# Theoretical Problems in Global Seismology and Geodynamics

Thesis submitted for the Degree of Doctor of Philosophy by
David Al-Attar



Department of Earth Sciences and Worcester College University of Oxford

Hilary Term, 2011

Supervised by
Professor John H. Woodhouse
and
Dr Colin J. Thomson

The tolling bell
Measures time not our time, rung by the unhurried
Ground swell, a time
Older than the time of chronometers, older
Than time counted by anxious worried women
Lying awake, calculating the future,
Trying to unweave, unwind, unravel
And piece together the past and the future,
Between midnight and dawn, when the past is all deception,
The future futureless, before the morning watch
When time stops and time is never ending;
And the ground swell, that is and was from the beginning,
Clangs
The bell.

T.S. Eliot, The Dry Salvages.

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#### Abstract

In Chapter 2, we consider the hydrostatic equilibrium figure of a rotating earth model with arbitrary radial density profile. We derive an exact non-linear partial differential equation describing the equilibrium figure. Perturbation theory is used to obtain approximate forms of this equation, and we show that the first-order theory is equivalent to Clairaut's equation.

In Chapter 3, a method for parametrizing the possible equilibrium stress fields of a laterally heterogeneous earth model is described. In this method a solution of the equilibrium equations is first found that satisfies some desirable physical property. All other solutions can be written as the sum of this equilibrium stress field and a divergence-free stress tensor field whose boundary tractions vanish.

In Chapter 4, we consider the minor vector method for the stable numerical solution of systems of linear ordinary differential equations. Results are presented for the application of the method to the calculation of seismic displacement fields in spherically symmetric, self-gravitating earth models.

In Chapter 5, we present a new implementation of the direct solution method for calculating normal mode spectra in laterally heterogeneous earth models. Numerical tests are presented to demonstrate the validity and effectiveness of this method for performing large mode coupling calculations.

In Chapter 6, we consider the theoretical basis for the viscoelastic normal mode method which is used in studies of seismic wave propagation, post-glacial rebound, and post-seismic deformation. We show how the time-domain solution to the viscoelastodynamic equation can be written as a normal mode sum in a rigorous manner.

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#### **Extended Abstract**

#### Equilibrium Structure of the Earth

In Chapter 2, we investigate the classical problem of determining the hydrostatic equilibrium figure of a rotating earth model possessing an arbitrary radial density profile. To do this, we first consider the calculation of the gravitational potential in an aspherical earth model. This is accomplished by defining a mapping which takes the given aspherical earth model into a spherical reference model. In terms of this mapping we can 'pull-back' Poisson's equation to obtain an equivalent equation for the gravitational potential defined in the reference model. We employ perturbation theory to obtain approximate forms of this new equation, carrying out the analysis to third-order in a small parameter. We next consider the relationship between the density and geometry of the earth model imposed by the hydrostatic equilibrium equations. From this relationship we derive a non-linear partial differential equation that describes a mapping from a given spherically symmetric reference model into an aspherical earth model which is in hydrostatic equilibrium subject to a given forcing-potential. We again employ perturbation theory up to third-order to obtain approximate forms of this equation, and show that the first-order theory is equivalent to Clairaut's equation.

In Chapter 3, a new method for parametrizing the possible equilibrium stress fields of a laterally heterogeneous earth model is described. In this method a solution of the equilibrium equations is first found that satisfies some desirable physical property. For example, we show that the equilibrium stress field with smallest norm relative to a given inner product can be obtained by solving a static linear elastic boundary value problem. We also show that the equilibrium stress field whose deviatoric component has smallest norm with

respect to a given inner product can be obtained by solving a steady-state incompressible viscous flow problem. Having found such a solution of the equilibrium equations, all other solutions can be written as the sum of this equilibrium stress field and a divergence-free stress tensor field whose boundary tractions vanish. Given n divergence-free and traction-free tensor fields, we then obtain a simple n-dimensional parametrization of equilibrium stress fields in the earth model. The practical construction of such divergence-free and traction-free tensor fields in the mantle of a spherically symmetric reference earth model is described using generalized spherical harmonics.

#### Seismic Wavefield Calculations

In Chapter 4, an account is given of the minor vector method that allows for the stable numerical integration of the systems of linear ordinary differential equations occurring in a number of geophysical problems. In particular, new results are presented that allow for the application of the method to the solution of six-dimensional inhomogeneous boundary value problems such as those encountered in the calculation of seismic displacement fields in spherically symmetric, self-gravitating earth models. In addition, the symplectic structure possessed by many of the ordinary differential equations of interest is described. It is shown how this structure can be used to simplify the numerical implementation of the minor vector method, and also to concisely derive a number of theoretical results about the eigenfrequencies and eigenfunctions of a linearly viscoelastic earth model.

In Chapter 5, we consider the calculation of synthetic normal mode spectra in laterally heterogeneous earth models using the direct solution method. In this method the so-called mode coupling equations are solved at a discrete range of frequencies, and the time-domain solution is obtained using a numerical inverse Fourier transform. Early implementations of this method made use of LU-decomposition to solve the mode coupling equations. However, as the number of coupled modes is increased this method of solution becomes very inefficient. To circumvent this problem we describe a new iterative implementation of the direct solution method which is able to solve the mode coupling equations in a significantly more efficient manner. We then use this method to investigate the effects of truncating the mode coupling equations on synthetic spectra.

In Chapter 6, we consider the theoretical basis for the viscoelastic normal mode method which is used in studies of seismic wave propagation, post-glacial rebound, and post-seismic deformation. Previous discussions of this topic have focused on either very simple earth models (e.g. those comprising a number of homogeneous layers), or have had to rely on a number of unproven assumptions (e.g. that only first-order poles of the Laplace transform domain solution occur). We present a rigorous formulation of viscoelastic normal mode theory which is applicable to a generally heterogeneous earth model, and which does not depend on any unproven assumptions. In particular, we show how to incorporate higher-order poles of the Laplace transform domain solution into the time-domain normal mode sum.

#### Acknowledgements

First and foremost, I would like to thank John Woodhouse. I have felt extremely fortunate to have been able to work with John over the past few years, and have greatly benefited from his knowledge and experience. I would also like to thank my co-supervisor Colin Thompson for the interest shown in my work during a number of visits to the Schlumbeger Research Center in Cambridge. Special thanks must be given to Shamita Das for the advice and encouragement she has provided since my time as an undergraduate student.

I gratefully acknowledge financial support for the project which came through a Natural Environment Research Council (NERC) grant tied to a Cooperative Award in the Science of the Environment (CASE) studentship with Schlumbeger. Additional funding was provided through the award of a Martin Senior Scholarship from Worcester College, while a Junior Research Fellowship at Merton College has provided support during the last few months of the project, and will enable me to continue my work in Oxford.

Conversations with Arwen Deuss, Ana Ferreira, Jeannot Trampert, Sir John Ball, and Andy Wathen, were very useful in developing various sections of the thesis. In particular, Arwen kindly allowed me to make use of a number of her mode coupling programs. I would also like to acknowledge the thoughtful and constructive reviews for my papers by Tony Dahlen, Awren Deuss, Jeroen Tromp, Bernard Vallete, and a number of anonymous reviewers.

My time as a student in Oxford has been enriched by a number of people. Firstly, I would like to thank the other members of the seismology group: Ben Fox, David Robinson, Eoin McMannus, Andrew Valentine, Tom O'Toole, and Cedric Twardzik. Special thanks must go to Andrew for being a sounding board for my ideas during the early stages of the project, and to Tom for kindly proof-reading this thesis. I would also like to express special thanks to Jonathan Edge, Ros Armytage, Alex Liu, and Teresa Kyrke-Smith for their kindness and friendship.

Finally, I would like to thank my parents and my brother, to whom I owe more than I can say.

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## Chapter 1

# Introduction

For the basic problem of philosophy seems to be to discover the forces of nature from the phenomena of motions and then to demonstrate other phenomena from these forces.

Isaac Newton, Philosophiae Naturalis Principia Mathematica.

But the total field is so underdetermined by its boundary conditions, experience, that there is much latitude of choice as to what statements to reevaluate in the light of any single contrary experience. No particular experiences are linked with any particular statements in the interior of the field, except indirectly through consideration of equilibrium affecting the field as a whole.

W.V. Quine, Two Dogmas of Empiricism.

#### 1.1 Background and Motivation

One of the central problems in the Earth Sciences is understanding the evolution and dynamics of the Earth. In addressing this problem we are immediately faced with the fact that while the dynamics of the Earth clearly involves processes occurring within its interior, there is no direct way of observing them. Instead, we have access only to observations of near-surface processes, and from these observations must make inferences about what is happening at depth. Amongst the various methods available for studying the Earth's interior, seismology is perhaps the most important, though much useful information also comes from other geophysical, geochemical, and petrological sources.

The spherically symmetric average structure of the Earth has long been known (Dziewonski & Anderson 1981), and more recent studies have focused on identifying lateral variations with respect to this structure using the methods of seismic tomography (see Romanowicz 2003 for a review). Though such studies show that the magnitude of lateral variations within the Earth are relatively small (e.g. typically a few percent), these variations are of great geodynamic significance. For example, the motion of tectonic plates is thought to represent the surface manifestation of convection within the Earth's mantle. Such convection is driven by buoyancy forces associated with lateral density variations, which, in turn, are due to lateral variations in either temperature or chemical composition (or some combination of the two factors). These thermal or compositional variations also induce lateral variations in seismic wave speeds, and it is (principally) these wave speed variations that tomographic studies seek to determine. It follows that tomographic images can potentially provide information about thermal and compositional properties of the mantle, and also about the driving forces and kinematics of mantle convection. For example, tomographic studies have played a key role in elucidating the mode of mantle convection (i.e. layered versus whole mantle convection) and the fate of subducted slabs (e.g. Woodhouse & Dziewonski 1989; van der Hilst 1997; Ritsema et al. 1999).

As noted above, the majority of tomographic studies focus on imaging lateral variations in seismic wave speed within the Earth. This is because while seismic observations are strongly sensitive to such wave speed perturbations, they are considerably less sensitive to variations in other model parameters such as density. As a result, the interpretation of tomographic velocity models in terms of geodynamically interesting parameters like density and temperature can be problematic. For example, a given low velocity anomaly could arise from either a positive temperature anomaly or from variations in chemical composition. While the first of these alternatives would correspond to a negative density anomaly, the latter situation could potentially be associated with either a positive or negative density anomaly. Consequently, the simple interpretation of tomographic velocity models in terms of temperature (and hence density and buoyancy) is not always possible. A practical example of this situation is given by the so-called Large Low-Shear-Velocity Provinces found in the lowermost mantle (e.g. Lay 2007). At present it is unclear whether the origin of these anomalies is due to elevated temperatures, and hence associated with the

presence of buoyant material at the base of the mantle, or if they result from compositional variations and are, in fact, dense stable features.

There are, however, some seismic observations that display non-negligible sensitivity to lateral density variations within the Earth, and so can help resolve some of the difficulties mentioned above. In particular, normal mode spectra can be used to provide constraints on lateral density variations. Such long-period waves, however, have correspondingly long wavelengths, and so can provide constraints on only very large-scale density variations within the Earth. Ishii & Tromp (1999, 2001) produced one of the first models of lateral density variations within the Earth using a combination of normal mode observations and measurements of the Earth's gravity field. An important conclusion of this pioneering study was that simple scaling relations between velocity and density perturbations (e.g. Karato 1993) do not seem to hold, this observation being consistent with both thermal and compositional changes playing major roles in generating the observed anomalies.

Though normal mode spectra do provide useful constraints on lateral density variations in the Earth, the sensitivity of such observations to density structure is still significantly less than their sensitivity to variations in seismic wave speed. As a result, the effects of lateral density variations on observed spectra is likely to be rather subtle, and the recovery of such variations is challenging. In particular, Duess & Woodhouse (2001) suggest the ability to extract reliable information on lateral density variations will require the use of very accurate methods for calculating synthetic normal mode spectra. Through a variety of example calculations, these authors have shown that the errors associated with a number of widely-used approximations in mode coupling calculations (such as the self- or group-coupling approximations) can be of the same order of magnitude as the expected effects of lateral heterogeneity within the Earth. Consequently the use of such approximations—as was done, for example, by Ishii & Tromp (1999, 2001)—casts at least some doubt as to the robustness of the density models obtained.

#### 1.2 Thesis Outline

This thesis describes a number of theoretical and computational problems relating, in broad terms, to normal mode seismology and the study of the Earth's internal structure. The first part of the thesis discusses two problems relating to the equilibrium structure of the Earth, while the second part is concerned primarily with the theory of seismic wave propagation. In terms of geophysical inverse theory (e.g. Backus 1967, 1968; Parker 1994; Tarantola 2005), the first part of the thesis is related to the description and parametrization of the earth model, while the second part focuses on the forward problem of calculating synthetic seismic data in a given earth model. Future work will apply these methods to the study of the Earth's internal structure, and, in particular, to the construction of robust models of lateral density variations.

# Part I

Equilibrium Structure of the Earth

## Chapter 2

# Hydrostatic Equilibrium of the Earth

#### 2.1 Introduction

In this chapter, we consider the problem of determining the equilibrium figure of a rotating, self-gravitating earth model. In the case that the earth model's density is assumed to be constant, this problem has received the attention of such distinguished mathematicians as Newton, Riemann, and Poincaré (Todhunter 1873; Chandrasekhar 1966, 1969). The geophysical application of this theory is, however, limited by the presence of density variations within the Earth. Of greater practical importance is the work of Clairaut (1743), who developed a theory of hydrostatic equilibrium for a planet having an arbitrary radial density profile. Clairaut's original theory is accurate to first-order in a dimensionless parameter representing the flattening of spherical surfaces in the reference model. Though this first-order theory is sufficiently accurate for most geophysical applications, the interpretation of some more recent geodetic and geophysical measurements require the use of a more accurate theory (e.g. Ricard et. al. 1984, Mitrovica et. al. 2005, Chambat et. al. 2010). Such extensions of Clairaut's theory accurate to second- and third-order have been derived by Kopal (1960), Lanzano (1962), Valette (1987), and Chambat et. al. (2010).

The main new result presented in this chapter is the derivation of an exact theory of hydrostatic equilibrium. Within this theory, the equilibrium figure of the rotating earth model is found by solving a non-linear partial differential equation. The direct solution of this equation is likely to require sophisticated numerical methods, and has not been considered in detail. Instead we show how approximate solutions to the equation can be constructed using perturbation theory, carrying out the necessary analysis up to thirdorder.

#### 2.2 Geometry of the Earth Model

Let the earth model occupy an open, bounded, and connected subset  $M \subseteq \mathbb{R}^3$  with smooth boundary  $\partial M$ . For simplicity we shall assume that the earth model possesses no additional internal boundaries; the necessary modifications to accommodate this complexity are, however, trivial. The closure  $M \cup \partial M$  of M will be denoted by  $\overline{M}$ . We write  $T_xM$  for the tangent space to M at a point x, and  $T_x^*M$  for the associated cotangent space. The corresponding tangent and cotangent bundles are written TM and  $T^*M$ , respectively, and we write  $T_x^*M$  for the bundle of r-times contravariant and s-times covariant tensors. The space of smooth real-valued functions on M is denoted by  $\mathcal{F}(M)$ , while the spaces of smooth sections of TM,  $T^*M$ , and  $T_x^*M$ , are denoted, respectively, by  $\mathcal{T}(M)$ ,  $\mathcal{T}^*(M)$ , and  $\mathcal{T}_s^*(M)$ . Finally, the space of smooth k-forms on M is denoted by  $\Omega^k(M)$ .

Let  $g \in \mathcal{T}_2^0(\mathbb{R}^3)$  denote the Euclidean metric tensor on  $\mathbb{R}^3$ , given in an orthonormal cartesian co-ordinate system  $x^i$  by

$$q = \delta_{ij} \, \mathrm{d}x^i \otimes \mathrm{d}x^j. \tag{2.1}$$

By restricting g to M, we make M a Riemannian manifold with boundary. We recall (e.g. Lee 1997, Chapter 3) that the volume-form  $\mu_M \in \Omega^3(M)$  associated with g is defined by the requirement that if the ordered-triple of tangent vectors  $\{v_1, v_2, v_3\}$  forms a positively-orientated orthonormal basis for  $T_xM$  at a point  $x \in M$ , then we have

$$\mu_M(v_1, v_2, v_3) = 1. (2.2)$$

Let  $\iota_M : \partial M \to M$  denote the inclusion mapping from  $\partial M$  into M. By assumption  $\iota_M$  is a smooth embedding (i.e. a diffeomorphism onto its image), and so has an injective tangent mapping  $(T\iota_M)_x : T_x \partial M \to T_x M$  at each point  $x \in \partial M$  (here, and in what follows, we have identified  $x \in \partial M$  with its image in M under the inclusion mapping). By pulling-back

the Euclidean metric  $g \in \mathcal{T}_2^0(M)$  to  $\partial M$  using  $\iota_M$ , we obtain a non-degenerate symmetric tensor field  $\iota_M^* g \in \mathcal{T}_2^0(\partial M)$ , which is used to define a Riemannian structure on  $\partial M$  (e.g. Lee 1997, Chapter 8).

At a point  $x \in \partial M$ , the image of  $T_x \partial M$  under  $(T \iota_M)_x$  spans a two-dimensional linear subspace of  $T_x M$ . Let  $N_x M$  denote the orthogonal complement to  $(T \iota_M)_x (T_x \partial M)$  so that

$$T_x M = N_x M \oplus (T \iota_M)_x (T_x \partial M). \tag{2.3}$$

We call  $N_xM$  the normal space to a point  $x \in \partial M$ , and write NM for the disjoint union of the spaces  $N_xM$  as x ranges over  $\partial M$ , which we call the normal bundle to  $\partial M$ . Clearly  $N_xM$  is one-dimensional. At each point  $x \in \partial M$ , let  $n_x$  be the unit outward normal vector which spans  $N_xM$ , and denote by  $n: \partial M \to NM$  the tangent vector field with  $n(x) = n_x$ .

We say that an ordered-pair of tangent vectors  $\{v_1, v_2\}$  in  $T_x \partial M$  is positively-oriented if the ordered-triple  $\{n_x, (T\iota_M)_x v_1, (T\iota_M)_x v_2\}$  in  $T_x M$  is positively-oriented in M. Having defined an orientation on  $\partial M$ , we can introduce a Riemannian volume-form  $\mu_{\partial M} \in \Omega^2(\partial M)$  in terms of the metric  $\iota_M^* g$  in a manner analogous to that done on M; if the ordered-pair  $\{v_1, v_2\}$  of tangent vectors in  $T_x \partial M$  forms a positively-oriented orthonormal basis at a point  $x \in \partial M$ , then we have

$$\mu_{\partial M}(v_1, v_2) = 1. \tag{2.4}$$

For a point  $x \in \partial M$ , suppose we are given a tangent vector  $w \in T_x M$ . If we form the interior product  $i_w \mu_M$ , we then have a two-form at x which we can pull-back to  $\partial M$  under the inclusion mapping  $\iota_M$  to give  $\iota_M^*(i_w \mu_M)$ . Let  $\{v_1, v_2\}$  form a positively-oriented orthonormal basis for  $T_x \partial M$ . By the definition of the pull-back, we have

$$\iota_M^*(i_w\mu_M)(v_1, v_2) = \mu_M(w, (T\iota_M)_x v_1, (T\iota_M)_x v_2). \tag{2.5}$$

Using eq.(2.3), we can write w uniquely in the form

$$w = w^{\parallel} + w^{\perp}, \tag{2.6}$$

where  $w^{\parallel} \in T_x \partial M$  and  $w^{\perp} \in N_x M$ . Moreover, we clearly have

$$w^{\perp} = (w, n_x)_{TM} \, n_x, \tag{2.7}$$

where we have written  $(\cdot, \cdot)_{TM}$  for the inner-product on TM induced by g. Inserting this decomposition into eq.(2.5), and using the anti-linearity of  $\mu_M$  we find

$$\iota_M^*(i_w\mu_M)(v_1, v_2) = (w, n_x)_{TM} \,\mu_M(n_x, (T\iota_M)_x v_1, (T\iota_M)_x v_2) = (w, n_x)_{TM} \,, \tag{2.8}$$

where in obtaining the last equality we have used the fact that  $\{n_x, (T\iota_M)_x v_1, (T\iota_M)_x v_2\}$ 

forms a positively-oriented orthonormal basis for  $T_xM$ . It follows that we have the useful identity

$$\iota_M^*(i_w\mu_M) = (w, n_x)_{TM} \mu_{\partial M}, \tag{2.9}$$

relating the volume-forms on M and  $\partial M$  (e.g Marsden & Hughes 1983, Proposition 7.16).

We now derive a number of identities which will be required in later sections. Firstly, for two smooth tangent vector fields  $v, w \in \mathcal{T}(M)$  we wish to show that

$$\iota_{M}^{*}\left(\mathcal{L}_{v}(i_{w}\mu_{M})\right) = \left\{ \left(\operatorname{div}(w)v, n\right)_{TM} + \operatorname{div}_{\partial M}\left[\left(w^{\perp}, n\right)_{TM}v^{\parallel} - \left(v^{\perp}, n\right)_{TM}w^{\parallel}\right] \right\} \mu_{\partial M}, \tag{2.10}$$

where  $\mathcal{L}_v$  denotes the autonomous Lie derivative along the flow of v, div is the divergence operator on M,  $\operatorname{div}_{\partial M}$  is the divergence operator on  $\partial M$ , and we have made use of the orthogonal decompositions

$$v|_{\partial M} = v^{\perp} + v^{\parallel}, \tag{2.11}$$

$$w|_{\partial M} = w^{\perp} + w^{\parallel}, \tag{2.12}$$

where  $v^{\perp}$  and  $w^{\perp}$  lie in NM, while  $v^{\parallel}$  and  $w^{\parallel}$  lie in  $T\partial M$ . To prove this identity we first recall (e.g. Abraham *et al.* 1988, Section 6.4) that for a tangent vector field w on an arbitrary Riemannian manifold M with volume-form  $\mu_M$ , the divergence operator is defined in terms of the autonomous Lie derivative by

$$\operatorname{div}(w)\mu_M = \mathcal{L}_w \mu_M. \tag{2.13}$$

Using Cartan's formula (e.g. Abraham et al. 1988, Theorem 6.4.8)

$$\mathcal{L}_w \alpha = d(i_w \alpha) + i_w (d\alpha), \quad \alpha \in \Omega^k(M), \tag{2.14}$$

we obtain

$$\mathcal{L}_v(i_w \mu_M) = d(i_v i_w \mu_M) + i_v d(i_w \mu_M). \tag{2.15}$$

We see that the second term on the right hand side reduces to

$$i_v d(i_w \mu_M) = \operatorname{div}(w) i_v \mu_M, \tag{2.16}$$

which we can pull-back to  $\partial M$  using eq.(2.9) to obtain

$$\iota_M^* \left( i_v d(i_w \mu_M) \right) = \left( div(w)v, n \right)_{TM} \mu_{\partial M}. \tag{2.17}$$

Turning now to the first term on the right hand side of eq.(2.15), we see from the above orthogonal decompositions of v and w that

$$i_v i_w \mu_M = i_{v\parallel} i_{w\perp} \mu_M - i_{w\parallel} i_{v\perp} \mu_M + i_{v\parallel} i_{w\parallel} \mu_M. \tag{2.18}$$

Recalling that the exterior derivative commutes with pull-backs (e.g. Abraham et al.

1988, Theorem 6.4.4), we find that

$$\iota_{M}^{*}\left(d(i_{v}i_{w}\mu_{M})\right) = d\left(\iota_{M}^{*}\left[i_{v}\|i_{w}^{\perp}\mu_{M} - i_{w}\|i_{v}^{\perp}\mu_{M} + i_{v}\|i_{w}\|\mu_{M}\right]\right) \tag{2.19}$$

For any tangent vector field w, say, lying in  $T\partial M$ , we have

$$\iota_M^* i_w = i_w \iota_M^*, \tag{2.20}$$

where we have identified  $w \in T\partial M$  with its image under the tangent mapping  $T\iota_M$  (e.g. Abraham *et al.* 1988, Proposition 6.4.10) . It follows that

$$\iota_{M}^{*} \left[ i_{v \parallel} i_{w \perp} \mu_{M} - i_{w \parallel} i_{v \perp} \mu_{M} + i_{v \parallel} i_{w \parallel} \mu_{M} \right] = i_{v \parallel} \iota_{M}^{*} \left( i_{w \perp} \mu_{M} \right) \\
- i_{w \parallel} \iota_{M}^{*} \left( i_{v \perp} \mu_{M} \right) \\
+ i_{v \parallel} \iota_{M}^{*} \left( i_{w \parallel} \mu_{M} \right), \tag{2.21}$$

which, on use of eq.(2.9), reduces to

$$\iota_{M}^{*} \left[ i_{v \parallel} i_{w \perp} \mu_{M} - i_{w \parallel} i_{v \perp} \mu_{M} + i_{v \parallel} i_{w \parallel} \mu_{M} \right] = \left( w^{\perp}, n \right)_{TM} i_{v \parallel} \mu_{\partial_{M}} - \left( v^{\perp}, n \right)_{TM} i_{w \parallel} \mu_{\partial_{M}}. \tag{2.22}$$

Using this result, we see that

$$\iota_{M}^{*}\left(d(i_{v}i_{w}\mu_{M})\right) = d\left[\left(w^{\perp}, n\right)_{TM}i_{v\parallel}\mu_{\partial_{M}} - \left(v^{\perp}, n\right)_{TM}i_{w\parallel}\mu_{\partial_{M}}\right],\tag{2.23}$$

which, applying the definition of the divergence operator to  $\partial M$ , gives

$$\iota_{M}^{*}\left(d(i_{v}i_{w}\mu_{M})\right) = \operatorname{div}_{\partial M}\left[\left(w^{\perp}, n\right)_{TM} v^{\parallel} - \left(v^{\perp}, n\right)_{TM} w^{\parallel}\right] \mu_{\partial M},\tag{2.24}$$

from which we obtain eq.(2.10). We note that in the special case that v and w are parallel, eq.(2.10) reduces to

$$\iota_M^* \left( \mathcal{L}_v(i_w \mu_M) \right) = (\operatorname{div}(w)v, n)_{TM} \mu_{\partial M}. \tag{2.25}$$

Next, we consider the reduction of the expression

$$\iota_M^* \left( \mathcal{L}_{v_1} \mathcal{L}_{v_2} (i_w \mu_M) \right), \tag{2.26}$$

where  $v_1$ ,  $v_2$  and w are smooth tangent vector fields on M. Using Cartan's formula twice, we find that

$$\mathcal{L}_{v_1} \mathcal{L}_{v_2}(i_w \mu_M) = i_{v_1} d(i_{v_2} d(i_w \mu_M)) + d(i_{v_1} d(i_{v_2} i_w \mu_M)) + d(i_{v_1} i_{v_2} d(i_w \mu_M)).$$
 (2.27)

$$= i_{v_1} \operatorname{d}(\operatorname{div}(w) i_{v_2} \mu_M) + \operatorname{d}(i_{v_1} \operatorname{d}(i_{v_2} i_w \mu_M)) + \operatorname{d}(\operatorname{div}(w) i_{v_1} i_{v_2} \mu_M). \quad (2.28)$$

We see readily that

$$i_{v_1} \operatorname{d}(\operatorname{div}(w) i_{v_2} \mu_M) = \operatorname{div}(\operatorname{div}(w) v_2) i_{v_1} \mu_M,$$
 (2.29)

which, using eq.(2.9), gives

$$\iota_{M}^{*}\left(i_{v_{1}}\operatorname{d}(\operatorname{div}(w)i_{v_{2}}\mu_{M})\right) = \left(\operatorname{div}\left(\operatorname{div}(w)v_{2}\right)v_{1}, n\right)_{TM}\mu_{\partial M}.$$
(2.30)

Similarly, using eq.(2.10), we find that

 $\iota_M^*\left(\operatorname{d}(\operatorname{div}(w)i_{v_1}i_{v_2}\mu_M)\right) = \operatorname{div}_{\partial M}\left[\left(\operatorname{div}(w)v_2^{\perp},n\right)_{TM}v_1^{\parallel} - \left(\operatorname{div}(w)v_1^{\perp},n\right)_{TM}v_2^{\parallel}\right]\mu_{\partial M},$  (2.31) which, we note, vanishes if  $v_1$  and  $v_2$  are parallel on  $\partial M$ . We have not been able to reduce  $\iota_M^*\left(\operatorname{d}(i_{v_1}i_{v_2}\operatorname{d}(i_w\mu_M))\right)$  into a simple expression involving  $\mu_{\partial M}$ . If, however,  $v_1$  and  $v_2$  are parallel this term vanishes, and this case will be sufficient for our applications. We can, therefore, write that

$$\iota_{M}^{*}\left(\mathcal{L}_{v_{1}}\mathcal{L}_{v_{2}}(i_{w}\mu_{M})\right) = \operatorname{div}_{\partial M}\left[\left(\operatorname{div}(w)v_{2}^{\perp},n\right)_{TM}v_{1}^{\parallel} - \left(\operatorname{div}(w)v_{1}^{\perp},n\right)_{TM}v_{2}^{\parallel}\right]\mu_{\partial M} + \left(\operatorname{div}\left(\operatorname{div}(w)v_{2}\right)v_{1},n\right)_{TM}\mu_{\partial M},$$

$$(2.32)$$

when  $v_1$  and  $v_2$  are parallel, and that

$$\iota_{M}^{*} \left( \mathcal{L}_{v_{1}} \mathcal{L}_{v_{2}} (i_{w} \mu_{M}) \right) = \left( \operatorname{div} \left( \operatorname{div}(w) v_{2} \right) v_{1}, n \right)_{TM} \mu_{\partial M}, \tag{2.33}$$

when w is also parallel to  $v_1$  and  $v_2$  on  $\partial M$ .

Finally, we consider the expression

$$\iota_M^* \left( \mathcal{L}_{v_1} \mathcal{L}_{v_2} \mathcal{L}_{v_3} (i_w \mu_M) \right), \tag{2.34}$$

for smooth tangent vector fields  $v_1$ ,  $v_2$ ,  $v_3$  and w, in the case that all these vector fields are parallel. Repeated application of Cartan's formula, the definition of the divergence operator on M, and use of eq.(2.9), eventually leads to the desired identity

$$\iota_{M}^{*}\left(\mathcal{L}_{v_{1}}\mathcal{L}_{v_{2}}\mathcal{L}_{v_{3}}(i_{w}\mu_{M})\right) = (\operatorname{div}(\operatorname{div}(\operatorname{div}(w)v_{3})v_{2})v_{1}, n)_{TM}\,\mu_{\partial M}. \tag{2.35}$$

#### 2.3 Poisson's Equation in Aspherical Earth Models

#### 2.3.1 Formulation of the problem

Let  $\rho^E$  denote the density in the earth model M; the reason for the inclusion of the superscript E will be clarified below. We assume that  $\rho^E$  is smooth and everywhere positive in M, and extend the definition of  $\rho^E$  to the whole of  $\mathbb{R}^3$  by requiring that  $\rho^E = 0$  exterior to  $\overline{M}$ . The gravitational potential of the earth model  $\varphi^E$  is a solution of Poisson's equation

$$\Delta \varphi^E = 4\pi G \rho^E, \quad x \in \mathbb{R}^3 \tag{2.36}$$

where  $\Delta$  denotes the Laplacian operator on M, subject to the boundary conditions

$$\left[\varphi^{E}\right]_{-}^{+} = 0, \quad x \in \partial M, \tag{2.37}$$

$$\left(\left[\operatorname{grad}\varphi^{E}\right]_{-}^{+}, n\right)_{TM} = 0, \quad x \in \partial M, \tag{2.38}$$

along with the condition that  $\varphi^E$  tends to zero at infinity. It may be shown that this boundary value problem admits a unique solution, and that the solution  $\varphi^E$  is smooth wherever  $\rho^E$  is. In fact, an explicit solution to this problem is given by

$$\varphi^{E}(x) = -G \int_{M} \frac{\rho^{E}(x')}{\|x - x'\|} \mu_{M}(x'), \qquad (2.39)$$

where  $\|\cdot\|$  denotes the standard Euclidean norm. The practical utility of this solution is, however, largely limited to spherical earth models where the expansion

$$\frac{1}{\|x - x'\|} = \begin{cases}
\frac{1}{r} \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \left(\frac{r'}{r}\right)^{l} \sum_{m=-l}^{l} \overline{Y_{lm}(\theta', \phi')} Y_{lm}(\theta, \phi), & r' < r, \\
\frac{1}{r'} \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} \left(\frac{r}{r'}\right)^{l} \sum_{m=-l}^{l} \overline{Y_{lm}(\theta', \phi')} Y_{lm}(\theta, \phi), & r < r'
\end{cases} ,$$
(2.40)

can be used to reduce eq.(2.39) into a series of radial integrals which can be evaluated numerically.

#### 2.3.2 Solutions in spherical earth models

In the case that the earth model is spherically symmetric, let us denote the volume it occupies by  $M_0$ , the associated density by  $\rho^0$ , and the gravitational potential by  $\varphi^0$ . For such an earth model, it may be shown that  $\varphi^0$  depends only on the radial co-ordinate r, and is given by

$$\varphi^{0}(r) = -4\pi G \left\{ \int_{r}^{b} \rho^{0}(s) s \, \mathrm{d}s + \frac{1}{r} \int_{0}^{r} \rho^{0}(s) s^{2} \, \mathrm{d}s \right\}, \tag{2.41}$$

where b is the radius of the model.

More generally, when the volume occupied by the earth model M is spherical, but the density  $\rho^E$  is not spherically symmetric, we can obtain the solution of Poisson's equation by expanding the gravitational potential in spherical harmonics. In detail, the (l, m)-th expansion coefficient of  $\varphi^E$  satisfies the equation

$$\partial_r^2 \varphi_{lm}^E + 2r^{-1} \partial_r \varphi_{lm}^E - l(l+1)r^{-2} \varphi_{lm}^E = 4\pi G \rho_{lm}^E, \quad r \in (0, \infty), \tag{2.42}$$

where  $\rho_{lm}^{E}$  is taken to be zero for r > b, subject to the boundary conditions

$$\left[\varphi_{lm}^{E}\right]_{-}^{+} = 0, \quad r = b,$$
 (2.43)

$$\left[\partial_r \varphi_{lm}^E\right]_-^+ = 0, \quad r = b, \tag{2.44}$$

along with the conditions that  $\varphi_{lm}^E$  be regular at r=0 and tend to zero as  $r\to\infty$ . A solution to this problem may be shown to be

$$\varphi_{lm}^{E}(r) = \frac{-4\pi G}{2l+1} \left\{ r^{l} \int_{r}^{b} \rho_{lm}^{E}(s) s^{-l+1} \, \mathrm{d}s + r^{-l-1} \int_{0}^{r} \rho_{lm}^{E}(s) s^{l+2} \, \mathrm{d}s \right\}, \tag{2.45}$$

for  $r \in (0, b]$ , while for  $r \ge b$  it is given by

$$\varphi_{lm}^E(r) = \frac{-4\pi G \, r^{-l-1}}{2l+1} \int_0^b \rho_{lm}^E(s) s^{l+2} \, \mathrm{d}s. \tag{2.46}$$

This solution can also be obtained from eq.(2.39) using the spherical harmonic expansion of the Newtonian potential in eq.(2.40).

#### 2.3.3 Solutions in aspherical earth models

Let us suppose that there exists a diffeomorphism  $\xi: M_0 \to M$  between a spherically symmetric earth model  $M_0$  and the aspherical earth model M we wish to consider. We make the simplifying assumption that this diffeomorphism is radial, so that in spherical polar co-ordinates

$$\xi(r,\theta,\phi) = (r + h^L(r,\theta,\phi),\theta,\phi), \tag{2.47}$$

where  $h^L$  is some given smooth function on  $M_0$  which vanishes at r = 0. It will be useful to assume that  $\xi$  has been extended continuously into a homeomorphism on  $\mathbb{R}^3$  in such a way that it is smooth in  $\mathbb{R}^3 \setminus \overline{M}$ , and that it tends to the identity mapping at infinity. Note that we have assumed that  $\xi$  is continuous across  $\partial M$ , but have allowed for the possibility that it is not smooth across this boundary.

Using the mapping  $\xi$ , we can pull-back the functions  $\rho^E$  and  $\varphi^E$  to  $M_0$  as

$$\rho^L \equiv \xi^* \rho^E, \tag{2.48}$$

$$\varphi^L \equiv \xi^* \varphi^E. \tag{2.49}$$

We note that the use of the superscripts L and E in these equations mimics the distinction between Lagrangian and Eulerian variables in continuum mechanics. We now wish to transform Poisson's equation for  $\varphi^E$  in M into an equivalent equation for  $\varphi^L$  on  $M_0$ . To do this, we first recall that the Laplacian operator  $\Delta : \mathcal{F}(M) \to \mathcal{F}(M)$  is defined by

$$\Delta = \operatorname{div} \circ \operatorname{grad},\tag{2.50}$$

where grad:  $\mathcal{F}(M) \to \mathcal{T}(M)$  is the gradient operator associated with the metric tensor g. Let w be some smooth tangent vector field on M. Using Cartan's formula we see that

$$\operatorname{div}(w)\mu_M = \operatorname{d}(i_w \mu_M). \tag{2.51}$$

Pulling-back this expression to  $M_0$  under  $\xi$ , we obtain for the left hand side

$$\xi^* (\operatorname{div}(w)\mu_M) = J\xi^* (\operatorname{div}(w)) \mu_{M_0},$$
(2.52)

where J is the Jacobian of  $\xi$ , and for the right hand side

$$\xi^* d(i_w \mu_M) = d(i_{J\xi^* w} \mu_0) = \text{div}(J\xi^* w) \mu_{M_0}. \tag{2.53}$$

Combining these results, we obtain

$$\xi^* (\operatorname{div}(w)) = J^{-1} \operatorname{div}(J\xi^* w),$$
 (2.54)

which is commonly known as the *Piola identity* (e.g. Marsden & Hughes 1983, Theorem 7.20). We recall that the gradient operator grad on a scalar field  $f \in \mathcal{F}(M)$  is defined such that

$$(\operatorname{grad} f, w)_{TM} = \langle df, w \rangle_{T^*M \times TM}, \qquad (2.55)$$

for any  $w \in \mathcal{T}(M)$ , where the angular bracket on the right hand side denotes the duality pairing between cotangent and tangent vectors (e.g. Abraham *et al.* 1988, Section 6.4). From this definition, we obtain

$$\operatorname{grad} f = g^{-1} \cdot \operatorname{d} f, \tag{2.56}$$

where  $g^{-1} \in \mathcal{T}_0^2(M)$  is the inverse of the metric tensor, and so find that

$$\xi^*(\operatorname{grad}\varphi^E) = a^{-1} \cdot \operatorname{grad}\varphi^L, \tag{2.57}$$

where we have introduced the tensor field

$$a = g^{-1} \cdot \xi^* g. \tag{2.58}$$

It follows that the pulled-back form of Poisson's equation can be written as

$$\operatorname{div}\left[Ja^{-1}\cdot\operatorname{grad}\varphi^{L}\right] = 4\pi G\rho^{L}J. \tag{2.59}$$

To complete the specification of this problem, we must consider the boundary conditions on  $\varphi^L$ . The continuity of  $\varphi^E$  across  $\partial M$  trivially leads to

$$\left[\varphi^L\right]_{-}^{+} = 0, \quad x \in \partial M_0. \tag{2.60}$$

Similarly, we obtain the condition that  $\varphi^L$  tends to zero at infinity. To deal with the boundary condition on the normal derivative of  $\varphi^E$ , it is useful to write eq.(2.38) as

$$\left(\left[\operatorname{grad}\varphi^{E}\right]_{-}^{+}, n\right)_{TM} \mu_{\partial M} = 0, \quad x \in \partial M.$$
(2.61)

From eq.(2.9), we can write this condition as

$$\iota_M^*(i_{\left[\operatorname{grad}\varphi^E\right]_-^+}\mu_M) = 0, \quad x \in \partial M, \tag{2.62}$$

which we can pull-back to  $\partial M_0$  using the restriction  $\xi|_{\partial M_0}$  of  $\xi$  to  $\partial M_0$ :

$$((\xi|_{\partial M_0})^* \circ \iota_M^*) (i_{[\text{grad } \varphi^E]^+} \mu_M) = (\iota_M \circ \xi|_{\partial M_0})^* (i_{[\text{grad } \varphi^E]^+} \mu_M)$$
(2.63)

$$= (\xi \circ \iota_{M_0})^* (i_{\lceil \operatorname{grad} \omega^E \rceil} + \mu_M)$$
 (2.64)

$$= (\iota_{M_0}^* \circ \xi^*)(i_{\lceil \operatorname{grad} \varphi^E \rceil} + \mu_M)$$
 (2.65)

$$= \iota_{M_0}^* (i_{[Ja^{-1} \cdot \operatorname{grad} \varphi^L]} + \mu_{M_0})$$
 (2.66)

$$= \left( \left[ Ja^{-1} \cdot \operatorname{grad} \varphi^L \right]_{-}^{+}, n_0 \right)_{TM_0} \mu_{\partial M_0}, \tag{2.67}$$

where  $n_0$  is the outward unit normal to  $\partial M_0$ , and we have made use of the obvious identity  $\iota_M \circ \xi|_{\partial M_0} = \xi \circ \iota_{M_0}$ . We can, therefore, express this boundary condition as

$$\left( \left[ Ja^{-1} \cdot \operatorname{grad} \varphi^L \right]_{-}^{+}, n_0 \right)_{TM_0} = 0, \quad x \in \partial M_0.$$
 (2.68)

This boundary value problem for  $\varphi^L$  is defined in the spherical earth model  $M_0$ . Consequently, we can use spherical harmonic expansions to reduce the problem into a coupled system of equations for the expansion coefficients  $\varphi^L_{lm}$ . Numerical solution of a truncated version of this system of equations should provide a method for calculating the gravitational potential in aspherical earth models to a high degree of accuracy.

#### 2.3.4 Perturbation series solutions

An alternative to the direct solution of the above boundary value problem is the expansion  $\varphi^L$  in a perturbation series. To do this, we introduce a one-parameter family of radial mappings  $\xi_s: M_0 \to M_s$  with  $M_s \equiv \xi_s(M_0)$  such that  $\xi_0$  is the identity mapping, and  $\xi_1 = \xi$ . One way of doing this is to let  $h^L$  be the function defined in eq.(2.47), and to then set

$$\xi_s(r,\theta,\phi) = (r + sh^L(r,\theta,\phi),\theta,\phi). \tag{2.69}$$

It will, however, be useful to consider a more general one-parameter family of radial mappings taking the form

$$\xi_s(r,\theta,\phi) = (r + h_s^L(r,\theta,\phi), \theta, \phi), \tag{2.70}$$

where  $h_s^L$  depends analytically on s about s=0, and is such that  $h_0^L=0$  and  $h_1^L=h^L$ . Similarly, we introduce a one-parameter family  $\rho_s^L$  such that  $\rho_0^L$  is equal to the density in a spherically symmetric earth model  $\rho^0$ , and  $\rho_1^L$  is equal to  $\rho^L$  as defined in eq.(2.49). For example, we could set

$$\rho_s^L = \rho^0 + s(\rho^L - \rho^0), \tag{2.71}$$

though, again, it will be useful to suppose that  $\rho_s^L$  has a more general dependence on s. In terms of  $\rho_s^L$ , it is also useful to introduce

$$\rho_s^E = (\xi_s)_* \rho_s^L, \tag{2.72}$$

where we note that  $\rho_1^E$  is simply the given density  $\rho^E$  in the aspherical earth model M.

In  $M_s$  we require that  $\varphi_s^E$  for  $s \in [0,1]$ , be a solution of Poisson's equation

$$\Delta \varphi_s^E = 4\pi G \rho_s^E, \tag{2.73}$$

along with the boundary conditions

$$\left[\varphi_s^E\right]_-^+ = 0, \quad x \in \partial M_s, \tag{2.74}$$

$$\left(\left[\operatorname{grad}\varphi_{s}^{E}\right]_{-}^{+}, n_{s}\right)_{TM_{s}} = 0, \quad x \in \partial M_{s}, \tag{2.75}$$

where  $n_s$  is the unit outward normal to  $\partial M_s$ , along with the condition that  $\varphi_s^E$  tends to zero at infinity. The results of the previous section show that this problem is equivalent to the equation

$$\operatorname{div}\left[J_{s}a_{s}^{-1}\cdot\operatorname{grad}\varphi_{s}^{L}\right]=4\pi G\rho_{s}^{L}J_{s},\tag{2.76}$$

with  $\varphi_s^L = \xi_s^* \varphi_s^E$ , subject to the boundary conditions

$$\left[\varphi_s^L\right]_-^+ = 0, \quad x \in \partial M_0, \tag{2.77}$$

$$\left( \left[ J_s a_s^{-1} \cdot \operatorname{grad} \varphi_s^L \right]_-^+, n_0 \right)_{TM_0} = 0, \quad x \in \partial M_0, \tag{2.78}$$

where  $J_s$  and  $a_s$  have been defined in terms of the mapping  $\xi_s$  in an obvious manner. In these equations the coefficients depend analytically on s about the point s = 0. From this it may be shown that  $\varphi_s^L$  also depends analytically on s about s = 0, and can, therefore, be expanded in a Taylor series about s = 0 as

$$\varphi_s^L = \sum_{n=0}^{\infty} \frac{1}{n!} s^n \varphi^{Ln}, \qquad (2.79)$$

where the expansion coefficients are give by

$$\varphi^{Ln} = \left. \frac{\partial^n \varphi_s^L}{\partial s^n} \right|_{s=0}. \tag{2.80}$$

The other s-dependent terms  $J_s$ ,  $a_s$ , and  $\rho_s^L$  can be similarly expanded in powers of s about s = 0. Inserting these expansions into the above equations and collecting powers of s, it is possible to derive a recursive system of boundary value problems satisfied by the expansion coefficients  $\varphi^{Ln}$ . This approach is, however, very involved algebraically, and we have found it more expedient to proceed using a different method.

For a fixed value of  $x \in M_0$ , we define  $\xi_x$  to be the mapping  $s \mapsto \xi_s(x)$  from a subinterval of  $\mathbb{R}$  into  $M_s$ . The Lagrangian velocity field  $v_s^L$  associated with  $\xi_s$  at a point  $x \in M_0$  is then defined by

$$v_s^L(x) = T\xi_x \left. \frac{\partial}{\partial s} \right|_s,\tag{2.81}$$

where we note that  $v_s^L(x)$  is an element of  $T_{\xi_s(x)}M_s$ . In spherical polar co-ordinates we find

that

$$v_s^L(x) = \frac{\partial h_s^L}{\partial s}(x) \left. \frac{\partial}{\partial r} \right|_{\xi_s(x)}$$
 (2.82)

We define the Eulerian velocity field associated with  $\xi_s$  to be

$$v_s^E = v_s^L \circ \xi_s^{-1}. (2.83)$$

Using the expression for  $v_s^L$  above, we see that at a point  $x \in M_s$ 

$$v_s^E(x) = \frac{\partial h_s^L}{\partial s}(\xi_s^{-1}(x)) \left. \frac{\partial}{\partial r} \right|_{x} = \frac{\partial h_s^E}{\partial s}(x) \left. \frac{\partial}{\partial r} \right|_{x}, \tag{2.84}$$

where we have defined  $h_s^E$  to be the function on  $M_s$  satisfying

$$\frac{\partial h_s^L}{\partial s} = \xi_s^* \frac{\partial h_s^E}{\partial s},\tag{2.85}$$

along with  $h_0^E = 0$ .

Recalling (e.g. Abraham *et al.* 1988, Section 5.4) that the 'time-dependent' Lie derivative  $L_{v_s^E}\varphi_s^E$  of  $\varphi_s^E$  along the flow of  $v_s^E$  is defined by

$$\xi_s^* \left( L_{v_s^E} \varphi_s^E \right) = \frac{\partial}{\partial s} (\xi_s^* \varphi_s^E), \tag{2.86}$$

we see from eq.(2.80) that

$$\varphi^{Ln} = \underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \left. \varphi_s^E \right|_{s=0}. \tag{2.87}$$

It will also be useful to define

$$\varphi^{En} = \left. \frac{\partial^n \varphi_s^E}{\partial s^n} \right|_{s=0}. \tag{2.88}$$

Using the identity (e.g. Abraham et al. 1988, Theorem 5.4.5)

$$L_{v_s^E} = \frac{\partial}{\partial s} + \mathcal{L}_{v_s^E},\tag{2.89}$$

we see that

$$\varphi^{L1} = \varphi^{E1} + \mathcal{L}_{v^{E1}}\varphi^0, \tag{2.90}$$

where we have set  $v^{E1} = v_0^E$  and have put  $\varphi^{E0} = \varphi^{L0} = \varphi^0$ . By repeated use of eq.(2.89) we obtain the useful relations

$$L_{v_s^E} L_{v_s^E} = \frac{\partial^2}{\partial s^2} + \mathcal{L}_{v_s^E} \frac{\partial}{\partial s} + \mathcal{L}_{\partial v_s^E/\partial s} + \mathcal{L}_{v_s^E} L_{v_s^E}, \qquad (2.91)$$

$$= \frac{\partial^2}{\partial s^2} + 2\mathcal{L}_{v_s^E} \frac{\partial}{\partial s} + \mathcal{L}_{\partial v_s^E/\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{v_s^E}, \qquad (2.92)$$

$$L_{v_s^E} L_{v_s^E} L_{v_s^E} = \frac{\partial^3}{\partial s^3} + 2\mathcal{L}_{v_s^E} \frac{\partial^2}{\partial s^2} + 2\mathcal{L}_{\partial v_s^E/\partial s} \frac{\partial}{\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{\partial v_s^E/\partial s} \frac{\partial}{\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{v_s^E} \mathcal{L}_{\partial v_s^E/\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{\partial v_s^E/\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{\partial v_s^E/\partial s} + \mathcal{L}_{v_s^E} \mathcal{L}_{$$

$$+\mathcal{L}_{\partial^2 v_z^E/\partial s^2} + 2\mathcal{L}_{v_z^E} \mathcal{L}_{\partial v_z^E/\partial s} + \mathcal{L}_{\partial v_z^E/\partial s} \mathcal{L}_{v_z^E} + \mathcal{L}_{v_z^E} \mathcal{L}_{v_z^E} \mathcal{L}_{v_z^E}, \tag{2.94}$$

from which we find

$$\varphi^{L2} = \varphi^{E2} + \mathcal{L}_{v^{E1}}\varphi^{E1} + \mathcal{L}_{v^{E2}}\varphi^{0} + \mathcal{L}_{v^{E1}}\varphi^{L1}, \tag{2.95}$$

$$= \varphi^{E2} + 2\mathcal{L}_{v^{E1}}\varphi^{E1} + \mathcal{L}_{v^{E2}}\varphi^0 + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}\varphi^0, \qquad (2.96)$$

$$\varphi^{L3} = \varphi^{E3} + 2\mathcal{L}_{v^{E1}}\varphi^{E2} + 2\mathcal{L}_{v^{E2}}\varphi^{E1} + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}\varphi^{E1}$$

$$+\mathcal{L}_{v^{E3}}\varphi^0 + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E2}}\varphi^0 + \mathcal{L}_{v^{E2}}\varphi^{L1} + \mathcal{L}_{v^{E1}}\varphi^{L2}, \tag{2.97}$$

$$= \varphi^{E3} + 3\mathcal{L}_{v^{E1}}\varphi^{E2} + 3\mathcal{L}_{v^{E2}}\varphi^{E1} + 3\mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}\varphi^{E1}$$

$$+\mathcal{L}_{vE3}\varphi^0 + 2\mathcal{L}_{vE1}\mathcal{L}_{vE2}\varphi^0 + \mathcal{L}_{vE2}\mathcal{L}_{vE1}\varphi^0 + \mathcal{L}_{vE1}\mathcal{L}_{vE1}\mathcal{L}_{vE1}\varphi^0, \tag{2.98}$$

where we have defined

$$v^{En} = \left. \frac{\partial^{n-1} v_s^E}{\partial s^{n-1}} \right|_{s=0}. \tag{2.99}$$

It follows from eq.(2.84) that

$$v^{En} = h^{En} \frac{\partial}{\partial r},\tag{2.100}$$

where

$$h^{En} = \left. \frac{\partial^n h_s^E}{\partial s^n} \right|_{s=0}. \tag{2.101}$$

Using eq.(2.85), we see that the functions  $h^{En}$  are related to the expansion coefficients

$$h^{Ln} = \frac{\partial h_s^L}{\partial s} \bigg|_{s=0}, \quad n \ge 1 \tag{2.102}$$

of  $h_s^L$  by

$$h^{Ln} = \underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{(n-1)-\text{terms}} \frac{\partial h_s^E}{\partial s} \bigg|_{s=0}, \quad n \ge 1.$$
 (2.103)

Up to third-order, this gives

$$h^{L1} = h^{E1}, (2.104)$$

$$h^{L2} = h^{E2} + \mathcal{L}_{vE1} h^{E1}, \tag{2.105}$$

$$h^{L3} = h^{E3} + 2\mathcal{L}_{v^{E1}}h^{E2} + \mathcal{L}_{v^{E2}}h^{E1} + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}h^{E1}. \tag{2.106}$$

As we have assumed that  $\xi$  (and therefore  $h^L$ ) is continuous across  $\partial M_0$ , we see that each of the coefficients  $h^{Ln}$  must be continuous. It follows that

$$[h^{E1}]_{-}^{+} = 0, \quad x \in \partial M_0,$$
 (2.107)

$$[h^{E2} + \mathcal{L}_{v^{E1}} h^{E1}]_{-}^{+} = 0, \quad x \in \partial M_0,$$
 (2.108)

$$\left[h^{E3} + 2\mathcal{L}_{v^{E1}}h^{E2} + \mathcal{L}_{v^{E2}}h^{E1} + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}h^{E1}\right]_{-}^{+} = 0, \quad x \in \partial M_0.$$
 (2.109)

It is noteworthy that neither  $h^{E2}$  nor  $h^{E3}$  is continuous across  $\partial M_0$  unless we also require

the continuity of the radial derivatives of  $h_s^E$  across  $\partial M_0$  up to first- and second-order, respectively.

Pulling-back Poisson's equation for  $\varphi_s^E$  to  $M_0$ , we obtain

$$\xi_s^* \left( \Delta \varphi_s^E - 4\pi G \rho_s^E \right) = 0. \tag{2.110}$$

Differentiating this equation n-times with respect to s and evaluating the resulting expression at s = 0, leads to

$$\underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \left( \Delta \varphi_s^E - 4\pi G \rho_s^E \right) \Big|_{s=0} = 0, \tag{2.111}$$

for all n. When n=0, this equation reduces to Poisson's equation in a spherically symmetric earth model whose solution is  $\varphi^0$ . Up to third-order, we find after some simple reduction that

$$\Delta \varphi^{En} = 4\pi G \rho^{En}, \tag{2.112}$$

and, in fact, it may be shown that this result holds for all  $n \ge 1$ .

Turning now to the boundary conditions, we can write the continuity of  $\varphi_s^E$  on  $\partial M_s$  as

$$\left[\xi_s^* \varphi_s^E\right]_-^+ = 0, \quad x \in \partial M_0, \tag{2.113}$$

while we have seen that the continuity of the normal derivative of  $\varphi_s^E$  can be expressed in the form

$$(\iota_{M_0}^* \circ \xi_s^*)(i_{[\operatorname{grad} \varphi_s^E]^+} \mu_{M_s}) = 0, \quad x \in \partial M_0.$$
 (2.114)

Differentiating these two conditions n-times with respect to s and evaluating the resulting expressions at s = 0, we obtain

$$[\underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \varphi_s^E \big|_{s=0}]_-^+ = 0, \quad x \in \partial M_0,$$
(2.115)

$$\iota_{M_0}^* \left( \underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \left( i_{\left[ \text{grad } \varphi_s^E \right]_-^+} \mu_{M_s} \right) \Big|_{s=0} \right) = 0, \quad x \in \partial M_0. \tag{2.116}$$
As we noted above,  $\underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{s} \left. \varphi_s^E \right|_{s=0}$  can be expressed in terms of  $\varphi^{En}$  along with various

terms of lower order in the perturbation series. It follows that the first of these boundary conditions takes the general form

$$\left[\varphi^{En}\right]_{-}^{+} = \text{lower-order terms.}$$
 (2.117)

Similarly, the second of the above conditions reduces to the general form

$$\left(\left[\operatorname{grad}\varphi^{En}\right]_{-}^{+}, n_{0}\right)_{TM_{0}} = \text{lower-order terms.}$$
 (2.118)

If follows that we can successively solve Poisson's equation for the 'Eulerian' expansion coefficients  $\varphi^{En}$ , computing the inhomogeneous boundary conditions for each of the problems from the results of previous calculations. It is noteworthy that the values of  $h^{En}$  and its radial derivatives are only required on  $\partial M_0$ , so that it is possible to make use of these formulae without having to explicitly construct the radial mapping  $\xi_s$  on the whole of  $M_0$ . This would not be the case if we had instead regarded the 'Lagrangian' expansion coefficients  $\varphi^{Ln}$  as the primary unknowns.

We now consider in detail the reduction of the above boundary conditions into a practically useful form, carrying out the analysis up to third-order.

### First-order boundary conditions

The first-order boundary conditions require that

$$[L_{v_s^E} \varphi_s^E|_{s=0}]_-^+ = 0, \quad x \in \partial M_0,$$
 (2.119)

$$\iota_{M_0}^* \left( L_{v_s^E} \left( i_{\left[ \operatorname{grad} \varphi_s^E \right]_-^+} \mu_{M_s} \right) \Big|_{s=0} \right) = 0, \quad x \in \partial M_0.$$
 (2.120)

From the first of these equations, we see that

$$\left[\varphi^{E1} + \mathcal{L}_{v^{E1}}\varphi^{0}\right]_{-}^{+} = 0, \tag{2.121}$$

on  $\partial M_0$ . Noting that

$$\mathcal{L}_{v^{E1}}\varphi^0 = h^{E1}\partial_r\varphi^0,\tag{2.122}$$

and using the continuity of  $h^{E1}$  and of  $\partial_r \varphi^0$ , we obtain

$$\left[\varphi^{E1}\right]_{-}^{+} = 0, \quad x \in \partial M_0.$$
 (2.123)

For the second of the boundary conditions, we have

$$L_{v_s^E} \left( i_{\left[ \operatorname{grad} \varphi_s^E \right]_-^+} \mu_{M_s} \right) \bigg|_{s=0} = i_{\left[ \operatorname{grad} \varphi^{E1} \right]_-^+} \mu_{M_0} + \mathcal{L}_{v^{E1}} \left( i_{\left[ \operatorname{grad} \varphi^0 \right]_-^+} \mu_{M_0} \right). \tag{2.124}$$

Using eq.(2.10) we see that

$$\mathcal{L}_{v^{E1}}(i_{\left[\operatorname{grad}\varphi^{0}\right]^{+}}\mu_{M_{0}}) = \left[\Delta\varphi^{0}\right]_{-}^{+}i_{v^{E1}}\mu_{M_{0}} = 4\pi G\left[\rho^{0}\right]_{-}^{+}i_{v^{E1}}\mu_{M_{0}}, \tag{2.125}$$

where we have made use of the fact that grad  $\varphi^0$  is parallel to  $v^{E1}$ . It follows that

$$\left( \left[ \operatorname{grad} \varphi^{E1} + 4\pi G \rho^0 v^{E1} \right]_{-}^{+}, n_0 \right)_{TM_0} = 0, \quad x \in M_0.$$
 (2.126)

### Second-order boundary conditions

For the second-order boundary conditions, we have

$$[L_{v_s^E} L_{v_s^E} \varphi_s^E \Big|_{s=0}]_-^+ = 0, \quad x \in \partial M_0,$$
 (2.127)

$$\iota_{M_0}^* \left( L_{v_s^E} L_{v_s^E} \left( i_{\left[ \text{grad } \varphi_s^E \right]_-^+} \mu_{M_s} \right) \right|_{s=0} \right) = 0, \quad x \in \partial M_0.$$
 (2.128)

The first of these conditions requires that

$$\left[\varphi^{E2} + 2h^{E1}\partial_r\varphi^{E1} + h^{E2}\partial_r\varphi^0 + h^{E1}\partial_r\left(h^{E1}\partial_r\varphi^0\right)\right]_{-}^{+} = 0, \quad x \in \partial M_0. \tag{2.129}$$

Using the continuity of  $\partial_r \varphi^0$  along with eq.(2.108), we obtain

$$\left[\varphi^{E2} - h^{E1}\partial_r h^{E1}\partial_r \varphi^0 + 2h^{E1}\partial_r \varphi^{E1} + h^{E1}\partial_r \left(h^{E1}\partial_r \varphi^0\right)\right]_-^+ = 0, \quad x \in \partial M_0. \tag{2.130}$$

From the identity

$$-h^{E1}\partial_r h^{E1}\partial_r \varphi^0 + h^{E1}\partial_r (h^{E1}\partial_r \varphi^0) = (h^{E1})^2 \partial_r^2 \varphi^0 = 4\pi G \rho^0 (h^{E1})^2 - 2r^{-1} (h^{E1})^2 \partial_r \varphi^0, \quad (2.131)$$

where we have used Poisson's equation for  $\varphi^0$ , we see that this boundary condition reduces to

$$\left[\varphi^{E2} + 2h^{E1}\partial_{r}\varphi^{E1} + 4\pi G\rho^{0}(h^{E1})^{2}\right]^{+} = 0, \quad x \in \partial M_{0}. \tag{2.132}$$

Using eq.(2.126) we see that

$$\left[\partial_r \varphi^{E1} + 4\pi G \rho^0 h^{E1}\right]_-^+ = 0, \tag{2.133}$$

on  $\partial M_0$ , which can be used to simplify eq.(2.132) to obtain

$$\left[\varphi^{E2} + h^{E1}\partial_r \varphi^{E1}\right]^+ = 0, \quad x \in \partial M_0,$$
 (2.134)

or, equivalently,

$$\left[\varphi^{E2} - 4\pi G \rho^0 (h^{E1})^2\right]_{-}^{+} = 0, \quad x \in \partial M_0.$$
 (2.135)

For the second of the boundary conditions, we have

$$\left. L_{v_s^E} L_{v_s^E} \left( i_{\left[ \operatorname{grad} \varphi_s^E \right]_{-}^{+}} \mu_{M_s} \right) \right|_{s=0} = i_{\left[ \operatorname{grad} \varphi^{E2} \right]_{-}^{+}} \mu_{M_0} + 2 \mathcal{L}_{v^{E1}} \left( i_{\left[ \operatorname{grad} \varphi^{E1} \right]_{-}^{+}} \mu_{M_0} \right) + \mathcal{L}_{v^{E2}} \left( i_{\left[ \operatorname{grad} \varphi^0 \right]_{-}^{+}} \mu_{M_0} \right) + \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E1}} \left( i_{\left[ \operatorname{grad} \varphi^{E1} \right]_{-}^{+}} \mu_{M_0} \right).$$

$$\left. + \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E1}} \left( i_{\left[ \operatorname{grad} \varphi^{E1} \right]_{-}^{+}} \mu_{M_0} \right).$$

$$(2.136)$$

Making use of eq.(2.10) we find that

$$\mathcal{L}_{v^{E2}}(i_{\left[\text{grad }\varphi^{0}\right]^{+}}\mu_{M_{0}}) = \left[\Delta\varphi^{0}\right]_{-}^{+}i_{v^{E2}}\mu_{M_{0}} = 4\pi G\left[\rho^{0}\right]_{-}^{+}i_{v^{E2}}\mu_{M_{0}}, \tag{2.137}$$

and from eq.(2.32) that

$$\mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}(i_{[\text{grad }\varphi^{E1}]^{+}}\mu_{M_{0}}) = 4\pi G \left[\operatorname{div}(\rho^{0}v^{E1})\right]_{-}^{+} i_{v^{E1}}\mu_{M_{0}}, \tag{2.138}$$

while from eq.(2.10) we see that

$$\mathcal{L}_{v^{E1}}(i_{\left[\text{grad }\varphi^{E1}\right]_{-}^{+}}\mu_{M_{0}}) = 4\pi G \left[\rho^{E1}\right]_{-}^{+} i_{v^{E1}}\mu_{M_{0}}$$
(2.139)

where we have used the fact that  $[\operatorname{grad} \varphi^{E1}]_{-}^{+}$  and  $v^{E1}$  are parallel (this follows easily from

the continuity of  $\varphi^{E1}$ ). Combining all these results, we finally obtain

$$\left( \left[ \operatorname{grad} \varphi^{E2} + 4\pi G \rho^0 v^{E2} + 8\pi G \rho^{E1} v^{E1} + 4\pi G \operatorname{div}(\rho^0 v^{E1}) v^{E1} \right]_{-}^{+}, n_0 \right)_{TM_0} = 0, \qquad (2.140)$$

on  $\partial M_0$ . Using the identity

$$\operatorname{div}(\rho^{0} v^{E1}) = \mathcal{L}_{v^{E1}} \rho^{0} + \rho^{0} \operatorname{div}(v^{E1}), \tag{2.141}$$

along with  $\rho^{L1} = \rho^{E1} + \mathcal{L}_{v^{E1}}\rho^0$ , we see that this boundary condition can equivalently be written

$$\left(\left[\operatorname{grad}\varphi^{E2}+4\pi G\left\{\rho^{0}v^{E2}+(\rho^{E1}+\rho^{L1})v^{E1}+\rho^{0}\operatorname{div}(v^{E1})v^{E1}\right\}\right]_{-}^{+},n_{0}\right)_{TM_{0}}=0,\qquad(2.142)$$
 on  $\partial M_{0}.$ 

### Third-order boundary conditions

For the third-order boundary conditions, we have

$$[L_{v_s^E}L_{v_s^E}L_{v_s^E}\varphi_s^E\big|_{s=0}]_{-}^+ = 0, \quad x \in \partial M_0,$$
 (2.143)

$$\iota_{M_0}^* \left( L_{v_s^E} L_{v_s^E} L_{v_s^E} \left( i_{\left[ \text{grad } \varphi_s^E \right]_-^+} \mu_{M_s} \right) \Big|_{s=0} \right) = 0, \quad x \in \partial M_0.$$
 (2.144)

From the first of these conditions we obtain

$$[\varphi^{E3}+3h^{E1}\partial_r\varphi^{E2}+3h^{E2}\partial_r\varphi^{E1}+3h^{E1}\partial_r(h^{E1}\partial_r\varphi^{E1})+h^{E3}\partial_r\varphi^{0}$$

$$+2h^{E1}\partial_r(h^{E2}\partial_r\varphi^0) + h^{E2}\partial_r(h^{E1}\partial_r\varphi^0) + h^{E1}\partial_r(h^{E1}\partial_r(h^{E1}\partial_r\varphi^0))|_{-}^{+} = 0, \quad (2.145)$$

on  $\partial M_0$ . Using eq.(2.109) along with the continuity of  $\partial_r \varphi^0$  we can write

$$\left[h^{E3}\varphi^{0}\right]_{-}^{+} = -\left[2h^{E1}\partial_{r}h^{E2} + h^{E2}\partial_{r}h^{E1} + h^{E1}\partial_{r}(h^{E1}\partial_{r}h^{E1})\right]_{-}^{+}.$$
 (2.146)

Substituting this relation into eq.(2.143) we find after some reduction that

$$[\varphi^{E3} + 3h^{E1}\partial_{r}\varphi^{E2} + 3h^{E2}\partial_{r}\varphi^{E1} + 3h^{E1}\partial_{r}(h^{E1}\partial_{r}\varphi^{E1}) +3h^{E1}h^{E2}\partial_{r}^{2}\varphi^{0} + 3(h^{E1})^{2}\partial_{r}h^{E1}\partial_{r}^{2}\varphi^{0} + (h^{E1})^{3}\partial_{r}^{3}\varphi^{0}]_{-}^{+} = 0.$$
(2.147)

Making use of Poisson's equation for  $\varphi^0$ , we find that

$$3h^{E2}\partial_{r}^{2}\varphi^{0} + 3h^{E1}\partial_{r}h^{E1}\partial_{r}^{2}\varphi^{0} + (h^{E1})^{2}\partial_{r}^{3}\varphi^{0} = 4\pi G\rho^{0}(h^{E2} + h^{E1}\partial_{r}h^{E1})$$
$$-2r^{-1}\varphi^{0}(h^{E2} + h^{E1}\partial_{r}h^{E1})$$
$$+4\pi G\partial_{r}\rho^{0}(h^{E1})^{2} + 2r^{-2}\varphi^{0}(h^{E1})^{2}$$
$$-2r^{-1}\partial_{r}\varphi^{0}(h^{E1})^{2}, \qquad (2.148)$$

from which we obtain

$$[3h^{E2}\partial_r^2\varphi^0 + 3h^{E1}\partial_r h^{E1}\partial_r^2\varphi^0 + (h^{E1})^2\partial_r^3\varphi^0]_{-}^{+} = 4\pi G [\rho^0]_{-}^{+} (h^{E2} + h^{E1}\partial_r h^{E1}) + 4\pi G [\partial_r \rho^0]_{-}^{+} (h^{E1})^2, \qquad (2.149)$$

where we have made use of eq.(2.107) and eq.(2.108) along with the continuity of  $\varphi^0$  and  $\partial_r \varphi^0$ . Using this relation we can simplify eq.(2.147) to obtain

$$[\varphi^{E3} + 3h^{E2}\partial_r\varphi^{E1} + 3h^{E1}\partial_r(h^{E1}\partial_r\varphi^{E1}) + 3h^{E1}\partial_r\varphi^{E2}$$

$$+12\pi G\rho^0 h^{E1}(h^{E2} + h^{E1}\partial_r h^{E1}) + 4\pi G\rho^0 (h^{E1})^3]_{-}^{+} = 0, \quad x \in \partial M_0.$$
(2.150)

For the second of the boundary conditions, we have that

$$\begin{aligned}
L_{v_{s}^{E}}L_{v_{s}^{E}}L_{v_{s}^{E}}\left(i_{\left[\operatorname{grad}\varphi_{s}^{E}\right]_{-}^{+}}\mu_{M_{s}}\right)\Big|_{s=0} &= i_{\left[\operatorname{grad}\varphi_{E3}\right]_{-}^{+}}\mu_{M_{0}} \\
&+3\mathcal{L}_{v_{E1}}\left(i_{\left[\operatorname{grad}\varphi_{E2}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+3\mathcal{L}_{v_{E2}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+\mathcal{L}_{v_{E1}}\mathcal{L}_{v_{E1}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+\mathcal{L}_{v_{E3}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+2\mathcal{L}_{v_{E1}}\mathcal{L}_{v_{E2}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+\mathcal{L}_{v_{E2}}\mathcal{L}_{v_{E1}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{M_{0}}\right) \\
&+\mathcal{L}_{v_{E1}}\mathcal{L}_{v_{E1}}\left(i_{\left[\operatorname{grad}\varphi_{E1}\right]_{-}^{+}}\mu_{E1}\right) \\
&+\mathcal{L}_{v_{E1}}\mathcal{L}_{v_{E1}}\left(i_$$

Using eq.(2.9) we see that

$$\iota_{M_0}^* \left( i_{\left[\operatorname{grad} \varphi^{E3}\right]_{-}^{+}} \mu_{M_0} \right) = \left( \left[\operatorname{grad} \varphi^{E3}\right]_{-}^{+}, n_0 \right)_{TM_0} \mu_{\partial M_0}.$$
 (2.152)

From eq.(2.10) we find that

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E1}} (i_{[\text{grad } \varphi^{E2}]_{-}^+} \mu_{M_0}) \right) = 4\pi G \left[ \rho^{E2} \right]_{-}^+ h^{E1} \mu_{M_0} 
- \left[ \text{div}_{\partial M_0} \left( h^{E1} \text{grad}_{\partial M_0} \varphi^{E2} \right) \right]_{-}^+ \mu_{\partial M_0}, \qquad (2.153)$$

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E2}}(i_{[\text{grad }\varphi^{E1}]_-^+} \mu_{M_0}) \right) = 4\pi G \left[ \rho^{E1} h^{E2} \right]_-^+ \mu_{M_0}, \tag{2.154}$$

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E3}} (i_{[\text{grad }\varphi^0]_-^+} \mu_{M_0}) \right) = 4\pi G \left[ \rho^0 h^{E3} \right]_-^+ \mu_{M_0}, \tag{2.155}$$

where  $\operatorname{grad}_{\partial M_0}$  is the gradient operator on  $\partial M_0$ . From eq.(2.32) we find that

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E1}} (i_{\left[ \operatorname{grad} \varphi^{E1} \right]_{-}^{+}} \mu_{M_0}) \right) = 4\pi G \left[ \operatorname{div}(\rho^{E1} v^{E1}) \right]_{-}^{+} h^{E1} \mu_{M_0}, \tag{2.156}$$

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E2}} (i_{[\text{grad }\varphi^0]^+} \mu_{M_0}) \right) = 4\pi G \left[ \text{div}(\rho^0 v^{E2}) \right]_-^+ h^{E1} \mu_{M_0}, \tag{2.157}$$

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E2}} \mathcal{L}_{v^{E1}} (i_{\left[ \operatorname{grad} \varphi^0 \right]_{-}^{+}} \mu_{M_0}) \right) = 4\pi G \left[ \operatorname{div}(\rho^0 v^{E1}) h^{E2} \right]_{-}^{+} \mu_{M_0}. \tag{2.158}$$

While from eq.(2.35) we obtain

$$\iota_{M_0}^* \left( \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E1}} \mathcal{L}_{v^{E1}} (i_{[\text{grad }\varphi^0]} + \mu_{M_0}) \right) = 4\pi G \left[ \text{div} (\text{div}(\rho^0 v^{E1}) v^{E1}) \right]_{-}^+ h^{E1}$$
(2.159)

Putting all these results together, we find that the boundary condition can be written as

$$\begin{split} & [ \left( \operatorname{grad} \varphi^{E3}, n_0 \right)_{TM_0} + 12\pi G \rho^{E2} h^{E1} - 3 \operatorname{div}_{\partial M_0} [h^{E1} \operatorname{grad}_{\partial M_0} \varphi^{E2}] \\ & + 12\pi G \rho^{E1} h^{E2} + 4\pi G \operatorname{div} (\rho^{E1} v^{E1}) h^{E1} + 4\pi G \rho^0 h^{E3} + 8\pi G \operatorname{div} (\rho^0 v^{E2}) h^{E1} \end{split}$$

$$+4\pi G \operatorname{div}(\rho^{0} v^{E1}) h^{E2} + 4\pi G \operatorname{div}(\operatorname{div}(\rho^{0} v^{E1}) v^{E1}) h^{E1}]_{-}^{+} = 0, \tag{2.160}$$

for  $x \in \partial M_0$ .

## 2.4 Hydrostatic Equilibrium Equations

The equations of hydrostatic equilibrium in an earth model M can be written

$$\operatorname{grad} p^E + \rho^E \operatorname{grad}(\varphi^E + \psi^E) = 0, \quad x \in M, \tag{2.161}$$

where  $p^E$  is the pressure,  $\rho^E$  the density,  $\varphi^E$  the gravitational potential, and  $\psi^E$  a forcing potential. The form of  $\psi^E$  will depend on the problem considered. For example, it could be the centrifugal potential associated with the steady rotation of the earth model about an axis through its center of mass. In a co-rotating spherical polar co-ordinates this forcing potential is given by

$$\psi^{E} = -\frac{1}{2}\Omega^{2}r^{2}\sin^{2}(\theta), \qquad (2.162)$$

where  $\Omega$  is the angular velocity of the earth model. Alternatively,  $\psi^E$  could be the tidal potential due to the Moon and the Sun. This equation is supplemented by the boundary condition

$$p^E = 0, \quad x \in \partial M. \tag{2.163}$$

Using the relation grad =  $g^{-1}$  · d, we can equivalently express eq.(2.161) in terms of exterior derivatives as

$$dp^{E} + \rho^{E} d(\varphi^{E} + \psi^{E}) = 0.$$
 (2.164)

It follows immediately that the hydrostatic equilibrium equations can be satisfied only if  $\rho^E d(\varphi^E + \psi^E)$  is an exact one-form. A necessary condition for this to be the case is that  $\rho^E d(\varphi^E + \psi^E)$  is closed, which means that

$$d\left[\rho^E d(\varphi^E + \psi^E)\right] = d\rho^E \wedge d(\varphi^E + \psi^E) = 0. \tag{2.165}$$

In fact, if we assume that M is contractible (i.e. homotopic to a point), it follows from Poincare's lemma (e.g. Lee 2002, Theorem 15.14) that this condition is also sufficient for  $\rho^E d(\varphi^E + \psi^E)$  to be exact. Supposing that  $\rho^E d(\varphi^R + \psi^E)$  is exact, a solution to eq.(2.164) can be given as

$$p(x) = \int_{c(x)} \rho^E d(\varphi^E + \psi^E), \qquad (2.166)$$

where c(x) is a piecewise-smooth curve in M going from x to an arbitrary point on  $\partial M$ .

The condition that  $d\rho^E \wedge d(\varphi^E + \psi^E) = 0$  implies that the level-surfaces of  $\rho^E$  and the geopotential  $\varphi^E + \psi^E$  must coincide within M. Moreover, taking the wedge product of eq.(2.164) with  $d\rho^E$ , we obtain

$$dp^E \wedge d(\varphi^E + \psi^E) = 0. \tag{2.167}$$

It follows that the level-surfaces of  $p^E$  and the geopotential also coincide. We conclude that in a hydrostatic earth model, the level-surfaces of  $p^E$ ,  $\rho^E$ , and  $\varphi^E + \psi^E$  are coincident. In particular, as  $p^E$  vanishes on  $\partial M$ , we see that  $\rho^E$  and  $\varphi^E + \psi^E$  must be constant there.

In the special case that  $\rho^E$  is constant throughout the earth model the one-form  $\rho^E d(\varphi^E + \psi^E)$  is trivially exact, and the only non-trivial constraint placed by the equilibrium equations is that  $\varphi^E + \psi^E$  is constant on  $\partial M$ .

### 2.4.1 Spherically symmetric earth models

We now consider the equilibrium equations in a spherically symmetric earth model for which the forcing potential vanishes. The pressure in such an earth model will be denoted by  $p^0$ . Due to the spherical symmetry, the density  $\rho^0$  depends only upon the radial coordinate r, and so is necessarily constant on  $\partial M_0$ . We have seen that the gravitational potential of such an earth model depends only upon the radial co-ordinate. Using the fact that both  $\rho^0$  and  $\varphi^0$  are functions of r alone, we calculate that

$$d\left[\rho^{0} d\varphi^{0}\right] = \partial_{r} \rho^{0} dr \wedge \partial_{r} \varphi^{0} dr = 0, \tag{2.168}$$

so that  $\rho^0 d\varphi^0$  is an exact one-form. A solution to the equilibrium equations can, therefore, be obtained from eq.(2.166) as

$$p(r) = \int_{r}^{b} \rho^{0}(s)\partial_{s}\varphi^{0}(s) ds.$$
 (2.169)

### 2.4.2 An Exact Theory of Hydrostatic Equilibrium

In this section, we wish to consider the structure of an earth model M that is in hydrostatic equilibrium under a non-zero forcing potential  $\psi^E$ . To simplify this problem, we again assume that M is diffeomorphic to a spherically symmetric earth model  $M_0$  under a mapping  $\xi: M_0 \to M$ . We shall further assume that the density in M is related to that in

 $M_0$  through

$$\rho^E = \xi_* \rho^0. \tag{2.170}$$

These assumptions are equivalent to those used in Clairaut's theory of hydrostatic equilibrium.

We can pull-back eq.(2.164) to  $M_0$  using  $\xi$  to obtain

$$dp^{L} + \rho^{0} d(\varphi^{L} + \psi^{L}) = 0, \tag{2.171}$$

where we have defined

$$p^L = \xi^* p^E, \tag{2.172}$$

$$\psi^L = \xi^* \psi^E, \tag{2.173}$$

and have used the fact that  $\xi^* \rho^E = \rho^0$ . Taking the exterior derivative of eq.(2.171) leads to the relation

$$\partial_r \rho^0 \, \mathrm{d}r \wedge \, \mathrm{d}(\varphi^L + \psi^L) = 0. \tag{2.174}$$

If we assume that  $\partial_r \rho^0$  is nowhere zero in the interval (0,b), then this equation implies

$$dr \wedge d(\varphi^L + \psi^L) = 0, \tag{2.175}$$

which requires that  $\varphi^L + \psi^L$  depends only upon the radial co-ordinate. If  $\partial_r \rho^0$  does vanish at a number of isolated points in (0,b), this conclusion still holds due to the continuity of  $\varphi^L$  and  $\psi^L$ . If, however,  $\partial_r \rho^0$  vanishes identically in some subinterval of (0,b), then we can draw no conclusions on the behaviour of  $\varphi^L + \psi^L$  there.

