $\mathbf{h}$ onto $\mathbf{h}'(u)$ with its axis orthogonal to the plane spanned by the vectors $\mathbf{h}$ and $\mathbf{h}'(u)$, and where therefore $p^*(u)$ is the inverse rotation mapping $\mathbf{h}'(u)$ onto $\mathbf{h}$, we get that $q(t)p^*(u)$ is the resulting quaternion mapping $\mathbf{h}'(u)$ onto $\mathbf{r}$. On the other side, due to Corollary 2, the sequence of rotations

$$\mathbf{h}\xrightarrow{q(t)}\mathbf{r}\xrightarrow{q(t)pq(t)^*}\mathbf{r}'(v) \tag{51}$$

gives us the resulting quaternion $q(t)p(u)$ mapping $\mathbf{h}$ onto $\mathbf{r}'(u+2t) = \mathbf{r}'(v)$. Let us show that $\{q(t)p(u); u\in[0,2\pi)\} = \{q(t)p^*(u); u\in[0,2\pi)\}$. Indeed, since $C(\mathbf{h},\rho)$ is a circle, it contains points $\mathbf{h}'(u)$ and $\mathbf{h}'(u+\pi)$ which are symmetric with respect to $\mathbf{h}$ for every u and all three vectors $\mathbf{h}'(u), \mathbf{h}$ and $\mathbf{h}'(u+\pi)$ are lying in the same plane. Then the quaternion $p^*(u)$ is mapping $\mathbf{h}$ onto $\mathbf{h}'(u+\pi)$. Hence, the set of all quaternions mapping $\mathbf{h}$ onto $\mathbf{h}'(u), u \in [0, 2\pi)$ can be represented by

$$\{p(u); u \in [0, 2\pi)\} = \{p(u); u \in [0, \pi)\} \cup \{p^*(u); u \in [0, \pi)\} \tag{52}$$

It gives us immediately that $\{p(u); u \in [0, 2\pi)\} = \{p^*(u); u \in [0, 2\pi)\}$, and therefore $\{q(t)p(u); u \in [0, 2\pi)\} = \{q(t)p^*(u); u \in [0, 2\pi)\}$. Thus,

$$\bigcup_{v \in [0,2\pi)} G(\mathbf{h}, \mathbf{r}'(v)) = \bigcup_{u \in [0,2\pi)} G(\mathbf{h}'(u), \mathbf{r}) \tag{53}$$

This completes the proof. □

Corollary 3
The set of all rotations mapping $\mathbf{h}$ on the spherical cap $\bigcup_{\varrho \in [0,\rho]} C(\mathbf{r}, \rho)$ is equal to the set of all rotations mapping the spherical cap $\bigcup_{\varrho \in [0,\rho]} C(\mathbf{h}, \rho)$ onto $\mathbf{r}$.

It should be noted that Proposition 7 leads to a completely geometrical proof of Ásgeirsson's mean value theorem [5,6,12–14] for Radon transforms $\mathscr{R}f$ of even functions defined on $\mathbb{S}^3$.

3.2. Mapping a pair of given vectors onto another pair

Now we consider the problem with two pairs of given unit vectors $(\mathbf{h}, \mathbf{r})$ and $(\mathbf{h}_1, \mathbf{r}_1)$ to be mapped onto each other by the same rotation. It is possible to solve the problem by a conditional extremum approach looking for the rotation which minimizes $\|\mathbf{h}-\mathbf{r}\|^2 + \|\mathbf{h}_1 - \mathbf{r}_1\|^2$ subject to the constraint $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$. However, we shall continue the geometric approach to find an exact solution.

Proposition 8
Given two pairs of unit vectors $(\mathbf{h}, \mathbf{r}), (\mathbf{h}_1, \mathbf{r}_1) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that $(\mathbf{h} \times \mathbf{r}) \times (\mathbf{h}_1 \times \mathbf{r}_1) \neq 0$. Then there exists a unique quaternion $q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } q\mathbf{h}_1 q^* = \mathbf{r}_1 \tag{54}$$

provided that $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$, as rotations preserve the geodetic distance of unit vectors.

