Seismic Redatuming with Transmission Loss Correction in Complex Media

Proefschrift

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In memory of my grandfather Prof. Henk Huisman, † 2005. *The man who taught me the meaning of the word ambivalence.*

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Glossary of notations

Notation p,P,\tilde{P}	Description Given the space-time domain field p , the capital P is the corresponding space-frequency field and the capital with tilde \tilde{P} is the corresponding wavenumber-frequency domain field.	17
·	In this thesis a number of linear operators appear, for example the Helmholtz operator \hat{H}_2 and related square root operator \hat{H}_1 . Their operator-character is indicated by the [^] -sign on top.	
iib	Acronym for Invariant ImBedding.	78
x	Scalar quantities will be denoted by plain symbols x .	
x	Matrix- and vector-quantities are denoted bold symbols x . Whether a matrix- or vector-quantity is denoted, is context dependent.	
.†	Adjoint of a matrix/operator. The adjoint of a matrix is equal to its complex conjugated transposed, for the definition of an adjoint operator see equation (A.14).	

Notation Description

 \cdot^t

- Transposed of a matrix/operator. For a matrix this comes down to interchanging rows and columns, for the definition of a transposed operator see equation (A.13).
- .[±] The ⁺-superscript denotes a down going field, the ⁻superscript an up going one.

Glossary

Symbol	Description	Page
Â,Ã	Operator matrix for the wave equation. Also-called	19, 29
	two way operator matrix.	
a	Top of the invariant imbedding domain	77
Ê,Ê	One-way wave operator matrix for pressure normal- ized wave fields.	30, 63
Ê,Ĩ	One-way wave operator matrix for flux normalized wave fields.	31, 63
b	Bottom of the invariant imbedding domain	77
C	The set of all complex numbers.	
c	Propagation velocity.	11
\mathbb{C}^n	The set all of <i>n</i> -vectors with components in \mathbb{C} .	
$\mathbb{C}^{n imes n}$	The set all of $n \times n$ square matrices with elements in	
	C.	
D,Ũ	Source vector for the wave equation.	19, 29
$\partial \mathbb{D}$	Integration boundary at the redatuming depth.	90
$\delta(t)$	Dirac delta function for scalar dependencies.	11
$\delta(\mathbf{x})$	$= \delta(x_1)\delta(x_2)\delta(x_3)$ Dirac delta function for vector	11
	dependencies.	
\tilde{E}_n, \tilde{E}_n	Global up going reflection response of interfaces at depths $x_{3,1}, x_{3,n-1}$, with sources and receivers just above depth $x_{3,n}$.	36

Symbol	Description	Page
$E_{\hat{H}}$	A measure for the error of the modal decomposition	67
	based on pressure normalized wave field composition.	
	In the ideal case $E_{\hat{H}} = 0$.	
$\hat{\mathcal{F}}, \hat{\mathcal{F}}^{-1}$	Operator notation for the Fourier integral transform.	14
$\hat{F}^{\pm}, \hat{F}^{\pm}, \mathbf{F}^{\pm}$	Inverse propagation operator for up going wave fields,	93, 98
	without the `the corresponding kernel is meant. The	
	bold symbol \mathbf{F}^{\pm} is the square matrix for the discrete	
	representation.	
$ ilde{f}^{\pm}$	The wavenumber frequency representation of inverse	28
	propagators for up and down going wave fields in ho-	
	mogeneous media, also see \tilde{w}^{\pm}	
f,F,Ĩ	External force. When we are not working in the	10
	space-time domain, f denotes unspecified vector	
~ . ~	function.	
F_n^{\pm},F_n	Flux normalized inverse propagator, the \pm -	42
$\sim + (V)$	superscript is redundant; also see W_n^{\pm} .	
$F_n^{+,(K)}$	Flux normalized inverse down propagator with K	42
A .	terms for transmission loss correction	
\tilde{F}_p^\pm	Operator for undoing primary propagation effects in	132
	the up/down direction.	
C	$- \begin{pmatrix} G^{+,+} & G^{+,-} \end{pmatrix}$ Green's function matrix for the	84
0	$= \left(\mathbf{G}^{-,+} \mathbf{G}^{-,-} \right)$ Siven s function matrix for the	04
~	one-way wave equation.	
\mathbb{G}	The part of 3D space containing the earth's Subsur-	91
	face or geology.	
$g_{l,m}$	Angle-depedent impedance ratio, used to relate pres-	40
a. ~	sure normalized up and down going propagators.	
g,G,G	Green's function. When we are not working in the	11
	space-time domain, g is an unspecified function.	
$H_{p}(\mathbf{x}_{H};\mathbf{x}_{H}^{'})$	Kernel representation of \hat{H}_p , i.e. the Helmholtz oper-	59
	ator to the power $p/2$	
\hat{H}_2	Helmholtz operator	52