Let us suppose that the density structure in  $M_0$  is such that eq.(2.175) does hold. We can then write

$$\varphi^L + \psi^L = \varphi^0 + \gamma, \tag{2.176}$$

where  $\gamma$  is some arbitrary function of r. Substituting this relation into eq.(2.171) we find

$$dp^{L} + \rho^{0} \partial_{r} (\varphi^{0} + \gamma) dr = 0, \qquad (2.177)$$

which implies that  $p^L$  is also a function of r alone. Making use of the hydrostatic equilibrium equations in  $M_0$ , we find that

$$\partial_r(p^L - p^0) + \rho^0 \partial_r \gamma = 0, \tag{2.178}$$

which has the solution

$$p^{L}(r) = p^{0}(r) + \int_{r}^{b} \rho^{0}(s)\partial_{s}\gamma(s) ds.$$

$$(2.179)$$

From eq.(2.176), we see that

$$\varphi^L = \varphi^0 + \gamma - \psi^L. \tag{2.180}$$

Assuming that  $\gamma$  has been specified and is sufficiently smooth, we can substitute this identity into eq.(2.59) to obtain

$$\operatorname{div}\left[Ja^{-1}\cdot\operatorname{grad}(\varphi^{0}+\gamma-\psi^{L})\right]=4\pi G\rho^{0}J,\tag{2.181}$$

along with the boundary condition

$$\left( \left[ Ja^{-1} \cdot \operatorname{grad}(\varphi^0 + \gamma - \psi^L) \right]_{-}^{+}, n_0 \right) = 0, \quad x \in \partial M_0, \tag{2.182}$$

and the condition that  $\xi$  is continuous across  $\partial M_0$ . In these equations the only unknown is  $\xi$ , so that we can regard them as comprising a sufficient condition on  $\xi$  for the earth model M to be in hydrostatic equilibrium.

As eq.(2.181) is a single partial differential equation, it cannot constrain the mapping  $\xi$  uniquely. For example, let  $\chi: M_0 \to M_0$  be a diffeomorphism that maps level surfaces of density in  $M_0$  onto themselves. It is easy to see that if a mapping  $\xi$  satisfies the above equation, then so does  $\xi \circ \chi$ . One way of eliminating this non-uniqueness is to assume that  $\xi$  is purely radial; i.e. in spherical polar co-ordinates, we would have

$$\xi(r,\theta,\phi) = (r + h^L(r,\theta,\phi),\theta,\phi), \tag{2.183}$$

where  $h^L$  is some scalar function. Clearly such a representation of  $\xi$  is not the most general possible. It should, however, be applicable to calculations in which the model M is fairly close to a spherically symmetric model. Making use of this assumption, it is possible to reduce eq.(2.181) and the associated boundary conditions into a non-linear boundary value problem for the unknown function  $h^L$ .

To express these equations in more detail, we require formulae for J and a in spherical polar co-ordinates. Due to the complexity of the general problem, we shall assume that the forcing potential  $\psi^E$  is equal to the centrifugal potential of a steadily rotating earth model as given in eq.(2.162). As this potential is axisymmetric, we can simplify the problem by assuming that the mapping  $\xi$  depends only on r and  $\theta$ . Let  $(r', \theta', \phi')$  be a spherical polar co-ordinate system on M, and  $(r, \theta, \phi)$  the corresponding system on  $M_0$ . Under this radial mapping, we find that the pulled-back centrifugal potential  $\psi^E$  is given by

$$\psi^{L} = -\frac{1}{2}\Omega^{2}(r+h^{L})^{2}\sin^{2}(\theta). \tag{2.184}$$

It may be shown that

$$g = dr' \otimes dr' + (r')^2 d\theta' \otimes d\theta' + (r')^2 \sin^2(\theta') d\phi' \otimes d\phi', \qquad (2.185)$$

and that

$$\mu_M = (r')^2 \sin(\theta') \, \mathrm{d}r' \wedge \mathrm{d}\theta' \wedge \mathrm{d}\phi'. \tag{2.186}$$

The pull-back of the contangent vectors dr,  $d\theta$ , and  $d\phi$  under the axisymmetric radial mapping

$$r' = r + h^L(r,\theta), \tag{2.187}$$

$$\theta' = \theta, \tag{2.188}$$

$$\phi' = \phi, \tag{2.189}$$

are readily found to be

$$\xi^* \, \mathrm{d}r' = (1 + \partial_r h^L) \, \mathrm{d}r + \partial_\theta h^L \, \mathrm{d}\theta, \qquad (2.190)$$

$$\xi^* d\theta' = d\theta, \tag{2.191}$$

$$\xi^* \, \mathrm{d}\phi' = \mathrm{d}\phi. \tag{2.192}$$

Using these formulae, we see that

$$\xi^* \mu_M = \frac{(r+h^L)^2}{r^2} \left(1 + \partial_r h^L\right) \mu_{M_0}, \tag{2.193}$$

from which it follows that

$$J = \frac{(r+h^L)^2}{r^2} \left(1 + \partial_r h^L\right). \tag{2.194}$$

Similarly, we find that

$$\xi^* g = \left(1 + \partial_r h^L\right)^2 dr \otimes dr$$

$$+ \left(1 + \partial_r h^L\right) \partial_\theta h^L \left(dr \otimes d\theta + d\theta \otimes dr\right)$$

$$+ \left[ (r + h^L)^2 + \left(\partial_\theta h^L\right)^2 \right] d\theta \otimes d\theta$$

$$+ (r + h^L)^2 \sin^2(\theta) d\phi \otimes d\phi. \tag{2.195}$$

The inverse metric tensor  $g^{-1}$  in  $M_0$  is given in spherical polar co-ordinates by

$$g^{-1} = \frac{\partial}{\partial r} \otimes \frac{\partial}{\partial r} + r^{-2} \frac{\partial}{\partial \theta} \otimes \frac{\partial}{\partial \theta} + r^{-2} \operatorname{cosec}^{2}(\theta) \frac{\partial}{\partial \phi} \otimes \frac{\partial}{\partial \phi}, \tag{2.196}$$

from which we obtain

$$a = \left(1 + \partial_r h^L\right)^2 \frac{\partial}{\partial r} \otimes dr$$

$$+ \left(1 + \partial_r h^L\right) \partial_\theta h^L \left(\frac{\partial}{\partial r} \otimes d\theta + r^{-2} \frac{\partial}{\partial \theta} \otimes dr\right)$$

$$+ r^{-2} \left[ (r + h^L)^2 + \left(\partial_\theta h^L\right)^2 \right] \frac{\partial}{\partial \theta} \otimes d\theta$$

$$+ r^{-2} (r + h^L)^2 \frac{\partial}{\partial \phi} \otimes d\phi. \tag{2.197}$$

From these expressions, we find that

$$Ja^{-1} = \frac{(r+h^L)^2 + (\partial_{\theta}h^L)^2}{r^2(1+\partial_r h^L)} \frac{\partial}{\partial r} \otimes dr$$
$$-\partial_{\theta}h^L \left(\frac{\partial}{\partial r} \otimes d\theta + r^{-2} \frac{\partial}{\partial \theta} \otimes dr\right)$$
$$+(1+\partial_r h^L) \frac{\partial}{\partial \theta} \otimes d\theta$$
$$+(1+\partial_r h^L) \frac{\partial}{\partial \phi} \otimes d\phi. \tag{2.198}$$

From the identity  $grad = g^{-1} \cdot d$ , we obtain

$$\operatorname{grad}(\varphi^0 + \gamma - \psi^L) = \partial_r(\varphi^0 + \gamma - \psi^L) \frac{\partial}{\partial r} - \frac{1}{r^2} \partial_\theta \psi^L \frac{\partial}{\partial \theta}, \tag{2.199}$$

where

$$\partial_r \psi^L = -\Omega^2 (r + h^L) (1 + \partial_r h^L) \sin^2(\theta), \qquad (2.200)$$

$$\partial_{\theta} \psi^{L} = -\Omega^{2} (r + h^{L}) [\sin^{2}(\theta) \partial_{\theta} h^{L} + (r + h^{L}) \sin(\theta) \cos(\theta)]. \tag{2.201}$$

Inserting these expressions into eq.(2.181), we finally obtain

$$\frac{\partial}{\partial r} \left\{ \frac{(r+h^L)^2 + (\partial_{\theta}h^L)^2}{1 + \partial_r h^L} \partial_r (\varphi^0 + \gamma - \psi^L) + \partial_{\theta} h^L \partial_{\theta} \psi^L \right\} 
- \frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left\{ \sin(\theta) \left[ \partial_{\theta} h^L \partial_r (\varphi^0 + \gamma - \psi^L) + (1 + \partial_r h^L) \partial_{\theta} \psi^L \right] \right\} 
= 4\pi G \rho^0 (r+h^L)^2 (1 + \partial_r h^L),$$
(2.202)

which is the desired exact non-linear partial differential equation for  $h^L$ . This equation must be solved in  $\mathbb{R}^2$  subject to the boundary conditions that  $h^L$  and  $Ja^{-1}$  are continuous across  $\partial M_0$ , along with the condition that  $h^L$  tends to zero at infinity.

### 2.4.3 Perturbation series solutions

We now consider how to obtain approximate solutions of the boundary value problem for  $h^L$  using perturbation theory. To do this, let  $\xi_s: M_0 \to M_s$  be a one-parameter family of radial mappings as introduced in the previous section. Let us define

$$\psi_s^E = s\psi^E, \tag{2.203}$$

and require that the mappings  $\xi_s$  are such that the earth model  $M_s$  is in hydrostatic equilibrium under the action of the forcing potential  $\psi_s^E$ ; note that this condition holds trivially in the case that s = 0. From eq.(2.176), we see that for each s we must have

$$\xi_s^*(\varphi_s^E + \psi_s^E) = \varphi^0 + \gamma_s, \tag{2.204}$$

where  $\gamma_s$  is some one-parameter family of sufficiently smooth functions of r such that  $\gamma_0 = 0$ . Differentiating this equation n-times with respect to s and evaluating the resulting

expression at s = 0 leads to

$$\underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \left( \varphi_s^E + \psi_s^E \right) \Big|_{s=0} = \gamma^n, \tag{2.205}$$

where we have defined

$$\gamma^n = \left. \frac{\partial^n \gamma_s}{\partial s^n} \right|_{s=0}. \tag{2.206}$$

Up to third-order, this equation gives

$$\varphi^{E1} + \psi^E + \mathcal{L}_{v^{E1}}\varphi^0 = \gamma^1, \tag{2.207}$$

$$\varphi^{E2} + \mathcal{L}_{vE1}(\varphi^{E1} + \psi^{E}) + \mathcal{L}_{vE2}\varphi^{0} + \mathcal{L}_{vE1}\gamma^{1} = \gamma^{2}, \tag{2.208}$$

$$\varphi^{E3} + 2\mathcal{L}_{v^{E1}}\varphi^{E2} + 2\mathcal{L}_{v^{E2}}(\varphi^{E1} + \psi^{E}) + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E1}}(\varphi^{E1} + \psi^{E})$$

$$+\mathcal{L}_{v^{E3}}\varphi^{0} + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E2}}\varphi^{0} + \mathcal{L}_{v^{E2}}\gamma^{1} + \mathcal{L}_{v^{E1}}\gamma^{2} = \gamma^{3}.$$
 (2.209)

Using eq.(2.100), we see that these relations can also be written as

$$\varphi^{E1} + \psi^E + h^{E1} \partial_r \varphi^0 = \gamma^1, \tag{2.210}$$

$$\varphi^{E2} + h^{E1} \partial_r (\varphi^{E1} + \psi^E) + h^{E2} \partial_r \varphi^0 + h^{E1} \partial_r \gamma^1 = \gamma^2, \tag{2.211}$$

$$\varphi^{E3} + 2h^{E1}\partial_r\varphi^{E2} + 2h^{E2}\partial_r(\varphi^{E1} + \psi^E) + h^{E1}\partial_r(h^{E1}\partial_r(\varphi^{E1} + \psi^E))$$

$$+h^{E3}\partial_r\varphi^0 + h^{E1}\partial_r(h^{E2}\partial_r\varphi^0) + h^{E2}\partial_r\gamma^1 + h^{E1}\partial_r\gamma^2 = \gamma^3.$$
 (2.212)

Assuming that  $\partial_r \varphi^0$  is non-zero, we can use these relations to express  $h^{E1}$ ,  $h^{E2}$ , and  $h^{E3}$  in terms of  $\varphi^{E1}$ ,  $\varphi^{E2}$ , and  $\varphi^{E3}$ :

$$h^{E1} = -\frac{1}{\partial_r \varphi^0} \left\{ \varphi^{E1} + \psi^E - \gamma^1 \right\}, \tag{2.213}$$

$$h^{E2} = -\frac{1}{\partial_r \varphi^0} \left\{ \varphi^{E2} + h^{E1} \partial_r (\varphi^{E1} + \psi^E) + h^{E1} \partial_r \gamma^1 - \gamma^2 \right\}, \qquad (2.214)$$

$$h^{E3} = -\frac{1}{\partial_r \varphi^0} \left\{ \varphi^{E3} + 2h^{E1} \partial_r \varphi^{E2} + 2h^{E2} \partial_r (\varphi^{E1} + \psi^E) \right\}$$

$$+h^{E1}\partial_r(h^{E1}\partial_r(\varphi^{E1}+\psi^E))+h^{E1}\partial_r(h^{E2}\partial_r\varphi^0)$$

$$+h^{E2}\partial_r\gamma^1 + h^{E1}\partial_r\gamma^2 - \gamma^3\}, \qquad (2.215)$$

Similarly, from the identity  $\xi_s^* \rho_s^E = \rho^0$ , we obtain

$$\underbrace{L_{v_s^E} \cdots L_{v_s^E}}_{n\text{-terms}} \rho_s^E \Big|_{s=0} = 0, \tag{2.216}$$

which can be written to third-order as

$$\rho^{E1} + \mathcal{L}_{n^{E1}}\rho^0 = 0, \tag{2.217}$$

$$\rho^{E2} + \mathcal{L}_{v^{E1}}\rho^{E1} + \mathcal{L}_{v^{E2}}\rho^{0} = 0, \tag{2.218}$$

$$\rho^{E3} + 2\mathcal{L}_{vE1}\rho^{E2} + 2\mathcal{L}_{vE2}\rho^{E1} + \mathcal{L}_{vE1}\mathcal{L}_{vE1}\rho^{E1}$$

$$+\mathcal{L}_{v^{E3}}\rho^0 + \mathcal{L}_{v^{E1}}\mathcal{L}_{v^{E2}}\rho^0 = 0, \tag{2.219}$$

or, equivalently, as

$$\rho^{E1} + h^{E1} \partial_r \rho^0 = 0, \tag{2.220}$$

$$\rho^{E2} + h^{E1}\partial_r \rho^{E1} + h^{E2}\partial_r \rho^0 = 0, \tag{2.221}$$

$$\rho^{E3} + 2h^{E1}\partial_{r}\rho^{E2} + 2h^{E2}\partial_{r}\rho^{E1} + h^{E1}\partial_{r}\left(h^{E1}\partial_{r}\rho^{E1}\right)$$

$$+h^{E3}\partial_{r}\rho^{0} + h^{E1}\partial_{r}\left(h^{E2}\partial_{r}\rho^{0}\right) = 0, (2.222)$$

Making use of equations (2.213)-(2.215) we find that

$$\rho^{E1} = \frac{\partial_r \rho^0}{\partial_r \varphi^0} \left\{ \varphi^{E1} + \psi^E - \gamma^1 \right\}, \tag{2.223}$$

$$\rho^{E2} = -h^{E1}\partial_{r}\rho^{E1} + \frac{\partial_{r}\rho^{0}}{\partial_{r}\varphi^{0}} \left\{ \varphi^{E2} + h^{E1}\partial_{r}(\varphi^{E1} + \psi^{E}) + h^{E1}\partial_{r}\gamma^{1} - \gamma^{2} \right\}, \qquad (2.224)$$

$$\rho^{E3} = -3h^{E1}\partial_{r}\rho^{E2} - 2h^{E2}\partial_{r}\rho^{E1} - h^{E1}\partial_{r}\left(h^{E1}\partial_{r}\rho^{E1}\right) - h^{E1}\partial_{r}\left(h^{E2}\partial_{r}\rho^{0}\right)$$

$$+ \frac{\partial_{r}\rho^{0}}{\partial_{r}\varphi^{0}}\left\{\varphi^{E3} + 2h^{E1}\partial_{r}\varphi^{E2} + 2h^{E2}\partial_{r}(\varphi^{E1} + \psi^{E})\right.$$

$$+ h^{E1}\partial_{r}(h^{E1}\partial_{r}(\varphi^{E1} + \psi^{E})) + h^{E1}\partial_{r}(h^{E2}\partial_{r}\varphi^{0})$$

$$+h^{E2}\partial_r\gamma^1 + h^{E1}\partial_r\gamma^2 - \gamma^3\}, \qquad (2.225)$$

which shows that  $\rho^{E1}$ ,  $\rho^{E2}$ , and  $\rho^{E3}$  can also be written in terms of  $\varphi^{E1}$ ,  $\varphi^{E2}$ , and  $\varphi^{E3}$ .

More generally, it may be shown that  $h^{En}$  and  $\rho^{En}$  can be expressed in terms of  $\varphi^{En}$  along with lower-order terms in the perturbation series. Substituting these expressions the boundary value problems for  $\varphi^{En}$  derived in section 2.3, we obtain a series of linear boundary value problems. In detail, the *n*th coefficient  $\varphi^{En}$  function satisfies the equation

$$\Delta \varphi^{En} - 4\pi G \frac{\partial_r \rho^0}{\partial_r \varphi^0} \varphi^{En} = 4\pi G f^{En}, \qquad (2.226)$$

subject to the boundary conditions

$$\left[\varphi^{En}\right]_{-}^{+} = \left[k^{En}\right]_{-}^{+}, \quad x \in \partial M_0,$$
 (2.227)

$$\left( \left[ \operatorname{grad} \varphi^{En} - \frac{4\pi G \rho^0}{\partial_r \varphi^0} \varphi^{En} n_0 \right]_{-}^{+}, n_0 \right)_{TM_0} = \left[ t^{En} \right]_{-}^{+}, \quad x \in \partial M_0, \tag{2.228}$$

where the functions  $f^{En}$ ,  $k^{En}$ , and  $t^{En}$  involve only lower-order terms in the perturbation series. The solution to this boundary value problem can be most easily determined by expanding the equations in spherical harmonics, and so obtaining a decoupled system of ordinary differential equations for the expansion coefficients  $\varphi_{lm}^{En}$ . For each value of (l,m)the solution can then be written as

$$\varphi_{lm}^{En}(r) = \int_0^b G_l^f(r, r') f_{lm}^{En}(r') dr' + G_l^k(r) \left[ k_{lm}^{En}(b) \right]_-^+ + G_l^t(r) \left[ t_{lm}^{En}(b) \right]_-^+, \qquad (2.229)$$

where the kernels  $G_l^f$ ,  $G_l^k$ , and  $G_l^t$  can be obtained by numerical integration of a twodimensional system of ordinary differential equations, or, alternatively, by the solution of a system of linear equations arising from the finite-element discretization of the weakform of this system ordinary differential equations. Having, in this way, determined the functions  $\varphi^{En}$  up to some desired order, it this then possible to calculate the coefficients  $h^{Ln}$  of the perturbation series for the radial mapping  $h_s^L$ . The general expression for these expansion coefficients can be written

$$h_{lm}^{Ln}(r) = H_{lm}^{Ln}(r) + \int_0^b H_l^f(r, r') f_{lm}^{En}(r') dr' + H_l^k(r) \left[ k_{lm}^{En}(b) \right]_-^+ + H_l^t(r) \left[ t_{lm}^{En}(b) \right]_-^+,$$
(2.230)

where  $H_{lm}^{Ln}(r)$  involves only lower-order terms of terms in the perturbation series, and where the kernels  $H_{lm}^f$ ,  $H_{lm}^k$ , and  $H_{lm}^t$  can be expressed in terms of  $G_{lm}^F$ ,  $G_{lm}^k$ , and  $G_{lm}^t$  by

$$H_l^f(r,r') = -\frac{1}{\partial_r \varphi^0(r)} G_l^f(r,r'),$$
 (2.231)

$$H_l^k(r,r') = -\frac{1}{\partial_r \varphi^0(r)} G_l^k(r,r'),$$
 (2.232)

$$H_l^t(r,r') = -\frac{1}{\partial_r \varphi^0(r)} G_l^t(r,r'). \tag{2.233}$$

We now state in detail the force-terms for the boundary value problems for the  $\varphi^{En}$  up to third-order:

#### First-order equations

For the first-order equations we have

$$f^{E1} = \frac{\partial_r \rho^0}{\partial_r \varphi^0} \left\{ \psi^E - \gamma^1 \right\}, \tag{2.234}$$

$$k^{E1} = 0, (2.235)$$

$$t^{E1} = \frac{4\pi G \rho^0}{\partial_r \varphi^0} \left\{ \psi^E - \gamma^1 \right\}. \tag{2.236}$$

### Second-order equations

For the second-order equations we have

$$f^{E2} = -h^{E1}\partial_{r}\rho^{E1} + \frac{\partial_{r}\rho^{0}}{\partial_{r}\phi^{0}} \left\{ h^{E1}\partial_{r}(\varphi^{E1} + \psi^{E}) + h^{E1}\partial_{r}\gamma^{1} - \gamma^{2} \right\}, \tag{2.237}$$

$$k^{E2} = -h^{E1} \partial_r \varphi^{E1},$$
 (2.238)

$$t^{E2} = \frac{4\pi G \rho^{0}}{\partial_{r} \varphi^{0}} \left\{ h^{E1} \partial_{r} (\varphi^{E1} + \psi^{E}) + h^{E1} \partial_{r} \gamma^{1} - \gamma^{2} \right\}$$

$$-4\pi G \left[ \rho^{E1} + \rho^{0} \operatorname{div}(v^{E1}) \right] h^{E1}.$$
(2.239)

### Third-order equations

For the third-order equations we have

$$f^{E3} = -3h^{E1}\partial_{r}\rho^{E2} - 2h^{E2}\partial_{r}\rho^{E1} - h^{E1}\partial_{r}\left(h^{E1}\partial_{r}\rho^{E1}\right) - h^{E1}\partial_{r}\left(h^{E2}\partial_{r}\rho^{0}\right) \\ + \frac{\partial_{r}\rho^{0}}{\partial_{r}\varphi^{0}} \left\{ 2h^{E1}\partial_{r}\varphi^{E2} + 2h^{E2}\partial_{r}(\varphi^{E1} + \psi^{E}) \right. \\ + h^{E1}\partial_{r}(h^{E1}\partial_{r}(\varphi^{E1} + \psi^{E})) + h^{E1}\partial_{r}(h^{E2}\partial_{r}\varphi^{0}) \\ + h^{E2}\partial_{r}\gamma^{1} + h^{E1}\partial_{r}\gamma^{2} - \gamma^{3} \right\},$$

$$(2.240)$$

$$k^{E3} = -3h^{E2}\partial_{r}\varphi^{E1} - 3h^{E1}\partial_{r}(h^{E1}\partial_{r}\varphi^{E1}) - 3h^{E1}\partial_{r}\varphi^{E2} \\ -12\pi G\rho^{0}h^{E1}(h^{E2} + h^{E1}\partial_{r}h^{E1}) - 4\pi G\rho^{0}(h^{E1})^{3},$$

$$(2.241)$$

$$t^{E3} = -12\pi G\rho^{E2}h^{E1} + 3\text{div}_{\partial M_{0}}[h^{E1}\text{grad}_{\partial M_{0}}\varphi^{E2}] \\ -12\pi G\rho^{E1}h^{E2} - 4\pi G\text{div}(\rho^{E1}v^{E1})h^{E1} - 8\pi G\text{div}(\rho^{0}v^{E2})h^{E1} \\ -4\pi G\text{div}(\rho^{0}v^{E1})h^{E2} - 4\pi G\text{div}(\text{div}(\rho^{0}v^{E1})v^{E1})h^{E1} \\ + \frac{4\pi G\rho^{0}}{\partial_{r}\varphi^{0}} \left\{ 2h^{E1}\partial_{r}\varphi^{E2} + 2h^{E2}\partial_{r}(\varphi^{E1} + \psi^{E}) \right. \\ + h^{E1}\partial_{r}(h^{E1}\partial_{r}(\varphi^{E1} + \psi^{E})) + h^{E1}\partial_{r}(h^{E2}\partial_{r}\varphi^{0}) \\ + h^{E2}\partial_{r}\gamma^{1} + h^{E1}\partial_{r}\gamma^{2} - \gamma^{3} \right\}.$$

$$(2.242)$$

As yet, we have not specified the arbitrary radial functions  $\gamma^n$  which enter into the theory. Inspection of the 'force-terms' in the boundary value problem for  $\varphi^{En}$  shows that each  $\gamma^n$  only influences the degree-zero (i.e. spherically symmetric) part of  $h^{Ln}$ . It is, therefore, possible to place constraints on the  $\gamma^n$  by requiring that the degree-zero coefficient of  $h^{Ln}_{00}$  vanishes at all depths. In particular, this constraint requires that the mean radius of the earth model remains constant. For  $f^{En}_{00}$  and  $t^{En}_{00}$  we can write

$$f_{00}^{En} = \tilde{f}_{00}^{En} - \sqrt{4\pi} \frac{\partial_r \rho^0}{\partial_r \varphi^0} \gamma^n, \qquad (2.243)$$

$$k_{00}^{En} = \tilde{k}_{00}^{En} - \sqrt{4\pi} \frac{4\pi G \rho^0}{\partial_r \varphi^0} \gamma^n,$$
 (2.244)

where we have defined  $\tilde{f}_{00}^{En}$  and  $\tilde{k}_{00}^{En}$  through these relations, and the factors of  $\sqrt{4\pi}$  occur because we are considering expansions in fully normalized spherical harmonics. From the degree-zero version of eq.(2.230) we find that

$$h_{00}^{Ln}(r) = H_{00}^{Ln}(r) + \int_{0}^{b} H_{0}^{f}(r, r') \tilde{f}_{00}^{En}(r') dr'$$

$$+ H_{0}^{k}(r) \left[ k_{00}^{En}(b) \right]_{-}^{+} + H_{0}^{t}(r) \left[ \tilde{t}_{00}^{En}(b) \right]_{-}^{+}$$

$$- \sqrt{4\pi} \int_{0}^{b} H_{0}^{f}(r, r') \frac{\partial_{r} \rho^{0}(r')}{\partial_{r} \varphi^{0}(r')} \gamma^{n}(r') dr'$$

$$-\sqrt{4\pi}H_0^t(r)\left[\frac{4\pi G\rho^0(b)}{\partial_r\varphi^0(b)}\gamma^n(b)\right]_-^+. \tag{2.245}$$

The requirement that  $h_{00}^{Ln}(r) = 0$  in [0, b] can, therefore, be written as

$$\sqrt{4\pi} \int_{0}^{b} H_{0}^{f}(r, r') \frac{\partial_{r} \rho^{0}(r')}{\partial_{r} \varphi^{0}(r')} \gamma^{n}(r') dr' 
+ \sqrt{4\pi} H_{0}^{t}(r) \left[ \frac{4\pi G \rho^{0}(b)}{\partial_{r} \varphi^{0}(b)} \gamma^{n}(b) \right]_{-}^{+} = H_{00}^{Ln}(r) + \int_{0}^{b} H_{0}^{f}(r, r') \tilde{f}_{00}^{En}(r') dr' 
+ H_{0}^{k}(r) \left[ k_{00}^{En}(b) \right]_{-}^{+} 
+ H_{0}^{t}(r) \left[ \tilde{t}_{00}^{En}(b) \right]_{-}^{+},$$
(2.246)

which can be regarded as an integral equation for  $\gamma^n$ . Both  $\varphi^0$  and  $\varphi^L_{00}$  must vanish at r=0, so it follows from eq.(2.176) that we have the boundary condition

$$\sqrt{4\pi}\gamma^n(0) = \psi_{00}^L(0) = \psi_{00}^E(0). \tag{2.247}$$

The boundary condition for  $\gamma^n$  at r=b can be chosen arbitrarily, though it is convenient to take

$$\sqrt{4\pi} \left[ \frac{4\pi G \rho^0(b)}{\partial_r \varphi^0(b)} \gamma^n(b) \right]_-^+ = \tilde{t}_{00}^{En}. \tag{2.248}$$

With these boundary conditions, the above integral equation for  $\gamma^n$  reduces to

$$\sqrt{4\pi} \int_{0}^{b} H_{0}^{f}(r, r') \frac{\partial_{r} \rho^{0}(r')}{\partial_{r} \varphi^{0}(r')} \gamma^{n}(r') dr' = H_{00}^{Ln}(r) + \int_{0}^{b} H_{0}^{f}(r, r') \tilde{f}_{00}^{En}(r') dr' + H_{0}^{k}(r) \left[k_{00}^{En}(b)\right]_{-}^{+}, \qquad (2.249)$$

which is a Fredholm equation of the first kind. In the case n = 1, we have  $H_{00}^{E1} = 0$  and  $k_{00}^{E1} = 0$ , so that this equation becomes

$$\sqrt{4\pi} \int_0^b H_0^f(r, r') \frac{\partial_r \rho^0(r')}{\partial_r \varphi^0(r')} \gamma^1(r') \, \mathrm{d}r' = \int_0^b H_0^f(r, r') \tilde{f}_{00}^{E1}(r') \, \mathrm{d}r', \tag{2.250}$$

which admits the solution

$$\gamma^{1} = \frac{1}{\sqrt{4\pi}} \frac{\partial_{r} \varphi^{0}}{\partial_{r} \rho^{0}} \tilde{f}_{00}^{E1} = \frac{1}{\sqrt{4\pi}} \psi_{00}^{E}, \tag{2.251}$$

which is also seen to satisfy the boundary conditions for the problem. That this solution is unique depends on whether the integral operator

$$A(\gamma)(r) \equiv \int_0^b H_0^f(r, r') \frac{\partial_r \rho^0(r')}{\partial_r \varphi^0(r')} \gamma(r') \, \mathrm{d}r', \qquad (2.252)$$

has a trivial kernel, and the same question applies to the uniqueness of solutions for  $n \ge 2$ . We have not, however, investigated this issue in any detail.

### 2.4.4 Reduction of the first-order theory to Clairaut's Equation

We conclude by showing that the results of our first-order theory are equivalent to those of Clairaut. In the case that the forcing-potential is equal to the centrifugal-potential

$$\psi^{E} = -\frac{1}{2}\Omega^{2}r^{2}\sin^{2}(\theta), \qquad (2.253)$$

we find that

$$\psi_{00}^{E} = -\frac{2}{3}\sqrt{\pi}\Omega^{2}r^{2}, \qquad (2.254)$$

$$\psi_{20}^{E} = \frac{2}{3} \sqrt{\frac{\pi}{5}} \Omega^{2} r^{2}, \qquad (2.255)$$

with all other expansion coefficients being equal to zero. From eq.(2.251) we see that the choice

$$\gamma^1 = -\frac{2}{6}\Omega^2 r^2, \tag{2.256}$$

leads to the mean radii of level-surfaces in the earth model remaining constant to first-order. From eq.(2.234) and (2.236) we then find that

$$f_{20}^{E1} = \frac{2}{3} \sqrt{\frac{\pi}{5}} \Omega^2 r^2 \frac{\partial \rho^0}{\partial_r \varphi^0}, \qquad (2.257)$$

$$t_{20}^{E1} = \frac{8\pi G}{3} \sqrt{\frac{\pi}{5}} \Omega^2 r^2 \frac{\rho^0}{\partial_r \varphi^0},$$
 (2.258)

with all other expansion coefficients being equal to zero. By the linearity of the equation for  $\varphi^{E1}$ , we see that only the coefficient function  $\varphi^{E1}_{20}$  is non-zero, and that it satisfies the equation

$$\partial_r^2 \varphi_{20}^{E1} + 2r^{-1} \partial_r \varphi_{20}^{E1} - \left(6r^{-2} + 4\pi G \frac{\partial_r \rho^0}{\partial_r \varphi^0}\right) \varphi_{20}^{E1} = \frac{8\pi G}{3} \sqrt{\frac{\pi}{5}} \Omega^2 r^2 \frac{\partial_r \rho^0}{\partial_r \varphi^0},\tag{2.259}$$

which is subject to the boundary conditions

$$\left[\varphi_{20}^{E1}\right]_{-}^{+} = 0, \quad r = b,$$
 (2.260)

$$\left[\partial_{r}\varphi_{20}^{E1} - \frac{4\pi G\rho^{0}}{\partial_{r}\varphi^{0}}\varphi_{20}^{E1}\right]_{-}^{+} = \left[\frac{8\pi G}{3}\sqrt{\frac{\pi}{5}}\Omega^{2}r^{2}\frac{\rho^{0}}{\partial_{r}\varphi^{0}}\right]_{-}^{+}, \quad r = b.$$
 (2.261)

To relate these equations to Clairaut's we define the ellipticity  $\epsilon$  of the earth model to be such that

$$h^{E1}(r,\theta,\phi) = -\frac{2}{3}r\epsilon(r)P_2(\cos(\theta)), \qquad (2.262)$$

where  $P_l$  denotes the Legendre polynomial of degree l. From this relation we see that

$$h_{20}^{E1} = -\frac{4}{3}\sqrt{\frac{\pi}{5}}r\epsilon. {(2.263)}$$

Using eq.(2.213) we have

$$h_{20}^{E1} = -\frac{1}{\partial_x \varphi^0} \left( \varphi_{20}^{E1} + \psi_{20}^E \right), \tag{2.264}$$

which leads to the relation

$$\varphi^{E1} = \frac{2}{3} \sqrt{\frac{\pi}{5}} \left( 2r \partial_r \varphi^0 \epsilon - \Omega^2 r^2 \right). \tag{2.265}$$

On substitution of this identity into eq.(2.259) we obtain after some algebra

$$\partial_r^2 \epsilon + 8\pi G \rho^0 g^{-1} (\partial_r \epsilon + r^{-1} \epsilon) - 6r^{-2} \epsilon = 0, \tag{2.266}$$

where we have set  $g = \partial_r \varphi^0$ , which is Clairaut's equation for the ellipticity (e.g. Dahlen & Tromp 1998, eq.(14.13)). Similarly, we find that the boundary condition on  $\partial_r \varphi_{20}^{E1}$  at r = b reduces to

$$\partial_r \epsilon(b) = b^{-1} \left( \frac{5}{2} \Omega^2 b^3 / GM - 2\epsilon(b) \right), \tag{2.267}$$

where M is the total mass of the earth model, and we have used the fact that  $\varphi^{E1}$  is harmonic outside of  $M_0$ ; again this result agrees with those of Dahlen & Tromp (1998) in their eq.(14.14).

# Chapter 3

# Parametrization of Equilibrium Stress Fields in the Earth

### 3.1 Introduction

In this chapter, we consider the problem of parametrizing the possible equilibrium stress fields in the Earth. These equilibrium stress fields are solutions of the equations of static equilibrium – or equilibrium equations for short – which express a balance between the forces of self-gravitation, rotation, and internal stresses in the Earth (e.g. Dahlen & Tromp 1998, Section 3.1). Implicit in the use of the equilibrium equations is the assumption that the dynamic component of any velocity field in the Earth associated with long-term geodynamic processes such as mantle convection is negligible. This assumption is justified for seismological applications by scaling analysis of the time-dependent momentum equations, which indicate that the Earth must be extremely close to a state of static equilibrium (e.g. Forte 2007, Section 1.23.2.3.1).

The seismological interest in the equilibrium stress field is due to its occurrence as a parameter in the elastodynamic equations that govern seismic wave propagation (e.g. Rayleigh 1906, Love 1911, Dahlen 1972a, Dahlen 1973, Dahlen & Smith 1975, Woodhouse & Dahlen 1979, Valette 1986, Vermeersen & Vlaar 1991, Dahlen & Tromp 1998). Consequently, it may be possible to make inferences about the equilibrium stress field from seismic observations. The feasibility of such an inverse problem depends upon the sensitivity of

seismic observations to variations in the equilibrium stress field relative to their sensitivity to variations in other model parameters such as seismic wave speeds, density, anisotropy, anelasticity, and boundary topography. This issue has previously been investigated by a number of authors including Dahlen (1972b,1972c) and Nikitin & Chesnokov (1984) who considered the effects of deviatoric equilibrium stress fields on body wave radiation patterns and travel-times. Using estimates of the magnitude of deviatoric stresses in the Earth, Dahlen concluded that the influence of the equilibrium stress field on these body-wave observations is likely small compared to the effects of other factors such as lateral variations in seismic wave speed. It is not, however, immediately clear that these conclusions also apply to longer period seismic observations such as normal mode spectra. For example, Valette (1986) determined an expression for the first-order perturbation to normal mode eigenfrequencies due to a deviatoric equilibrium stress field using the isolated mode approximation, and from examination of the resulting sensitivity kernel, concluded that there is no a priori reason to neglect the effects of deviatoric equilibrium stress fields.

Determining the effects of the equilibrium stress field on seismic wave propagation is complicated by the fact the perturbations to the density structure, to boundary topography, and to the equilibrium stress field cannot be made independently. This is because any perturbations to these parameters must be such that the equilibrium equations are satisfied in the perturbed earth model. As a result, the construction of a range of equilibrium stress fields for a given laterally heterogeneous earth model (i.e. one in which the density and boundary topography perturbations have been specified) is a non-trivial problem. Similarly, if we wish to include the equilibrium stress field as an unknown in a tomographic inversion, we require a method for parametrizing the perturbations to the equilibrium stress field consistent with given perturbations to the density structure and boundary topography.

The problem of parametrizing the possible equilibrium stress fields of an earth model has been considered previously by Backus (1967) whose method has, for example, been applied practically by Dahlen (1982) and Valette & Chambat (2004). Backus's method makes use of a representation theorem for symmetric second-order tensor fields in terms of six scalar potential functions (Backus 1966), and is based on the observation that the equilibrium equations place only three constraints on these six scalar potential functions. It follows

that we can specify three of these scalar potential functions arbitrarily (subject to certain compatibility conditions), and then solve the equilibrium equations for the remaining three scalar potential functions. In this way we see that a unique equilibrium stress field corresponds to each possible choice of the three arbitrary scalar potential functions.

In this work we approach the problem in a different manner. Our starting point is the observation that the difference between any two equilibrium stress fields is a divergence-free stress field whose boundary tractions vanish; the vector space of such stress fields is denoted by  $\ker(\operatorname{Div}_0)$ , this notation being fully explained in Section 3.1. It follows that if, by some means, we have obtained a particular equilibrium stress field  $\mathbf{T}_m$ , then all other equilibrium stress fields can be written in the form  $\mathbf{T}_m + \mathbf{S}$ , where  $\mathbf{S}$  is an element of  $\ker(\operatorname{Div}_0)$ . Consequently, given such an equilibrium stress field  $\mathbf{T}_m$ , along with a finite set  $\{\mathbf{S}_i\}_{i=1}^n$  of elements of  $\ker(\operatorname{Div}_0)$ , we can then consider the expression

$$\mathbf{T} = \mathbf{T}_m + a_1 \mathbf{S}_1 + \dots + a_n \mathbf{S}_n, \tag{3.1}$$

where  $a_i, \ldots, a_n$  are scalar constants, as forming an n-dimensional parametrization of equilibrium stress fields in the earth model (more formally, we can regard this expression as defining an affine mapping from  $\mathbb{R}^n$  into the space of equilibrium stress fields). It is clear that by including a sufficiently large set of elements of  $\ker(\operatorname{Div}_0)$  in the above expression we can, in principle, express any equilibrium stress field in this form.

Using this approach, we have separated the problem of parametrizing the possible equilibrium stress fields into two sub-problems: (i) determining a particular solution  $\mathbf{T}_m$  of the equilibrium equations, and (ii) constructing a suitably large number of elements of  $\ker(\mathrm{Div}_0)$ . In solving the first of these problems there are a number of possibilities. One method would be to use an equilibrium stress field obtained from a geodynamic model of viscous mantle flow (e.g. Forte & Peltier 1990). Alternatively, we can seek a solution of the equilibrium equations that satisfies some physically desirable property. For example, we can attempt to find the equilibrium stress field with smallest norm with respect to a given inner product. Using an orthogonal decomposition theorem for second order symmetric tensor fields (e.g. Berger & Ebin 1969, Ting 1977, Georgescu 1980, Cantor 1981) we show that there is a unique solution to this problem, and that this equilibrium stress field – which we call the minimum equilibrium stress field for the earth model – can be constructed by solving a boundary value problem that has exactly the same form as

a static linear elastic displacement problem. Alternatively, we can seek the equilibrium stress field whose deviatoric component has the smallest norm with respect to the given inner product. This problem can be solved using the method of Lagrange multipliers, and we show that the resulting equilibrium stress field – which we call the *minimum deviatoric* equilibrium stress field – can be obtained by solving a boundary value problem of the same form as the steady-state incompressible Navier-Stokes equations.

The idea of determining the equilibrium stress field with the minimum deviatoric components has previously been considered by Dahlen (1981,1982) in studies of isostasy in the oceanic lithosphere. However, Dahlen's approach to this problem differs from ours in a number of ways. Firstly, his method is less general due to his use of a number of assumptions about the form of the equilibrium stress field derived from consideration of local isostasy. Secondly, he adopts a 'local definition' of the minimum deviatoric equilibrium stress field (for example, see eq.(21) in Dahlen 1981 or eq.(47) in Dahlen 1982) in contrast to our 'global definition' in terms of an inner product on the space of second-order symmetric tensor fields. Because of these differences, Dahlen was not led to the interesting relationship between the minimum deviatoric equilibrium stress field and the steady-state incompressible Navier-Stokes equations described in this work.

In generating elements of the vector space  $\ker(\operatorname{Div_0})$  for use in eq.(3.1) there are a number of available methods (e.g. Truesdell 1959, Gurtin 1963). However, because we need only consider the construction of such tensor fields in a spherically symmetric reference model it is simplest to use Backus's method specialized to the case of divergence-free tensor fields. In doing this we shall not use the scalar representation theorem of Backus (1966), but instead employ the generalised spherical harmonic formalism of Phinney & Burridge (1973) which, we feel, is more suited to practical calculations.

The method for parametrizing equilibrium stress fields described above provides an alternative to that given by Backus (1967). It will be useful to consider some of the merits of these two approaches. A disadvantage of our method is that the calculation of either the minimum equilibrium stress field or the minimum deviatoric equilibrium stress field requires the solution of a system of linear partial differential equations. This is in contrast to Backus's method which involves largely algebraic calculations. Consequently, the

practical implementation of Backus's parametrization is simpler than ours. This disadvantage is not, however, very severe because the calculations involved in producing either minimum equilibrium stress field or the minimum deviatoric equilibrium stress field can be performed efficiently using a range of existing numerical techniques (see section 3.5).

To illustrate a potential advantage of our method, it will useful to consider the problem of estimating the likely effects of deviatoric equilibrium stress fields on seismic wave propagation. To do this we must be able to produce a number of realistic equilibrium stress fields for a given earth model in which seismic calculations can be performed. Stating here precisely what is meant by 'realistic' is difficult because the state of stress within the Earth's interior is not well understood. Physical arguments and information derived from geodynamic simulations do, however, suggest some general properties of a realistic equilibrium stress field (e.g. Karato & Wu 1993). For example, it is reasonable to expect that the deviatoric component of the equilibrium stress field should be small relative to its hydrostatic component. This is because rocks in the Earth's interior would be expected to undergo some form of deformation (e.g. fracture or plastic flow) if the deviatoric stresses became too large, and any such deformation would in turn act to lower the magnitude of the deviatoric stress. Using Backus's method it is not immediately clear how we could (other than by trial-and-error) determine equilibrium stress fields in the earth model having deviatoric components small in magnitude. The minimum deviatoric equilibrium stress field for an earth model, on the other hand, provides an immediate solution to this problem.

As a further example, suppose that we wished to perform a tomographic inversion in which density and boundary topography are free-parameters, but do not wish to include the equilibrium stress field as a free-parameter in the inversion. In such cases it has been usual to employ the so-called quasi-hydrostatic approximation in which the deviation of the equilibrium stress field away from its hydrostatic reference value is neglected; clearly this approximation results in a perturbed earth model that will not be in static equilibrium (e.g. Dahlen & Tromp 1998, Section 3.11). An alternative to using the quasi-hydrostatic approximation would be to set the equilibrium stress field during the tomographic inversion equal to either the minimum equilibrium stress field or the minimum deviatoric equilibrium stress field (i.e. regard it as a functional of the specified density and boundary topogra-

phy perturbations). Though in doing this we would be making an essentially arbitrary assumption, this process would at least lead to a self-consistent model parametrization in which the equilibrium stress field used was physically plausible. More generally, if we wished to include the equilibrium stress field as a parameter in a tomographic inversion, then either the minimum equilibrium stress field or the minimum deviatoric equilibrium stress field would provide a sensible a priori equilibrium stress field about which to make small perturbations at each step of the tomographic inversion.

## 3.2 A Review of Equilibrium Equations

### 3.2.1 Statement of the basic equations

The earth model is supposed to occupy an open bounded subset  $M \subseteq \mathbb{R}^3$  with smooth boundary  $\partial M$ , and is further divided into a number of solid and fluid sub-regions which are separated by smooth, non-intersecting, closed surfaces called internal boundaries. The union of the solid regions will be denoted  $M_S$  and that of all fluid regions  $M_F$ . The union  $\Sigma$  of all internal and external boundaries is split into the four subsets  $\Sigma_{SS}$ ,  $\Sigma_{SF}$ ,  $\Sigma_{FS}$ , and  $\Sigma_{FF}$  where the first subscript denotes whether the region on the inside of the boundary is solid S or fluid S, while the second subscript specifies whether the region on the outside of boundary is solid or fluid. We note that if the earth model has an ocean, then its free-surface is regarded, by definition, as a fluid-fluid boundary. A generic point in the earth model will be denoted  $\Sigma$  in what follows. The equilibrium stress tensor in the model will be written  $\Sigma$ , or in component form  $\Sigma$ . This stress tensor is symmetric, and satisfies the equilibrium equations

$$Div \mathbf{T} = \rho \nabla \varphi. \tag{3.2}$$

In this equation, Div is the divergence operator on second-order tensor fields whose action on **T** may be written in index notation as

$$(\operatorname{Div}\mathbf{T})_i = T_{ji,j},\tag{3.3}$$

where we have made use of the summation convention, and the 'comma' notation for partial derivatives. The boundary conditions on **T** are that the traction vector be continuous on

all boundaries so that

$$[\hat{\mathbf{n}} \cdot \mathbf{T}]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma,$$
 (3.4)

where  $\hat{\mathbf{n}}$  is the outward unit normal vector to a boundary, and the notation  $[\cdot]_{-}^{+}$  denotes the jump in a quantity on crossing a boundary in the direction of the outward normal. The other terms in eq.(3.2) are the density  $\rho$ , and the gravitational potential  $\varphi$  which is a solution of the equation

$$\Delta \varphi = 4\pi G \rho, \tag{3.5}$$

where  $\Delta$  is the Laplacian operator, G is the universal gravitational constant,  $\rho$  is taken to be identically zero outside of M, and  $\varphi$  is subject to the boundary conditions

$$[\varphi]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.6}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi\right]^+ = 0, \quad \mathbf{x} \in \Sigma, \tag{3.7}$$

along with the condition that  $\varphi$  vanish at infinity.

In a spherically symmetric earth model with radius b it may be shown that

$$\varphi(r) = -4\pi G \left\{ \int_r^b \rho(s)s \, \mathrm{d}s + \frac{1}{r} \int_0^r \rho(s)s^2 \, \mathrm{d}s \right\},\tag{3.8}$$

and that a solution of the equilibrium equations exists in the form  $\mathbf{T} = -p\mathbf{1}$  with the pressure given by

$$p(r) = \int_{r}^{b} \rho(s)g(s) \,\mathrm{d}s,\tag{3.9}$$

where  $g = \partial_r \varphi$  is the gravitational acceleration in the earth model. A solution of the equilibrium equations taking the form  $\mathbf{T} = -p\mathbf{1}$  is said to be hydrostatic. It may be shown that in a hydrostatic earth model the level surfaces of the three scalar fields  $\rho$ ,  $\varphi$ , and p must all coincide, and that (in the absence of rotation) each such level surface must be spherical (e.g. Dahlen & Tromp 1998, Section 13.11.1, and also Chapter 3). Because of this constraint it is not possible to find an everywhere hydrostatic solution to the equilibrium equations in an earth model with a laterally heterogeneous density structure. In the fluid regions of a model, however, it is necessary for the stress tensor to be hydrostatic because a stationary fluid cannot support deviatoric stresses. We shall see shortly that this condition in fluid regions places a strong constraint on the possible density structures of laterally heterogeneous earth models. For simplicity, the effects of rotation have not been included in the above discussion. However rotational effects can be incorporated into the hydrostatic reference model described below using the theory of hydrostatic ellipticity

(Jeffreys 1976, Dahlen & Tromp 1998, Section 14.1).

# 3.2.2 Linearized equations in a slightly laterally heterogeneous earth model

Let us now consider an earth model that is obtained from a spherically symmetric reference model possessing a hydrostatic equilibrium stress field by adding small perturbations to the density and to the boundary surfaces. The density in the perturbed model will be written

$$\rho = \rho^{(0)} + \rho^{(1)},\tag{3.10}$$

where  $\rho^{(0)}$  is the density in the spherically symmetric reference model and  $\rho^{(1)}$  is the density perturbation; in what follows the superscripts (0) and (1) will be used to distinguish between quantities in the reference model and their (first-order) perturbations. Each of the spherical boundaries in the reference model is deformed so that a point with spherical polar coordinates  $(r, \theta, \varphi)$  on the reference boundary is moved to the point  $(r + h(\theta, \varphi), \theta, \varphi)$  on the perturbed boundary. We may assume without loss of generality that the density and boundary perturbations are such that their average over any spherical surface vanishes, so, for example, the spherical average

$$\bar{\rho}^{(1)}(r) = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} \rho^{(1)}(r, \theta, \phi) \sin(\theta) \, d\theta \, d\phi$$
 (3.11)

of the density perturbation over a spherical surface with radius r is equal to zero; this condition is equivalent to requiring that the degree-zero spherical harmonic expansion coefficients of  $\rho^{(1)}$  and h are equal to zero.

The stress tensor in the perturbed model takes the form

$$\mathbf{T} = -p^{(0)}\mathbf{1} + \mathbf{T}^{(1)},\tag{3.12}$$

in solid regions, and

$$\mathbf{T} = -p^{(0)}\mathbf{1} - p^{(1)}\mathbf{1},\tag{3.13}$$

in fluid regions. Upon cancelling out the zeroth-order terms and ignoring any products of the perturbed quantities, the equilibrium equations in the perturbed model become

$$Div \mathbf{T}^{(1)} = \rho^{(0)} \nabla \varphi^{(1)} + \rho^{(1)} \nabla \varphi^{(0)}, \tag{3.14}$$

in solid regions, and

$$-\nabla p^{(1)} = \rho^{(0)} \nabla \varphi^{(1)} + \rho^{(1)} \nabla \varphi^{(0)}, \tag{3.15}$$

in fluid regions. Linearizing the continuity of traction condition in the perturbed earth model leads to the following boundary conditions for  $\mathbf{T}^{(1)}$  and  $p^{(1)}$  which are applied on the unperturbed boundaries of the reference earth model

$$\left[\hat{\mathbf{n}} \cdot \mathbf{T}^{(1)} + \rho^{(0)} g h \hat{\mathbf{n}}\right]^{+} = 0, \quad \mathbf{x} \in \Sigma_{SS}, \tag{3.16}$$

$$\hat{\mathbf{n}} \cdot \mathbf{T}^{(1)} + p^{(1)}\hat{\mathbf{n}} - \left[\rho^{(0)}\right]^{+} gh\hat{\mathbf{n}} = 0, \quad \mathbf{x} \in \Sigma_{SF}, \tag{3.17}$$

$$\hat{\mathbf{n}} \cdot \mathbf{T}^{(1)} + p^{(1)}\hat{\mathbf{n}} + \left[\rho^{(0)}\right]_{-}^{+} gh\hat{\mathbf{n}} = 0, \quad \mathbf{x} \in \Sigma_{FS}, \tag{3.18}$$

$$[p^{(1)} - \rho^{(0)}gh]^+ = 0, \quad \mathbf{x} \in \Sigma_{FF},$$
 (3.19)

where  $g = \partial_r \varphi^{(0)}$  (e.g. Dahlen & Tromp 1998, section 13.7.1) . The perturbed gravitational potential  $\varphi^{(1)}$  in the above equations is a solution of the equation

$$\Delta \varphi^{(1)} = 4\pi G \rho^{(1)},\tag{3.20}$$

subject to the linearized boundary conditions

$$\left[\varphi^{(1)}\right]^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.21}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} + 4\pi G \rho^{(0)} h\right]^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.22}$$

along with the requirement that  $\varphi^{(1)}$  vanish at infinity.

By considering the degree-zero spherical harmonic component of the above equation for  $\varphi^{(1)}$  it is clear that because the degree-zero components of  $\rho^{(1)}$  and h both vanish the same is true of  $\varphi^{(1)}$ . Similarly we see from eq.(3.15) that the spherically averaged part  $\bar{p}^{(1)}$  of the pressure perturbation  $p^{(1)}$  is constrained to be constant in each connected component of  $M_F$ . The remaining aspherical part of the pressure perturbation is defined by

$$\hat{p}^{(1)} = p^{(1)} - \bar{p}^{(1)}, \tag{3.23}$$

and is seen to satisfy exactly the same equations and boundary conditions as  $p^{(1)}$ .

# 3.2.3 Constraints on the model perturbations due to the hydrostatic condition in fluid regions

We now consider in detail how the hydrostatic condition on the stress tensor in fluid regions constrains the possible model perturbations; the results of this section have been previously described by Backus (1967), Dahlen (1974), Woodhouse & Dahlen (1979), and

Wahr & de Vries (1989). It will be useful to write the density perturbation as

$$\rho^{(1)} = \rho^{(1,S)} + \rho^{(1,F)}, \tag{3.24}$$

where  $\rho^{(1,S)}$  is non-zero only in  $M_S$  and  $\rho^{(1,F)}$  is non-zero only in  $M_F$ . Corresponding to this decomposition of  $\rho^{(1)}$  we write  $\varphi^{(1)}$  as

$$\varphi^{(1)} = \varphi^{(1,S)} + \varphi^{(1,F)}, \tag{3.25}$$

with the functions  $\varphi^{(1,S)}$  and  $\varphi^{(1,F)}$  defined to be solutions of the boundary value problems

$$\Delta \varphi^{(1,S)} = 4\pi G \rho^{(1,S)},\tag{3.26}$$

and

$$\Delta \varphi^{(1,F)} = 4\pi G \rho^{(1,F)},\tag{3.27}$$

subject to the boundary conditions

$$\left[\varphi^{(1,S)}\right]^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.28}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,S)} + 4\pi G \rho^{(0)} h^{(S)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma^{(S)}, \tag{3.29}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,S)}\right]^{+} = 0, \quad \mathbf{x} \in \Sigma^{(F)}, \tag{3.30}$$

and

$$\left[\varphi^{(1,F)}\right]^{+} = 0, \quad \mathbf{x} \in \Sigma,\tag{3.31}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,F)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma^{(S)}, \tag{3.32}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,F)} + 4\pi G \rho^{(0)} h^{(F)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma^{(F)}, \tag{3.33}$$

where we have defined  $\Sigma^{(S)} = \Sigma_{SS} \cup \Sigma_{SF} \cup \Sigma_{FS}$ , and  $\Sigma_{FF} = \Sigma^{(F)}$ . The superscripts (S) and (F) on the boundary perturbations h have also been introduced to indicate whether a given boundary perturbation acts on a boundary in  $\Sigma^{(S)}$  or  $\Sigma^{(F)}$ .

Making use of these notations, we can write eq.(3.15) as

$$-\nabla \hat{p}^{(1)} = \rho^{(0)} \nabla \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) + g \rho^{(1,F)} \hat{\mathbf{r}}, \tag{3.34}$$

where we have used the fact that  $\nabla \varphi^{(0)} = g\hat{\mathbf{r}}$  with  $\hat{\mathbf{r}}$  the unit vector in the radial direction. Taking the cross product of this equation with  $\hat{\mathbf{r}}$  we obtain the relation

$$0 = \hat{\mathbf{r}} \times \left\{ \nabla \hat{p}^{(1)} + \rho^{(0)} \nabla \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) + g \rho^{(1,F)} \hat{\mathbf{r}} \right\}$$

$$= \hat{\mathbf{r}} \times \left\{ \nabla \left[ \hat{p}^{(1)} + \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) \right] - \partial_r \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) \hat{\mathbf{r}} \right\}$$

$$= \hat{\mathbf{r}} \times \nabla \left\{ \hat{p}^{(1)} + \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) \right\}, \tag{3.35}$$

from which we readily deduce that the quantity  $\hat{p}^{(1)} + \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right)$  depends only upon the coordinate r. However, we know that  $\hat{p}^{(1)}$ ,  $\varphi^{(1,S)}$ , and  $\varphi^{(1,F)}$  all have zero mean

over any spherical surface, so we conclude that the identity

$$\hat{p}^{(1)} = -\rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right), \tag{3.36}$$

holds in  $M_F$ . The above equation shows that the aspherical part of the pressure perturbation in fluid-regions of the model is fully specified by knowledge of the perturbation in gravitational potential. From this relation and the boundary conditions for  $\hat{p}^{(1)}$  on  $\Sigma^{(F)}$  we also obtain the identity

$$h^{(F)} = -g^{-1} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right), \tag{3.37}$$

showing that the fluid-fluid boundary perturbations are also fully determined by the gravitational potential perturbation. Returning to eq.(3.34) we take the curl of both sides to obtain the relation

$$0 = \nabla \times \left\{ \rho^{(0)} \nabla \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) + g \rho^{(1,F)} \hat{\mathbf{r}} \right\}$$

$$= \partial_r \rho^{(0)} \mathbf{r} \times \nabla \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) + g \nabla \rho^{(1,F)} \times \hat{\mathbf{r}}$$

$$= \hat{\mathbf{r}} \times \nabla \left\{ \partial_r \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) - g \rho^{(1,F)} \right\}. \tag{3.38}$$

By an argument similar to that leading to eq.(3.36) we see that this equation implies the equality

$$\rho^{(1,F)} = g^{-1} \partial_r \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right), \tag{3.39}$$

showing that the density perturbation in fluid regions is also fully determined by the gravitational potential perturbation. Making use of eq.(3.39) and (3.37) the equation for  $\varphi^{(1,F)}$  can now be transformed into the equation

$$\Delta \varphi^{(1,F)} = \begin{cases} 4\pi G g^{-1} \partial_r \rho^{(0)} \left( \varphi^{(1,S)} + \varphi^{(1,F)} \right) & \mathbf{x} \in M_F \\ 0 & \mathbf{x} \in \mathbb{R}^3 \setminus M_F \end{cases} , \tag{3.40}$$

subject to the boundary conditions

$$\left[\varphi^{(1,F)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.41}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,F)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma^{(S)}, \tag{3.42}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1,F)} - 4\pi G g^{-1} \rho^{(0)} \left(\varphi^{(1,S)} + \varphi^{(1,F)}\right)\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma^{(F)}.$$
 (3.43)

From the above results, we conclude that in perturbing a spherically symmetric reference model with a hydrostatic equilibrium stress field the only free-parameters are:

- 1. the density perturbation in solid regions;
- 2. boundary perturbations to solid-solid and fluid-solid boundaries;

3. constant pressure perturbations in each connected component of the fluid regions.

Having specified these perturbations, the density perturbation in fluid regions, the pressure perturbation in fluid regions, and the fluid-fluid boundary perturbations are fully determined.

An interesting consequence of the above analysis is that lateral variations in density or boundary topography in the mantle or inner core of the Earth will induce lateral variations in density within the fluid outer core. As discussed in detail by Wahr & de Viers (1989), such lateral variations in the outer core are consistent with the conclusions of Stevenson (1987) who employed fluid-dynamical arguments to show that within the outer core surfaces of constant material properties should closely coincide with surfaces of constant gravitational potential. Based upon Stevenson's arguments, the existence of lateral heterogeneities within the outer core other than those induced by lateral density or boundary variations in the mantle or inner core seems unlikely. Indeed, any such density variations would be inconsistent with our assumption of stresses being hydrostatic in the outer core.

## 3.3 Solutions of the Equilibrium Equations

In this section, we shall be concerned with describing two ways of determining physically plausible particular solutions to the equilibrium equations. These equilibrium stress fields, once determined, can then be used as the stress field  $\mathbf{T}_m$  occurring in eq.(3.1) of the introduction.

In addressing this problem, it will be useful to generalize and simplify the form of the equilibrium equations given in the previous section. To do this we consider the problem of finding a symmetric tensor field  $\mathbf{T}$  defined in an open bounded region  $M \subseteq \mathbb{R}^3$  satisfying the equation

$$Div \mathbf{T} = \mathbf{f}, \tag{3.44}$$

for a given vector field f, subject to the inhomogeneous boundary conditions

$$[\hat{\mathbf{n}} \cdot \mathbf{T}]_{-}^{+} = \mathbf{t},\tag{3.45}$$

with  $\mathbf{t}$  a given vector field on  $\Sigma$ . Here M is now an arbitrary open bounded subset of  $\mathbb{R}^3$  with smooth external boundary denoted by  $\Sigma$ ; the modifications to the theory arising

from the presence of internal boundaries are, however, trivial.

### 3.3.1 Some notations and preliminary results

With the region M as above, we write  $L^2(M; \mathbb{R}^3)$  for the Hilbert space of real-valued vector fields defined in M that are square-integrable with respect to the inner product

$$(\mathbf{u}, \mathbf{v})_{L^2(M; \mathbb{R}^3)} = \int_M u_i v_i \, \mathrm{d}V. \tag{3.46}$$

Let  $L_s(\mathbb{R}^3)$  denote the vector space of real-valued symmetric second-order tensors. We shall write  $L^2(M; L_s(\mathbb{R}^3))$  for the Hilbert space of real-valued second-order symmetric tensor fields defined on M that are square integrable with respect to the inner product

$$(\mathbf{S}, \mathbf{T})_{L^{2}(M; L_{s}(\mathbb{R}^{3}))} = \int_{M} \frac{1}{2\eta} S_{ij} T_{ij} \, dV, \tag{3.47}$$

where  $\eta$  is a real-valued, everywhere positive (i.e. there exists a positive constant K such that  $\eta(\mathbf{x}) > K$  for all  $\mathbf{x} \in M$ ), and piecewise continuously differentiable function; The reason for introducing this weighting factor  $\eta$  will be clarified below.

The divergence operator Div was introduced informally in Section 2. To define this operator more precisely we must specify the domain D(Div) of second-order symmetric tensor fields on which it can act. To do this we let D(Div) be the linear subspace of  $L^2(M; L_s(\mathbb{R}^3))$  comprising those elements  $\mathbf{T} \in L^2(M; L_s(\mathbb{R}^3))$  for which  $Div\mathbf{T}$ , defined in the distributional sense, is an element of  $L^2(M; \mathbb{R}^3)$ . Clearly all elements  $\mathbf{T} \in L^2(M; L_s(\mathbb{R}^3))$  whose components have continuous first-order partial derivatives will be contained in D(Div). More generally, it may be shown that D(Div) is equal to the Sobolev space  $H^1(M; L_s(\mathbb{R}^3))$  comprising those elements of  $L^2(M; L_s(\mathbb{R}^3))$  whose first partial derivatives, taken in the distributional sense, are square integrable. It may also be shown that  $H^1(M; L_s(\mathbb{R}^3))$  is dense in  $L^2(M; L_s(\mathbb{R}^3))$ , and that the boundary tractions  $\hat{\mathbf{n}} \cdot \mathbf{T}$  on  $\Sigma$  of elements  $\mathbf{T} \in D(Div)$  are well-defined elements of the fractional Sobolev space  $H^{1/2}(\Sigma; \mathbb{R}^3)$  (e.g. Ting 1977, Georgescu 1980). Corresponding to the divergence operator we define its image to be the linear subspace of  $L^2(M; \mathbb{R}^3)$  given by

$$\operatorname{im}(\operatorname{Div}) = \{\operatorname{Div}\mathbf{T} \in L^2(M; \mathbb{R}^3) \mid \mathbf{T} \in \operatorname{D}(\operatorname{Div})\}, \tag{3.48}$$

and the kernel of Div to be the linear subspace of D(Div) defined by

$$\ker(\operatorname{Div}) = \{ \mathbf{T} \in \operatorname{D}(\operatorname{Div}) \mid \operatorname{Div}\mathbf{T} = 0 \}. \tag{3.49}$$

Similar definitions of the image and kernel apply to any linear operator between two vector

spaces.

The final concept we need to introduce is the adjoint of the divergence operator in the case that we restrict the action of Div to those elements of D(Div) satisfying the boundary condition  $[\hat{\mathbf{n}} \cdot \mathbf{T}]_{-}^{+} = \mathbf{0}$  on  $\Sigma$ . We denote the restriction of the divergence operator to this subspace as Div<sub>0</sub> and write D(Div<sub>0</sub>) for its domain. It follows from the continuity of the trace mapping that D(Div<sub>0</sub>) is a closed subset of  $H^{1}(M; L_{s}(\mathbb{R}^{3}))$ , and it may be shown that it is also dense in  $L^{2}(M; L_{s}(\mathbb{R}^{3}))$ . The adjoint operator Div<sub>0</sub>\* corresponding to Div<sub>0</sub> is defined as follows (e.g. Yosida 1980, Chapter VII, Section 2, Theorem 1): We say that a  $\mathbf{u} \in L^{2}(M; \mathbb{R}^{3})$  is in D(Div<sub>0</sub>\*) if there exists a  $\mathbf{u}^{*} \in L^{2}(M; L_{s}(\mathbb{R}^{3}))$  such that for all  $\mathbf{T} \in D(\text{Div}_{0})$  we have

$$(\text{Div}_0 \mathbf{T}, \mathbf{u})_{L^2(M:\mathbb{R}^3)} = (\mathbf{T}, \mathbf{u}^*)_{L^2(M:L_2(\mathbb{R}^3))}.$$
 (3.50)

For such  $\mathbf{u} \in D(Div_0^*)$  we define  $Div_0^*\mathbf{u}$  to equal  $\mathbf{u}^*$ , and so can write

$$\left(\operatorname{Div}_{0}\mathbf{T},\mathbf{u}\right)_{L^{2}(M;\mathbb{R}^{3})} = \left(\mathbf{T},\operatorname{Div}_{0}^{*}\mathbf{u}\right)_{L^{2}(M;L_{s}(\mathbb{R}^{3}))},\tag{3.51}$$

for all  $\mathbf{T} \in D(\operatorname{Div}_0)$ . From this identity it may be shown using the divergence theorem that  $D(\operatorname{Div}_0^*)$  is equal to  $H^1(M; \mathbb{R}^3)$ , and that the action of  $\operatorname{Div}_0^*$  on an element  $\mathbf{u} \in D(\operatorname{Div}_0^*)$  can be written

$$\operatorname{Div}_{0}^{*}\mathbf{u} = -2\eta \nabla_{s}\mathbf{u}, \tag{3.52}$$

where  $\nabla_s: H^k(M; \mathbb{R}^3) \to H^{k-1}(M; L_s(\mathbb{R}^3))$  denotes the symmetric gradient operator which is given in component form by

$$(\nabla_s \mathbf{u})_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}). \tag{3.53}$$

### 3.3.2 Orthogonal decomposition of the equilibrium stress fields

In this subsection, we describe an orthogonal decomposition theorem for second-order symmetric tensor fields which will allow us to determine a particular solution of the equilibrium equations. This decomposition theorem is a special case of a more general theorem for linear partial differential operators which may also be used to prove the Helmholtz decomposition theorem for vector fields, and the Hodge decomposition theorem for differential forms (Berger & Ebin 1969, Cantor 1981, Abraham et al.1991).

Particularly useful for our purposes are the results of Ting (1977) and Georgescu (1980),

who consider the decomposition of  $L^2(M; L_s(\mathbb{R}^3))$  in an open bounded region possessing a smooth boundary. The main result of interest is that  $L^2(M; L_s(\mathbb{R}^3))$  can be written as the orthogonal direct sum

$$L^{2}(M; L_{s}(\mathbb{R}^{3})) = \ker(\operatorname{Div}_{0}) \oplus \operatorname{im}(\operatorname{Div}_{0}^{*}), \tag{3.54}$$

where the operators  $\mathrm{Div}_0$  and  $\mathrm{Div}_0^*$  have been defined above (see Theorem 3.1 of Ting 1997, and Theorems 4.2 and 4.9 of Georgescu 1980). This result says that any element  $\mathbf{T} \in L^2(M; L_s(\mathbb{R}^3))$  can be written uniquely in the form

$$\mathbf{T} = -\mathrm{Div}_0^* \mathbf{u} + \mathbf{S},\tag{3.55}$$

for some  $\mathbf{u} \in \mathrm{D}(\mathrm{Div}_0^*)$  and  $\mathbf{S} \in \ker(\mathrm{Div}_0)$ , and that the two terms in the sum are orthogonal with respect to the inner product on  $L^2(M; L_s(\mathbb{R}^3))$  (we include a minus sign in the first term of this expression for later convenience). In particular, Theorem 4.9 of Georgescu (1980) shows that if  $\mathbf{T} \in \mathrm{D}(\mathrm{Div})$ , then the vector field  $\mathbf{u} \in \mathrm{D}(\mathrm{Div}_0^*)$  occurring in the above decomposition is such that  $\mathrm{Div}_0^*\mathbf{u} \in \mathrm{D}(\mathrm{Div})$ , which implies that  $\mathbf{u} \in H^2(M; \mathbb{R}^3)$ .

Because of this we can substitute the above expression for  $\mathbf{T} \in D(Div)$  into the boundary value problem at the start of this section and, making use of the expression for  $Div_0^*$  given above, obtain the equation

$$Div(2\eta\nabla_s\mathbf{u}) = \mathbf{f},\tag{3.56}$$

with the boundary conditions

$$[2\eta \hat{\mathbf{n}} \cdot \nabla_s \mathbf{u}]_{-}^{+} = \mathbf{t}, \tag{3.57}$$

on  $\Sigma$ . This boundary value problem for  $\mathbf{u}$  has exactly the same form as the static linear elastic displacement problem in M for a material with shear modulus  $\eta$  and bulk modulus  $\kappa = \frac{2}{3}\eta$  subject to the body force  $\mathbf{f}$  and surface tractions  $\mathbf{t}$ . The minus sign in the first term in eq.(3.55) and the form of the weighting factor used in the inner product on  $L^2(M; L_s(\mathbb{R}^3))$  were chosen so that this direct correspondence would arise.

As  $\eta$  has been assumed to be everywhere positive, we can use standard existence and uniqueness theorems (e.g. Marsden & Hughes 1983, Chapter 6, Theorem 1.11) to show that a solution  $\mathbf{u} \in H^2(M; L_s(\mathbb{R}^3))$  to this boundary value problem exists so long as the identity

$$\int_{M} \mathbf{f} \cdot (\mathbf{a} + \mathbf{B}\mathbf{x}) \, dV = -\int_{\Sigma} \mathbf{t} \cdot (\mathbf{a} + \mathbf{B}\mathbf{x}) \, dS, \tag{3.58}$$

holds for all constant vector fields  $\mathbf{a}$  and all constant anti-symmetric matrix fields  $\mathbf{B}$ . Physically this condition implies that the body forces and surface tractions apply no net force nor net torque to body. It may be shown that the solution  $\mathbf{u}$  to this boundary value problem is defined uniquely up to the addition of an element of  $\ker(\nabla_s)$  (i.e. a rigid rotation or translation). Consequently, solution of this boundary value problem yields a unique equilibrium stress field  $2\eta\nabla_s\mathbf{u}$ .

### 3.3.3 Minimum equilibrium stress fields

If we write  $||\mathbf{T}||_{L^2(M;L_s(\mathbb{R}^3))}$  for the norm on  $L^2(M;L_s(\mathbb{R}^3))$  induced by the given inner product, using eq.(3.54), we see that the squared norm of an equilibrium stress field  $\mathbf{T}$  is given by

$$||\mathbf{T}||_{L^{2}(M;L_{s}(\mathbb{R}^{3}))}^{2} = ||-\operatorname{Div}_{0}^{*}\mathbf{u}||_{L^{2}(M;L_{s}(\mathbb{R}^{3}))}^{2} + ||\mathbf{S}||_{L^{2}(M;L_{s}(\mathbb{R}^{3}))}^{2}, \tag{3.59}$$

where  $\mathbf{S} = \mathbf{T} + \mathrm{Div}_0^* \mathbf{u} \in \ker(\mathrm{Div}_0)$ , and  $\mathbf{u}$  is a solution of the boundary value problem just described. From this relation it is clear that the equilibrium stress field  $-\mathrm{Div}_0^* \mathbf{u}$  is the solution of the equilibrium equations that minimizes the norm-functional.

This result may also be established in a less formal manner by considering the variational problem to minimize the functional

$$I = \frac{1}{2} ||\mathbf{T}||_{L^2(M; L_s(\mathbb{R}^3))}^2, \tag{3.60}$$

subject to the constraint that  $\mathbf{T} \in D(Div)$  is also a solution of the equilibrium equations. To solve this problem, we introduce a Lagrange multiplier vector field  $\mathbf{u} \in D(Div_0^*)$ , and construct the augmented functional

$$I' = \frac{1}{2} ||\mathbf{T}||_{L^2(M; L_s(\mathbb{R}^3))}^2 + (\mathbf{u}, \text{Div}\mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)},$$
(3.61)

which incorporates the constraint that  $\mathbf{T}$  be a solution of the equilibrium equations. The first variation of functional with respect to the admissible variations  $\delta \mathbf{T} \in D(Div_0)$  and  $\delta \mathbf{u} \in D(Div_0^*)$  is found to be

$$\delta I' = (\mathbf{T}, \delta \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))} + (\mathbf{u}, \operatorname{Div}_0 \delta \mathbf{T})_{L^2(M; \mathbb{R}^3)} + (\delta \mathbf{u}, \operatorname{Div} \mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)}$$

$$= (\mathbf{T} + \operatorname{Div}_0^* \mathbf{u}, \delta \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))} + (\delta \mathbf{u}, \operatorname{Div} \mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)},$$
(3.62)

from which we see, using the density of  $D(Div_0)$  in  $L^2(M; L_s(\mathbb{R}^3))$  and of  $D(Div_0^*)$  in  $L^2(M; \mathbb{R}^3)$ , that the vanishing of  $\delta I'$  for all  $\delta \mathbf{T} \in D(Div_0)$  and  $\delta \mathbf{u} \in D(Div_0^*)$  does, as expected, lead to the relation  $\mathbf{T} = -Div_0^*\mathbf{u}$ , along with the boundary value problem for  $\mathbf{u}$  described above.

We shall call the resulting equilibrium stress field  $\mathbf{T} = -\mathrm{Div}_0^*\mathbf{u}$  the minimum equilibrium stress field for the earth model. Because, however, this equilibrium stress field depends upon the choice of inner product on  $L^2(M; L_s(\mathbb{R}^3))$  – as expressed by the function  $\eta$  – it is important to remember that this stress field is only a 'minimum' with respect to the given norm on  $L^2(M; L_s(\mathbb{R}^3))$ , and not in any absolute sense. It is readily seen that the equilibrium stress field obtained by the above method does not change if  $\eta$  is replaced by some positive scalar multiple of itself. It does depend upon spatial variations of  $\eta$ , and this property allows us to build in further a priori preferences into the minimum equilibrium stress field. For example, we might expect that the departure of the equilibrium stress field from its hydrostatic reference value would be larger (relative to the magnitude of the ambient hydrostatic stress) in the lithosphere than in the underlying mantle due to the occurrence of tectonic deformation. To incorporate this preference into the minimization problem, we can simply set the magnitude of  $\eta$  in the lithosphere larger than in the mantle, and so down-weight the effects of lithospheric stresses.

A modification of the above approach is to determine a solution of the equilibrium equations which minimizes the norm of its deviatoric component. Such an equilibrium stress field is of physical interest because it is likely that the deviatoric part of the equilibrium stress field in the Earth is relatively small due to its magnitude being strongly limited by the strength of rocks in the Earth's interior. To do this, we shall write  $\pi: L^2(M; L_s(\mathbb{R}^3)) \to L^2(M; L_s(\mathbb{R}^3))$  for the bounded linear operator mapping symmetric second-order tensor fields onto the linear subspace of trace-free symmetric second order tensor fields given by

$$\pi \mathbf{T} = \mathbf{T} - \frac{1}{3} \operatorname{tr}(\mathbf{T}) \mathbf{1}, \tag{3.63}$$

where  $tr(\mathbf{T}) = T_{ii}$  is the trace of a tensor field. It is clear that  $\pi$  is *idempotent* (i.e.  $\pi\pi = \pi$ ) so that it defines a projection operator. Moreover, a simple calculation shows that

$$(\pi \mathbf{S}, \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))} = (\mathbf{S}, \pi \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))},$$
 (3.64)

for any  $\mathbf{S}, \mathbf{T} \in L^2(M; L_s(\mathbb{R}^3))$ , so that  $\pi$  is self-adjoint and thus defines an orthogonal projection operator.

We wish to find the solution of the equilibrium equations that minimizes the functional

$$J = \frac{1}{2} ||\pi \mathbf{T}||_{L^2(M; L_s(\mathbb{R}^3))}^2.$$
 (3.65)

To solve this problem, we again introduce a Lagrange multiplier vector field  $\mathbf{u} \in D(Div_0^*)$ , and form the augmented functional

$$J' = \frac{1}{2} ||\pi \mathbf{T}||_{L^2(M; L_s(\mathbb{R}^3))}^2 + (\mathbf{u}, \text{Div}\mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)},$$
(3.66)

to incorporate the constraint that  $\mathbf{T}$  be an equilibrium stress field. The first variation of this functional with respect to the admissible variations  $\delta \mathbf{T} \in D(Div_0)$  and  $\delta \mathbf{u} \in D(Div_0^*)$  is found to be

$$\delta J' = (\pi \mathbf{T}, \pi \delta \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))} + (\mathbf{u}, \operatorname{Div}_0 \delta \mathbf{T})_{L^2(M; \mathbb{R}^3)} + (\delta \mathbf{u}, \operatorname{Div} \mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)}$$

$$= (\pi \mathbf{T} + \operatorname{Div}_0^* \mathbf{u}, \delta \mathbf{T})_{L^2(M; L_s(\mathbb{R}^3))} + (\delta \mathbf{u}, \operatorname{Div} \mathbf{T} - \mathbf{f})_{L^2(M; \mathbb{R}^3)}, \tag{3.67}$$

where we have made use of the fact that  $\pi$  is self-adjoint and idempotent. The vanishing of  $\delta J'$  for arbitrary  $\delta \mathbf{T} \in D(Div_0)$  implies the relation

$$\pi \mathbf{T} = -\mathrm{Div}_0^* \mathbf{u},\tag{3.68}$$

which in turn implies that

$$\operatorname{tr}(\operatorname{Div}_{0}^{*}\mathbf{u}) = 0. \tag{3.69}$$

Making use of the expression for the adjoint operator  $\operatorname{Div}_0^*$  given above, we see that the first of these equations can be written

$$\pi \mathbf{T} = 2\eta \nabla_s \mathbf{u},\tag{3.70}$$

while the second becomes

$$\operatorname{div}\mathbf{u} = 0. \tag{3.71}$$

Because eq.(3.70) only specifies the trace-free part of the stress tensor  $\mathbf{T}$ , it follows that the full relation between  $\mathbf{T}$  and  $\mathbf{u}$  takes the form

$$\mathbf{T} = -p\mathbf{1} + 2\eta \nabla_s \mathbf{u},\tag{3.72}$$

where p is a scalar field which is defined such that  $p = -\frac{1}{3} \text{tr}(\mathbf{T})$  but is otherwise unconstrained. Inspection of eq.(3.71) and eq.(3.72) shows that the relationship between the stress tensor  $\mathbf{T}$  and the Lagrange multiplier field  $\mathbf{u}$  has exactly the same form as the constitutive equation of an incompressible Newtonian fluid with velocity vector  $\mathbf{u}$ , pressure p, and viscosity  $\eta$  (e.g. Batchelor 1967).