Proof
Algebraically, q is given as the solution of the system of the two equations

$$q\mathbf{h} - \mathbf{r}q = 0 \tag{55}$$

$$q\mathbf{h}_1 - \mathbf{r}_1 q = 0 \tag{56}$$

subject to $\mathbf{h} \cdot \mathbf{h}_1 = \mathbf{r} \cdot \mathbf{r}_1$. By geometrical reasoning the solution is given as follows. The axis $\mathbf{q}$ of the rotation q is given by the intersection of the two planes of rotation axes corresponding to the circle Equation (55) and the circle Equation (56), respectively. The intersection of two planes is provided by the vector product of their normals, thus

$$\mathbf{q} = \left[\left(\frac{\mathbf{h}\times\mathbf{r}}{\|\mathbf{h}\times\mathbf{r}\|}\right)\times\left(\frac{\mathbf{h}+\mathbf{r}}{\|\mathbf{h}+\mathbf{r}\|}\right)\right]\times\left[\left(\frac{\mathbf{h}_1\times\mathbf{r}_1}{\|\mathbf{h}_1\times\mathbf{r}_1\|}\right)\times\left(\frac{\mathbf{h}_1+\mathbf{r}_1}{\|\mathbf{h}_1+\mathbf{r}_1\|}\right)\right]$$

$$= \frac{\mathbf{h}-\mathbf{r}}{\|\mathbf{h}-\mathbf{r}\|}\times\frac{\mathbf{h}_1-\mathbf{r}_1}{\|\mathbf{h}_1-\mathbf{r}_1\|} \tag{57}$$

If the vectors $\mathbf{h}-\mathbf{r}$ and $\mathbf{h}_1-\mathbf{r}_1$ are not collinear, Equation (57) yields the unique axis of the required rotation. The angle ω of the rotation q is provided by Equation (22). The required quaternion of rotation is

$$q = \cos\frac{\omega}{2} + \frac{\mathbf{q}}{\|\mathbf{q}\|}\sin\frac{\omega}{2} \tag{58}$$

If the vectors $\mathbf{h}-\mathbf{r}$ and $\mathbf{h}_1-\mathbf{r}_1$ are collinear, two possibilities arise.

In the first case $\mathbf{h} = -\mathbf{h}_1$. Then it follows that all vectors $\mathbf{h}, \mathbf{r}, \mathbf{h}_1, \mathbf{r}_1$ are lying in the same plane. The axis of rotation coincides with the vector $(\mathbf{h}\times\mathbf{r})/\|\mathbf{h}\times\mathbf{r}\|$ and the angle of rotation ω is equal to the angle η between $\mathbf{h}$ and $\mathbf{r}$.

In the second case $\mathbf{h} \neq -\mathbf{h}_1$. Then, due to symmetry, the axis of rotation coincides with the line of intersection of two planes: the plane spanned by the vectors $\mathbf{h}, \mathbf{h}_1$ and the plane spanned by the vectors $\mathbf{r}, \mathbf{r}_1$, i.e. it is the vector product of two normals

$$\mathbf{q} = \frac{\mathbf{h}\times\mathbf{h}_1}{\|\mathbf{h}\times\mathbf{h}_1\|}\times\frac{\mathbf{r}\times\mathbf{r}_1}{\|\mathbf{r}\times\mathbf{r}_1\|} \tag{59}$$

and the angle of rotation ω is again given by Equation (22). □

Remark

The condition of collinearity has a simple quaternion analogue. Two arbitrary vectors $\mathbf{h}, \mathbf{r}$ are collinear if the corresponding pure quaternions h, r are commutative, i.e. $hr - rh = 0$.

Next, the factorization, Equation (34), is applied to control the degree of freedom when specifying and representing a particular rotation mapping $\mathbf{h}$ onto $\mathbf{r}$. Instead of using two pairs of unit vectors mapped onto each other, the condition now is that we have two unit vectors in the tangential plane of the radius vector $\mathbf{r}\in\mathbb{S}^2$—one of them arbitrarily given, the other one subjected to a rotation $r(t)\in\mathbb{S}^3$ about $\mathbf{r}$ by $t\in[0, 2\pi)$—enclose a given angle, say t_0.