Symbol	Description	Page
\hat{H}_p	Should be read as \hat{H}_2^p , i.e. the Helmholtz operator to	59
	the power $p/2$, for $p = 0, \pm 1/2, \pm 1$.	
$\hat{\mathcal{H}}$	Non-relativistic quantum mechanical Hamiltonian	52
	operator	
\hat{H}_2, \tilde{H}_2	Pseudo Helmholtz-operator.	19, 26
$ ilde{H}_1, \hat{H}_1$	The square root of the pseudo Helmholtz-operator	27, 51
	\hat{H}_2 .	
\hat{H}_{-1}	Inverse of the square root of the pseudo Helmholtz	58
	operator	
$H^s(\mathbb{R}^n)$	Sobolev space, set of functions on \mathbb{R}^n that are square	169
	integrable and whose s-order derivatives are also	
	square integrable.	
Ι	Square unit matrix.	
Л	$=\begin{pmatrix} 1 & 0 \end{pmatrix}$	
0	$- \begin{pmatrix} 0 & -1 \end{pmatrix}$.	
j	Imaginary unit.	
K	Bulk modulus.	10
К	$= \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}$	
	$\begin{pmatrix} 1 & 0 \end{pmatrix}$	
$k(\mathbf{x})$	Wave number in laterally varying medium.	52
k_0	Wavenumber corresponding to background velocity.	52
\mathbf{k}_{H}	$= (k_1, k_2)$. Horizontal wave-vector, also see k .	10
k	$= (k_1, k_2, k_3)$. Wave-vector, see x for specification	10
	of vector character.	
. ~		
Ĺ,Ĺ	Pressure normalized one-way composition operator	30, 61
^ ~	matrix.	
L,L	Flux normalized one-way composition operator ma-	30, 62
	trix.	
\mathbb{L}	Lower half space below overburden.	91

Symbol	Description	Page
ĩ,ĩ	Building blocks for (de)composition matrices in the wavenumber frequency domain,	29
	\tilde{l} : pressure normalized (de)composition,	
	\tilde{l} : flux normalized (de)composition.	
<i>î</i> ,î	Building blocks for (de)composition matrices in the	61
	space frequency domain,	
	\hat{l} : pressure normalized (de)composition,	
	\hat{l} : flux normalized (de)composition.	
L_2	Set of square integrable functions.	13
N	= $\{1, 2, \ldots\}$. The set all of natural numbers.	
Ν	$= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$	
\mathbb{N}^n	The set of all <i>n</i> -vectors with components in \mathbb{N} .	
0	The part of 3D space containing the overburden	91
Р,Р	Flux normalized one-way wave field vector.	31, 63
Р,Р	Pressure normalized one-way wave field vector.	30, 62
p, P, \tilde{P}	Acoustic pressure.	10
$P_{l,n}^{\pm}$	Wave fields recorded at an infinitesimal distance <i>be</i> - low depth $x_{3,n}$.	32
$P_{u,n}^{\pm}$	Wave fields recorded at an infinitesimal distance	32
<i>u</i> , <i>n</i>	above depth $x_{3,n}$.	
Q,Q	The wave field vector $\mathbf{Q} = (P, V)^t$ contains the pres-	19, 29
	sure and vertical particle velocity fields.	
q , Q , $ ilde{Q}$	Volume-injection rate.	10
$\tilde{R}^+_{n,N}$	Given interfaces at depths $x_{3,n}, x_{3,n+1}, \ldots, x_{3,N}$.	44
	Then $\ddot{R}_{n,N}^+$ is the reflection response with sources and	
	receivers directly above $x_{3,n}$.	