Assuming that the fields  $\mathbf{u}$  and p are sufficiently well-behaved, we can insert these expressions into the boundary value problem at the start of this section to obtain the equation

$$-\nabla p + \text{Div}(2\eta \nabla_s \mathbf{u}) = \mathbf{f},\tag{3.73}$$

which is subject to the incompressibility condition in eq. (3.71) and to the boundary con-

ditions

$$[-p\hat{\mathbf{n}} + 2\eta\hat{\mathbf{n}} \cdot \nabla_s \mathbf{u}]_{-}^{+} = \mathbf{t}, \tag{3.74}$$

on  $\Sigma$ . This boundary value problem is formally identical to the steady-state Navier-Stokes equations for an incompressible viscous fluid subject to the given body forces and surface tractions. Using existence and uniqueness theorems for the steady-state Navier-Stokes equations (e.g. Sohr 2000) we can conclude that solution of this problem leads to an uniquely determined equilibrium stress field so long as the conditions on  $\mathbf{f}$  and  $\mathbf{t}$  given in eq.(3.58) hold.

We shall refer to the resulting equilibrium stress field as the minimum deviatoric equilibrium stress field for the earth model. As with the case of the minimum equilibrium stress field, the equilibrium stress field obtained by solving this problem does not depend on the absolute magnitude of  $\eta$ , but only upon its spatial variations. Because of this, we can again make use of spatial variations in  $\eta$  to incorporate further a priori preferences about the form of the equilibrium stress field into the minimization problem.

To conclude this section, we consider a particularly interesting property of the minimum deviatoric equilibrium stress field. To do this, we first recall some basic facts about the elastic tensor of an earth model with a non-zero equilibrium stress field following the discussion given in Section 3.6 of Dahlen & Tromp (1998). Let us denote by s the infinitesimal displacement vector describing the deformation of the earth model away from its equilibrium configuration, and by  $\mathbf{T}^{L1}$  the incremental Lagrangian stress tensor resulting from this deformation (though there are a number of other measures of stress that can be used, the incremental Lagrangian stress tensor is most useful for our present purposes). It may be shown that s and  $\mathbf{T}^{L1}$  are related by the constitutive equation

$$T_{ij}^{L1} = \Upsilon_{ijkl} s_{k,l}, \tag{3.75}$$

where  $\Upsilon_{ijkl}$  is a tensor with the symmetries  $\Upsilon_{ijkl} = \Upsilon_{klij}$  (see eq.(3.121) and eq.(3.125) of Dahlen & Tromp 1998), while the *principle of material frame indifference* leads to the relation

$$\Upsilon_{ijkl} = \Gamma_{ijkl} + \frac{1}{2} \left( T_{kl} \delta_{ij} - T_{ij} \delta_{kl} + T_{ik} \delta_{jl} - T_{jl} \delta_{ik} + T_{jk} \delta_{il} - T_{il} \delta_{jk} \right), \tag{3.76}$$

where  $\Gamma_{ijkl}$  is a tensor possessing the symmetries

$$\Gamma_{ijkl} = \Gamma_{iikl} = \Gamma_{ijlk} = \Gamma_{klij}, \tag{3.77}$$

and  $T_{ij}$  denotes the components of the equilibrium stress field in the earth model (see eq.(3.141) of Dahlen & Tromp 1998, and also eq.(4) of Dahlen 1972c). This expression can be regarded as splitting the elastic tensor  $\Upsilon_{ijkl}$  into the sum of an *intrinsic elastic tensor*  $\Gamma_{ijkl}$  and a second term which depends explicitly upon the equilibrium stress field. It is not difficult to show that the second term on the right hand side of eq.(3.76) does not depend on the hydrostatic component of the equilibrium stress field, so that we can replace  $T_{ij}$  in the above expression with its deviatoric component for which we write  $\tau_{ij}$ . We recall that the elastic tensor  $\Upsilon_{ijkl}$  is said to be *isotropic* if it takes the form

$$\Upsilon_{ijlk} = (\kappa - \frac{2}{3}\mu)\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{3.78}$$

where  $\kappa$  and  $\mu$  are, respectively, the bulk and shear moduli of the earth model. When this condition is not met we say that  $\Upsilon_{ijkl}$  is anisotropic. From eq.(3.76) we see that anisotropy in  $\Upsilon_{ijkl}$  can be due to either (i) intrinsic anisotropy of the tensor  $\Gamma_{ijkl}$  arising from, for example, the preferential alignment of crystallographic axes, or (ii) stress-induced anisotropy due to the deviatoric component of the equilibrium stress field. A simple measure of the magnitude of any stress-induced anisotropy in the earth model is

$$\int_{M} (\Upsilon_{ijkl} - \Gamma_{ijkl}) (\Upsilon_{ijkl} - \Gamma_{ijkl}) \, dV, \tag{3.79}$$

and a routine calculation shows that this is equal to

$$\frac{9}{4} \int_{M} \tau_{ij} \tau_{ij} \, \mathrm{d}V. \tag{3.80}$$

This implies that the equilibrium stress field which minimizes the magnitude of stressinduced anisotropy in the earth model (in the sense just defined) is precisely the *minimum* deviatoric equilibrium stress field in the case that the weighting function  $\eta$  in the definition of the scalar product on  $L^2(M; L_s(\mathbb{R}^3))$  is equal to an arbitrary positive constant.

# 3.4 Divergence-Free Tensor Fields in Spherically Symmetric Earth Models

In this section, we consider how elements of the vector space  $ker(Div_0)$  can be practically constructed. The results of section 2 show that for our purposes such tensor fields need only be generated in the solid regions of a spherically symmetric reference earth model. Taking PREM of Dziewonski & Anderson (1981) as an example, we shall suppose that the earth model has a solid inner core, a fluid outer core, a solid mantle and crust, and a fluid

ocean. Consequently we require a method for generating elements of  $\ker(\operatorname{Div}_0)$  within the inner core and solid mantle of the earth model. For simplicity we shall focus attention on the construction of elements of  $\ker(\operatorname{Div}_0)$  within the mantle and crust of the earth model. Essentially the same method can be used in the inner core, though in this case we must deal with the added complication of insuring that the tensor fields are regular at the center of the earth model.

We assume that the mantle and crust of the earth model occupies the spherical shell with inner radius  $r_1$  and outer radius  $r_n$ , and that there are n-2 internal spherical boundaries with radii  $r_1 < r_2 < \ldots < r_{n-1} < r_n$ . Denoting this spherical shell by M and the union of all internal and external boundaries by  $\Sigma$ , we then wish to generate symmetric second-order tensor fields  $\mathbf{T} \in D(\mathrm{Div}_0)$ . To do this we shall, essentially, use the method of Backus (1967) specialized to the case of divergence-free and traction-free tensor fields. In doing this we shall not, however, make use of Backus's representation theorem for the tensor fields in terms of six scalar potential functions (Backus 1966). Instead we express our results in terms of the generalized spherical harmonic functions of Phinney & Burridge (1973) whose use is now more common (see also Dahlen & Tromp 1998, Appendix C).

In this formalism, an arbitrary element  $\mathbf{T} \in D(Div_0)$  can be expanded in terms of generalized spherical harmonics as

$$\mathbf{T}(r,\theta,\varphi) = \sum_{lm} T_{lm}^{\alpha\beta}(r) Y_{lm}^{N}(\theta,\varphi) \hat{\mathbf{e}}_{\alpha} \otimes \hat{\mathbf{e}}_{\beta}, \tag{3.81}$$

where the coefficient functions  $T_{lm}^{\alpha\beta}$  are piecewise continuously differentiable functions of r, summation over repeated Greek indices is implied in the range  $\{-,0,+\}$ ,  $\mathbf{e}_{\alpha}$  is a unit vector in the canonical basis, and  $Y_{lm}^{N}$  is a generalized spherical harmonic of degree l, order m, and upper index  $N = \alpha + \beta$ . Because  $\mathbf{T}$  is a symmetric tensor field the radial expansion coefficients  $T_{lm}^{\alpha\beta}$  have the symmetry

$$T_{lm}^{\alpha\beta} = T_{lm}^{\beta\alpha}. (3.82)$$

In addition, the requirement that T be real-valued implies

$$T_{l-m}^{-\alpha-\beta} = (-1)^m \overline{T_{lm}^{\alpha\beta}}, \tag{3.83}$$

where the over-line denotes complex-conjugation (this relationship follows from (C.107) of Dahlen & Tromp (1998)). Due to these conditions we see that for each  $l \geq 0$  we need only consider values of m in the range  $0, 1, \ldots, l$ , and that for each l and m there are only six independent coefficient functions  $T_{lm}^{\alpha\beta}$ .

The condition that  $Div \mathbf{T} = \mathbf{0}$  is expressed for each value of l and m in terms of the three ordinary differential equations

$$\partial_r T_{lm}^{-0} + 3r^{-1} T_{lm}^{-0} - \Omega_l^0 r^{-1} T_{lm}^{-+} - \Omega_l^2 r^{-1} T_{lm}^{--} = 0, (3.84)$$

$$\partial_r T_{lm}^{00} + 2r^{-1} \left( T_{lm}^{00} + T_{lm}^{-+} \right) - \Omega_l^0 r^{-1} \left( T_{lm}^{-0} + T_{lm}^{0+} \right) = 0, \tag{3.85}$$

$$\partial_r T_{lm}^{0+} + 3r^{-1} T_{lm}^{0+} - \Omega_l^0 r^{-1} T_{lm}^{-+} - \Omega_l^2 r^{-1} T_{lm}^{++} = 0, (3.86)$$

where  $\Omega_l^N = \sqrt{(l+N)(l-N+1)/2}$ . Similarly, the traction free-boundary conditions for the problem become

$$[T_{lm}^{-0}(r_i)]_{-}^{+} = 0, (3.87)$$

$$\left[T_{lm}^{00}(r_i)\right]_{-}^{+} = 0, (3.88)$$

$$\left[T_{lm}^{0+}(r_i)\right]_{-}^{+} = 0, (3.89)$$

where i = 1, ..., n, and it is understood that the radial coefficient functions vanish for r outside the interval  $[r_1, r_n]$ .

At this stage it will be useful to introduce six new radial coefficient functions for each l and m through the equations

$$T_{lm}^{--} = 2\Omega_l^0 \Omega_l^2 (M_{lm} - iN_{lm}),$$
 (3.90)

$$T_{lm}^{-0} = \Omega_l^0 (S_{lm} - iT_{lm}), \qquad (3.91)$$

$$T_{lm}^{-+} = L_{lm},$$
 (3.92)

$$T_{lm}^{00} = R_{lm}, (3.93)$$

$$T_{lm}^{0+} = \Omega_l^0 \left( S_{lm} + i T_{lm} \right),$$
 (3.94)

$$T_{lm}^{++} = 2\Omega_l^0 \Omega_l^2 \left( M_{lm} + i N_{lm} \right), \tag{3.95}$$

which correspond to the toroidal and poloidal combinations of Phinney & Burridge (1973). In terms of these new functions, equations (3.84) to (3.86) are seen to decouple into the two-dimensional system

$$\partial_r R_{lm} + 2r^{-1} \left( R_{lm} + L_{lm} \right) - \zeta^2 r^{-1} S_{lm} = 0, \tag{3.96}$$

$$\partial_r S_{lm} + 3r^{-1} S_{lm} - r^{-1} L_{lm} - (\zeta^2 - 2)r^{-1} M_{lm} = 0, \tag{3.97}$$

and the one-dimensional system

$$\partial_r T_{lm} + 3r^{-1} T_{lm} - (\zeta^2 - 2)r^{-1} N_{lm} = 0, \tag{3.98}$$

where  $\zeta = \sqrt{l(l+1)}$ , while the boundary conditions become

$$[R_{lm}(r_i)]_{-}^{+} = 0, (3.99)$$

$$[S_{lm}(r_i)]_{-}^{+} = 0, (3.100)$$

$$[T_{lm}(r_i)]_{-}^{+} = 0, (3.101)$$

for i = 1, ..., n. We shall call any tensor field for which  $T_{lm} = N_{lm} = 0$  a spheroidal tensor field, and any tensor field for which  $R_{lm} = S_{lm} = L_{lm} = M_{lm} = 0$  a toroidal tensor field. In deriving the equations (3.96) to (3.98) we have assumed that  $l \ge 1$  so that  $\Omega_l^0 \ne 0$ . In the special case l = 0 only  $T_{00}^{00}$  and  $T_{00}^{-+}$  can be non-zero due to the fact that  $Y_{lm}^N = 0$  if |N| > l. From this we see that in the case l = 0 eq.(3.84) and eq.(3.86) are satisfied identically, while eq.(3.85) becomes

$$\partial_r R_{00} + 2r^{-1} (R_{00} + L_{00}) = 0.$$
 (3.102)

Let us first consider how to generate toroidal elements of ker(Div<sub>0</sub>). It is clear from eq.(3.98) that if we let  $T_{lm}$  be an arbitrarily piecewise differentiable function in  $[r_1, r_n]$  we can obtain a divergence-free toroidal tensor field by setting

$$N_{lm} = \frac{1}{\zeta^2 - 2} \left( r \partial_r T_{lm} + 3T_{lm} \right), \tag{3.103}$$

where we have assumed that  $l \geq 2$ . Moreover, by requiring that the given function  $T_{lm}$  be continuous across all internal boundaries  $r_2, \ldots, r_{n-1}$ , and that it vanish at  $r_1$  and  $r_n$ , we obtain a toroidal element of ker(Div<sub>0</sub>). We have seen above that there are no toroidal tensor fields in the case l = 0. Similarly in the case l = 1 it follows from  $Y_{1m}^{\pm 2} = 0$  that  $N_{1m} = 0$ , so we can solve eq.(3.98) to obtain  $T_{1m} = cr^{-3}$  where c is an arbitrary constant. However, it is clear that  $T_{1m} = cr^{-3}$  cannot satisfy the boundary conditions  $T_{1m}(r_1) = T_{1m}(r_n) = 0$  for any non-zero value of the constant c, and we conclude that there are no non-trivial toroidal elements of ker(Div<sub>0</sub>) for l = 1.

We can construct spheroidal elements of  $ker(Div_0)$  by a similar process. From eq.(3.96) and (3.97) it is readily seen that  $L_{lm}$  and  $M_{lm}$  can be expressed in terms of  $R_{lm}$  and  $S_{lm}$  by the expressions

$$L_{lm} = \frac{1}{2} \left[ \zeta^2 S_{lm} - r \partial_r R_{lm} - 2R_{lm} \right], \qquad (3.104)$$

$$M_{lm} = \frac{1}{2(\zeta^2 - 2)} \left[ r \partial_r R_{lm} + 2R_{lm} + 2r \partial_r S_{lm} - (\zeta^2 - 6) S_{lm} \right], \tag{3.105}$$

where we have again assumed  $l \geq 2$ . From this we see that if we arbitrarily specify  $R_{lm}$  and  $S_{lm}$  to be piecewise differentiable functions in  $[r_1, r_n]$  such that they are continuous at each internal boundary  $r_2, \ldots, r_{n-1}$  and vanish at the end points  $r_1$  and  $r_n$ , then we obtain a spheroidal element of  $\ker(\text{Div}_0)$ . In the case l = 0 we have seen that only eq.(3.102) need

be satisfied, and this may be achieved by setting

$$L_{00} = -\frac{1}{2} \left( r \partial_r R_{00} + 2R_{00} \right), \tag{3.106}$$

for any function  $R_{00}$  that is continuous, piecewise differentiable in  $[r_1, r_n]$ , and vanishes at the endpoints of the interval. In the case l = 1 we must have  $M_{1m} = 0$ , and eq.(3.96) and eq.(3.97) reduce to

$$\partial_r R_{1m} + 2r^{-1} \left( R_{1m} + L_{1m} \right) - 2r^{-1} S_{1m} = 0, \tag{3.107}$$

$$\partial_r S_{1m} + 3r^{-1}S_{1m} - r^{-1}L_{1m} = 0. (3.108)$$

Solving the second of these equations for  $L_{1m}$  leads to

$$L_{1m} = r\partial_r S_{1m} + 3S_{1m}, (3.109)$$

which, when substituted in eq.(3.96), gives

$$\partial_r \left( R_{1m} + 2S_{1m} \right) + 2r^{-1} \left( R_{1m} + 2S_{1m} \right) = 0. \tag{3.110}$$

Using the required continuity of  $R_{1m}$  and  $S_{1m}$ , we see that this latter equation implies that

$$R_{1m} + 2S_{1m} = cr^{-2}, (3.111)$$

with c some constant. However, the boundary conditions on  $R_{1m}$  and  $S_{1m}$  are such that this constant c must equal zero, and we conclude that the identity

$$R_{1m} = -2S_{1m}, (3.112)$$

must hold for all spheroidal elements of ker(Div) in the case l = 1. If we choose the function  $S_{1m}$  in eq.(3.112) to be continuous, piecewise differentiable in  $[r_1, r_n]$ , and to vanish at  $r_1$  and  $r_n$ , then the above formulae give a spheroidal element of ker(Div<sub>0</sub>) for l = 1.

Let us denote by  $\mathscr{C}$  the vector space of complex-valued scalar functions defined on  $[r_1, r_n]$  that are piecewise continuously differentiable, vanish at the endpoints  $r_1$  and  $r_n$ , and are continuous across the internal boundaries  $r_2, \ldots, r_{n-1}$ . In terms of these functions we can summarize the above results as follows:

- 1. For l=0 there is one spheroidal element of  $\ker(\operatorname{Div}_0)$  corresponding to each element of  $\mathscr{C}$ .
- 2. For l=1 and for each m=0,1 there is one spheroidal element of  $\ker(\operatorname{Div}_0)$  corresponding to each element of  $\mathscr C$ .
- 3. For  $l \geq 2$  and each m = 0, 1, ..., l there is one toroidal element of  $\ker(\operatorname{Div}_0)$  corresponding to each element of  $\mathscr{C}$ , and there is one spheroidal element of  $\ker(\operatorname{Div}_0)$  corresponding to each pair of elements of  $\mathscr{C}$ .

To apply these results practically we must be able to generate a number of elements of  $\mathscr{C}$ . Clearly there are many possible ways of doing this. For example, elements of  $\mathscr{C}$  can be readily produced using cubic spline interpolation, or with Lagrange polynomial interpolation.

# 3.5 Numerical Methods and Example Calculations

To illustrate the theory presented, we now consider the numerical calculation of minimum equilibrium stress fields in a laterally heterogeneous earth model. A similar approach can be used to determine minimum deviatoric equilibrium stress fields, though, as yet, this has not been implemented.

# 3.5.1 The laterally heterogeneous earth model

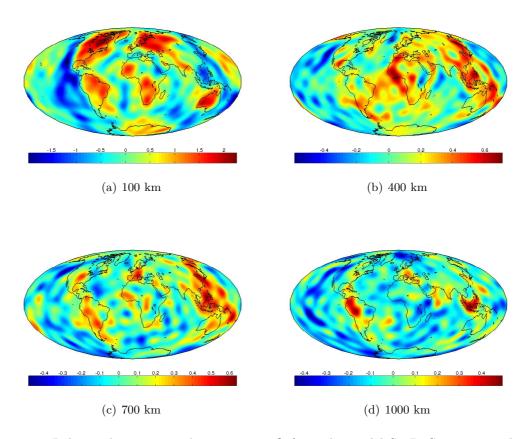


Figure 3.1: Relative density perturbations  $100 \times \delta \rho/\rho$  in the model S20RTS at various depths. Note that the scale differs from figure to figure, with the largest density variations being present at shallower depths.

For the calculations we use the mantle model S20RTS of Ritsema *et al.*(1999). This model specifies perturbations in shear wave velocity in the mantle relative to the spherically symmetric reference model PREM. These perturbations are parametrized radially in spline functions, and angularly in spherical harmonics up to degree twenty. To obtain density perturbations, we use the scaling relation

$$\delta \rho / \rho = 0.3 \, \delta v_s / v_s, \tag{3.113}$$

whose plausibility is suggested by mineral physics experiments (e.g. Karato 1993). Unfortunately, this scaling relation is not likely to be applicable to the whole of the mantle. In particular, under continental cratons there are large positive shear velocity anomalies in S20RTS, which correspond – through the above relation – to positive density perturbations. It is, however, more probable that there exist *negative* density perturbations under continental cratons associated with buoyant crustal material. Nonetheless, it is thought that the density model used in the calculations is sufficiently realistic to allow for preliminary estimates of the magnitude of realistic equilibrium stress fields, and to assess the likely significance for seismic wave propagation.

We have also incorporated a simplified version of the crustal model CRUST5.0 (Mooney et al. 1998). This crustal model was obtained from CRUST5.0 by vertically averaging the specified seven-layer crustal model into a three-layer crustal model corresponding to that used in PREM, retaining topography on the Moho, a mid-crustal discontinuity, and the sea-floor. In this process we insured that the total mass of the crust was conserved in each vertical column. The averaged crustal model was then expanded up to degree twenty in spherical harmonics to match the parametrization of the mantle model. In figure 3.1 is shown a number of depth slices of the density model used in the calculations.

# 3.5.2 Calculation of the gravitational potential

To calculate the perturbed gravitational potential, we must solve the boundary value problems stated in equations (3.26) and (3.40) along with the associated boundary conditions. Let us define a function  $\chi_M$  on  $\mathbb{R}^3$  such that

$$\chi_M = \begin{cases} 1 & \mathbf{x} \in M_F \\ 0 & \mathbf{x} \in \mathbb{R}^3 \setminus M_F \end{cases} , \tag{3.114}$$

and another function  $\chi_{\Sigma}$  on  $\Sigma$  such that

$$\chi_{\Sigma} = \begin{cases} 1 & \mathbf{x} \in \Sigma^{(F)} \\ 0 & \mathbf{x} \in \Sigma^{(S)} \end{cases}$$
 (3.115)

We can then combine the above two boundary value problems into the single equation

$$\Delta \varphi^{(1)} - 4\pi G \chi_M g^{-1} \partial_r \rho^{(0)} \varphi^{(1)} = 4\pi G (1 - \chi_M) \rho^{(1)}, \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.116}$$

subject to the boundary conditions

$$\left[\varphi^{(1)}\right]_{-}^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.117}$$

$$\left[\hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} - 4\pi G \rho^{(0)} \left\{ \chi_{\Sigma} g^{-1} \varphi^{(1)} - (1 - \chi_{\Sigma}) h^{(S)} \right\} \right]^{+} = 0, \quad \mathbf{x} \in \Sigma, \tag{3.118}$$

along with the condition that  $\varphi^{(1)}$  vanishes at infinity.

To solve this boundary value problem, we first express the equations in their weak form. Let  $\zeta$  be a complex-valued function defined in  $\mathbb{R}^3$  that is continuous in M and vanishes identically in  $\mathbb{R}^3 \setminus M$ . Multiplying eq.(3.116) by  $\overline{\zeta}$  (where here the overline denotes complex conjugation), and integrating over M, we obtain

$$\int_{M} \Delta \varphi^{(1)} \overline{\zeta} \, dV - 4\pi G \int_{M_F} g^{-1} \partial_r \rho^{(0)} \varphi^{(1)} \overline{\zeta} \, dV = 4\pi G \int_{M_S} \rho^{(1)} \overline{\zeta} \, dV. \tag{3.119}$$

Using the divergence theorem, we see that

$$\int_{M} \Delta \varphi^{(1)} \overline{\zeta} \, dV = -\int_{M} \nabla \varphi^{(1)} \cdot \nabla \overline{\zeta} \, dV - \int_{\Sigma} \left[ \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \overline{\zeta} \right]_{-}^{+} dS, \tag{3.120}$$

and as  $\zeta$  vanishes outside of M, the surface integral above can be written

$$\int_{\Sigma} \left[ \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \overline{\zeta} \right]_{-}^{+} dS = \int_{\Sigma \setminus \partial M} \left[ \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \overline{\zeta} \right]_{-}^{+} dS - \int_{\partial M} \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \Big|_{-} \overline{\zeta} dS, \tag{3.121}$$

where  $\nabla \varphi^{(1)}|_{-}$  denotes the value of  $\nabla \varphi^{(1)}$  on the underside of  $\partial M$ . From the boundary condition in eq.(3.118), we find that

$$\int_{\Sigma} \left[ \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \overline{\zeta} \right]_{-}^{+} = 4\pi G \int_{\Sigma^{(F)}} g^{-1} \left[ \rho^{(0)} \right]_{-}^{+} \varphi^{(1)} \overline{\zeta} \, dS$$

$$-4\pi G \int_{\Sigma^{(S)}} \left[ \rho^{(0)} \right]_{-}^{+} h^{(S)} \overline{\zeta} \, dS$$

$$- \int_{\partial M} \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \Big|_{+} \overline{\zeta} \, dS, \tag{3.122}$$

where  $\nabla \varphi^{(1)}|_{+}$  denotes the value of  $\nabla \varphi^{(1)}$  on the outside of  $\partial M$ . Substituting this expression into eq.(3.119), we obtain

$$-\int_{M} \nabla \varphi^{(1)} \cdot \nabla \overline{\zeta} \, dV - 4\pi G \int_{\Sigma^{(F)}} g^{-1} \left[ \rho^{(0)} \right]_{-}^{+} \varphi^{(1)} \overline{\zeta} \, dS$$

$$+ \int_{\partial M} \hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \Big|_{+} \overline{\zeta} \, dS - 4\pi G \int_{M_{F}} g^{-1} \partial_{r} \rho^{(0)} \varphi^{(1)} \overline{\zeta} \, dV$$

$$= 4\pi G \int_{M_{S}} \rho^{(1)} \overline{\zeta} \, dV - 4\pi G \int_{\Sigma^{(S)}} \left[ \rho^{(0)} \right]_{-}^{+} h^{(S)} \overline{\zeta} \, dS. \tag{3.123}$$

To deal with the term  $\nabla \varphi^{(1)}|_+$  we recall that  $\varphi^{(1)}$  is harmonic in  $\mathbb{R}^3 \setminus M$  and vanishes at

infinity. From this condition, we find that exterior to the earth model

$$\varphi^{(1)}(r,\theta,\phi) = \sum_{lm} \left(\frac{b}{r}\right)^{l+1} \varphi_{lm}^{(1)}(b) Y_{lm}^{(0)}(\theta,\phi), \quad r \ge b, \tag{3.124}$$

where  $\varphi_{lm}^{(1)}(b)$  is the (l,m)-th spherical harmonic expansion coefficient of  $\varphi^{(1)}|_{\partial M}$ , and so we obtain

$$\hat{\mathbf{n}} \cdot \nabla \varphi^{(1)} \big|_{+} = -\sum_{lm} \frac{l+1}{b} \varphi_{lm}^{(1)}(b) Y_{lm}^{0}(\theta, \phi). \tag{3.125}$$

Substituting this formula into eq.(3.123), we find after some reduction

$$-\int_{M} \nabla \varphi^{(1)} \cdot \nabla \overline{\zeta} \, dV - 4\pi G \int_{\Sigma^{(F)}} g^{-1} \left[ \rho^{(0)} \right]_{-}^{+} \varphi^{(1)} \overline{\zeta} \, dS$$

$$-\sum_{lm} (l+1)b \varphi_{lm}^{(1)}(b) \overline{\zeta_{lm}(b)} - 4\pi G \int_{M_{F}} g^{-1} \partial_{r} \rho^{(0)} \varphi^{(1)} \overline{\zeta} \, dV$$

$$= 4\pi G \int_{M_{S}} \rho^{(1)} \overline{\zeta} \, dV - 4\pi G \int_{\Sigma^{(S)}} \left[ \rho^{(0)} \right]_{-}^{+} h^{(S)} \overline{\zeta} \, dS, \qquad (3.126)$$

where  $\zeta_{lm}(b)$  are the spherical harmonic expansion coefficients of  $\zeta_{l\partial M}$ . We have seen that a solution  $\varphi^{(1)}$  of the boundary problem satisfies the above equation. Conversely, it may be shown that if this equation is satisfied for all suitably smooth functions  $\zeta$ , then  $\varphi^{(1)}$  is a solution of the boundary value problem.

To simplify the problem, we now expand  $\varphi^{(1)}$  in terms of spherical harmonics as

$$\varphi^{(1)}(r,\theta,\phi) = \sum_{lm} \varphi_{lm}^{(1)}(r) Y_{lm}^{(0)}(\theta,\phi), \qquad (3.127)$$

while, making use of the rules for contravariant differentiation (Phinney & Burridge 1973, Dahlen & Tromp 1998), we obtain

$$\nabla \varphi^{(1)}(r,\theta,\phi) = \sum_{l'm'} \varphi_{lm}^{(1)|\alpha}(r) Y_{lm}^{\alpha}(\theta,\phi) \hat{\mathbf{e}}_{\alpha}, \qquad (3.128)$$

where

$$\varphi_{lm}^{(1)|0} = \partial_r \varphi_{lm}^{(1)}, \qquad (3.129)$$

$$\varphi_{lm}^{(1)|\pm} = \Omega_l^0 r^{-1} \varphi_{lm}^{(1)}. \tag{3.130}$$

Setting

$$\zeta(r,\theta,\phi) = \zeta_{lm}(r)Y_{lm}^0(\theta,\phi), \tag{3.131}$$

for a given value of (l, m), we find that eq. (3.126) reduces to

$$-\int_{I} \partial_{r} \varphi_{lm}^{(1)}(r) \, \overline{\partial_{r} \zeta_{lm}}(r) \, r^{2} \, dr - l(l+1) \int_{I} \varphi_{lm}^{(1)}(r) \, \overline{\zeta_{lm}(r)} \, dr$$

$$-4\pi G \sum_{r \in d_{F}} g(r)^{-1} \left[ \rho^{(0)}(r) \right]_{-}^{+} \varphi_{lm}^{(1)}(r) \, \overline{\zeta_{lm}(r)} r^{2} - (l+1) b \, \varphi_{lm}^{(1)}(b) \overline{\zeta_{lm}}(b)$$

$$-4\pi G \int_{I_{F}} g(r)^{-1} \partial_{r} \rho(r) \varphi_{lm}^{(1)}(r) \, \overline{\zeta_{lm}(r)} r^{2} \, dr$$

$$= 4\pi G \int_{I_{S}} \rho_{lm}^{(1)}(r) \overline{\zeta_{lm}(r)} \, r^{2} \, dr - 4\pi G \sum_{r \in d_{S}} \left[ \rho^{(0)}(r) \right]_{-}^{+} h_{lm}^{(S)} \, \overline{\zeta}_{lm}(r) r^{2}, \qquad (3.132)$$

where I = (0, b),  $I_S$  and  $I_F$  denote the subsets of I lying in  $M_S$  and  $M_F$ , respectively, and  $d_S$  and  $d_F$  comprise, respectively, the radii of boundaries in  $\Sigma^{(S)}$  and  $\Sigma^{(F)}$ .

We have now reduced calculation of  $\varphi^{(1)}$  to the solution of eq.(3.132) for those values of (l,m) for which either  $\rho_{lm}^{(1)}$  or  $h_{lm}^{(S)}$  are non-zero. To numerically solve this equation we expand  $\varphi_{lm}^{(1)}$  in a finite set of radial basis functions

$$\varphi_{lm}^{(1)}(r) = \sum_{n=1}^{N} \varphi_{lmn}^{(1)} \eta_n(r), \tag{3.133}$$

such that each function  $\eta_n(r)$  is continuous in I. Taking in turn  $\zeta_{lm}(r) = \eta_n(r)$ , we then obtain a system of N linear equations for the expansion coefficients  $\varphi_{lmn}^{(1)}$ . In practice, we use Lagrange polynomials defined on a grid, the nodes of which are taken to be the so-called GLL-points used in the Spectral Element Method (e.g. Komatitsch & Tromp 1998). The resulting system of linear equations has a banded structure, so that its numerical solution is very efficient.

## 3.5.3 Radial sensitivity kernels for gravitational potential perturbations

In the previous subsection we described a numerical method for calculating the perturbation in the gravitational potential  $\varphi^{(1)}$  associated with a given laterally heterogeneous earth model. The surface value of the potential perturbation can be compared with the observations, and so provide constraints on density and boundary perturbations in the Earth's interior. Suppose that we have observationally determined the surface values of  $\varphi^{(1)}$  on the Earth in terms of its spherical harmonic expansion coefficients  $\varphi^{(1)}_{lm}(b)$  up to some maximum order. We have seen that  $\varphi^{(1)}_{lm}(b)$  depends linearly on the radial function  $\rho^{(1)}_{lm}(r)$  in solid regions of the earth model and on the boundary perturbation expansion coefficients  $h^{(S)}_{lm}$  on the solid-solid and fluid-solid boundaries of the model. In this subsection we shall describe a simple numerical method for calculating the radial sensitivity kernels relating  $\rho^{(1)}_{lm}(r)$  and  $h^{(S)}_{lm}$  to  $\varphi^{(1)}_{lm}(r)$ .

Let us define the operator

$$A = \Delta - 4\pi G \chi_M g^{-1} \partial_r \rho^{(0)}, \tag{3.134}$$

for suitably regular scalar functions in M, along with the boundary operator

$$B = \hat{\mathbf{n}} \cdot \nabla - 4\pi G \chi_{\Sigma} g^{-1} \rho^{(0)}, \tag{3.135}$$

which is defined on  $\Sigma$ . We also introduce the space  $L^2(M;\mathbb{C})$  of complex-valued scalar

functions on M that are square-integrable with respect to the inner product

$$(\varphi,\zeta)_{L^2(M;\mathbb{R}^3)} = \int_M \varphi \,\overline{\zeta} \,\mathrm{d}V,\tag{3.136}$$

along with the space  $L^2(\Sigma; \mathbb{C})$  comprising complex-valued scalar functions defined on  $\Sigma$  which are square-integrable with respect to the inner product

$$(\varphi, \zeta)_{L^2(\Sigma; \mathbb{C})} = \int_{\Sigma} \varphi \,\overline{\zeta} \,\mathrm{d}S. \tag{3.137}$$

In terms of these definitions, the boundary value problem for  $\varphi^{(1)}$  described in the previous subsection can be written

$$A\varphi^{(1)} = f, \quad x \in M, \tag{3.138}$$

where we have defined

$$f = 4\pi G(1 - \chi_M)\rho^{(1)},\tag{3.139}$$

subject to the boundary conditions that

$$\left[\varphi^{(1)}\right]_{-}^{+} = 0, \quad x \in \Sigma,$$
 (3.140)

$$[B\varphi^{(1)}]^+ = [k]_-^+, \quad x \in \Sigma,$$
 (3.141)

where we have defined

$$k = -4\pi G(1 - \chi_{\Sigma})g^{-1}\rho^{(0)}h^{(S)}.$$
(3.142)

Making use of the divergence theorem it is easily seen that the operator A satisfies the identity

$$(A\varphi,\zeta)_{L^2(M;\mathbb{C})} = (\varphi,A\zeta)_{L^2(M;\mathbb{C})} - \left( [B\varphi]_-^+,\zeta \right)_{L^2(\Sigma;\mathbb{C})} + \left( \varphi, [B\zeta]_-^+ \right)_{L^2(\Sigma;\mathbb{C})}, \tag{3.143}$$

for all subitably regular scalar fields  $\varphi$  and  $\zeta$  defined in  $\mathbb{R}^3$  which are continuous across  $\Sigma$ .

We can express  $\varphi_{lm}^{(1)}(b)$  in terms of the inner product on  $L^2(\Sigma;\mathbb{C})$  as

$$\varphi_{lm}^{(1)}(b) = (\varphi^{(1)}, \xi)_{L^2(\Sigma; \mathbb{C})}, \qquad (3.144)$$

where we have defined the function  $\xi$  to be

$$\xi = \begin{cases} \frac{1}{b^2} Y_{lm} & x \in \partial M \\ 0 & x \in \Sigma \setminus \partial M \end{cases}$$
 (3.145)

Let  $\zeta$  be a subitably regular function on  $\mathbb{R}$  that is continuous across  $\Sigma$ . Then from eq.(3.138) we see that

$$\left(A\varphi^{(1)},\zeta\right)_{L^2(M;\mathbb{C})} = (f,\zeta)_{L^2(M;\mathbb{C})}.$$
(3.146)

From eq.(3.143) and the boundary conditions on  $\varphi^{(1)}$  we find that

$$(A\varphi^{(1)},\zeta)_{L^{2}(M;\mathbb{C})} = (\varphi^{(1)},A\zeta)_{L^{2}(M;\mathbb{C})} - ([k]_{-}^{+},\zeta)_{L^{2}(\Sigma;\mathbb{C})} + (\varphi^{(1)},[B\zeta]_{-}^{+})_{L^{2}(\Sigma;\mathbb{C})},$$
 (3.147)

which implies that

$$\left(\varphi^{(1)}, A\zeta\right)_{L^{2}(M;\mathbb{C})} - \left(\left[k\right]_{-}^{+}, \zeta\right)_{L^{2}(\Sigma;\mathbb{C})} + \left(\varphi^{(1)}, \left[B\zeta\right]_{-}^{+}\right)_{L^{2}(\Sigma;\mathbb{C})} = (f, \zeta)_{L^{2}(M;\mathbb{C})}. \tag{3.148}$$

If we require that  $\zeta$  satisfies the equation

$$A\zeta = 0, (3.149)$$

in  $\mathbb{R}^3$  along with the boundary condition

$$\left[B\zeta\right]_{-}^{+} = \xi,\tag{3.150}$$

then we see that

$$\left(\varphi^{(1)},\xi\right)_{L^{2}(\Sigma;\mathbb{C})} = \left(f,\zeta\right)_{L^{2}(M;\mathbb{C})} + \left([k]_{-}^{+},\zeta\right)_{L^{2}(\Sigma;\mathbb{C})},\tag{3.151}$$

and, by definition of  $\xi$ , obtain

$$\varphi_{lm}^{(1)}(b) = (f,\zeta)_{L^2(M;\mathbb{C})} + ([k]_-^+,\zeta)_{L^2(\Sigma;\mathbb{C})}. \tag{3.152}$$

It is easy to see that the solution  $\zeta$  of the above boundary value problem takes the form  $\zeta_l(r)Y_{lm}(\theta,\phi)$  with the radial coefficient function  $\zeta_l(r)$  being readily calculated using the finite-element method described in the previous subsection. Inserting this form of  $\zeta$  into eq.(3.152) we find that

$$\varphi_{lm}^{(1)}(b) = 4\pi G \int_{I_S} \rho_{lm}^{(1)}(r) \overline{\zeta_l(r)} r^2 \, dr - 4\pi G \sum_{d \in d_S} g(d)^{-1} \left[ \rho^{(0)} \right]_-^+ h_{lm}^{(S)} \overline{\zeta_l(d)} d^2, \tag{3.153}$$

where  $I_S$  denotes the subset of [0, b] occupied by solid parts of the earth model, and  $d_S$  denotes the set of radii of solid-solid and fluid-solid boundaries.

### 3.5.4 Calculation of the minimum equilibrium stress field

To calculate the minimum equilibrium stress field, we must solve the boundary value problem in eq.(3.56) and the associated boundary conditions. For simplicity, we shall assume that the weighting function  $\eta$  occurring in the inner-product on  $L^2(M; L_s(\mathbb{R}^3))$  depends only on the radial co-ordinate. To solve this problem, we first express it in its weak form. Let  $\mathbf{v}$  be a complex-valued vector field defined in M which is continuous across  $\Sigma$ . We find from eq.(3.56) that

$$\int_{M} \operatorname{Div}(2\eta \nabla_{s} \mathbf{u}) \cdot \overline{\mathbf{v}} \, dV = \int_{M} \mathbf{f} \cdot \overline{\mathbf{v}} \, dV, \tag{3.154}$$

and application of the divergence theorem and the boundary conditions, leads to

$$-\int_{M} 2\eta \nabla_{s} \mathbf{u} : \overline{\nabla}_{s} \mathbf{v} \, dV - \int_{\Sigma} \mathbf{t} \cdot \overline{\mathbf{v}} \, dS = \int_{M} \mathbf{f} \cdot \overline{\mathbf{v}} \, dV. \tag{3.155}$$

If eq.(3.155) holds for all sufficiently smooth  $\mathbf{v}$ , then it may be shown that  $\mathbf{u}$  is a solution of the eq.(3.56) and the associated boundary conditions – this is the weak-form of the

boundary value problem.

To simplify this equation we expand  ${\bf u}$  in generalized spherical harmonics as

$$\mathbf{u}(r,\theta,\phi) = \sum_{lm} u_{lm}^{\alpha}(r) Y_{lm}^{\alpha}(\theta,\phi) \hat{\mathbf{e}}_{\alpha}.$$
 (3.156)

It will be convenient to express the expansion coefficients  $u_{lm}^{\alpha}$  of  ${\bf u}$  in the form

$$u_{lm}^- = \Omega_l^0(V_{lm} - iW_{lm}),$$
 (3.157)

$$u_{lm}^0 = U_{lm},$$
 (3.158)

$$u_{lm}^+ = \Omega_l^0(V_{lm} + iW_{lm}),$$
 (3.159)

and similarly for f

$$f_{lm}^- = \Omega_l^0 (G_{lm} - iH_{lm}),$$
 (3.160)

$$f_{lm}^0 = F_{lm}, (3.161)$$

$$f_{lm}^+ = \Omega_l^0 (G_{lm} + iH_{lm}),$$
 (3.162)

and for t

$$t_{lm}^- = \Omega_l^0(B_{lm} - iC_{lm}),$$
 (3.163)

$$t_{lm}^0 = A_{lm}, (3.164)$$

$$t_{lm}^+ = \Omega_l^0(B_{lm} + iC_{lm}).$$
 (3.165)

Taking

$$\mathbf{v} = v_{lm}^{\alpha} Y_{lm}^{\alpha} \hat{\mathbf{e}}_{\alpha},\tag{3.166}$$

for a given value of (l, m), with

$$v_{lm}^{-} = \Omega_l^0(V_{lm}' - iW_{lm}'), \tag{3.167}$$

$$v_{lm}^0 = U_{lm}', (3.168)$$

$$v_{lm}^+ = \Omega_l^0(V_{lm}' + iW_{lm}'),$$
 (3.169)

we find after some reduction that

$$\int_{M} 2\eta \nabla_{s} \mathbf{u} : \overline{\nabla_{s} \mathbf{v}} \, dV = \zeta^{2} (\zeta^{2} - 2) \int_{I} \eta \left( V_{lm} \overline{V'_{lm}} + W_{lm} \overline{W'_{lm}} \right) dr 
+ 2 \int_{I} \eta \partial_{r} U_{lm} \overline{\partial_{r} U'_{lm}} r^{2} dr 
+ \int_{I} \eta \left( \zeta^{2} V_{lm} - 2U_{lm} \right) \overline{\left( \zeta^{2} V'_{lm} - 2U'_{lm} \right)} dr 
+ \zeta^{2} \int_{I} \eta \left( r \partial_{r} V_{lm} - V_{lm} + U_{lm} \right) \overline{\left( r \partial_{r} V'_{lm} - V'_{lm} + U'_{lm} \right)} dr 
+ \zeta^{2} \int_{I} \eta \left( r \partial_{r} W_{lm} - W_{lm} \right) \overline{\left( r \partial_{r} W'_{lm} - W'_{lm} \right)} dr,$$
(3.170)

that

$$\int_{\Sigma} \mathbf{t} \cdot \overline{\mathbf{v}} \, dS = \sum_{r \in d} \left[ A_{lm} \overline{U'_{lm}} + \zeta^2 (B_{lm} \overline{V'_{lm}} + C_{lm} \overline{W'_{lm}}) \right] r^2, \tag{3.171}$$

where d denotes the set of radii of boundaries in  $\Sigma$ , and that

$$\int_{M} \mathbf{f} \cdot \overline{\mathbf{v}} \, dV = \int_{I} \left[ F_{lm} \overline{U'_{lm}} + \zeta^{2} \left( G_{lm} \overline{V'_{lm}} + H_{lm} \overline{W'_{lm}} \right) \right] r^{2} \, dr. \tag{3.172}$$

From these equations it is seen that the problem decouples into a toroidal equation

$$-(\zeta^{2} - 2) \int_{I} \eta W_{lm} \overline{W'_{lm}} dr$$

$$- \int_{I} \eta \left( r \partial_{r} W_{lm} - W_{lm} \right) \overline{\left( r \partial_{r} W'_{lm} - W'_{lm} \right)} dr$$

$$- \sum_{r \in d} C_{lm} \overline{W'_{lm}} r^{2}$$

$$= \int_{I} H_{lm} \overline{W'_{lm}} r^{2} dr, \qquad (3.173)$$

and a spheroidal equation

$$-\zeta^{2}(\zeta^{2}-2)\int_{I}\eta V_{lm}\overline{V_{lm}'}\,\mathrm{d}r$$

$$-2\int_{I}\eta \partial_{r}U_{lm}\overline{\partial_{r}U_{lm}'}r^{2}\,\mathrm{d}r$$

$$-\int_{I}\eta\left(\zeta^{2}V_{lm}-2U_{lm}\right)\overline{\left(\zeta^{2}V_{lm}'-2U_{lm}'\right)}\,\mathrm{d}r$$

$$-\zeta^{2}\int_{I}\eta\left(r\partial_{r}V_{lm}-V_{lm}+U_{lm}\right)\overline{\left(r\partial_{r}V_{lm}'-V_{lm}'+U_{lm}'\right)}\,\mathrm{d}r$$

$$-\sum_{r\in d}\left(A_{lm}\overline{U_{lm}'}+\zeta^{2}B_{lm}\overline{V_{lm}'}\right)r^{2}$$

$$=\int_{I}\left(F_{lm}\overline{U_{lm}'}+\zeta^{2}G_{lm}\overline{V_{lm}'}\right)r^{2}\,\mathrm{d}r.$$
(3.174)

For the minimum stress calculations, we have

$$\mathbf{f} = \rho^{(1)} \nabla \varphi^{(0)} + \rho^{(0)} \nabla \varphi^{(1)}, \tag{3.175}$$

and

$$\mathbf{t} = \begin{cases} -\left[\rho^{(0)}\right]_{-}^{+} g h \hat{\mathbf{n}} & \mathbf{x} \in \Sigma_{SS} \\ -\left[\rho^{(0)}\right]_{-}^{+} g h + p^{(1)} \hat{\mathbf{n}} & \mathbf{x} \in \Sigma_{SF} \end{cases}$$

$$\left[\rho^{(0)}\right]_{-}^{+} g h + p^{(1)} \hat{\mathbf{n}} & \mathbf{x} \in \Sigma_{FS} \end{cases}$$
(3.176)

Reducing these expressions into generalized spherical harmonic coefficients, leads to

$$F_{lm} = \rho_{lm}^{(1)} g + \rho^{(0)} \partial_r \varphi_{lm}^{(1)}, \tag{3.177}$$

$$G_{lm} = r^{-1} \rho^{(0)} \varphi_{lm}^{(1)}, \tag{3.178}$$

$$H_{lm} = 0,$$
 (3.179)

and

$$A_{lm} = \begin{cases} -\left[\rho^{(0)}\right]_{-}^{+} g h_{lm} & r \in d_{SS} \\ -\left[\rho^{(0)}\right]_{-}^{+} g h_{lm} + p_{lm}^{(1)} & r \in d_{SF} \end{cases},$$

$$\left[\rho^{(0)}\right]_{-}^{+} g h_{lm} + p_{lm}^{(1)} & r \in d_{FS} \end{cases}$$
(3.180)

$$B_{lm} = 0, (3.181)$$

$$C_{lm} = 0, (3.182)$$

where  $d_{SS}$ ,  $d_{SF}$ , and  $d_{FF}$  are, respectively, the set of radii of boundaries in  $\Sigma_{SS}$ ,  $\Sigma_{SF}$ , and  $\Sigma_{FS}$ .

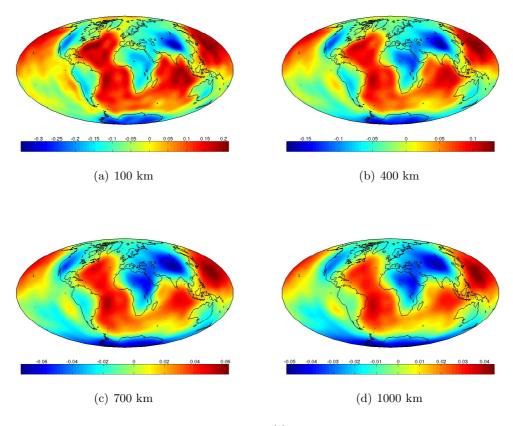


Figure 3.2: Relative pressure perturbations  $100 \times p^{(1)}/\mu$  in the model S20RTS at various depths. In the calculations the weighting factor  $\eta$  was set equal to 1 in solid regions.

In the above formulae, the force and traction terms for the toroidal equation vanish, so that we need only solve the spheroidal equations to determine the minimum equilibrium stress field. To solve these equations numerically, we expand the coefficients  $U_{lm}$ , and  $V_{lm}$  in radial basis functions, and so convert the above equations into a system of linear equations for the expansion coefficients. To do this, we again use Lagrange polynomials on a radial grid defined in terms of the GLL-points used in the Spectral Element Method.

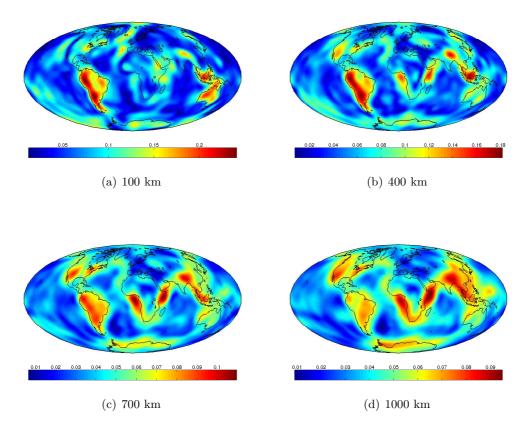


Figure 3.3: Relative deviatoric stress perturbations  $100 \times ||\tau||/\mu$  in the model S20RTS at various depths. In the calculations the weighting factor  $\eta$  was set equal to 1 in solid regions.

Having found  $\mathbf{u}$ , the expansion coefficients of the minimum equilibrium stress field can then be calculated using the formulae

$$L_{lm} = \eta r^{-1} \left[ \zeta^2 V_{lm} - 2U_{lm} \right], \tag{3.183}$$

$$M_{lm} = \eta r^{-1} V_{lm}, (3.184)$$

$$N_{lm} = 0,$$
 (3.185)

$$R_{lm} = 2\eta \partial_r U_{lm}, \tag{3.186}$$

$$S_{lm} = \eta \left[ \partial V_{lm} - r^{-1} V_{lm} + r^{-1} U_{lm} \right] \tag{3.187}$$

$$T_{lm} = 0, (3.188)$$

where the coefficients  $L_{lm}$ ,  $M_{lm}$ ,  $N_{lm}$ ,  $R_{lm}$ ,  $S_{lm}$ , and  $T_{lm}$  are related to the coefficients  $T_{lm}^{\alpha\beta}$  through the formulae in eq.(3.90).

Some results from a minimum stress field calculation are shown in figures 3.2 and 3.3. For this calculation the norm-weighting factor  $\eta$  was set equal to one in both the mantle and

inner core of the earth model. Figure 3.2 shows a number of depth slices of  $100 \times p^{(1)}/\mu$ , where  $p^{(1)} = -\frac{1}{3} \text{tr} \mathbf{T}^{(1)}$  is the pressure perturbation and  $\mu$  is the shear modulus of the earth model at the given depth. It is seen that the pressure perturbation is strongly correlated with the position of oceans and continents. This is because the crustal model used is not in isostatic equilibrium. Figure 3.3 shows corresponding depth slices of  $100 \times ||\tau||/\mu$  where  $\|\tau\|$  is the norm of the deviatoric stress field. Spatial variations of the deviatoric stress perturbation seem to be largely sensitive to density variations in the mantle, being largest in the vicinity of strong density anomalies such as under continental cratons (repeating the calculations with the crustal model removed shows that, at the depths plotted, the crustal model has very little effect on  $\|\tau\|$ ). The values of  $100 \times \|\tau\|/\mu$  in the upper mantle are around 0.1-0.2%, which is an order of magnitude smaller than the corresponding variations  $100 \times \delta v_s/v_s$  in shear wave velocity. It follows that the effects of the deviatoric stress field on seismic wave propagation is likely to be correspondingly smaller when compared with the effects of shear wave velocity variations. However, the relative magnitudes of these perturbations are not so different that the influence of the deviatoric equilibrium stress field on seismic observations should be dismissed without further quantitative investigation.

# 3.6 Discussion

In this chapter we have described a method of parametrizing the possible equilibrium stress fields in a slightly laterally heterogeneous earth model. The primary difference between our method and that described by Backus (1967) is that we have considered how to construct particular solutions of the equilibrium equations possessing desirable physical characteristics. In particular, we have shown how to construct the equilibrium stress field possessing the smallest norm with respect to a given inner product, and the equilibrium stress field whose deviatoric component has smallest norm with respect to a given inner product. These particular solutions of the equilibrium equations have a number of potential applications. For example, we have seen that the minimum deviatoric equilibrium stress field is the solution of the equilibrium equations which leads to the smallest (in the sense previously defined) amount of stress-induced anisotropy in the earth model. Consequently, determination of the minimum deviatoric equilibrium stress field

provides a useful 'lower-bound' on the amount of stress-induced anisotropy associated with a given laterally heterogeneous earth model.

# Part II

# Seismic Wavefield Calculations

# Chapter 4

# Synthetic Seismograms in Spherical Earth Models Using the Direct Radial Integration Method

# 4.1 Introduction

It is well known that geometric symmetries allow many of the partial differential equations occurring in geophysics to be reduced to systems of ordinary differential equations. Such equations occur, for example, in seismic calculations in both flat and spherical earth problems when the material parameters of the earth model depend only upon a 'vertical' co-ordinate (e.g. Aki & Richards 1980, chapters 7 and 8, Dahlen & Tromp 1998, chapter 8). The numerical integration of the resulting systems of ordinary differential equations potentially provides a simple method of solution to the partial differential equations. However, it has been observed that many of the equations occurring in geophysical problems cannot be stably solved numerically by standard methods (Gilbert & Backus 1966). This is largely due to the need to compute determinants of linearly-independent sets of solutions to the differential equations; the values of such determinants are frequently many orders of magnitude smaller than the solutions from which they are formed, so that they cannot be computed accurately using finite precision arithmetic.

An elegant solution to this problem was given by Gilbert & Backus (1966) who showed that these determinants could be calculated directly by the integration of a related system of differential equations for the so-called *minor vectors* of the system. This theory was extended by Woodhouse (1980) to include a method for the the solution of boundary value problems for four-dimensional systems of ordinary differential equations, and then later in Woodhouse (1988) where the calculation of the eigenfrequencies and eigenfunctions of an even-dimensional system of differential equations was considered and the algebraic theory of minor vectors was described in detail. These results form the basis of the *direct radial integration method* of Friederich & Dalkolmo (1995) for the calculation of synthetic seismograms in non-self-gravitating spherically symmetric earth models, and also for the standard methods by which the eigenfrequencies and eigenfunctions of spherical earth models are calculated.

The main purpose of this chapter is to provide the necessary theoretical extensions of the minor vector method to allow for the stable numerical solution of boundary value problems for six-dimensional systems of linear ordinary differential equations (in fact, the theory is given with essentially no extra effort for an arbitrary even-dimensional system of equations). The practical importance of this result is that it allows for the application of the direct radial integration method to the case of a self-gravitating earth model. The theory developed is also directly applicable to a number of other problems such as the calculation of static and post-seismic displacement fields in self-gravitating spherically symmetric earth models (e.g. Pollitz 1992, 1996), post-glacial rebound problems (e.g. Peltier 1974), and also to mantle flow calculations in a spherical earth model (e.g. Forte 2007).

In addition to these results on minor vectors, we consider the application of symmetries possessed by the differential equations occurring in a number of problems of interest. These symmetries arise because the equations are particular cases of Hamilton's canonical equations (Chapman & Woodhouse 1979). It is shown that these symmetries may be used to significantly simplify the numerical implementation of the minor vector method, and also to derive many of the important properties of the normal modes of an earth model.

### 4.2 The Spheroidal Motion Equations

To motivate the general theory present below, we consider the calculation of spheroidal displacement fields in an earth model which is everywhere solid. The ordinary differential equations governing spheroidal motions of a self-gravitating earth model have been derived by several of authors, and can be stated in a number of different forms (e.g. Alterman et. al. 1959, Takeuchi & Saito 1974, Phinney & Burridge 1978, Dahlen & Tromp 1998, Woodhouse & Deuss 2007). A large part of this work is based upon a symmetry exhibited by these equations which arises because they may be written in the form of Hamilton's canonical equations (Chapman & Woodhouse 1979, Woodhouse 1988); we shall follow the notation of Woodhouse (1980) and Woodhouse & Deuss (2007) which displays this symmetry in a particularly useful form.

The symbol  $\omega$  denotes angular frequency throughout this work, and we use the Fourier transform convention

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt, \quad f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(\omega) e^{i\omega t} d\omega, \tag{4.1}$$

for any function f(t). For notational simplicity we shall often not explicitly distinguish between a function f and its Fourier transform  $\hat{f}$ , using the symbol f for both. The distinction between these two functions should, however, be clear from context. We shall often consider causal functions for which f(t) = 0 for t < 0. For such functions it is useful to extend the definition of the Fourier transform so that  $\omega$  can be complex-valued. The resulting transformation is sometimes known as the Fourier-Laplace transform (e.g. Friedlander & Joshi 1998, Chapter 10), and is related to the Laplace transform by a rotation of the transformation variable by 90° in the complex-plane.

### 4.2.1Statement of the boundary value problem

We begin by defining the notations used for the vector spherical harmonic expansions of the frequency domain displacement vector  $\mathbf{u}(\mathbf{x},\omega)$  and the perturbation in gravitational potential  $\phi(\mathbf{x}, \omega)$ . In a spherical polar co-ordinate system  $(r, \theta, \varphi)$  we write

$$u_r(r,\theta,\varphi,\omega) = \sum_{lm} U_{lm}(r,\omega)Y_{lm}(\theta,\varphi),$$
 (4.2)

$$u_{r}(r,\theta,\varphi,\omega) = \sum_{lm} U_{lm}(r,\omega)Y_{lm}(\theta,\varphi), \qquad (4.2)$$

$$u_{\theta}(r,\theta,\varphi,\omega) = \sum_{lm} V_{lm}(r,\omega)\partial_{\theta}Y_{lm}(\theta,\varphi), \qquad (4.3)$$

$$u_{\varphi}(r,\theta,\varphi,\omega) = \sum_{lm} V_{lm}(r,\omega)\operatorname{cosec}(\theta)\partial_{\varphi}Y_{lm}(\theta,\varphi), \qquad (4.4)$$

$$\phi(r,\theta,\varphi,\omega) = \sum_{lm} \phi_{lm}(r,\omega)Y_{lm}(\theta,\varphi), \qquad (4.5)$$

$$\phi(r,\theta,\varphi,\omega) = \sum_{lm}^{lm} \phi_{lm}(r,\omega) Y_{lm}(\theta,\varphi), \tag{4.5}$$

where the function  $Y_{lm}(\theta,\varphi)$  is the fully normalized surface spherical harmonic of degree land order m as defined in Appendix B of Dahlen & Tromp (1998). It will also be useful to expand the traction vector,  $\mathbf{t}(\mathbf{x}, \omega)$ , acting on spherical surfaces of the earth model as

$$t_r(r,\theta,\varphi,\omega) = \sum_{lm} P_{lm}(r,\omega) Y_{lm}(\theta,\varphi),$$
 (4.6)

$$t_{\theta}(r,\theta,\varphi,\omega) = \sum_{lm} S_{lm}(r,\omega)\partial_{\theta}Y_{lm}(\theta,\varphi),$$
 (4.7)

$$t_{\varphi}(r,\theta,\varphi,\omega) = \sum_{lm} S_{lm}(r,\omega) \operatorname{cosec}(\theta) \partial_{\varphi} Y_{lm}(\theta,\varphi).$$
 (4.8)

The constitutive relation of the earth model is assumed to be transversely isotropic and linear viscoelastic, in which case the expansion coefficients of the traction vector are related to those of the displacement vector by the equations

$$P_{lm}(r,\omega) = F(r,\omega)r^{-1}\left[2U_{lm}(r,\omega) - \zeta^2V_{lm}(r,\omega)\right] + C(r,\omega)\partial_r U_{lm}(r,\omega), \tag{4.9}$$

$$S_{lm}(r,\omega) = L(r,\omega) \left[ \partial_r V_{lm}(r,\omega) - r^{-1} V_{lm}(r,\omega) + r^{-1} U_{lm}(r,\omega) \right],$$
 (4.10)

where  $\zeta = \sqrt{l(l+1)}$ , and C, F, and L are three of the five 'viscoelastic moduli' A, C, F, L, and N of a transversely isotropic material (Love 1944, Woodhouse & Deuss 2007). From the theory of linear viscoelasticity and our Fourier transform convention we know that the functions  $\omega \mapsto A(r,\omega)$ , etc, are holomorphic in the lower half of the complex-plane (e.g. Dahlen & Tromp 1998, chapter 6).

It is found that the above vector spherical harmonic expansions decouple the elastodynamic equation into a system of ordinary differential equations for the expansion coefficients of each spherical harmonic order m and degree l. These ordinary differential equations may be written in the general form

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{y}(r,\omega) = \mathbf{A}(r,\omega)\mathbf{y}(r,\omega) + \mathbf{f}(r,\omega),\tag{4.11}$$

where the six-dimensional displacement-stress vector is given by

$$\mathbf{y} = \begin{pmatrix} rU \\ r\zeta V \\ r\phi \\ rP \\ r\zeta S \\ r\psi/(4\pi G) \end{pmatrix}, \tag{4.12}$$

with G the gravitational constant, and the variable  $\psi$  defined by

$$\psi = \partial_r \phi + (l+1)r^{-1}\phi + 4\pi G\rho U. \tag{4.13}$$

The important symmetry alluded to above is that the coefficient matrix  $\mathbf{A}(r,\omega)$  in eq.(4.11) has the structure

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & \mathbf{K} \\ \mathbf{S} & -\mathbf{T}^T \end{pmatrix},\tag{4.14}$$

where each submatrix is in  $\mathbb{C}^{3\times 3}$ , and **K** and **S** are symmetric. For the spheroidal motion

$$\mathbf{T} = \begin{pmatrix} (1 - 2F/C)r^{-1} & \zeta F/Cr^{-1} & 0 \\ -\zeta r^{-1} & 2r^{-1} & 0 \\ -4\pi G\rho & 0 & -lr^{-1} \end{pmatrix}, \tag{4.15}$$

$$\mathbf{K} = \begin{pmatrix} 1/C & 0 & 0 \\ 0 & 1/L & 0 \\ 0 & 0 & 4\pi G \end{pmatrix}, \tag{4.16}$$

$$g(r) = \frac{4\pi G}{r^2} \int_0^r \rho(r')r'^2 dr', \qquad (4.18)$$

and  $\gamma = A - N - F^2/C$ . In the static or quasi-static displacement problems the differential equations are identical to those above except for the neglect of the inertial term  $\rho\omega^2$  in the matrix components  $S_{11}$  and  $S_{22}$ .

The vector **f** in equation (4.11) represents the force term in the problem resulting from the vector spherical harmonic expansion of the body force in the elastodynamic equation. In the case of a moment tensor point source it may be shown that this vector takes the form

$$\mathbf{f}(r,\omega) = \mathbf{a}(r,\omega)\delta(r - r_s) + \mathbf{b}(r,\omega)\frac{\mathrm{d}}{\mathrm{d}r}\delta(r - r_s),\tag{4.19}$$

where  $r_s$  is the radius of the source point and **a** and **b** are given vectors (see Woodhouse & Deuss 2007 for full expressions). This force vector is only valid if the vector a is continuous and b is differentiable as functions of r in some neighborhood of  $r_s$  because this is the only case in which the products with delta functions are well defined. Physically, this result means that a moment tensor point source cannot be located at a depth in the earth model at which a jump in material properties occurs (Woodhouse 1981).

We now describe the boundary conditions that the displacement-stress vector must satisfy. Suppose the earth model's radius lies in the interval  $[0, r_2]$  and that the various material parameters are continuously differentiable within this interval except for a finite number of jump discontinuities. It may be shown that the continuity conditions on displacements, tractions, and perturbation in gravitational potential are such that the displacement-stress vector must be continuous at each material discontinuity of the earth model. Clearly the point r=0 is a regular singular point of the system of equations, and we shall require that the displacement-stress vector be bounded as it is approached. The simplest means of incorporating this boundary condition is to use the fact that three linearly independent closed-form solutions of the spheroidal motion equations are known in the case of an isotropic homogeneous earth model (Takeuchi & Saito 1972). If we assume that within an arbitrarily small radius, say  $r_1$ , the earth model is isotropic, homogeneous, and that no body force acts, then the displacement-stress vector within this radius must lie in the three-dimensional linear subspace spanned by the three solutions mentioned above. We may, therefore, restrict the interval of interest in numerical integrations to  $[r_1, r_2]$ , where  $r_1$ can be made as small as we desire, and use the values of the closed-form solutions at  $r=r_1$ to define a three-dimensional linear subspace in which the solution must lie at  $r = r_1$ . At the surface of the earth model the free-surface boundary conditions of the problem are such that the two traction terms  $y_4$  and  $y_5$  vanish, and it may be shown that  $y_6$  must vanish also here. Consequently we see that at  $r = r_2$  the displacement-stress vector must lie in the three-dimensional linear subspace spanned by the columns of the matrix

$$\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.$$
(4.20)

The above boundary conditions can be summarized by saying that at either of the two endpoints of the interval of integration we require the displacement-stress vector to lie in a given three-dimensional linear subspace. These linear subspaces will be denoted by  $V^{(1)}(\omega)$  and  $V^{(2)}(\omega)$  with the superscript referring to the end points  $r_1$  and  $r_2$ , respectively. The functional argument  $\omega$  in the notation for the linear subspaces reflects the fact that the

 $V^{(1)}(\omega)$  subspace varies with frequency – although not really needed, we choose to retain the argument in the case of  $V^{(2)}(\omega)$  in the interests of notational symmetry and generality.

# 4.2.2 A simple solution to the boundary value problem

We shall postpone discussion of the solution in the case of a general force term until a later section and, for the moment, consider the case of a moment tensor point source as given in eq.(4.19). For such a point source, the force term in the equations can be replaced by a discontinuity condition on the displacement-stress vector at the source radius; this is a familiar result (e.g. Hudson 1969, Takeuchi & Saito 1972), but we repeat the derivation for completeness and also because it is a convenient point to introduce the propagator matrix for equation (4.11). Following Gilbert & Backus (1966), we define the propagator matrix for eq.(4.11) between the points  $r', r \in [r_1, r_2]$  to be the continuous matrix function  $\mathbf{P}(r, r', \omega) \in \mathbb{C}^{6 \times 6}$  satisfying the equations

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{P}(r,r',\omega) = \mathbf{A}(r,\omega)\mathbf{P}(r,r',\omega), \quad \mathbf{P}(r',r',\omega) = \mathbf{1}.$$
(4.21)

From the definition of the propagator matrix it is not difficult to see that a particular integral of eq.(4.11) is given by

$$\mathbf{y}(r,\omega) = \int_{r_1}^{r} \mathbf{P}(r,r',\omega)\mathbf{f}(r') dr.$$
 (4.22)

To find the actual solution to the problem we would have to add to the right hand side of the above expression some linear combination of solutions to the homogeneous form of eq.(4.11) so that the boundary conditions are satisfied; these additional terms are continuous at  $r_s$  and so, for our present purposes, can be ignored. If we substitute eq.(4.19) into the above equation and make use of the properties of the Dirac delta function and its distributational derivatives along with the easily proven relation  $\mathbf{P}(r, r', \omega)^{-1} = \mathbf{P}(r', r, \omega)$ , we find that

$$\mathbf{y}(r,\omega) = \begin{cases} \mathbf{0} & r \in [r_1, r_s) \\ \mathbf{P}(r, r_s, \omega) \mathbf{a}(r_s, \omega) + \mathbf{P}(r, r_s, \omega) \mathbf{A}(r_s, \omega) \mathbf{b}(r_s, \omega) - \mathbf{P}(r, r_s, \omega) \frac{\mathrm{d}}{\mathrm{d}r} \mathbf{b}(r_s, \omega) & r \in (r_s, r_2] \end{cases}$$
(4.23)

From this result we can see that a point source leads to a jump discontinuity in the displacement-stress vector at the source radius given by

$$\lim_{\epsilon \searrow 0} [\mathbf{y}(r_s + \epsilon, \omega) - \mathbf{y}(r - \epsilon, \omega)] = \mathbf{a}(r_s, \omega) + \mathbf{A}(r_s, \omega)\mathbf{b}(r_s, \omega) - \frac{\mathrm{d}}{\mathrm{d}r}\mathbf{b}(r_s, \omega) = \mathbf{s}(\omega), \tag{4.24}$$

where the 'discontinuity-vector'  $\mathbf{s}(\omega)$  is defined by the above equality and is not to be confused with the displacement vector defined earlier. Combining this observation with the fact that the point source obviously has support equal to  $\{r_s\}$ , we see that the boundary value problem may be expressed by requiring that the displacement-stress vector be a continuous solution of the homogeneous (i.e. unforced) form of eq.(4.11) on either side of the source radius  $r_s$ , and be required to undergo the jump prescribed by eq.(4.24) at  $r = r_s$ .

We can now outline a very simple method of solution for the boundary value problem. Let the matrix  $\mathbf{Y}_0^{(1)}(\omega) \in \mathbb{C}^{6\times 3}$  be such that its columns span the linear subspace  $V^{(1)}(\omega)$ , and, similarly, let  $\mathbf{Y}_0^{(2)}(\omega) \in \mathbb{C}^{6\times 3}$  be such that its columns span the linear subspace  $V^{(2)}(\omega)$ ; an example of such a matrix  $\mathbf{Y}_0^{(2)}(\omega)$  was given in the previous subsection in eq.(4.20). In terms of these matrices we can define two matrix functions taking values in  $\mathbb{C}^{6\times 3}$  by

$$\mathbf{Y}^{(1)}(r,\omega) = \mathbf{P}(r,r_1,\omega)\mathbf{Y}_0^{(1)}(\omega), \quad \mathbf{Y}^{(2)}(r,\omega) = \mathbf{P}(r,r_2,\omega)\mathbf{Y}_0^{(2)}(\omega). \tag{4.25}$$

The action of the propagator matrix on a vector is equivalent to numerical integration of the homogeneous form of eq.(4.11) from the second radial argument to the first, so that the above pair of matrices can be obtained by six different numerical integrations of the homogeneous form of eq.(4.11). It is apparent that in the interval  $[r_1, r_s)$  a solution to the problem, if it exists, must be some linear combination of the three columns of  $\mathbf{Y}^{(1)}(r,\omega)$ , and, similarly, in the interval  $(r_s, r_2]$ , a solution must be a linear combination of the three columns of  $\mathbf{Y}^{(2)}(r,\omega)$ . Let us define a matrix function in  $\mathbb{C}^{6\times 6}$  by

$$\mathbf{Y}(r,\omega) = (\mathbf{Y}^{(1)}(r,\omega) \quad \mathbf{Y}^{(2)}(r,\omega)), \qquad (4.26)$$

and also introduce two matrices in  $\mathbb{C}^{6\times 6}$  by

$$\mathbf{J}_{-} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathbf{J}_{+} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}. \tag{4.27}$$

In terms of these definitions we can summarize the above remarks by stating that, if a solution exists, then it must take the form

$$\mathbf{y}(r,\omega) = \begin{cases} \mathbf{Y}(r,\omega)\mathbf{J}_{-}\mathbf{c}(\omega) & r \in [r_{1}, r_{s}) \\ \mathbf{Y}(r,\omega)\mathbf{J}_{+}\mathbf{c}(\omega) & r \in (r_{s}, r_{2}] \end{cases}, \tag{4.28}$$

where  $\mathbf{c}(\omega) \in \mathbb{C}^6$  is a vector independent of r. From the required discontinuity condition at the source radius, we find that  $\mathbf{c}(\omega)$  is given by

$$\mathbf{c}(\omega) = (\mathbf{J}_{+} - \mathbf{J}_{-})\mathbf{Y}(r_{s}, \omega)^{-1}\mathbf{s}(\omega), \tag{4.29}$$

where we have assumed that

$$\det[\mathbf{Y}(r_s,\omega)] \neq 0,\tag{4.30}$$

which constitutes a necessary and sufficient condition for a solution of the problem to exist. Supposing that this condition is met, the unique solution to the boundary value problem can be written as

$$\mathbf{y}(r,\omega) = \begin{cases} -\mathbf{Y}(r,\omega)\mathbf{J}_{-}\mathbf{Y}(r_{s},\omega)^{-1}\mathbf{s}(\omega) & r \in [r_{1}, r_{s}) \\ \mathbf{Y}(r,\omega)\mathbf{J}_{+}\mathbf{Y}(r_{s},\omega)^{-1}\mathbf{s}(\omega) & r \in (r_{s}, r_{2}] \end{cases}$$
(4.31)

A practical numerical process for computing this solution can be summarized as follows:

- 1. Integrate a set of three solutions spanning  $V^{(1)}(\omega)$  from the center of the earth model to the source radius,
- 2. Integrate a set of three solutions spanning  $V^{(2)}(\omega)$  from the surface of the earth model to the source radius.
- 3. Apply the discontinuity condition at the source radius to find the displacement-stress vector on either side of  $r_s$  by solving a sixth-order system of linear equations
- 4. Integrate the solution at the source radius to the desired receiver locations.

As will be discussed in detail in section 4.5, there are numerical instabilities associated with the implementation of steps (3) and (4) in the above method which limit its practical utility, and necessitate the use of the minor vector method that is described in section 4.4.

# 4.3 Hamilton's Equations and Symplectic Geometry

# 4.3.1 Linear Hamiltonian systems

The general form of the spheroidal motion equations introduced in the previous section may be written as

$$\frac{\mathrm{d}}{\mathrm{d}r} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{T} & \mathbf{K} \\ \mathbf{S} & -\mathbf{T}^T \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} + \begin{pmatrix} \mathbf{g} \\ \mathbf{h} \end{pmatrix}, \tag{4.32}$$

where  $\mathbf{q}, \mathbf{p}, \mathbf{g}, \mathbf{h} \in \mathbb{C}^n$ , for some integer n, and the submatrices are in  $\mathbb{C}^{n \times n}$ . As is readily checked by direct calculation, all systems of equations possessing the above structure may

be expressed as Hamilton's canonical equations (e.g. Arnold 1989)

$$\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}r} = \frac{\partial H}{\partial \mathbf{p}}, \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}r} = -\frac{\partial H}{\partial \mathbf{q}},\tag{4.33}$$

for the quadratic Hamiltonian

$$H(\mathbf{q}, \mathbf{p}) = -\frac{1}{2}\mathbf{q}^{T}\mathbf{S}\mathbf{q} + \mathbf{p}^{T}\mathbf{T}\mathbf{q} + \frac{1}{2}\mathbf{p}^{T}\mathbf{K}\mathbf{p} - \mathbf{q}^{T}\mathbf{h} + \mathbf{p}^{T}\mathbf{g}.$$
 (4.34)

The above Hamiltonian is, excepting an irrelevant constant term, the most general quadratic Hamiltonian which is 'real' in the sense that the expression does not involve the complex conjugates of **q** nor **p**; systems of ordinary differential equations possessing this structure will be called real linear Hamiltonian systems in what follows. The above result is essentially a restatement of that given by Chapman & Woodhouse (1979) who showed that a system of second-order linear equations expressible in variational form with a 'real' quadratic Lagrangian could be written in the above form so long as the Lagrangian satisfied a certain non-degeneracy condition – the two statements are equivalent because a non-degenerate 'real' quadratic Lagrangian transforms into a 'real' quadratic Hamiltonian upon the use of a Legendre transform (e.g. Arnold 1989, chapter 4).

# 4.3.2 Propagation invariants and symplectic vector spaces

To motivate the definition of a symplectic vector space let us consider the above real linear Hamiltonian system in the case that the force term is equal to zero. Suppose we have two solutions  $\mathbf{y}_1$  and  $\mathbf{y}_2$ , and define a matrix in  $\mathbb{C}^{2n\times 2n}$  by

$$\Sigma = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix},\tag{4.35}$$

where each of the submatrices is in  $\mathbb{C}^{n\times n}$ . We shall show that the scalar quantity  $\mathbf{y}_1^T \mathbf{\Sigma} \mathbf{y}_2$  is independent of r, and so can be regarded as a *propagation invariant* of the equations (e.g. Thomson *et. al.* 1986). This fact is most easily demonstrated by noting that the coefficient matrix of the linear equations satisfies the identity

$$(\mathbf{\Sigma}\mathbf{A})^T = \mathbf{\Sigma}\mathbf{A} = -\mathbf{A}^T\mathbf{\Sigma}.$$
 (4.36)

We then compute that

$$\frac{\mathrm{d}}{\mathrm{d}r} \left( \mathbf{y}_1^T \mathbf{\Sigma} \mathbf{y}_2 \right) = \mathbf{y}_1^T \mathbf{A}^T \mathbf{\Sigma} \mathbf{y}_2 + \mathbf{y}_1^T \mathbf{\Sigma} \mathbf{A} \mathbf{y}_2 = \mathbf{y}_1^T (\mathbf{A}^T \mathbf{\Sigma} + \mathbf{\Sigma} \mathbf{A}) \mathbf{y}_2 = 0, \tag{4.37}$$

and so  $\mathbf{y}_1^T \mathbf{\Sigma} \mathbf{y}_2$  is indeed independent of r. The existence of such a propagation invariant for these equations is not surprising as it is known that Hamiltonian systems are always associated with an invariant related to their symplectic structure. We shall follow Arnold

(1988, chapter 8) by defining a skew-scalar product mapping  $\mathbb{C}^{2n} \times \mathbb{C}^{2n}$  into  $\mathbb{C}$  by

$$[\mathbf{y}_1, \mathbf{y}_2] = \mathbf{y}_1^T \mathbf{\Sigma} \mathbf{y}_2, \tag{4.38}$$

where  $\mathbf{y}_1$  and  $\mathbf{y}_2$  are now arbitrary vectors in  $\mathbb{C}^{2n}$ . This skew-scalar product is linear in each of its arguments, and it is anti-symmetric in the sense that  $[\mathbf{y}_2, \mathbf{y}_1] = -[\mathbf{y}_1, \mathbf{y}_2]$ , so that it defines a two-form on  $\mathbb{C}^{2n}$  (e.g. Lang 2000, chapter XV, section 8). In addition  $[\mathbf{y}_1, \mathbf{y}] = 0$  for all  $\mathbf{y}$  implies that  $\mathbf{y}_1 = \mathbf{0}$ , so we say that  $[\cdot, \cdot]$  is non-degenerate. This non-degenerate two-form makes  $\mathbb{C}^{2n}$  into a symplectic vector space (Arnold 1988, Hörmander 2000b); in the remainder of this subsection we shall describe two basic concept of such spaces that will be important in later sections.