Let q be the quaternion defined in Equation (58), i.e $q\mathbf{h}q^* = \mathbf{r}$ and $q\mathbf{h}_1q^* = \mathbf{r}_1$. Defining the orthogonal projection $(\mathbf{v})_T$ of an arbitrary unit vector $\mathbf{v}\in\mathbb{S}^2$ onto the tangential plane of the radius vector $\mathbf{r}$ (see Figure 3)

$$(\mathbf{v})_T(\mathbf{r}) = \mathbf{v} - (\mathbf{v}\cdot\mathbf{r})\ \mathbf{r}$$

we get

$$(\mathbf{r}_1)_T(\mathbf{r}) = \mathbf{r}_1 - (\mathbf{r}_1\cdot\mathbf{r})\mathbf{r} = q\mathbf{h}_1q^* - (q\mathbf{h}_1q^*\cdot\mathbf{r})\ \mathbf{r}$$

where the latter yields

$$(\mathbf{r}_1)_T(\mathbf{r}) = q\mathbf{h}_1q^* - (q\mathbf{h}_1q^*\cdot q\mathbf{h}q^*)q\mathbf{h}q^*$$

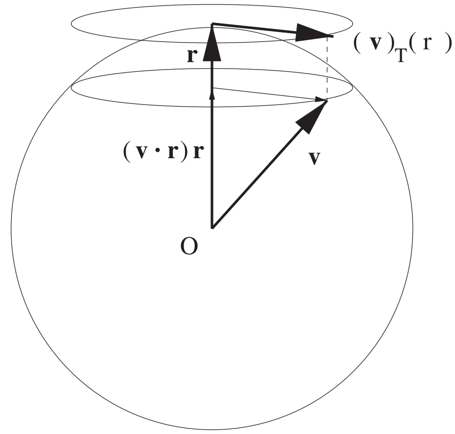

Figure 3. Projection $(\mathbf{v})_T$.

$$= q\mathbf{h}_1 q^* - (\mathbf{h}_1 \cdot \mathbf{h}) q\mathbf{h}q^*$$

$$= q(\mathbf{h}_1 - (\mathbf{h}_1 \cdot \mathbf{h})\mathbf{h})q^* = q(\mathbf{h}_1)_T(\mathbf{h})q^*$$

Then the projection $(\mathbf{v})_T(\mathbf{r})$ of an arbitrary vector $\mathbf{v}$ may be thought of as the result of a rotation of $(\mathbf{r}_1)_T(\mathbf{r})$ about $\mathbf{r}$ by the angle $\alpha = \arccos((\mathbf{v})_T \cdot (\mathbf{r}_1)_T)$.

Proposition 9
Given a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$, and two additional unit vectors $\mathbf{h}_1, \mathbf{v} \in \mathbb{S}^2$. Then there exists a unique quaternion $q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } (\mathbf{v})_T(\mathbf{r}) \cdot (q\mathbf{h}_1 q^*)_T(\mathbf{r}) = \cos t_0 \tag{60}$$

where $t_0 \in [0, 2\pi)$ denotes the angle between the orthogonal projection of $\mathbf{v}$ and the orthogonal projection of $q\mathbf{h}_1 q^*$ onto the tangential plane of $\mathbf{r}$.

Proof
Let p be a quaternion obtained like in Proposition 8 such that

$$p\mathbf{h}p^* = \mathbf{r}$$

$$p\mathbf{h}_1 p^* = \mathbf{v}$$

When a vector is rotating about the vector $\mathbf{r}$ by the angle t_0, its projection on the tangential plane of $\mathbf{r}$ is also rotating about $\mathbf{r}$ by the same angle by definition.

Now, the quaternion we are looking for is $q = r(t_0)p$, where $r(t_0) = \cos(t_0/2) + \mathbf{r}\sin(t_0/2)$. Indeed,

$$q\mathbf{h}q^* = r(t_0)p\mathbf{h}p^* r^*(t_0) = r(t_0)\mathbf{r}r^*(t_0) = \mathbf{r} \tag{61}$$

as a rotation of a vector about itself does not change the vector, and

$$q\mathbf{h}_1 q^* = r(t_0)p\mathbf{h}_1 p^* r^*(t_0) = r(t_0)\mathbf{v}r^*(t_0) \tag{62}$$

The angle between $(\mathbf{v})_T(\mathbf{r})$ and $(r(t_0)\mathbf{v}r^*(t_0))_T(\mathbf{r})$ is just t_0. □

For mutually orthogonal unit quaternions $q, p_1, p_2, p_3 \in \mathbb{S}^3$ let $S(p_1, p_2, p_3)$ denote the orthogonally complementary sphere of a given quaternion $q \in \mathbb{S}^3$, i.e. $S(p_1, p_2, p_3) := q^{\perp} \cap \mathbb{S}^3$. Due to Proposition 1 we can write

$$S(p_1, p_2, p_3) = \mathbb{S}^2 q \tag{63}$$

Since $\mathbb{S}^2$ consists of all pure unit quaternions, Equation (63) means that the orthogonal complement of q consists of all quaternions representing rotations composed of a first rotation represented by q and a second rotation by the angle π about an arbitrary axes in $\mathbb{S}^2$.