Symbol	Description	Page
$\hat{R}^+,\hat{R}^+,\mathbf{R}^+$	Global reflection operator for down going wave fields,	78, 108
	without the `the corresponding kernel is meant. The	
	bold symbol \mathbf{R}^+ is the square matrix for the discrete	
	representation.	
\hat{R}^-, \hat{R}^-	Global reflection operator for up going wave fields,	78
	without the `the corresponding kernel is meant.	
$\tilde{R}_n^+, \tilde{R}_n^+$	Given interfaces at depths $x_{3,1}, x_{3,2}, \ldots, x_{3,n}$. Then	34
	for a down going source function plus receivers at $x_{3,0}$	
	these are the global reflection coefficients for pressure	
	and flux normalized down going wave fields, respec-	
	tively.	
$\tilde{R}_n^-, \tilde{R}_n^-$	Given interfaces at depths $x_{3,1}, x_{3,2}, \ldots, x_{3,n}$. Then	34
	for an up going source function and receivers directly	
	below $x_{3,n}$ these are the global reflection coefficients	
	for pressure and flux normalized down going wave	
	fields, respectively.	
$ ilde{r}^{\pm}, ilde{r}^{\pm}$	Local reflection coefficient for pressure and flux nor-	32
	malized wave fields, respectively. Called a local coef-	
	ficient because they correspond to a single interface.	
$\hat{r}^{\pm},\hat{\mathbf{r}}^{\pm}$	local reflection operators, analogous to the reflection	65
	coefficients in horizontally layered media	
\mathbb{R}	The set of all real numbers.	
$\tilde{R}_{dat,n}$	Redatuming result for horizontally layered media. An	45
	estimate of the response of a thought experiment with	
	down going sources and receivers for up going wave	
	fields buried in the subsurface at depth b , obtained	
	from the reflection response at the surface a , by un-	
	doing the propagation effects of the medium between	
	these two levels. The bold symbol is the discrete ma-	
	trix representation.	
$\hat{\mathbf{D}}$ $(1,1)$ $\hat{\mathbf{D}}$ $(1,1)$		

 $R_{dat}(b;b)$, $R_{dat}(b;b)$,

Symbol	Description	Page
$\mathbf{R}_{dat}(b;b)$	Redatuming result. An estimate of the response of a	94
	thought experiment with down going sources and re-	
	ceivers for up going wave fields buried in the subsur-	
	face at depth $x_3 = b$, obtained from the reflection re-	
	sponse at the surface $x_3 = a$ by undoing the propaga-	
	tion effects of the medium between these two levels.	
	The bold symbol is the discrete matrix representation.	
\mathbb{R}^n	The set all of <i>n</i> -vectors with components in \mathbb{R} .	
$\mathbb{R}^{n imes n}$	The set all of $n \times n$ square matrices with elements in	
	$\mathbb{R}.$	
$\tilde{R}_{thght,n}$	Given interfaces at depths $x_{3,1}, x_{3,2}, \ldots, x_{3,N}, n < \infty$	44
	N. Then $\tilde{R}_{thght,n}$ is the up going response due to a	
	down going source field, both located just above depth	
	$x_{3,n}$.	
$\hat{R}_{thght}(b;b)$	Operator representing a thought experiment with	93
	down going sources and up going receivers buried in	
	the subsurface at depth b.	
ρ	Mass-density	10
Ŝ,S	Flux normalized one-way source vector	31
Ŝ,S	Pressure normalized one-way source vector	30
$\partial \mathbb{S}$	Integration boundary coinciding with the measure-	90
	ment surface.	
$\hat{\mathbf{S}}_{scat}$	Scattering operator matrix	78
$\hat{T}^{\pm}, \hat{T}^{\pm}, \mathbf{T}^{\pm}$	Global transmission operator for down going wave	78, 98
	fields, without the `the corresponding kernel is meant.	
	The bold symbol \mathbf{T}^{\pm} is the square matrix for the dis-	
	crete representation.	
$\tilde{T}_n^{\pm}, \tilde{T}_n^{\pm}$	Given interfaces at depths $x_{3,1}, x_{3,2}, \ldots, x_{3,n}$. Then	34
	for a down going source function at $x_{3,0}$ and receivers	
	directly below $x_{3,n}, \tilde{T}_n^+$, and \tilde{T}_n^+ are the global trans-	
	mission coefficients for pressure and flux normalized	
	down going wave fields, respectively. Their up going	
	counterparts are \tilde{T}_n^- , and \tilde{T}_n^- .	