Following Hörmander (2000b), a linear mapping  $\mathbf{X}: \mathbb{C}^{2n} \to \mathbb{C}^{2n}$  is said to be a *symplectic* isomorphism if its action leaves the skew-scalar product invariant, that is

$$[\mathbf{X}\mathbf{y}_1, \mathbf{X}\mathbf{y}_2] = [\mathbf{y}_1, \mathbf{y}_2],\tag{4.39}$$

for all  $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{C}^{2n}$ . The above result about propagation invariants for real linear Hamiltonian systems implies the identity

$$[\mathbf{P}(r,r')\mathbf{y}_1,\mathbf{P}(r,r')\mathbf{y}_2] = [\mathbf{y}_1,\mathbf{y}_2],\tag{4.40}$$

for all  $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{C}^{2n}$ , and so we see that the propagator matrices of such equations are all symplectic isomorphisms. From the above definition it can readily be shown that a symplectic isomorphism  $\mathbf{X}$  must satisfy the relation

$$\mathbf{X}^T \mathbf{\Sigma} \mathbf{X} = \mathbf{\Sigma},\tag{4.41}$$

and, in addition, that such transformations form a group known as the (complex) symplectic group which is often denoted by  $\mathbf{Sp}(2n,\mathbb{C})$ , where the first argument indicates the dimensions of the vector space and the second the field of scalars it is defined over (e.g. Hall 2004). That the propagator matrices of a real linear Hamiltonian system are elements of the symplectic group has a number of important consequences, for example, it leads to the useful relation

$$\mathbf{P}(r,r')^{-1} = \mathbf{\Sigma}^T \mathbf{P}(r,r')^T \mathbf{\Sigma},\tag{4.42}$$

which allows the inverse of a propagator matrix to be calculated very easily.

The second concept to be introduced in this subsection concerns the linear subspaces of a symplectic vector space. A p-dimensional linear subspace V of  $\mathbb{C}^{2n}$  is said to be isotropic

(Hörmander 2000b) if, for any two of its elements  $\mathbf{y}_1, \mathbf{y}_2 \in V$ , the identity

$$[\mathbf{y}_1, \mathbf{y}_2] = 0, \tag{4.43}$$

holds. An isotropic subspace in  $\mathbb{C}^{2n}$  that has dimension n is said to be a Lagrangian subspace; it is not difficult to show that these are the isotropic subspaces of  $\mathbb{C}^{2n}$  of maximum dimension. Suppose that the columns of the matrix  $\mathbf{Y} \in \mathbb{C}^{2n \times p}$  span a given p-dimensional linear subspace V of  $\mathbb{C}^{2n}$ , then it is easy to see that V is isotropic if and only if the identity

$$\mathbf{Y}^T \mathbf{\Sigma} \mathbf{Y} = \mathbf{0},\tag{4.44}$$

holds. An important, and obvious, property of isotropic subspaces is that they are mapped into isotropic subspaces by symplectic isomorphisms. It follows that if V is an isotropic subspace of  $\mathbb{C}^{2n}$ , and  $\mathbf{Y}$  is a matrix whose columns span V, then the linear subspace obtained by integrating the columns of  $\mathbf{Y}$  from r' to r according to the homogeneous form of eq.(4.32) will also be isotropic.

In the next section when we describe the general form of the linear differential equations to be solved, the boundary conditions are stated by requiring that the solution lie in a given Lagrangian subspace at either end of the interval  $[r_1, r_2]$ . We shall conclude this section by demonstrating that the linear subspaces defined previously for the boundary conditions of the spheroidal motion equations are indeed Lagrangian. First we consider the boundary condition at the earth model's surface, which is described by the subspace  $V^{(2)}(\omega)$  spanned by the columns of the matrix shown in eq.(4.20). That this linear subspace is Lagrangian follows from a simple computation using eq.(4.44) and the fact that it is three-dimensional. At the center of the earth model we recall that the boundary conditions are that the solution be bounded as  $r \to 0$ , and we saw previously that this condition can be stated as requiring that the solution at  $r = r_1$  lie in the three-dimensional linear subspace  $V^{(1)}(\omega)$  defined by the known closed-form solutions to the problem in an isotropic (in the sense of constitutive relations) homogeneous earth model. To show that this subspace is Lagrangian we need simply show that it is isotropic, which may be done as follows. Fix  $r_1$ , and let  $\mathbf{Y}^{(1)}(r,\omega) \in \mathbb{C}^{6\times 3}$  be a matrix whose columns span the three-dimensional linear subspace of closed-form solutions in  $[0, r_1]$ . We have seen that  $\mathbf{Y}^{(1)}(r, \omega)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(r, \omega)$ is independent of r in  $[0, r_1]$ . The closed-form solutions to the spheroidal motion equations given by Takeuchi & Saito (1972) are such that each of the three solutions tends to the zero vector as  $r \to 0$ . Thus  $\mathbf{Y}^{(1)}(0,\omega)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(0,\omega) = \mathbf{0}$ , and, we see that this equality must hold throughout  $[0, r_1]$ , showing that the subspace  $V^{(1)}(\omega)$  at  $r_1$  is indeed Lagrangian. The above arguments may also be applied to the toroidal and radial motion equations of a spherical earth model (though all one-dimensional linear subspaces of  $\mathbb{C}^2$  are trivially Lagrangian), and may also be adapted to deal with the radiation conditions imposed at infinity on solutions in certain 'flat-earth' problems whose differential equations also have the form of real linear Hamiltonian systems.

# 4.4 Solution of the Boundary Value Problem

In this section, we describe a method of solution for two-point boundary value problems associated with a real linear Hamiltonian system of ordinary differential equations whose numerical implementation does not possess the instabilities associated with the solution given in section 4.2. We shall firstly state the problem to be solved in a general form, of which the spheroidal motion equations are a specific example. The reason for considering the problem in general terms is that by doing so we simultaneously develop the theory required for a number of different problems including the toroidal and radial motions of a spherical earth model. In addition, it will be seen that there is essentially no extra effort required in dealing with the equations in the general case.

# 4.4.1 Statement of the problem

Let m be an even natural number such that m=2n. We seek solutions  $\mathbf{y}(r,\omega) \in \mathbb{C}^m$  of the ordinary differential equation

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{y}(r,\omega) = \mathbf{A}(r,\omega)\mathbf{y}(r,\omega) + \mathbf{f}(r,\omega),\tag{4.45}$$

in the interval  $[r_1, r_2]$ , where  $\mathbf{A}(r, \omega) \in \mathbb{C}^{m \times m}$  is a piecewise continuous function of r, and  $\mathbf{f}(r, \omega)$  is a given vector function. The force vector  $\mathbf{f}(r, \omega)$  may be a generalized function such as a delta function, though in this case we require that its singular support (see Hörmander 2000a, section 2.2) does not intersect the points of discontinuity of the coefficient matrix. The coefficient matrix of the problem is assumed to have the structure of a real linear Hamiltonian system

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & \mathbf{K} \\ \mathbf{S} & -\mathbf{T}^T \end{pmatrix},\tag{4.46}$$

where the submatrices are in  $\mathbb{C}^{n\times n}$ , with **K** and **S** symmetric. We equip  $\mathbb{C}^m = \mathbb{C}^{2n}$  with the skew-scalar product of section 4.3 making it a symplectic vector space. The boundary conditions on the problem are that at  $r = r_1$  the solution lie in a given Lagrangian subspace  $V^{(1)}(\omega)$ , while at the point  $r = r_2$  the solution lie in a Lagrangian subspace  $V^{(2)}(\omega)$ . In addition, the displacement-stress vector  $\mathbf{y}(r,\omega)$  is required to be continuous across any discontinuities of the coefficient matrix.

As functions of the parameter  $\omega$  we shall require that for each  $r \in [r_1, r_2]$  the coefficient matrix be a holomorphic function in an open subset  $\Omega_A$  of the complex-plane which contains the lower half-plane, and that the linear subspaces  $V^{(1)}(\omega)$  and  $V^{(2)}(\omega)$  are spanned by vectors that depend holomorphically on  $\omega$  in  $\Omega_A$ . In addition,  $\mathbf{f}(r,\omega)$  is supposed to be a holomorphic function of  $\omega$  in an open subset  $\Omega_f$  of the complex-plane which also contains the lower half-plane.

# 4.4.2 A simple method of solution

By a similar method to that given in section 4.2, we can quite easily obtain a solution to the above system of differential equations. For some  $\omega \in \Omega_A$ , let  $\mathbf{P}(r, r', \omega) \in \mathbb{C}^{m \times m}$  be the propagator matrix for the homogeneous form of eq.(4.45), and suppose that the matrices  $\mathbf{Y}_0^{(1)}(\omega), \mathbf{Y}_0^{(2)}(\omega) \in \mathbb{C}^{m \times n}$  span, respectively, the Lagrangian subspaces  $V^{(1)}(\omega)$  and  $V^{(2)}(\omega)$ . As  $\omega \in \Omega_A$ , it follows from a standard theorem of ordinary differential equations that  $\omega \mapsto \mathbf{P}(r, r', \omega)$  is holomorphic in some neighborhood of the point  $\omega$  for all  $r, r' \in [r_1, r_2]$ . We define the matrices

$$\mathbf{Y}^{(1)}(r,\omega) = \mathbf{P}(r,r_1,\omega)\mathbf{Y}_0^{(1)}(\omega), \quad \mathbf{Y}^{(2)}(r,\omega) = \mathbf{P}(r,r_2,\omega)\mathbf{Y}_0^{(2)}(\omega), \tag{4.47}$$

and, by analogy with section 4.2, introduce the matrices  $\mathbf{J}_{-}, \mathbf{J}_{+} \in \mathbb{C}^{m \times m}$ , along with the matrix function  $\mathbf{Y}(r,\omega) \in \mathbb{C}^{m \times m}$ . For a given r, the columns of  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$  each span Lagrangian subspaces which we shall denote by  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$ , respectively. In addition, let us suppose that  $\det[\mathbf{Y}(r,\omega)] \neq 0$  for all  $r \in [r_1, r_2]$ , so that the interior sum of these subspaces spans  $\mathbb{C}^m$ . We seek a solution to eq.(4.45) of the form

$$\mathbf{y}(r,\omega) = \mathbf{Y}(r,\omega)\mathbf{v}(r,\omega),$$
 (4.48)

where  $\mathbf{v}(r,\omega) \in \mathbb{C}^m$  is some vector function to be determined. Substituting the above solution into eq.(4.45) and canceling common terms, we find that

$$\mathbf{Y}(r,\omega)\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{v}(r,\omega) = \mathbf{f}(r,\omega). \tag{4.49}$$

As, by assumption,  $\mathbf{Y}(r,\omega)$  is non-singular, we can write the solution to this equation as

$$\mathbf{v}(r,\omega) = \mathbf{v}(r_1,\omega) + \int_{r_1}^{r} \mathbf{Y}(r',\omega)^{-1} \mathbf{f}(r',\omega) \, \mathrm{d}r', \qquad (4.50)$$

where the initial value  $\mathbf{v}(r_1,\omega)$  is to be determined. At this point it is useful to observe that the structure of  $\mathbf{A}$  is such that  $\text{tr}[\mathbf{A}]$  vanishes identically in  $[r_1, r_2]$ . By making use of the well known relation (Gilbert & Backus 1966),

$$\frac{\mathrm{d}}{\mathrm{d}r} \det[\mathbf{Y}(r,\omega)] = \operatorname{tr}[\mathbf{A}(r,\omega)] \det[\mathbf{Y}(r,\omega)], \tag{4.51}$$

we see that if  $\mathbf{Y}(r,\omega)$  is non-singular at some point in  $[r_1, r_2]$  then it is non-singular throughout the interval and  $\det[\mathbf{Y}(r,\omega)]$  is independent of r (note that even if  $\operatorname{tr}[\mathbf{A}]$  did not vanish, if  $\mathbf{Y}$  were non-singular at some point, then it would still be non-singular throughout  $[r_1, r_2]$ ). Putting the above solution for  $\mathbf{v}(r,\omega)$  into eq.(4.48) we obtain

$$\mathbf{y}(r,\omega) = \mathbf{Y}(r,\omega)\mathbf{v}(r_1,\omega) + \int_{r_1}^{r} \mathbf{Y}(r,\omega)\mathbf{Y}(r',\omega)^{-1}\mathbf{f}(r',\omega)\,\mathrm{d}r'. \tag{4.52}$$

and, by changing the roles of  $r_1$  and  $r_2$ , that

$$\mathbf{y}(r,\omega) = \mathbf{Y}(r,\omega)\mathbf{v}(r_2,\omega) - \int_{-\infty}^{r_2} \mathbf{Y}(r,\omega)\mathbf{Y}(r',\omega)^{-1}\mathbf{f}(r',\omega)\,\mathrm{d}r'. \tag{4.53}$$

The boundary conditions on the solution are such that we must have

$$\mathbf{y}(r_1, \omega) = \mathbf{Y}(r_1, \omega)\mathbf{v}(r_1, \omega)$$

$$= \mathbf{Y}(r_1, \omega)\mathbf{v}(r_2, \omega)$$

$$-\int_{r_1}^{r_2} \mathbf{Y}(r_1, \omega)\mathbf{Y}(r', \omega)^{-1}\mathbf{f}(r', \omega) dr' \in V^{(1)}(\omega), \tag{4.54}$$

and

$$\mathbf{y}(r_2, \omega) = \mathbf{Y}(r_2, \omega)\mathbf{v}(r_2, \omega)$$

$$= \mathbf{Y}(r_2, \omega)\mathbf{v}(r_1, \omega)$$

$$+ \int_{r_1}^{r_2} \mathbf{Y}(r_2, \omega)\mathbf{Y}(r', \omega)^{-1}\mathbf{f}(r', \omega) dr' \in V^{(2)}(\omega), \qquad (4.55)$$

which imply that for some  $\mathbf{c}(\omega) \in \mathbb{C}^m$  we have

$$\mathbf{Y}(r_1, \omega)\mathbf{v}(r_1, \omega) = \mathbf{Y}(r_1, \omega)\mathbf{v}(r_2, \omega) - \int_{r_1}^{r_2} \mathbf{Y}(r_1, \omega)\mathbf{Y}(r', \omega)^{-1}\mathbf{f}(r', \omega) dr'$$

$$= \mathbf{Y}(r_1, \omega)\mathbf{J}_{-}\mathbf{c}(\omega), \qquad (4.56)$$

$$\mathbf{Y}(r_2, \omega)\mathbf{v}(r_2, \omega) = \mathbf{Y}(r_2, \omega)\mathbf{v}(r_1, \omega) + \int_{r_1}^{r_2} \mathbf{Y}(r_2, \omega)\mathbf{Y}(r', \omega)^{-1}\mathbf{f}(r', \omega) dr'$$

$$= \mathbf{Y}(r_2, \omega)\mathbf{J}_{+}\mathbf{c}(\omega). \tag{4.57}$$

From these equations we see that  $\mathbf{v}(r_1,\omega) = \mathbf{J}_{-}\mathbf{c}(\omega)$  and  $\mathbf{v}(r_2,\omega) = \mathbf{J}_{+}\mathbf{c}(\omega)$ , and that we must have

$$\mathbf{c}(\omega) = (\mathbf{J}_{+} - \mathbf{J}_{-}) \int_{r_{1}}^{r_{2}} \mathbf{Y}(r', \omega)^{-1} \mathbf{f}(r', \omega) \, \mathrm{d}r', \qquad (4.58)$$

which leads to

$$\mathbf{v}(r_1, \omega) = -\mathbf{J}_{-} \int_{r_1}^{r_2} \mathbf{Y}(r', \omega)^{-1} \mathbf{f}(r', \omega) \, \mathrm{d}r', \qquad (4.59)$$

$$\mathbf{v}(r_2,\omega) = \mathbf{J}_+ \int_{r_1}^{r_2} \mathbf{Y}(r',\omega)^{-1} \mathbf{f}(r',\omega) \, \mathrm{d}r'. \tag{4.60}$$

Putting all these results together we can write the solution to eq.(4.45) as

$$\mathbf{y}(r,\omega) = \int_{r_1}^{r} \mathbf{Y}(r,\omega) \mathbf{J}_{+} \mathbf{Y}(r',\omega)^{-1} \mathbf{f}(r',\omega) \, dr' - \int_{r}^{r_2} \mathbf{Y}(r,\omega) \mathbf{J}_{-} \mathbf{Y}(r',\omega)^{-1} \mathbf{f}(r',\omega) \, dr'.$$
(4.61)

If we wish to restrict attention to the point source in eq.(4.19) of section 4.2 we can substitute this force vector into the above expression to obtain the solution

$$\mathbf{y}(r,\omega) = \begin{cases} -\mathbf{Y}(r,\omega)\mathbf{J}_{-}\mathbf{Y}(r_{s},\omega)^{-1}\mathbf{s}(\omega) & r \in [r_{1}, r_{s}) \\ \mathbf{Y}(r,\omega)\mathbf{J}_{+}\mathbf{Y}(r_{s},\omega)^{-1}\mathbf{s}(\omega) & r \in (r_{s}, r_{2}] \end{cases}, \tag{4.62}$$

in agreement with the earlier result. We can also define a *Green's function* for the problem by

$$\mathbf{G}(r, r', \omega) = \begin{cases} -\mathbf{Y}(r, \omega)\mathbf{J}_{-}\mathbf{Y}(r', \omega)^{-1} & r \in [r_1, r') \\ \mathbf{Y}(r, \omega)\mathbf{J}_{+}\mathbf{Y}(r', \omega)^{-1} & r \in (r', r_2] \end{cases}, \tag{4.63}$$

and so write the solution concisely as

$$\mathbf{y}(r,\omega) = \int_{r_1}^{r_2} \mathbf{G}(r,r',\omega)\mathbf{f}(r',\omega)\,\mathrm{d}r'. \tag{4.64}$$

# 4.4.3 Applications of the symplectic structure of the equations

Up to this point we have made use of none of the special properties belonging to real linear Hamiltonian systems, nor have we used the fact that the linear subspaces  $V^{(1)}(\omega)$  and  $V^{(2)}(\omega)$  are Lagrangian. We now exploit these properties to transform the solution just found into an equivalent form that is of greater use for both numerical and theoretical work.

It was shown in the previous subsection that in the case of a real linear Hamiltonian system  $det[\mathbf{Y}(r,\omega)]$  is independent of r, and we shall write

$$\Delta(\omega) = \det[\mathbf{Y}(r,\omega)],\tag{4.65}$$

for this quantity. We now demonstrate that the identities

$$\Delta(\omega) = \det[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^T \mathbf{Y}^{(1)}(r,\omega)] = (-1)^n \det[\tilde{\mathbf{Y}}^{(1)}(r,\omega)^T \mathbf{Y}^{(2)}(r,\omega)], \tag{4.66}$$

hold, where  $\tilde{\mathbf{Y}}^{(2)}(r,\omega) = \mathbf{\Sigma}\mathbf{Y}^{(2)}(r,\omega)$ , and  $\tilde{\mathbf{Y}}^{(1)}(r,\omega) = \mathbf{\Sigma}\mathbf{Y}^{(1)}(r,\omega)$ . To do this we shall need to make use of some of the properties of the Pfaffian of an anti-symmetric matrix (e.g. Lang 2000, chapter XV, section 9) which we now briefly review. For any anti-symmetric matrix  $\mathbf{X} \in \mathbb{C}^{2n \times 2n}$  it may be shown that its determinant can be written as the square of an nth order polynomial in the matrix coefficients. The Pfaffian of X, written Pf[X], is defined to be equal to this polynomial, that is,

$$\det[\mathbf{X}] = \Pr[\mathbf{X}]^2,\tag{4.67}$$

with the sign of Pf[X] fixed by a certain convention that we need not consider. For any matrix  $\mathbf{Z} \in \mathbb{C}^{2n \times 2n}$  it may be shown that

$$Pf[\mathbf{Z}^T \mathbf{X} \mathbf{Z}] = \det[\mathbf{Z}] Pf[\mathbf{X}], \tag{4.68}$$

while for any matrix  $\mathbf{V} \in \mathbb{C}^{n \times n}$  we have

To proceed with the proof of eq.(4.66), we compute that for the matrix 
$$\mathbf{Y}(r,\omega)$$
 we have 
$$\mathbf{Y}^T \mathbf{\Sigma} \mathbf{Y} = \begin{pmatrix} \mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(1)} & \mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} \\ \mathbf{Y}^{(2)T} \mathbf{\Sigma} \mathbf{Y}^{(1)} & \mathbf{Y}^{(2)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} \end{pmatrix}. \tag{4.69}$$
 From the fact that the subspaces  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$  are Lagrangian, we see by eq.(4.44)

$$\mathbf{Y}^{T} \mathbf{\Sigma} \mathbf{Y} = \begin{pmatrix} \mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(1)} & \mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} \\ \mathbf{Y}^{(2)T} \mathbf{\Sigma} \mathbf{Y}^{(1)} & \mathbf{Y}^{(2)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} \end{pmatrix}. \tag{4.70}$$

that 
$$\mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(1)} = \mathbf{Y}^{(2)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} = \mathbf{0}$$
, and so, using the anti-symmetry of  $\mathbf{\Sigma}$ , we obtain 
$$\mathbf{Y}^T \mathbf{\Sigma} \mathbf{Y} = \begin{pmatrix} \mathbf{0} & \mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(2)} \\ -(\mathbf{Y}^{(1)T} \mathbf{\Sigma} \mathbf{Y}^{(2)})^T & \mathbf{0} \end{pmatrix}. \tag{4.71}$$
 We can combine this result with the Pfaffian identities stated above to show that

$$Pf[\mathbf{Y}^{T}\boldsymbol{\Sigma}\mathbf{Y}] = \det[\mathbf{Y}]Pf[\boldsymbol{\Sigma}]$$

$$= (-1)^{n(n-1)/2} \det[\mathbf{Y}^{(1)T}\boldsymbol{\Sigma}\mathbf{Y}^{(2)}]$$

$$= (-1)^{n(n-1)/2} \det[\mathbf{Y}^{(1)T}\tilde{\mathbf{Y}}^{(2)}]$$

$$= (-1)^{n(n-1)/2} \det[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}], \qquad (4.72)$$

where the first equality follows from eq.(4.68), and the second equality follows from (4.69)and eq.(4.71). The proof of the first identity in eq.(4.66) is then completed by using (4.69)to calculate that  $Pf[\Sigma] = (-1)^{n(n-1)/2}$ . The second identity in eq.(4.66) then follows from the first by the well known property of determinants that  $det[-\mathbf{X}] = (-1)^n det[\mathbf{X}]$  for any matrix  $\mathbf{X} \in \mathbb{C}^{n \times n}$ .

We shall also require the following identity 
$$\operatorname{adj}[\mathbf{Y}(r,\omega)] = \begin{pmatrix} \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^T \mathbf{Y}^{(1)}(r,\omega)] \tilde{\mathbf{Y}}^{(2)}(r,\omega)^T \\ (-1)^n \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r,\omega)^T \mathbf{Y}^{(2)}] \tilde{\mathbf{Y}}^{(1)}(r,\omega)^T \end{pmatrix}, \tag{4.73}$$
 which may be verified by checking that

which may be verified by checking that

$$\operatorname{adj}[\mathbf{Y}]\mathbf{Y} = \mathbf{Y}\operatorname{adj}[\mathbf{Y}] = \Delta \mathbf{1}. \tag{4.74}$$

that 
$$\Delta \neq 0$$
, we can make use of eq.(4.44) along with eq.(4.66) to calculate that
$$\begin{pmatrix} \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}]\tilde{\mathbf{Y}}^{(2)T} \\ (-1)^{n}\operatorname{adj}[\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(2)}]\tilde{\mathbf{Y}}^{(1)T} \end{pmatrix} (\mathbf{Y}^{(1)} \quad \mathbf{Y}^{(2)})$$

$$= \begin{pmatrix} \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}]\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)} & \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}]\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(2)} \\ (-1)^{n}\operatorname{adj}[\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(2)}]\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(1)} & (-1)^{n}\operatorname{adj}[\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(2)}]\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(2)} \end{pmatrix}$$

$$= \begin{pmatrix} \operatorname{det}[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}]\mathbf{1} & \mathbf{0} \\ \mathbf{0} & (-1)^{n}\operatorname{det}[\tilde{\mathbf{Y}}^{(1)T}\mathbf{Y}^{(2)}]\mathbf{1} \end{pmatrix}$$

$$= \begin{pmatrix} \Delta \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \Delta \mathbf{1} \end{pmatrix} = \Delta \mathbf{1}, \tag{4.75}$$

so that the first of the above identities,  $\operatorname{adj}[\mathbf{Y}]\mathbf{Y} = \Delta \mathbf{1}$ , holds, and the second then follows from the associativity of matrix multiplication. When  $\Delta = 0$  the result holds (so long as  $\omega \in \Omega_A$ ) from the case just proven and the fact that the adjugate matrix is a holomorphic function of  $\omega$ . If we now substitute eq.(4.73) into eq.(4.61), we can write the solution as

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \int_{r_1}^r \mathbf{Y}^{(2)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega)^T \mathbf{Y}^{(2)}(r',\omega)] \tilde{\mathbf{Y}}^{(1)}(r',\omega)^T \mathbf{f}(r',\omega) dr'$$

$$\frac{-1}{\Delta(\omega)} \int_{r}^{r_2} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r',\omega)^T \mathbf{Y}^{(1)}(r',\omega)] \tilde{\mathbf{Y}}^{(2)}(r',\omega)^T \mathbf{f}(r',\omega) dr', \quad (4.76)$$

$$\mathbf{y}(r,\omega) = \begin{cases} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r_s,\omega)^T \mathbf{Y}^{(1)}(r_s,\omega)] \tilde{\mathbf{Y}}^{(2)}(r_s,\omega)^T \mathbf{s}(\omega) & r \in [r_1, r_s) \\ \frac{(-1)^n}{\Delta(\omega)} \mathbf{Y}^{(2)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r_s,\omega)^T \mathbf{Y}^{(2)}(r_s,\omega)] \tilde{\mathbf{Y}}^{(1)}(r_s,\omega)^T \mathbf{s}(\omega) & r \in (r_s, r_2] \end{cases}$$
The Creen's function for the problem can now be written as

The Green's function for the problem can now be written as 
$$\mathbf{G}(r,r',\omega) = \begin{cases} \frac{-1}{\Delta(\omega)}\mathbf{Y}^{(1)}(r,\omega)\mathrm{adj}[\tilde{\mathbf{Y}}^{(2)}(r',\omega)^T\mathbf{Y}^{(1)}(r',\omega)]\tilde{\mathbf{Y}}^{(2)}(r',\omega)^T & r \in [r_1,r') \\ \frac{(-1)^n}{\Delta(\omega)}\mathbf{Y}^{(2)}(r,\omega)\mathrm{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega)^T\mathbf{Y}^{(2)}(r',\omega)]\tilde{\mathbf{Y}}^{(1)}(r',\omega)^T & r \in (r',r_2] \end{cases}$$
 and a relatively simple computation demonstrates the source-receiver reciprocity relation

$$\mathbf{G}(r', r, \omega) = \mathbf{\Sigma}\mathbf{G}(r, r', \omega)^{T}\mathbf{\Sigma}.$$
(4.79)

#### 4.4.4 A review of minor vectors

The algebra of minor vectors has been described in detail in Woodhouse (1988). In this subsection we shall simply state a number of definitions and results that are needed below.

Let Y be an m-by-n complex valued matrix with  $n \leq m$ . We define the nth order minor vector of this matrix to be the  $\frac{m!}{n!(m-n)!}$  dimensional vector whose components comprise the independent n-by-n subdeterminants of  $\mathbf{Y}$ . This minor vector is denoted by  $[\mathbf{Y}:n]$ , and its components may be labeled by sets of n distinct integers  $(i_1, \ldots, i_n)$  in the range

1 to n identifying the rows of **Y** the particular subdeterminant is formed from; using this notation, we can write

$$[\mathbf{Y}:n]_{(i_{1},\dots,i_{n})} = \begin{vmatrix} Y_{i_{1}1} & Y_{i_{1}2} & \dots & Y_{i_{1}n} \\ Y_{i_{2}1} & Y_{i_{2}2} & \dots & Y_{i_{2}n} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{i_{n}1} & Y_{i_{n}2} & \dots & Y_{i_{n}n} \end{vmatrix}.$$

$$(4.80)$$

We observe that if two sets of integers  $(i_1,\ldots,i_n)$  and  $(j_1,\ldots,j_n)$  are related by a permutation, then the corresponding minor vector elements will be equal up to their signs – this is why the minor vectors are  $\frac{m!}{n!(m-n)!}$  dimensional and not  $m^n$  dimensional. In practical calculations it is necessary to define a 'basis' for the minor vector by choosing an ordered set of  $\frac{m!}{n!(m-n)!}$  independent sets of n integers to label the different components of the minor vector. It is common to make use of the ordering in which, for any  $(i_1,\ldots,i_n)$ , we require that  $i_1 < i_2 < \cdots < i_n$ , and, for any two  $(i_1,\ldots,i_n)$  and  $(j_1,\ldots,j_n)$ , we say that the second set of integers is 'greater' than the first if, for some  $1 \le k \le n-1$ , the first k numbers are equal, i.e.  $i_m = j_m$  for  $1 \le m \le k$ , and for the k+1th numbers  $i_{k+1} < j_{k+1}$ . As an example, in the case that m=4 and n=2, the second order minor vectors are six dimensional, and the sets of integers labeling the components of the minor vectors using the above ordering are (1,2), (1,3), (1,4), (2,3), (2,4), (3,4).

We may generalize the above definition of an nth-order minor vector of  $\mathbf{Y}$  to define a pth order minor matrix of  $\mathbf{Y} \in \mathbb{C}^{m \times n}$ , written  $[\mathbf{Y}:p]$ , where p is an natural number less than or equal to n and m (in the case of p=n this definition reduces to that of a minor vector). This pth order minor matrix of  $\mathbf{Y}$  is an  $\frac{m!}{p!(m-p)!}$ -by- $\frac{n!}{p!(n-p)!}$  dimensional matrix whose components consist of p-dimensional subdeterminants of  $\mathbf{Y}$ . We can label the rows of this matrix by sets of p integers in the range 1 to m, and the columns of the matrix may be labeled by sets of p integers in the range 1 to n; a general component of the minor matrix can be written

$$[\mathbf{Y}:p]_{(i_{1},\dots,i_{p})(j_{1},\dots,j_{p})} = \begin{vmatrix} Y_{i_{1}j_{1}} & Y_{i_{1}j_{2}} & \dots & Y_{i_{1}j_{p}} \\ Y_{i_{2}j_{1}} & Y_{i_{2}j_{2}} & \dots & Y_{i_{2}j_{p}} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{i_{p}j_{1}} & Y_{i_{p}j_{2}} & \dots & Y_{i_{p}j_{p}} \end{vmatrix}.$$

$$(4.81)$$

As above, we introduce a basis for the minor matrix by choosing sets of integers to label the rows and columns of the matrix. Suppose that  $\mathbf{X} \in \mathbb{C}^{m \times q}$  and  $\mathbf{Y} \in \mathbb{C}^{q \times n}$  so that the matrix product  $\mathbf{X}\mathbf{Y}$  can be formed to give an m-by-n dimensional matrix. Given a natural number p less than or equal to m, q, and n, we can form the minor matrices  $[\mathbf{X}:p]$ ,  $[\mathbf{Y}:p]$ , and  $[\mathbf{X}\mathbf{Y}:p]$ . If orderings for the rows and columns of these matrices have been defined in a consistent manner then the product of the minor matrices  $[\mathbf{X}:p]$  and  $[\mathbf{Y}:p]$  is defined, and it may be shown (e.g. Gantmacher 1959) that

$$[\mathbf{X}:p][\mathbf{Y}:p] = [\mathbf{XY}:p]. \tag{4.82}$$

This result forms a generalization of the well known multiplication rule for determinants, and of the Cauchy-Binet formula that applies to the minors of matrices whose product is square. A corollary of this result is that if  $\mathbf{Y}$  is a non-singular m-dimensional square matrix, then for any  $1 \leq p \leq m$ , the minor matrix  $[\mathbf{Y}:p]$  is also non-singular and has inverse given by  $[\mathbf{Y}^{-1}:p]$ . This implies, as a special case, that identity matrices are carried into identity matrices by the operation of 'taking minors', and so all the necessary conditions are satisfied for 'taking minors' to define a group homomorphism between the general linear groups  $\mathbf{Gl}(m,\mathbb{C})$  and  $\mathbf{Gl}(m!/(p!(m-p)!),\mathbb{C})$ . An important consequence of eq.(4.82) is that the minor vector corresponding to an n-dimensional linear subspace of  $\mathbb{C}^m$ , with  $n \leq m$ , is, up to a non-zero scalar multiple, independent of the basis chosen for the subspace (Woodhouse 1988, Result 2.1). This means that when dealing with the minor vectors of linear subspaces we are essentially proceeding in a basis independent manner. We also note the readily verified fact that 'taking minors' respects matrix transposition in the sense that

$$[\mathbf{Y}:p]^T = [\mathbf{Y}^T:p],\tag{4.83}$$

whenever the above minor matrices are defined.

In addition to minor vectors it is necessary to define related quantities known as spanning matrices. For a matrix  $\mathbf{Y} \in \mathbb{C}^{m \times n}$ , with  $n \leq m$ , we define the its spanning matrix, written  $\operatorname{sp}[\mathbf{Y}:n]$ , to be the m-by-  $\frac{m!}{(n-1)!(m-n+1)!}$  dimensional matrix with components given by

$$\operatorname{sp}[\mathbf{Y}:n]_{(i_1)(i_2,\ldots,i_n)} = \begin{cases} 0 & \text{if } i_1 = i_k \text{ for } 2 \leq k \leq n \\ \pm [\mathbf{Y}:n]_{(j_1,\ldots,j_n)} & \text{where } (j_1,\ldots,j_n) \text{ is the even } (+) \\ & \text{or odd } (-) \text{ permutation of } (i_1,\ldots,i_n) \end{cases}$$
that places them in increasing order

Note that in this equation  $(i_1)$  acts as the row index for the spanning matrix, and  $(i_2, \ldots, i_n)$  acts as the column index – we chose to order these bases in the same manner done for the minor vectors. Suppose that  $\mathbf{Y} \in \mathbb{C}^{m \times n}$  is transformed into a new matrix  $\mathbf{Y}' \in \mathbb{C}^{m \times n}$  by a transformation  $\mathbf{Y}' = \mathbf{X}\mathbf{Y}$ . It may be shown that the spanning matrices for  $\mathbf{Y}$  and  $\mathbf{Y}'$  are related by the rule

$$\operatorname{sp}[\mathbf{Y}':n] = \mathbf{X}\operatorname{sp}[\mathbf{Y}:p][\mathbf{X}^T:n-1], \tag{4.85}$$

which is given in eq.(3.25) of Woodhouse (1988).

Having introduced minor vectors and spanning matrices we now turn to stating Result 2.3 of Woodhouse (1988) that is essential to the theory of Section 4.4 of this chapter. We shall first describe this result in its full form, and then give the specialized form that is used in Section 4.4. First we recall that, for a given p-dimensional linear subspace V of  $\mathbb{C}^m$  with p < m, the *orthogonal space*, which we write as  $\tilde{V}$ , is the (n-p)-dimensional linear subspace of vectors in  $\mathbb{C}^m$  whose elements are orthogonal to each element of V under the usual Hermitian inner product; that is, for all  $\mathbf{y} \in V$  and  $\mathbf{z} \in \tilde{V}$ , we have

$$\mathbf{z}^{\dagger}\mathbf{y} = 0,\tag{4.86}$$

where the † symbol denotes Hermitian conjugation.

**Theorem 4.4.1** (Woodhouse 1988) Let  $V^{(1)}$  and  $V^{(2)}$  be two disjoint linear subspaces of  $\mathbb{C}^m$  of dimension n and m-n, respectively, so that their union spans the whole space. Let  $\mathbf{m}^{(1)}$  and  $\mathbf{m}^{(2)}$  be the minor vectors of these subspaces, and furthermore, let  $\tilde{\mathbf{m}}^{(1)}$  and  $\tilde{\mathbf{m}}^{(2)}$  be the minor vectors of the subspaces  $\tilde{V}^{(1)}$  and  $\tilde{V}^{(2)}$  orthogonal to  $V^{(1)}$  and  $V^{(2)}$ , respectively. The projection operators  $\mathbb{P}^{(1)}$  and  $\mathbb{P}^{(2)}$  onto the spaces  $V^{(1)}$  and  $V^{(2)}$  can be written

$$\mathbb{P}^{(1)} = \frac{1}{\Lambda} \mathbf{M}^{(1)} \tilde{\mathbf{M}}^{(2)\dagger}, \quad \mathbb{P}^{(2)} = \pm \frac{1}{\Lambda} \mathbf{M}^{(2)} \tilde{\mathbf{M}}^{(1)\dagger}, \tag{4.87}$$

where  $\mathbf{M}^{(1)}$  and  $\mathbf{M}^{(2)}$  are the spanning matrices for  $V^{(1)}$  and  $V^{(2)}$ ,  $\tilde{\mathbf{M}}^{(1)}$  and  $\tilde{\mathbf{M}}^{(2)}$  are the spanning matrices for  $\tilde{V}^{(1)}$  and  $\tilde{V}^{(2)}$ ,  $\Delta$  is defined as

$$\Delta = \tilde{\mathbf{m}}^{(2)\dagger} \mathbf{m}^{(1)},\tag{4.88}$$

and the negative sign in the expression for  $\mathbb{P}^{(2)}$  is taken only if n and m-n are odd.

**Theorem 4.4.2** Let  $V^{(1)}$  and  $V^{(2)}$  be disjoint Lagrangian subspaces of  $\mathbb{C}^m = \mathbb{C}^{2n}$  with minor vectors  $\mathbf{m}^{(1)}$  and  $\mathbf{m}^{(2)}$ , and spanning matrices  $\mathbf{M}^{(1)}$  and  $\mathbf{M}^{(2)}$ . The projection operators

 $\mathbb{P}^{(1)}$  and  $\mathbb{P}^{(2)}$  onto these subspaces can be written

$$\mathbb{P}^{(1)} = \frac{1}{\Delta} \mathbf{M}^{(1)} \tilde{\mathbf{M}}^{(2)T}, \quad \mathbb{P}^{(2)} = \frac{(-1)^n}{\Delta} \mathbf{M}^{(2)} \tilde{\mathbf{M}}^{(1)T}, \tag{4.89}$$

where  $\tilde{\mathbf{M}}^{(1)}$  and  $\tilde{\mathbf{M}}^{(2)}$  are defined by

$$\tilde{\mathbf{M}}^{(1)} = \mathbf{\Sigma} \mathbf{M}^{(1)} [\mathbf{\Sigma}^T : n-1], \tag{4.90}$$

$$\tilde{\mathbf{M}}^{(2)} = \mathbf{\Sigma} \mathbf{M}^{(2)} [\mathbf{\Sigma}^T : n - 1], \tag{4.91}$$

and  $\Delta$  is given by

$$\Delta = \tilde{\mathbf{m}}^{(2)T} \mathbf{m}^{(1)}, \tag{4.92}$$

where  $\tilde{\mathbf{m}}^{(2)} = [\mathbf{\Sigma} : n] \mathbf{m}^{(2)}$ .

To see that this result follows from Theorem 4.4.1 we recall from Section 4.3 that a Lagrangian subspace of  $\mathbb{C}^{2n}$  is a n-dimensional linear subspace such that for any two of its elements  $\mathbf{y}_1$  and  $\mathbf{y}_2$  we have

$$[\mathbf{y}_1, \mathbf{y}_2] = \mathbf{y}_1^T \mathbf{\Sigma} \mathbf{y}_2 = 0. \tag{4.93}$$

If  $V^{(1)}$  is a Lagrangian subspace then the above equation clearly implies that the orthogonal space  $\tilde{V}^{(1)}$  to  $V^{(1)}$  consists of elements of the form  $\Sigma \mathbf{y}^*$ , where  $\mathbf{y}$  is in  $V^{(1)}$ , and the \* notation denotes complex conjugation. This observation shows that the expression for  $\Delta$  in the general form of Theorem 4.4.1 does reduce to the form given in the specialized case of the result. In the same way we may use the explicit forms for the orthogonal space just given, along with the transformation rule for spanning matrices in eq.(4.85) to show that the spanning matrix of  $\tilde{V}^{(1)}$  is given by

$$\Sigma \mathbf{M}^{(1)*}[\Sigma:n-1],\tag{4.94}$$

and similarly for  $\tilde{V}^{(2)}$ . We note that the 'tilded' terms in the two statements of the result do not correspond exactly due to the fact that the complex conjugations that occur in the general result have 'undone themselves' in the special case.

### 4.4.5 Theoretical development of the minor vector method

We now consider how the solutions obtained above can be calculated numerically in a stable and efficient manner. This will be done by making use of the theory of minor vectors as developed by Gilbert & Backus (1966), Woodhouse (1980), and Woodhouse (1988). In this subsection we focus on the algebraic manipulations required to express

the previously obtained solutions in terms of minor vectors and related quantities. The practical implementation of the numerical method, along with a discussion of why it provides improved numerical stability, is given in the next section.

We begin by showing how the term  $\Delta(\omega)$  may be calculated in terms of the minor vectors of the system. Using the notations described in the previous subsection, let us define the *n*th-order *minor vectors* 

$$\mathbf{m}^{(\alpha)}(r,\omega) = [\mathbf{Y}^{(\alpha)}(r,\omega):n], \quad \alpha = 1, 2, \tag{4.95}$$

which are each of dimension  $m!/(n!)^2$ . If we make use of these definitions along with eq.(4.66) and eq.(4.82) we find that

$$\Delta(\omega) = \tilde{\mathbf{m}}^{(2)}(r,\omega)^T \mathbf{m}^{(1)}(r,\omega) = (-1)^n \tilde{\mathbf{m}}^{(1)}(r,\omega)^T \mathbf{m}^{(2)}(r,\omega), \tag{4.96}$$

where we have defined

$$\tilde{\mathbf{m}}^{(\alpha)}(r,\omega) = [\mathbf{\Sigma}\mathbf{Y}^{(\alpha)}(r,\omega):n] = [\mathbf{\Sigma}:n]\mathbf{m}^{(\alpha)}(r,\omega), \quad \alpha = 1,2.$$
(4.97)

The importance of eq. (4.96) lies in the fact that the relevant minor vectors may be directly calculated by the numerical integration of a system of ordinary differential equations (Gilbert & Backus 1966). To see that this is the case, we write the differential equation satisfied by  $\mathbf{Y}^{(1)}(r,\omega)$  as the infinitesimal linear transformation

$$\mathbf{Y}^{(1)}(r+\epsilon,\omega) = (\mathbf{1} + \epsilon \mathbf{A}(r,\omega)) \,\mathbf{Y}^{(1)}(r,\omega) + O(\epsilon^2). \tag{4.98}$$

Using eq.(4.82) to form nth order minors of either side of the above expression, shows that

$$\mathbf{m}^{(1)}(r+\epsilon,\omega) = [\mathbf{1} + \epsilon \mathbf{A}(r,\omega) : n]\mathbf{m}^{(1)}(r,\omega) + O(\epsilon^2). \tag{4.99}$$

From this relation we find that  $\mathbf{m}^{(1)}(r,\omega)$  satisfies the linear differential equation

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{m}^{(1)}(r,\omega) = \mathbf{A}^{(n)}(r,\omega)\mathbf{m}^{(1)}(r,\omega), \tag{4.100}$$

where the coefficient matrix is defined by

$$\mathbf{A}^{(n)}(r,\omega) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{1} + \epsilon \mathbf{A}(r,\omega) : n] \bigg|_{\epsilon=0}.$$
(4.101)

The differential equation satisfied by  $\mathbf{m}^{(2)}(r,\omega)$  is of exactly the same form. Gilbert & Backus (1966) and Woodhouse (1988) have described simple rules for constructing this coefficient matrix from  $\mathbf{A}$ .

We now consider how to express the other parts of equations (4.76) and (4.77) in terms of the minor vectors. Let us first make use of the propagator matrix for the system to write eq.(4.76) as

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \int_{r_1}^r \mathbf{P}(r,r',\omega) \mathbf{Y}^{(2)}(r',\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega)^T \mathbf{Y}^{(2)}(r',\omega)] \tilde{\mathbf{Y}}^{(1)}(r',\omega)^T \mathbf{f}(r',\omega) dr'$$

$$\frac{-1}{\Delta(\omega)} \int_{r}^{r_2} \mathbf{P}(r, r', \omega) \mathbf{Y}^{(1)}(r', \omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r', \omega)^{T} \mathbf{Y}^{(1)}(r', \omega)] \tilde{\mathbf{Y}}^{(2)}(r', \omega)^{T} \mathbf{f}(r', \omega) \operatorname{d}r',$$
(4.102)

and define the matrices  $\mathbb{P}^{(1)}(r,\omega)$  and  $\mathbb{P}^{(2)}(r,\omega)$  by

$$\mathbb{P}^{(1)}(r,\omega) = \frac{1}{\Delta(\omega)} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^T \mathbf{Y}^{(1)}(r,\omega)] \tilde{\mathbf{Y}}^{(2)}(r,\omega)^T, \tag{4.103}$$

$$\mathbb{P}^{(2)}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \mathbf{Y}^{(2)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r,\omega)^T \mathbf{Y}^{(2)}(r,\omega)] \tilde{\mathbf{Y}}^{(1)}(r,\omega)^T, \tag{4.104}$$

so that the solution can be written

$$\mathbf{y}(r,\omega) = \int_{r_1}^{r} \mathbf{P}(r,r',\omega) \mathbb{P}^{(2)}(r',\omega) \mathbf{f}(r',\omega) \, \mathrm{d}r' - \int_{r}^{r_2} \mathbf{P}(r,r',\omega) \mathbb{P}^{(1)}(r',\omega) \, \mathrm{d}r'. \quad (4.105)$$

We shall show that the matrices defined in eq.(4.103) and eq.(4.104) act, respectively, as projection operators onto the Lagrangian subspaces  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$ . We recall that such projection operators must have the defining properties that

$$\mathbb{P}^{(1)}(r,\omega)\mathbf{y} \in V^{(1)}(r,\omega), \quad \forall \mathbf{y} \in \mathbb{C}^m, \tag{4.106}$$

$$\mathbb{P}^{(2)}(r,\omega)\mathbf{y} \in V^{(2)}(r,\omega), \quad \forall \mathbf{y} \in \mathbb{C}^m, \tag{4.107}$$

which is to say the image of each operator is contained in the subspace it projects onto, and, further, on this subspace the projection operator acts as the identity so that we have

$$\mathbb{P}^{(1)}(r,\omega)\mathbf{y} = \mathbf{y}, \quad \forall \mathbf{y} \in V^{(1)}(r,\omega), \tag{4.108}$$

$$\mathbb{P}^{(2)}(r,\omega)\mathbf{y} = \mathbf{y}, \quad \forall \mathbf{y} \in V^{(2)}(r,\omega). \tag{4.109}$$

That the matrices  $\mathbb{P}^{(1)}(r,\omega)$  and  $\mathbb{P}^{(2)}(r,\omega)$  defined in eq.(4.103) and eq.(4.104) have their images contained, respectively, in  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$  is clear from their definition, and we need only check the second property for each operator. For any  $\mathbf{y} \in V^{(1)}(r,\omega)$  we know that there is some  $\mathbf{c} \in \mathbb{C}^n$  such that  $\mathbf{y} = \mathbf{Y}^{(1)}(r,\omega)\mathbf{c}$ . Using this fact along with eq.(4.66) and the definition of the adjoint of a matrix, we then compute that

$$\mathbb{P}^{(1)}(r,\omega)\mathbf{y} = \frac{1}{\Delta(\omega)}\mathbf{Y}^{(1)}(r,\omega)\operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T}\mathbf{Y}^{(1)}(r,\omega)]\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T}\mathbf{y}$$

$$= \frac{1}{\Delta(\omega)}\mathbf{Y}^{(1)}(r,\omega)\operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T}\mathbf{Y}^{(1)}(r,\omega)]\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T}\mathbf{Y}^{(1)}(r,\omega)\mathbf{c}$$

$$= \frac{1}{\Delta(\omega)}\mathbf{Y}^{(1)}(r,\omega)(\Delta(\omega)\mathbf{1})\mathbf{c} = \mathbf{Y}^{(1)}(r,\omega)\mathbf{c} = \mathbf{y}, \tag{4.110}$$

confirming that  $\mathbb{P}^{(1)}(r,\omega)$  is the projection operator for  $V^{(1)}(r,\omega)$ ; the proof for  $\mathbb{P}^{(2)}(r,\omega)$  is identical.

Having now established the fact that  $\mathbb{P}^{(1)}(r,\omega)$  and  $\mathbb{P}^{(2)}(r,\omega)$  are projection operators on  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$  we can make use of Theorem 4.4.2 given in the previous subsection to represent these operators in terms of the *spanning matrices* for the system. Following

the notations of the previous subsection, we define the nth-order spanning matrices

$$\mathbf{M}^{(\alpha)}(r,\omega) = \operatorname{sp}[\mathbf{Y}^{(\alpha)}(r,\omega):n], \quad \alpha = 1, 2, \tag{4.111}$$

each of which is an element of  $\mathbb{C}^{m \times \frac{m!}{(n-1)!(n+1)!}}$ , and is expressible in terms of the *n*th-order minor vectors of the system. The projection operators onto  $V^{(1)}(r,\omega)$  and  $V^{(2)}(r,\omega)$  can be written in terms of these spanning matrices as

$$\mathbb{P}^{(1)}(r,\omega) = \frac{1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \tilde{\mathbf{M}}^{(2)}(r,\omega)^T, \tag{4.112}$$

$$\mathbb{P}^{(2)}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \mathbf{M}^{(2)}(r,\omega) \tilde{\mathbf{M}}^{(1)}(r,\omega)^T, \tag{4.113}$$

where

$$\tilde{\mathbf{M}}^{(\alpha)}(r,\omega) = \operatorname{sp}[\mathbf{\Sigma}\mathbf{Y}^{(\alpha)}(r,\omega):n] = \mathbf{\Sigma}\mathbf{M}^{(\alpha)}(r,\omega)[\mathbf{\Sigma}^T:n-1], \quad \alpha = 1, 2.$$
 (4.114)

Putting these results into eq.(4.105) gives

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \int_{r_1}^r \mathbf{P}(r,r',\omega) \mathbf{M}^{(2)}(r',\omega) \tilde{\mathbf{M}}^{(1)}(r',\omega)^T \mathbf{f}(r',\omega) \, \mathrm{d}r'$$

$$\frac{-1}{\Delta(\omega)} \int_{r_1}^{r_2} \mathbf{P}(r,r',\omega) \mathbf{M}^{(1)}(r',\omega) \tilde{\mathbf{M}}^{(2)}(r',\omega)^T \mathbf{f}(r',\omega) \, \mathrm{d}r', \qquad (4.115)$$

or, in the case of a point source

$$\mathbf{y}(r,\omega) = \begin{cases} \frac{-1}{\Delta(\omega)} \mathbf{P}(r, r_s, \omega) \mathbf{M}^{(1)}(r_s, \omega) \tilde{\mathbf{M}}^{(2)}(r_s, \omega)^T \mathbf{s}(\omega), & r \in [r_1, r_s) \\ \\ \frac{(-1)^n}{\Delta(\omega)} \mathbf{P}(r, r_s, \omega) \mathbf{M}^{(2)}(r_s, \omega) \tilde{\mathbf{M}}^{(1)}(r_s, \omega)^T \mathbf{s}(\omega), & r \in (r_s, r_2] \end{cases}$$
(4.116)

It will be seen in the next section that use of the above expressions to compute the solution of the boundary value problem can lead to numerical instabilities due to the need to propagate the solution from a 'source position' r' (or  $r_s$ ) to the 'receiver position' r by integration of the homogeneous form of the eq.(4.45). This problem can be circumvented by making use of the transformation rules for the spanning matrices given by Woodhouse (1988) to express the solution in a form that displays greater numerical stability. By making use of eq.(4.85), we can write

$$\mathbf{P}(r, r', \omega)\mathbf{M}^{(\alpha)}(r', \omega) = \mathbf{M}^{(\alpha)}(r, \omega)[\mathbf{P}(r, r', \omega)^T : n - 1]^{-1}, \quad \alpha = 1, 2, \tag{4.117}$$

so that the solution in eq.(4.115) becomes

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \int_{r_1}^r \mathbf{M}^{(2)}(r,\omega) [\mathbf{P}(r,r',\omega)^T : n-1]^{-1} \tilde{\mathbf{M}}^{(1)}(r',\omega)^T \mathbf{f}(r',\omega) \, \mathrm{d}r'$$

$$\frac{-1}{\Delta(\omega)} \int_{r}^{r_2} \mathbf{M}^{(1)}(r,\omega) [\mathbf{P}(r,r',\omega)^T : n-1]^{-1} \tilde{\mathbf{M}}^{(2)}(r',\omega)^T \mathbf{f}(r',\omega) \, \mathrm{d}r'. \tag{4.118}$$

Let us now define two matrices in  $\mathbb{C}^{\frac{m!}{(n-1)!(n+1)!} \times m}$  by

$$\mathbf{B}^{(\alpha)}(r, r', \omega) = [\mathbf{P}(r, r', \omega)^T : n - 1]^{-1} \tilde{\mathbf{M}}^{(\alpha)}(r', \omega)^T, \quad \alpha = 1, 2, \tag{4.119}$$

which, for want of a better name, we shall refer to as the *B-matrices* for the system. We

can show by a computation similar to that leading to eq.(4.100) that

$$\frac{\mathrm{d}}{\mathrm{d}r}[\mathbf{P}(r,r',\omega):n-1] = \mathbf{A}^{(n-1)}(r,\omega)[\mathbf{P}(r,r',\omega):n-1], \tag{4.120}$$
 where  $\mathbf{A}^{(n-1)}(r,\omega) \in \mathbb{C}^{\frac{m!}{(n-1)!(n+1)!} \times \frac{m!}{(n-1)!(n+1)!}}$  is defined by analogy with eq.(4.101) as

$$\mathbf{A}^{(n-1)}(r,\omega) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{1} + \epsilon \mathbf{A}(r,\omega) : n-1] \bigg|_{\epsilon=0}. \tag{4.121}$$

From this equation we can show that

$$\frac{\mathrm{d}}{\mathrm{d}r} [\mathbf{P}(r, r', \omega)^T : n - 1]^{-1} = -\mathbf{A}^{(n-1)} (r, \omega)^T [\mathbf{P}(r, r', \omega)^T : n - 1]^{-1}, \tag{4.122}$$

and so see the B-matrices satisfy the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{B}^{(\alpha)}(r,r',\omega) = -\mathbf{A}^{(n-1)}(r,\omega)^T\mathbf{B}^{(\alpha)}(r,r',\omega), \quad \alpha = 1, 2, \tag{4.123}$$

with initial conditions at r = r'

$$\mathbf{B}^{(\alpha)}(r', r', \omega) = \tilde{\mathbf{M}}^{(\alpha)}(r', \omega)^T, \quad \alpha = 1, 2. \tag{4.124}$$

Putting these B-matrices into eq.(4.118) we obtain

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \int_{r_1}^r \mathbf{M}^{(2)}(r,\omega) \mathbf{B}^{(1)}(r,r',\omega) \mathbf{f}(r',\omega) dr'$$
$$-\frac{1}{\Delta(\omega)} \int_{r}^{r_2} \mathbf{M}^{(1)}(r,\omega) \mathbf{B}^{(2)}(r,r',\omega) \mathbf{f}(r',\omega) dr', \tag{4.125}$$

which is the final form of the solution that we shall use in numerical calculations. By making the same replacements as above, we also obtain the corresponding solution in the case of a point force as

$$\mathbf{y}(r,\omega) = \begin{cases} \frac{-1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \mathbf{B}^{(2)}(r,r_s,\omega) \mathbf{s}(\omega) & r \in [r_1, r_s) \\ \\ \frac{(-1)^n}{\Delta(\omega)} \mathbf{M}^{(2)}(r,\omega) \mathbf{B}^{(1)}(r,r_s,\omega) \mathbf{s}(\omega) & r \in (r_s, r_2] \end{cases} , \tag{4.126}$$

$$\mathbf{y}(r,\omega) = \begin{cases} \frac{-1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \mathbf{B}^{(2)}(r,r_s,\omega) \mathbf{s}(\omega) & r \in [r_1,r_s) \\ \frac{(-1)^n}{\Delta(\omega)} \mathbf{M}^{(2)}(r,\omega) \mathbf{B}^{(1)}(r,r_s,\omega) \mathbf{s}(\omega) & r \in (r_s,r_2] \end{cases}$$
along with the expression
$$\mathbf{G}(r,r',\omega) = \begin{cases} \frac{-1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \mathbf{B}^{(2)}(r,r',\omega) & r \in [r_1,r') \\ \frac{(-1)^n}{\Delta(\omega)} \mathbf{M}^{(2)}(r,\omega) \mathbf{B}^{(1)}(r,r',\omega) & r \in (r',r_2] \end{cases}$$
for the Green's function for the problem

for the Green's function for the pro

#### 4.4.6Extension of the method to a general linear system

While the theory of Subsection 4.4.5 presented the minor vector method as specialized to a real linear Hamiltonian system this circumstance is not necessary for its use. An example of a more general problem is the calculation of synthetic seismograms in a fully anisotropic half-space, for which the governing differential equations may be shown (e.g. Woodhouse 1974, Fryer & Frazer 1984) to have a coefficient matrix with the structure

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & \mathbf{K} \\ \mathbf{S} & \mathbf{T}^T \end{pmatrix}. \tag{4.128}$$

In the case that the wavenumbers and elastic parameters of the problem are all real the above equations can be written in Hamiltonian form, though this Hamiltonian is not 'real' in the sense that it involves complex conjugation, and the coefficient matrix is found to posses the structure

$$\mathbf{A} = \begin{pmatrix} \mathbf{T} & \mathbf{K} \\ \mathbf{S} & -\mathbf{T}^{\dagger} \end{pmatrix},\tag{4.129}$$

where † denotes Hermitian conjugation. Systems with the above structure may be shown to possess many similar properties to the real linear Hamiltonian systems described in this work (e.g. Thomson et. al. 1986). Interestingly, we observe that the corresponding equations in the case of a transversely isotropic half space are expressible in the form of a real linear Hamiltonian system (e.g. Aki & Richards, 1980, chapter 7); the physical significance of this fact is not fully understood, but it may be that the symplectic structure of the equations does in some way depend on the additional symmetries present when the constitutive relation is transversely isotropic.

To make the required generalizations to the above method we return to the equation (4.61) which was derived without any use of the special properties of a real linear Hamiltonian system, and write it as

$$\mathbf{y}(r,\omega) = \int_{r_1}^{r} \mathbf{P}(r,r',\omega)\mathbf{Y}(r',\omega)\mathbf{J}_{+}\mathbf{Y}(r',\omega)^{-1}\mathbf{f}(r',\omega)\,\mathrm{d}r'$$
$$-\int_{r}^{r_2} \mathbf{P}(r,r',\omega)\mathbf{Y}(r',\omega)\mathbf{J}_{-}\mathbf{Y}(r',\omega)^{-1}\mathbf{f}(r',\omega)\,\mathrm{d}r'. \tag{4.130}$$

Proceeding as in section 4.4.5 we show that the matrices

$$\mathbb{P}^{(1)}(r,\omega) = \mathbf{Y}(r',\omega)\mathbf{J}_{-}\mathbf{Y}(r',\omega)^{-1}, \tag{4.131}$$

$$\mathbb{P}^{(2)}(r,\omega) = \mathbf{Y}(r',\omega)\mathbf{J}_{+}\mathbf{Y}(r',\omega)^{-1}, \tag{4.132}$$

are the projection operators onto the linear subspaces spanned by the columns of the matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$ . Having made this identification, we can make use of Theorem 4.4.1 of Woodhouse (1988) which shows how these projection operators may be constructed in terms of the spanning matrices of  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$ . The final result of this analysis gives a formula very similar to eq.(4.125) except for the fact that the determinant term  $\Delta(\omega)$  now depends on r and so must be brought within the integral sign, and that the terms like  $\tilde{\mathbf{m}}^{(1)}(r,\omega)$ ,  $\tilde{\mathbf{m}}^{(2)}(r,\omega)$  etc, are no longer defined by formulae

involving the matrix  $\Sigma$  but rather through eq.(2.38) of Woodhouse (1988).

# 4.5 Numerical Implementation and Stability

# 4.5.1 Numerical implementation of the minor vector method

In this subsection we shall describe the numerical implementation of the minor vector method. We focus on the case of a point source given in eq.(4.126) as this is likely to be of greatest practical importance, and also because it provides the basis for calculations with a general force vector. To fix attention, let  $r > r_s$ , that is, the receiver position is above the source, with the other case being handled in essentially the same manner. For the given geometry the displacement-stress vector is given by

$$\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \mathbf{M}^{(2)}(r,\omega) \mathbf{B}^{(1)}(r,r_s,\omega) \mathbf{s}(\omega), \tag{4.133}$$

so that we need to calculate  $\Delta(\omega)$ ,  $\mathbf{M}^{(2)}(r,\omega)$ , and  $\mathbf{B}^{(1)}(r,r_s,\omega)$ . The process for computing these terms is as follows:

- 1. Numerically integrate the *n*th order minor vector equations from  $r_1$  to  $r_s$  to obtain  $\mathbf{m}^{(1)}(r_s,\omega)$ . From this vector we can compute  $\mathbf{M}^{(1)}(r_s,\omega)$  and store its value. We then continue the numerical integration of the *n*th order minor vector equations up to the receiver depth r to obtain  $\mathbf{m}^{(1)}(r,\omega)$  which we store.
- 2. Numerically integrate the *n*th order minor vector equations from  $r_2$  to r to obtain  $\mathbf{m}^{(2)}(r,\omega)$  and  $\mathbf{M}^{(2)}(r,\omega)$ . Using  $\mathbf{m}^{(2)}(r,\omega)$  along with  $\mathbf{m}^{(1)}(r,\omega)$ , we then calculate  $\Delta(\omega)$  by eq.(4.96). If  $\Delta(\omega) \neq 0$  then  $\omega$  is not an eigenfrequency of the equations, and a solution to the problem will exist.
- 3. Using the value of  $\mathbf{M}^{(1)}(r_s, \omega)$  previously found, we compute by eq.(4.124) the initial conditions for  $\mathbf{B}^{(1)}(r_s, r_s, \omega)$ . We then numerically integrate the (n-1)th minor vector equations in the form of eq.(4.123) from  $r_s$  to r to obtain  $\mathbf{B}^{(1)}(r, r_s, \omega)$ .

Having performed these various steps, the solution is then calculated using eq.(4.133). The number of computations in step (iii) may be reduced if we first compute  $\mathbf{B}^{(1)}(r_s, r_s, \omega)\mathbf{s}(\omega)$ , and then integrate the (n-1)th minor vector equations only once to obtain  $\mathbf{B}^{(1)}(r, r_s, \omega)\mathbf{s}(\omega)$  directly, rather than performing m integrations of these equations so as to compute the full

B-matrix. In the case of a general force vector the required computations are essentially the same as above, except for the fact that the B-matrices must now be tabulated throughout  $[r_1, r_2]$  at a sufficient number of points for accurate numerical evaluation of the integrals occurring in eq.(4.125).

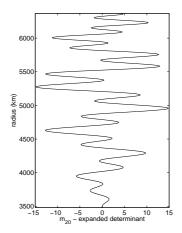
For the spheroidal motion equations the third-order minor vector equations are twenty dimensional. However, Result 4.2 of Woodhouse (1988) shows that in the case of real linear Hamiltonian system, the third-order minor vectors possess symmetries that allow the number of equations to be reduced to fourteen. The second-order minor vector equations that the B-matrices satisfy are fifteen-dimensional, though it may be shown that for a real linear Hamiltonian system there exists a symmetry such that the B-matrices may be calculated by solving a reduced set of fourteen equations. In the case that n = 2, such as for spheroidal motions in a fluid layer or spheroidal motions in a non-self-gravitating earth model, the B-matrices are four-by-four dimensional, and eq.(4.123) becomes

$$\frac{\mathrm{d}}{\mathrm{d}r}\mathbf{B}^{(\alpha)}(r,r',\omega) = -\mathbf{A}(r,\omega)^T\mathbf{B}^{(\alpha)}(r,r',\omega), \quad \alpha = 1,2,$$
(4.134)

so that step (iii) of the above algorithm essentially involves integration of the original system of equations. This specific result for four-dimensional systems of equations was given by Woodhouse (1980), and forms part of the theoretical basis for the method used to compute synthetic seismograms in a non-self-gravitating earth model by Friederich & Dalkolmo (1995).

## 4.5.2 Numerical stability of the minor vector method

In this subsection we consider why the minor vector method presented above is able to produce accurate solutions to the boundary value problem of spheroidal motions in a self-gravitating earth model while the simpler method of section 4.2 cannot. To this end a number of example calculations have been performed with the two methods of solution to demonstrate some of the problems observed and how they are remedied by the minor vector method. The earth model PREM of Dziewonski & Anderson (1981) has been used in all calculations. Because we are primarily interested in the implementation of the minor vector method for six-dimensional systems of equations we have chosen to restrict attention to the solid mantle of the PREM model, and have used a stress-free



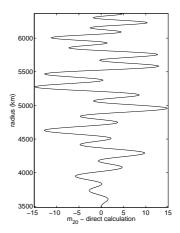


Figure 4.1: This figure shows two plots of the minor vector component  $m_{20}(r,\omega)$  for l=2 and  $\omega=20\,\mathrm{mHz}$  as calculated either by evaluation of the necessary sub-determinant of the  $\mathbf{Y}(r,\omega)$  matrix (the plot on the left) or by integration of the minor vector equations (the plot on the right). As can be seen the two versions of  $m_{20}(r,\omega)$  look very similar, and, in fact, they are in complete agreement to the level of accuracy of the calculations.

boundary condition at the core-mantle boundary. All numerical integrations have been performed using a fourth-order Runge-Kutta method described by Press *et. al.* (1986). During these numerical integrations the continuity of the displacement-stress vector  $\mathbf{y}(r,\omega)$  is imposed explicitly at those radii for which the coefficient matrix  $\mathbf{A}(r,\omega)$  is discontinuous. For calculations in which a source discontinuity-vector  $\mathbf{s}(\omega)$  was needed, it was taken as  $\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \end{pmatrix}^T$  – this arbitrary choice is not important for any of the observations made below.

The first problem with the solution presented in section 4.2 and given in eq.(4.31) is that, though the relevant matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$  can be calculated accurately by numerical integration of the sixth-order system of differential equations, the inverse of the resulting six-by-six matrix  $\mathbf{Y}(r,\omega)$  cannot be computed accurately. To illustrate this point we can consider the calculation of the third-order minors of the matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$ , from which the inverse of  $\mathbf{Y}(r,\omega)$  may be calculated using the results of the previous section. In Figures 4.1 and 4.2 plots of the  $m_{20}^{(1)}(r,\omega)$  component of the minor

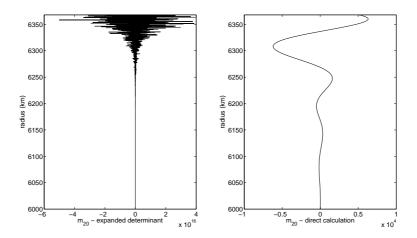


Figure 4.2: This figure shows two plots of the minor vector component  $m_{20}(r,\omega)$  for l=100 and  $\omega=30\,\mathrm{mHz}$  as calculated either by evaluation of the necessary sub-determinant of the  $\mathbf{Y}(r,\omega)$  matrix (the plot on the left) or by integration of the minor vector equations (the plot on the right). We observe that only the radius range 6000–6368 km is shown because the solution is vanishingly small lower in the mantle.

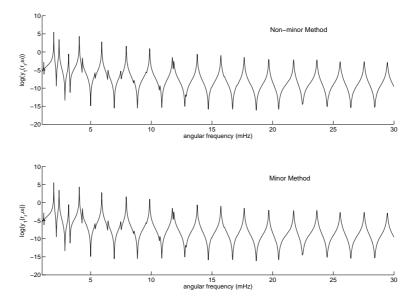


Figure 4.3: Plots of  $\log(|y_1(r_r,\omega)|)$  against  $\omega$  for the l=2 spheroidal motion equations as calculated either by the non-minor method using eq.(4.62) in the upper plot, and the minor vector method using eq.(4.126) in the lower plot. The source depth for the calculation was 10 km, and the receiver depth was also 10 km.

vector  $\mathbf{m}^{(1)}(r,\omega)$ , which is defined by the determinant

$$m_{20}^{(1)} = \begin{vmatrix} Y_{41}^{(1)} & Y_{42}^{(1)} & Y_{43}^{(1)} \\ Y_{51}^{(1)} & Y_{52}^{(1)} & Y_{53}^{(1)} \\ Y_{61}^{(1)} & Y_{62}^{(1)} & Y_{63}^{(1)} \end{vmatrix}, \tag{4.135}$$

are shown for two different values of  $(\omega, l)$  as calculated either by expansion of the above determinant, or by direct integration of the differential equations satisfied by the minor vector  $\mathbf{m}^{(1)}(r,\omega)$  given in eq.(4.101). As can be seen from Figure 4.2, for certain values of  $(\omega, l)$  there can be very large differences between the minors calculated by the two methods, with the solution obtained by direct expansion of the determinant showing extremely erratic behaviour, and being many orders of magnitude larger than the correct solution obtained by direct integration of the minor vector equations. To understand these observations we recall that for a given value of  $(\omega, l)$  the solutions to the homogeneous form of eq.(4.11) may have either exponentially growing or decreasing solutions in portions of the interval of integration (e.g. Dahlen & Tromp 1998, chapter 12). Due to the exponential behaviour of the solutions, it is possible for the columns of  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$  to have very large magnitudes, yet still, in principle, contain the contributions of those solutions that have been exponentially decreasing. These exponentially decreasing contributions to the columns of the Y-matrices can have magnitudes far smaller than the total magnitude of the columns of the matrix, and, when using finite precision arithmetic, may be totally lost if their relative magnitudes becomes smaller than the relative accuracy of the integration. If such an 'underflow' process occurs, then while the resulting Y-matrices will still be correct to a number of significant figures determined by the relative accuracy of the integration, it will no longer be possible to accurately calculate the minors of the Y-matrices. To see that this is the case, we recall that the minors of a matrix are, in a sense, functions of the linear subspace spanned by the columns of the matrix, and, up to a scalar multiple, are independent of the basis chosen for this subspace. Because of this, the exponentially small components of the columns of the Y-matrices are just as important for the calculation of the minors as the exponentially large components. In Figure 4.2 we are seeing the results of exactly such an underflow problem which leads to the values of  $m_{20}^{(1)}(r,\omega)$  calculated by the expansion of the required determinant being grossly incorrect. It is worth noting that though the above discussion has focused on the inversion of  $\mathbf{Y}(r,\omega)$ by the calculation of its minors, the same numerical instabilities affect other numerical methods for computing the inverse such as LU decomposition (Press et al. 1986).

The effects of these numerical instabilities on the calculated solutions to the boundary value problems are shown clearly in Figure 4.3 and 4.4. Here the calculated values of the  $y_1$  component of the displacement-stress vector are plotted as a function of frequency for two different values of l as calculated either with or without the use of the minor vector method. For these calculations, the source and receiver depth was located at 10 km so that integration of the B-matrix equations was not needed to compute the solution. When l=2 in Figure 4.3, there is no difficulty in the expansion of the minors required to compute the solution given in eq.(4.31), and in this case there is perfect agreement between the non-minor and minor vector solutions to the problem. For l = 100 in Figure 4.4, however, it is seen that while the two solutions are in agreement for lower frequencies, for values of  $\omega$  greater than around 20 mHz the two methods of solution diverge, with the non-minor solution behaving extremely erratically. This example illustrates the general observation that, for a given value of l, there is usually a 'transition frequency' below which the non-minor vector method is stable, and above which the minor vector method is essential. Numerical investigations have shown that this transition frequency usually occurs a little above the fundamental mode frequency for the given l. In Figure 4.5 is shown the  $y_1$  component of the displacement-stress vector for the static deformation problem  $(\omega = 0 \, \mathrm{mHz})$  when the source and receiver depths are located at 10 km depth. It is seen that for l less than around 2000 the non-minor and minor vector methods of calculation are in agreement, but for larger values of l the non-minor vector method becomes unstable.

Next we consider why the B-matrices were introduced into the problem, and why, as is done in eq.(4.116), we cannot simply propagate the solution obtained at the source depth to the receiver depth by integrating the original system of differential equations. Suppose we are solving a point source problem, and that the receiver is located above the source. Then we know from eq.(4.116) the solution to the problem can be written

 $\mathbf{y}(r,\omega) = \frac{(-1)^n}{\Delta(\omega)} \mathbf{P}(r,r_s,\omega) \mathbf{M}^{(2)}(r_s,\omega) \tilde{\mathbf{M}}^{(1)}(r_s,\omega)^T \mathbf{s}(\omega) = \mathbf{P}(r,r_s,\omega) \mathbb{P}^{(2)}(r_s,\omega) \mathbf{s}(\omega), \qquad (4.136)$ where we have recalled the definition of the projection operator  $\mathbb{P}^{(2)}(r,\omega)$  in eq.(4.104). From this equation we see that the solution to the problem is obtained by projecting the source discontinuity-vector  $\mathbf{s}(\omega)$  onto the linear subspace  $V^{(2)}(r_s,\omega)$ , and then propagating this vector up to the receiver position. As we shall now explain, when the source and

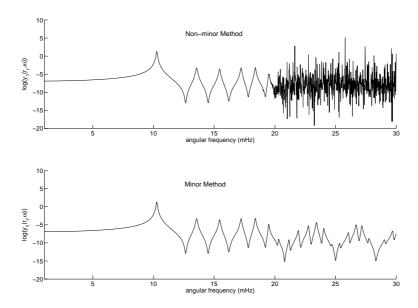


Figure 4.4: Plots of  $\log(|y_1(r_r,\omega)|)$  against  $\omega$  for the l=100 spheroidal motion equations as calculated either by the non-minor method using eq.(4.62) in the upper plot, and the minor vector method using eq.(4.126) in the lower plot. The source depth  $d_s$  for the calculation was 10 km, and the receiver depth  $d_r$  was also 10 km.

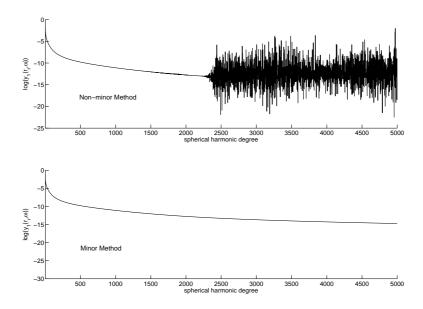


Figure 4.5: Plots of  $\log(|y_1(r_r,\omega)|)$  against l for the static deformation problem as calculated either by the non-minor method using eq.(4.62) in the upper plot, and the minor vector method using eq.(4.126) in the lower plot.

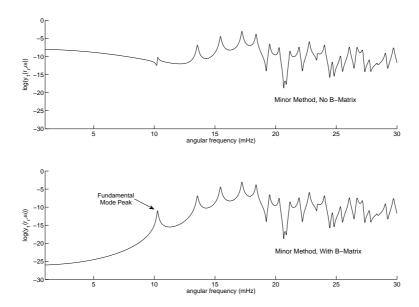


Figure 4.6: Plots of  $\log(|y_1(r_r,\omega)|)$  against  $\omega$  for the l=100 equations as calculated either by the minor method without the use of B-matrices given in eq.(4.116) in the upper plot, and the minor vector method using the B-matrices as in eq.(4.126) in the lower plot. The source  $d_s$  for the calculation was 670 km, and the receiver depth  $d_r$  was 10 km.

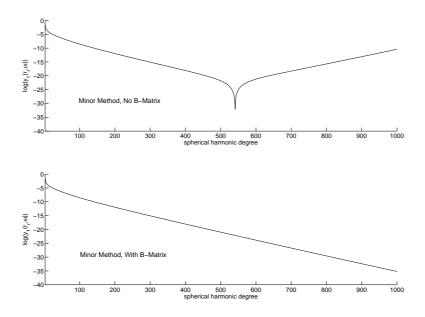


Figure 4.7: Plots of  $\log(|y_1(r_r,\omega)|)$  against l for the static deformation problem as calculated either by the minor method without the use of B-matrices given in eq.(4.116) in the upper plot, and the minor vector method using the B-matrices as in eq.(4.126) in the lower plot. The source  $d_s$  for the calculation was 100 km, and the receiver depth  $d_r$  was 10 km.

receiver depths are significantly different the propagation of the displacement-stress vector to the source position can lead to numerical instabilities. Consider the case when the source depth is, for the given  $(l,\omega)$ , positioned well below the turning point of the equations where the solution changes from exponential to oscillatory behaviour (e.g. Dahlen & Tromp 1998, chapter 12). In this case the linear subspace  $V^{(1)}(r_s,\omega)$  is effectively spanned by the set of three solutions that grow exponentially upwards, while the linear space  $V^{(2)}(r,\omega)$  is the spanned by the set of solutions that decrease exponentially upwards. In practice, the projection operator given in the above equation will act to produce a vector that only lies in  $V^{(2)}(r_s,\omega)$  to a finite number of significant figures determined by the accuracy of the numerical integration method. Beyond these significant figures the displacement-stress vector obtained will, in general, have some component in  $V^{(1)}(r_s,\omega)$  that grows exponentially during the upwards integration. By the time the integration gets to the source position, this upwards growing error term may have become larger than the 'true' solution, and so all accuracy may be lost.

In Figure 4.6 and Figure 4.7 two examples of the above problem are shown, the first for the dynamic problem for l = 100 and frequencies in the range 1 to  $30 \,\mathrm{mHz}$  for a source depth of 670 km and receiver depths of 10 km, and the second for the static deformation problem for l in the range 2 to 1000 for a source depth of 100 km and receiver depth of  $10\,\mathrm{km}$ . In each of these two figures, the upper plot shows the  $y_1$  component of the displacement-stress vector calculated using the minor vector method to give the solution at the source depth, and this solution was then propagated up to the receiver by integrating the original system of differential equations. In the lower plot of each figure is again shown the  $y_1$  component of the displacement-stress vector, but now calculated by using the 'full' minor vector method described in the previous subsection involving the integration of the (n-1)th minor vector equations to solve for  $\mathbf{B}^{(1)}(r,r_s,\omega)$ . In Figure 4.6 it is seen that the two methods of calculation agree for the higher frequencies present, but as the frequency decreases the two solutions diverge dramatically (note the logarithmic scale), with the 'non B-matrix' solution becoming exponentially large as frequency tends to zero, and the B-matrix solution becoming exponentially small. Physically we would expect that the Bmatrix solution is correct because such a deep source is known to poorly excite fundamental or low overtone surface waves. The non-physical exponential growth of the non B-matrix solution for lower frequencies is a clear example of the problem described above during the propagation of the solution from the source to the receiver for a deep source. A very similar phenomena is seen in Figure 4.7 for the static deformation problem, where the non B-matrix solution is seen to grow exponentially with l for large values of l, while the B-matrix solution decreases exponentially with increasing l as would be physically expected.