Moreover, for every quaternion $q \in C(q_1, q_2)$, the circle $C(q_3, q_4) \subset q^{\perp}$, i.e. if $q\mathbf{h}q^* = \mathbf{r}$, then the set of all rotations $p\mathbf{h}p^* = -\mathbf{r}$ is completely contained in the sphere $q^{\perp}$.

Proposition 10
Given an arbitrary quaternion $q_0 \in \mathbb{S}^3$ and denote $S(p_1, p_2, p_3)$ the orthogonally complementary sphere of q_0. For each choice of $p_3 \in q_0^{\perp}$ there exists a unique pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r}, \ \ \forall \ q \in C(p_1, p_2) \tag{64}$$

Proof
Of course, the statement holds true for

$$\mathbf{h} = \mathrm{Vec}(p_1^* p_2)$$

$$\mathbf{r} = \mathrm{Vec}(p_2 p_1^*)$$

because of Proposition 4. However, here we would like to find $\mathbf{h}$ and $\mathbf{r}$ in terms of q_0 and p_3.

First, remember that $q_0^{\perp} = \mathbb{S}^2 q_0$. Then, because of Proposition 1 every three mutually orthonormal quaternions $p_1, p_2, p_3 \in q_0^{\perp} \cap \mathbb{S}^3$, which are assumed to build a right-handed system in this order, can always be written as

$$p_i = \mathbf{v}_i q_0$$

where $\mathbf{v}_i = p_i q_0^* \in \mathbb{S}^2, \ \ i = 1, 2, 3$. Hence

$$p_i p_j^* = v_i q_0 q_0^* v_j^* = \mathbf{v}_i \cdot \mathbf{v}_j - \mathbf{v}_i \times \mathbf{v}_j$$

The orthonormality of p_1, p_2, p_3 implies for the associated vectors that $\mathrm{Sc}(p_i p_j^*) = \mathbf{v}_i \cdot \mathbf{v}_j = 0$, i.e. the vectors $\mathbf{v}_i, i = 1, 2, 3$, build an orthonormal basis with no handedness assigned yet. Furthermore, using Equation (4) we get

$$2(\mathbf{v}_i \cdot \mathbf{v}_j) = v_i v_j + v_j v_i = 0$$

thus $v_i v_j = -v_j v_i$. A (right) handedness is assigned to $\mathbf{v}_i, i = 1,2,3$, by setting

$$v_3 = v_1 v_2 = -v_2 v_1$$

Now, we define h as following

$$h = p_1^* p_2 = q_0^* v_1^* v_2 q_0 = -q_0^* v_1 v_2 q_0 = -q_0^* v_3 q_0 = q_0^* v_3^* q_0 = p_3^* q_0$$

and

$$r = p_2 p_1^* = v_2 q_0 q_0^* v_1^* = -v_2 v_1 = v_3 = p_3 q_0^*$$

Thus, a quaternion $q(t) = p_1 \cos t + p_2 \sin t \in C(p_1, p_2)$ maps the vector $\mathbf{h} = q_0^* p_3$ on the vector $\mathbf{r} = q_0 p_3^*$. To check the result one can use the quaternion multiplication $q(t)hq^*(t)$. □

The parametrization of $C(p_1, p_2)$ in terms of q_0, p_3 proves instrumental in integration, e.g. as with respect to spherical Radon transforms of order 1, 2 [14]. Moreover, this parametrization implies that each circle contained in $q_0^\perp$ refers to a different unique pair of unit vectors related to one another by the corresponding rotations.

Corollary 4
Let $C(q_1, q_2)$ and $C(q_3, q_4)$ be defined like in Proposition 5. If $q_0 \in C(q_1, q_2)$, then $C(q_3, q_4)$ is the only circle representing all rotations acting on $\mathbf{h}$ which is completely contained in $q_0^\perp$.

Thus, the major property of the sphere $q_0^\perp = \mathbb{S}^2 q_0 \subset \mathbb{S}^3 \subset \mathbb{H}$ is that it contains the circle representing all rotations mapping $\mathbf{h}$ on $-\mathbf{r}$ and that it does not contain any other circle representing all rotations mapping $\mathbf{h}$ on a direction different of $-\mathbf{r}$.