Symbol	Description	Page
$ ilde{t}^{\pm}, ilde{t}^{\pm}, ilde{t}$	Local transmission coefficient for pressure and flux normalized wave fields, respectively. Called a local coefficient because they correspond to a single interface. Because $\tilde{t}^- = \tilde{t}$, the ±-superscript can be omitted.	32
$\hat{t}^{\pm},$ î $^{\pm}$	local transmission operators, analogous to the trans- mission coefficients in horizontally layered media	65
t	Time.	9
t_s	Cental time-value of Green's function source field; in most realizations/approximation this is also the time of the peak value.	11
\mathbf{T}_w	Diagonal matrix with taper weights.	173, 175
v,V,Ũ	= (v_1, v_2, v_3) . Particle velocity vector; see x for specification of vector character. See glossary of no- tation for v vs. V.	10
V	Vertical particle velocity in the space frequency do- main.	18
$ ilde W_n^\pm, ilde W_n^\pm, ilde W_n.$	Given a down going source at $x_{3,0}$ and receivers just above $x_{3,n}$ with interfaces at depths $x_{3,1}, x_{3,n-1}$. \tilde{W}_n^+ and \tilde{W}_n^+ are the global down going propagators of pressure and flux normalized wave fields, respec- tively. For the up going counterparts the positions of sources and receivers are interchanged. Because $\tilde{W}_n^- = \tilde{W}_n^+$, the \pm -superscript can be omitted.	36
$\tilde{w}_n^{\pm}, \tilde{w}_n$	\tilde{w}_n^+ is the wavenumber frequency representation of the down going propagator in homogeneous layer be- tween depths $x_{3,n-1}$ and $x_{3,n}$, \tilde{w}_n^- the upgoing prop- agator. The \pm -superscript is redundant.	27
\hat{W}_p^{\pm}	Operator describing primary propagation effects in the up/down direction.	132
$\mathbb{X}(a,b)$	Open domain, <i>not</i> including its boundaries at $x_3 = a$ and $x_3 = b$.	77

Symbol	Description	Page
$\mathbb{X}[a,b]$	Closed domain, including its boundaries at $x_3 = a$	77
	and $x_3 = b$.	
x_i	Spatial coordinates:	9
	i = 1: horizontal in line direction,	
	i = 2: horizontal cross line direction,	
	i = 3: depth direction.	
$\partial \mathbb{X}\{a\}, \partial \mathbb{X}\{b\}$	Boundaries of the domain X .	77
\mathbf{x}_H	$= (x_1, x_2)$. Horizontal coordinate-vector, also see x.	9
$x_{3,l}$	A depth level which lies directly below x_3 .	32
$x_{3,u}$	A depth level which lies directly <i>above</i> x_3 .	32
x	$= (x_1, x_2, x_3)$. Spatial coordinate-vector.	9
∇	$= (\partial_1, \partial_2, \partial_3)$. Nabla-operator.	10
$ abla_H$	= (∂_1, ∂_2) . Nabla-operator for horizontal coordi-	10
	nates.	
\mathbf{X}_{S}	Source position for Green's function.	11

Chapter 1

Introduction

The subject of thesis belongs to the discipline of exploration geophysics, which aims to assist in the exploration of oil and natural gas. To do so geophysicists use, amongst others, seismic reflection measurements performed at the surface to construct structural images of the earth's subsurface, in order to locate the interfaces between different layers. The technical name for the construction of such images is migration. It is the ultimate goal of this thesis to devise a migration algorithm that preserves the amplitude information of the recorded wave fields, in order to make the migration output useful as input for inversion. Different approaches can be taken to reach this goal, but here we will aim to let the migration algorithm obey the law of energy conservation. All early developed migration algorithms and many algorithms currently in use mainly focus on travel time information; they can seriously distort the amplitude information and actually do so in most cases. In the geophysical literature, migration algorithms that aim to preserve amplitude information are commonly referred to as True Amplitude migration. We will however avoid this term for two reasons. First there is the philosophical question What is truth ?, and the second reason is that already a wide range of approaches has been labeled True Amplitude migration. In our opinion the term has therefore lost much of its precision and meaning.

Before we start discussing science in sections 1.2 and 1.3, we first present some historical context of global oil demand and exploration geophysics, which are both marked by the First World War (WWI), lasting from 1914 to 1918.

1.1 Exploration geophysics, oil and the First World War

The combustion of hydrocarbons provides us with heat, electricity and mobility. In principle there are also other energy sources that can supply us with these three ingredients for prosperity, but in particular for mobility there was, and still is, no economically viable alternative. By 1905 engineers had demonstrated that vehicles with gasoline-powered engines were superior to those driven by coal, steam or electricity. Similar to numerous other technologies, it still took (the threat of) a major war to spread the use and accelerate further development. In 1911 the looming conflict with Germany urged the British Navy to switch from coal to oil for fueling their ships in order to stay ahead of their opponents, see Yergin [99]. On land the change was triggered by the WWI-battles taking place at the Western front running from the Belgium North Sea to the French border with Switzerland. Here it became obvious that in the late 19th century the development of battlefield tactics had not kept pace with the technological advances of weaponry. In particular the destructive power of machine guns and heavy artillery was unprecedented. They gave defenders in trenches a tremendous advantage over the classic infantry rushes; despite the sacrifice of millions of soldiers on both sides, the Western front shifted only a few miles in the period 1914-1917. But in 1917 the tide turned in favor of the Allies, partly due to their large scale deployment of armored, gasoline-powered tanks; Fletcher [29] describes how these vehicles were able to break through the Western front.