The reason that the B-matrix method removes this instability may be understood heuristically by regarding the method as postponing the action of the projection operator on the discontinuity-vector until the receiver position has been reached. In this way the solution obtained at the receiver position is calculated to the same relative accuracy as the numerical integrations. A more formal approach to the stability of the calculations is to consider the ostensible order of magnitude of the solution obtained by the two methods in the case that the solutions behave in an exponential manner throughout the earth model. To simplify the geometry of the problem we take the receiver position at the surface  $r = r_2$  and the source position at  $r = r_s$  with  $r_s < r$ . We shall assume that the solutions to the homogeneous form of eq.(4.45) all have exponential behaviour, and that the three upwards increasing solutions have the growth rates  $\lambda_1 > \lambda_2 > \lambda_3 \ge 0$ . We first determine the ostensible order of magnitude of the non-B-matrix solution as follows: The solution to the problem obtained at the source position can be written

$$\mathbf{y}(r_s, \omega) = \mathbb{P}^{(2)}(r_s, \omega)\mathbf{s}(\omega), \tag{4.137}$$

where  $\mathbb{P}^{(2)}(r_s,\omega)$  is the projection operator onto the subspace  $V^{(2)}(r_s,\omega)$ . We are free to assume that the source-discontinuity vector has unit magnitude, and recalling that projection operators have norm less than or equal to one, we see that the solution at the source position has magnitude of order 1. To obtain the solution at the receiver position using the non-B-matrix method we need to propagate  $\mathbf{y}(r_s,\omega)$  to  $r=r_2$  by integrating the original system of differential equations for the problem. During this upward integration the displacement-stress vector will grow exponentially at the largest exponential rate  $\lambda_1$  so that

$$\mathbf{y}(r_2,\omega) \sim e^{\lambda_1(r_2 - r_s)},\tag{4.138}$$

where the notation  $\sim$  means order of magnitude. For the B-matrix solution to the problem

we have

$$\mathbf{y}(r,\omega) = \frac{-1}{\Delta(\omega)} \mathbf{M}^{(2)}(r_2,\omega) \mathbf{B}^{(1)}(r_2,r_s,\omega) \mathbf{s}(\omega), \tag{4.139}$$

so that we need to determine the order of magnitude of each of the various terms. The determinant  $\Delta(\omega)$  depends on the minor vector  $\mathbf{m}^{(1)}(r_2,\omega)$  which was obtained by integrating the third-order minor vector equations from  $r_1$  to  $r_2$ . This integration has largest growth rate  $\lambda_1 + \lambda_2 + \lambda_3$ , so that we obtain

$$\Delta(\omega) \sim e^{(\lambda_1 + \lambda_2 + \lambda_3)(r_2 - r_1)}. (4.140)$$

Similarly the initial value of  $\mathbf{B}^{(1)}(r_s, r_s, \omega)$  depends on  $\mathbf{m}^{(1)}(r_s, \omega)$ , and we obtain

$$\mathbf{B}^{(1)}(r_s, r_s, \omega) \sim e^{(\lambda_1 + \lambda_2 + \lambda_3)(r_s - r_1)}$$
 (4.141)

During the integration of the second-order minor vector equations from  $r_s$  to  $r_2$  the largest growth rate is  $\lambda_1 + \lambda_2$  so that

$$\mathbf{B}^{(1)}(r_2, r_s, \omega) \sim e^{(\lambda_1 + \lambda_2 + \lambda_3)(r_s - r_1)} e^{(\lambda_1 + \lambda_2)(r_2 - r_s)},$$
 (4.142)

$$= e^{(\lambda_1 + \lambda_2)(r_2 - r_1)} e^{\lambda_3(r_s - r_1)}. \tag{4.143}$$

Finally, we can take  $\mathbf{M}^{(2)}(r_2,\omega) \sim 1$ , and by putting all these results together we find

$$\mathbf{y}(r_2, \omega) \sim e^{-(\lambda_1 + \lambda_2 + \lambda_3)(r_2 - r_1)} e^{(\lambda_1 + \lambda_2)(r_2 - r_1)} e^{\lambda_3(r_s - r_1)} = e^{-\lambda_3(r_2 - r_s)}. \tag{4.144}$$

We can conclude that the non B-matrix method leads to a solution with ostensible order of magnitude  $e^{\lambda_1(r_2-r_s)}$  while the B-matrix method gives a solution of order  $e^{-\lambda_3(r_2-r_s)}$  which is exponentially smaller. The results of these order-of-magnitude calculations show that the non-B-matrix method leads to a solution of an exponentially larger order than the B-matrix solution, in accordance with the numerical examples. Because the order of magnitude of the exact solution cannot be larger than that of the ostensible order calculated, we can conclude that the B-matrix solution will have a far greater stability than the non-B-matrix solution. Though this argument does not demonstrate that the solution obtained by the B-matrix method is necessarily correct, that this is the case is strongly suggested by the physically plausible behaviour of the solution seen in the example calculation described above.

# 4.6 Calculation of the time-domain solution

In this section we turn our attention to the evaluation of the inverse Fourier transforms needed to compute the time domain solution of the boundary value problems we have been considering. The discussion will focus on the case of seismic displacement fields in spherically symmetric earth models, though the general results presented will be applicable to a wide range of boundary value problems that have the structure of real linear Hamiltonian systems.

We first consider the application of numerical inverse Fourier transforms to calculate the time-domain solution. In this method the solution of the frequency-domain equations are determined at a discrete range of frequencies, and the fast Fourier transform (FFT) algorithm is used to calculate the corresponding time-domain solution. This method has been used previously by Friedrich & Dalkolmo (1995) in non-self gravitating earth models, and also in the *direct solution method* of Cummins *et al.* (1994) who employed a finite-element method for calculating solutions of the frequency-domain equations.

We next consider the analytical evaluation of the inverse Fourier transform using the methods of contour integration. This approach leads to a concise expression for the time-domain solution as a sum over the normal modes of the earth model along with additional terms related to viscoelastic relaxation processes. For simplicity, in this chapter we focus only on simple poles of the frequency-domain solution associated with normal modes of the earth model, and postpone the detailed discussion of other kinds of singularity to Chapter 6.

## 4.6.1 Numerical inverse Fourier transforms

The minor vector method can be applied to the solution of the spheroidal, toroidal, and radial systems of inhomogeneous differential equations in a more realistic earth model which includes a solid inner core, a fluid outer core, a solid mantle and crust, and a fluid ocean. In this way, the complete solution of the elastodynamic equation can be determined in the *spectral-domain* in which the time-dependence of the solution has been transformed into the frequency-domain, and the angular-dependence of the solution has been expanded in vector spherical harmonics. In figures 4.8 to 4.11 the form of such *spectral solutions* are shown for spheroidal and toroidal equations.

Having obtained the spectral solution of the problem for a suitable range of l's and  $\omega$ 's, we can sum the appropriate aspherical harmonic series to obtain the frequency-domain solu-

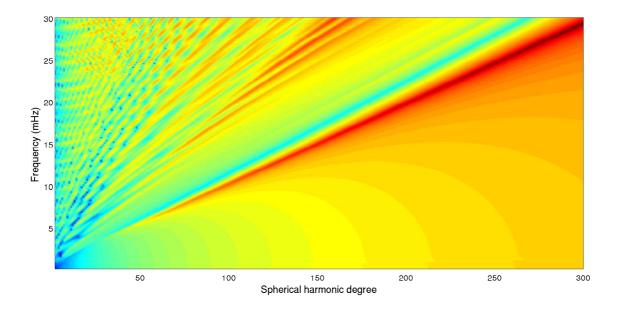


Figure 4.8: A plot of the logarithmic amplitude of the  $G_{12}$  component of the spheroidal Green's function for a source located at 10km depth and receiver at the sea-floor. The colour scale is such that red denotes high values, and blue low values. The high-amplitudes on the plot can clearly be seen to delineate the mode branches found on spheroidal dispersion diagrams.

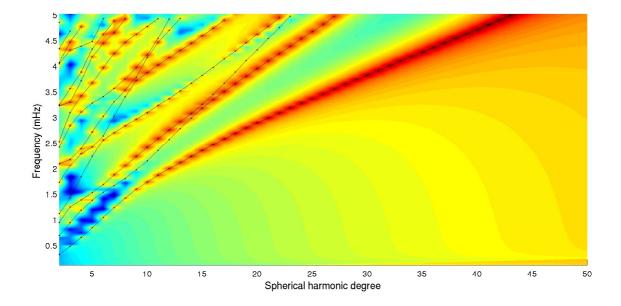


Figure 4.9: A close up of the lower frequency and angular order portion of the previous figure showing the structure of the spectral solution more clearly. Also plotted is the location of the spheroidal eigenfrequencies for the earth model, which are denoted by black dots.

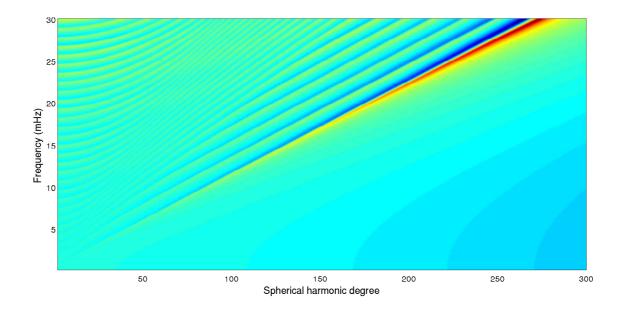


Figure 4.10: A plot of the logarithmic amplitude of the  $G_{11}$  component of the toroidal Green's function for a source located at 10km depth and receiver at the sea-floor. The colour scale is such that red denotes high values, and blue low values. The high-amplitudes on the plot can clearly be seen to deliniate the mode branches found on toroidal dispersion diagrams.

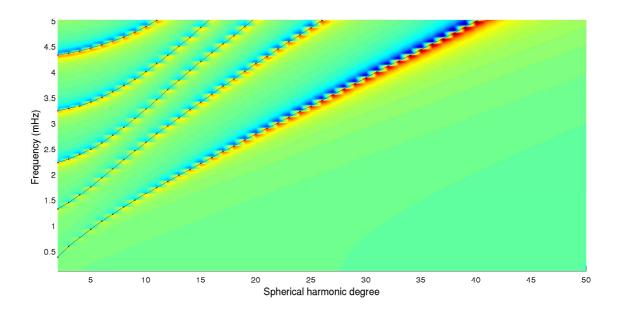


Figure 4.11: A close up of the lower frequency and angular order portion of a portion of the previous figure showing the structure of the spectral solution more clearly. Also plotted is the location of the toroidal eigenfrequencies for the earth model.

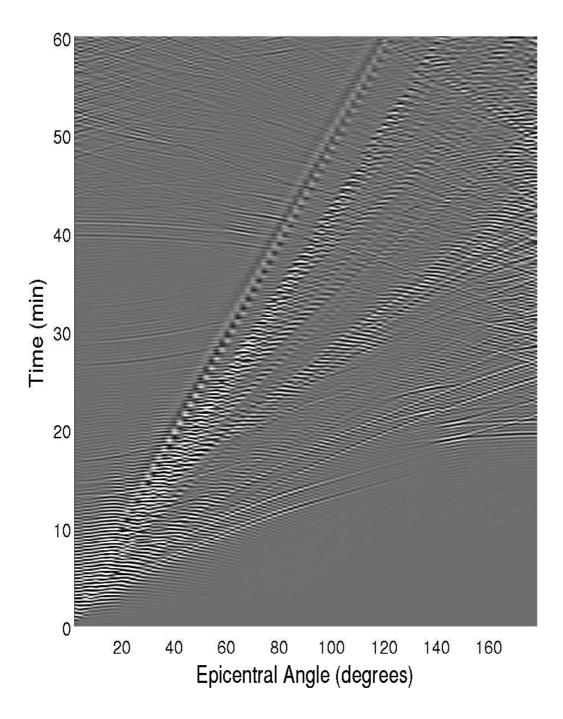


Figure 4.12: Vertical component synthetic acceleration seismograms at a range of epicentral angles from a moment tensor point source. The source depth was chosen to be  $300\,\mathrm{km}$  so as to suppress the occurrance of large amplitude surface waves. In the plot light shades correspond to positive amplitudes and dark shades to negative amplitudes. These calculations were done using frequencies from  $0.1\,\mathrm{mHz}$  to  $60\,\mathrm{mHz}$  and l in the range 0-800.

tion at a discrete range of frequencies. The time-domain solution can then be computed by performing a numerical Fourier transform using the fast Fourier transform (FFT) algorithm (e.g. Press et al. 1986). A complication arising in this process is that the frequency-domain solution may be singular for certain frequencies lying on the real-axis. This is because the solution of the elastodynamic equations is, in general, not integrable, and so does not have a well-defined Fourier transform in the classical sense. To circumvent this problem we instead consider the inverse Fourier-Laplace transform for which values of the frequency-domain solution lying in the lower-half of the complex-plane are used. It may be shown that for such values of  $\omega$  the solution is holomorphic and that it is square integrable along any line parallel to the real axis. For definiteness, let us consider the calculation of the radial component  $u_r(t)$  at a given receiver position The inversion formula for the Fourier-Laplace transform gives for any  $\epsilon > 0$ 

$$u_r(t) = \frac{1}{2\pi} \int_{-\infty - i\epsilon}^{\infty - i\epsilon} \hat{u}_r(\omega) e^{i\omega t} d\omega = \frac{e^{\epsilon t}}{2\pi} \int_{-\infty}^{\infty} \hat{u}_r(\omega - i\epsilon) e^{i\omega t} d\omega.$$
 (4.145)

From this expression we see that  $u_r(t)$  can be found by first computing the normal inverse Fourier transform of  $\omega \mapsto \hat{u}_r(\omega - \mathrm{i}\epsilon)$  using the FFT algorithm, and then multiplying the result by the growing exponential  $\mathrm{e}^{\epsilon t}$ . The larger the value of  $\epsilon$  used, the further away the integration contour will lie from any singularities of  $\hat{u}_r(\omega)$ , and so the smoother the integrand occurring in the numerical inverse Fourier transform. Consequently, by choosing  $\epsilon$  to be large, we can reduce the number of frequencies at which we determine the spectral solution. Noting that

$$u_r(t)e^{-\epsilon t} = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}_r(\omega - i\epsilon)e^{i\omega t} d\omega, \qquad (4.146)$$

we see that the time-series corresponding to  $\hat{u}_r(\omega - i\epsilon)$  under the inverse Fourier transform is  $u_r(r)e^{-\epsilon t}$ , and so for large values of  $\epsilon$  the later portions of this time-series will be strongly attenuated. If  $\epsilon$  is taken to be too large, the computed values of  $u_r(t)e^{-\epsilon t}$  for large times may be zero to the numerical precision of the calculations. In practice it is found that if the desired length of the time series is T, then taking  $\epsilon$  such that  $\epsilon T \approx 0.2$  is a good choice (Friedrich & Dalkolmo 1995). Given a value of  $\epsilon$ , the frequency-spacing of the values of  $\hat{u}_r(\omega - i\epsilon)$  to be tabulated can then be chosen from the requirement that the exponential  $e^{i\omega t}$  is sufficiently well-sampled in the given time-range, and also from estimates of the width of the 'spectral peaks' of  $\hat{u}_r(\omega - i\epsilon)$  which may be shown to be approximately proportional to  $\epsilon$ . To illustrate this method, figures 4.12 and 4.13 show example synthetic seismograms. The

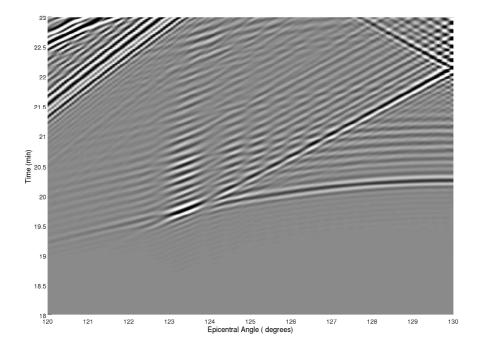


Figure 4.13: A close up of the PKP-triplication shown in a vertical component synthetic seismogram. For this calculation the range of frequencies used was 0.1-300 mHz and the range of *l*'s was 0-10000.

accuracy of these calculations has been verified by comparing the calculated seismograms with those produced using normal mode summation.

# 4.6.2 Eigenfrequencies and eigenfunctions of the equations

We consider the evaluation of the inverse Fourier transform

$$\mathbf{y}(r,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{\mathbf{y}}(r,\omega) e^{i\omega t} d\omega, \qquad (4.147)$$

for positive times, where  $\hat{\mathbf{y}}(r,\omega)$  is the solution of the boundary value problem considered in section 4.4; in accordance with our earlier notational simplifications, in what follows we write  $\mathbf{y}(r,\omega)$  for the Fourier transform  $\hat{\mathbf{y}}(r,\omega)$ . To begin with we consider the evaluation of this integral when the solution given in eq.(4.76) is used. Substituting this form of the solution into the above expression and interchanging the order of integration shows that we need to evaluate the vector-valued integrals

$$\mathbf{I}_{1}(r,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r',\omega)^{T} \mathbf{Y}^{(1)}(r',\omega)] \tilde{\mathbf{Y}}^{(2)}(r',\omega)^{T} \mathbf{f}(r',\omega) e^{\mathrm{i}\omega t} d\omega,$$
(4.148)

$$\mathbf{I}_{2}(r,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(2)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega)^{T} \mathbf{Y}^{(2)}(r',\omega)] \tilde{\mathbf{Y}}^{(1)}(r',\omega)^{T} \mathbf{f}(r',\omega) e^{i\omega t} d\omega.$$

$$(4.149)$$

These integrals can be simplified by supposing for the moment that the force vector is independent of frequency (so that the time dependence of  $\mathbf{f}(t)$  is that of a delta function), and later allowing a more general time dependence of the force vector by using a convolution in the time domain. Because of this, we focus on evaluation of the two matrix-valued integrals

$$\mathbf{J}_{1}(r,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r',\omega)^{T} \mathbf{Y}^{(1)}(r',\omega)] \tilde{\mathbf{Y}}^{(2)}(r',\omega)^{T} e^{\mathrm{i}\omega t} d\omega,$$

$$(4.150)$$

$$\mathbf{J}_{2}(r,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(2)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega)^{T} \mathbf{Y}^{(2)}(r',\omega)] \tilde{\mathbf{Y}}^{(1)}(r',\omega)^{T} e^{\mathrm{i}\omega t} d\omega.$$

$$(4.151)$$

In order to evaluate the integrals in eq.(4.150) and eq.(4.151) we form an infinite semicircular integration contour in the upper half-plane, and then use the residue theorem to sum the contributions of the various singularities enclosed within the contour. In forming this integration contour it may be necessary to take account of branch cuts of the integrands associated with linearly viscoelastic constitutive relations (e.g. Dahlen & Tromp 1998). Though general results are not known for the analytical evaluation of the resulting branch cut integrals, it is possible to compute such integrals numerically, and we shall not consider them further. Instead we concentrate on the poles of the integrand inclosed within the integration contour.

Recalling from section 4.4 that  $\Omega_A$  was defined to be the subset of the complex plane where the coefficient matrix  $\mathbf{A}(r,\omega)$  is holomorphic, we know that within this subset the matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$  are holomorphic. In addition,  $\Delta(\omega)$  and the adjugate matrices occurring in the integrands of eq.(4.150) and eq.(4.151) must also be holomorphic in  $\Omega_A$  because they are expressible as polynomials in the components of  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$ . We see, therefore, that within  $\Omega_A$  the integrands of eq.(4.150) and eq.(4.151) are meromorphic, and it follows that within any compact subset of the complex plane the only singularities that can occur are a finite number of poles. This means that within  $\Omega_A$  the only singularities of the integrands are finite order poles, and these poles cannot have any finite accumulation points.

If  $\omega \notin \Omega_A$  then the situation is far more complex because the matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$  may or may not be holomorphic. An example of such complexities comes from consideration of the spheroidal motion equations for a self-gravitating earth model with a fluid core (or outer core) for which the coefficient matrix  $\mathbf{A}(r,\omega) \in \mathbb{C}^{4\times 4}$  possess a second order pole at  $\omega = 0$  (e.g. Woodhouse & Deuss 2007). It is known that the solution to the spheroidal motion boundary value problem in this case is holomorphic at  $\omega = 0$  so long as the fluid portions of the earth model are neutrally stratified (e.g. Longman 1963). However, if any part of the fluid portions of the earth model are non-neutrally stratified then it may be shown that the solution to the boundary value problem possesses an essential singularity at  $\omega = 0$  which is an accumulation point of finite order poles associated with so-called core undertone modes (Wunsch 1974, Dahlen 1974, Dahlen & Fels 1978).

Due to the potential complexities of the problem when  $\omega \notin \Omega_A$ , we choose to restrict attention to the case that  $\omega \in \Omega_A$ , and, in doing so, possibly ignore contributions to the solution from other singularities. This assumption is in accordance with previous treatments of the modes of an elastic or viscoelastic earth model. A further approximation we make is that all poles of the integrand in  $\Omega_A$  are of first-order. This is because it is not clear at present how the residue of the integrands in eq.(4.150) and eq.(4.151) can be evaluated at higher-order poles. However, it is thought that for realistic earth models the effects of linear viscoelasticity are sufficiently small that this assumption is likely to be valid.

Taking into account the above discussion, we shall now show how the residue of the integrands in eq.(4.150) and eq.(4.151) can be calculated at a first-order pole. Let  $\omega = \omega_p$  be a first-order zero of  $\Delta(\omega_p)$ , i.e.  $\Delta(\omega_p) = 0$  and  $\partial_\omega \Delta(\omega_p) \neq 0$ . From eq.(4.66) we see that the matrix  $\mathbf{Y}(r,\omega)$  defined in section 4.4 is singular (i.e. has vanishing determinant) at this frequency, so that the Lagrangian subspaces  $V^{(1)}(r,\omega_p)$  and  $V^{(2)}(r,\omega_p)$  must have non-empty intersection. It may be shown that in the case of a first-order zero of  $\Delta(\omega)$ , the intersection of these subspaces is necessarily one-dimensional. Let us fix a particular  $r' \in [r_1, r_2]$  for which  $V^{(1)}(r,\omega_p) \cap V^{(2)}(r,\omega_p)$  is spanned by a vector  $\mathbf{y}_p$ . In terms of this vector we may define a solution of the homogeneous form of eq.(4.45) by

$$\mathbf{y}_p(r) = \mathbf{P}(r, r', \omega_p) \mathbf{y}_p. \tag{4.152}$$

This function must span  $V^{(1)}(r,\omega_p) \cap V^{(2)}(r,\omega_p)$  at all r, for otherwise this subspace would not be one-dimensional as we have assumed. It is clear that  $\mathbf{y}_p(r)$  is a continuous solution of the homogeneous form of eq.(4.45) that lies in  $V^{(1)}(\omega_p)$  and  $V^{(2)}(\omega_p)$ . We say that  $\mathbf{y}_p(r)$ is an eigenfunction of the boundary value problem, and  $\omega_p$  is said to be its eigenfrequency.

The subspace  $V^{(1)}(r,\omega_p)$  may be spanned by the columns of the partitioned matrix

$$\mathbf{Y}^{(1)}(r,\omega) = (\mathbf{y}_p(r) \quad \mathbf{Y}_r^{(1)}(r)), \qquad (4.153)$$

where  $\mathbf{Y}_r^{(1)}(r) \in \mathbb{C}^{m \times (n-1)}$  is an arbitrary matrix whose columns span the linear subspace obtained from  $V^{(1)}(r,\omega_p)$  by removing  $\mathbf{y}_p(r)$  from the basis set. Similarly we may write

$$\mathbf{Y}^{(2)}(r,\omega) = (\mathbf{y}_p(r) \quad \mathbf{Y}_r^{(2)}(r)), \qquad (4.154)$$

and can calculate that

and can calculate that
$$\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)} = \begin{pmatrix}
-\mathbf{y}_p^T \mathbf{\Sigma} \mathbf{y}_p & -\mathbf{y}_p^T \mathbf{\Sigma} \mathbf{Y}_r^{(1)} \\
-\mathbf{y}_p^T \mathbf{\Sigma} \mathbf{Y}_r^{(2)} & -\mathbf{Y}_r^{(2)T} \mathbf{\Sigma} \mathbf{Y}_r^{(1)}
\end{pmatrix}.$$
(4.155)
As  $\mathbf{y}_p(r)$  lies in both  $V^{(1)}(r, \omega_p)$  and  $V^{(2)}(r, \omega_p)$ , we see that

$$\mathbf{y}_{p}^{T} \mathbf{\Sigma} \mathbf{y}_{p} = 0, \quad \mathbf{y}_{p}^{T} \mathbf{\Sigma} \mathbf{Y}_{r}^{(1)} = \mathbf{0}, \quad \mathbf{y}_{p}^{T} \mathbf{\Sigma} \mathbf{Y}_{r}^{(2)} = \mathbf{0},$$
 (4.156)

while  $\mathbf{Y}_r^{(2)T} \mathbf{\Sigma} \mathbf{Y}_r^{(1)}$  must be non-singular, for otherwise the isotropic subspaces spanned by the columns of  $\mathbf{Y}_r^{(1)}$  and  $\mathbf{Y}_r^{(2)}$  would have a non-empty intersection, and this would imply that  $V^{(1)}(r,\omega_p)\cap V^{(2)}(r,\omega_p)$  had dimension greater than one. Using these observations we may write

$$\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)} = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0} & -\mathbf{Y}_r^{(2)T}\mathbf{\Sigma}\mathbf{Y}_r^{(1)} \end{pmatrix}, \tag{4.157}$$

and it is easy to see that this matrix has a one-dimensional kernel spanned by the column vector  $\mathbf{r} = \begin{pmatrix} 1 & \mathbf{0} \end{pmatrix}^T \in \mathbb{C}^{n \times 1}$  and the row vector  $\mathbf{r}^T \in \mathbb{C}^{n \times 1}$ , where the notation used is such that the first component of the vector equals one and all other elements equal zero. Using, for example, the result described in the appendix of Al-Attar (2007b), we see that the adjugate of this matrix is given by

$$\operatorname{adj}[\tilde{\mathbf{Y}}^{(2)T}\mathbf{Y}^{(1)}] = \kappa \mathbf{r} \mathbf{r}^{T} = \kappa \begin{pmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{4.158}$$

where  $\kappa$  is a non-zero constant.

Putting all the above results together, we can compute that

$$\mathbf{Y}^{(1)}(r,\omega_p)\operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r',\omega_p)^T\mathbf{Y}^{(1)}(r',\omega_p)]\tilde{\mathbf{Y}}^{(2)}(r',\omega_p)^T = -\kappa \mathbf{y}_p(r)\mathbf{y}_p(r')^T\mathbf{\Sigma}, \tag{4.159}$$

and also

$$\mathbf{Y}^{(2)}(r,\omega_p)\operatorname{adj}[\tilde{\mathbf{Y}}^{(1)}(r',\omega_p)^T\mathbf{Y}^{(2)}(r',\omega_p)]\tilde{\mathbf{Y}}^{(1)}(r',\omega_p)^T = (-1)^n\kappa\mathbf{y}_p(r)\mathbf{y}_p(r')^T\mathbf{\Sigma},\tag{4.160}$$

by use of the identity  $\operatorname{adj}[-\mathbf{X}^T] = (-1)^{(n-1)}\operatorname{adj}[\mathbf{X}]^T$  which holds for any  $\mathbf{X} \in \mathbb{C}^{n \times n}$ . Making

use of the above two formulae and the residue theorem, we may write expressions for the integrals in eq.(4.150) and eq.(4.151) as

$$\mathbf{J}_{1}(r,t) = \sum_{p} \frac{\kappa}{\mathrm{i}\partial_{\omega}\Delta(\omega_{p})} \mathbf{y}_{p}(r) \mathbf{y}_{p}(r')^{T} \mathbf{\Sigma} \mathrm{e}^{\mathrm{i}\omega_{p}t}, \tag{4.161}$$

$$\mathbf{J}_{2}(r,t) = \sum_{p} \frac{(-1)^{n} \kappa}{\mathrm{i} \partial_{\omega} \Delta(\omega_{p})} \mathbf{y}_{p}(r) \mathbf{y}_{p}(r')^{T} \mathbf{\Sigma} \mathrm{e}^{\mathrm{i} \omega_{p} t}. \tag{4.162}$$

where the summation is over all first-order poles contained in the upper half plane.

We shall now show that the term  $\partial_{\omega}\Delta(\omega_{p})$  in the above expression is given by

$$\partial_{\omega} \Delta(\omega_p) = -\kappa \int_{r_1}^{r_2} \mathbf{y}_p(r)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_p) \mathbf{y}_p(r) \, \mathrm{d}r + B(\omega_p), \tag{4.163}$$

where  $B(\omega_p)$  vanishes if the linear subspaces  $V^{(1)}(r_1,\omega)$  and  $V^{(2)}(r_2,\omega)$  are independent of frequency. To prove this result we first make use of eq.(4.66) to calculate that

$$\partial_{\omega} \Delta(\omega_{p}) = \partial_{\omega} \det[\tilde{\mathbf{Y}}^{(2)}(r, \omega_{p})^{T} \mathbf{Y}^{(1)}(r, \omega_{p})]$$

$$= \operatorname{tr}[\partial_{\omega} \{\tilde{\mathbf{Y}}^{(2)}(r, \omega_{p})^{T} \mathbf{Y}^{(1)}(r, \omega_{p})\} \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r, \omega)^{T} \mathbf{Y}^{(1)}(r, \omega)]], \qquad (4.164)$$

and use the expression for the adjoint matrix given in equation (4.158) to obtain

$$\partial_{\omega} \Delta(\omega_p) = \kappa \mathbf{r}^T \partial_{\omega} \{ \tilde{\mathbf{Y}}^{(2)}(r, \omega_p)^T \mathbf{Y}^{(1)}(r, \omega_p) \} \mathbf{r}. \tag{4.165}$$

Considering the term

$$\partial_{\omega} \{ \tilde{\mathbf{Y}}^{(2)T}(r, \omega_p) \mathbf{Y}^{(1)}(r, \omega_p) \} = -\partial_{\omega} \mathbf{Y}^{(2)}(r, \omega_p)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(r, \omega_p)$$
$$-\mathbf{Y}^{(2)}(r, \omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{Y}^{(1)}(r, \omega_p), \tag{4.166}$$

a simple calculation using eq.(4.45) shows that

$$\frac{\mathrm{d}}{\mathrm{d}r} [\partial_{\omega} \mathbf{Y}^{(2)}(r, \omega_p)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(r, \omega_p)] = -\mathbf{Y}^{(2)}(r, \omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_p) \mathbf{Y}^{(1)}(r, \omega_p), \quad (4.167)$$

$$\frac{\mathrm{d}}{\mathrm{d}r} [\mathbf{Y}^{(2)}(r,\omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{Y}^{(1)}(r,\omega_p)] = \mathbf{Y}^{(2)}(r,\omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r,\omega_p) \mathbf{Y}^{(1)}(r,\omega_p). \tag{4.168}$$

By integrating these relations we obtain

$$\partial_{\omega} \mathbf{Y}^{(2)}(r, \omega_{p})^{T} \mathbf{\Sigma} \mathbf{Y}^{(1)}(r, \omega_{p}) = -\int_{r_{2}}^{r} \mathbf{Y}^{(2)}(r, \omega_{p})^{T} \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_{p}) \mathbf{Y}^{(1)}(r, \omega_{p}) dr$$

$$+ \partial_{\omega} \mathbf{Y}^{(2)}(r_{2}, \omega_{p})^{T} \mathbf{\Sigma} \mathbf{Y}^{(1)}(r_{2}, \omega_{p}), \qquad (4.169)$$

$$\mathbf{Y}^{(2)}(r,\omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{Y}^{(1)}(r,\omega_p) = \int_{r_1}^r \mathbf{Y}^{(2)}(r,\omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r,\omega_p) \mathbf{Y}^{(1)}(r,\omega_p) dr$$

$$+ \mathbf{Y}^{(2)}(r_1,\omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{Y}^{(1)}(r_1,\omega_p), \qquad (4.170)$$

which shows that

$$\partial_{\omega} \{ \tilde{\mathbf{Y}}^{(2)T}(r, \omega_p) \mathbf{Y}^{(1)}(r, \omega_p) \} = -\int_{r_1}^{r_2} \mathbf{Y}^{(2)}(r, \omega_p)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_p) \mathbf{Y}^{(1)}(r, \omega_p) \, \mathrm{d}r$$
$$-\partial_{\omega} \mathbf{Y}^{(2)}(r_2, \omega_p)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(r_2, \omega_p)$$
$$-\mathbf{Y}^{(2)}(r_1, \omega_p) T \mathbf{\Sigma} \partial_{\omega} \mathbf{Y}^{(1)}(r_1, \omega_p). \tag{4.171}$$

By putting this result into eq.(4.165), and making use of equations (4.153) and (4.154),

we arrive at eq.(4.163), with an explicit expression for the boundary term

$$B(\omega_p) = -\kappa \mathbf{r}^T \partial_\omega \mathbf{Y}^{(2)}(r_2, \omega_p)^T \mathbf{\Sigma} \mathbf{Y}^{(1)}(r_2, \omega_p) \mathbf{r} - \kappa \mathbf{r}^T \mathbf{Y}^{(2)}(r_1, \omega_p)^T \mathbf{\Sigma} \partial_\omega \mathbf{Y}^{(1)}(r_1, \omega_p) \mathbf{r},$$

$$(4.172)$$

which clearly vanishes if  $V^{(1)}(r_1,\omega)$  and  $V^{(2)}(r_2,\omega)$  are independent of frequency. We recall that for the case of the spheroidal motion equations, the boundary conditions at the free surface are independent of frequency so that the first term in the above expression for  $B(\omega_p)$  does indeed vanish. However, the boundary conditions at  $r_1$  described in section 4.2 are frequency dependent, so that the second term in the expression for  $B(\omega_p)$  may be non-zero. However, we know that the radius  $r_1$  may be made arbitrarily close to zero, and that the matrix  $\mathbf{Y}^{(1)}(r_1,\omega)$  tends to zero as  $r_1 \to 0$ , so that for the spheroidal motion equations we have

$$\partial_{\omega} \Delta(\omega_p) = -\kappa \int_0^{r_2} \mathbf{y}_p(r)^T \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_p) \mathbf{y}_p(r) \, \mathrm{d}r.$$
 (4.173)

By making use of this result we can write the expressions for  $J_1$  and  $J_2$  as

$$\mathbf{J}_{1}(r,t) = \sum_{p} \frac{1}{2i\omega_{p}} \hat{\mathbf{y}}_{p}(r) \hat{\mathbf{y}}_{p}(r')^{T} \mathbf{\Sigma} e^{i\omega_{p}t}, \qquad (4.174)$$

$$\mathbf{J}_{2}(r,t) = \sum_{p} \frac{(-1)^{p}}{2i\omega_{p}} \hat{\mathbf{y}}_{p}(r) \hat{\mathbf{y}}_{p}(r')^{T} \mathbf{\Sigma} e^{i\omega_{p}t}, \qquad (4.175)$$

where we have introduced normalized eigenfunctions by

$$\int_{r_1}^{r_2} \hat{\mathbf{y}}_p(r)^T [-\mathbf{\Sigma} \partial_{\lambda} \mathbf{A}(r, \omega_p)] \hat{\mathbf{y}}_p(r) \, \mathrm{d}r = 1, \tag{4.176}$$

with  $\lambda = \omega^2$ . If desired, the spheroidal mode normalization integral may be found using the above equation and the coefficient matrices given in section 4.2. In the case of an elastic earth model, the rather cumbersome formula for the normalization integral reduces to the familiar expression

$$\int_{0}^{r_2} \rho(U^2 + \zeta^2 V^2) r^2 \, \mathrm{d}r = 1. \tag{4.177}$$

By adding the effects of the force vector into the solution by means of a convolution in the time domain, and putting the resulting expressions into eq.(4.76) we find that the time domain solution to the boundary value problem may be written as a sum over the normal modes as

$$\mathbf{y}(r,t) = \sum_{p} \frac{1}{2i\omega_p} \hat{\mathbf{y}}_p(r) \int_0^t \int_0^{r_2} [-\hat{\mathbf{y}}_p(r')^T \mathbf{\Sigma} \mathbf{f}(r',t')] e^{i\omega_p(t-t')} dr' dt', \qquad (4.178)$$

or in the case of a point force

$$\mathbf{y}(r,t) = \sum_{p} \frac{1}{2i\omega_p} \hat{\mathbf{y}}_p(r) \int_0^t [-\hat{\mathbf{y}}_p(r_s)^T \mathbf{\Sigma} \mathbf{s}(t')] e^{i\omega_p(t-t')} dt'.$$
 (4.179)

In these expressions we observe that the 'mode excitation coefficients', such as  $\hat{\mathbf{y}}_p(r_s)^T \mathbf{\Sigma} \mathbf{s}(t')$  in the case of a point force, involve the skew-scalar product of the force term with the eigenfunction. This is because the eigenfunctions of a real linear Hamiltonian system satisfy a biorthogonality relation involving the skew-scalar product. If  $\omega_p$  and  $\omega_q$  are distinct eigenfrequencies with normalized eigenfunctions  $\hat{\mathbf{y}}_p(r)$  and  $\hat{\mathbf{y}}_q(r)$ , then we may show that the relation

$$\int_{0}^{r_2} \hat{\mathbf{y}}_q(r)^T \mathbf{\Sigma} [\mathbf{A}(r, \omega_p) - \mathbf{A}(r, \omega_q)] \hat{\mathbf{y}}_p(r) dr = 0,$$
(4.180)

holds. To prove this result we start from the fact that  $\hat{\mathbf{y}}_p(r)$  and  $\hat{\mathbf{y}}_q(r)$  satisfy the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}r}\hat{\mathbf{y}}_p(r) = \mathbf{A}(r,\omega_p)\hat{\mathbf{y}}_p(r), \quad \frac{\mathrm{d}}{\mathrm{d}r}\hat{\mathbf{y}}_q(r) = \mathbf{A}(r,\omega_q)\hat{\mathbf{y}}_q(r). \tag{4.181}$$

From the identity  $\Sigma \mathbf{A} = -\mathbf{A}^T \Sigma$ , we find that

$$\frac{\mathrm{d}}{\mathrm{d}r}[\hat{\mathbf{y}}_q(r)^T \mathbf{\Sigma} \hat{\mathbf{y}}_p(r)] = \hat{\mathbf{y}}_q(r)^T \mathbf{\Sigma} [\mathbf{A}(r, \omega_p) - \mathbf{A}(r, \omega_q)] \hat{\mathbf{y}}_p(r), \tag{4.182}$$

which we integrate over  $[r_1, r_2]$  to give

$$\hat{\mathbf{y}}_q(r_2)^T \mathbf{\Sigma} \hat{\mathbf{y}}_p(r_2) - \hat{\mathbf{y}}_q(r_1)^T \mathbf{\Sigma} \hat{\mathbf{y}}_p(r_1) = \int_{r_1}^{r_2} \hat{\mathbf{y}}_q(r)^T \mathbf{\Sigma} [\mathbf{A}(r,\omega_p) - \mathbf{A}(r,\omega_q)] \hat{\mathbf{y}}_p(r) \, \mathrm{d}r.$$
(4.183)

The first term on the left hand side is equal to zero because the boundary conditions at the free-surface  $r = r_2$  are independent of frequency, meaning  $\hat{\mathbf{y}}_p(r_2)$  and  $\hat{\mathbf{y}}_q(r_2)$  lie in the same Lagrangian subspace. As with the normalization integral discussed above, the second term on the left hand side may not be zero as the boundary conditions at  $r = r_1$  are frequency dependent for the spheroidal motion equations. However, if we let  $r_1 \to 0$  then this term does tend to zero, and we obtain the result given in eq.(4.180).

Earlier work on the modes of an anelastic earth model by Tromp & Dahlen (1990) and Lognonné (1991) started from the assumption that the time domain solution to the problem could be written as a sum over the eigenfunctions of the earth model, and then made use of the above biorthogonality relation to determine the mode excitation coefficients of the expansion. From the expressions for the spheroidal motion coefficient matrices given in section 4.2 we can give an explicit formula for the biorthogonality relation for the spheroidal motion equations, though, as the result is lengthy, we will not write it down (the equivalent formula in the case of an isotropic earth model may be found in Tromp &

Dahlen 1990). In the case of an elastic earth model the biorthogonality relation takes the simple form

$$\int_{0}^{r_2} \rho(U_p U_q + \zeta^2 V_p V_q) r^2 \, \mathrm{d}r = \delta_{pq}, \tag{4.184}$$

which is the usual statement of the *orthogonality* of the spheroidal eigenfunctions (e.g. Dahlen & Tromp 1998).

As a final result in this subsection, we shall re-derive the method of Woodhouse (1988) for the reconstruction of the normalized eigenfunctions from the minor vectors of the system in a simple manner. Let  $\omega_p$  be an eigenfrequency of the equations associated with a firstorder zero of  $\Delta(\omega)$ , and let C be a positively-oriented closed contour encircling no other eigenfrequencies but  $\omega_p$ . From what was proven above, we know that

$$\frac{1}{2\pi} \int_{C} \frac{1}{\Delta(\omega)} \mathbf{Y}^{(1)}(r,\omega) \operatorname{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T} \mathbf{Y}^{(1)}(r',\omega)] \tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T} d\omega = \frac{1}{2i\omega_{p}} \hat{\mathbf{y}}_{p}(r) \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma},$$
(4.185)

where  $\hat{\mathbf{y}}_p(r)$  is the normalized eigenfunction associated with the eigenfrequency. However, from section 4.4 we have

$$\mathbf{Y}^{(1)}(r,\omega)\text{adj}[\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T}\mathbf{Y}^{(1)}(r',\omega)]\tilde{\mathbf{Y}}^{(2)}(r,\omega)^{T} = \mathbf{M}^{(1)}(r,\omega)\tilde{\mathbf{M}}^{(2)}(r,\omega)^{T}, \tag{4.186}$$

so that the above result may be written

$$\frac{1}{2\pi} \int_{C} \frac{1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \tilde{\mathbf{M}}^{(2)}(r,\omega)^{T} d\omega = \frac{1}{2i\omega_{p}} \hat{\mathbf{y}}_{p}(r) \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma}.$$
 (4.187)

Within the interior of the contour C the spanning matrices are holomorphic as they can be written as polynomial functions of the components of the matrices  $\mathbf{Y}^{(1)}(r,\omega)$  and  $\mathbf{Y}^{(2)}(r,\omega)$ . Because of this, the only singularity of the integrand on the left hand side is at  $\omega = \omega_p$  when  $\Delta(\omega)$  vanishes. By applying the residue theorem we find that

$$\frac{1}{2\pi} \int_{C} \frac{1}{\Delta(\omega)} \mathbf{M}^{(1)}(r,\omega) \tilde{\mathbf{M}}^{(2)}(r,\omega)^{T} d\omega = \frac{\mathrm{i}}{\partial_{\omega} \Delta(\omega)} \mathbf{M}^{(1)}(r,\omega_{p}) \tilde{\mathbf{M}}^{(2)}(r,\omega_{p})^{T}, \tag{4.188}$$

and from eq.(4.187) we obtain the identity

$$\hat{\mathbf{y}}_p(r)\hat{\mathbf{y}}_p(r)^T = \frac{1}{\partial_\lambda \Delta(\omega_p)} \mathbf{M}^{(1)}(r,\omega_p) \tilde{\mathbf{M}}^{(2)}(r,\omega_p)^T \mathbf{\Sigma}, \tag{4.189}$$

where  $\lambda = \omega^2$ . This formula, stating that the dyad of an eigenfunction is expressible in terms of the spanning matrices of the system, was first derived by Woodhouse (1988) using algebraic methods, and forms the basis for the calculation of eigenfunctions in the normal mode program OBANI and in its widely used modification MINOS due to Guy Masters.

### 4.6.3 An application to mode perturbation theory

We shall conclude by deriving a compact formula for the first order perturbation in an eigenfrequency of a real linear Hamiltonian system due to a change in the coefficient matrix of the equations including perturbations in the position of any discontinuities of the matrix. To do this we shall make use of the 'brute force' method described by Dahlen & Tromp (1998) which eschews Rayleigh's principle (e.g. Woodhouse 1976) and instead works directly with the perturbed differential equations satisfied by the eigenfunctions. The concise notation used in this chapter means that this approach is actually rather straightforward, and it also has the advantage of applying directly to problems in anelastic earth models where Rayleigh's principle, in its usual form, does not hold.

Suppose that  $\omega_p$  is an eigenfrequency of the unperturbed equations with normalized eigenfunction  $\hat{\mathbf{y}}_p(r)$ . Let the discontinuities of the unperturbed coefficient matrix  $\mathbf{A}(r,\omega)$  in the interval  $[r_1, r_2]$  be labeled as  $d_1, d_2, \ldots, d_{N-1}, d_N$  where  $d_1 = r_1$  and  $d_N = r_2$ . Suppose now that the coefficient matrix is perturbed by a small amount such that it becomes  $\mathbf{A}(r,\omega) + \delta \mathbf{A}(r,\omega)$ , and that the positions of each discontinuity are modified to  $d_i + \delta d_i$  with  $\delta d_i$  small. We expect that these small perturbations in the coefficient matrix will lead to small perturbations in both the eigenfunction  $\hat{\mathbf{y}}_p + \delta \mathbf{y}_p$ , and to the eigenfrequency  $\omega_p + \delta \omega_p$ . These perturbed quantities must satisfy the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}r}[\hat{\mathbf{y}}_p(r) + \delta \mathbf{y}_p(r)] = [\mathbf{A}(r, \omega_p + \delta \omega_p) + \delta \mathbf{A}(r, \omega_p + \delta \omega_p)][\hat{\mathbf{y}}_p(r) + \delta \mathbf{y}_p(r)], \tag{4.190}$$

along with the boundary and continuity conditions

$$\hat{\mathbf{y}}_p(d_1 + \delta d_1) + \delta \mathbf{y}_p(d_1 + \delta d_1) \in V^{(1)}(\omega_p + \delta \omega_p),$$
 (4.191)

$$[\hat{\mathbf{y}}_n(d_i + \delta d_i) + \delta \mathbf{y}_n(d_i + \delta d_i)]^+ = 0, \quad i = 2, \dots, N - 1,$$
 (4.192)

$$\hat{\mathbf{y}}_{p}(d_{N} + \delta d_{N}) + \delta \mathbf{y}_{p}(d_{N} + \delta d_{N}) \in V^{(2)}(\omega_{p} + \delta \omega_{p}). \tag{4.193}$$

At this stage it will be useful to make the assumptions that the linear subspaces  $V^{(1)}(\omega)$  and  $V^{(2)}(\omega)$  are independent of frequency. We know that this assumption is true of  $V^{(2)}(\omega)$ , and while not true of  $V^{(1)}(\omega)$ , we have seen previously that any additional terms at  $r = r_1$  will tend to zero as we let  $r_1 \to 0$ . By making use of this assumption, we can expand the above equations and boundary conditions to first order in perturbed quantities to obtain

$$\frac{\mathrm{d}}{\mathrm{d}r}\delta\mathbf{y}_{p}(r) = \mathbf{A}(r,\omega_{p})\delta\mathbf{y}_{p}(r) + \delta\omega_{p}\partial_{\omega}\mathbf{A}(r,\omega_{p})\hat{\mathbf{y}}_{p}(r) + \delta\mathbf{A}(r,\omega_{p})\hat{\mathbf{y}}_{p}(r), \tag{4.194}$$

along with the boundary conditions

$$\delta d_1 \mathbf{A}(d_1, \omega_p) \hat{\mathbf{y}}_p(d_1) + \delta \mathbf{y}_p(d_1) \in V^{(1)}, \tag{4.195}$$

$$\left[\delta d_i \mathbf{A}(d_i, \omega_p) \hat{\mathbf{y}}_p(d_i) + \delta \mathbf{y}_p(d_i)\right]_{-}^{+} = 0, \tag{4.196}$$

$$\delta d_N \mathbf{A}(d_N, \omega_p) \hat{\mathbf{y}}_p(d_N) + \delta \mathbf{y}_p(d_N) \in V^{(2)}. \tag{4.197}$$

Pre-multiplying eq.(4.194) by  $\hat{\mathbf{y}}_p(r)^T \mathbf{\Sigma}$  and making use of the identity  $\mathbf{\Sigma} \mathbf{A} = -\mathbf{A}^T \mathbf{\Sigma}$ , we obtain

$$\frac{\mathrm{d}}{\mathrm{d}r}[\hat{\mathbf{y}}_p(r)^T \mathbf{\Sigma} \delta \mathbf{y}_p(r)] = \delta \omega_p \hat{\mathbf{y}}_p(r)^T \mathbf{\Sigma} \partial_\omega \mathbf{A}(r, \omega_p) \hat{\mathbf{y}}_p(r) + \hat{\mathbf{y}}_p(r)^T \mathbf{\Sigma} \delta \mathbf{A}(r, \omega_p) \hat{\mathbf{y}}_p(r). \tag{4.198}$$

Integrating this equation over  $[r_1, r_2]$  we find

$$\hat{\mathbf{y}}_{p}(d_{N})^{T} \mathbf{\Sigma} \delta \mathbf{y}_{p}(d_{N}) - \sum_{i=2}^{N-1} \left[ \hat{\mathbf{y}}_{p}(d_{i})^{T} \mathbf{\Sigma} \delta \mathbf{y}_{p}(d_{i}) \right]_{-}^{+} - \hat{\mathbf{y}}_{p}(d_{1})^{T} \mathbf{\Sigma} \delta \mathbf{y}_{p}(d_{1})$$

$$= \delta \omega_{p} \int_{r_{i}}^{r_{2}} \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_{p}) \hat{\mathbf{y}}_{p}(r) dr + \int_{r_{i}}^{r_{2}} \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma} \delta \mathbf{A}(r, \omega_{p}) \hat{\mathbf{y}}_{p}(r) dr. \qquad (4.199)$$

If we make use of the boundary conditions for  $\delta \mathbf{y}_p(r)$  and the continuity of  $\hat{\mathbf{y}}_p(r)$ , we see that

$$\hat{\mathbf{y}}_p(d_1)^T \mathbf{\Sigma} \delta \mathbf{y}_p(d_1) = -\delta d_1 \hat{\mathbf{y}}_p(d_1)^T \mathbf{\Sigma} \mathbf{A}(d_1, \omega_p) \hat{\mathbf{y}}_p(d_1), \tag{4.200}$$

$$\left[\hat{\mathbf{y}}_{p}(d_{i})^{T} \mathbf{\Sigma} \delta \mathbf{y}_{p}(d_{i})\right]^{+} = -\delta d_{i} \hat{\mathbf{y}}_{p}(d_{i})^{T} \mathbf{\Sigma} \left[\mathbf{A}(d_{i}, \omega_{p})\right]^{+} \hat{\mathbf{y}}_{p}(d_{i}), \tag{4.201}$$

$$\hat{\mathbf{y}}_p(d_N)^T \mathbf{\Sigma} \delta \mathbf{y}_p(d_N) = -\delta d_N \hat{\mathbf{y}}_p(d_N)^T \mathbf{\Sigma} \mathbf{A}(d_N, \omega_p) \hat{\mathbf{y}}_p(d_N). \tag{4.202}$$

Using these relations in the above formula, and combining all boundary terms into one summation, we obtain

$$\sum_{i=1}^{N} \delta d_{i} \hat{\mathbf{y}}_{p}(d_{i})^{T} \mathbf{\Sigma} \left[ \mathbf{A}(d_{i}, \omega_{p}) \right]_{-}^{+} \hat{\mathbf{y}}_{p}(d_{i}) = \delta \omega_{p} \int_{r_{1}}^{r_{2}} \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma} \partial_{\omega} \mathbf{A}(r, \omega_{p}) \hat{\mathbf{y}}_{p}(r) dr + \int_{r_{1}}^{r_{2}} \hat{\mathbf{y}}_{p}(r)^{T} \mathbf{\Sigma} \delta \mathbf{A}(r, \omega_{p}) \hat{\mathbf{y}}_{p}(r) dr.$$

$$(4.203)$$

If we now make use of the normalization condition on the unperturbed eigenfunction, this formula can be rearranged to give the desired result

$$\delta\omega_p = \frac{1}{2\omega_p} \int_{r_1}^{r_2} \mathbf{y}_p(r)^T \mathbf{\Sigma} \delta \mathbf{A}(r, \omega_p) \mathbf{y}_p(r) \, \mathrm{d}r - \frac{1}{2\omega_p} \sum_{i=1}^N \delta d_i \mathbf{y}(d_i)^T \left[ \mathbf{\Sigma} \mathbf{A}(d_i, \omega_p) \right]_{-}^+ \mathbf{y}_p(d_i), \quad (4.204)$$

where, as above, we observe that expressions involving the skew-scalar product naturally arise.

### 4.7 Discussion

The main theoretical result of this chapter is the method described in section 4.4 for the numerical integration of a six-dimensional inhomogeneous system of ordinary differential equations using minor vectors. The example calculations presented show that this method

is able to produce stable and accurate solutions to the equations while simpler methods cannot. Except for the need to transcribe the lengthy minor vector formulae, the numerical implementation of this method is very simple, and involves only a marginal increase in computation time compared to the simple methods of solution.

We have also presented a new implementation of the direct radial integration method of Friedrich & Dalkolmo (1995) which allows for the incorporation of self-gravitation into the calculations. This method provides a useful alternative to normal mode summation for the calculation of complete synthetic seismograms in spherically symmetric earth models. In particular, it is well suited to calculations at high frequencies where the application of normal mode summation becomes problematic due to the computational difficulties in generating complete mode catalogs.

## Chapter 5

# Calculation of Normal Mode Spectra in Laterally Heterogeneous Earth Models Using an Iterative Direct Solution Method

### 5.1 Introduction

Normal mode spectra provide a valuable data set for global seismic tomography. In particular, mode spectra are amongst the few geophysical observables that provide constraints on lateral density variations within the Earth (e.g. Ishhi & Tromp 1999, 2001). Accurate modelling of synthetic mode spectra in laterally heterogeneous earth models is, therefore, an important problem in computational seismology (e.g. Dahlen 1968, 1969; Woodhouse & Dahlen 1979; Woodhouse 1980, 1983; Woodhouse & Giardini 1986; Park 1986, 1990; Hara et. al. 1991, 1993). A comprehensive overview of normal mode theory can be found in Dahlen & Tromp (1998).

Recent work by Deuss & Woodhouse (2001, 2004) and Irving et. al. (2008), has high-lighted the need to include large numbers of modes into coupling calculations in order to produce accurate spectra. Traditional methods for performing such 'full-coupling' calculations involve the diagonalization of coupling matrices; a process which rapidly becomes computationally inefficient as the number of coupled modes is increased. In addition, the exact incorporation of rotation of the earth model into these calculations requires

the dimension of the eigenvalue problem to be doubled, while linear viscoelasticity can only be included in an approximate manner. To circumvent these problems, Deuss and Woodhouse (2004) introduced an *iteration method* (IM) which provides a computationally efficient numerical method for the calculation of the eigenfunctions and eigenfrequencies of a rotating, linear viscoelastic, laterally heterogeneous earth model without the need to diagonalize the coupling matrix.

An alternative method for calculating mode spectra is the direct solution method (DSM) introduced by Hara et al. (1993). In this method, the eigenfunctions and eigenfrequencies of the laterally heterogeneous earth model are not calculated. Instead, solutions of the inhomogeneous (i.e. with a force-term) mode-coupling equations are computed at a range of discrete frequencies to directly produce the synthetic spectra (in detail, such synthetic spectra must be processed using discrete Fourier transforms prior to comparison with data). An advantage of the DSM is that the effects of rotation and linear viscoelasticity can be included in the calculations in an exact and simple manner. In addition, the computational efficiency of the DSM is, potentially, greater than methods based on the diagonalization of the coupling matrix (see Hara et al. 1993 for a discussion).

In previous implementations of the DSM the inhomogeneous mode-coupling equations were solved by performing an LU-decomposition of the coupling matrix followed by back-substitution. Though this method is effective for small coupling calculations, the computation time increases rapidly with the dimension of the coupling matrix. In this chapter we describe a new implementation of the DSM that employs an iterative method to solve the inhomogeneous mode coupling equations. An advantage of this *iterative direct solution method* (IDSM) is that it does not require the LU-decomposition of the whole coupling matrix, but instead involves only the LU-decomposition of small submatrices and the calculation of matrix-vector products. This fact means that the numerical implementation of the IDSM can readily be parallelized, and so be used to perform coupling calculations at higher frequencies than previously attempted. In particular, the IDSM may prove to be a useful tool for generating accurate long-period surface wave seismograms in laterally heterogeneous earth models.

## 5.2 Theoretical Background and Method

### 5.2.1 Mode coupling equations

By expanding the displacement vector field in terms of the eigenfunctions of a spherically symmetric earth model, the elastodynamic equation in a rotating, laterally heterogeneous, and slightly aspherical earth model can be expressed as the initial value-problem

$$\mathbf{P}\ddot{\mathbf{u}}(t) + \mathbf{W}\dot{\mathbf{u}}(t) + \mathbf{H}\mathbf{u}(t) = \mathbf{f}(t), \quad \mathbf{u}(0) = \dot{\mathbf{u}}(0) = \mathbf{0}. \tag{5.1}$$

Here **u** is a vector containing the expansion coefficients of the displacement vector, **P** is the kinetic energy operator, **W** is the Coriolis operator, **H** is the elastodynamic operator, and **f** is a vector containing the expansion coefficients of the body-force equivalent of the seismic source. Detailed expressions for these various terms can be found in Woodhouse & Dahlen (1978), Woodhouse (1980), Mochizuki (1986) and Dahlen & Tromp (1998). If the effects of linear viscoelasticity are included, then the elastodynamic operator involves a convolution in the time-domain, though for simplicity we leave this possibility implicit in the notation.

In principle, the above equation should incorporate coupling of all the eigenfunctions of the spherically symmetric earth model, and so involve infinite-dimensional vectors and matrices. We note that this formulation excludes the possibility of a continuous component to the normal mode spectrum of the spherically symmetric earth model due to the presence of a non-neutrally stratified fluid outer core (e.g. Rogister & Valette 2008). In practice we can, of course, only deal with finite-dimensional systems of equations, and so we shall suppose that a finite set of eigenfunctions has been chosen for use in the coupling calculations.

### 5.2.2 Diagonalization and the direct solution method

To solve this equation we shall work in the frequency-domain, using the Fourier-Laplace transform (e.g. Friedlander & Joshi 1998, Chapter 10)

$$\tilde{\mathbf{u}}(\omega) = \int_0^\infty \mathbf{u}(t) e^{-i\omega t} dt, \qquad (5.2)$$

where  $\omega$  is complex-valued. For suitably regular functions the inverse Fourier-Laplace transform is given by

$$\mathbf{u}(t) = \frac{1}{2\pi} \int_{-\infty - i\epsilon}^{\infty - i\epsilon} \tilde{\mathbf{u}}(\omega) e^{i\omega t} d\omega, \qquad (5.3)$$

where  $\epsilon$  is an arbitrary real number such that all singularities of  $\tilde{\mathbf{u}}(\omega)$  lie above the line  $\mathrm{Im}(\omega) = -\mathrm{i}\epsilon$ . The transformed version of eq.(5.1) can be written

$$[-\omega^2 \mathbf{P} + i\omega \mathbf{W} + \mathbf{H}(\omega)] \,\tilde{\mathbf{u}}(\omega) = \tilde{\mathbf{f}}(\omega), \tag{5.4}$$

where we have now explicitly allowed for the frequency-dependence of the elastodynamic operator arising from viscoelastic effects. This equation can be written more concisely as

$$\mathbf{A}(\omega)\tilde{\mathbf{u}}(\omega) = \tilde{\mathbf{f}}(\omega),\tag{5.5}$$

where we have defined the *coupling matrix*  $\mathbf{A}(\omega)$  in an obvious manner.

Solutions of eq.(5.5) can be sought in a number of ways. One approach is to consider the eigenvalue-problem

$$\mathbf{A}(\omega)\mathbf{u} = \mathbf{0},\tag{5.6}$$

which has non-trivial solutions  $\mathbf{u}$ , called eigenfunctions, only for  $\omega$  equal to the eigenfrequencies of the laterally heterogeneous earth model. Having solved this eigenvalue problem, the time-domain solution  $\mathbf{u}(t)$  can be expressed in a relatively simple manner in terms of these eigenfrequencies and eigenfunctions (e.g. Dahlen & Tromp 1998, Chapter 7) Deuss & Woodhouse 2004; Al-Attar 2007; see also the theory of Chapter 6). A complication associated with this method is that the above eigenvalue problem is of non-standard form, so that the usual methods based on matrix-diagonalization are not directly applicable to its solution. If the effects of viscoelasticity are neglected, this problem can be circumvented by doubling the size of the eigenvalue problem, and so reducing it to the standard-form (Wahr 1981, Deuss & Woodhouse 2001). A number of approximate methods have also been developed for reducing eq.(5.6) into a standard eigenvalue problem; see Deuss & Woodhouse (2001) for a concise summary of such approximations. An attractive feature of the iteration method of Deuss & Woodhouse (2004) is that it allows for the solution of the non-standard eigenvalue problem in eq.(5.6) directly in a theoretically exact manner.

An alternative approach to solving eq.(5.5) is the direct solution method (DSM) introduced

by Hara et. al. (1993). In this method, solutions of eq.(5.5) are calculated directly at a discrete range of frequencies. In the previous implementations of the DSM, these linear equations were solved using LU-decomposition. The numerical cost of this method rises, roughly, like the third power of the dimension of the linear system (e.g. Press et. al. 1986), so that its application rapidly becomes unfeasible as the number of coupled modes is increased. In order for the DSM to be applied to large coupling calculations, we shall now describe an iterative method for the solution of the inhomogeneous mode coupling equations.

### 5.2.3 Iterative solution of the mode coupling equations

To solve the linear system eq.(5.5) iteratively we make use of the preconditioned biconjugate gradient algorithm (BCG) (e.g. Saad 2000). In this method, an initial guess  $\tilde{\mathbf{u}}_0$  for the solution is given, and this solution is iteratively updated until convergence to the actual solution is obtained (here and in the following, we have neglected the dependence of the various terms on  $\omega$  for notational clarity). The efficiency of this method depends crucially on the choice of the preconditioner for the linear system. We recall that a preconditioner for eq.(5.5) is a matrix  $\mathbf{B}$ , say, which is an approximate inverse of  $\mathbf{A}$ , i.e. we have  $\mathbf{B}\mathbf{A}\approx\mathbf{1}$ . In choosing a suitable preconditioner an important consideration is the trade-off between the effectiveness of the preconditioner and the effort required in its construction (e.g. Chen 2005).

To develop an efficient preconditioner for eq.(5.5) it is helpful to consider the structure of the coupling matrix in further detail. A is partitioned into a number of sub-matrices, each of which involves the coupling of a pair of multiplets of the spherical earth model. The diagonal sub-matrices represent the effects of self-coupling between multiplets, while the off-diagonal sub-matrices represent cross-coupling. It may be shown that

$$P = 1 + P^{(1)}, \quad H = \Omega^2 + H^{(1)},$$
 (5.7)

where  $\Omega$  is a diagonal matrix whose non-zero entries in each of the self-coupling submatrices are equal to the degenerate eigenfrequency of the associated multiplet. We can, therefore, write

$$\mathbf{A} = (\mathbf{\Omega}^2 - \omega^2 \mathbf{1}) + \mathbf{A}^{(1)},\tag{5.8}$$

where we have defined,

$$\mathbf{A}^{(1)} = -\omega^2 \mathbf{P}^{(1)} + \mathrm{i}\omega \mathbf{W} + \mathbf{H}^{(1)}. \tag{5.9}$$

For the frequency-range of interest to seismology, the norm of  $\mathbf{A}^{(1)}$  can be shown to be small compared to  $|\omega|^2$ . It follows that  $\mathbf{A}$  is diagonally dominant except within those self-coupling sub-matrices corresponding to multiplets having eigenfrequencies close to  $\omega$ . This suggests a preconditioner for eq.(5.5) can be constructed as follows:

- 1. Select a frequency bandwidth  $\Delta\omega$ , and determine which multiplets have eigenfrequencies lying in  $(\omega \Delta\omega, \omega + \Delta\omega)$ . Such multiplets are grouped into a target block, and remaining multiplets into a residual block.
- 2. According to the above decomposition, we write  $\mathbf{A} = \begin{pmatrix} (\mathbf{\Omega}_{TT}^2 \omega^2 \mathbf{1}_{TT}) + \mathbf{A}_{TT}^{(1)} & \mathbf{0}_{TR} \\ \mathbf{0}_{RT} & (\mathbf{\Omega}_{RR}^2 \omega^2 \mathbf{1}_{RR}) \end{pmatrix} + \begin{pmatrix} \mathbf{0}_{TT} & \mathbf{A}_{TR}^{(1)} \\ \mathbf{A}_{RT}^{(1)} & \mathbf{A}_{RR}^{(1)} \end{pmatrix}, \quad (5.10)$ where the subscript TT is used to denote the target block, RR the residual block, and TR and RT the off-diagonal blocks coupling the target and residual blocks.
- 3. The preconditioner for the system is then defined as the inverse of the first of the above matrices  $\mathbf{B} = \begin{pmatrix} \left\{ (\mathbf{\Omega}_{TT}^2 \omega^2 \mathbf{1}_{TT}) + \mathbf{A}_{TT}^{(1)} \right\}^{-1} & \mathbf{0}_{TR} \\ \mathbf{0}_{RT} & (\mathbf{\Omega}_{RR}^2 \omega^2 \mathbf{1}_{RR})^{-1} \end{pmatrix}. \tag{5.11}$

By varying  $\Delta\omega$ , we can seek a frequency bandwidth which generates an efficient preconditioner. For small values of  $\Delta\omega$ , the size of the target-block will be small, so that construction of the preconditioner is inexpensive. However, such a preconditioner may be a poor approximate inverse of  $\mathbf{A}$ , and many iterations may be required for the BCG algorithm to converge. We note that in the extreme case of  $\Delta\omega = 0$  the preconditioner is simply the 'spherical earth solution' of the elastodynamic equations. Conversely, for larger values of  $\Delta\omega$ , the preconditioner will be a better approximate inverse to  $\mathbf{A}$  and fewer iterations of the BCG will be required. However, as  $\Delta\omega$  is increased the construction of the preconditioner may become prohibitively expensive. Indeed, if  $\Delta\omega$  is made sufficiently large, all multiplets will lie in the target-block.

Each iteration of the BCG requires two multiplications of a vector by  $\mathbf{B}\mathbf{A}$  and one multiplication of a vector by  $\mathbf{A}^T\mathbf{B}^T$ . To perform these matrix-vector multiplications it is not

necessary to explicitly construct the preconditioning matrix **B**. To see this, let  $\mathbf{v} = \mathbf{B}\mathbf{A}\mathbf{w}$ for a given vector  $\mathbf{w}$ . This relation is equivalent to the linear system  $\mathbf{B}^{-1}\mathbf{v} = \mathbf{A}\mathbf{w}$ , where the matrix  $\mathbf{B}^{-1}$  is, by definition, equal t

the matrix 
$$\mathbf{B}^{-1}$$
 is, by definition, equal to
$$\mathbf{B}^{-1} = \begin{pmatrix} \left\{ (\mathbf{\Omega}_{TT}^2 - \omega^2 \mathbf{1}_{TT}) + \mathbf{A}_{TT}^{(1)} \right\} & \mathbf{0}_{TR} \\ \mathbf{0}_{RT} & (\mathbf{\Omega}_{RR}^2 - \omega^2 \mathbf{1}_{RR}) \end{pmatrix}. \tag{5.12}$$
If we set  $\mathbf{z} = \mathbf{A}\mathbf{w}$ , and partition  $\mathbf{v}$  and  $\mathbf{z}$  as

$$\mathbf{v} = \begin{pmatrix} \mathbf{v}_T \\ \mathbf{v}_R \end{pmatrix}, \quad \mathbf{z} = \begin{pmatrix} \mathbf{z}_T \\ \mathbf{z}_R \end{pmatrix}, \tag{5.13}$$

then the above linear system is equivalent to the two decoupled systems

$$\left\{ (\mathbf{\Omega}_{TT}^2 - \omega^2 \mathbf{1}_{TT}) + \mathbf{A}_{TT}^{(1)} \right\} \mathbf{v}_T = \mathbf{z}_T, \tag{5.14}$$

$$(\mathbf{\Omega}_{RR}^2 - \omega^2 \mathbf{1}_{RR}) \mathbf{v}_R = \mathbf{z}_R. \tag{5.15}$$

It follows that we can compute  $\mathbf{v} = \mathbf{B}\mathbf{A}\mathbf{w}$  by forming one matrix-vector product with  $\mathbf{A}$  to compute  $\mathbf{z}$ , and by solving the above two linear systems for  $\mathbf{v}_T$  and  $\mathbf{v}_R$ . The linear system for  $\mathbf{v}_R$  is diagonal, so that its solution may be found trivially. To solve the system for  $\mathbf{v}_T$ the LU-decomposition of the matrix  $\left\{ (\mathbf{\Omega}_{TT}^2 - \omega^2 \mathbf{1}_{TT}) + \mathbf{A}_{TT}^{(1)} \right\}$  is formed, and the solution is then found using back-substitution. A similar argument applies to the calculation of matrix-vector products with  $\mathbf{A}^T \mathbf{B}^T$ . Importantly, the LU-decomposition of the targetblock portion of the coupling matrix need only be performed once per frequency.

#### 5.3 Example Calculations

In this section we present a range of calculations to demonstrate the validity and effectiveness of the IDSM. In all calculations the spherical earth eigenfunctions used were calculated for the earth model PREM of Dziewonski & Anderson (1981). As a laterally heterogeneous earth model we use the S-wave model S20RTS of Ritsema et. al. (1999) scaling the S-wave velocity perturbations to give P-wave velocity and density perturbations. For these scaling relations we take

$$\delta V_p / V_p = 0.5 \, \delta V_s / V_s, \quad \delta \rho / \rho = 0.3 \, \delta V_s / V_s, \tag{5.16}$$

these values being suggested by mineral physics (e.g. Karato 1993).

### 5.3.1 Validation of the iterative method

The accuracy of the IDSM can be most easily verified by comparing its results with those of the traditional DSM. In figure 5.1 such a comparison is shown for a small portion of synthetic spectra, and it is seen that the IDSM rapidly converges to the DSM solution. In numerical tests it is found that typically only three to four iterations of the method are required for convergence.

### 5.3.2 Choice of $\Delta\omega$ for the target-block

The efficiency of the preconditioner used in the IDSM depends on the choice of the frequency bandwidth  $\Delta\omega$  used for the target block. In figure 5.2 we plot the variation with  $\Delta f = \frac{1}{2\pi}\Delta\omega$  in (a) total calculation time, (b) mean number of iterations for convergence, and (c) mean calculation time per iteration. It is seen that as  $\Delta\omega$  increases the number of iterations needed for convergence of the BCG algorithm decreases monotonically; this is because as  $\Delta\omega$  increases the preconditioner **B** becomes a closer approximation to  $\mathbf{A}^{-1}$ . However, as  $\Delta\omega$  is increased more work must be done to construct the preconditioner, and it is seen that the mean time per iteration increases correspondingly. In 5.2 (a) it is seen that due to these opposing effects, the total calculation time initially decreases with increasing  $\Delta\omega$ , reaches a minimum at around  $\Delta f \approx 0.05\,\mathrm{mHz}$ , and then starts to rise again. The precise value of this minimum is found to depend on the details of the calculation (such as number of modes coupled, and length of the time-series), though the choice  $\Delta f \approx 0.05\,\mathrm{mHz}$  seems, in general, to work well.

### 5.3.3 Comparison of the traditional and iterative DSM

To demonstrate the advantage of the iterative solution method, it is useful to investigate how the computation time required in the DSM and IDSM scales with frequency. To do this we computed synthetic spectra using the two methods coupling all modes having eigenfrequencies less than a given value  $f_{\rm max}$  for  $f_{\rm max}=0.5$  through to  $2.0\,{\rm mHz}$  in  $0.25\,{\rm mHz}$  intervals. In each calculation the length of the time-series produced was 96 hours, and the number of frequency steps was chosen based on this time to achieve good spectral

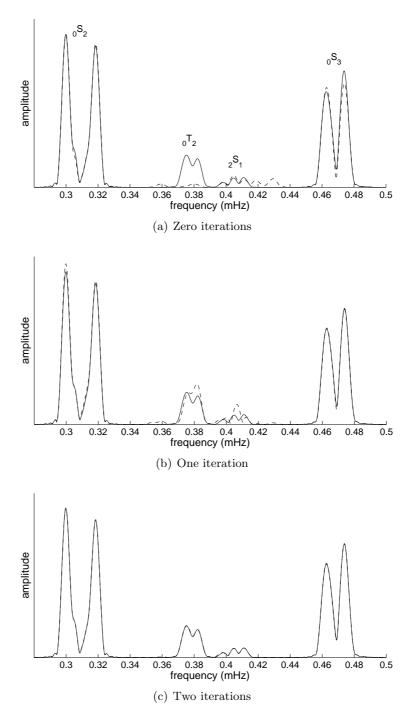


Figure 5.1: These figures show a portion of synthetic spectra for different numbers of iterations of the BCG to demonstrate its rapid convergence. In each figure the solid line is the reference synthetic spectra calculated by the traditional DSM, while the broken line is the result of the IDSM for the stated number of iterations. In these calculations the frequency bandwidth  $\Delta f$  for the target block was taken to be 0.05 mHz.

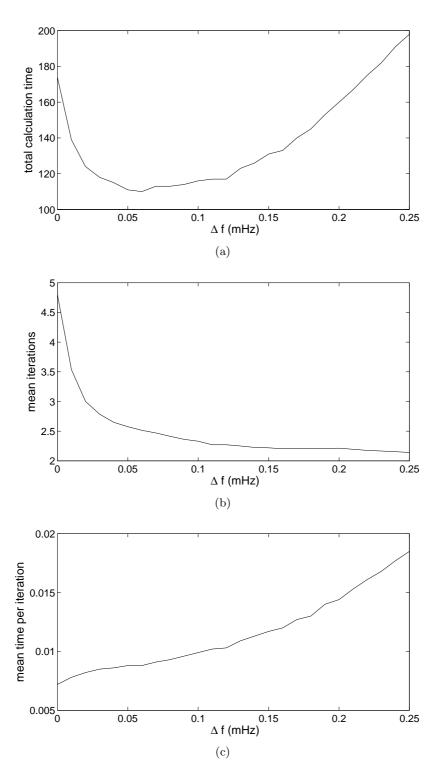


Figure 5.2: Plots showing the variation in (a) total calculation time (in seconds), (b) mean number of iterations per frequency, and (c) mean calculation time per iteration (in seconds), with choice of the frequency bandwidth parameter  $\Delta f = \frac{1}{2\pi}\Delta\omega$ . For these calculation all modes with eigenfrequencies less than 2 mHz where included, and a 96 hour time series were generated.

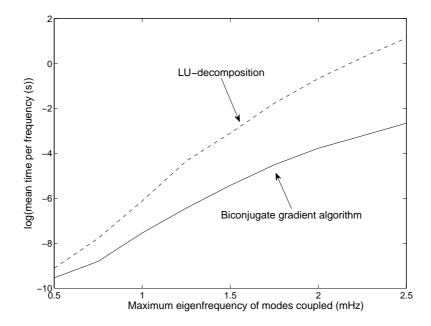


Figure 5.3: Comparison of the mean calculation time per frequency between the traditional and iteration DSM as the size the coupling matrix is increased. It is seen that the calculation time for the iterative DSM scales roughly like  $f_{max}^3$ , while the traditional DSM scales like  $f_{max}^5$ .

resolution. The results of these calculations are summarized in fig 5.3. In this figure it is seen that IDSM is more computationally efficient than the DSM at all frequencies considered. From these plots it is found that the calculation time for the DSM scales roughly like  $f_{\text{max}}^5$ , while for the IDSM the scaling is roughly like  $f_{\text{max}}^3$ . This implies that the advantages of the IDSM over the DSM are greatest for large coupling calculations.

### 5.3.4 Effects of truncating the coupling equations

In setting up the mode coupling equations we must select a finite subset of spherical earth multiplets we wish to consider. This truncation of the infinite-dimensional mode coupling equations necessarily introduces an error into the calculations. An important question therefore arises: suppose we wish to calculate synthetic spectra in a given frequency-range  $(\omega_1, \omega_2)$ , then which multiplets must be included in the coupling calculations in order for the resulting spectra to be sufficiently accurate? Here by 'sufficiently accurate' we mean, roughly speaking, that the difference between calculated spectra and the exact spectra are smaller than the expected differences between synthetic and observed spectra for the real

Earth.

This issue has previously been considered in the work of Deuss & Woodhouse (2001, 2004), and Irving et al. (2008). An important conclusion of this work was that the use of so-called 'full-coupling calculations' is essential for the accurate calculation of synthetic spectra. These 'full-coupling calculations' involve large numbers of multiplets, and stand opposed to the so-called self-coupling and group-coupling approximations that have been widely used. However, an assumption that seems to be more or less implicit in these papers is that if one wishes to calculate accurate spectra up to some maximum frequency, then the corresponding 'full-coupling calculation' should include all mulitplets having eigenfrequencies less than or equal to this frequency. To test this assumption, we generated a number of synthetic spectra for the same frequency band with varying numbers of multiplets included in the calculations. The results of such a calculation are shown in figure 5.4 in which the synthetic spectra around the mode  ${}_{0}T_{3}$  are plotted for a number of different coupling calculations. From these figures it is seen that in order for the spectra to converge to the exact answer a remarkably large number of multiplets need be included in the calculations. It should be stressed that the behaviour of this mode is atypical, and for most modes convergence occurs significantly more rapidly. Nonetheless, this example reiterates the conclusions of Deuss & Woodhouse (2001) on the importance of wide-band coupling in the generation of accurate synthetic spectra.

### 5.4 Discussion

In this chapter we have described a new iterative implementation of the direct solution method for the calculation of synthetic seismograms in laterally heterogeneous earth models. Numerical tests show that this method is significantly more efficient than the traditional DSM for performing large coupling calculations. We have also employed this method to investigate the effects of truncating the mode coupling equations. Example calculations demonstrate the importance of using large numbers of modes in coupling calculations, and, in particular, show that calculation of accurate synthetics in a given frequency band often requires the inclusion of a surprisingly large number of modes lying outside of the frequency band of interest.

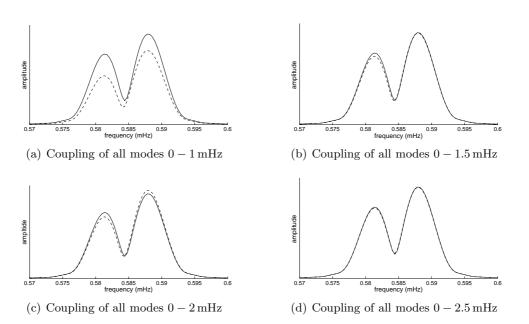


Figure 5.4: Synthetic spectra for the mode  ${}_{0}T_{3}$  for different numbers of coupled modes. In each plot the solid line is the result of coupling all modes with eigenfrequencies less than 3 mHz, while the broken line shows the results of performing the calculations with a smaller subset of modes. It is seen that a surprisingly large number of modes are required for the spectra to converge. We note also that the converge of the spectra as the size of the coupling matrix is increased is somewhat irregular, with the fit being slightly better in subfigure (b) than in (c).

## Chapter 6

# Viscoelastic Normal Mode Theory

Empirical evidence can never establish mathematical existence—nor can the mathematician's demand for existence be dismissed by the physicist as useless rigor. Only a mathematical existence proof can ensure that the mathematical description of a physical phenomenon is meaningful.

Richard Courant.

### 6.1 Introduction

Over a range of time scales from seconds to thousands of years, and for deformations involving sufficiently small strain-rates, the rheology of the Earth is commonly assumed to be described by a linear viscoelastic constitutive relation. For example, linear viscoelasticity is used in studies of seismic wave propagation to incorporate the effects of attenuation and anelastic dispersion, and also in studies of post-seismic deformation and post-glacial rebound. In each of these applications it is necessary to calculate solutions of the so-called viscoelastodynamic equation, though in the latter two cases this problem is usually simplified by use of the quasi-static approximation in which inertial terms in the equation are set equal to zero.

A widely used method for solving the viscoelastodynamic equation is the viscoelastic normal mode method in which the response of the earth model is expanded in terms of its viscoelastic eigenfunctions. The derivation of this normal mode solution has been considered previously by a number of authors for both the dynamic form of the equation (e.g. Yuen & Peltier 1980; Tromp & Dahlen 1990; Lognonné 1991; Dahlen & Tromp 1998; Deuss & Woodhouse 2004; Al-Attar 2007a, 2007b; Al-Attar & Woodhouse 2008) and for the quasi-static approximation (e.g. Peltier 1974, 1976; Peltier & Andrews 1976; Wu & Peltier 1980; Pollitz 1992; Boschi et al. 1995; Tromp & Mitrovica 1999a, 1999b, 2000; Pollitz 2003). However, the complexity of the viscoelastodynamic equation has meant that in deriving the normal mode solution it has been common to employ a number of simplifying assumptions. For example, in many previous studies attention has been limited to spherically symmetric earth models comprising a finite number of homogeneous layers, and having a linear viscoelastic constitutive relation of a specific simple form such as that of a Maxwell solid or a standard linear solid. While consideration of such simple earth models is undoubtedly useful for practical purposes, from a theoretical point of view this approach is unsatisfactory because we cannot infer the general validity of the normal mode solution to the viscoelastodynamic equation from any number of specific cases. That the simple form of these normal mode solutions of the viscoelastodynamic equations may indeed be invalid for general earth models has been suggested by the work of Fang & Hager (1995) and Han & Wahr (1995). In the context of the quasi-static approximation, these authors have shown that as the number of homogeneous layers in an earth model is increased to a 'continuum limit' the number of viscoelastic eigenfrequencies in a bounded portion of the negative real axis of the Laplace transform domain becomes dense, forming a feature that Fang & Hager (1995) call a 'continuum of poles'. The contribution of this feature to the time-domain solution cannot be represented as a discrete normal mode sum, but instead takes a more general form of a continuous sum (i.e. an integral) of decaying exponentials. A further assumption that has usually been made in developing viscoelastic normal mode theory is that the only singularities of the Laplace transform domain solution of the viscoelastoelastodynamic equation are isolated simple poles associated with eigenfrequencies of the earth model. Though this assumption is known to hold for the elastodynamic equation, there exists no corresponding proof for the viscoelastodynamic equation. In fact, there is much evidence to suggest that this assumption is not generally valid. For example, singularities of the Laplace transform domain solution other than isolated simple poles have been observed by a number of authors including: the presence of branch-cuts

for earth models with an absorption-band-solid constitutive relation noted by Yuen & Peltier (1981), Tromp & Dahlen (1990), and Dahlen & Tromp (1998); the 'continuous poles' of Fang & Hager (1995) and Han & Wahr (1995) discussed above; and also the occurrence of accumulation points of simple poles in earth models that incorporate the effects of self-gravitation as described by Tanaka et al. (2006, 2007) and Cambiotti et al. (2009). Moreover, by considering the simple analogue problem of a linear viscoelastic string, it is possible to construct situations in which higher-order poles of the Laplace transform domain solution occur (e.g. Al-Attar 2007a).