Proposition 11
Given a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$, there exists a pair of orthogonal unit quaternions $p, q \in \mathbb{S}^3$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } p\mathbf{h}p^* \in \mathbf{r}^\perp \cap \mathbb{S}^2. \tag{65}$$

Proof
Let $q \in \mathbb{S}^3$ be an arbitrary unit quaternion such that $q\mathbf{h}q^* = \mathbf{r}$. For any $p \in \mathbb{S}^3$ it holds

$$p\mathbf{h}p^* = pq^*q\mathbf{h}q^*qp^* = pq^*\mathbf{r}(pq^*)^*$$

Thus, $p \in \mathbb{S}^3$ has to be constructed to satisfy the orthogonality condition $\mathrm{Sc}(pq^*) = 0$ and it has to be

$$pq^*\mathbf{r}(pq^*)^* = \mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$$

Hence, for any $\mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$ we get

$$\mathrm{Vec}(pq^*) = \frac{\mathbf{r} + \mathbf{r}_1}{\|\mathbf{r} + \mathbf{r}_1\|}$$

and the angle of rotation is π. Thus

$$pq^* = 0 + \frac{\mathbf{r} + \mathbf{r}_1}{\|\mathbf{r} + \mathbf{r}_1\|}$$

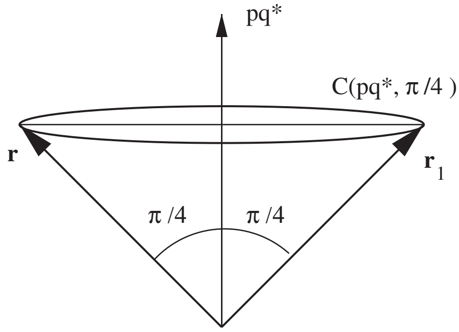

Figure 4. Rotation of $\mathbf{r}$ by pq^*.

Eventually the quaternion we are looking for is

$$p = \frac{\mathbf{r} + \mathbf{r}_1}{\|\mathbf{r} + \mathbf{r}_1\|} q \tag{66}$$

If $\mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$ and $q \in \mathbb{S}^3$ are fixed, then p is uniquely defined by Equation (66). Since the set $G(\mathbf{h}, \mathbf{r})$ is represented by the circle $C(q_1, q_2)$ of Proposition 3 spanned by two linearly independent quaternions $q_1, q_2 \in \mathbb{S}^3$, there are also two linearly independent solutions $p_i = (\mathbf{r} + \mathbf{r}_1)/(\|\mathbf{r} + \mathbf{r}_1\|)q_i$, $i = 1, 2$, of Equation (66). □

The inverse assertion holds also.

Proposition 12
Given a pair of unit orthonormal quaternions $p, q \in \mathbb{S}^3$, there exists a pair of unit vectors $(\mathbf{h}, \mathbf{r}) \in \mathbb{S}^2 \times \mathbb{S}^2$ such that

$$q\mathbf{h}q^* = \mathbf{r} \text{ and } p\mathbf{h}p^* \in \mathbf{r}^\perp \cap \mathbb{S}^2 \tag{67}$$

Proof
Since p and q are assumed to be orthonormal, $\mathrm{Sc}(pq^*) = 0$. Thus, $pq^* \in \mathbb{S}^2$ is a pure quaternion. Choosing $\mathbf{r}$ as a unit vector of the small circle $C(pq^*, \pi/4)$ with centre pq^* and $(pq^*) \cdot \mathbf{r} = \cos \pi/4$, it holds that $(pq^*)\mathbf{r}(pq^*)^* = \mathbf{r}_1$ is a vector orthonormal to $\mathbf{r}$, i.e. $\mathbf{r}_1 \in \mathbf{r}^\perp$, since pq^* represents a rotation about $pq^* \in \mathbb{S}^2$ by the angle π, see Figure 4. Next, defining $\mathbf{h} = q^*\mathbf{r}q$, we get, obviously, $q\mathbf{h}q^* = \mathbf{r}$ and

$$p\mathbf{h}p^* = pq^*\mathbf{r}qp^* = (pq^*)\mathbf{r}(pq^*)^* = \mathbf{r}_1 \in \mathbf{r}^\perp \tag{68}$$

If $\mathbf{r}_1 \in \mathbf{r}^\perp \cap \mathbb{S}^2$ is fixed, then $\mathbf{h}$ is uniquely defined by Equation (68). □

The propositions proved above lead to the following final result.

Proposition 13
Let q_1, q_2, q_3, q_4 denote four mutually orthonormal quaternions; let $C(q_1, q_2)$ denote the circle of quaternions $q(s), s \in [0, 2\pi)$, representing the rotations $\boldsymbol{g} \in G(\mathbf{h}, \mathbf{r})$, and $C(q_3, q_4)$ the circle $q(t), t \in [0, 2\pi)$, representing the rotations $\boldsymbol{g} \in G(-\mathbf{h}, \mathbf{r})$. Then the spherical torus

$T(q_1, q_2, q_3, q_4; \Theta) \subset S^3$ defined as the set of quaternions

$$q(s,t;\Theta) = (q_1 \cos s + q_2 \sin s)\cos \Theta + (q_3 \cos t + q_4 \sin t)\sin \Theta$$
$$s,t \in [0, 2\pi), \quad \Theta \in [0, \pi/2]$$

represents all rotations mapping $\mathbf{h}$ on the small circle $C(\mathbf{r}, 2\Theta) \subset \mathbb{S}^2$.

In particular, $q(s, -s; \Theta)$ maps $\mathbf{h}$ for all $s \in [0, 2\pi)$ onto $\mathbf{r}'_0$ in the plane spanned by $\mathbf{h}$ and $\mathbf{r}$ with $\mathbf{h} \cdot \mathbf{r}'_0 = \cos(\eta - 2\Theta)$,

$$q(s, -s; \Theta)\mathbf{h}q^*(s, -s; \Theta) = \mathbf{r}'_0 \text{ for all } s \in [0, 2\pi)$$

Moreover, for an arbitrary $s_0 \in [0, 2\pi)$, $q(s_0, t - s_0; \Theta)$ (or $q(s_0 + t, -s_0; \Theta)$, respectively,) maps $\mathbf{h}$ on $\mathbf{r}' \in C(\mathbf{r}, 2\Theta)$ which results from a positive (counter-clockwise) rotation of $\mathbf{r}'_0$ about $\mathbf{r}$ by the angle $t \in [0, 2\pi)$,

$$q(s_0, t - s_0; \Theta)\mathbf{h}q^*(s_0, t - s_0; \Theta) = r(t)\mathbf{r}'_0 r^*(t), \text{ for all } s \in [0, 2\pi).$$

Proof

It can be shown by using Equation (27) and straightforward quaternion multiplication that

$$q_1\mathbf{h}q_2^* = -q_2\mathbf{h}q_1^* = 1$$
$$q_1\mathbf{h}q_3^* = -q_3\mathbf{h}q_1^* = -\mathbf{n}_1 \times \mathbf{r}$$
$$q_1\mathbf{h}q_4^* = -q_4\mathbf{h}q_1^* = -\mathbf{n}_1$$
$$q_2\mathbf{h}q_3^* = -q_3\mathbf{h}q_2^* = -\mathbf{n}_1$$
$$q_2\mathbf{h}q_4^* = -q_4\mathbf{h}q_2^* = \mathbf{n}_1 \times \mathbf{r}$$
$$q_3\mathbf{h}q_4^* = -q_4\mathbf{h}q_3^* = -1$$

where $\mathbf{n}_1$ is defined in Equation (16). Appropriate substitution of terms in the expression for $q(s, t; \Theta)$ results in

$$\begin{aligned} \mathbf{r}' &= q(s,t;\Theta)\mathbf{h}q^*(s,t;\Theta) \\ &= \mathbf{r} \cos 2\Theta - (\mathbf{n}_1 \times \mathbf{r}) \sin 2\Theta \cos(s+t) - \mathbf{n}_1 \sin 2\Theta \sin(s+t) \end{aligned} \tag{69}$$

Since $\mathbf{r}$ is orthogonal to $\mathbf{n}_1 \times \mathbf{r}$ and $\mathbf{n}_1$, the angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$ is 2Θ (up to the sign) for every s and t. It means that the quaternion $q(s, t; \Theta)$ maps the vector $\mathbf{h}$ onto the small circle $C(\mathbf{r}, 2\Theta)$.