In this chapter, we investigate the theoretical foundations of viscoelastic normal mode theory. In doing this we do not consider the most general form of the viscoelastodynamic equations of interest to geophysics, but instead consider a simplified form of the equation which retains essentially all of the pertinent features. In particular, we neglect the effects of initial stress, rotation, and gravitation. We further assume that the earth model is everywhere solid, that it possesses no internal boundaries, and that the boundary conditions on the surface are that displacements and not tractions vanish. Of these various neglected features, it is only the presence of fluid regions in the earth model which presents significant complications to the theory. In fact, even in the case of the elastodynamic equation, the presence of fluid regions in the earth model presents a major theoretical difficulty. Briefly, the problem is that our theory depends on the strong ellipticity of the elastodynamic and viscoelastodynamic operators, and if the earth model possess fluid regions this property ceases to hold. At the end of the chapter we briefly outline the modifications to the theory needed to incorporate these neglected features, focusing on the inclusion of self-gravitation into the problem.

### 6.2 Statement of the Problem

### 6.2.1 Equations of motion

Let  $\Omega$  be an open bounded subset of  $\mathbb{R}^n$  with  $n \geq 1$ . The boundary of  $\Omega$  is denoted by  $\partial \Omega$  and is assumed to be smooth. Points in  $\Omega$  will be denoted by x, and their components with respect to a fixed cartesian reference frame by  $x_i$ . We consider the linearized momentum

equation

$$\frac{\partial^2 u_i}{\partial t^2} - \frac{1}{\rho} \frac{\partial T_{ji}}{\partial x_j} = f_i, \quad x \in \Omega, \quad t \in (0, \infty)$$
(6.1)

where  $u_i$  are the components of the *n*-dimensional displacement vector u,  $\rho$  is the density,  $T_{ij}$  are the components of the symmetric Cauchy stress tensor T, and  $f_i$  are the components of an applied body-force f. This equation is to be solved subject to the homogeneous Dirichlet boundary conditions

$$u_i(x,t) = 0, \quad t \in (0,\infty), \quad x \in \partial\Omega,$$
 (6.2)

and the initial conditions

$$u_i(x,0) = \frac{\partial u_i}{\partial t}(x,0) = 0, \quad x \in \Omega.$$
 (6.3)

Physically u, T, and f should have real-valued components. It will, however, be convenient from the outset to allow these terms to be complex-valued. We assume that  $\rho$  is real-valued, smooth in  $\Omega$ , everywhere positive, and that it can be extended to a continuous function on the closure  $\Omega^{cl} = \Omega \cup \partial \Omega$  of  $\Omega$ .

To complete the description of this problem we must specify the constitutive relation between the displacement vector and the stress tensor. We recall that the (linearized) strain tensor e in the body is defined as

$$e_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right). \tag{6.4}$$

We shall consider two types of constitutive relation:

### Linear hyperelastic solids

The first constitutive relation we consider is that of a linear hyperelastic solid. In such a material the stress and strain tensors are related through *Hooke's Law* 

$$T_{ij} = a_{ijkl}e_{kl}, (6.5)$$

where  $a_{ijkl}$  are the components of the elastic tensor a for the body. These  $a_{ijkl}$  are assumed to be real-valued and satisfy the symmetry relations

$$a_{ijkl} = a_{jikl} = a_{ijlk} = a_{klij}. (6.6)$$

An elastic tensor a is said to be strongly elliptic (e.g. Marsden & Hughes 1983, section

4.3) if for all  $x \in \Omega^{\operatorname{cl}}$  and for all  $u, v \in \mathbb{C}^n$  we have

$$a_{ijkl}(x)u_i\overline{u_k}v_j\overline{v_k} \ge K\|u\|_{\mathbb{C}^n}^2\|v\|_{\mathbb{C}^n}^2, \tag{6.7}$$

where the constant K > 0 can be chosen independently of x. Similarly, we say that a is uniformly pointwise stable (e.g. Marsden & Hughes 1983, section 4.3) if for all  $x \in \Omega^{cl}$  and for all symmetric  $e \in \mathbb{C}^{n \times n}$  we have

$$a_{ijkl}(x)e_{ij}\overline{e_{kl}} \ge Ke_{ij}\overline{e_{ij}},$$
 (6.8)

where the constant K > 0 can be chosen independently of x. By taking  $e_{ij} = u_i v_j$ , it is easy to see that the uniform pointwise stability of a implies its strong ellipticity; the converse result, however, may be shown not to hold (e.g. Marsden & Hughes 1983, Chapter 4, Proposition 3.10). For an isotropic material the elastic tensor can be written

$$a_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{il} + \delta_{il} \delta_{jk}), \tag{6.9}$$

where  $\lambda$  and  $\mu$  are the two Lamé moduli. In this case it may be shown (e.g. Marsden & Hughes 1983, Chapter 4) that the strong ellipticity of a is equivalent to the conditions

$$\mu > 0, \quad \lambda + 2\mu > 0,$$
 (6.10)

for all  $x \in \Omega^{cl}$ , while uniform pointwise stability of a is equivalent to

$$\mu > 0, \quad \lambda + \frac{2}{3}\mu > 0,$$
 (6.11)

for all  $x \in \Omega^{cl}$ . We note that the strong ellipticity condition for an isotropic material is equivalent to the requirement that the squared p-wave and s-wave speeds, given by

$$v_p^2 = \frac{\lambda + 2\mu}{\rho}, \quad v_s^2 = \frac{\mu}{\rho},$$
 (6.12)

respectively, are everywhere positive, while the uniform pointwise stability condition requires that the shear modulus  $\mu$  and bulk moduls  $\kappa = \lambda + \frac{2}{3}\mu$  are everywhere positive.

With the above constitutive relation, we obtain from eq.(6.1) the elastodynamic equation

$$\frac{\partial^2 u_i}{\partial t^2} - \frac{1}{\rho} \frac{\partial}{\partial x_i} \left( a_{jikl} \frac{\partial u_l}{\partial x_k} \right) = f_i, \tag{6.13}$$

where we assume that a is smooth in  $\Omega$  and can be extended to a continuous function on  $\Omega^{\text{cl}}$ . We further assume that a is uniformly pointwise stable. Formally defining a linear operator by

$$(Au)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{i}} \left( a_{jikl}(x) \frac{\partial u_{l}}{\partial x_{k}}(x) \right), \tag{6.14}$$

we can write eq.(6.13) concisely as

$$\frac{\partial^2 u}{\partial t^2} + Au = f. \tag{6.15}$$

We shall refer to A as the *elastodynamic operator* in what follows. Note that in the above equation we regard u and f as being functions of t taking values in appropriate function spaces.

#### Linear viscoelastic solids

In a linear viscoelastic material Hooke's Law is generalized to allow the stress tensor at a given time to depend linearly on the entire strain history of the material. This idea is expressed through *Boltzmann's superposition principle* 

$$T_{ij}(x,t) = \int_{-\infty}^{t} b_{ijkl}(x,t-t') \frac{\partial e_{ij}}{\partial t'}(x,t') \,\mathrm{d}t', \tag{6.16}$$

where  $b_{ijkl}$  are the components of the so-called relaxation tensor b for the material (e.g. Coleman & Noll 1962; Day 1972; Fabrizio & Morro 1992). In this equation values of  $b_{ijkl}(x,t)$  for t < 0 are not needed, so we are free to set  $b_{ijkl}(x,t) = 0$  for all negative times. Having done this, eq.(6.16) can be written more concisely as

$$T_{ij} = b_{ijkl} * \frac{\partial e_{ij}}{\partial t}, \tag{6.17}$$

where the convolution is understood to be taken with respect to t. We shall assume that the components of  $b_{ijkl}$  are real-valued, and that they satisfy the symmetry relations

$$b_{ijkl} = b_{jikl} = b_{ijlk} = b_{klij}. (6.18)$$

We note that by taking

$$b_{ijkl}(x,t) = H(t)a_{ijkl}(x),$$
 (6.19)

where H(t) is the Heavyside step function, and  $a_{ijkl}$  is a tensor with appropriate symmetries, then eq.(6.16) reduces to Hooke's Law. It follows that linear elastic materials can be regarded as a special case of linear viscoelastic materials

In the case that the reference body is linear viscoelastic, we assume that  $b_{ijkl}(x,t)$  is smooth as a function of x in  $\Omega$ , and that it may be extended to a continuous function on  $\Omega^{cl}$ . Further assumptions on the time-dependence of the relaxation tensor are given in the

next subsection. Substituting eq.(6.17) into eq.(6.1) we obtain

$$\frac{\partial^2 u_i}{\partial t^2} - \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( b_{jikl} * \frac{\partial}{\partial x_k} \frac{\partial u_l}{\partial t} \right) = f_i, \tag{6.20}$$

which we shall call the *viscoelastodynamic equation*. Formally defining an operator-valued function  $t \mapsto B(t)$  by

$$(B(t)u)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{j}} \left( b_{jikl}(x,t) \frac{\partial u_{l}}{\partial x_{k}}(x) \right), \tag{6.21}$$

we can write eq.(6.20) concisely as

$$\frac{\partial^2 u}{\partial t^2} + B * \frac{\partial u}{\partial t} = f, \tag{6.22}$$

where we again think of u and f as being functions of time taking values in appropriate function spaces. We will refer to B as the relaxation operator.

### 6.2.2 Completely monotone relaxation tensors

In this chapter we focus attention on those materials whose relaxation tensors satisfy the condition of being *completely monotone* (e.g. Day 1971, 1972; Hanyga 2005; Hanyga & Seredyńska 2007). This class of relaxation tensors includes all those commonly employed in geophysics, such as Maxwell solids, standard linear solids, and absorption band solids (e.g. Dahlen & Tromp 1998, Chapter 6).

We first recall that a function  $f:(0,\infty)\to\mathbb{R}$  is said to be completely monotone if it is infinitely differentiable and if

$$(-1)^n f^{(n)}(t) \ge 0, (6.23)$$

for all  $n \in \mathbb{N}$  and all t > 0, where  $f^{(n)}$  denotes the *n*th derivative of f (e.g. Widder 1941, Chapter IV). A result known as Bernstein's theorem (e.g. Widder 1941, Theorem 12a; Pollard 1944) states that all completely monotone functions can be written in the form

$$f(t) = \int_{[0,\infty)} e^{-st} m(\mathrm{d}s), \tag{6.24}$$

where m is a non-negative Radon measure on  $[0, \infty)$  (note that this result can alternatively be formulated in terms of Stieltjes integrals of monotonically increasing functions). From this result, we see that  $\lim_{t\searrow 0} f(t)$  exists if and only if  $m([0,\infty))$  is finite. In this case, f extends to a bounded continuous function on  $[0,\infty)$  satisfying

$$f(0) = m([0, \infty)). \tag{6.25}$$

We recall that the support  $\operatorname{supp}(m)$  of a measure m on  $[0,\infty)$  is defined to be the complement of the largest measurable open subset  $E\subseteq [0,\infty)$  on which m(E)=0. A Radon measure (being by definition locally-finite) necessarily satisfies the condition  $m([0,\infty))<\infty$  if it has compact support. We also note the relation

$$\lim_{t \to \infty} f(t) = m(\{0\}),\tag{6.26}$$

showing that a completely monotone function f tends to zero as  $t \to \infty$  unless its associated measure m has an atom at 0.

A relaxation tensor b is completely monotone if for all  $x \in \Omega^{\text{cl}}$  and all symmetric  $e \in \mathbb{C}^{n \times n}$  the real-valued function  $b_{ijkl}(x,t)e_{ij}\overline{e_{kl}}$  is completely monotone for  $t \in (0,\infty)$ . A generalization of Bernstein's theorem to tensor-valued functions (Gripenberg *et al.* 1990; Hanyga & Seredyńska 2007) shows that for  $t \in (0,\infty)$  a completely monotone relaxation tensor can be written

$$b_{ijkl}(x,t) = \int_{[0,\infty)} e^{-st} m_{ijkl}(x,ds),$$
 (6.27)

where, for each fixed  $x \in \Omega^{\text{cl}}$ ,  $m_{ijkl}(x,\cdot)$  are the components of a tensor-valued Radon measure  $m(x,\cdot)$  on  $[0,\infty)$ . These components are real-valued and satisfy the relations

$$m_{ijkl}(x, E) = m_{jikl}(x, E) = m_{ijlk}(x, E) = m_{klij}(x, E),$$
 (6.28)

along with

$$m_{ijkl}(x, E)e_{ij}\overline{e_{kl}} \ge 0,$$
 (6.29)

for each measurable subset  $E \subseteq [0, \infty)$  and all symmetric  $e \in \mathbb{C}^{n \times n}$ . We shall suppose further that for each  $x \in \Omega^{\text{cl}}$  the measure  $m(x, \cdot)$  has compact support, and write  $[s_1, s_2]$  for the smallest closed interval such that

$$\operatorname{supp}(m(x,\cdot)) \subseteq [s_1, s_2], \tag{6.30}$$

for all  $x \in \Omega^{\text{cl}}$ . Because of this assumption, the relaxation tensor b is defined for all  $t \in [0, \infty)$ , and

$$b_{ijkl}(x,0) = m_{ijkl}(x,[0,\infty)).$$
 (6.31)

We further assume that the tensor-valued measure m is such that  $m(\cdot, [0, \infty))$  is uniformly pointwise stable.

For each measurable subset  $E \subseteq [0, \infty)$  we can formally define a linear operator M(E) by

$$(M(E)u)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{i}} \left( m_{jikl}(x, E) \frac{\partial u_{l}}{\partial x_{k}}(x) \right), \tag{6.32}$$

and so think of the function  $E \to M(E)$  as defining an operator-valued measure on  $[0, \infty)$ . We can then write the relaxation operator B(t) associated with a completely monotone relaxation tensor formally as

$$B(t) = \int_{[0,\infty)} e^{-st} M(ds), \quad t \ge 0.$$
 (6.33)

## 6.3 The elastodynamic and relaxation operators

In the previous section we introduced in a formal manner the elastodynamic operator A in terms of which the elastodynamic equation can be written

$$\frac{\partial^2 u}{\partial t^2} + Au = f, (6.34)$$

subject to certain initial and boundary conditions. We also introduced an operator-valued function  $t \mapsto B(t)$ , which we called the relaxation operator, in terms of which the viscoelastodynamic equation can be written

$$\frac{\partial^2 u}{\partial t^2} + B * \frac{\partial u}{\partial t} = f, \tag{6.35}$$

again subject to certain initial and boundary conditions. Moreover, we showed formally that for a material with a completely monotone relaxation function, the relaxation operator takes the form

$$B(t) = \int_{[0,\infty)} e^{-st} M(ds), \quad t \ge 0,$$
 (6.36)

where M is an operator-valued Radon measure on  $[0, \infty)$ . In this section we shall consider how these various ideas can be formulated in a rigorous manner.

### 6.3.1 Sobolev spaces

We begin by recalling some useful definitions and results from the theory of Sobolev spaces (e.g. Lions & Magenes 1972; Dautray & Lions 1984; Friedman 1997; Wloka 1997; Trèves 2003). In stating these results we do not specify in detail any smoothness requirements on the boundary of the region  $\partial\Omega$ . Instead we simply say that the boundary is 'sufficiently

smooth', which can be taken to mean that  $\partial\Omega$  is a smooth (n-1)-dimensional submanifold of  $\mathbb{R}^n$ .

With the region  $\Omega$  as above, let  $L^2(\Omega; \mathbb{C}^n)$  denote the Hilbert space of measurable functions  $u: \Omega \to \mathbb{C}^n$  that are square-integrable with respect to the inner-product

$$(u,v)_{L^2(\Omega;\mathbb{C}^n)} = \int_{\Omega} (u(x), v(x))_{\mathbb{C}^n} dx,$$
 (6.37)

where  $(\cdot,\cdot)_{\mathbb{C}^n}$  denotes the standard Hermitian inner-product on  $\mathbb{C}^n$  given by

$$(u,v)_{\mathbb{C}^n} = u_i \overline{v_i}. \tag{6.38}$$

The associated norm on  $L^2(\Omega; \mathbb{C}^n)$  will be written  $\|\cdot\|_{L^2(\Omega; \mathbb{C}^n)}$  and is defined by

$$||u||_{L^{2}(\Omega;\mathbb{C}^{n})}^{2} = (u,u)_{L^{2}(\Omega;\mathbb{C}^{n})}.$$
(6.39)

We recall that an *n*-dimensional multi-index  $\alpha$  is an *n*-tuple of natural numbers  $(\alpha_1, \dots, \alpha_n)$ , and that the space of such multi-indices is denoted by  $\mathbb{N}^n$ . The length of a multi-index  $\alpha$  is defined to be

$$|\alpha| = \alpha_1 + \dots + \alpha_n. \tag{6.40}$$

Given a multi-index, we define the differential operator  $\partial^{\alpha}$  by

$$\partial^{\alpha} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_n}}.$$
(6.41)

The Sobolev space  $H^s(\Omega; \mathbb{C}^n)$  for positive integer s is defined to be

$$H^{s}(\Omega; \mathbb{C}^{n}) = \{ u \in L^{2}(\Omega; \mathbb{C}^{n}) \mid \partial^{\alpha} u \in L^{2}(\Omega; \mathbb{C}^{n}), |\alpha| \leq s \}$$

$$(6.42)$$

where the partial derivatives are understood in the distributional sense. On  $H^s(\Omega; \mathbb{C}^n)$  we can define an inner-product

$$(u,v)_{H^s(\Omega;\mathbb{C}^n)} = \sum_{|\alpha| \le s} (\partial^{\alpha} u, \partial^{\alpha} v)_{L^2(\Omega;\mathbb{C}^n)}, \qquad (6.43)$$

and associated norm  $\|\cdot\|_{H^s(\Omega;\mathbb{C}^n)}$ . It may be shown that  $H^s(\Omega;\mathbb{C}^n)$  is complete with respect to this norm, and so becomes a Hilbert space. The definition of  $H^s(\Omega;\mathbb{C}^n)$  can be extended to non-integral and non-positive values of s using Fourier transforms (e.g. Trèves 2003, Section 25).

We now state without proof a number of properties of Sobolev spaces which will be required below:

**Proposition 6.3.1** For  $s, s' \in \mathbb{R}$ , if s > s' then  $H^s(\Omega; \mathbb{C}^n)$  is contained in  $H^{s'}(\Omega; \mathbb{C}^n)$ , and the injection is continuous.

**Proposition 6.3.2** For each  $\alpha \in \mathbb{N}^n$  and  $s \in \mathbb{R}$ , the differential operator  $\partial^{\alpha}$  defines a continuous mapping from  $H^s(\Omega; \mathbb{C}^n)$  into  $H^{s-|\alpha|}(\Omega; \mathbb{C}^n)$ .

Let  $\mathscr{D}(\mathbb{R}^n;\mathbb{C}^n)$  denote the space of infinitely differentiable  $\mathbb{C}^n$ -valued functions in  $\mathbb{R}^n$  with compact support and given the usual topology. We write  $\mathscr{D}(\Omega^{\text{cl}};\mathbb{C}^n)$  for the space of restrictions to  $\Omega$  of elements of  $\mathscr{D}(\mathbb{R}^n;\mathbb{C}^n)$ .

**Proposition 6.3.3** If  $\Omega$  is a sufficiently smooth open subset of  $\mathbb{R}^n$ , then  $\mathcal{D}(\Omega^{\operatorname{cl}}; \mathbb{C}^n)$  is dense in  $H^s(\Omega; \mathbb{C}^n)$ .

Combining this result with Proposition 6.3.1 we see that:

**Corollary 6.3.4** If  $\Omega$  is a sufficiently smooth open subset of  $\mathbb{R}^n$  and  $s, s' \in \mathbb{R}$  with s > s', then the injection of  $H^s(\Omega; \mathbb{C}^n)$  into  $H^{s'}(\Omega; \mathbb{C}^n)$  is dense.

Let  $\mathscr{D}(\Omega; \mathbb{C}^n)$  denote the space of infinitely differentiable  $\mathbb{C}^n$ -valued functions defined in  $\Omega$  having compact support and given the usual topology. The space  $H_0^s(\Omega; \mathbb{C}^n)$  is defined to be the closure of  $\mathscr{D}(\Omega; \mathbb{C}^n)$  in the  $\|\cdot\|_{H^s(\Omega; \mathbb{C}^n)}$ -norm topology.

**Proposition 6.3.5** Let  $\Omega$  be a bounded subset of  $\mathbb{R}^n$ , and s and integer greater than zero. Then  $H_0^s(\Omega; \mathbb{C}^n) \neq H^s(\Omega; \mathbb{C}^n)$ .

Let  $\Omega$  be an open subset of  $\mathbb{R}^n$  with sufficiently smooth boundary  $\partial\Omega$ . The Sobolev spaces  $H^s(\partial\Omega;\mathbb{C}^n)$  for  $s\in\mathbb{R}$  can be defined in the above manner by employing partitions of unity and local co-ordinate charts on  $\partial\Omega$  (e.g. Trèves 2003; Section 26). For a function  $u\in\mathcal{D}(\Omega^{cl};\mathbb{C}^n)$ , let  $\gamma_0$  denote the *trace mapping* that takes u to its restriction  $u|_{\partial\Omega}$  on the boundary  $\partial\Omega$ .

**Theorem 6.3.6** If  $\partial\Omega$  is sufficiently smooth, then for each  $s \in \mathbb{R}$  the trace mapping  $\gamma_0$  extends to a continuous mapping from  $H^s(\Omega; \mathbb{C}^n)$  onto  $H^{s-1/2}(\partial\Omega; \mathbb{C}^n)$ .

**Proposition 6.3.7** The kernel of the trace mapping  $\gamma_0 : H^1(\Omega; \mathbb{C}^n) \to H^{1/2}(\partial\Omega; \mathbb{C}^n)$  is equal to  $H^1_0(\Omega; \mathbb{C}^n)$ .

Let  $\Omega$  be a sufficiently smooth bounded open subset of  $\mathbb{R}^n$ . We denote by  $C^k(\mathbb{R}^n; \mathbb{C}^n)$  the space of k-times continuously differentiable  $\mathbb{C}^n$ -valued functions on  $\mathbb{R}^n$ , and by  $C^k(\Omega^{\text{cl}}; \mathbb{C}^n)$  the space of restrictions of such functions to  $\Omega$ . On  $C^k(\Omega^{\text{cl}}; \mathbb{C}^n)$  we can define the norm

$$||u||_{C^k(\Omega^{\mathrm{cl}};\mathbb{C}^n)} = \sup_{|\alpha| \le k} \left( \sup_{x \in \Omega^{\mathrm{cl}}} |\partial^{\alpha} u(x)| \right). \tag{6.44}$$

It may be shown that  $C^k(\Omega^{cl}; \mathbb{C}^n)$  is complete with respect to this norm, and so defines a Banach space.

**Theorem 6.3.8** Let  $\Omega$  be a sufficiently smooth bounded open subset of  $\mathbb{R}^n$ . If  $s > \frac{n}{2} + k$ , the elements of  $H^s(\Omega; \mathbb{C}^n)$  are k-fold continuously differentiable functions, and the embedding of  $H^s(\Omega; \mathbb{C}^n)$  into  $C^k(\Omega^{cl}; \mathbb{C}^n)$  is continuous.

We recall that a linear mapping between metric spaces is said to be *compact* if the image of a bounded set under the mapping is pre-compact (i.e. has compact closure).

**Theorem 6.3.9** Let  $\Omega$  be a sufficiently smooth bounded open subset of  $\mathbb{R}^n$ . Then the injection of  $H^{s+1}(\Omega;\mathbb{C}^n)$  into  $H^s(\Omega;\mathbb{C}^n)$  is compact.

### 6.3.2 The elastodynamic operator

Recalling that the density  $\rho$  on  $\Omega$  is assumed to be smooth and everywhere positive, we can define a Hilbert space  $L^2(\Omega, \rho; \mathbb{C}^n)$  which comprises those measurable functions  $u: \Omega \to \mathbb{C}^n$  that are square-integrable with respect to the inner-product

$$(u,v)_{L^2(\Omega,\rho;\mathbb{C}^n)} = \int_{\Omega} \rho(x) (u(x), v(x))_{\mathbb{C}^n} dx, \qquad (6.45)$$

with associated norm  $\|\cdot\|_{L^2(\Omega,\rho;\mathbb{C}^n)}$ . Clearly  $L^2(\Omega;\mathbb{C}^n)$  and  $L^2(\Omega,\rho;\mathbb{C}^n)$  are equal as point-sets. As  $\rho$  is continuous and positive on the compact set  $\Omega^{\text{cl}}$ , it satisfies

$$0 < \rho_m = \min_{x \in \Omega^{cl}} \rho(x) \le \rho(x) \le \max_{x \in \Omega^{cl}} \rho(x) = \rho_M < \infty.$$
 (6.46)

It follows that for all  $u \in L^2(\Omega; \mathbb{C}^n)$  we have

$$\sqrt{\rho_m} \|u\|_{L^2(\Omega;\mathbb{C}^n)} \le \|u\|_{L^2(\Omega,\rho;\mathbb{C}^n)} \le \sqrt{\rho_M} \|u\|_{L^2(\Omega;\mathbb{C}^n)},\tag{6.47}$$

so that the norms on  $L^2(\Omega; \mathbb{C}^n)$  and  $L^2(\Omega, \rho; \mathbb{C}^n)$  are equivalent, and we conclude that these two Hilbert spaces are homeomorphic.

For suitably smooth  $\mathbb{C}^n$ -valued functions on  $\Omega$  we have defined the elastodynamic operator by

$$(Au)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{j}} \left( a_{jikl}(x) \frac{\partial u_{l}}{\partial x_{k}}(x) \right). \tag{6.48}$$

In particular, this operator makes classical sense if  $u \in C^2(\Omega^{\text{cl}}; \mathbb{C}^n)$ , and in this case the Dirichlet boundary conditions  $u|_{\partial\Omega} = 0$  are also well-defined. We now consider how to extend the definition of A to (a subset of) functions defined in  $L^2(\Omega, \rho; \mathbb{C}^n)$ . The resulting linear operator  $A: D(A) \to L^2(\Omega, \rho; \mathbb{C}^n)$  with domain  $D(A) \subseteq L^2(\Omega, \rho; \mathbb{C}^n)$  will be called the realization of A in  $L^2(\Omega, \rho; \mathbb{C}^n)$  (e.g. Browder 1961). Our motivation for considering this density-weighted Hilbert space  $L^2(\Omega, \rho; \mathbb{C}^n)$  can be seen as follows. We recall that the formal adjoint of A in  $L^2(\Omega, \rho; \mathbb{C}^n)$  is defined to be the partial differential operator A' such that

$$(Au, v)_{L^2(\Omega, \rho; \mathbb{C}^n)} = (u, A'v)_{L^2(\Omega, \rho; \mathbb{C}^n)}, \tag{6.49}$$

for all  $u, v \in \mathcal{D}(\Omega; \mathbb{C}^n)$ . A simple calculation using integration by parts shows that A' is equal to A, and so we say that A is formally self-adjoint in  $L^2(\Omega, \rho; \mathbb{C}^n)$ . Had we instead worked in the space  $L^2(\Omega; \mathbb{C}^n)$  we would not have obtained this result except in the relatively uninteresting case that  $\rho$  is a constant in  $\Omega$ . We will see later that the formal self-adjointness of A along with its strong ellipticity actually implies that A is a self-adjoint operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

Roughly speaking, we wish to define the domain of A to be the subspace  $D(A) \subseteq L^2(\Omega, \rho; \mathbb{C}^n)$  for which Au, when suitably interpreted, is an element of  $L^2(\Omega, \rho; \mathbb{C}^n)$ , and for which the Dirichlet boundary conditions  $u|_{\partial\Omega}=0$  hold in a generalized sense. Noting that the definition of A in eq.(6.48) involves only partial derivatives of order less than or equal to two, we see from Proposition 6.3.2 that if we regard these derivatives as being taken in the distributional sense, then  $Au \in L^2(\Omega, \rho; \mathbb{C}^n)$  whenever  $u \in H^2(\Omega; \mathbb{C}^n)$ . For  $u \in H^2(\Omega; \mathbb{C}^n)$  the restriction to  $\partial\Omega$  is not well-defined. We can, however, consider its generalization given by the trace-mapping  $\gamma_0$  introduced in Proposition 6.3.6. In this manner the Dirichlet boundary condition is generalized to  $\gamma_0 u = 0$  for  $u \in D(A)$ . Making use of Proposition 6.3.7

it follows that

$$D(A) = H^{2}(\Omega; \mathbb{C}^{n}) \cap H_{0}^{1}(\Omega; \mathbb{C}^{n}), \tag{6.50}$$

where we here think of  $H^2(\Omega; \mathbb{C}^n) \cap H^1_0(\Omega; \mathbb{C}^n)$  as being a dense subset of  $L^2(\Omega, \rho; \mathbb{C}^n)$ . For notation convenience we define

$$H_{\partial}^{2}(\Omega; \mathbb{C}^{n}) = H^{2}(\Omega; \mathbb{C}^{n}) \cap H_{0}^{1}(\Omega; \mathbb{C}^{n}), \tag{6.51}$$

so that  $D(A) = H_{\partial}^2(\Omega; \mathbb{C}^n)$ . As the trace-mapping  $\gamma_0 : H^2(\Omega; \mathbb{C}^n) \to H^{3/2}(\Omega; \mathbb{C}^n)$  is continuous, we see that  $D(A) = H^2(\Omega; \mathbb{C}^n) \cap H_0^1(\Omega; \mathbb{C}^n)$  is closed in  $H^2(\Omega; \mathbb{C}^n)$ , and so becomes a Hilbert space when given the induced topology. It follows that we can alternatively think of A as being a continuous operator from  $H_{\partial}^2(\Omega; \mathbb{C}^n)$  into  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

### 6.3.3 The relaxation operator

For sufficiently smooth functions we have defined the relaxation operator to be

$$(B(t)u)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{j}} \left( b_{jikl}(x,t) \frac{\partial u_{l}}{\partial x_{k}}(x) \right), \tag{6.52}$$

where we note that  $b_{ijkl}(x,t) = \text{for } t < 0$ , so that B(t) is equal to the zero-operator for t < 0. For  $t \ge 0$ , we form the realization of B(t) in  $L^2(\Omega, \rho; \mathbb{C}^n)$  by taking

$$D(B(t)) = H_{\partial}^{2}(\Omega; \mathbb{C}^{n}). \tag{6.53}$$

We can again think of B(t) as being either a linear operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$  with dense domain, or as a continuous linear operator from  $H^2_{\partial}(\Omega; \mathbb{C}^n)$  into  $L^2(\Omega, \rho; \mathbb{C}^n)$ . This latter point of view is particularly useful when considering  $t \mapsto B(t)$  as an operator-valued function.

Let us set  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$  for notational simplicity. We write L(Y; X) for the Banach space of bounded linear operators from Y into X with operator-norm denoted by  $\|\cdot\|_{L(Y;X)}$ . With this notation, we see that  $t \mapsto B(t)$  is a well-defined function on  $\mathbb{R}$  taking values in L(Y;X). From eq.(6.27) it is clear that for all  $x \in \Omega$  the mapping  $t \mapsto b(x,t)$  is continuous for  $t \in (0,\infty)$  and bounded for  $t \in [0,\infty)$ . It follows that the operator-valued function  $t \mapsto B(t)$  is continuous for  $t \in (0,\infty)$  and bounded for  $t \in [0,\infty)$  in the operator-norm topology on L(Y;X).

Let  $t \mapsto u(t)$  be a Y-valued function that is locally integrable, i.e. such that

$$\left\| \int_{U} u(t) \, \mathrm{d}t \right\|_{Y} < \infty, \tag{6.54}$$

where U is an arbitrary bounded subset of  $\mathbb{R}$ . For such  $u : \mathbb{R} \to Y$  having  $\operatorname{supp}(u) \subseteq [\alpha, \infty)$  with  $\alpha > -\infty$ , it follows from the boundedness of  $t \mapsto B(t)$  that the convolution

$$(B * u)(t) = \int_{\alpha}^{t} B(t - t')u(t') dt', \qquad (6.55)$$

is a well-defined X-valued function. In particular, if  $t \mapsto u \in X$  is such that  $\frac{\partial u}{\partial t}$  exists, is locally integrable, and has support in some right half-line, then the convolution  $B * \frac{\partial u}{\partial t}$  occurring in the viscoelastodynamic equation is well-defined.

For each measurable  $E \subseteq [0, \infty)$  we have defined an operator M(E) formally by

$$(M(E)u)_i(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_j} \left( m_{jikl}(x, E) \frac{\partial u_l}{\partial x_k}(x) \right). \tag{6.56}$$

We see readily that M(E) can be extended to a bounded linear operator from Y into X. We can, therefore, consider  $E \mapsto M(E)$  as being an L(Y; X)-valued measure, and write

$$B(t) = \int_{[0,\infty)} e^{-st} M(\mathrm{d}s), \tag{6.57}$$

for  $t \in [0, \infty)$ , where the convergence of this integral is understood in the operator-norm topology on L(Y; X).

## 6.4 Vector-Valued Convolution Equations

### 6.4.1 Spaces of test functions and distributions

We begin by recalling some basic notations for scalar- and vector-valued distributions. Further details can be found in the books by Dautray & Lions (1984), Hörmander (1990), Friedlander & Joshi (1998), and Trèves (2003, 2009).

We write  $\mathscr{D}$  for the space of smooth complex-valued test-functions on  $\mathbb{R}$  having compact support and given the usual topology, and denote its topological dual space by  $\mathscr{D}'$ . The action of a distribution  $T \in \mathscr{D}'$  on a test-function  $\varphi \in \mathscr{D}$  will be denoted by  $\langle T, \varphi \rangle$ . We write  $\mathscr{E}$  for the space of smooth test-functions on  $\mathbb{R}$ , and  $\mathscr{E}'$  for its topological dual space which may be shown to comprises those elements of  $\mathscr{D}'$  having compact support. We also write  $\mathscr{S}$  for the Schwartz space of rapidly decreasing test-functions on  $\mathbb{R}$ , and  $\mathscr{S}'$  for its topological dual space of Schwartz distributions. The dual pairings between  $\mathscr{E}$  and  $\mathscr{E}'$  and

between  $\mathscr{S}$  and  $\mathscr{S}'$  are also denoted by  $\langle \cdot, \cdot \rangle$ . We recall the inclusions

$$\mathscr{D} \subseteq \mathscr{S} \subseteq \mathscr{E},\tag{6.58}$$

$$\mathcal{E}' \subseteq \mathcal{S}' \subseteq \mathcal{D}',\tag{6.59}$$

each of which is continuous and dense.

For a Banach space Z, we write  $\mathscr{D}'(Z)$  for the space of Z-valued continuous linear functionals on  $\mathscr{D}$ , denoting the action of such a vector-valued distribution  $T \in \mathscr{D}'(Z)$  on a test-function  $\varphi \in \mathscr{D}$  by  $\langle T, \varphi \rangle \in Z$ . The space  $\mathscr{D}'(Z)$  is given the weak-topology induced from  $\mathscr{D}$ , and will be referred to as the space of Z-valued distributions. The subspace of  $\mathscr{D}'(Z)$  comprising distributions having support contained in some right half-line  $[\alpha, \infty)$  with  $\alpha > -\infty$  will be written  $\mathscr{D}'_{+}(Z)$ . We can define the spaces  $\mathscr{E}'(Z)$ ,  $\mathscr{F}'(Z)$ , and  $\mathscr{F}'_{+}(Z)$  in an analogous manner. Given a vector  $u \in Z$  and a distribution  $T \in \mathscr{D}'$ , we define their tensor-product to be the Z-valued distribution  $T \otimes u \in \mathscr{D}'(Z)$  given by

$$\langle T \otimes u, \varphi \rangle = \langle T, \varphi \rangle u, \tag{6.60}$$

for any test-function  $\varphi \in \mathcal{D}$ .

### 6.4.2 The Laplace transform

In this subsection we recall the definition of the distributional Laplace transform, and describe a number of its properties (e.g. Dautray & Lions (1984); Fattorini 1980; Trèves 2003). For a Banach space Z, let  $f \in \mathscr{D}'_{+}(Z)$  be such that  $fe^{-\xi_0 t} \in \mathscr{S}'(Z)$  for some  $\xi_0 \in \mathbb{R}$ . Then for  $\text{Re}(p) \geq \xi_0$  we can define the Laplace transform  $p \mapsto \mathscr{L}(f)(p) \in Z$  of f by

$$\mathcal{L}(f)(p) = \mathcal{F}\left(fe^{-\xi t}\right)(\eta), \quad p = \xi + i\eta, \ \xi, \eta \in \mathbb{R},\tag{6.61}$$

where  $\mathscr{F}$  denotes the distributional Fourier transform on  $\mathscr{S}'(Z)$ . We will often write  $\tilde{f}(p)$  as a shorthand for the Laplace transform  $\mathscr{L}(f)(p)$ . A central property of the Laplace transform is given in the following result (e.g. Dautray & Lions 1984, Chapter XVI, Theorem 2):

**Theorem 6.4.1** A function  $p \mapsto F(p)$  with values in a Banach space Z is the Laplace transform of a distribution  $f \in \mathcal{D}'_{+}(Z)$  having support in  $[\alpha, \infty)$  if and only if there exists an  $\xi_0 \in \mathbb{R}$  such that for  $\text{Re}(p) > \xi_0$  the function  $p \mapsto F(p)$  is holomorphic and satisfies the

estimate

$$||F(p)||_Z \le e^{-\xi \alpha} \operatorname{Pol}(|p|), \quad p = \xi + i\eta, \quad \xi, \eta \in \mathbb{R},$$
 (6.62)

where  $Pol(\cdot)$  denotes a polynomial with positive coefficients.

A related result is (e.g. Dautray & Lions 1984, Chapter XVI, Lemma 2):

**Lemma 6.4.2** Let Z be a Banach space, and suppose that  $p \mapsto F(p) \in Z$  is a holomorphic function for  $\text{Re}(p) > \xi_0 > 0$  and for such p satisfies the estimate

$$||F(p)||_Z \le \frac{Ce^{-\xi\alpha}}{|p|^2}, \quad p = \xi + i\eta.$$
 (6.63)

Then F is the Laplace transform of a continuous function  $t \mapsto f(t) \in Z$  with  $\operatorname{supp}(f) \subseteq [\alpha, \infty)$ .

The next result shows how a distribution may be recovered from its Laplace transform:

**Proposition 6.4.3** For a Banach space Z, let  $f \in \mathcal{D}'_{+}(Z)$  have Laplace transform  $p \mapsto \tilde{f}(p)$  defined for  $\text{Re}(p) > \xi_0$ . Then f can be expressed in terms of  $\tilde{f}(p)$  by the inverse Laplace transform

$$f(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{f}(p) e^{pt} dp, \qquad (6.64)$$

where  $\xi > \xi_0$  is arbitrary, the notation f(t) here means that the distribution f acts on the variable t, and the convergence of the integral is in  $\mathcal{D}'_{+}(Z)$ .

**Proof** By definition  $\eta \mapsto \tilde{f}(\xi + i\eta)$  for  $\xi > \xi_0$  is the distributional Fourier transform of  $f(t)e^{-\xi t} \in \mathcal{S}'(Z)$ , and so is itself an element of  $\mathcal{S}'(Z)$ . For  $\xi > \xi_0$ , let us define a sequence of functions by

$$\eta \mapsto \tilde{f}_n(\xi + i\eta) = \begin{cases} \tilde{f}(\xi + i\eta) & |\eta| \le n \\ 0 & |\eta| \ge n \end{cases}, \tag{6.65}$$

for n = 1, 2, ... It is clear that  $\eta \mapsto \tilde{f}_n(\xi + i\eta)$  tends to  $\eta \mapsto \tilde{f}(\xi + i\eta)$  in  $\mathscr{S}'(Z)$ , and it follows from the continuity of the inverse Fourier transform on  $\mathscr{S}'(Z)$  that

$$\lim_{n \to \infty} \mathscr{F}_{\eta}^{-1} \left( \tilde{f}_n(\xi + i\eta) \right) = \mathscr{F}_{\eta}^{-1} \left( \tilde{f}(\xi + i\eta) \right) = e^{-\xi t} f(t), \tag{6.66}$$

where the notation  $\mathscr{F}_{\eta}^{-1}$  here means that the inverse Fourier transform acts on the  $\eta$ -

variable. As  $\eta \mapsto \tilde{f}_n(\xi + i\eta)$  is continuous and has compact support, we have

$$\mathscr{F}_{\eta}^{-1}\left(\tilde{f}_{n}(\xi+\mathrm{i}\eta)\right) = \frac{1}{2\pi}\left\langle\tilde{f}_{n}(\xi+\mathrm{i}\eta),\mathrm{e}^{\mathrm{i}\eta t}\right\rangle = \frac{1}{2\pi}\int_{-n}^{n}\tilde{f}(\xi+\mathrm{i}\eta)\mathrm{e}^{\mathrm{i}\eta t}\,\mathrm{d}\eta. \tag{6.67}$$

Changing integration variables from  $\eta$  to  $p = \xi + i\eta$ , we then find

$$\mathscr{F}_{\eta}^{-1}\left(\tilde{f}_{n}(\xi+\mathrm{i}\eta)\right) = \frac{1}{2\pi\mathrm{i}} \int_{\xi-\mathrm{i}n}^{\xi+\mathrm{i}n} \tilde{f}(p) \mathrm{e}^{pt} \mathrm{e}^{-\xi t} \,\mathrm{d}p,\tag{6.68}$$

which leads to

$$e^{-\xi t} f(t) = \lim_{n \to \infty} \frac{1}{2\pi i} \int_{\xi - in}^{\xi + in} \tilde{f}(p) e^{pt} e^{-\xi t} dp,$$
 (6.69)

with the limit being taken in  $\mathscr{S}'(Z)$ . Cancelling the common factors of  $e^{-\xi t}$ , we finally obtain

$$f(t) = \lim_{n \to \infty} \frac{1}{2\pi i} \int_{\xi - in}^{\xi + in} \tilde{f}(p) e^{pt} dp, \tag{6.70}$$

with the limit now being in  $\mathcal{D}'_{+}(Z)$ .

It will be useful to consider in further detail the sense in which the integral in eq.(6.64) converges to the distribution  $f \in \mathcal{D}'_{+}(Z)$ . Let us define a sequence of distributions  $f_n \in$ 

 $\mathcal{D}'(Z)$  for  $n = 1, 2, \dots$  by

$$f_n(t) = \frac{1}{2\pi i} \int_{\xi - in}^{\xi + in} \tilde{f}(p) e^{pt} dp, \qquad (6.71)$$

with  $\xi > \xi_0$  arbitrary. We note that these distributions do not have support contained in a right half-line. Proposition 6.4.3 shows that  $f_n$  converges to f in the topology of  $\mathscr{D}'(Z)$ . This means that for each test-function  $\varphi \in \mathscr{D}$  we have

$$\lim_{n \to \infty} \langle f_n, \varphi \rangle = \langle f, \varphi \rangle. \tag{6.72}$$

As each  $f_n$  is a continuous function, we can write

$$\langle f_n, \varphi \rangle = \int_{-\infty}^{\infty} f_n(t) \varphi(t) \, dt = \frac{1}{2\pi i} \int_{\xi - in}^{\xi + in} \tilde{f}(p) \, \langle e^{pt}, \varphi(t) \rangle \, dp, \tag{6.73}$$

where in obtaining the second equality we have interchanged the order of integration, and where

$$\langle e^{pt}, \varphi(t) \rangle = \int_{-\infty}^{\infty} e^{pt} \varphi(t) dt.$$
 (6.74)

To see that the integrals  $\langle f_n, \varphi \rangle$  converge to a limit as  $n \to \infty$  we require the following result:

**Lemma 6.4.4** For  $\varphi \in \mathscr{D}$  having  $\operatorname{supp}(\varphi) \subseteq (-\infty, \tau]$  with  $\tau < \infty$  and each  $m \in \mathbb{N}$  there exists a constant C > 0 such that

$$|\langle e^{pt}, \varphi(t) \rangle| \le C e^{\operatorname{Re}(p)\tau} |p|^{-m} \sup_{t \in \mathbb{R}} |\partial_t^m \varphi(t)|.$$
 (6.75)

**Proof** By defintion we have

$$\langle e^{pt}, \varphi(t) \rangle = \int_{-\infty}^{\infty} e^{pt} \varphi(t) dt.$$
 (6.76)

Using the identity  $e^{pt} = p^{-1}\partial_t e^{pt}$ , and integrating by parts we obtain

$$\langle e^{pt}, \varphi(t) \rangle = -p^{-1} \langle e^{pt}, \partial_t \varphi(t) \rangle.$$
 (6.77)

Repeating this argument m-times give

$$\langle e^{pt}, \varphi(t) \rangle = (-1)^m p^{-m} \langle e^{pt}, \partial_t^m \varphi(t) \rangle.$$
 (6.78)

For  $t \in \text{supp}(\varphi)$  we have  $|e^{pt}| \leq e^{\text{Re}(p)\tau}$  so that

$$|\langle e^{pt}, \partial_t^m \varphi(t) \rangle| \le C e^{\operatorname{Re}(p)\tau} \sup_{t \in \mathbb{R}} |\partial_t^m \varphi(t)|,$$
 (6.79)

from which we obtain the desired result.

Using this lemma we obtain the estimate

$$|\langle f_{n}, \varphi \rangle| \leq \frac{1}{2\pi} \int_{\xi-\mathrm{i}n}^{\xi+\mathrm{i}n} ||\tilde{f}(p)||_{Z} |\langle e^{pt}, \varphi(t) \rangle| |dp|$$

$$\leq C e^{\xi(\tau-\alpha)} \sup_{t \in \mathbb{R}} |\partial_{t}^{m} \varphi(t)| \frac{1}{2\pi} \int_{\xi-\mathrm{i}n}^{\xi+\mathrm{i}n} |p|^{-m} \mathrm{Pol}(|p|) |dp|, \qquad (6.80)$$

where we have used Theorem 6.4.1 with  $\operatorname{supp}(f) \subseteq [\alpha, \infty)$ . If q is the order of the polynomial  $\operatorname{Pol}(|p|)$ , then by taking m > q+2 in our estimate for  $|\langle f_n, \varphi \rangle|$  we see that the integral  $\int_{\xi-\mathrm{i}n}^{\xi+\mathrm{i}n} |p|^{-m} \operatorname{Pol}(|p|) |\mathrm{d}p|$  converges as  $n \to \infty$ , and so obtain

$$|\langle f, \varphi \rangle| = \lim_{n \to \infty} |\langle f_n, \varphi \rangle| \le C e^{\xi(\tau - \alpha)} \sup_{t \in \mathbb{D}} |\partial_t^m \varphi(t)|, \tag{6.81}$$

for some C > 0 showing that the limit f of the sequence  $f_n$  is a well-defined distribution of finite-order. We note that if  $\tau < \alpha$ , then by taking  $\xi > \xi_0$  sufficiently large we can make  $|\langle f, \varphi \rangle|$  as small as we like, and so can conclude that  $\operatorname{supp}(f) \subseteq [\alpha, \infty)$  as expected.

# 6.4.3 Convolution equations and the Green distribution

Let X and Y be Banach spaces, with norms  $\|\cdot\|_X$  and  $\|\cdot\|_Y$ , respectively. We recall that L(Y;X) denotes the Banach space of bounded linear operators from Y into X, and that the associated operator-norm is written  $\|\cdot\|_{L(Y;X)}$ . Let  $S \in \mathscr{D}'_{+}(L(Y;X))$  be a given operator-valued distribution having

$$supp(S) \subseteq [0, \infty). \tag{6.82}$$

We assume that there exists a  $\xi_0 \in \mathbb{R}$  such that  $e^{-\xi_0 t} S \in \mathscr{S}'_+(L(Y;X))$ , from which it follows that S has a Laplace transform  $p \mapsto \tilde{S}(p)$  for  $\text{Re}(p) > \xi_0$ . We write  $\pi(S)$  for the largest open subset of  $\mathbb{C}$  for which  $p \mapsto \tilde{S}(p)$  can be extended by analytic continuation.

Associated with S, we can consider the convolution equation

$$S * u = f, (6.83)$$

for  $u \in \mathcal{D}'_{+}(Y)$ , where  $f \in \mathcal{D}'_{+}(X)$  is a given force-term. Following Lions (1960) and Fattorini (1976, 1980), eq.(6.83) is said to be well-posed if:

1. For every  $f \in \mathscr{D}'_{+}(X)$  there exists a unique  $u \in \mathscr{D}'_{+}(Y)$  satisfying eq.(6.83) such that

$$supp(u) \subseteq supp(f) + [0, \infty). \tag{6.84}$$

2. The corresponding mapping  $f \mapsto u$  from  $\mathscr{D}'_{+}(X)$  into  $\mathscr{D}'_{+}(Y)$  is continuous in the following sense: Let  $\{f_i\}$  be a sequence in  $\mathscr{D}'_{+}(X)$  such that  $\operatorname{supp}(f_i) \in [\alpha, \infty)$  for fixed  $\alpha > -\infty$  and  $f_i \to 0$  in  $\mathscr{D}'_{+}(X)$ , then the sequence  $\{u_i\}$  in  $\mathscr{D}'_{+}(Y)$  with  $S * u_i = f_i$ , is such that  $u_i \to 0$ .

We require the following result:

**Theorem 6.4.5** The convolution equation in eq.(6.83) is well-posed if and only if there exists a distribution  $G \in \mathcal{D}'_{+}(L(X;Y))$  such that

$$supp(G) \subseteq [0, \infty), \tag{6.85}$$

and

$$G * S = \delta \otimes 1_Y, \quad S * G = \delta \otimes 1_X,$$
 (6.86)

where  $1_X$  and  $1_Y$  denote, respectively, the identity operators on X and on Y. We shall call

G the Green distribution for S.

The full proof of this result can be found in Fattorini (1983), and we only outline the sufficiency of the condition.

**Proof (Sufficiency of the condition)** Suppose that such a G exists. Then putting u = G \* f, we obtain

$$S * u = S * (G * f) = (S * G) * f = (\delta \otimes 1_X) * f = f,$$
(6.87)

showing that u is a solution of the convolution equation. On the other hand, if u is a solution of eq.(6.83), then

$$G * f = G * (S * u) = (G * S) * u = (\delta \otimes 1_Y) * u = u, \tag{6.88}$$

so that u = G \* f is the unique solution to the equation. That u satisfies the condition in eq.(6.84), and that u depends continuously on f in the indicated manner, follow from eq.(6.85) along with standard properties of the convolution of two distributions.

The existence of a Green distribution G for a given S depends on the behaviour of the Laplace transform  $\tilde{S}(p)$ . We denote by  $\varrho(S) \subseteq \pi(S)$  the subset of  $\mathbb{C}$  on which the inverse operator  $\tilde{S}(p)^{-1}$  exists in L(X;Y).

**Proposition 6.4.6** The subset  $\varrho(S) \subseteq \pi(S)$  is open, and in this set the mapping  $p \mapsto \tilde{S}(p)^{-1}$  is holomorphic.

The proof of this result follows directly from:

**Lemma 6.4.7** Let X,Y be Banach spaces, and  $p \mapsto f(p)$  be an L(Y;X)-valued function that is holomorphic in some neighborhood of the point  $p_0 \in \mathbb{C}$ . Suppose that  $f(p_0)^{-1}$  exists in L(X;Y). Then there exists a neighborhood of  $p_0$  for which  $f(p)^{-1}$  exists in L(X;Y) and for which the function  $p \mapsto f(p)^{-1} \in L(X;Y)$  is holomorphic.

**Proof** Let U be a neighborhood of  $p_0$  in which  $p \mapsto f(p)$  is holomorphic. For  $p \in U$ , consider

$$f(p) = f(p_0) + [f(p) - f(p_0)] = f(p_0) \{1 + f(p_0)^{-1} [f(p) - f(p_0)]\},$$
(6.89)

where we have used that fact that  $f(p_0)^{-1}$  exists in L(X,Y). If we can show that the operator

$$1 + f(p_0)^{-1} [f(p) - f(p_0)], (6.90)$$

is invertible and that its inverse is bounded in the topology of L(Y,Y), it will follow that  $f(p)^{-1}$  exists in L(X,Y). To do this we note that

$$||f(p_0)^{-1}[f(p) - f(p_0)]||_{L(Y,Y)} \le ||f(p_0)^{-1}||_{L(X,Y)} ||f(p) - f(p_0)||_{L(Y,X)}, \tag{6.91}$$

and that the holomorphy of f(p) implies that by taking p sufficiently close to  $p_0$  we can make the term  $||f(p) - f(p_0)||_{L(Y,X)}$  as small as we like. In particular, for any  $0 < \epsilon < 1$  we can find an open neighborhood  $U_0 \subseteq U$  of  $p_0$  such that for all  $p \in U_0$  we have

$$||f(p_0)^{-1}[f(p) - f(p_0)]||_{L(Y,Y)} < \epsilon.$$
(6.92)

It then follows that in  $U_0$  the desired inverse operator is given by the uniformly convergent Neumann series

$$\{1 + f(p_0)^{-1} [f(p) - f(p_0)]\}^{-1} = \sum_{n=0}^{\infty} (-1)^n \{f(p_0)^{-1} [f(p) - f(p_0)]\}^n,$$
 (6.93)

and that

$$\|\{1 + f(p_0)^{-1} [f(p) - f(p_0)]\}^{-1}\|_{L(Y,Y)} \le (1 - \epsilon)^{-1}.$$
(6.94)

That the mapping  $p \mapsto f(p)^{-1}$  is holomorphic in  $U_0$  follows easily from the fact that each term in the Neumann series depends holomorphically on p.

We can characterize the existence of a Green distribution G for S by the following theorem (Fattorini 1976, 1983):

**Theorem 6.4.8** Let  $S \in \mathscr{D}'_{+}(L(Y;X))$  with  $\operatorname{supp}(S) \subseteq [0,\infty)$ . Then there exists a Green distribution  $G \in \mathscr{D}'_{+}(L(X;Y))$  satisfying the conditions in Theorem 6.4.5 if and only if  $\varrho(S)$  contains a logarithmic region

$$\Lambda(\alpha, \beta, \xi_0) = \{ p \in \mathbb{C} \mid \text{Re}(p) \ge \max(\alpha \ln |p| + \beta, \xi_0) \}, \tag{6.95}$$

where  $\alpha, \beta \geq 0$ ,  $|\xi_0| < \infty$ , and if the estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le C(1+|p|)^m,\tag{6.96}$$

holds when  $p \in \Lambda(\alpha, \beta, \xi_0)$  for some C > 0, and some integer m.

If these conditions hold, then letting  $\Gamma$  denote the boundary of the region  $\Lambda(\alpha, \beta + 1, \xi_0 + 1)$ , the Green distribution is given by

$$G(t) = \frac{1}{2\pi i} \int_{\Gamma} \tilde{S}(p)^{-1} e^{pt} dp,$$
 (6.97)

where the convergence of this integral is understood in  $\mathcal{D}'_{+}(L(X;Y))$ .

From Theorem 6.4.1 and Proposition 6.4.3 we obtain the useful corollary:

**Corollary 6.4.9** Suppose  $\varrho(S)$  contains a right half-plane  $\{p \in \mathbb{C} \mid \operatorname{Re}(p) > \xi_0\}$  for some  $|\xi_0| < \infty$ , and that for such p we have

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le C(1+|p|)^m,\tag{6.98}$$

for some C > 0 and integer m. Then the Green distribution  $G \in \mathscr{D}'_{+}(L(X;Y))$  has a Laplace transform  $\tilde{G}(p)$  for  $Re(p) > \xi_0$  which is given by

$$\tilde{G}(p) = \tilde{S}(p)^{-1}.$$
 (6.99)

In this case, G can be obtained through the inverse Laplace transform

$$G(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{G}(p) e^{pt} dp, \qquad (6.100)$$

where  $\xi > \xi_0$  is arbitrary.

# 6.5 Applications to the elastodynamic equation

# 6.5.1 Formulation as a convolution equation

Let us again write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$  for notation simplicity. We have seen that the elastodynamic equation can be expressed in the form

$$\frac{\partial^2 u}{\partial t^2} + Au = f, (6.101)$$

where  $t \mapsto u(t)$  is a Y-valued function,  $A \in L(Y;X)$  is the elastodynamic operator, and  $t \mapsto f(t)$  is a X-valued force-term. In this formulation of the problem, the boundary conditions on u have been incorporated into the definition of the Hilbert space Y, while the initial conditions become

$$u(0) = \frac{\partial u}{\partial t}(0) = 0. \tag{6.102}$$

To derive existence and uniqueness theorems for the elastodynamic equation, we first express the above problem as a convolution equation of the type considered in the previous section. Defining an operator-valued distribution  $S \in \mathcal{D}'_{+}(L(Y;X))$  by

$$S = \frac{\partial^2 \delta}{\partial t^2} \otimes 1 + \delta \otimes A, \tag{6.103}$$

we see that for any  $u \in \mathcal{D}'_{+}(Y)$ 

$$S * u = \frac{\partial^2 u}{\partial t^2} + Au. \tag{6.104}$$

It follows that we can generalize the elastodynamic equation to finding a  $u \in \mathcal{D}'_{+}(Y)$  such that

$$S * u = f, \tag{6.105}$$

for a given  $f \in \mathscr{D}'_{+}(X)$ . In making this generalization we have to abandon the given initial conditions on u as, in general, the pointwise values of distributions are not meaningful. We will later see that if the given force-term f is sufficiently regular, then the solution u to this problem has well-defined pointwise-values, and that the initial conditions do indeed hold.

As the support of S defined in eq.(6.103) is compact, we see that its Laplace transform  $p \mapsto \tilde{S}(p)$  is an entire function (i.e.  $\pi(S) = \mathbb{C}$ ), and a simple calculation shows that

$$\tilde{S}(p) = p^2 1 + A.$$
 (6.106)

To show that a Green distribution G exists for this S, it follows from Theorem 6.4.8 that we must show that the inverse operator  $\tilde{S}(p)^{-1}$  exists in L(X;Y) in some logarithmic region  $\Lambda(\alpha,\beta,\xi_0)$  as defined in eq.(6.95), and that in this region  $\|\tilde{S}(p)\|^{-1}$  satisfies an estimate of the form given in eq.(6.96). In fact, we shall prove that:

**Proposition 6.5.1** For the elastodynamic operator A, the operator-valued function  $\tilde{S}(p) = p^2 1 + A$  is such that:

- 1. The inverse operator  $\tilde{S}(p)^{-1}$  exists in L(X;Y) for all  $p \in \mathbb{C}$  with Re(p) > 0.
- 2. For any  $\xi_0 > 0$ , when  $Re(p) > \xi_0$  we have the estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;y)} \le C(1+|p|),$$
 (6.107)

for some C > 0.

It follows that the Green distribution G for the elastodynamic equation exists, that it has a Laplace transform

$$\tilde{G}(p) = \tilde{S}(p)^{-1} = (p^2 1 + A)^{-1},$$
(6.108)

for all Re(p) > 0, and that it can be expressed through the inverse Laplace transform

$$G(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{G}(p) e^{pt} dp, \qquad (6.109)$$

where  $\xi > \xi_0$  is arbitrary. To prove Proposition 6.5.1 we must consider in further detail the properties of the elastodynamic operator.

# 6.5.2 The elastodynamic operator revisited

# Strong ellipticity of A

Expanding out the definition of A given in eq. (6.48), we find that

$$(Au)_{i}(x) = -\frac{1}{\rho(x)} \left\{ a_{jikl}(x) \frac{\partial^{2}}{\partial x_{k} \partial x_{j}} + \frac{\partial a_{jikl}}{\partial x_{j}}(x) \frac{\partial}{\partial x_{k}} \right\} u_{l}(x). \tag{6.110}$$

The *principal part* of A is defined to be the negative of those terms in the above expression involving the highest-order partial derivatives (i.e. those of second-order), and is readily seen to equal

$$\frac{1}{\rho(x)}a_{jikl}(x)\frac{\partial^2}{\partial x_k \partial x_j}. (6.111)$$

Making the replacement  $\frac{\partial}{\partial x_i} \to k_i$ , where  $k \in \mathbb{R}^n$  is an arbitrary non-zero vector, in the principal part of A gives

$$A_{il}(x,k) = \frac{1}{\rho(x)} a_{jikl}(x) k_j k_k \tag{6.112}$$

which is known as the *characteristic matrix* associated with A for the given k (e.g. Nirenberg 1955; Agmon *et al.* 1959, 1964; Browder 1961).

We say that A is strongly elliptic at a point x if there exists a complex number  $\gamma$ , and a positive constant c, such that

$$\operatorname{Re}\left(\gamma A_{il}(x,k)u_{i}\overline{u_{l}}\right) \geq c\|u\|_{\mathbb{C}^{n}}^{2},\tag{6.113}$$

for all  $k \in \mathbb{R}^n$  and all  $u \in \mathbb{C}^n$ . If A is strongly elliptic at each point  $x \in \Omega^{\text{cl}}$  in such a way that the numbers  $\gamma$  and c above can be chosen independently of x, then we say that A is strongly elliptic (e.g. Nirenberg 1955; Browder 1961). From our assumption that the

elastic tensor a is uniformly pointwise stable, it is readily seen that eq.(6.113) holds for any  $\gamma > 0$ , so that A is indeed strongly elliptic. In fact, for this condition to hold it is sufficient to assume that a satisfies the weaker condition of being strongly elliptic in the sense previously defined (e.g. Marsden & Hughes 1983; Section 6.1).

If  $A_1$  denotes any linear partial differential operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$  involving only partial derivatives of order less than two, it follows that  $A + A_1$  has the same principal part as A, and so is also strongly elliptic. More generally, this statement applies to the case in which  $A_1$  is an arbitrary bounded operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$ , such as an integral operator with sufficiently smooth kernel. In particular, we see that  $\lambda 1 - A$  for any  $\lambda \in \mathbb{C}$  is strongly elliptic.

## A priori estimates

A consequence of the strong ellipticity of A is the existence of a number of so-called a priori estimates (e.g. Nirenberg 1955; Agmon et al. 1959, 1964; Browder 1961; Wloka 1997). Of these estimates, the most important for our purposes is that if  $u \in D(A)$  and  $Au \in H^s(\Omega; \mathbb{C}^n)$  for  $s \geq 0$ , then  $u \in D(A) \cap H^{s+2}(\Omega; \mathbb{C}^n)$  and

$$||u||_{H^{s+2}(\Omega;\mathbb{C}^n)} \le K\left(||Au||_{H^s(\Omega;\mathbb{C}^n)} + ||u||_{H^s(\Omega;\mathbb{C}^n)}\right),\tag{6.114}$$

where K is some positive constant. In particular, for the case s=0, this implies that if  $u \in D(A)$  then

$$||u||_{H^{2}(\Omega;\mathbb{C}^{n})} \le K(||Au||_{L^{2}(\Omega,\varrho;\mathbb{C}^{n})} + ||u||_{L^{2}(\Omega,\varrho;\mathbb{C}^{n})}),$$
 (6.115)

for some positive constant K. Applying eq.(6.114) recursively, we obtain the further estimate

$$||u||_{H^{s+2}(\Omega;\mathbb{C}^n)} \le K(||Au||_{H^s(\Omega;\mathbb{C}^n)} + ||u||_{L^2(\Omega;\mathbb{C}^n)}),$$
 (6.116)

for some K > 0.

A number of important properties of A can be derived from these a priori estimates. Here we again write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$  for notation simplicity.

**Proposition 6.5.2** A is a closed unbounded operator on X.

**Proof** Let  $\{u_i\}$  be a sequence in Y such that  $u_i \to u$  and  $Au_i \to v$  in X. To show that A is

closed, we must demonstrate that  $u \in Y$ , and that Au = v. By assumption  $\{u_i\}$  and  $\{Au_i\}$  are Cauchy sequences in X, while eq.(6.115) implies that

$$||u_i - u_j||_Y \le K \left( ||Au_i - Au_j||_X + ||u_i - u_j||_X \right), \tag{6.117}$$

for any i, j, showing that  $\{u_i\}$  is also Cauchy in Y. It follows that  $u_i \to u$  in Y, and by the continuity of A from Y into X, that Au = v. As A is closed, and as Y is a proper subset of X, the closed graph theorem implies that A is an unbounded operator on X.

For the moment let  $A: D(A) \to X$  be an arbitrary linear operator. We recall that the kernel of A is defined to be the linear subspace

$$\ker(A) = \{ u \in D(A) \mid Au = 0 \}, \tag{6.118}$$

and that its dimension is called the *nullity* of A which is written nul(A). Similarly, the image of A is defined to be

$$im(A) = \{Au \in X \mid u \in D(A)\},$$
(6.119)

while we define the *cokernel* of A to be the quotient space

$$\operatorname{coker}(A) = X/\operatorname{im}(A), \tag{6.120}$$

whose dimension is called the *defect* of A and is denoted by def(A). If im(A) is closed and one of either nul(A) or def(A) is finite, we say that A is a *semi-Fredholm operator*, and define its index as

$$\operatorname{ind}(A) = \operatorname{nul}(A) - \operatorname{def}(A). \tag{6.121}$$

If im(A) is closed and both nul(A) and def(A) are finite, we say that A is a Fredholm operator (e.g. Wloka 1997; Edmunds & Evans 1987). We now return to consideration of the elastodynamic operator:

**Theorem 6.5.3** The kernel of A is finite-dimensional, and its image is closed in X.

**Remark** This result shows that A is a semi-Fredholm operator. We shall see shortly that A is in fact a Fredholm operator.

**Proof** To prove that ker(A) is finite-dimensional, we recall that a Hilbert space Z is finite-

dimensional if and only if its closed unit-ball  $\{x \in Z \mid ||x||_Z \le 1\}$  is compact. As A is closed, it is easy to see that  $\ker(A)$  is a closed subset of X, and so becomes a Hilbert space when given the induced topology. It follows that if we can show that the closed unit-ball  $\{u \in \ker(A) \mid ||u||_X \le 1\}$  is compact, then  $\ker(A)$  must be finite-dimensional.

For  $u \in \ker(A)$ , we see from eq.(6.115) that  $||u||_Y \leq K||u||_X$ , while as the inclusion  $Y \to X$  is continuous, we also have  $||u||_X \leq K'||u||_Y$  for some constant K' > 0. It follows that on  $\ker(A)$  the norms  $||\cdot||_X$  and  $||\cdot||_Y$  are equivalent. This implies that  $\{u \in \ker(A) \mid ||u||_X \leq 1\}$  is the image under this inclusion of a bounded set in Y. Recalling from Theorem 6.3.9 that this inclusion is compact, it follows that the closed unit-ball  $\{u \in \ker(A) \mid ||u||_X \leq 1\}$  is compact in X.

We have seen that  $\ker(A)$  is finite-dimensional, and therefore closed in Y. Recalling that in a Hilbert space each finite-dimensional subspace has a closed complement, we can write  $Y = \ker(A) \oplus Y_1$ , with  $Y_1$  closed. Let us define  $A_1 : Y_1 \to \operatorname{im}(A)$  to be the restriction of A to  $Y_1$ . By defintion,  $A_1$  is a continuous bijection. If we can show that its inverse  $A_1^{-1} : \operatorname{im}(A) \to Y_1$  is also continuous, then  $\operatorname{im}(A) - \operatorname{being}$  the pre-image of the closed set  $Y_1$  under a continuous mapping – must itself be closed.

For  $A_1^{-1}$  to be continuous, the inequality

$$||u||_Y \le C||A_1 u||_X,\tag{6.122}$$

must hold for all  $u \in Y_1$ . Suppose this is not the case. Then we can find a sequence  $\{u_n\}$  in  $Y_1$  such that  $||u_n||_Y = 1$ , and

$$1 = ||u_n||_Y > n||A_1 u_n||_X. (6.123)$$

We note, in particular, that for such a sequence  $||A_1u_n||_X \to 0$ , which implies that  $A_1u_n \to 0$  in X. As this sequence is bounded in  $Y_1$ , and as the inclusion  $Y \to X$  is compact, it follows that the image of this sequence in X is compact, and so possesses a convergent subsequence, which we again denote by  $\{u_n\}$ . Arguing as in the proof of Proposition 6.5.3, we see from eq.(6.115) that this subsequence is Cauchy in Y, and so converges to a limit  $u \in Y_1$ . As the norm  $||\cdot||_Y$  is continuous on Y, we must have  $||u||_Y = \lim_{n\to\infty} ||u_n||_Y = 1$ . On the other hand, as  $A_1: Y_1 \to \operatorname{im}(A)$  is continuous, we find that  $||A_1u||_X = \lim_{n\to\infty} ||A_1u_n||_X = 0$ , which implies u = 0 as  $A_1$  is a bijection. This contradiction shows that  $A_1^{-1}$  must be continuous,

and so concludes our proof.

#### The resolvent of A

We noted at the end of the previous subsection that the operator  $\lambda 1 - A$  is strongly elliptic for any  $\lambda \in \mathbb{C}$ . It follows that  $\lambda 1 - A$  also satisfies analogous a priori estimates to those for A. In fact, we obtain readily from eq.(6.114) that if  $u \in D(\lambda 1 - A)$  and if  $(\lambda 1 - A)u \in H^s(\Omega; \mathbb{C}^n)$ for  $s \geq 0$ , then  $u \in D(\lambda 1 - A) \cap H^{s+2}(\Omega; \mathbb{C}^n)$  and

$$||u||_{H^{s+2}(\Omega;\mathbb{C})} \le K\left(||(\lambda 1 - A)u||_{H^{s}(\Omega;\mathbb{C}^{n})} + (1 + |\lambda|)||u||_{H^{s}(\Omega;\mathbb{C}^{n})}\right),\tag{6.124}$$

where K is a positive constant that does not depend on  $\lambda$ . Specializing this result to the case s = 0, we obtain

$$||u||_{H^{2}(\Omega;\mathbb{C})} \le K\left(||(\lambda 1 - A)u||_{L^{2}(\Omega,\rho;\mathbb{C}^{n})} + (1 + |\lambda|)||u||_{L^{2}(\Omega,\rho;\mathbb{C}^{n})}\right),\tag{6.125}$$

for all  $u \in D(\lambda 1 - A)$ . Adapting the proofs of Propositions 6.5.2 and 6.5.3, we find from eq.(6.125) that:

**Theorem 6.5.4** For any  $\lambda \in \mathbb{C}$ , the linear operator  $\lambda 1 - A$  on  $L^2(\Omega, \rho; \mathbb{C}^n)$  with dense domain  $D(\lambda 1 - A) = H^2_{\partial}(\Omega; \mathbb{C}^n)$ , is closed, has finite-dimensional kernel, and closed image.

We recall that the resolvent operator of A is defined by

$$R(A;\lambda) = (\lambda 1 - A)^{-1},$$
 (6.126)

for those  $\lambda \in \mathbb{C}$  for which the inverse operator exists in  $L(L^2(\Omega, \rho; \mathbb{C}^n); L^2(\Omega, \rho; \mathbb{C}^n))$ . The set of  $\lambda \in \mathbb{C}$  for which  $R(A; \lambda)$  exists is called the *resolvent set* of A and is denoted by  $\varrho(A)$ , while its complement is known as the *spectrum* of A and is written  $\varsigma(A)$ .

**Proposition 6.5.5** For  $\lambda \in \varrho(A)$ , the resolvent operator  $R(A; \lambda)$  maps  $H^s(\Omega; \mathbb{C}^n)$  continuously into  $H^{s+2}_{\partial}(\Omega; \mathbb{C}^n) \equiv H^{s+2}(\Omega; \mathbb{C}^n) \cap H^1_0(\Omega; \mathbb{C}^n)$  for  $s \geq 0$ , and satisfies the estimates

$$||R(A;\lambda)||_{L(H^s;H^{s+2})} \le K[1+(1+|\lambda|)||R(A;\lambda)||_{L(H^s;H^s)}], \tag{6.127}$$

$$||R(A;\lambda)||_{L(H^{s+2}:H^{s+2})} \le K[1+(1+|\lambda|)||R(A;\lambda)||_{L(H^{s}:H^{s})}], \tag{6.128}$$

where we have written  $H^s$  for  $H^s(\Omega; \mathbb{C}^n)$  for notational clarity, and where K > 0 is inde-

pendent of  $\lambda$ . In particular, for even s, we obtain

$$||R(A;\lambda)||_{L(H^s;H^{s+2})} \le K \left[1 + (1+|\lambda|)^{s/2+1} ||R(A;\lambda)||_{L(L^2;L^2)}\right], \tag{6.129}$$

$$||R(A;\lambda)||_{L(H^{s+2};H^{s+2})} \le K \left[1 + (1+|\lambda|)^{s/2+1} ||R(A;\lambda)||_{L(L^2;L^2)}\right], \tag{6.130}$$

where we have written  $L^2$  for  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

Moreover, for  $s \geq 0$  and  $\lambda \in \varrho(A)$ , the resolvent operator  $R(A; \lambda)$  maps  $H^s(\Omega; \mathbb{C}^n)$  compactly into itself.

**Proof** That for  $\lambda \in \varrho(A)$ , the resolvent operator  $R(A; \lambda)$  maps  $H^s(\Omega; \mathbb{C}^n)$  into  $H^{s+2}_{\partial}(\Omega; \mathbb{C}^n)$  for  $s \geq 0$  follows directly from the a priori estimate for  $\lambda 1 - A$  in eq.(6.124). For  $u \in H^s(\Omega; \mathbb{C}^n)$  we then have  $R(A; \lambda)u \in H^{s+2}_{\partial}(\Omega; \mathbb{C}^n)$ , and from eq.(6.124) find that

$$||R(A;\lambda)u||_{H^{s+2}} \leq K[||u||_{H^{s}} + (1+|\lambda|)||R(A;\lambda)u||_{H^{s}}]$$

$$\leq K[1+(1+|\lambda|)||R(A;\lambda)||_{L(H^{s},H^{s})}] ||u||_{H^{s}}$$

$$\leq K[1+(1+|\lambda|)||R(A;\lambda)||_{L(H^{s},H^{s})}] ||u||_{H^{s+2}}, \tag{6.131}$$

where in obtaining the last inequality we have used  $||u||_{H^s} \leq ||u||_{H^{s+2}}$ . From the second of the above inequalities we obtain

$$||R(A;\lambda)||_{L(H^s:H^{s+2})} \le K \left[1 + (1+|\lambda|)||R(A;\lambda)||_{L(H^s,H^s)}\right],\tag{6.132}$$

while the third gives

$$||R(A;\lambda)||_{L(H^{s+2}:H^{s+2})} \le K \left[1 + (1+|\lambda|)||R(A;\lambda)||_{L(H^{s},H^{s})}\right]. \tag{6.133}$$

Repeated use of these two inequalities leads readily to eq.(6.129) and eq.(6.130). The final result of the proposition follows from the above results and Theorem 6.3.9.

# Self-adjointness of A and the spectral theorem

Let T be an unbounded operator on a Hilbert space X with dense domain D(T). We recall that the adjoint of T is the linear operator  $T^*: D(T^*) \to X$  defined as follows (e.g. Browder 1961; Yoisda 1980): The domain of  $T^*$  comprises those  $u^* \in X$  for which  $u \mapsto (Tu, u^*)_X$  is a bounded linear functional on the dense subset  $D(T) \subseteq X$ . For  $u^* \in D(T)$  it may be shown that there exists a unique  $v \in X$  such that  $(Tu, u^*)_X = (u, v)_X$ , and we set  $T^*u^* = v$ .

It follows that for any  $u \in D(T)$  and  $u^* \in D(T^*)$  we have

$$(Tu, u^*)_X = (u, T^*u^*)_X.$$
 (6.134)

If T is a closed operator it may be shown that  $D(T^*)$  is dense in X, and that  $(T^*)^* = T$ . The following result will be required below (e.g. Dautray & Lions 1984, Chapter VI, Section 2.1):

**Proposition 6.5.6** Let  $T: D(T) \to X$  be a closed operator on a Hilbert space X with dense domain, and let  $T^*: D(T^*) \to X$  be its adjoint operator. Then we have the orthogonality relations

$$\ker(T^*) = \operatorname{im}(T)^{\perp}, \quad \ker(T) = \operatorname{im}(T^*)^{\perp}, \tag{6.135}$$

where  $\perp$  denotes the operation of taking orthogonal complements in X. If, moreover,  $\operatorname{im}(T)$  is closed in X, we have the reciprocal orthogonality relations

$$\operatorname{im}(T) = \ker(T^*)^{\perp}, \quad \operatorname{im}(T^*) = \ker(T)^{\perp}.$$
 (6.136)

If  $T: D(T) \to X$  and  $S: D(S) \to X$  are two operators on X, we recall that S is said to be an extension of T, written  $T \subseteq S$ , if  $D(T) \subseteq D(S)$  and if for  $u \in D(T)$  we have Tu = Su. An operator  $T: D(T) \to X$  is said to be symmetric if its adjoint  $T^*: D(T^*) \to X$  is an extension of T. If T is symmetric, and if  $D(T) = D(T^*)$ , then we say that T is self-adjoint.

An important result for self-adjoint operators is the *spectral theorem* which may be formulated in the following manner (e.g. Dautray & Lions 1984, Chapter VIII, Section 3; Davies 1995, Chapter 2):

**Theorem 6.5.7** Let  $T: D(T) \to X$  be a self-adjoint operator on a Hilbert space X. Then there exists an associated operator-valued measure P on  $\mathbb{R}$  such that:

- 1. The support supp $(P) \subseteq \mathbb{R}$  of the measure P, when regarded as a subset of  $\mathbb{C}$ , is equal to the spectrum of T.
- 2. For any measurable  $E \subseteq \mathbb{R}$ , the operator P(E) is an orthogonal projection operator on X which commutes with T, i.e.

$$TP(E) = P(E)T. (6.137)$$

3. If  $E_1$  and  $E_2$  are two measurable subsets of  $\mathbb{R}$ , then

$$P(E_1)P(E_2) = P(E_2)P(E_1) = P(E_1 \cap E_2). \tag{6.138}$$

4. The measure P is a resolution of the identity in the sense that

$$P(\mathbb{R}) = 1. \tag{6.139}$$

5. The domain of T is equal to

$$D(T) = \left\{ u \in X \mid \left\| \int_{\mathbb{R}} \zeta P(d\zeta) u \right\|_{X} < \infty \right\}, \tag{6.140}$$

and for  $u \in D(T)$  we have

$$Tu = \int_{\mathbb{D}} \zeta P(\mathrm{d}\zeta) u, \tag{6.141}$$

where this integral is strongly convergent in X. We can formally write this expression for T as

$$T = \int_{\mathbb{R}} \zeta P(\mathrm{d}\zeta),\tag{6.142}$$

which is known as the spectral decomposition of T.

Let  $f: \mathbb{C} \to \mathbb{C}$  be a function that is holomorphic in a neighborhood of  $\varsigma(T)$ , then we can define an operator f(T) by

$$f(T)u = \int_{\mathbb{D}} f(\zeta)P(\mathrm{d}\zeta)u, \tag{6.143}$$

which has domain

$$D(f(T)) = \left\{ u \in X \mid \left\| \int_{\mathbb{R}} f(\zeta) P(d\zeta) u \right\|_{Y} < \infty \right\}.$$
 (6.144)

Again, we can write this operator formally as

$$f(T) = \int_{\mathbb{R}} f(\zeta) P(d\zeta). \tag{6.145}$$

We note that if f is bounded on  $\varsigma(T)$ , then we have

$$\left\| \int_{\mathbb{R}} f(\zeta) P(\mathrm{d}\zeta) u \right\|_{X} \le \sup_{\zeta \in \varsigma(T)} |f(\zeta)| \left\| \int_{\mathbb{R}} P(\mathrm{d}\zeta) u \right\|_{X}$$

$$\le \sup_{\zeta \in \varsigma(T)} |f(\zeta)| \|u\|_{X}, \tag{6.146}$$

showing that f(T) is a bounded operator on X, and that the integral in eq.(6.145) is convergent in the norm-topology of L(X;X). An important result is that the mapping  $f \mapsto f(T)$  defines a functional calculus in the following sense (e.g. Dautray & Lions 1984; Chapter VII, Section 4; Davies 1995, Theorem 2.3.1):

**Theorem 6.5.8** Let  $T: D(T) \to X$  be a self-adjoint operator on a Hilbert space X. Let  $f,g: \mathbb{C} \to \mathbb{C}$  be two functions that are holomorphic in a neighborhood of  $\varsigma(T)$ , and write fg for the function  $(fg)(\zeta) = f(\zeta)g(\zeta)$ , and similarly for gf. If the operators f(T), g(T), (fg)(T), (gf)(T) are defined as above, then

$$(fg)(T) = (gf)(T) = f(T)g(T) = g(T)f(T).$$
 (6.147)

In particular, if  $f: \mathbb{C} \to \mathbb{C}$  is such that 1/f is also holomorphic in some neighborhood of  $\varsigma(T)$ , then the inverse operator  $f(T)^{-1}$  exists and is given by

$$f(T)^{-1} = (1/f)(T).$$
 (6.148)

A direct corollary of this result is:

**Corollary 6.5.9** Let  $T: D(T) \to X$  be a self-adjoint operator on a Hilbert space X. Then for  $\lambda \notin \varsigma(T)$ , the resolvent operator  $R(T; \lambda) = (\lambda 1 - T)^{-1}$  is given by

$$R(T;\lambda) = \int_{\mathbb{R}} (\lambda - \zeta)^{-1} P(d\zeta), \tag{6.149}$$

and satisfies the norm-estimate

$$||R(T;\lambda)||_{L(X;X)} \le \frac{1}{\operatorname{dist}(\lambda,\varsigma(T))},\tag{6.150}$$

where for any closed  $U \subseteq \mathbb{C}$  we write  $\operatorname{dist}(\lambda, U)$  for the minimum euclidean distance from  $\lambda$  to U.

For a symmetric operator T, it is clear that the sesquilinear-form  $u\mapsto (Tu,u)_X$  defined for  $u\in \mathrm{D}(T)$  is real-valued. We say that such an operator is bounded from below if there exists a  $c>-\infty$  such that

$$(Tu, u)_{x} \ge c||u||^{2},$$
 (6.151)

for all  $u \in D(T)$ . In particular, we say that such a T is non-negative if this c can be taken equal to 0, and that it is positive-definite if

$$(Tu, u)_{x} > 0,$$
 (6.152)

for all non-zero  $u \in D(T)$ . It may be shown that if T is self-adjoint, and if T is bounded from below with for some  $c > -\infty$ , then  $\varsigma(T) \subseteq [c, \infty)$ . We may similarly define symmetric operators that are bounded from above, are non-positive, and are negative-definite.

An important subclass of self-adjoint operators are those that are bounded from below and have compact resolvents. For such operators it may be shown that the spectrum comprises a countable set of real eigenvalues  $\{\zeta_n\}_{n=1}^{\infty}$  which is bounded from below and has a single accumulation point at infinity (e.g. Davies 1995, Corollary 4.2.3). We may assume with out loss of generality that the eigenvalues  $\zeta_n$  have been ordered so that  $\zeta_{n+1} > \zeta_n$  for all n. In this case the associated projection-valued measure P is given by

$$P = \sum_{n=1}^{\infty} \delta_{\zeta_n} P_n, \tag{6.153}$$

where  $\delta_{\zeta_n}$  denotes the Dirac measure at  $\zeta_n$ , and where  $P_n$  is the orthogonal projection operator onto the finite-dimensional eigenspace of T associated with  $\zeta_n$ . The orthogonal projection operators  $P_n$  may be shown to satisfy

$$TP_n = P_n T = \zeta_n P_n, \tag{6.154}$$

are mutually orthogonal in the sense that

$$P_n P_m = P_m P_n = \delta_{nm} P_n, \tag{6.155}$$

and form a resolution of the identity

$$\sum_{n=1}^{\infty} P_n = 1. \tag{6.156}$$

As above, for a function  $f: \mathbb{C} \to \mathbb{C}$  holomorphic in a neighborhood of  $\varsigma(T)$  we can define the operator f(T) in terms of the projection valued measure P by

$$f(T) = \sum_{n=1}^{\infty} f(\zeta_n) P_n, \tag{6.157}$$

with this mapping  $f \mapsto f(T)$  forming a functional calculus. In particular, for  $\lambda \notin \varsigma(T)$  we can write the resolvent operator as

$$R(T;\lambda) = \sum_{n=1}^{\infty} (\lambda - \zeta_n)^{-1} P_n.$$
 (6.158)

This expression shows that for such a T, the resolvent operator is a meromorphic function of  $\lambda \in \mathbb{C}$  having a countable number of simple poles at each of the eigenvalues of T, and such that the residue of  $R(T;\lambda)$  at the eigenvalue  $\lambda_n$  is equal to the orthogonal projection operator onto the finite-dimensional eigenspace of  $\lambda_n$ .

**Theorem 6.5.10** The elastodynamic operator A is self-adjoint in  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

**Proof** We noted in subsection 6.3.2 that the elastodynamic operator  $A: D(A) \to L^2(\Omega, \rho; \mathbb{C}^n)$ 

was formally self-adjoint in the sense that

$$(Au, v)_{L^2(\Omega, \rho; \mathbb{C}^n)} = (u, Av)_{L^2(\Omega, \rho; \mathbb{C}^n)},$$

$$(6.159)$$

for all  $u, v \in \mathcal{D}(\Omega; \mathbb{C}^n)$ , where we recall that  $\mathcal{D}(\Omega; \mathbb{C}^n)$  denotes the space of smooth  $\mathbb{C}^n$ -valued functions having compact support in  $\Omega$ . In fact, this identity motivated our introduction of the density-weighted space  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

More generally, let A denote an arbitrary strongly-elliptic partial differential operator and A' its formal adjoint defined through

$$(Au, v)_{L^{2}(\Omega, o; \mathbb{C}^{n})} = (u, A'v)_{L^{2}(\Omega, o; \mathbb{C}^{n})}, \tag{6.160}$$

for all  $u, v \in \mathcal{D}(\Omega; \mathbb{C}^n)$ . Write  $A_2$  for the  $L^2(\Omega, \rho; \mathbb{C}^n)$  realization of A subject to homogeneous Dirichlet boundary conditions, and similarly write  $(A')_2$  for the  $L^2(\Omega, \rho; \mathbb{C}^n)$  realization of A' again subject to homogeneous Dirichlet boundary conditions. Theorem 5 of Browder (1961) shows that  $A_2^* = (A')_2$  (note that Browder's theorem applies to a single strongly elliptic differential operator, but the modifications to the proof required for its application to strongly elliptic systems are straightforward). Applying this result to the elastodynamic operator, we see that it is indeed self-adjoint.

Corollary 6.5.11 The elastodynamic operator A is a Fredholm operator with ind(A) = 0.

**Proof** We have already seen that A is semi-Fredholm with  $\operatorname{nul}(A) < \infty$ , so we need only show that  $\operatorname{def}(A) = \operatorname{nul}(A)$ . By definition,  $\operatorname{coker}(A)$  is isomorphic to  $\operatorname{im}(A)^{\perp}$ . From eq.(6.135) and the self-adjointness of A we obtain  $\operatorname{im}(A)^{\perp} = \ker(A^*) = \ker(A)$ , which implies  $\operatorname{def}(A) = \operatorname{nul}(A)$  as desired.

**Proposition 6.5.12** The elastodynamic operator A is positive-definite.

**Proof** For any  $u \in \mathcal{D}(\Omega^{cl}; \mathbb{C}^n)$  satisfying  $u|_{\partial\Omega} = 0$  we find using integration by parts

$$(Au, u)_{L^{2}(\Omega, \rho; \mathbb{C}^{n})} = \int_{\Omega} a_{ijkl}(x) e_{ij}(x) \overline{e_{kl}(x)} dx$$

$$\geq K \int_{\Omega} e_{ij}(x) \overline{e_{ij}(x)} dx, \qquad (6.161)$$

where we have written  $e_{ij}$  for the components of the strain tensor associated with u, and where we have made use of the uniform pointwise stability of the elastic tensor a in obtaining the final inequality. The integrals on either side of this inequality are well-defined for  $u \in D(A)$ , and as  $\mathscr{D}(\Omega^{cl}; \mathbb{C}^n) \cap D(A)$  is dense in D(A), it follows that this inequality also holds for  $u \in D(A)$ . From Korn's first inequality (e.g. Marsden & Hughes 1983, Chapter 6, Section 1.12) we have

$$\int_{\Omega} e_{ij}(x) \overline{e_{ij}(x)} \, \mathrm{d}x \ge \|u\|_{H^1(\Omega;\mathbb{C}^n)}^2 \ge C \|u\|_{L^2(\Omega,\rho;\mathbb{C}^n)},\tag{6.162}$$

for all  $u \in H_0^1(\Omega; \mathbb{C}^n)$  with some C > 0, which implies

$$(Au, u)_{L^{2}(\Omega, \rho; \mathbb{C}^{n})} \ge C \|u\|_{L^{2}(\Omega, \rho; \mathbb{C}^{n})}^{2},$$
 (6.163)

for all  $u \in D(A)$  showing that A is indeed positive-definite.

From the spectral theorem along with Proposition 6.5.5 we can conclude that:

**Theorem 6.5.13** The spectrum  $\varsigma(A)$  of the elastodynamic operator comprises a countable set of eigenvalues  $\{\zeta_n\}_{n=1}^{\infty}$  contained in  $(0,\infty)$  and accumulating to  $\infty$ . Corresponding to each eigenvalue  $\zeta_n$ , there is a finite-dimensional eigenspace with orthogonal projection operator  $P_n$ . For  $\lambda \notin \varsigma(A)$  the resolvent operator is a meromorphic function of  $\lambda$  given by

$$R(A;\lambda) = \sum_{n=1}^{\infty} (\lambda - \zeta_n)^{-1} P_n, \qquad (6.164)$$

and we have the norm estimate

$$||R(A;\lambda)||_{L(X;X)} \le \frac{1}{\operatorname{dist}(\lambda,\varsigma(A))},\tag{6.165}$$

where we have again set  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  for notational clarity.

### Proof of Proposition 6.5.1

We have now assembled all the results required to prove Proposition 6.5.1, and so conclude that a Green distribution for the convolution-form of the elastodynamic equation does exist.

# **Proof** Noting that

$$\tilde{S}(p)^{-1} = (p^2 1 + A)^{-1} = R(-A; p^2), \tag{6.166}$$

we can conclude from Theorem 6.5.13 that  $\tilde{S}(p)^{-1}$  is defined in L(X;X) for all  $p \in \mathbb{C}$  such that  $p^2 \notin \varsigma(-A) \subseteq (-\infty,0)$ , and satisfies

$$\|\tilde{S}(p)^{-1}\|_{L(X;X)} \le \frac{1}{\operatorname{dist}(p^2,\varsigma(-A))}.$$
 (6.167)

In particular,  $\tilde{S}(p)^{-1}$  is defined in L(X;X) for Re(p) > 0, and a simple geometric argument (e.g. Dautray & Lions 1984, Chapter XVI, Proposition 1) shows that for such p we have

$$\|\tilde{S}(p)^{-1}\|_{L(X;X)} \le \frac{1}{\operatorname{Re}(p)|p|}.$$
 (6.168)

From Proposition 6.5.5 we see that for Re(p) > 0, the operator  $\tilde{S}(p)^{-1}$  is in fact in L(X;Y), and that it satisfies the norm estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le K \left[ 1 + \frac{1 + |p|^2}{\operatorname{Re}(p)|p|} \right]. \tag{6.169}$$

Letting  $\xi_0 > 0$  be arbitrary, we see readily that if  $\text{Re}(p) > \xi_0$ , then the above inequality reduces to

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le C(1+|p|),\tag{6.170}$$

for some positive constant C.

### 6.5.3 Regularity of the solution

We have now shown that a unique solution  $u \in \mathcal{D}'_{+}(H^{2}_{\partial}(\Omega; \mathbb{C}^{n}))$  of the convolution-form

$$S * u = f, \tag{6.171}$$

of the elastodynamic equation exists for each force term  $f \in \mathcal{D}'_{+}(L^{2}(\Omega, \rho; \mathbb{C}^{n}))$ , and that this solution is given by

$$u = G * f, \tag{6.172}$$

where G is the Green distribution for eq.(6.171). For a general force term, this solution will be a  $H^2_{\partial}(\Omega; \mathbb{C}^n)$ -valued distribution, and so will satisfy neither the elastodynamic equation, the homogeneous Dirichlet boundary conditions, nor the given initial conditions in a classical sense. In this subsection, we shall investigate the conditions on the force term required for the solution u to have various regularity properties. In particular, we will show that if f is sufficiently regular, then the solution given in eq.(6.172) is in fact a

classical solution of the elastodynamic equations satisfying the given initial and boundary conditions.

In what follows it will be useful to write  $L^2$  for  $L^2(\Omega, \rho; \mathbb{C}^n)$ ,  $H^s$  for  $H^s(\Omega; \mathbb{C}^n)$ , and  $H^s_{\partial}$  for  $H^s_{\partial}(\Omega; \mathbb{C}^n) \equiv H^s(\Omega; \mathbb{C}^n) \cap H^1_0(\Omega; \mathbb{C}^n)$  when  $s \geq 1$ , and to identify  $H^0$  with  $L^2$ . Supposing that the force term  $f \in \mathscr{D}'_+(L^2)$  has a Laplace transform  $p \mapsto \tilde{f}(p)$  defined for  $\text{Re}(p) > \xi_0$  for some  $\xi_0 > 0$ , we can use the convolution theorem for Laplace-transforms to conclude that the solution  $u \in \mathscr{D}'_+(H^2_{\partial})$  given in eq.(6.172) also has a Laplace transform  $p \mapsto \tilde{u}(p)$  for  $\text{Re}(p) > \xi_0$ , and that

$$\tilde{u}(p) = \tilde{G}(p)\tilde{f}(p). \tag{6.173}$$

Let us suppose that the given force term is in fact an  $H^s$ -valued distribution for some even  $s \geq 0$  (the case of odd s can be handled similarly), then from Proposition 6.5.5 we can conclude that u is a  $H^{s+2}_{\partial}$ -valued distribution. We can estimate the  $H^{s+2}$ -norm of the solution in the Laplace transform domain by

$$\|\tilde{u}(p)\|_{H^{s+2}} = \|\tilde{G}(p)\tilde{f}(p)\|_{H^{s+2}}$$

$$\leq \|\tilde{G}(p)\|_{L(H^s:H^{s+2})}\|f\|_{H^s}. \tag{6.174}$$

From eq.(6.129) and eq.(6.168) we see that when  $Re(p) > \xi_0$  we have

$$\|\tilde{G}(p)\|_{L(H^s;H^{s+2})} \leq K \left[ 1 + \frac{(1+|p|^2)^{s/2+1}}{\operatorname{Re}(p)|p|} \right]$$

$$\leq C|p|^{s+1}, \tag{6.175}$$

for some C > 0. From this we obtain the estimate

$$\|\tilde{u}(p)\|_{H^{s+2}} \le C|p|^{s+1}\|\tilde{f}\|_{H^s},\tag{6.176}$$

which holds for all  $Re(p) > \xi_0$ . From Lemma 6.4.2, we see that if for  $Re(p) > \xi_0$  we have

$$\|\tilde{f}(p)\|_{H^s} \le C|p|^{-(k+2)},$$

$$(6.177)$$

then  $t \mapsto f(t) \in H^s$  is a continuous function having k continuous time-derivatives with  $\operatorname{supp}(f) \subseteq [0, \infty)$ , and

$$\|\tilde{u}(p)\|_{H^{s+2}} \le C|p|^{s-(k+1)},\tag{6.178}$$

for some C > 0. If k is such that

$$k \ge s + 1 + l,\tag{6.179}$$

for some  $l \geq 0$ , then we would have

$$\|\tilde{u}(p)\|_{H^{s+2}} \le C|p|^{-(l+2)},$$
(6.180)

and could conclude from Lemma 6.4.2 that  $t \mapsto u \in H^{s+2}_{\partial}$  is a continuous function having l continuous time-derivatives. We note that if the solution u to eq.(6.171) is continuous as a function of time then it must satisfy the initial condition u(0) = 0 as we know that  $\sup u(u) \subseteq [0, \infty)$ . Similarly, if u has a continuous first time-derivative, then we also obtain  $\partial u/\partial t(0) = 0$ . We summarize these result as:

**Theorem 6.5.14** Let the force term in eq.(6.171) be an  $H^s$ -valued distribution for some even  $s \ge 0$  with  $\operatorname{supp}(f) \subseteq [0, \infty)$ , and suppose that f has a Laplace transform  $\tilde{f}(p)$  defined for  $\operatorname{Re}(p) > \xi_0 > 0$  which satisfies

$$\|\tilde{f}(p)\|_{H^s} \le C|p|^{-(k+2)},\tag{6.181}$$

for some C > 0 and integer  $k \ge 0$ . Then if

$$k - s - 1 \ge 0, (6.182)$$

the solution  $u \in \mathcal{D}'_+(H^{s+2}_{\partial})$  to eq.(6.171) is a continuous function having k+1-s continuous derivatives. In particular, if

$$k - s - 1 \ge 1,\tag{6.183}$$

then the solution u of eq. (6.171) satisfies the initial conditions

$$u(0) = \frac{\partial u}{\partial t}(0) = 0, \tag{6.184}$$

while if

$$k - s - 1 \ge 2, (6.185)$$

the time-derivatives in the elastodynamic equation can be understood in the classical sense.

From Theorem 6.3.8 we obtain the corollary:

Corollary 6.5.15 Let the force term f in eq.(6.171) be as in Theorem 6.5.14. Then if

$$s > \frac{n}{2} + l,\tag{6.186}$$

for some integer  $l \geq 0$ , and if

$$k - s - 1 \ge 0, (6.187)$$

the solution u of eq.(6.171) as a function of x is continuous with l continuous spatial derivatives, and as a function of time is continuous with k+1-s continuous time-derivatives. In particular, if

$$s > \frac{n}{2} + 2, (6.188)$$

and

$$k - s - 1 \ge 2, (6.189)$$

then u is a classical solution of the elastodynamic equations satisfying the homogeneous Dirichlet boundary conditions and the given initial conditions.

A further regularity result of interest is a sufficient condition on the force term f for the solution u of eq.(6.171) to be a square-integrable function of time. We shall now prove:

**Theorem 6.5.16** Let  $L^2(H^s)$  denote the Hilbert space of measurable  $H^s$ -valued functions defined on  $\mathbb{R}$  that are square-integrable with respect to the inner product

$$(u,v)_{L^2(H^s)} = \int_{-\infty}^{\infty} (u(t), v(t))_{H^s} dt.$$
(6.190)

If for some even integer  $s \ge 0$  the force term f in eq.(6.171) is such that

$$e^{-\xi_0 t} \frac{\partial^n f}{\partial t^n} \in L^2(H^s),$$
 (6.191)

for  $\xi_0 > 0$ , and all  $0 \le n \le s + 1$ , then

$$e^{-\xi_0 t} u \in L^2(H_{\partial}^{s+2}),$$
 (6.192)

$$e^{-\xi_0 t} \frac{\partial u}{\partial t} \in L^2(H^{s+1}),$$
 (6.193)

$$e^{-\xi_0 t} \frac{\partial^2 u}{\partial t^2} \in L^2(H^s). \tag{6.194}$$

**Proof** We recall that on  $L^2(H^s)$  the distributional Fourier transform acts as a homeomorphism. It follows from the definition of the Laplace transform of f that the functions

$$\eta \mapsto \mathcal{L}(\partial^n f/\partial t^n)(\xi + i\eta),$$
 (6.195)

defined for  $\eta \in \mathbb{R}$ , with  $\xi \geq \xi_0$  and  $n \leq s+1$ , are elements of  $L^2(H^s)$ . Using the relation  $\mathcal{L}(\partial f/\partial t)(p) = p\mathcal{L}(f)(p)$ , we see in particular that

$$\eta \mapsto (\xi + i\eta)^{s+1} \tilde{f}(\xi + i\eta),$$
(6.196)

is in  $L^2(H^s)$  for  $\xi \geq \xi_0$ . From eq.(6.176) we obtain

$$\|\tilde{u}(\xi + i\eta)\|_{H^{s+2}} \leq C|\xi + i\eta|^{s+1} \|\tilde{f}(\xi + i\eta)\|_{H^{s}}$$

$$= C\|(\xi + i\eta)^{s+1} \tilde{f}(\xi + i\eta)\|_{H^{s}}, \tag{6.197}$$

which implies that

$$\eta \mapsto \tilde{u}(\xi + i\eta),$$
(6.198)

is in  $L^2(H^{s+2}_{\partial})$  for  $\xi \geq \xi_0$ , and it follows that  $e^{-\xi_0 t}u \in L^2(H^{s+2}_{\partial})$  as desired. From the elastodynamic equation we have

$$e^{-\xi_0 t} \frac{\partial^2 u}{\partial t^2} = e^{-\xi_0 t} f - A \left( e^{-\xi_0 t} u \right),$$
 (6.199)

and as the two terms on the right hand side are in  $L^2(H^s)$ , we can conclude that  $e^{-\xi_0 t} \partial^2 u / \partial t^2 \in L^2(H^s)$ . To complete the proof we must show that  $e^{-\xi_0} \partial u / \partial t \in L^2(H^{s+1})$ . However, this result follows from  $e^{-\xi_0 t} u \in L^2(H^{s+2})$  and  $e^{-\xi_0 t} \partial^2 u / \partial t^2 \in L^2(H^s)$  through a theorem of Lions & Magenes (1972, Vol. 1, Section 2.1) on intermediate derivatives.

Corollary 6.5.17 Let the conditions given in Theorem 6.5.16 on the force term in eq.(6.171) hold. Then  $t \mapsto u(t) \in H^{s+2}_{\partial}$  and  $t \mapsto \partial u/\partial t(t) \in H^{s+1}_{\partial}$  are continuous functions, and the initial conditions

$$u(0) = \frac{\partial u}{\partial t}(0) = 0, \tag{6.200}$$

are satisfied.

The proof of this corollary follows directly from:

**Lemma 6.5.18** Let Z be a Banach space and  $f \in \mathcal{D}'_{+}(Z)$  be such that  $\partial_t f = g$  for some  $g \in L^2(Z)$ . Then  $t \mapsto f(t)$  is a continuous function given by

$$f(t) = f(0) + \int_0^t g(t') dt', \qquad (6.201)$$

where  $f(0) \in Z$ .

**Remark** We note that this result is, in fact, a special case of the Sobolev embedding theorem.

**Proof** Let us define a function

$$h(t) = \int_0^t g(t') \, \mathrm{d}t', \tag{6.202}$$

which is well-defined as  $g \in L^2(Z)$  is locally integrable. For h > 0, we have

$$||h(t+h) - h(t)||_{Z} \le \int_{t}^{t+h} ||g(t')||_{Z} dt' \le h^{1/2} ||g||_{L^{2}}, \tag{6.203}$$

where we have employed the Cauchy-Schwarz inequality, and a similar result can be given for h < 0. It follows that  $t \mapsto h(t)$  is continuous.

We now show that the distributional derivative of h is equal to g. Having done so, our desired result follows from the fact that two distributions having the same derivative differ by a constant. Let  $\varphi \in \mathscr{D}$  be a test-function with compact support. By definition, the distributional derivative  $\partial_t h$  of h is such that

$$\langle \partial_t h, \varphi \rangle = -\langle h, \partial_t \varphi \rangle, \tag{6.204}$$

where, as h is continuous, we have

$$\langle h, \partial_t \varphi \rangle = \int_{-\infty}^{\infty} h(t) \partial_t \varphi(t) \, dt.$$
 (6.205)

The definition of h(t) gives

$$\langle h, \partial_t \varphi \rangle = \int_{-\infty}^{\infty} \int_0^t g(t') \, \mathrm{d}t' \partial_t \varphi(t) \, \mathrm{d}t, \tag{6.206}$$

and interchanging the order of integration we obtain

$$\langle h, \partial_t \varphi \rangle = -\int_{-\infty}^{\infty} g(t)\varphi(t) dt = -\langle g, \varphi \rangle.$$
 (6.207)

This gives

$$\langle \partial_t h, \varphi \rangle = \langle g, \varphi \rangle, \tag{6.208}$$

showing  $\partial_t h = g$  as desired.

# 6.5.4 Eigenfunction expansions

We have seen that the Green distribution for the elastodynamic equation is given by the inverse Laplace transform

$$G(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{G}(p) e^{pt} dp, \qquad (6.209)$$

where  $\tilde{G}(p) = (p^21 + A)^{-1}$ , and  $\xi > 0$  is arbitrary. Moreover, by the spectral theorem, we know that  $\tilde{G}(p)$  can be written

$$\tilde{G}(p) = \sum_{n=1}^{\infty} (p^2 + \zeta_n)^{-1} P_n, \tag{6.210}$$

where  $\{\zeta_n\}_{n=1}^{\infty}$  are the eigenvalues of A, and  $\{P_n\}_{n=1}^{\infty}$  are the orthogonal projection operators onto the finite-dimensional eigenspaces of A associated with the eigenvalues  $\zeta_n$ . We now consider how the integral in eq.(6.209) can be evaluated using the spectral representation of  $\tilde{G}(p)$  given in eq.(6.210).

Let  $\{\eta_N\}_{N=1}^{\infty}$  be a sequence of real numbers such that

$$\sqrt{\zeta_N} < \eta_N < \sqrt{\zeta_{N+1}},\tag{6.211}$$

$$|\eta_N^2 - \zeta_N| \ge \delta,\tag{6.212}$$

$$|\eta_N^2 - \zeta_{N+1}| \ge \delta \tag{6.213}$$

for all N and some  $\delta > 0$ ; the existence of such a  $\delta > 0$  follows from the fact that the eigenvalues  $\{\zeta_N\}_{N=1}^{\infty}$  have no finite accumulation points. Let  $\xi > 0$  be given, and consider the following sequence  $\{\Gamma_N\}_{N=1}^{\infty}$  of closed positively oriented contours in the complex p-plane: The contour  $\Gamma_N$  consists of (1) the line vertical segment from  $\xi - i\eta_N$  to  $\xi + i\eta_N$ , and (2) the left semi-circle with radius  $\eta_N$  and center  $\xi$ . We first show that:

**Lemma 6.5.19** The Green distribution G for the elastodynamic equation is given by

$$G(t) = \lim_{N \to \infty} \frac{1}{2\pi i} \int_{\Gamma_N} \tilde{G}(p) e^{pt} dp, \qquad (6.214)$$

with this limit being understood in the sense of distributions having support contained in  $[0,\infty)$ . That is, for any  $\varphi \in \mathscr{D}$  having  $\operatorname{supp}(\varphi) \subset [0,\infty)$ , we have

$$\langle G, \varphi \rangle = \lim_{N \to \infty} \left\langle \frac{1}{2\pi i} \int_{\Gamma_N} \tilde{G}(p) e^{pt} dp, \varphi(t) \right\rangle.$$
 (6.215)

**Proof** We again write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$  for notational clarity. For every test-function  $\varphi \in \mathcal{D}$  having  $\operatorname{supp}(\varphi) \subseteq [0, \infty)$  we must show that

$$\langle G, \varphi \rangle = \lim_{N \to \infty} \left\langle \frac{1}{2\pi i} \int_{\Gamma_N} \tilde{G}(p) e^{pt} dp, \varphi(t) \right\rangle$$
$$= \lim_{N \to \infty} \frac{1}{2\pi i} \int_{\Gamma_N} \tilde{G}(p) \langle e^{pt}, \varphi(t) \rangle dp, \qquad (6.216)$$

with this limit being taken in L(X;Y). Let  $\Gamma'_N$  denote the semi-circular portion of the contour  $\Gamma_N$ . From the remarks after the proof of Proposition 6.4.3, we need only show

that

$$\lim_{N \to \infty} \frac{1}{2\pi i} \int_{\Gamma_N'} \tilde{G}(p) \langle e^{pt}, \varphi(t) \rangle dp = 0.$$
 (6.217)

By construction, on  $\Gamma'_N$  we have

$$|p^2 + \zeta_N| \ge \delta,\tag{6.218}$$

for all N, and it follows from eq.(6.210) that

$$\|\tilde{G}(p)\|_{L(X:X)} \le 1/\delta,$$
 (6.219)

for  $p \in \Gamma_N'$ , and making use of Proposition 6.5.5 we find

$$\|\tilde{G}(p)\|_{L(X;Y)} \le \frac{1+|p|^2}{\delta},$$
(6.220)

on  $\Gamma_N'$ . From Lemma 6.4.4 we know that

$$|\langle e^{pt}, \varphi(t) \rangle| \le C e^{\operatorname{Re}(p)\tau} |p|^{-m} \sup_{t \in \mathbb{R}} |\partial_t^m \varphi(t)|,$$
 (6.221)

where C>0,  $\mathrm{supp}(\varphi)\in(-\infty,\tau]$ , and m is any positive integer. By assumption  $\varphi$  has support contained in  $[0,\infty)$  so that  $\tau\geq 0$ , and on  $\Gamma'_N$  we have

$$|\langle e^{pt}, \varphi(t) \rangle| \le C e^{\xi \tau} |p|^{-m} \sup_{t \in \mathbb{R}} |\partial_t^m \varphi(t)|, \tag{6.222}$$

for any integer  $m \geq 0$ . Combining these various estimates we obtain

$$\left\| \frac{1}{2\pi i} \int_{\Gamma_N'} \tilde{G}(p) \langle e^{pt}, \varphi(t) \rangle dp \right\|_{L(X,Y)} \le C|p|^{-m+2}$$
(6.223)

for some C > 0. On  $\Gamma'_N$  for large enough N it is clear that  $|p| > C'\eta_N$  for some constant C' > 0, so that

$$\left\| \frac{1}{2\pi i} \int_{\Gamma_N'} \tilde{G}(p) \langle e^{pt}, \varphi(t) \rangle dp \right\|_{L(X;Y)} \le C |\eta_N|^{-m+2}, \tag{6.224}$$

for some C > 0, and the result follows by taking  $m \ge 3$ , and letting  $N \to \infty$ .

We have now seen that G(t) can be obtained as the distributional limit of a sequence of semi-circular contour integrals closed in the left half plane. By construction, for large enough N, the contour  $\Gamma_N$  contains the simple poles of  $\tilde{G}(p)$  associated with the first N eigenvalues of A. From eq.(6.210) and an application of Cauchy's residue theorem we readily calculate

$$\frac{1}{2\pi i} \int_{\Gamma_n} \tilde{G}(p) e^{pt} dp = \sum_{n=1}^N \frac{1}{\zeta_n} \sin(\sqrt{\zeta_n} t) P_n.$$
 (6.225)

We have now shown:

**Theorem 6.5.20** The Green distribution G for the elastodynamic equation is given by

$$G(t) = \sum_{n=1}^{\infty} \frac{1}{\zeta_N} \sin(\sqrt{\zeta_n}t) H(t) P_n, \qquad (6.226)$$

where H(t) is the Heaviside step function, and where the convergence of this infinite sum is understood in the distributional sense. Recalling the functional calculus notation, we can alternatively write the Green distribution as

$$G(t) = \frac{1}{\sqrt{A}}\sin(\sqrt{A}t)H(t). \tag{6.227}$$

If f is the force term in eq.(6.171), then using eq.(6.225) we can write the solution u = G\*f to the elastodynamic equations as

$$u = \sum_{n=1}^{\infty} \frac{1}{\sqrt{\zeta_n}} s_n * P_n f,$$
 (6.228)

where  $s_n \in \mathcal{D}'_+$  is the distribution defined by

$$\langle s_n, \varphi \rangle = \int_0^\infty \sin(\sqrt{\zeta_n} t) \varphi(t) \, \mathrm{d}t,$$
 (6.229)

for all  $\varphi \in \mathscr{D}$ . Let  $\{u_{nk}\}_{k=1}^{N_n}$  form a basis for the  $N_n$ -dimensional eigenspace of A associated with the eigenvalue  $\zeta_n$ . Assuming without loss of generality that these eigenvectors  $u_{nk}$  are mutually orthonormal, the action of the projection operator  $P_n$  on f can be written

$$P_n f = \sum_{k=1}^{N_n} (f, u_{nk})_X u_{nk}. \tag{6.230}$$

We can now write the above expression for u explicitly in terms of the eigenfunctions of A as

$$u = \sum_{n=1}^{\infty} \sum_{k=1}^{N_n} \frac{1}{\sqrt{\zeta_n}} f_{nk} \otimes u_{nk}, \tag{6.231}$$

where  $f_{nk} \in \mathcal{D}'_+$  is the distribution defined by

$$f_{nk} = s_n * (f, u_{nk})_{\mathbf{v}}. ag{6.232}$$

Eq.(6.231) is the eigenfunction expansion solution of the elastodynamic equation.

# 6.6 Applications to the Viscoelastodynamic Equation

# 6.6.1 Formulation as a convolution equation

Again we write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$  for notational clarity. We have seen that the viscoelastodynamic equation can be written

$$\frac{\partial^2 u}{\partial t^2} + B * \frac{\partial u}{\partial t} = f, \tag{6.233}$$

where  $t \mapsto u(t) \in Y$ ,  $t \mapsto f(t) \in X$  is the given force term, and  $t \mapsto B(t) \in L(Y;X)$  is the relaxation operator. If we allow u, f, and B to be vector-valued distributions with support contained in some right half line, then this equation can be written

$$S * u = f, \tag{6.234}$$

with  $u \in \mathcal{D}'_{+}(Y)$ ,  $f \in \mathcal{D}'_{+}(X)$ , and where we have defined an operator-valued distribution  $S \in \mathcal{D}'_{+}(L(Y;X))$  by

$$S = \frac{\partial^2 \delta}{\partial t^2} \otimes 1 + \frac{\partial B}{\partial t}.$$
 (6.235)

Recalling that for a material with a completely monotone relaxation function

$$B(t) = H(t) \int_{[0,\infty)} e^{-st} M(ds),$$
 (6.236)

with M an L(Y; X)-valued measure on  $[0, \infty)$ , we see that

$$\frac{\partial B}{\partial t}(t) = \delta(t) \otimes A - H(t) \int_{[0,\infty)} s e^{-st} M(ds), \tag{6.237}$$

where we have defined

$$A = M([0, \infty)), \tag{6.238}$$

which, by assumption, is a well-defined operator in L(Y; X).

As the Dirac delta distribution has compact support, and as  $\int_{[0,\infty)} se^{-st} M(ds)$  is bounded for  $t \in [0,\infty)$ , we see that  $Se^{-\xi t}$  is an L(Y;X)-valued Schwartz distribution for all  $\xi > 0$ , and a simple calculation shows that for such p we have

$$\tilde{S}(p) = p^2 1 + \tilde{A}(p),$$
(6.239)

where we have defined the viscoelastodynamic operator to be

$$\tilde{A}(p) = p\tilde{B}(p). \tag{6.240}$$

Using Fubini's theorem to interchange the order of integration, we see from eq. (6.236) that

for Re(p) > 0 we have

$$\tilde{B}(p) = \int_{[0,\infty)} \frac{1}{p+s} M(\mathrm{d}s),$$
(6.241)

which implies that for Re(p) > 0 the viscoelastodynamic operator can be written

$$\tilde{A}(p) = \int_{[0,\infty)} \frac{p}{p+s} M(\mathrm{d}s). \tag{6.242}$$

The existence of a unique solution to eq.(6.234) depends on there being a Green distribution  $G \in \mathcal{D}'_{+}(L(X;Y))$  with  $\operatorname{supp}(G) \subseteq [0,\infty)$  such that

$$G * S = \delta \otimes 1, \quad S * G = \delta \otimes 1.$$
 (6.243)

We have seen that the existence of this Green distribution depends on the properties of the operator-valued function  $\tilde{S}(p)^{-1}$  in the complex p-plane. We shall show that:

**Proposition 6.6.1** The operator-valued function  $\tilde{S}(p)^{-1} = (p^21 + \tilde{A}(p))^{-1}$  is holomorphic in L(X;Y) for all Re(p) > 0, and for  $\text{Re}(p) > \xi$  with  $\xi > 0$  arbitrary we have the estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le C(1+|p|). \tag{6.244}$$

From Corollary 6.4.9 it then follows that the Green distribution G for eq.(6.234) exists, that it has a Laplace transform  $\tilde{G}(p)$  defined for Re(p) > 0 given by

$$\tilde{G}(p) = \tilde{S}(p)^{-1},$$
(6.245)

and that it can be expressed in terms of  $\tilde{G}(p)$  through the inverse Laplace transform

$$G(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{G}(p) e^{pt} dp, \qquad (6.246)$$

where  $\xi > 0$  is arbitrary. To prove Proposition 6.6.1 we must consider the properties of the viscoelastodynamic operator  $\tilde{A}(p)$  in further detail.

## 6.6.2 The viscoelastodynamic operator

## Domain of holomorphy

We have defined the viscoelastodynamic operator for Re(p) > 0 by

$$\tilde{A}(p) = \int_{[0,\infty)} \frac{p}{p+s} M(\mathrm{d}s). \tag{6.247}$$

For fixed p, this is a linear partial differential operator whose action on sufficiently smooth functions is given by

$$(\tilde{A}(p)u)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{j}} \left( \tilde{a}_{jikl}(x, p) \frac{\partial u_{l}}{\partial x_{k}}(x) \right). \tag{6.248}$$

Here we have defined

$$\tilde{a}_{ijkl}(x,p) = \int_{[0,\infty)} \frac{p}{p+s} m_{ijkl}(x,ds),$$
(6.249)

with m the tensor-valued Radon measure associated with the relaxation tensor b though Bernstein's theorem. As above, we can think of this operator as either defining a continuous linear mapping from  $H^2_{\partial}(\Omega; \mathbb{C}^n)$  into  $L^2(\Omega, \rho; \mathbb{C}^n)$  or as an unbounded linear operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$  with dense domain  $D(\tilde{A}(p))$  equal to  $H^2_{\partial}(\Omega; \mathbb{C}^n)$ .

In discussing the properties of  $\tilde{A}(p)$  further we require the following result:

**Lemma 6.6.2** Let  $\mu$  be a non-negative Radon measure on  $[0,\infty)$  with compact support

$$\operatorname{supp}(\mu) \subseteq [s_1, s_2], \tag{6.250}$$

where  $s_1 = \min(\operatorname{supp}(\mu))$  and  $s_2 = \max(\operatorname{supp}(\mu))$ . The function  $p \mapsto f(p)$  defined by

$$f(p) = \int_{[0,\infty)} \frac{p}{p+s} \mu(\mathrm{d}s),$$
 (6.251)

satisfies the following properties:

- 1. It is holomorphic for  $p \in \mathbb{C} \setminus -\text{supp}(\mu)$ .
- 2. It is bounded at  $\infty$  and satisfies

$$\lim_{p \to \infty} f(p) = \mu([0, \infty)). \tag{6.252}$$

3. For  $-\pi < \theta < \pi$  we have

$$\lim_{r \searrow 0} f(re^{i\theta}) = \mu(\{0\}). \tag{6.253}$$

4. Let  $p = \xi + i\eta$  with  $\xi, \eta \in \mathbb{R}$ . Re(f(p)) is positive in the open subset of  $\mathbb{C}$  defined by

$$(\xi + s_2/2)^2 + \eta^2 > (s_2/2)^2,$$
 (6.254)

which describes the exterior of the circle of radius  $s_2/2$  centered at the point  $-s_2/2$ , while Re(f(p)) is negative in the bounded open subset of  $\mathbb{C}$  defined by

$$(\xi + s_1/2)^2 + \eta^2 < (s_1/2)^2, \tag{6.255}$$

which describes the interior of a circle of radius  $s_1/2$  centered at the point  $-s_1/2$ .

- 5. Im(f(p)) is positive when Im(p) > 0, negative for Im(p) < 0, and is equal to 0 for Im(p) = 0.
- 6. If the set  $[s_2, s_1] \setminus \text{supp}(\mu)$  is non-empty, then f(p) has a single first-order zero in the interior of each connected component of  $[-s_2, -s_1] \setminus -\text{supp}(\mu)$ .

**Proof** Properties (1) to (3) are readily established. To prove properties (4) and (5) we write

$$f(p) = \int_{[0,\infty)} \frac{|p|^2 + s\operatorname{Re}(p)}{|p+s|^2} \mu(\mathrm{d}s) + i \int_{[0,\infty)} \frac{s\operatorname{Im}(p)}{|p+s|^2} \mu(\mathrm{d}s), \tag{6.256}$$

which gives

$$\operatorname{Re}(f(p)) = \int_{[0,\infty)} \frac{|p|^2 + s\operatorname{Re}(p)}{|p+s|^2} \mu(ds),$$
 (6.257)

$$\operatorname{Im}(f(p)) = \int_{[0,\infty)} \frac{s \operatorname{Im}(p)}{|p+s|^2} \mu(ds).$$
 (6.258)

Putting  $p = \xi + i\eta$ , we see that

$$|p|^2 + s\operatorname{Re}(p) = (\xi + s/2)^2 + \eta^2 - (s/2)^2.$$
 (6.259)

It follows that if

$$(\xi + s_2/2)^2 + \eta^2 > (s_2/2)^2,$$
 (6.260)

then Re(f(p)) > 0, while if

$$(\xi + s_1/2)^2 + \eta^2 < (s_1/2)^2, \tag{6.261}$$

then Re(f(p)) < 0. We obtain property (5) similarly.

From properties (3), (4), and (5) we see that f(p) is non-zero except possibly at 0 and in the interval  $[-s_2, -s_1]$  of the negative real axis. In the interval  $[-s_2, -s_1]$  of the negative real axis, f(p) is only well-defined in  $[-s_2, -s_1] \setminus -\text{supp}(p)$ . Supposing that this set is non-empty, let the open interval  $(-s'_2, -s'_1)$  denote one of its connected components. For  $p \in (-s'_2, -s'_1)$  with  $s'_1 \neq 0$  (the case with  $s'_1 = s_1 = 0$  can be handled similarly) we can write

$$f(p) = \int_{[s_1, s_1']} \frac{p}{p+s} \mu(\mathrm{d}s) + \int_{[s_2', s_2]} \frac{p}{p+s} \mu(\mathrm{d}s). \tag{6.262}$$

As  $p \to -s'_1$  from the left, the first of the terms on the right hand side of the above expression tends to  $\infty$  while the second term remains bounded. It follows that f(p) is positive for p sufficiently close to  $-s'_1$ . Similarly, we see that f(p) is negative for p sufficiently close to  $-s'_2$ . It follows that f(p) must have at least one zero in  $(-s'_2, -s'_1)$ . To see that

there is only one such zero, we calculate that

$$\frac{\mathrm{d}f}{\mathrm{d}p}(p) = \int_{[s_1, s_2]} \frac{s}{(p+s)^2} \mu(\mathrm{d}s) \ge 0, \tag{6.263}$$

which shows that f(p) is monotonically increasing in  $(-s'_2, -s'_1)$ , and the desired result follows.

For the tensor-valued Radon measure  $m(x,\cdot)$  associated with the relaxation function b through Bernstein's theorem, we recall that  $[s_1, s_2]$  was defined to be the smallest closed interval such that

$$\operatorname{supp}(m(x,\cdot)) \subseteq [s_1, s_2], \tag{6.264}$$

for all  $x \in \Omega^{\text{cl}}$ . It follows from the above lemma that for  $p \notin [-s_2, -s_1]$  the tensor-valued function  $p \mapsto \tilde{a}_{ijkl}(x,p)$  defined in eq.(6.249) is holomorphic for all  $x \in \Omega^{\text{cl}}$ . We can, therefore, extend the definition of the relaxation operator  $\tilde{A}(p)$  to a holomorphic operator-valued function in  $\mathbb{C} \setminus [-s_2, -s_1]$ . Within  $[-s_2, -s_1]$  there may be some values of p for which  $p \mapsto \tilde{A}(p)$  is well-defined and holomorphic, though whether or not this is the case will depend in detail on the form of the viscoelastic tensor  $\tilde{a}_{ijkl}(x,p)$ . Let us define

 $\Sigma_h = \{ p \in \mathbb{C} \mid \text{ for each } x \in \Omega^{\text{cl}} \text{ the function } p \mapsto \tilde{a}_{ijkl}(x,p) \text{ is holomorphic} \},$  (6.265) which is the largest subset of  $\mathbb{C}$  in which the operator-valued function  $p \mapsto \tilde{A}(p)$  is holomorphic. From the above remarks it is clear that we have the inclusion

$$\mathbb{C} \setminus [-s_2, -s_1] \subseteq \Sigma_h. \tag{6.266}$$

We also define

$$\Sigma_s = \mathbb{C} \setminus \Sigma_h, \tag{6.267}$$

which is the set of all  $p \in \mathbb{C}$  for which there exists an  $x \in \Omega^{\text{cl}}$  such that the function  $p \mapsto \tilde{a}_{ijkl}(x,p)$  is singular at p. On  $\Sigma_s$  the operator-valued function  $p \mapsto \tilde{A}(p)$  is singular.

## Strong ellipticity of $\tilde{A}(p)$

**Proposition 6.6.3** For  $p \notin [-s_2, -s_1]$  the viscoelastodynamic operator  $\tilde{A}(p)$  is strongly elliptic.

**Proof** Let  $p \notin [-s_2, -s_1]$ . That  $\tilde{A}(p)$  is strongly elliptic means that for every  $k \in \mathbb{R}^n$  with  $k \neq 0$ ,  $u \in \mathbb{C}^n$ , and  $x \in \Omega^{cl}$ , we have

$$\operatorname{Re}(\gamma A_{il}(x, p, k) u_i \overline{u_l}) \ge c \|u\|_{\mathbb{C}^n}^2, \tag{6.268}$$

for some  $\gamma \in \mathbb{C}$  and c > 0, where we have defined the characteristic matrix

$$A_{il}(x, p, k) = \frac{1}{\rho(x)} \tilde{a}_{jikl}(x, p) k_j k_k.$$
 (6.269)

From eq.(6.249) we find that

$$A_{il}(x, p, k)u_i\overline{u_l} = \int_{[s_1, s_2]} \frac{p}{p+s}\mu(\mathrm{d}s),$$
 (6.270)

where we have defined a real-valued Radon measure  $\mu$  on  $[0,\infty)$  by

$$\mu(\cdot) = \frac{1}{\rho(x)} m_{jikl}(x, \cdot) u_i k_j \overline{u}_l k_k. \tag{6.271}$$

It is readily seen that  $\mu$  is non-negative, and that

$$\mu([s_1, s_2]) \ge c \|u\|_{\mathbb{C}^n}^2 \tag{6.272}$$

for some c > 0, where we have recalled that  $m_{ijkl}(x, [s_1, s_2])$  has, by assumption, the properties of a strongly elliptic elastic tensor. The strong ellipticity of  $\tilde{A}(p)$  now follows easily from eq.(6.270) and the results of Lemma 6.6.2.

**Remark** Within the set  $[-s_2, -s_1]$  there may be some values of p for which  $\tilde{A}(p)$  is well-defined and strongly elliptic. We, therefore, define the set

$$\Sigma_e = \left\{ p \in \mathbb{C} \mid \tilde{A}(p) \text{ is strongly elliptic} \right\},$$
(6.273)

and from the above result have the inclusion

$$\mathbb{C} \setminus [-s_2, -s_1] \subseteq \Sigma_e. \tag{6.274}$$

We can also define a set

$$\Sigma_{ne} = \mathbb{C} \setminus \Sigma_e \tag{6.275}$$

which comprises those values of p for which  $p \mapsto \tilde{A}(p)$  is not strongly elliptic. In particular, if  $\Sigma_{ne} \cap \Sigma_h \neq \emptyset$ , then this set comprises those  $p \in [-s_2, -s_1]$  for which  $p \mapsto \tilde{A}(p)$  is holomorphic at p, but for which the operator  $\tilde{A}(p)$  fails to be strongly elliptic.

As with the case of the elastodynamic operator, the strong ellipticity of  $\tilde{A}(p)$  for  $p \in \Sigma_e$ 

implies the existence of a number of a priori estimates. The most important of these estimates is that if  $u \in D(\tilde{A}(p))$  and  $\tilde{A}(p)u \in H^s(\Omega; \mathbb{C}^n)$  for  $s \geq 0$ , then  $u \in D(\tilde{A}(p)) \cap H^{s+2}(\Omega; \mathbb{C}^n)$  and

$$||u||_{H^{s+2}(\Omega;\mathbb{C}^n)} \le K\left(||\tilde{A}(p)u||_{H^s(\Omega;\mathbb{C}^n)} + ||u||_{H^s(\Omega;\mathbb{C}^n)}\right),$$
 (6.276)

for some K > 0 which will, in general, depend on p. If we assume that the distance of p from  $\Sigma_{ne}$  is greater than some fixed number  $\delta > 0$ , then it may be shown that the constant K occurring in the a priori estimate can be taken independent of p. We will not give a proof of this result, but note that it follows from the general methods for obtaining such a priori estimates (e.g. Agmon  $et\ al.\ 1959,\ 1964$ ; Browder 1961) and the fact that for such p there exists positive constants c and c' independent of x and of p such that

$$c||u||_{\mathbb{C}^n}^2 \le \operatorname{Re}(\gamma A_{il}(x, p, k) u_i \overline{u_l}) \le c' ||u||_{\mathbb{C}^n}^2 \tag{6.277}$$

for some  $\gamma \in \mathbb{C}$ , all  $x \in \Omega^{\text{cl}}$ , all  $k \in \mathbb{R}^n$ , and all  $u \in \mathbb{C}^n$ . In the particular case that s = 0, the above estimate gives

$$||u||_{H^{2}(\Omega;\mathbb{C}^{n})} \le K\left(||\tilde{A}(p)u||_{L^{2}(\Omega,\rho;\mathbb{C}^{n})} + ||u||_{L^{2}(\Omega,\rho;\mathbb{C}^{n})}\right),$$

$$(6.278)$$

for all  $u \in D(\tilde{A}(p))$ . From these a priori estimates we can derive a number of important properties of the viscoelastodynamic operator. In particular, we can show that:

**Proposition 6.6.4** For  $p \in \Sigma_e$  and any  $\lambda \in \mathbb{C}$ , the operator  $\lambda 1 - \tilde{A}(p)$  on  $L^2(\Omega, \rho; \mathbb{C}^n)$  is closed, unbounded, has finite-dimensional kernel, and closed image.

# The adjoint of $\tilde{A}(p)$

We recall that the formal adjoint  $\tilde{A}(p)'$  of  $\tilde{A}(p)$  is defined such that

$$\left(\tilde{A}(p)u,v\right)_{L^{2}(\Omega,\rho;\mathbb{C}^{n})} = \left(u,\tilde{A}(p)'v\right)_{L^{2}(\Omega,\rho;\mathbb{C}^{n})},\tag{6.279}$$

for all  $u, v \in \mathcal{D}(\Omega; \mathbb{C}^n)$ . A simple calculation using integration by parts shows that the formal adjoint  $\tilde{A}(p)'$  is given by

$$(\tilde{A}(p)'u)_{i}(x) = -\frac{1}{\rho(x)} \frac{\partial}{\partial x_{j}} \left( \frac{\tilde{a}_{jikl}(x,p)}{\partial x_{k}} \frac{\partial u_{l}}{\partial x_{k}}(x) \right)$$

$$(6.280)$$

$$= -\frac{1}{\rho(x)} \frac{\partial}{\partial x_i} \left( \tilde{a}_{jikl}(x, \overline{p}) \frac{\partial u_l}{\partial x_k}(x) \right) = \tilde{A}(\overline{p}), \tag{6.281}$$

where in obtaining the second equality we have made use of the identity

$$\overline{\tilde{a}_{ijkl}(x,p)} = \tilde{a}_{ijkl}(x,\overline{p}), \tag{6.282}$$

which follows from eq.(6.249). Recalling Browder's (1961) result on the  $L^2$ -realizations of strongly elliptic operators, we see that the adjoint of the viscoelastodynamic operator is given by

$$\tilde{A}(p)^* = \tilde{A}(\overline{p}). \tag{6.283}$$

It follows that when  $\text{Im}(p) \neq 0$  the viscoelastodynamic operator is not self-adjoint. The operator-valued function  $p \mapsto \tilde{A}(p)$  does, however, define a *self-adjoint holomorphic family* in the sense of Kato (1980, Chapter VII, Section 3.1).

Though  $\tilde{A}(p)$  is not a self-adjoint operator,  $\tilde{A}(p)$  and  $\tilde{A}(p)^*$  are still closely related. To see this, let us define a *conjugate linear* operator J on  $L^2(\Omega, \rho; \mathbb{C}^n)$  by

$$Ju = \overline{u}. ag{6.284}$$

In terms of J we see that the formal adjoint of  $\tilde{A}(p)$  can be written

$$\tilde{A}(p)' = J\tilde{A}(p)J. \tag{6.285}$$

Again making use of Browder's (1961) result, we see that this relation implies that

$$\tilde{A}(p)^* = J\tilde{A}(p)J,\tag{6.286}$$

and we say that  $\tilde{A}(p)$  is a *J-self-adjoint* operator on  $L^2(\Omega, \rho; \mathbb{C}^n)$  (e.g. Edmunds & Evans 1987, Chapter III, Section 5). From eq.(6.286) we obtain for any  $\lambda \in \mathbb{C}$  the useful relations

$$\ker(\lambda 1 - \tilde{A}(p)) = J \ker(\overline{\lambda} 1 - \tilde{A}(p)^*), \tag{6.287}$$

$$\ker(\overline{\lambda}1 - \tilde{A}(p)^*) = J \ker(\lambda 1 - \tilde{A}(p)), \tag{6.288}$$

$$\operatorname{im}(\lambda 1 - \tilde{A}(p)) = J \operatorname{im}(\overline{\lambda} 1 - \tilde{A}(p)^*), \tag{6.289}$$

$$\operatorname{im}(\overline{\lambda}1 - \tilde{A}(p)^*) = J\operatorname{im}(\lambda 1 - \tilde{A}(p)). \tag{6.290}$$

**Proposition 6.6.5** For  $p \in \Sigma_e$  and any  $\lambda \in \mathbb{C}$  the operator  $\lambda 1 - \tilde{A}(p)$  is Fredholm with  $\operatorname{ind}(\lambda 1 - \tilde{A}(p)) = 0$ .

**Remark** If the set  $\Sigma_{ne} \cap \Sigma_h$  is non-empty, then for  $p \in \Sigma_{ne} \cap \Sigma_h$  the operator  $\lambda 1 - \tilde{A}(p)$  may fail to be Fredholm for certain values of  $\lambda \in \mathbb{C}$ .

**Proof** We have already seen that  $\lambda 1 - \tilde{A}(p)$  is semi-Fredholm with  $\operatorname{nul}(\lambda 1 - \tilde{A}(p)) < \infty$ , so we need only show that  $\operatorname{def}(\lambda 1 - \tilde{A}(p)) = \operatorname{nul}(\lambda 1 - \tilde{A}(p))$ . We know that  $\operatorname{coker}(\lambda 1 - \tilde{A}(p))$  is isomorphic to  $\operatorname{im}(\lambda 1 - \tilde{A}(p))^{\perp}$ , and from eq.(6.135) and eq.(6.288) obtain

$$\operatorname{im}(\lambda 1 - \tilde{A}(p))^{\perp} = \ker(\overline{\lambda} 1 - \tilde{A}(p)^{*}) = J \ker(\lambda 1 - \tilde{A}(p)), \tag{6.291}$$

which implies that

$$\dim \operatorname{coker}(\lambda 1 - \tilde{A}(p)) = \dim \ker(\lambda 1 - \tilde{A}(p)), \tag{6.292}$$

as desired.

# Resolvent of $\tilde{A}(p)$

Adapting the proof of Proposition 6.5.5 we obtain:

**Proposition 6.6.6** Let  $p \in \Sigma_e$  with  $\operatorname{dist}(p, \Sigma_{ne}) > \delta$  for some  $\delta > 0$ . Then for any  $\lambda \in \varrho(\tilde{A}(p))$ , the resolvent operator  $R(\tilde{A}(p); \lambda)$  maps  $H^s(\Omega; \mathbb{C}^n)$  continuously into  $H^{s+2}_{\partial}(\Omega; \mathbb{C}^n)$  for  $s \geq 0$ , and satisfies the estimates

$$||R(\tilde{A}(p);\lambda)||_{L(H^s;H^{s+2})} \le K \left[1 + (1+|\lambda|)||R(\tilde{A}(p);\lambda)||_{L(H^s;H^s)}\right],$$
 (6.293)

$$||R(\tilde{A}(p);\lambda)||_{L(H^{s+2};H^{s+2})} \leq K\left[1 + (1+|\lambda|)||R(\tilde{A}(p);\lambda)||_{L(H^{s};H^{s})}\right], \tag{6.294}$$

where we have written  $H^s$  for  $H^s(\Omega; \mathbb{C}^n)$  for notational clarity, and where K > 0 is independent of  $\lambda$  and of p. In particular, for even s, we obtain

$$||R(\tilde{A}(p);\lambda)||_{L(H^s;H^{s+2})} \leq K \left[1 + (1+|\lambda|)^{s/2+1} ||R(\tilde{A}(p);\lambda)||_{L(L^2;L^2)}\right], \qquad (6.295)$$

$$||R(\tilde{A}(p);\lambda)||_{L(H^{s+2};H^{s+2})} \leq K\left[1+(1+|\lambda|)^{s/2+1}||R(\tilde{A}(p);\lambda)||_{L(L^2;L^2)}\right], \qquad (6.296)$$

where we have written  $L^2$  for  $L^2(\Omega, \rho; \mathbb{C}^n)$ .

Moreover, for such  $\lambda \in \varrho(\tilde{A}(p))$ , the resolvent operator  $R(\tilde{A}(p); \lambda)$  maps  $H^s(\Omega; \mathbb{C}^n)$  compactly into itself.

To obtain further information on the resolvent set of  $\tilde{A}(p)$  it will be useful to recall the definition of the *numerical range* of a linear operator on a Hilbert space (e.g. Kato 1980, Chapter V, Section 3; Edmunds & Evans 1987, Chapter III, Section 2). Let  $T: D(T) \mapsto X$ 

be a closed linear operator on a Hilbert space X. The numerical range of T is the closed subset of  $\mathbb{C}$  defined by

$$\Gamma(T) = \{ (Tu, u)_X \mid u \in D(T), ||u||_X = 1 \}^{cl}.$$
(6.297)

The motivation for considering this set is the following result (e.g. Edmunds & Evans 1987, Chapter III, Theorem 2.3):

**Lemma 6.6.7** Let  $T: D(T) \to X$  be a closed operator on a Hilbert space X with numerical range  $\Gamma(T)$ . If for some  $\lambda \in \mathbb{C}$ , we have  $\lambda \notin \Gamma(T)$  then  $\ker(\lambda 1 - T) = \{0\}$ . Moreover, if in addition  $\operatorname{im}(\lambda 1 - T) = X$ , then  $\lambda \in \varrho(T)$  and

$$||R(T;\lambda)||_{L(X;X)} \le \frac{1}{\operatorname{dist}(\lambda,\Gamma(T))}.$$
(6.298)

The numerical range of  $\tilde{A}(p)$  for  $p \in \Sigma_e$  is described in the following result:

**Proposition 6.6.8** For  $q \in \Gamma(\tilde{A}(p))$  let us write  $q = \alpha + i\beta$  with  $\alpha, \beta \in \mathbb{R}$ , and similarly write  $p = \xi + i\eta$  with  $\xi, \eta \in \mathbb{R}$ .

1. For  $\xi \geq 0$  and  $\eta > 0$ , we have

$$\alpha > 0, \quad \beta > 0, \tag{6.299}$$

along with the estimate

$$0 < \frac{s_1 \eta}{\xi^2 + \eta^2 + s_1 \xi} \le \frac{\beta}{\alpha} \le \frac{s_2 \eta}{\xi^2 + \eta^2 + s_2 \xi} \le \frac{s_2}{\eta}. \tag{6.300}$$

2. For  $\xi \geq 0$  and  $\eta = 0$ , we have

$$\alpha > 0, \quad \beta = 0. \tag{6.301}$$

3. For  $\xi \geq 0$  and  $\eta < 0$ , we have

$$\alpha > 0, \quad \beta < 0, \tag{6.302}$$

along with the estimate

$$\frac{s_2}{\eta} \le \frac{s_2 \eta}{\xi^2 + \eta^2 + s_1 \xi} \le \frac{\beta}{\alpha} \le \frac{s_1 \eta}{\xi^2 + \eta^2 + s_2 \xi} < 0. \tag{6.303}$$

4. For  $\xi < 0$  and  $\eta > 0$  such that

$$\xi^2 + \eta^2 + s_2 \xi > 0, \tag{6.304}$$

we have

$$\alpha > 0, \quad \beta > 0, \tag{6.305}$$

along with the estimate

$$0 < \frac{s_1 \eta}{\xi^2 + \eta^2 + s_1 \xi} \le \frac{\beta}{\alpha} \le \frac{s_2 \eta}{\xi^2 + \eta^2 + s_2 \xi}.$$
 (6.306)

5. For  $\xi < 0$  and  $\eta = 0$  such that  $\xi < -s_2$ , we have

$$\alpha > 0, \quad \beta = 0. \tag{6.307}$$

6. For  $\xi < 0$  and  $\eta < 0$  such that

$$\xi^2 + \eta^2 + s_2 \xi > 0, \tag{6.308}$$

we have

$$\alpha > 0, \quad \beta < 0, \tag{6.309}$$

along with the estimate

$$\frac{s_2\eta}{\xi^2 + \eta^2 + s_2\xi} \le \frac{\beta}{\alpha} \le \frac{s_1\eta}{\xi^2 + \eta^2 + s_1\xi} < 0. \tag{6.310}$$

7. For  $\xi < 0$  and  $\eta > 0$  such that

$$\xi^2 + \eta^2 + s_1 \xi < 0, \tag{6.311}$$

we have

$$\alpha < 0, \quad \beta > 0, \tag{6.312}$$

along with the estimate

$$\frac{s_1 \eta}{\xi^2 + \eta^2 + s_2 \xi} \le \frac{\beta}{\alpha} \le \frac{s_2 \eta}{\xi^2 + \eta^2 + s_1 \xi} \tag{6.313}$$

8. For  $\xi < 0$  and  $\eta = 0$  such that  $\xi > -s_1$ , we have

$$\alpha < 0, \quad \beta = 0. \tag{6.314}$$

9. For  $\xi < 0$  and  $\eta < 0$  such that

$$\xi^2 + \eta^2 + s_1 \xi < 0, \tag{6.315}$$

we have

$$\alpha < 0, \quad \beta < 0, \tag{6.316}$$

along with the estimate

$$\frac{s_2\eta}{\xi^2 + \eta^2 + s_1\xi} \le \frac{\beta}{\alpha} \le \frac{s_1\eta}{\xi^2 + \eta^2 + s_2\xi}.$$
 (6.317)

**Proof** For  $u \in D(\tilde{A}(p))$  we calculate that

$$(Au, u)_{L^{2}(\Omega, \rho; \mathbb{C}^{n})} = \int_{\Omega} \tilde{a}_{jikl}(x, p) \frac{\partial u_{i}}{\partial x_{j}}(x) \frac{\partial u_{l}}{\partial x_{k}}(x) dx.$$
 (6.318)

Making use of eq.(6.249) and interchanging the order of integration, we find that

$$(Au, u)_{L^{2}(\Omega, \rho; \mathbb{C}^{n})} = \int_{[s_{1}, s_{2}]} \frac{p}{p+s} \mu(\mathrm{d}s), \tag{6.319}$$

where we have defined a non-negative Radon measure on  $[0, \infty)$  by

$$\mu(E) = \int_{\Omega} m_{jikl}(x, E) \frac{\partial u_i}{\partial x_j}(x) \frac{\partial u_l}{\partial x_k}(x) dx, \qquad (6.320)$$

for each measurable subset  $E \subseteq [0, \infty)$ . We note, in particular, that

$$\mu([0,\infty)) \ge c \|u\|_{L^2(\Omega,\rho;\mathbb{C}^n)}^2.$$
 (6.321)

Splitting eq.(6.319) into its real and imaginary parts gives

$$(Au, u)_{L^{2}(\Omega, \rho; \mathbb{C}^{n})} = \int_{[s_{1}, s_{2}]} \frac{|p|^{2} + s\operatorname{Re}(p)}{|p + s|^{2}} \mu(\mathrm{d}s) + i \int_{[s_{1}, s_{2}]} \frac{s\operatorname{Im}(p)}{|p + s|^{2}} \mu(\mathrm{d}s). \tag{6.322}$$

Defining  $q=(Au,u)_{L^2(\Omega,\rho;\mathbb{C}^n)}=\alpha+\mathrm{i}\beta$  with  $\alpha,\beta\in\mathbb{R},$  and recalling that  $p=\xi+\mathrm{i}\eta,$  we obtain

$$\alpha = \int_{[s_1, s_2]} \frac{\xi^2 + \eta^2 + s\xi}{(\xi + s)^2 + \eta^2} \mu(\mathrm{d}s), \tag{6.323}$$

$$\beta = \int_{[s_1, s_2]} \frac{s\eta}{(\xi + s)^2 + \eta^2} \mu(\mathrm{d}s), \tag{6.324}$$

(6.325)

For  $\xi \ge 0$  and  $\eta > 0$ , we see readily that  $\alpha > 0$  and  $\beta > 0$ . Moreover, we have the estimates

$$0 < (\xi^2 + \eta^2 + s_1 \xi) I(\xi, \eta) \le \alpha \le (\xi^2 + \eta^2 + s_2 \xi) I(\xi, \eta), \tag{6.326}$$

$$s_1 \eta I(\xi, \eta) \leq \beta \leq s_2 \eta I(\xi, \eta) \tag{6.327}$$

where we have defined

$$I(\xi, \eta) = \int_{[s_1, s_2]} \frac{1}{(\xi + s)^2 + \eta^2} \mu(\mathrm{d}s). \tag{6.328}$$

This implies that

$$0 < \frac{s_1 \eta}{\xi^2 + \eta^2 + s_2 \xi} \le \frac{\beta}{\alpha} \le \frac{s_2 \eta}{\xi^2 + \eta^2 + s_1 \xi} \le \frac{s_2}{\eta},\tag{6.329}$$

which proves case (1) of the proposition. The other cases are proven in an analogous manner.

**Proposition 6.6.9** Let  $p \in \Sigma_e$ . A sufficient condition for  $\lambda \in \mathbb{C}$  to be in  $\varrho(\tilde{A}(p))$  is that  $\lambda \notin \Gamma(\tilde{A}(p))$ .

**Proof** From Lemma 6.6.7 we see that  $\lambda \notin \Gamma(\tilde{A}(p))$  implies that  $\ker(\lambda 1 - \tilde{A}(p)) = \{0\}$ , and that, in this case,  $\lambda \in \varrho(\tilde{A}(p))$  if  $\operatorname{im}(\lambda 1 - \tilde{A}(p)) = L^2(\Omega, \rho; \mathbb{C}^n)$ . As  $\tilde{A}(p)$  has closed image, we can use eq.(6.136) to obtain

$$\operatorname{im}(\lambda 1 - \tilde{A}(p)) = \ker(\overline{\lambda} 1 - \tilde{A}(p)^*)^{\perp}. \tag{6.330}$$

It follows that  $\operatorname{im}(\lambda 1 - \tilde{A}(p)) = L^2(\Omega, \rho; \mathbb{C}^n)$  if and only if  $\ker(\overline{\lambda} 1 - \tilde{A}(p)^*) = \{0\}$ . To see that this is the case, we note that as  $\tilde{A}(p)$  and  $\tilde{A}(p)^*$  have common domains their numerical ranges are related by

$$\Gamma(\tilde{A}(p)^*) = \overline{\Gamma(\tilde{A}(p))}.$$
(6.331)

By assumption  $\lambda \notin \Gamma(\tilde{A}(p))$ , and so we can conclude that  $\overline{\lambda} \notin \Gamma(\tilde{A}(p)^*)$ , and a second application of Lemma 6.6.7 shows that  $\ker(\overline{\lambda}1 - \tilde{A}(p)^*) = \{0\}$  as desired.

Putting these various results together we can now give the proof of Proposition 6.6.1:

**Proof of Proposition 6.6.1** As above we write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$ . We first note the idenity

$$\tilde{S}(p)^{-1} = (p^2 1 + \tilde{A}(p))^{-1} = R(-\tilde{A}(p); p^2), \tag{6.332}$$

relating  $\tilde{S}(p)^{-1}$  to the resolvent operator of  $-\tilde{A}(p)$ . It follows from Proposition 6.6.9 that  $\tilde{S}(p)^{-1}$  exists in L(X;X) so long as  $p^2 \notin \Gamma(-\tilde{A}(p)) = -\Gamma(\tilde{A}(p))$ . Suppose first that Re(p) > 0 and Im(p) > 0. Then from Proposition 6.6.8 part (1) we see that  $-\Gamma(\tilde{A}(p))$  is contained in the quadrant  $\{p \in \mathbb{C} \mid \text{Re}(p) < 0, \text{Im}(p) < 0\}$ , while  $p^2$  lies in the upper half plane Im(p) > 0. It follows that  $\tilde{S}(p)^{-1}$  exists in L(X;X), and from

$$\operatorname{dist}(p^2, -\Gamma(\tilde{A}(p))) \ge |p|^2, \quad 0 < \arg(p) \le \pi/4,$$
 (6.333)

$$\operatorname{dist}(p^2, -\Gamma(\tilde{A}(p))) \ge \operatorname{Im}(p^2), \quad \pi/4 < \arg(p) < \pi/2,$$
 (6.334)

and from Lemma 6.6.7 we obtain the estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;X)} \le \frac{1}{|p|\operatorname{Re}(p)},$$
(6.335)

where we have used a simple geometric argument to combine the above two estimates for  $\operatorname{dist}(p^2, -\Gamma(\tilde{A}(p)))$ . The corresponding results for  $\operatorname{Im}(p) = 0$  and for  $\operatorname{Im}(p) < 0$  can be established in a similar manner.

Let  $\operatorname{Re}(p) > \xi_0$  for some  $\xi_0 > 0$ . Then  $\operatorname{dist}(p, [-s_2, -s_1]) > \xi_0$ , and from Proposition 6.6.6 we can conclude that for such p the operator  $\tilde{S}(p)^{-1}$  exists in L(X;Y) and satisfies the estimate

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le K \left[ 1 + \frac{1 + |p|^2}{\operatorname{Re}(p)|p|} \right],$$
 (6.336)

which can be simplified to give

$$\|\tilde{S}(p)^{-1}\|_{L(X;Y)} \le C(1+|p|),\tag{6.337}$$

for some positive constant C.

## 6.6.3 Regularity of the solution

We have now shown that a unique solution  $u \in \mathscr{D}'_{+}(H^{2}_{\partial}(\Omega; \mathbb{C}^{n}))$  of the convolution-form

$$S * u = f, \tag{6.338}$$

of the viscoelastodynamic equation exists for each force term  $f \in \mathscr{D}'_{+}(L^{2}(\Omega, \rho; \mathbb{C}^{n}))$ , and that this solution is given by

$$u = G * f, \tag{6.339}$$

where G is the Green distribution for eq.(6.338). As with the case of the elastodynamic equation, this solution will not, in general, be a classical solution of the viscoelastodynamic equations. We now state a number of regularity theorems for the viscoelastodynamic equation, the proof of these results being completely analogous to those for the elastodynamic equations given above. In what follows we write  $L^2$  for  $L^2(\Omega, \rho; \mathbb{C}^n)$ ,  $H^s$  for  $H^s(\Omega; \mathbb{C}^n)$  and  $H^s_{\partial}$  for  $H^s_{\partial}(\Omega; \mathbb{C}^n)$  when  $s \geq 1$ , and identify  $H^0$  with  $L^2$ .

**Theorem 6.6.10** Let the force term in eq.(6.338) be an H<sup>s</sup>-valued distribution for some

even  $s \ge 0$  with  $\operatorname{supp}(f) \subseteq [0, \infty)$ , and suppose that f has a Laplace transform  $\tilde{f}(p)$  defined for  $\operatorname{Re}(p) > \xi_0 > 0$  which satisfies

$$\|\tilde{f}(p)\|_{H^s} \le C|p|^{-(k+2)},\tag{6.340}$$

for some C > and integer  $k \ge 0$ . Then if

$$k - s - 1 \ge 0, (6.341)$$

the solution  $u \in \mathcal{D}'_{+}(H^{s+2}_{\partial})$  to eq.(6.338) is a continuous function having k+1-s continuous derivatives. In particular, if

$$k - s - 1 \ge 1, (6.342)$$

then the solution u of eq. (6.171) satisfies the initial conditions

$$u(0) = \frac{\partial u}{\partial t}(0) = 0, (6.343)$$

while if

$$k - s - 1 \ge 2, (6.344)$$

the time-derivatives in the elastodynamic equation can be understood in the classical sense.

Corollary 6.6.11 Let the force term f in eq.(6.338) be as in Theorem 6.6.10. Then if

$$s > \frac{n}{2} + l,\tag{6.345}$$

for some integer  $l \geq 0$ , and if

$$k - s - 1 \ge 0, (6.346)$$

the solution u of eq.(6.338) as a function of x is continuous with l continuous spatial derivatives, and as a function of time is continuous with k+1-s continuous time-derivatives. In particular, if

$$s > \frac{n}{2} + 2,$$
 (6.347)

and

$$k - s - 1 \ge 2, (6.348)$$

then u is a classical solution of the elastodynamic equations satisfying the homogeneous Dirichlet boundary conditions and the given initial conditions.

**Theorem 6.6.12** If for some even integer  $s \ge 0$  the force term f in eq.(6.338) is such

that

$$e^{-\xi_0 t} \frac{\partial^n f}{\partial t^n} \in L^2(H^s),$$
 (6.349)

for  $\xi_0 > 0$ , and all  $0 \le n \le s + 1$ , then

$$e^{-\xi_0 t} u \in L^2(H_{\partial}^{s+2}),$$
 (6.350)

$$e^{-\xi_0 t} \frac{\partial u}{\partial t} \in L^2(H^{s+1}),$$
 (6.351)

$$e^{-\xi_0 t} \frac{\partial^2 u}{\partial t^2} \in L^2(H^s).$$
 (6.352)

Corollary 6.6.13 Let the conditions given in Theorem 6.6.12 on the force term in eq.(6.338) hold. Then  $t \mapsto u(t) \in H^{s+2}_{\partial}$  and  $t \mapsto \partial u/\partial t(t) \in H^{s+1}_{\partial}$  are continuous functions, and the initial conditions

$$u(0) = \frac{\partial u}{\partial t}(0) = 0, \tag{6.353}$$

are satisfied.

## 6.6.4 Eigenfunction expansions

### Analytic continuation of $\tilde{G}(p)$ into the left half plane

As above we write  $X = L^2(\Omega, \rho; \mathbb{C}^n)$  and  $Y = H^2_{\partial}(\Omega; \mathbb{C}^n)$ . We have seen that the Green distribution G for the convolution-form of the viscoelastodynamic equation exists, and that it has a Laplace transform  $\tilde{G}(p)$  defined for all Re(p) > 0 given by

$$\tilde{G}(p) = (p^2 1 + \tilde{A}(p))^{-1}.$$
(6.354)

This expression for  $\tilde{G}(p)$  can be extended by analytic continuation into a subset of the closed left half-plane for which the inverse operator  $(p^21 + \tilde{A}(p))^{-1}$  exists.

### Proposition 6.6.14 Let

$$D_2 = \{ p \in \mathbb{C} \mid |p|^2 + s_2 \operatorname{Re}(p) < 0 \}$$
(6.355)

denote the subset of  $\mathbb{C}$  comprising points within the closed circular disk of radius  $s_2/2$  with center  $-s_2/2$ . Then the function  $p \mapsto \tilde{G}(p) \in L(X;Y)$  is holomorphic in the open set

$$\{p \in \mathbb{C} \mid \text{Re}(p) > -s_1/2 \text{ or } \text{Re}(p) < -s_2/2\} \setminus D_2,$$
 (6.356)

which is shown schematically in fig 6.1 If the distance of  $p \in \mathbb{C}$  from the complement of

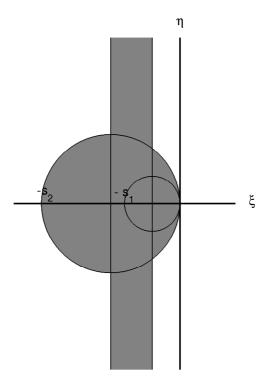


Figure 6.1: A schematic diagram of the subset (which is shaded in grey) of the complex plane in which the function  $p \mapsto \tilde{G}(p)$  may be singular.

this subset is greater than some arbitrary  $\delta > 0$ , we have the estimate

$$\|\tilde{G}(p)\|_{L(X;Y)} \le \text{Pol}(|p|),$$
 (6.357)

where  $Pol(\cdot)$  denotes a polynomial with positive coefficients.

**Proof** We write  $p = \xi + i\eta$  with  $\xi, \eta \in \mathbb{R}$  and consider first the case  $\eta > 0$ . We have seen in Proposition 6.6.1 that  $\tilde{G}(p)$  is defined and holomorphic for  $\xi > 0$ , so we may assume that  $\xi < 0$  (the case  $\xi = 0$  is handled similarly). We recall that if  $p \notin D_2$  we must have

$$\xi^2 + \eta^2 + s_2 \xi > 0. \tag{6.358}$$

From 6.6.9 we know that a sufficient condition for  $\tilde{G}(p)$  to exists for a given  $p \in \mathbb{C}$  is that  $-p^2 \notin \Gamma(\tilde{A}(p))$ . We put  $-p^2 = \alpha + \mathrm{i}\beta$  so that

$$\alpha = \eta^2 - \xi^2, \quad \beta = -2\xi\eta. \tag{6.359}$$

Using Proposition 6.6.8 part (4), we see that for  $\xi < 0$  and  $\eta > 0$  the point  $-p^2$  lies in  $\Gamma(\tilde{A}(p))$  if and only if only if

$$\frac{s_1\eta}{\xi^2 + \eta^2 + s_1\xi} \le \frac{-2\xi\eta}{\eta^2 - \xi^2} \le \frac{s_2\eta}{\xi^2 + \eta^2 + s_2\xi}.$$
(6.360)

As we have assumed that  $\eta > 0$ , we can simplify these inequalities to give

$$\frac{s_1}{\xi^2 + \eta^2 + s_1 \xi} \le \frac{-2\xi}{\eta^2 - \xi^2} \le \frac{s_2}{\xi^2 + \eta^2 + s_2 \xi}.$$
 (6.361)

Considering the first of these inequalities, we note that as  $\frac{s_1}{\xi^2 + \eta^2 + s_1 \xi}$  is non-negative, this inequality can only hold if  $\eta^2 - \xi^2 > 0$ , which implies that  $\pi/2 < \arg(p) < 3\pi/4$ . For such p we can rearrange this first inequality to give

$$s_1(\eta^2 - \xi^2) \le -2\xi \left(\xi^2 + \eta^2 + s_1 \xi\right),\tag{6.362}$$

which simplifies to

$$(s_1 + 2\xi)\eta^2 \le -(s_1 + 2\xi)\xi^2. \tag{6.363}$$

If  $s_1 + 2\xi > 0$ , then this inequality would imply that  $\eta^2 < 0$ , which cannot be true. It follows that  $s_1 + 2\xi \le 0$ , which implies  $\xi \le -s_1/2$ . From the second of the above inequalities we obtain by a similar argument that  $\xi \ge -s_2/2$ , and the result follows by forming the intersection of the appropriate regions. The case  $\eta < 0$  is handled in the same manner. Finally, the norm estimate on  $\|\tilde{G}(p)\|_{L(X;Y)}$  follows straightforwardly from Lemma 6.6.7 and Proposition 6.6.6.