In particular, for $t = -s$ Equation (69) simplifies to

$$q(s, -s; \Theta)\mathbf{h}q^*(s, -s; \Theta) = \mathbf{r} \cos 2\Theta - (\mathbf{n}_1 \times \mathbf{r}) \sin 2\Theta = \mathbf{r}'_0 \tag{70}$$

where the right-hand side can be seen to be equal to $\mathbf{r}'_0$ by simple trigonometry, as $\mathbf{r}'_0$ can be decomposed into the sum of its corresponding orthogonal projections. Hence, we can assume $s_0 = 0$. Since the small circle may be thought of as the result of rotating $\mathbf{r}'_0$ about $\mathbf{r}$ by the angle $t \in [0, 2\pi)$, it can be written

$$q(0, t; \Theta)\mathbf{h}q^*(0, t; \Theta) = r(t)\mathbf{r}'_0 r^*(t) \tag{71}$$

which is easily verified using Equations (8) and (70).

Conversely, if $q \in \mathbb{S}^3$ maps $\mathbf{h}$ on $\mathbf{r}' \in C(\mathbf{r}, 2\Theta)$, then its distance from the circle $C(q_1, q_2) = \{q(s) | s \in [0, 2\pi)\}$ representing all rotations mapping $\mathbf{h}$ on $\mathbf{r}$ is $d(q, C) = \inf_{s \in [0,2\pi)}$ $\arccos(\mathrm{Sc}(qq^*(s)) = \frac{1}{2} \arccos((qhq^*) \cdot r) = \Theta$ [15], which implies that q is an element of the torus $T(q_1, q_2, q_3, q_4, \Theta)$.

This completes the proof. □

Concludingly, the torus $T(q_1, q_2, q_3, q_4; \Theta)$ consisting of all quaternions with distance Θ from $C(q_1, q_2)$ essentially consists of all circles with distance Θ from $C(q_1, q_2)$ representing all rotations $\bigcup_{\mathbf{r}' \in C(\mathbf{r},2\Theta)} G(\mathbf{h}, \mathbf{r}')$ mapping $\mathbf{h}$ on $C(\mathbf{r}, 2\Theta)$, which was shown to be equal to $\bigcup_{\mathbf{h}' \in C(\mathbf{h},2\Theta)} G(\mathbf{h}', \mathbf{r})$ mapping $C(\mathbf{h}, 2\Theta)$ on $\mathbf{r}$ in Proposition 7, i.e.

$$\begin{aligned} T(q_1, q_2, q_3, q_4; \Theta) &= \bigcup_{\mathbf{r}' \in C(\mathbf{r},2\Theta)} C(q_1(\mathbf{h}, \mathbf{r}'), q_2(\mathbf{h}, \mathbf{r}')) \\ &= \bigcup_{\mathbf{h}' \in C(\mathbf{h},2\Theta)} C(q_1(\mathbf{h}', \mathbf{r}), q_2(\mathbf{h}', \mathbf{r})) \end{aligned}$$

which is essential to the inversion of the spherical Radon transform [6].

Corollary 5

All unit quaternions $q(s, t; \pi/4)$ with the same distance (of $\pi/4$) to $C(q_1, q_2)$ and $C(q_3, q_4)$ map $\mathbf{h}$ on the great circle $\mathbf{r}^\perp \subset \mathbb{S}^2$.

Obviously, for the special choice of $\Theta = \pi/4$ it holds

$$q\left(s, t - s; \frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(q_1 \cos s + q_2 \sin s + q_3 \cos(t - s) + q_4 \sin(t - s))$$

$$q(0, t; \frac{\pi}{4}) = \frac{1}{\sqrt{2}}(q_1 + q_3 \cos t + q_4 \sin t)$$

and in particular

$$q(0, 0; \frac{\pi}{4}) = \frac{1}{\sqrt{2}}(q_1 + q_3) =: p_1$$

$$q\left(\frac{\pi}{2}, 0; \frac{\pi}{4}\right) = \frac{1}{\sqrt{2}}(q_2 + q_3) =: p_2$$

$$q\left(0,\frac{\pi}{2};\frac{\pi}{4}\right)=\frac{1}{\sqrt{2}}(q_1+q_4)=:p_3$$

$$q\left(\frac{\pi}{2},\frac{\pi}{2};\frac{\pi}{4}\right)=\frac{1}{\sqrt{2}}(q_2+q_4)=:p_4$$

Any three out of the four unit quaternions p_i are linearly independent, e.g. $p_2+p_3-p_1=p_4$.