#### Singularities of $\tilde{G}(p)$

Proposition 6.6.14 implies that any singularities of  $\tilde{G}(p)$  are contained in the set

$$D_2 \cup \{ p \in \mathbb{C} \mid -s_2/2 \le \operatorname{Re}(p) \le -s_1/2 \}.$$
 (6.364)

We note that this set contains the subset  $\Sigma_{ne}$  of the negative real axis on which  $\tilde{A}(p)$  is either not well-defined, or is well-defined but is not strongly elliptic. For  $p \in \Sigma_e$ , however, we know that  $\tilde{S}(p)$  is a Fredholm operator with index equal to zero, and that its inverse  $\tilde{G}(p) = \tilde{S}(p)^{-1}$  is well-defined whenever  $\ker(\tilde{S}(p)) = \{0\}$ . If for such p we have  $\ker(\tilde{S}(p)) \neq \{0\}$  then  $\tilde{G}(p)$  is not-defined, and these points are singularities of the function  $p \mapsto \tilde{G}(p)$ . The following result – which is adapted from Theorem (1.1) of Mennicken & Möller (1984) – characterizes these singular points of  $\tilde{G}(p)$ :

**Theorem 6.6.15** The set of points  $p \in \Sigma_e$  for which  $p \mapsto \tilde{G}(p)$  is singular is discrete and may accumulate only at  $\infty$  or to points lying in  $\Sigma_{ne}$ . If  $p_0$  is such a singular point, then

 $\tilde{G}(p)$  is meromorphic in some neighborhood of  $p_0$ , and admits the Laurent expansion

$$\tilde{G}(p) = \sum_{k=-s}^{\infty} (p - p_0)^k G_k,$$
(6.365)

for some  $s > \infty$ , where for  $-s \le k \le -1$  each of the operators  $G_k \in L(X;Y)$  has a finite-dimensional image.

**Remark** If  $\Sigma_{ne} \cap \Sigma_h \neq \emptyset$ , then we can also consider the function  $p \mapsto \tilde{G}(p)$  within this subset. The conclusions of the above theorem need not, however, apply in this case due to the operator  $\tilde{S}(p)$  not necessarily being Fredholm.

**Proof** Let  $p_0 \in \Sigma_e$  be a point with  $\ker(\tilde{S}(p_0)) \neq \{0\}$ . As  $\tilde{S}(p_0) \in L(Y;X)$  is a Fredholm operator with index equal to zero, we can write

$$Y = Y_1 \oplus Y_2, \quad X = X_1 \oplus X_2,$$
 (6.366)

where  $Y_2 = \ker(\tilde{S}(p_0))$  is finite-dimensional,  $Y_1 = Y_2^{\perp}$  is closed,  $X_1 = \operatorname{im}(\tilde{S}(p_0))$  is closed, and  $X_2 = \operatorname{im}(\tilde{S}(p_0))^{\perp}$  is finite-dimensional with

$$\dim Y_2 = \dim X_2. \tag{6.367}$$

Corresponding to this decomposition we can write  $\tilde{S}(p)$  in a neighborhood of  $p_0$  in matrixform as

$$\tilde{S}(p) = \begin{pmatrix} \tilde{S}_{11}(p) & \tilde{S}_{12}(p) \\ \tilde{S}_{21}(p) & \tilde{S}_{22}(p) \end{pmatrix}, \tag{6.368}$$

where  $\tilde{S}_{11}(p)$  denotes the restriction of  $\tilde{S}(p)$  to a linear mapping from  $Y_1 \to X_1$ , and the other matrix elements are defined correspondingly. By assumption,  $\tilde{S}_{11}(p_0)$  is invertible at  $p_0$ , and so by Lemma 6.4.7, is invertible for all p in some neighborhood of  $p_0$ . Consequently, we can factor the above expression for  $\tilde{S}(p)$  as

$$\begin{pmatrix} \tilde{S}_{11} & \tilde{S}_{12} \\ \tilde{S}_{21} & \tilde{S}_{22} \end{pmatrix} = \begin{pmatrix} \tilde{S}_{11} & 0 \\ \tilde{S}_{21} & \tilde{S}_{22} - \tilde{S}_{21}\tilde{S}_{11}^{-1}\tilde{S}_{12} \end{pmatrix} \begin{pmatrix} 1_{11} & \tilde{S}_{11}^{-1}\tilde{S}_{12} \\ 0 & 1_{22} \end{pmatrix}, \tag{6.369}$$

where  $1_{11}$  and  $1_{22}$  denote, respectively, the identity operators on  $Y_1$  and  $Y_2$ , and where we have suppressed the explicit dependence of the matrix elements on p for notational clarity. From this decomposition we see that  $\tilde{S}(p)$  is invertible if and only if

$$\tilde{T}(p) = \tilde{S}_{22}(p) - \tilde{S}_{21}(p)\tilde{S}_{11}(p)^{-1}\tilde{S}_{12}(p), \tag{6.370}$$

is invertible, and that in this case

$$\begin{pmatrix} \tilde{S}_{11} & \tilde{S}_{12} \\ \tilde{S}_{21} & \tilde{S}_{22} \end{pmatrix}^{-1} = \begin{pmatrix} 1_{11} & -\tilde{S}_{11}^{-1}\tilde{S}_{12} \\ 0 & 1_{22} \end{pmatrix} \begin{pmatrix} \tilde{S}_{11}^{-1} & 0 \\ -\tilde{T}^{-1}\tilde{S}_{21}\tilde{S}_{11}^{-1} & \tilde{T}^{-1} \end{pmatrix}. \tag{6.371}$$

 $\tilde{T}(p)$  is a linear mapping between the finite-dimensional vector spaces  $Y_2$  and  $X_2$ , which we noted above have  $\dim Y_2 = \dim X_2$ . It follows that  $\tilde{T}(p)$  is invertible if and only if its determinant  $\det \tilde{T}(p)$  relative to some arbitrary bases for  $Y_2$  and  $X_2$  is non-zero. We know the function  $p \mapsto \tilde{S}_{11}(p)^{-1}$  depends holomorphically on p in some neighborhood of  $p_0$ , which implies that  $p \mapsto \det \tilde{T}(p)$  is holomorphic in some neighborhood of  $p_0$ . As  $\tilde{S}(p)$  is invertible for some  $p \in \mathbb{C}$ , we see that  $\det \tilde{T}(p)$  does not vanish identically in a neighborhood of  $p_0$ , and so can conclude that in any bounded neighborhood of  $p_0$  the zeros of  $\det \tilde{T}(p)$  form a discrete set with no accumulation points. It follows that the points  $p \in \Sigma_e$  for which  $p \mapsto \tilde{G}(p)$  is singular form a discrete set, and that they may accumulate only at  $\infty$  or to points lying in  $\Sigma_{ne}$ .

Let  $p_0$  be such an isolated singular point of  $p \mapsto \tilde{G}(p)$ . From the above argument we see that  $\tilde{G}(p)$  is defined in some open punctured region of  $p_0$ , and can be decomposed as

$$\tilde{G} = \begin{pmatrix} 1_{11} & -\tilde{S}_{11}^{-1}\tilde{S}_{12} \\ 0 & 1_{22} \end{pmatrix} \begin{pmatrix} \tilde{S}_{11}^{-1} & 0 \\ -\tilde{T}^{-1}\tilde{S}_{21}\tilde{S}_{11}^{-1} & \tilde{T}^{-1} \end{pmatrix}, \tag{6.372}$$

where we have again suppressed the dependence of the various terms on p for notational clarity. At  $p = p_0$  the singularity of  $\tilde{G}(p)$  arises from the singularity of finite-dimensional operator  $\tilde{T}(p)^{-1}$ , and it follows that the coefficients of the principal part of the Laurent series for  $\tilde{G}(p)$  at  $p_0$  will all have finite-dimensional images. Recalling that, with respect to some arbitrary bases of  $Y_2$  and  $X_2$ , the inverse of  $\tilde{T}(p)$  can be written

$$\tilde{T}(p)^{-1} = \frac{1}{\det \tilde{T}(p)} \operatorname{adj} \tilde{T}(p), \tag{6.373}$$

where  $\operatorname{adj}\tilde{T}(p)$  is adjugate matrix of  $\tilde{T}(p)$  which is holomorphic at  $p_0$ , we see that at  $p_0$  the function  $p \mapsto \tilde{T}(p)^{-1}$  can have at most a finite-order pole, and that the order of this pole is less than or equal to the order of the zero of  $\det \tilde{T}(p)$  at this point. It follows that  $\tilde{G}(p)$  can also have at most a finite-order pole at  $p_0$ .

#### 

#### Root functions and residues

Let  $p_0 \in \Sigma_e$  be an sth-order pole of  $\tilde{G}(p)$ . Following Gohberg & Sigal (1971) and Mennicken & Möller (1984), a Y-valued function  $p \mapsto u(p)$  which is holomorphic in some neighborhood of  $p_0$  is said to be a root function of  $\tilde{S}$  at  $p_0$  if  $u(p_0) \neq 0$  and  $(\tilde{S}u)(p_0) = 0$ , where we have

written  $(\tilde{S}u)(p) = \tilde{S}(p)u(p)$ . If u is such a root function at  $p_0$ , we write  $\nu(u)$  for the order of the zero of  $(\tilde{S}u)(p)$  at  $p_0$  which we call the *multiplicity* of u. To illustrate this idea, let u be such a root function at  $p_0$  which admits the Taylor expansion

$$u(p) = \sum_{l=0}^{\infty} (p - p_0)^l u_l, \tag{6.374}$$

while  $\tilde{S}(p)$  can be similarly written

$$\tilde{S}(p) = \sum_{k=0}^{\infty} (p - p_0)^k S_k. \tag{6.375}$$

As both these series are uniformly convergent in some neighborhood of  $p_0$ , we can write

$$(\tilde{S}u)(p) = \sum_{k=0}^{\infty} (p - p_0)^k \sum_{l=0}^k S_l u_{k-l}, \tag{6.376}$$

and the vanishing of  $(\tilde{S}u)(p)$  to  $\nu(u)$ th-order implies

$$S_0 u_0 = 0, (6.377)$$

$$S_0 u_1 + S_1 u_0 = 0, (6.378)$$

:

$$S_0 u_{\nu(u)-1} + S_1 u_{\nu(u)-2} + \dots + S_{\nu(u)} u_0 = 0. \tag{6.379}$$

These equations imply that  $u_0 \in \ker(\tilde{S}(p_0))$ , and that the vectors  $u_l$  for  $l = 1, ..., \nu(u) - 1$  are defined recursively through

$$S_0 u_l + S_1 u_{l-1} + \dots + S_l u_0 = 0. (6.380)$$

We say that the ordered set of vectors  $\{u_0, u_1, \dots, u_{\nu(v)-1}\}$  forms a chain of eigenvectors and associated vectors (CEAV) for  $\tilde{S}$  at  $p_0$ . It follows that to every root function we can associate a CEAV, and conversely, that to any such chain  $\{u_0, u_1, \dots, u_h\}$  we can define a root function

$$u(p) = \sum_{l=0}^{h} (p - p_0)^l u_l, \tag{6.381}$$

having  $\nu(u) \geq h+1$ . In particular, we see that we can, without loss of generality, assume that root functions are always polynomials of order at most one less than their multiplicity. Given an element  $u_0 \in \ker(\tilde{S}(p_0))$ , we define its  $\operatorname{rank} \rho(u_0)$  to be the maximum value of  $\nu(u)$  as u ranges over root functions at  $p_0$  with  $u(p_0) = u_0$ . From this definition, we see that for each  $u_0 \in \ker(\tilde{S}(p_0))$  with  $\rho(u_0) = \nu$ , we can associate a CEAV  $\{u_0, u_1, \ldots, u_h\}$  with  $h \leq \nu - 1$ .

A system  $\{u_1, \ldots, u_r\}$  of root functions of  $\tilde{S}$  at  $p_0$  is called a *canonical system of root functions* (CSRF) if:

- 1. The set of vectors  $\{u_1(p_0), \ldots, u_r(p_0)\}$  forms a basis for  $\ker(\tilde{S}(p_0))$ .
- 2.  $\nu(u_i)$  is the maximum of all  $\nu(u)$  where u varies in the set of the root functions of  $\tilde{S}$  at  $p_0$  with  $u(p_0) \in \ker(\tilde{S}(p_0)) \setminus \operatorname{span}\{u_1(p_0), \dots, u_{i-1}(p_0)\}.$

The existence of such a CSRF at  $p_0$  can be seen as follows. For each integer  $\nu \geq 1$ , let  $L_{\nu}$  denote the subspace of  $\ker(\tilde{S}(p_0))$  comprising the zero-vector along with the set of all  $u_0 \in Y$  for which there exists a root function u of  $\tilde{S}$  at  $p_0$  with  $u(p_0) = u_0$  and  $\nu(u) \geq \nu$ . Clearly we have the inclusions  $\ker(\tilde{S}(p_0)) \supseteq L_1 \supseteq L_2 \supseteq \cdots$ . Also, from the results of the previous paragraph, we see that if  $u_0 \in \ker(\tilde{S}(p_0))$ , then  $p \mapsto u(p) = u_0$  is a root function at  $p_0$  with  $\nu(u) \geq 1$ , so that  $\ker(\tilde{S}(p_0)) = L_1$ . For p in some punctured neighborhood of  $p_0$  we have  $\tilde{G}(p)(\tilde{S}u_i)(p) = u_i(p)$  for each  $i = 1, \ldots, r$ . It follows that the singularity of  $p \mapsto \tilde{G}(p)(\tilde{S}u_i)(p)$  at  $p_0$  is removable and that this function is non-zero there. As we have assumed that  $\tilde{G}(p)$  has an sth-order pole at  $p_0$ , this implies that the multiplicity of  $u_i$  cannot be greater than s. We conclude that

$$\ker(\tilde{S}(p_0)) = L_1 \supseteq L_2 \supseteq \dots \supseteq L_s \supseteq L_{s+1} = \{0\}. \tag{6.382}$$

Let us set  $r_s = \dim L_s$ , and suppose  $\{u_1^0, \dots, u_{r_s}^0\}$  is an arbitrary basis for  $L_s$ . For each  $u_j^0$  with  $1 \leq j \leq r_s$  there exists a root function  $p \mapsto u_j(p)$  such that  $u_j(p_0) = u_j^0$ , and  $\nu(u_j) = s$ . If  $r_s = \text{nul}(\tilde{S}(p_0))$ , the set of functions  $\{u_1, \dots, u_{r_s}\}$  forms a CSRF for  $\tilde{S}$  at  $p_0$ . Otherwise, we consider the quotient space  $L_{s-1}/L_s$ , and construct root functions  $u_{r_s+1}, \dots, u_{r_{s-1}}$  with multiplicity s-1 from arbitrary basis elements of  $L_{s-1}/L_s$ . Continuing this process for the space  $L_{s-1}/L_{s-2}$ , and so on, we eventually obtain the desired CSRF for  $\tilde{S}$  at  $p_0$ .

We saw above that the coefficients  $G_k \in L(X;Y)$  for  $-s \le k \le -1$  of the principal part of the Laurent series for  $\tilde{G}(p)$  at an sth-order pole  $p_0$  have finite-dimensional images. If the vectors  $\{u_1, \ldots, u_r\} \subseteq Y$  form a basis of  $\operatorname{im}(G_k)$  for a given k with  $-s \le k \le -1$ , then it is clear that

$$G_k = \sum_{i=1}^r u_i \otimes v_i, \tag{6.383}$$

for some  $\{v_1,\ldots,v_r\}\in X$ , where we have defined the linear operator  $u_i\otimes v_i\in L(X;Y)$  by

$$(u_i \otimes v_i)u = (u, v_i)_X u_i, \tag{6.384}$$

for any  $u \in X$ . We note that under this definition, the mapping  $(u, w) \mapsto u \otimes v$  is linear in the first argument and conjugate linear in the second. It follows that if the function  $p \mapsto$ 

 $u(p) \in Y$  is holomorphic in some neighborhood of a point  $p_0 \in \mathbb{C}$ , and and if  $p \mapsto v(p) \in X$  is holomorphic in a neighborhood of  $\overline{p_0}$ , then the operator-valued function  $p \mapsto u(p) \otimes v(\overline{p})$  is holomorphic in some neighborhood of  $p_0$ . We will require the following result which is equivalent to Proposition (1.11) of Mennicken & Möller (1984):

**Lemma 6.6.16** Let X and Y be Hilbert spaces, and U be an open neighborhood of a point  $p \in \mathbb{C}$ . Suppose that the functions  $u_1, \ldots, u_r : U \to Y$  are holomorphic in U, and such that the vectors  $u_1(p_0), \ldots, u_r(p_0)$  are linearly independent. If  $v_1, \ldots, v_r : U \to X$  is a set of functions that are meromorphic at  $\overline{p_0}$ , and if the function

$$\sum_{j=1}^{r} u_j(p) \otimes v_j(\overline{p}), \tag{6.385}$$

is holomorphic at  $p_0$ , then each of the functions  $v_j(p)$  is holomorphic at  $\overline{p_0}$ .

Following Mennicken & Möller (1984) we now shall show:

**Theorem 6.6.17** Let  $p_0$  be an sth-order pole of  $\tilde{G}(p)$ ,  $\{u_1, \ldots, u_r\}$  a CSRF for  $\tilde{S}$  at  $p_0$ , and set  $m_j = \nu(u_j)$ . There exist unique polynomials  $v_j : \mathbb{C} \to X$  for  $j = 1, \ldots, r$  of degree less than  $m_j$  and a unique function  $p \mapsto \tilde{G}_+(p) \in L(X;Y)$  holomorphic in an neighborhood of  $p_0$  such that

$$\tilde{G}(p) = \sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes v_j(\overline{p}) + \tilde{G}_+(p), \tag{6.386}$$

in some punctured neighborhood of  $p_0$ .

**Proof** We prove the result by induction. We wish to show that for q = 0, ..., s there are polynomials  $v_j^q : \mathbb{C} \to X$  of degree less than  $m_j$  such that the order of the pole at  $p_0$  of the function

$$\tilde{G}(p) - \sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes v_j^q(\overline{p}), \tag{6.387}$$

does not exceed s - q.

For q = 0 this result holds trivially by taking  $v_j^0 = 0$  for j = 1, ..., r. Assuming that the above result holds for some  $0 \le q < s$ , we wish to show that it also holds for q + 1. To do this we define the meromorphic function

$$H(p) = \sum_{l=-s+q}^{\infty} (p - p_0)^l H_l = \tilde{G}(p) - \sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes v_j^q(\overline{p}),$$
 (6.388)

for p in some punctured neighborhood of  $p_0$ . We note that for j = 1, ..., r, the function  $p \mapsto (p - p_0)^{-m_j} \tilde{S}(u_j)(p)$  is holomorphic at  $p_0$  as  $m_j = \nu(u_j)$ . For p in some punctured neighborhood of  $p_0$  we have

$$\tilde{S}(p)H(p) = 1 - \sum_{j=1}^{r} (p - p_0)^{-m_j} (\tilde{S}u_j)(p) \otimes v_j^q(\overline{p}),$$
 (6.389)

and it follows that the singularity of this function at  $p_0$  is removable. Let  $u_0$  be a non-zero element of  $\operatorname{im}(H_{-s+q})$  such that  $u_0 = H_{-s+q}w$  for some  $w \in Y$ , and define  $u(p) = (p-p_0)^{s-q}H(p)w$ . From eq.(6.389) we see that

$$(\tilde{S}u)(p) = (p - p_0)^{s-q}w - \sum_{i=1}^{r} (p - p_0)^{-m_j + s - q} \left(w, v_j^q(\overline{p})\right)_X (\tilde{S}u_j)(p), \tag{6.390}$$

and as s-q>0, we conclude that u is a root function for  $\tilde{S}$  at  $p_0$  having  $\nu(u)\geq s-q$ . It follows that  $u_0$  is an element of the finite-dimensional subspace  $L_{s-q}$ , and we can conclude that  $\operatorname{im}(H_{-s+q})\subseteq L_{s-q}$ . Recalling that  $L_{s-q}\subseteq \ker(\tilde{S}(p_0))$  and that  $\{u_1(p_0),\ldots,u_r(p_0)\}$  forms a basis for  $\ker(\tilde{S}(p_0))$  we see that

$$H_{-s+q} = \sum_{j=1}^{r} u_j(p_0) \otimes v_j, \tag{6.391}$$

for some  $v_j \in X$  such that  $v_j = 0$  if  $m_j < s - q$ . We now define

$$v_i^{q+1}(p) = v_i^q(p) + (p - \overline{p_0})^{m_j - s + q} v_j, \tag{6.392}$$

for j = 1, ..., r which are seen to be polynomials of degree less than  $m_j$ . In terms of these polynomials we can now calculate

$$\tilde{G}(p) - \sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes v_j^{q+1}(\overline{p})$$

$$= (p - p_0)^{-s+q} H_{-s+q} + \sum_{l=-s+q+1}^{\infty} (p - p_0)^l H_l - \sum_{j=1}^{r} (p - p_0)^{-s+q} u_j(p) \otimes v_j$$

$$= \sum_{l=-s+q+1}^{\infty} (p - p_0)^l H_l - \sum_{j=1}^{r} (p - p_0)^{-s+q} [u_j(p) - u_j(p_0)] \otimes v_j. \tag{6.393}$$

It is clear that the final term has at most a (s-q-1)th-order pole at  $p_0$ , which completes the induction step. By taking  $v_j(p) = v_j^s(p)$  we obtain eq.(6.386).

To see that the polynomials  $v_j$  in eq.(6.386) are unique, suppose that this equation holds for two different sets of polynomials  $\{v_1, \ldots, v_r\}$  and  $\{v'_1, \ldots, v'_r\}$ . We would then have

$$\sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes [v_j(\overline{p}) - v_j'(\overline{p})], \tag{6.394}$$

equal to a holomorphic function. However, as  $v_j$  and  $v'_j$  are polynomials of order less than  $m_j$ , the only way this can happen is if  $v_j = v'_j$  identically. We similarly see that the function

 $p \mapsto \tilde{G}_+(p)$  is unique.

**Lemma 6.6.18** The polynomials  $v_j : \mathbb{C} \to X$  for j = 1, ..., r occurring in eq.(6.386) take their values in Y.

**Proof** For any  $u \in Y$ ,  $v \in X$ , we have defined the operator  $u \otimes v \in L(X;Y)$  by

$$(u \otimes v)w = (w, v)_{x} u. \tag{6.395}$$

Recalling that Y is a dense subspace of X, we can also regard  $u \otimes v$  as being a bounded operator on X. The adjoint  $(u \otimes v)^*$  of this operator in X is defined so that

$$((u \otimes v)w_1, w_2)_X = (w_1, (u \otimes v)^*w_2)_X,$$
 (6.396)

for all  $w_1, w_2 \in X$ , and a simple calculation shows that

$$(u \otimes v)^* = v \otimes u. \tag{6.397}$$

For  $-s \le k \le -1$  let  $G_k$  denote the coefficients of the principal part of the Laurent series for  $\tilde{G}(p)$  about  $p_0$ . From eq.(6.386) and eq.(6.397) we see that  $\operatorname{im}(G_k^*)$  is contained in the space spanned by the coefficients of the polynomials  $v_j(p)$  for  $j=1,\ldots,r$ , and, in particular, that every such coefficient is in  $\operatorname{im}(G_k^*)$  for some  $-s \le k \le -1$ . For p in some punctured neighborhood of  $p_0$  we have  $\tilde{G}(p)\tilde{S}(p)=1$  which implies that

$$\operatorname{im}(\tilde{S}(p_0)) \subseteq \ker(G_k), \tag{6.398}$$

for  $-s \le k \le -1$ . Taking orthogonal complements of this inclusion in X gives

$$\ker(G_k)^{\perp} \subseteq \operatorname{im}(\tilde{S}(p))^{\perp}, \tag{6.399}$$

and using the eq.(6.135) and eq.(6.136) we obtain

$$\operatorname{im}(G_k^*) \subseteq \ker(\tilde{S}(p_0)^*) \subseteq Y. \tag{6.400}$$

We noted above that  $\bigoplus_{-s \leq k \leq -1} \operatorname{im}(G_k^*)$  coincides with the vector space spanned by the coefficients of the polynomials  $v_j(p)$  for  $j = 1, \ldots, r$ . It follows that each such polynomial coefficient is an element of Y, and hence that the polynomials  $v_j(p)$  take values in Y.

**Theorem 6.6.19** The polynomials  $\{v_1(p), \ldots, v_r(p)\}$  occurring in eq.(6.386) form a CSRF for  $\tilde{S}$  at the point  $\overline{p_0}$ , and satisfy the biorthogonality relations

$$\frac{1}{l!} \frac{\mathrm{d}^l}{\mathrm{d}p^l} \left( (p - p_0)^{-h} (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X \bigg|_{p = p_0} = \delta_{ij} \delta_{m_i - h, l}, \tag{6.401}$$

for  $1 \le i, j \le r, \ 1 \le h \le m_i, \ and \ 0 \le l \le m_j - 1.$ 

**Proof** For p in some punctured neighborhood of  $p_0$  we have  $\tilde{G}(p)\tilde{S}(p) = 1$ , and so from eq.(6.386) can write

$$\sum_{j=1}^{r} (p - p_0)^{-m_j} (u_j(p) \otimes v_j(\overline{p})) \tilde{S}(p) + \tilde{G}_+(p) \tilde{S}(p) = 1.$$
 (6.402)

If follows that the function

$$\sum_{j=1}^{r} (p - p_0)^{-m_j} (u_j(p) \otimes v_j(\overline{p})) \tilde{S}(p), \tag{6.403}$$

is holomorphic in some neighborhood of  $p_0$ . From the definition of  $u_j \otimes v_j$  and Lemma 6.6.18, we see that for any  $w \in Y$ 

$$(p-p_0)^{-m_j}(u_j(p)\otimes v_j(p))\tilde{S}(p)w = \left(w,\overline{(p-p_0)}^{-m_j}\tilde{S}(\overline{p})v_j(\overline{p})\right)_{X}u_j(p), \tag{6.404}$$

where we have recalled the identity  $\tilde{S}(p)^* = \tilde{S}(\overline{p})$ . From eq.(6.403) we now see that the function

$$\sum_{j=1}^{r} u_{j}(p) \otimes \left[ \overline{(p-p_{0})}^{-m_{j}} \tilde{S}(\overline{p}) v_{j}(\overline{p}) \right], \tag{6.405}$$

is holomorphic in some neighborhood of  $p_0$ , and Lemma 6.6.16 implies that each of the functions

$$p \mapsto (p - \overline{p_0})^{-m_j} \tilde{S}(p) v_i(p), \tag{6.406}$$

is holomorphic in some neighborhood of  $\overline{p_0}$ . It follows that  $(\tilde{S}v_j)(p)$  has a zero of at least  $m_j$ th-order at  $\overline{p_0}$ . We cannot, however, conclude that  $v_j$  is a root function at  $\overline{p_0}$  as we have yet to show that  $v_j(\overline{p_0})$  is non-zero.

Acting eq.(6.402) on  $u_i(p)$  for some  $1 \le i \le r$ , we find that

$$u_i(p) = \sum_{j=1}^r (p - p_0)^{-m_j} \left( (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X u_j(p) + \tilde{G}_+(p)(\tilde{S}u_i)(p).$$
 (6.407)

At  $p_0$  the function  $p \mapsto (\tilde{S}u_i)(p)$  has a zero of order  $m_i$ , which implies that

$$\sum_{i=1}^{r} (p - p_0)^{-m_i} \left[ (p - p_0)^{-m_j} \left( (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X - \delta_{ij} \right] u_j(p), \tag{6.408}$$

is holomorphic at  $p_0$ , and it follows from a simple variation of Lemma 6.6.16 that each of

the functions

$$f_{ij}(p) = (p - p_0)^{-m_i} \left[ (p - p_0)^{-m_j} \left( (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X - \delta_{ij} \right]$$
(6.409)

is holomorphic at  $p_0$ . Noting that we can also write

$$f_{ij}(p) = (p - p_0)^{-m_j} \left[ (p - p_0)^{-m_i} \left( (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X - \delta_{ij} \right], \tag{6.410}$$

we see that for any  $1 \le h \le m_i$ 

$$\left( (p - p_0)^{-h} (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_{X} - (p - p_0)^{m_i - h} \delta_{ij} = (p - p_0)^{m_i + m_j - h} f_{ij}(p), \tag{6.411}$$

which implies that the term on the left hand side has a zero at  $p_0$  of order greater than or equal to  $m_j$ . Differentiating eq.(6.411) l times with  $0 \le l \le m_j - 1$  we then obtain

$$\frac{1}{l!} \frac{\mathrm{d}^l}{\mathrm{d}p^l} \left( (p - p_0)^{-h} (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X \bigg|_{p = p_0} = \delta_{ij} \delta_{m_i - h, l}. \tag{6.412}$$

Taking  $h = m_i$  and l = 0, this gives

$$\left( (p - p_0)^{-m_i} (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X \Big|_{p = p_0} = \delta_{ij}, \tag{6.413}$$

which implies that the vectors  $v_j(\overline{p_0})$  for  $j=1,\ldots,r$  are linearly independent, and so we can conclude that the polynomials  $\{v_1(p),\cdots,v_r(p)\}$  form a CSRF for  $\tilde{S}$  at  $\overline{p_0}$ . Following an argument in Mennicken & Möller (1984), it may also be shown that the multiplicities of each  $v_j$  is in fact equal to  $m_j$ .

Theorem 6.6.17 can be equivalently expressed in terms of chains of eigenvectors and associated vectors for  $\tilde{S}$  at  $p_0$  and at  $\overline{p_0}$ . We say that a system of vectors  $\{u_j^l | 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  defines a canonical system of eigenvectors and associated vectors (CSEAV) of  $\tilde{S}$  at  $p_0$  if:

- 1. The vectors  $\{u_1^0, \ldots, u_r^0\}$  form a basis of  $\ker(\tilde{S}(p_0))$ .
- 2. For each  $j=1,\ldots,r$  the vectors  $\{u_j^0,u_j^1,\ldots,u_j^{m_j-1}\}$  form a CEAV for  $\tilde{S}$  at  $p_0$ .
- 3. The numbers  $m_i$  are given by

$$m_i = \sup\{\rho(u^0) \mid u^0 \in \ker(\tilde{S}(p_0)) \setminus \operatorname{span}\{u_b^0 \mid k < j\}\},$$
 (6.414)

where we recall that  $\rho(u^0)$  denotes the rank of  $u^0$ .

Let  $\{u_j^l | 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  be a CSEAV for  $\tilde{S}$  at  $p_0$ . Then it is clear that the functions

$$u_j(p) = \sum_{l=0}^{m_j - 1} (p - p_0)^l u_j^l, \quad 1 \le j \le r,$$
(6.415)

form a CSRF for  $\tilde{S}$  at  $p_0$ . Conversely, if  $\{u_1, \ldots, u_r\}$  is a CSRF for  $\tilde{S}$  at  $p_0$ , then we can assume without loss of generality that each of the root functions  $u_j$  takes the form

$$u_j(p) = \sum_{l=0}^{m_j-1} (p - p_0)^l u_j^l, \tag{6.416}$$

for some vectors  $\{u_j^l \mid 0 \le l \le m_j - 1\}$  with  $m_j = \nu(u_j)$ , and it is easy to see that  $\{u_j^l \mid 1 \le j \le r, 0 \le l \le m_j - 1\}$  is a CSEAV for  $\tilde{S}$  at  $p_0$ . Adapting Theorem (3.4) of Mennicken & Möller (1984) we have:

**Theorem 6.6.20** Let  $p_0 \in \Sigma_e$  be an sth-order pole of  $p \mapsto \tilde{G}(p)$ , and  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  a CSEAV for  $\tilde{S}$  at  $p_0$ . Then there exists a CSEAV  $\{v_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  for  $\tilde{S}$  at  $\overline{p_0}$  such that in some punctured neighborhood of  $p_0$  we have

$$\tilde{G}(p) = \sum_{j=1}^{r} \sum_{k=1}^{m_j} (p - p_0)^{-k} \sum_{l=0}^{m_j - k} u_j^l \otimes v_j^{m_j - l - k} + \tilde{G}_+(p), \tag{6.417}$$

where  $p \mapsto \tilde{G}_+(p)$  is holomorphic at  $p_0$ . The vectors  $u_i^l$  and  $v_j^l$  occurring in this expression satisfy the biorthogonality relations

$$\sum_{k=0}^{l} \left( \sum_{q=1}^{m_i} S_{q+k} u_i^{m_i - q}, v_j^{l-k} \right)_X = \delta_{ij} \delta_{l0}$$
 (6.418)

for  $1 \le i, j \le r$ , and  $0 \le l \le m_i - 1$ .

**Proof** Let  $\{u_1, \ldots, u_r\}$  be the CSRF for  $\tilde{S}$  at  $p_0$  associated with the CSEAV  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  by

$$u_j(p) = \sum_{l=0}^{m_j - 1} (p - p_0)^l u_j^l.$$
 (6.419)

From Theorem 6.6.17 we know that there is a unique CSRF  $\{v_1, \ldots, v_r\}$  for  $\tilde{S}$  at  $\overline{p_0}$  whose members are polynomials, such that

$$\tilde{G}(p) = \sum_{j=1}^{r} (p - p_0)^{-m_j} u_j(p) \otimes v_j(\overline{p}) + \tilde{G}_+(p), \tag{6.420}$$

with  $p \mapsto G_+(p)$  holomorphic at  $p_0$ . For  $1 \le j \le r$  we have

$$v_j(p) = \sum_{l=0}^{m_j-1} (p - \overline{p_0})^l v_j^l, \tag{6.421}$$

where, as we noted above, the vectors  $\{v_j^l | 1 \le j \le r, 0 \le l \le m_j - 1\}$  form a CSEAV for  $\tilde{S}$  at  $\overline{p_0}$ . Substituting the above expressions for  $u_i$  and  $v_j$  into eq.(6.420) and collecting like

powers of  $(p - p_0)$  we obtain eq.(6.417).

From Theorem 6.6.19 we know that the functions  $u_i$  and  $v_j$  must satisfy the biorthogonality relations

$$\frac{1}{l!} \frac{\mathrm{d}^l}{\mathrm{d}p^l} \left( (p - p_0)^{-h} (\tilde{S}u_i)(p), v_j(\overline{p}) \right)_X \bigg|_{p = p_0} = \delta_{ij} \delta_{m_i - h, l}, \tag{6.422}$$

for  $1 \le i, j \le r$ ,  $1 \le h \le m_i$ , and  $0 \le l \le m_j - 1$ . Expanding  $\tilde{S}$  into a Taylor series about  $p_0$ , using the above expressions for  $u_i$  and  $v_j$ , collecting like powers of  $(p - p_0)$ , and using eq.(6.377), we find that

$$\left( (p - p_0)^{-h} \tilde{S}(p) u_i(p), v_j(\overline{p}) \right)_X = \sum_{n=0}^{m_j - 1} (p - p_0)^{m_i + n - h} \sum_{k=m_i}^{m_i + n} \eta_{ij}^{nk} + \sum_{n=m_j}^{\infty} (p - p_0)^{m_i + n - h} \sum_{k=m_i + n - (m_j - 1)}^{m_i + n} \eta_{ij}^{nk}, \quad (6.423)$$

where, for notational clarity, we have defined

$$\eta_{ij}^{nk} = \sum_{q=k-(m_i-1)}^{k} \left( S_q u_i^{k-q}, v_j^{m_i+n-k} \right)_X.$$
 (6.424)

From this expression we find that for  $0 \le l \le m_i - 1$  and  $1 \le h \le m_i$ 

$$\frac{1}{l!} \frac{\mathrm{d}^{l}}{\mathrm{d}p^{l}} \left( (p - p_{0})^{-h} (\tilde{S}u_{i})(p), v_{j}(\overline{p}) \right)_{X} \Big|_{p = p_{0}} = \begin{cases}
\sum_{k=m_{i}}^{h+l} \eta_{ij}^{h+l-m_{i},k} & h+l \geq m_{i} \\
0 & h+l < m_{i}
\end{cases}, (6.425)$$

which, using eq.(6.422), gives

$$\sum_{k=m_i}^{l+h} \left( \sum_{q=k-(m_i-1)}^k S_q u_i^{k-q}, v_j^{l+h-k} \right)_Y = \delta_{ij} \delta_{m_i,l+h}, \tag{6.426}$$

for  $1 \le i, j \le r$ ,  $1 \le h \le m_i$ ,  $0 \le l \le m_j - 1$ , and  $l + h \ge m_i$ . Noting that in the above expression l and h only occur in the combination l + h, we see that, given values of i and j, there are  $m_j - 1$  independent equations corresponding to  $l + h = m_i, m_i + 1, \dots m_i + m_j - 1$ . Setting  $h = m_i$ , and letting  $l = 0, 1, \dots, m_j - 1$ , we obtain eq.(6.418) after re-labeling the summation indices.

**Proposition 6.6.21** Let  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  be a CSEAV for  $\tilde{S}$  at  $p_0$ , and

$$w(p) = \sum_{l=0}^{m_j-1} (p - p_0)^l w^l, \tag{6.427}$$

be a root function for  $\tilde{S}$  at  $p_0$  with multiplicity equal to  $m_j$  for some  $1 \leq j \leq r$ . Then there

exists unique coefficients  $C_k^l$  for  $1 \le k \le r$  and  $0 \le l \le m_j - 1$  such that

$$w^{l} = \sum_{n=0}^{l} \sum_{k=1}^{r} C_{k}^{n} u_{k}^{l-n}, \tag{6.428}$$

where  $C_k^0 = 0$  for  $k > \dim L_{m_j}$ .

**Proof** As  $w^0$  is in  $L_{m_j}$ , and as  $\{u_1^0, \ldots, u_{r_j}^0\}$  with  $r_j = \dim L_{m_j}$  forms a basis for this subspace, we see that there are unique coefficients  $C_k^0$  such that

$$w^0 = \sum_{k=1}^{r_j} C_k^0 u_k^0, \tag{6.429}$$

which proves eq.(6.428) in the case  $m_j = 1$ . For  $m_j > 1$  we proceed by induction. Assuming that eq.(6.428) holds for some  $0 \le l \le m_j - 2$ , we wish to show that it also holds for l + 1. From eq.(6.377) we see that

$$S_0 w^m + \ldots + S_m w^0 = 0, (6.430)$$

$$S_0 u_i^m + \ldots + S_m u_i^0 = 0, \quad 1 \le j \le r, \tag{6.431}$$

for each  $0 \le m \le l+1$ . From these equations we obtain

$$S_{0}w^{l+1} + \dots + S_{l+1}w^{0} - \sum_{k=1}^{r} C_{k}^{0} \left[ S_{0}u_{k}^{l+1} + \dots + S_{l+1}u_{k}^{0} \right]$$

$$- \sum_{k=1}^{r} C_{k}^{1} \left[ S_{0}u_{k}^{l} + \dots + S_{l}u_{k}^{0} \right]$$

$$\vdots$$

$$- \sum_{k=1}^{r} C_{k}^{l} \left[ S_{0}u_{k}^{1} + S_{1}u_{k}^{0} \right] = 0, \qquad (6.432)$$

which, by grouping terms, gives

$$S_{0}\left(w^{l+1} - \sum_{n=0}^{l} \sum_{k=1}^{r} C_{k}^{n} u_{k}^{l+1-n}\right)$$

$$+ S_{1}\left(w^{l} - \sum_{n=0}^{l} \sum_{k=1}^{r} C_{k}^{n} u_{k}^{l-n}\right)$$

$$\vdots$$

$$+ S_{l+1}\left(w^{0} - \sum_{k=1}^{r} C_{k}^{0} u_{k}^{0}\right) = 0.$$

$$(6.433)$$

Making use of eq.(6.428) this expression reduces to

$$S_0\left(w^{l+1} - \sum_{n=0}^l \sum_{k=1}^r C_k^n u_k^{l+1-n}\right) = 0.$$
(6.434)

It follows that there are unique coefficients  $C_k^{l+1}$  such that

$$w^{l+1} - \sum_{n=0}^{l} \sum_{k=1}^{r} C_k^n u_k^{l+1-n} = \sum_{k=1}^{r} C_k^{l+1} u_k^0, \tag{6.435}$$

which implies that eq.(6.428) does hold for l + 1.

Corollary 6.6.22 Let  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  and  $\{w_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  be two CSEAV for  $\tilde{S}$  at  $p_0$ . Then for each  $1 \leq j \leq r$  there exists unique coefficients  $C_{jk}^l$  for  $0 \leq l \leq m_j - 1$  and  $1 \leq k \leq r$  such that

$$w_j^l = \sum_{n=0}^l \sum_{k=1}^r C_{jk}^n u_k^{l-n}, \tag{6.436}$$

where  $C_{jk}^0 = 0$  if  $k > \dim L_{m_j}$ .

**Lemma 6.6.23** Let  $\{u_1, \ldots, u_r\}$  be a CSRF for  $\tilde{S}$  at  $p_0$ . Then the functions  $\{v_1, \ldots, v_r\}$  defined by

$$v_j(p) = Ju_j(\overline{p}), \tag{6.437}$$

form a CSRF for  $\tilde{S}$  at  $\overline{p_0}$ .

**Proof** The result follows easily from the identity  $\tilde{S}(\overline{p}) = J\tilde{S}(p)J$ .

Combining Corollary 6.6.22, Lemma 6.6.23, and Theorem 6.6.20 we obtain

**Theorem 6.6.24** Let  $p_0 \in \Sigma_e$  be an sth-order pole of  $p \mapsto \tilde{G}(p)$ , and  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  a CSEAV for  $\tilde{S}$  at  $p_0$ . If  $\{v_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  is the CSEAV for  $\tilde{S}$  at  $\overline{p_0}$  associated with  $\{u_j^l \mid 1 \leq j \leq r, 0 \leq l \leq m_j - 1\}$  through Theorem 6.6.20, then for each  $1 \leq j \leq r$  there exist unique coefficients  $C_{jt}^l$  for  $0 \leq l \leq m_j - 1$  and  $1 \leq t \leq r$  such that

$$v_j^l = \sum_{n=0}^l \sum_{t=1}^r \overline{C_{jt}^n} J u_t^{l-n}, \tag{6.438}$$

where  $C_{jt}^0 = 0$  for  $t > \dim L_{m_j}$ . In terms of these coefficients, we can express eq. (6.417) as

$$\tilde{G}(p) = \sum_{j=1}^{r} \sum_{k=1}^{m_j} (p - p_0)^{-k} \sum_{l=0}^{m_j - k} \sum_{n=0}^{m_j - l - k} \sum_{t=1}^{r} C_{jt}^n u_j^l \otimes J u_t^{m_j - l - k - n} + \tilde{G}_+(p).$$

$$(6.439)$$

The values of the  $C_{it}^l$  can be determined from the system of linear equations

$$\sum_{k=0}^{l} \sum_{n=0}^{l-k} \sum_{t=1}^{r} C_{jt}^{n} \left( \sum_{q=1}^{m_{i}} S_{q+k} u_{i}^{m_{i}-q}, J u_{t}^{l-k-n} \right)_{Y} = \delta_{ij} \delta_{l0}, \tag{6.440}$$

for  $1 \le i, j \le r$ , and  $0 \le l \le m_j - 1$ .

If we define

$$D_{ti}^{kl} = \left(\sum_{q=1}^{m_i} S_{q+k} u_i^{m_i - q}, J u_t^l\right)_{Y}, \tag{6.441}$$

then we may write eq.(6.440) concisely as

$$\sum_{k=0}^{l} \sum_{n=0}^{l-k} \sum_{t=1}^{r} C_{jt}^{n} D_{ti}^{k,l-k-n} = \delta_{ij} \delta_{l0}.$$
(6.442)

For fixed  $1 \le j \le r$ , we see that when l = 0

$$\sum_{t=1}^{r} C_{jt}^{0} D_{ti}^{00} = \delta_{ij}, \tag{6.443}$$

while for  $1 \le l \le m_j - 1$  we have the recursive formulae

$$\sum_{t=1}^{r} C_{jt}^{l} D_{ti}^{00} = -\sum_{k=0}^{l-1} \sum_{n=0}^{l-k} \sum_{t=1}^{r} C_{jt}^{n} D_{ti}^{k,l-k-n}.$$

$$(6.444)$$

The above systems of linear equations has a unique solution if and only if the  $r \times r$  matrix with components

$$D_{ij}^{00} = \left(\sum_{q=1}^{m_i} S_q u_j^{m_i - q}, J u_i^0\right)_X, \tag{6.445}$$

is non-singular.

We note, in particular, that at a first-order pole

$$D_{ij}^{00} = \left(S_1 u_j^0, J u_i^0\right)_X, \tag{6.446}$$

and it follows that a necessary condition for a point  $p_0 \in \Sigma_e$  with  $\ker(\tilde{S}(p_0)) \neq \{0\}$  to be a first-order pole of  $p \mapsto \tilde{G}(p)$  is that this matrix is non-singular. This condition can be seen to be sufficient as follows. Suppose that the matrix  $(S_1u_j^0, Ju_i^0)_X$  is non-singular, and that  $p_0$  is a pole of  $\tilde{G}(p)$  of order greater than one. It follows that the vector  $u_1^0 \in \ker(\tilde{S}_0)$  has rank greater than or equal to two, and from eq.(6.377) we can conclude that there exists a vector  $u_1^1$  such that

$$S_0 u_1^1 + S_1 u_1^0 = 0. (6.447)$$

This equation implies that  $S_1u_1^0 \in \operatorname{im}(S_0)$ , which from eq.(6.136) shows that  $S_1u_1^0 \perp J \ker(S_0)$ . However, this condition implies that the first row of the matrix  $(S_1u_j^0, Ju_i^0)_X$  vanishes identically in contradiction with our assumption that this matrix is non-singular. We summarize the above arguments as:

**Proposition 6.6.25** Let  $p_0 \in \Sigma_e$  be a pole of  $p \mapsto \tilde{G}(p)$ , and suppose that the vectors  $\{u_1^0, \ldots, u_r^0\}$  form a basis for  $\ker(\tilde{S}(p_0))$ . A necessary and sufficient condition for  $p_0$  to be a

first-order pole is that the  $r \times r$  matrix with components  $\left(S_1 u_j^0, J u_i^0\right)_X$  is non-singular.

From  $\tilde{S}(p) = p^2 1 + \tilde{A}(p)$  we can write

$$S_1 = 2p_0 1 + A_1, (6.448)$$

where

$$A_1 = \left. \frac{\mathrm{d}}{\mathrm{d}p} \tilde{A}(p) \right|_{p=p_0},\tag{6.449}$$

and so obtain

$$(S_1 u_i^0, J u_i^0)_{X} = 2p_0 (u_i^0, J u_i^0)_{X} + (A_1 u_i^0, J u_i^0)_{X}.$$

$$(6.450)$$

Using  $A_0 u_j^0 = -p_0^2 u_j^0$  we have

$$(u_j^0, Ju_i^0)_X = -\frac{1}{p_0^2} (A_0 u_j^0, Ju_i^0)_X,$$
 (6.451)

and so find

$$(S_1 u_j^0, J u_i^0)_X = -\frac{1}{p_0} ([2A_0 - p_0 A_1] u_j^0, J u_i^0)_X.$$
 (6.452)

From eq.(6.242) we obtain

$$A_0 = \int_{[s_1, s_2]} \frac{p_0}{p_0 + s} M(\mathrm{d}s), \tag{6.453}$$

$$A_1 = \int_{[s_1, s_2]} \frac{s}{(p_0 + s)^2} M(\mathrm{d}s), \tag{6.454}$$

which gives

$$\left(S_1 u_j^0, J u_i^0\right)_X = -\frac{1}{p_0} \int_{[s_1, s_2]} \frac{p_0}{p_0 + s} \left(2 - \frac{s}{p_0 + s}\right) \left(M(\mathrm{d}s) u_j^0, u_i^0\right)_X. \tag{6.455}$$

For  $|p_0| \gg s_2$  we see that the term  $2 - s/(p_0 + s)$  is approximately equal to 2, and so obtain

$$(S_1 u_j^0, J u_i^0)_X \approx 2p_0 (u_j^0, J u_i^0)_X.$$
 (6.456)

In the linear elastic case we have  $JA_0J = A_0$ , which implies that if  $u_i^0 \in \ker(A_0)$  then so is  $Ju_i^0$  and we can write

$$Ju_i^0 = \sum_{k=1}^r \overline{\alpha_{ik}} u_k^0, \tag{6.457}$$

where  $\overline{\alpha_{ik}}$  are the components of a non-singular matrix. In the viscoelastic case this result does not hold, but for large  $|p_0|$  the operator  $A_0$  tends to

$$A_{\infty} = M([s_1, s_2]), \tag{6.458}$$

which does satisfy  $JA_{\infty}J=A_{\infty}$ . Proceeding informally, this suggests that for large  $|p_0|$  we

have

$$Ju_i^0 = \sum_{k=1}^r \overline{\alpha_{ik}} u_k^0 + v_i, \tag{6.459}$$

where  $\overline{\alpha_{ik}}$  are again the components of a non-singular matrix and  $v_j$  are some vectors lying in  $\ker(S_0)^{\perp}$ . We do not, however, have a complete proof of this result. Using this expression we see that for large values of  $|p_0|$ 

$$(S_1 u_j^0, J u_i^0)_X \approx 2p_0 \sum_{k=1}^r \alpha_{jk} (u_j^0, u_k^0)_X,$$
 (6.460)

which implies that the matrix  $(S_1u_j^0, Ju_i^0)_X$  is non-singular. From these arguments we conjecture that for sufficiently large values of |p| all poles of  $p \mapsto \tilde{G}(p)$  are simple.

#### Calculation of the Green distribution

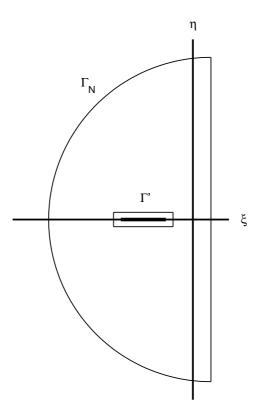


Figure 6.2: A schematic diagram of the contours used in the evaluation of the Green distribution for the viscoelastodynamic equation. In this figure the interval  $\Sigma_{ne}$  of the negative real axis is indicated by a thick line.

To determine the Green distribution for the viscoelastodynamic equation we must evaluate the integral

$$G(t) = \frac{1}{2\pi i} \int_{\xi - i\infty}^{\xi + i\infty} \tilde{G}(p) e^{pt} dp, \qquad (6.461)$$

where  $\tilde{G}(p) = (p^21 + \tilde{A}(p))^{-1}$ , and  $\xi > 0$  is arbitrary. As with the case of the elastodynamic equation, this integral can be approximated by a sequence  $\{\Gamma_N\}_{N=1}^{\infty}$  of semi-circular contour integrals closed in the left half plane with radii tending to infinity. Using Cauchy's theorem, each such contour can be deformed so that the subset  $\Sigma_{ne}$  of the negative real axis is enclosed within a closed contour  $\Gamma'$  of finite length which can be defined independently of N; this situation is shown schematically in fig 6.2. We can then write

$$G(t) = \frac{1}{2\pi i} \int_{\Gamma_{\infty} - \Gamma'} \tilde{G}(p) e^{pt} dp + \frac{1}{2\pi i} \int_{\Gamma'} \tilde{G}(p) e^{pt} dp, \qquad (6.462)$$

for  $t \geq 0$ , the convergence of these integrals being understood in the distributional sense. Within the interior of the contour  $\Gamma_N - \Gamma'$  the function  $p \mapsto \tilde{G}(p)$  is meromorphic, and expressions for the principal part of its Laurent series about each pole are given in Theorem 6.6.24. It follows that the integral

$$\frac{1}{2\pi i} \int_{\Gamma_{\infty} - \Gamma'} \tilde{G}(p) e^{pt} dp, \qquad (6.463)$$

can be expressed as a sum over the eigenvectors and associated vectors of  $\tilde{A}(p)$  corresponding to each of these poles. Let  $\{p_q\}_{q=1}^{\infty}$  denote the set of singularities of  $\tilde{G}(p)$  contained in the exterior of the contour  $\Gamma'$  having  $\mathrm{Im}(p_q) \geq 0$ , this sequence being ordered so that  $\mathrm{Im}(p_{q+1}) \geq \mathrm{Im}(p_q)$ . Note that to each  $p_q$  with  $\mathrm{Im}(p_q) > 0$  there is a corresponding singularity of  $\tilde{G}(p)$  at the point  $\overline{p_q}$ .

At  $p_q$  let  $\{u_j^{lq} | 1 \le j \le r_q, 0 \le l \le m_j^q - 1\}$  be a CSEAV for  $\tilde{S}$ . From Theorem 6.6.24, the principal part of the Laurent series for  $\tilde{G}(p)$  at  $p_q$  can be written

$$\sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} (p - p_0)^{-k} \sum_{l=0}^{m_j^q - k} \sum_{n=0}^{m_j^q - l - k} \sum_{j'=1}^{r_q} C_{jj'}^{n_q} u_j^{lq} \otimes J u_{j'}^{m_j^q - l - k - n, q}, \tag{6.464}$$

where  $C_{jj'}^{nq}$  are constants determined through eq.(6.440) which we here write as

$$\sum_{k=0}^{l} \sum_{n=0}^{l-k} \sum_{j'=1}^{r_q} C_{jj'}^{nq} \left( \sum_{v=1}^{m_i^q} S_{v+k} u_i^{m_i^q - v, q}, J u_{j'}^{l-k-n, q} \right)_X = \delta_{ij} \delta_{l0}, \tag{6.465}$$

for  $1 \le i, j \le r_q$  and  $0 \le l \le m_j^q - 1$ . For an integer  $k \ge 1$  the residue of  $(p - p_q)^{-k} e^{pt}$  at  $p_q$  is equal to  $\frac{1}{(k-1)!} t^{k-1} e^{p_q t}$ , and so the pole of  $\tilde{G}(p)$  at the point  $p_q$  contributes the term

$$\sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \frac{1}{(k-1)!} t^{k-1} e^{p_q t} \sum_{l=0}^{m_j^q - k} \sum_{n=0}^{m_j^q - l - k} \sum_{j'=1}^{r_q} C_{jj'}^{m_q^q} u_j^{lq} \otimes J u_{j'}^{m_j^q - l - k - n, q}, \tag{6.466}$$

to the integral in eq.(6.463).

At the point  $\overline{p_q}$  a CSEAV is given by  $\{Ju_j^{lq} | 1 \leq j \leq r_q, 0 \leq l \leq m_j^q - 1\}$ , and the principal

part of the Laurent series for  $p \mapsto \tilde{G}(p)$  at  $\overline{p_q}$  can be written

$$\sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} (p - \overline{p_0})^{-k} \sum_{l=0}^{m_j^q - k} \sum_{n=0}^{m_j^q - l - k} \sum_{j'=1}^{r_q} C'^{nq}_{jj'} J u_j^{lq} \otimes u_{j'}^{m_j^q - l - k - n, q}, \tag{6.467}$$

for some constants  $C_{jj'}^{'nq}$  which are determined through the modified form of eq.(6.465)

$$\sum_{k=0}^{l} \sum_{n=0}^{l-k} \sum_{j'=1}^{r_q} C_{jj'}^{'nq} \left( \sum_{v=1}^{m_i^q} S_{v+k}^* J u_i^{m_i^q-v,q}, u_{j'}^{l-k-n,q} \right)_{V} = \delta_{ij} \delta_{l0}, \tag{6.468}$$

for  $1 \leq i, j \leq r_q$  and  $0 \leq l \leq m_j^q - 1$ , where in obtaining this equation we have used the identity  $\tilde{S}(\overline{p}) = \tilde{S}(p)^*$ . From  $J\tilde{S}(p)J = \tilde{S}(\overline{p})$  we see that  $S_{q+k}^*J = JS_{q+k}$ , and using the relation  $(Ju, v)_X = \overline{(u, Jv)_X}$ , obtain

$$\sum_{k=0}^{l} \sum_{n=0}^{l-k} \sum_{j'=1}^{r_q} C_{jj'}^{'nq} \overline{\left(\sum_{v=1}^{m_i^q} S_{v+k} u_i^{m_i^q-v,q}, J u_{j'}^{l-k-n,q}\right)_X} = \delta_{ij} \delta_{l0}, \tag{6.469}$$

which, from comparison with eq.(6.465), shows that

$$C_{ij'}^{\prime nq} = \overline{C_{ij'}^{nq}}. (6.470)$$

We note, in particular, that if  $\text{Im}(p_q) = 0$ , then this result implies that the coefficients  $C_{jj'}^{nq}$  are real-valued. We can now write the principal part of the Laurent series for  $\tilde{G}(p)$  at  $\overline{p_q}$  as

$$\sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} (p - \overline{p_0})^{-k} \sum_{l=0}^{m_j^q - k} \sum_{n=0}^{m_j^q - l - k} \sum_{j'=1}^{r_q} \overline{C_{jj'}^{nq}} J u_j^{lq} \otimes u_{j'}^{m_j^q - l - k - n, q}, \tag{6.471}$$

and write the contribution of this pole to the integral in eq.(6.463)

$$\sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \frac{1}{(k-1)!} t^{k-1} e^{\overline{p_q}t} \sum_{l=0}^{m_j^q - k} \sum_{n=0}^{m_j^q - l - k} \sum_{j'=1}^{r_q} \overline{C_{jj'}^{nq}} J u_j^{lq} \otimes u_{j'}^{m_j^q - l - k - n, q}.$$
 (6.472)

Combining these results, we can write

$$\frac{1}{2\pi i} \int_{\Gamma_{\infty}-\Gamma'} \tilde{G}(p) e^{pt} dp = \sum_{q=1}^{N} \sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \sum_{l=0}^{m_j^q-k} \sum_{n=0}^{m_j^q-l-k} \sum_{j'=1}^{r_q} \frac{t^{k-1} C_{jj'}^{nq} e^{p_q t} u_j^{lq} \otimes J u_{j'}^{m_j^q-l-k-n,q}}{(k-1)!} + \sum_{q=N+1}^{\infty} \sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \sum_{n=0}^{m_j^q-k} \sum_{n=0}^{m_j^q-l-k} \sum_{j'=1}^{r_q} \frac{t^{k-1} \left\{ C_{jj'}^{nq} e^{p_q t} u_j^{lq} \otimes J u_{j'}^{m_j^q-l-k-n,q} + \overline{C_{jj'}^{nq}} e^{\overline{p_q} t} J u_j^{lq} \otimes u_{j'}^{m_j^q-l-k-n,q} \right\}}{(k-1)!},$$

$$(6.473)$$

where here we have written N for the (necessarily finite) number of poles  $p_q$  of  $\tilde{G}(p)$  contained within the contour  $\Gamma_{\infty} - \Gamma'$  having  $\text{Im}(p_q) = 0$ . Finally, adding the term arising from the contour  $\Gamma'$ , we obtain:

**Theorem 6.6.26** The Green distribution for the viscoelastodynamic equation can be writ-

ten in terms of the eigenvectors and associated vectors of  $\tilde{S}$  in the form

$$G(t) = \sum_{q=N+1}^{\infty} \sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \sum_{l=0}^{m_j^q-k} \sum_{n=0}^{m_j^q-l-k} \sum_{j'=1}^{r_q} \frac{t^{k-1} \left\{ C_{jj'}^{nq} e^{p_q t} u_j^{lq} \otimes J u_{j'}^{m_j^q-l-k-n,q} + \overline{C_{jj'}^{nq}} e^{\overline{p_q} t} J u_j^{lq} \otimes u_{j'}^{m_j^q-l-k-n,q} \right\}}{(k-1)!} + \sum_{q=1}^{N} \sum_{j=1}^{r_q} \sum_{k=1}^{m_j^q} \sum_{l=0}^{m_j^q-k} \sum_{n=0}^{m_j^q-l-k} \sum_{j'=1}^{r_q} \frac{t^{k-1} C_{jj'}^{nq} e^{p_q t} u_j^{lq} \otimes J u_{j'}^{m_j^q-l-k-n,q}}{(k-1)!} + \frac{1}{2\pi i} \int_{\Gamma'} \tilde{G}(p) e^{pt} dp, \quad (6.474)$$

where the convergence of this expression is understood in the sense of L(X;Y)-valued distributions having support contained in  $[0,\infty)$ .

A simpler expression is obtained if we assume that all the poles of  $\tilde{G}(p)$  enclosed in  $\Gamma_{\infty} - \Gamma'$  are of first-order

$$G(t) = \sum_{q=1}^{N} \sum_{j=1}^{r_q} \sum_{j'=1}^{r_q} C_{jj'}^{0q} e^{p_q t} u_j^{0q} \otimes J u_{j'}^{0q} + \frac{1}{2\pi i} \int_{\Gamma'} \tilde{G}(p) e^{pt} dp$$

$$+ \sum_{q=N+1}^{\infty} \sum_{j=1}^{r_q} \sum_{j'=1}^{r_q} \left\{ C_{jj'}^{0q} e^{p_q t} u_j^{0q} \otimes J u_{j'}^{0q} + \overline{C_{jj'}^{0q}} e^{\overline{p_q} t} J u_j^{0q} \otimes u_{j'}^{0q} \right\}, \qquad (6.475)$$

for  $t \ge 0$ . If we further assume that for each first-order pole the kernel is one-dimensional we obtain

$$G(t) = \sum_{q=1}^{N} C^{0q} e^{p_q t} u^{0q} \otimes J u^{0q} + \frac{1}{2\pi i} \int_{\Gamma'} \tilde{G}(p) e^{pt} dp + \sum_{q=N+1}^{\infty} \left\{ C^{0q} e^{p_q t} u^{0q} \otimes J u^{0q} + \overline{C^{0q}} e^{\overline{p_q} t} J u^{0q} \otimes u^{0q} \right\},$$

$$(6.476)$$

for  $t \geq 0$ , which is equivalent to the results of Al-Attar (2007b). If we neglect the contribution of the integral around  $\Gamma'$  in the above expression, then this expression is equivalent to those obtained by Lognonné (1991), Tromp & Dahlen (1990), Dahlen & Tromp (1998), and Deuss & Woodhouse (2004). We note also that the above expressions reduce to the previously obtained results for the elastodynamic equation in the special case of linear hyperelasticity.

We have not considered in detail the behaviour of  $\tilde{G}(p)$  in the subset  $\Sigma_{ne}$  of the negative real axis, and so have been left with the unevaluated integral  $\frac{1}{2\pi i} \int_{\Gamma'} \tilde{G}(p) e^{pt} dp$  in eq.(6.474). For such p, the operator  $\tilde{S}(p)$  need not be well defined, and even when it is, it may fail to be Fredholm. Consequently, our previous methods for studying the singularities of  $\tilde{G}(p)$  may not be applicable. Within  $\Sigma_{ne}$ , these singularities can, potentially, be very complicated, and do not seem to be ameanable to a simple analysis. For practical calculations, however, the contribution of these singularities can be included through numerical evaluation of the contour integral (e.g. Tanaka *et al.* 2006, 2007).

# 6.7 Discussion

# 6.7.1 Summary of main results

In this chapter we have made a detailed study of viscoelastic normal mode theory. In doing so we have focused on a form of the viscoelastodynamic equation that is slightly simpler than that usually applied in geophysical problems. In particular, we neglected the Earth's initial stress field, its rotation, and the effects of self-gravitation. We also assumed that the earth model is everywhere solid, that it has no internal boundaries, and applied a zero-displacement boundary condition at the surface instead of the usual zero-traction condition. As will be discussed further below, the incorporation of such features into the theory is, for the most part, straightforward, and most results carry over with only minor modifications. Before, however, considering such extensions of the theory, we shall summarize the main results of this chapter:

- 1. We derived existence, uniqueness, and regularity theorems for both the elastodynamic and viscoelastodynamic equations. While such results have long been known for the elastodynamic equation, it is thought that the results presented for the viscoelastodynamic equation are largely new.
- 2. We derived precise bounds on the locations of singularities of the Laplace transform domain Green operator  $p \mapsto \tilde{G}(p)$  in the complex plane. In doing so, we identified two main types of singularity: (i) points at which  $p \mapsto \tilde{S}(p)$  is holomorphic, but for which  $\text{nul}(\tilde{S}(p)) \neq 0$ , and (ii) points at which  $p \mapsto \tilde{S}(p)$  is itself singular, so that  $p \mapsto \tilde{G}(p)$  is not well-defined.
- 3. At points where  $p \mapsto \tilde{S}(p)$  is holomorphic, we showed that all singularities of  $p \mapsto \tilde{G}(p)$  are isolated finite-order poles so long as the operator  $\tilde{S}(p)$  is Fredholm. It was shown that a sufficient condition for  $\tilde{S}(p)$  to be Fredholm is the strong ellipticity of the viscoelastodynamic operator  $\tilde{A}(p)$ , and that this latter condition holds everywhere in  $\mathbb{C}$  except for a bounded subset of the negative real axis.
- 4. We derived a general expression for the residue of  $p \mapsto \tilde{G}(p)$  at an isolated finite-order pole, and gave a necessary and sufficient condition for such a pole to be simple. These

results extend those obtained in earlier studies of viscoelastic normal mode theory which restricted attention to first-order poles. In addition, we conjectured that for sufficiently large values of |p| all poles of  $p \mapsto \tilde{G}(p)$  will be simple.

5. We showed how the Green distribution for the viscoelastodynamic equation can be written as a normal mode sum involving the eigenvectors and assoicated vectors of the operator  $\tilde{S}$ . The expression for G also incorporates the effects of more complicated singularities of  $p \mapsto \tilde{G}(p)$  contained in a bounded portion of the negative real axis.

### 6.7.2 Extensions of the theory

As noted above, the form of the viscoelastodynamic equation considered in this chapter is somewhat simpler than that usually applied in geophysics. In this subsection, we shall outline how the theory presented can be extended to more general problems. Though, in detail, the effects of these various modifications do interact, it will be useful to consider them individually:

1. Boundary conditions: In this chapter we made use of zero-displacement boundary conditions at the surface of the earth model. In addition, we assumed that the earth model possessed no internal boundaries. In geophysical problems, however, the correct boundary conditions at the surface should be that tractions vanish (or equal some prescribed value due to surface loading), and the earth model should incorporate a number of internal boundaries across which displacement and traction should be continuous (discussion of fluid-solid boundaries is given below).

The necessary extensions of the theory to incorporate these more general boundary conditions are essentially straightforward, and only involve slightly more intricate arguments and notations.

2. Initial stress and self-gravitation: For studies of large-scale deformation of the Earth – such as normal mode seismology or post-glacial rebound – it is necessary to incorporate the effects of the Earth's initial stress field and self-gravitation into calculations (e.g. Dahlen 1972a; Valette 1986; Wolf 1991; Dahlen & Tromp 1998). The vis-

coelastodynamic equation is modified in two main ways by the incorporation of such effects: (i) the viscoelastic tensor  $\tilde{a}_{ijkl}$  of the earth model shows an explicit dependence on the initial stress field, (ii) additional terms occur in the viscoelastodynamic equation assoicated with gravitational forces.

From a mathematical point of view, the incorporation of initial stress and self-gravitation into the viscoelastodynamic equation is very simple. This is because the additional terms introduced in the viscoelastodynamic equation depend boundedly on u in the topology of  $L^2(\Omega, \rho; \mathbb{C}^n)$  (e.g. Valette 1989a). Consequently, the results derived in this chapter remain valid with essentially no modification. In detail, however, the incorporation of gravitation into the problem does have some interesting physical consequences. This is because the gravitational terms in the viscoelastodynamic equation, though bounded in  $L^2(\Omega, \rho; \mathbb{C}^n)$ , are not non-negative. As a result, it is possible for the gravitational terms to shift singularities of  $p \mapsto \tilde{G}(p)$  into the right half plane. Such singularities contribute exponentially growing terms to the mode sum solution of the viscoelastodynamic equations, and are associated with gravitational instability of the earth model (e.g. Wolf 1991; Dahlen & Tromp 1998; Vermeersen & Mitrovica 2000).

- 3. Rotation: For studies of the Earth's free oscillations it is necessary to include the effects of the Earth's rotation in the viscoelastodynamic equation in the form of centrifugal and Coriolis forces. The basic results of this chapter can be carried over to the case of a rotating earth model. However, in determining the residue of  $p \mapsto \tilde{G}(p)$  at an isolated pole in a rotating earth model it is necessary to also consider the eigenvectors and associated vectors of the viscoelastodynamic operator corresponding to an earth model with the opposite sense of rotation. Results of this form are familiar from earlier studies of both the elastodynamic and viscoelastodynamic equations in rotating earth models (e.g. Dahlen & Tromp 1998; Al-Attar 2007b).
- 4. Fluid regions: In modeling seismic wave propagation in the Earth, it is usual to regard the outer core and oceans as inviscid fluids. At the boundaries between solid and fluid regions it is then required that tractions and normal displacements are continuous, but that tangential slip is permissible. The extension of the the-

ory presented in this chapter to earth models possessing such fluid regions is not straightforward. This is because we have made extensive use of the strong ellipticity of the viscoelastodynamic operator  $\tilde{A}(p)$ . If the earth model contains fluid regions this operator is never strongly elliptic, so that many of our results need not hold.

A detailed study of the elastodynamic operator in the case of a rotating, self-gravitating, earth model possessing fluid regions has been made by Valette (1986; 1987; 1989a; 1989b). This work shows that the spectral properties of the elastodynamic operator can be significantly complicated by the presence of fluid regions. In particular, fluid regions can result in a continuous component of the spectrum located in a bounded neighborhood of zero. Physically, this portion of the spectrum is associated with the existence of internal waves within the outer core and oceans. It would be of interest in future work to attempt to adapt the methods of this chapter to incorporate fluid regions, and so extend the earlier results of Valette to the viscoelastic case.

We conclude by mentioning a number of further extensions and open questions relating to viscoelastic normal mode theory:

- 1. Behaviour of  $p \mapsto \tilde{G}(p)$  in  $\Sigma_{ne}$ : In this chapter we have been unable to give any concrete results about the behaviour of the Laplace transform domain Green operator  $p \mapsto \tilde{G}(p)$  in the subset  $\Sigma_{ne}$  of the negative real axis where the viscoelastodynamic operator  $\tilde{A}(p)$  fails to be strongly elliptic. Examples of the behaviour of  $p \mapsto \tilde{G}(p)$  in this region found in studies of simple example problems include accumulation points of finite-order poles, essential singularities, and branch-cut like features lying along portions of the negative real axis. It is not yet clear how to proceed with the study of  $p \mapsto \tilde{G}(p)$  in  $\Sigma_{ne}$ , though the study of simple problems suggests that methods borowed from the theory of singular integral equations may be of use (e.g. Muskhelishvili 1992).
- 2. Perturbation theory: In this chapter we have made a detail study of both the elasto-dynamic and viscoelastodynamic equations, and have seen that the former equation is, in fact, a special case of the latter. A practically important problem that we have not directly addressed is the development of a perturbation theory for the vis-

coelastodynamic equation during small changes to the relaxation tensor. Using the methods of this chapter, the development of such a perturbation theory should not be difficult. In particular, the proof of Theorem 6.6.15 can readily be adapted to study the behaviour of singularities of the Green operator  $p \mapsto \tilde{G}(p)$  under perturbations to the relaxation tensor using existing methods for finite-dimensional problems (e.g. Hryniv & Lancaster 1999).

- 3. Completeness of the eigenvectors and associated vectors: In the case of the elastodynamic equation, we know that the algebraic span of the eigenvectors of the elastodynamic operator is dense in  $L^2(\Omega, \rho; \mathbb{C}^n)$ . It is, therefore, natural to ask whether the set of eigenvectors and associate vectors for the viscoelastodynamic operator also forms a complete set. A proof of this result is not yet known, though it may be possible to adapt the methods of Agmon (1962) to establish one.
- 4. Genericity of simple poles: We have seen that the Green operator p → G̃(p) for the viscoelastodynamic equation can possess higher-order poles. This is in contrast to the corresponding operator for the elastodynamic equation which can only have simple poles. The occurrence of such higher-order poles in the viscoelastic string problem is found to depend crucially on the parameters of the string, and 'almost all' perturbations to these parameters result in the higher-order pole splitting into a corresponding number of simple poles. Such results suggest that simple poles may be a so-called generic feature for the viscoelastic normal mode problem. If so, from a numerical point of view, higher-order poles cannot occur, and are consequently of little practical interest. This situation would be analogous to the genericity of one-dimensional eigenspaces for elliptic operators on compact manifolds (e.g. Albert 1975; Uhlenbeck 1976), and the methods used for establishing such results may also be applicable to the viscoelastic normal mode problem.

#### Chapter 7

#### Discusion of Results

You can also collect butterflies and make many observations. If you like butterflies, that's fine; but such work must not be confounded with research, which is concerned to discover explanatory principles of some depth and fails if it does not do so.

Noam Chomsky, On Language.

In this final chapter we summarize the main results presented in this thesis. In doing so we focus on the relevance and utility of these results within geophysics and related fields. In addition, we outline a number of possible extensions of the work which will be investigated in the future.

#### 7.1 Chapter 2: Hydrostatic Equilibrium of the Earth

This chapter reconsidered the classic problem of determining the hydrostatic equilibrium figure of a steadily rotating earth model. The theory developed is also directly applicable to calculation of equilibrium figures of a range of astronomical bodies subject to either rotational or tidal forces.

Following the basic idea of Clairaut's original investigation of this problem (Clairaut 1743), we defined the hydrostatic equilibrium structure in terms of a mapping  $\xi: M_0 \to M$  from a spherical reference earth model  $M_0$  possessing a radial density profile into the desired

hydrostatic equilibrium model M. The main result of this chapter is the derivation of an exact non-linear boundary value problem from which this mapping  $\xi$  can be determined. To our knowledge, this is the first time such a result has been obtained.

Direct solution of the non-linear boundary value problem has not been attempted, though this would be a possible area for future work. Instead we showed how approximate solutions of this equation can be determined using perturbation theory. The end result of this analysis is a 'perturbation series' of linear boundary value problems defined in  $M_0$  whose solution can be obtained readily using standard methods. We have demonstrated explicitly that the first term in this perturbation series is equivalent to Clairaut's equation which is widely used within geophysics. It is thought that second- and third-order terms in the perturbation series are also equivalent to the extensions of Clairaut's equation obtained by a number of authors (e.g. Kopal 1960; Lanzano 1962; Chambat 2010), but have not verified this conjecture in detail due to the algebraic labor involved.

For applications to the Earth, the first-order theory (which, as noted, is equivalent to Clairaut's equation) is sufficiently accurate for most geophysical applications. With the increasing precision of geodetic observations there are, however, some circumstances in which use of the second-order theory may be required (e.g. Chambat 2010). For applications to the Earth there is not (and will almost certainly never be) a need for the exact theory of hydrostatic equilibrium we have described. There may, however, be some useful applications of this theory outside of the Earth sciences. For example, the theory can also be applied to studies of astronomical bodies such as rapidly rotating planets and stars for which more accurate theories may be necessary.

# 7.2 Chapter 3: Parametrization of Equilibrium Stress Fields in the Earth

This chapter investigated the possible forms of the equilibrium stress field in an earth model possessing lateral variations in density and boundary topography. It was shown that in such an earth model the equilibrium stress field must contain some deviatoric component, and that this equilibrium stress field is not determined uniquely by the equations of static

equilibrium. The interest in this equilibrium stress field arises from its occurrence as a parameter in the equations describing seismic wave propagation, and so, potentially, could be estimated using the techniques of seismic tomography.

In order to estimate the possible effects of the equilibrium stress field on seismic observations, it is necessary to perform seismic calculations in a range of earth models with realistic equilibrium stress fields. To do this, we showed how solutions of the equilibrium equations could be determined that possess physically appealing characteristics. In particular, we showed how to determine the equilibrium stress field which is, in a certain sense, the smallest possible, and also the equilibrium stress field whose deviatoric component is smallest. It was also shown that this latter equilibrium stress field is associated with the smallest amount of stress induced anisotropy in the earth model.

A number of numerical calculations were presented to illustrate the theory, and a preliminary conclusion obtained was that while the effects of the equilibrium stress field are likely to be small, they may not be completely negligible. Future work will focus on the quantification of the effects of equilibrium stress fields on seismic observations. In particular, the incorporation of these effects into calculations of normal mode spectra will be examined, as scaling analysis suggests that it will be at long periods that the effects of the equilibrium stress field are most pronounced.

### 7.3 Chapter 4: Synthetic Seismograms in Spherical Earth Models Using the Direct Radial Integration Method

This chapter considered the computational problem of calculating synthetic seismograms in spherically symmetric, self-gravitating earth models using the direct radial integration method introduced by Friedrich and Dalkolmo (1995). The main new result is an extension of the theory of Woodhouse (1980) for the stable numerical solution of two-point boundary value problems for systems of linear ordinary differential equations using minor vectors. A computer program implementing the theory has been written which is able to efficiently calculate synthetic seismograms in spherically symmetric earth models. This method provides a useful alternative to normal mode summation, and is particularly

suited for performing calculations at high frequencies (e.g. greater than 100 mHz) where mode calculations are not currently possible. In addition, this method is able to include the effects of linear viscoelasticity in a simple and exact manner. Along with its application to the calculation of synthetic seismograms, this method can be employed in a wide range of geophysically interesting problems including calculation of static and post-seismic displacement fields (e.g. Pollitz 1992, 1996), and in mantle flow calculations (e.g. Forte 2007).

# 7.4 Chapter 5: Calculation of Normal Mode Spectra in Laterally Heterogeneous Earth Models Using an Iterative Direct Solution Method

This chapter describes a numerical method for calculating normal mode spectra in laterally heterogeneous earth models. The method used is a new implementation of the direct solution method first introduced by Hara et al. (1993). In early implementations of this method the inhomogeneous mode coupling equations were solved using LU-decomposition. However, as the number of coupled modes is increased this method becomes very inefficient. To circumvent this problem we have employed the pre-conditioned conjugate gradient method to solve these equations. A number of numerical tests have been performed to demonstrate the accuracy and efficiency of this new approach.

The accurate calculation of synthetic spectra in laterally heterogeneous earth models is a necessary step in using normal mode observations to study the Earth's broad-scale structure. In spite of much recent progress in the computation of synthetic seismograms in laterally heterogeneous earth models (e.g. Komatitsch and Tromp 1998, 2002), mode coupling theory still seems to be the method of choice for calculating synthetic spectra. This is because of the need to incorporate self-gravitation fully into the calculations, and also the great length of the time-series required for normal mode studies which is prohibitively expensive for time-domain methods. Of existing methods for performing mode coupling calculations, the iterative direct solution method we have described seems to be the most efficient for performing large 'full-coupling' calculations. It also has the advantage that

it can incorporate the effects of rotation and linear viscoelasticity in an exact and simple manner. Future work on this method will focus on improving its implementation (e.g. through parallelization) and on the development of frequency-domain adjoint methods that can be used to calculate sensitivity kernels for normal mode observations in laterally heterogeneous earth models. Having done this, it will be possible to formulate and an inverse problem for determining earth structure from normal mode observations.

#### 7.5 Chapter 6: Viscoelastic Normal Mode Theory

In this chapter we considered the solution of the viscoelastodynamic equation in a bounded domain. We derived existence, uniqueness, and regularity theorems for the equation. We then showed how the solution could be written as a sum over the viscoelastic normal modes of the earth model. The theory developed generalizes those of earlier studies of viscoelastic normal mode theory in a number of ways. In particular, we proceeded in a mathematically rigorous manner throughout, so that the our results do not rely on any unproven assumptions or simplifications.

There remain a number of open questions in viscoelastic normal mode theory. Notably the development of a viscoelastic perturbation theory, and issues relating to the completeness of the viscoelastic eigenfunctions. In addition, there is significant work to be done on the numerical calculation of viscoelastic normal modes (e.g. Al-Attar 2007a). It is felt, however, that for practical calculations viscoelastic normal mode theory is probably not the best method. Instead, variants of the direct solution methods described in Chapters 4 and 5 are simpler to implement and likely to be more computationally efficient.

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