Eventually, the set of all circles $C(p_1,p_2)\subset\mathbb{S}^3$ with a fixed distance Θ of a given $q\in\mathbb{S}^3$ is characterized by

$$\Theta=d(q,C(p_1,p_2))=\frac{1}{2}\arccos(q\mathbf{h}q^*\cdot\mathbf{r})$$

where $\mathbf{r}\in\mathbb{S}^2$ is uniquely defined in terms of $\mathbf{h}$ and p_1,p_2 by $\mathbf{r}:=p(t)\mathbf{h}p^*(t)$ for all $p(t)\in C(p_1,p_2)$ and any arbitrary $\mathbf{h}\in\mathbb{S}^2$, i.e. each circle represents all rotations mapping some $\mathbf{h}\in\mathbb{S}^2$ onto an element of the small circle $C(q\mathbf{h}q^*,2\Theta)$. Thus, for each $q\in\mathbb{S}^3$ and $\Theta\in[0,\pi)$

$$\{C(p_1,p_2)|d(q,C(p_1,p_2))=\Theta\}=\bigcup_{\mathbf{h}\in\mathbb{S}^2}\ \bigcup_{\mathbf{r}\in C(q\mathbf{h}q^*,2\Theta)}C(p_1(\mathbf{h},\mathbf{r}),p_2(\mathbf{h},\mathbf{r}))$$

4. APPLICATIONS

Let $f:\mathbb{S}^3\mapsto[0,\infty)$ be an even probability density function of random unit quaternions representing random rotations. For any given direction $\mathbf{h}\in\mathbb{S}^2$ the probability density function of the random direction $q\mathbf{h}q^*\in\mathbb{S}^2$ is provided by the spherical Radon transform $(\mathscr{R}f):\mathbb{S}^2\times\mathbb{S}^2\mapsto[0,\infty)$ defined as

$$(\mathscr{R}f)(\mathbf{h},\mathbf{r})=\frac{1}{2\pi}\int_{C(q_1,q_2)}f(q)\,\mathrm{d}q=\frac{1}{2\pi}\int_0^{2\pi}f(q(t))\,\mathrm{d}t$$

Then Propositions 7 and 13 amount to

$$\int_{C(\mathbf{h},2\Theta)}(\mathscr{R}f)(\mathbf{h}',\mathbf{r})\,\mathrm{d}\mathbf{h}'=\int_{C(\mathbf{r},2\Theta)}(\mathscr{R}f)(\mathbf{h},\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$$=\int_{C(\mathbf{r},2\Theta)}\int_{C(q_1(\mathbf{h},\mathbf{r}'),q_2(\mathbf{h},\mathbf{r}'))}f(q)\,\mathrm{d}q\,\mathrm{d}\mathbf{r}' \tag{72}$$

$$=\int_{T(q_1,q_2,q_3,q_4;\Theta)}f(q)\,\mathrm{d}q$$

$$=\int_{d(q,C(q_1(\mathbf{h},\mathbf{r}),q_2(\mathbf{h},\mathbf{r})))=\Theta}f(q)\,\mathrm{d}q \tag{73}$$

where Equation (72) is an Ásgeirsson-type mean value theorem, and where Equation (73) is instrumental to the inversion of the spherical Radon transform as given by Helgason [6,16] and its relationship with the inversion formula as derived in texture analysis [17–19]. Details will be elaborated on in a forthcoming paper [20].

5. CONCLUSIONS

We have considered relations between geometrical objects—circles, spheres and tori—of unit quaternions representing rotations and geometrical objects—points, pairs of points, small and great circles—of unit vectors in three-dimensional space which have been subjected to these rotations. The geometrical approach to the description of some particular sets of quaternions is very useful with respect to Radon transforms of real-valued functions defined for rotations.

In a companion paper [3] the quaternion geometry will be applied to characterize the different cases of the Bingham distribution for $\mathbb{S}^3$, in particular it will be shown that all cases of ideal orientation patterns (cf. [21]) except for cone and ring fibre textures can be represented as special cases of the Bingham distribution.

In spite of the crystallographic background of our results, their featured geometrical approach may prove useful in other fields when one has to deal with rotations of spherical objects in three-dimensional space.

ACKNOWLEDGEMENTS

The author H.S. would like to thank Gerald van den Boogaart, now with the Mathematics Department of Greifswald University, Germany, for many helpful and clarifying discussions on the subject of quaternions.

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