Mobility has always been crucial in warfare, so once the mobility-boosting merits of oil had become clear, it severely changed the ways the navy and army operated, and even enabled the emergence of a new branch of military service: the air force. Oil hence became a decisive factor in battle, and subsequently a cause of war on its own. Besides raising oil demand, WWI also had a great influence on the development of tools for reflection seismics, see Bates et al. [3].

Heavy artillery caused large numbers of casualties directly at the front lines as well as kilometers behind. It was therefore just a matter of time before the principle of locating earthquake-origins was also tried at the blast waves caused by these big guns. This idea emerged on both sides: Germany ordered some 100 seismic troops in 1917, which never became fully operational, while 500 Englishmen and 700 Americans were employed in Sound Ranging at the end of WWI. Artillery detectors were of course only interested in the big blast waves traveling directly from its origin to the receivers, but these were not the only events registered by the seismic sensors. The readouts also showed a long train of weaker events, the down going part of the blast wave that is reflected in the up going direction by the subsurface of the Earth. Figure 1.1 shows the response of measurements made



Figure 1.1: Unprocessed seismic data, produced with a dynamite source at offset= 0m and receivers arranged in a straight line starting close to the source point. This post-WWI seismogram shows the comparatively strong direct wave on the line (0.5s,650m)-(1.0s,1750m). Since the top layers of the subsurface have lower velocities than the lower layers, the so-called refracted waves traveling via these lower layers arrive earlier than the direct wave.

on land with a dynamite source. Supporting the necessary technical developments for artillery detection, the Sound Section of the U.S. Bureau of Standards employed among others the four men that would later form the "Geological Engineering Company"; Haseman, Karcher, Eckhardt, and McCollum. The basic patents were filed in January 1919 and they performed the first fully valid field test in June 1921. Also in 1919 a related patent was filed by the scientist Mintrop, involved with artillery detection on the German side. Mintrop set up the company Seismos Limited in 1921, and in 1924 one of its crews located the Orchard salt dome in Texas. This was probably the first discovery of commercial amounts of oil instigated by seismic reflection measurements.

Such reflection measurements can in general not provide a direct answer to the question whether hydrocarbons are present or not. After performing their reflection measurements, exploration geophysicists typically apply so-called migration algorithms to undo the wave propagation effects and obtain an image of the subsurface. Finally geologists can use it, amongst other sources of information, to judge if the presence of hydrocarbons is likely or not. Neither the amount of measurements nor the resources for processing and analyzing them are unlimited, so migration algorithms necessarily make a lot of simplifying assumptions about the subsurface and the physics of wave propagation.

But the amount of measurements that one can acquire has grown steadily since the early seismic experiments, and in the last decades the computing resources for processing and analysis have grown exponentially. Various migration algorithms have been developed to use these increased amounts of information and resources in order to reduce the number of assumptions and the degree of neglect mentioned above; Bednar [4] gives a historical overview of these developments. Sections 1.2 and 1.3 will zoom in on the particular approach of this thesis.

1.2 Context of this thesis

Crude oil is formed in the subsurface roughly between the depths 2.5 km and 5 km. In this so-called "oil-window" temperature and pressure are high enough for organic matter to break down (or "crack") into liquid oil, below 5 km an even further reduction to natural gas occurs. Once they are formed, oil and natural gas usually have a lower density than their surroundings and tend to rise to the surface. Fortunately for us, some of it actually completed this journey, and gave mankind a first taste of crude oil (or bitumen as it was styled in earlier times). However, all easy to reach hydrocarbons were quickly recovered after industrial exploration started in 1860. The bulk of hydrocarbons ran into something

they could not penetrate, for example a salt body, and got trapped before reaching the surface. Ideally, exploration geophysicists can deduce the presence of such oil-traps, or less ideally but more likely, they make a seismic image for geologists to judge if oil-traps are likely to be present. See Deffeyes [21] for an accessible and detailed description of the science of hydrocarbon formation and recovery.

The principle of non destructive probing with (sound) waves of an object with a still unknown interior, and trying to infer information on the interior from the response, is applied in a number of fields besides seismic exploration. One can find clear analogies between sound scans of pregnant women in medical imaging and the reflection measurements of exploration geophysics; the former produces an image of the shape of the baby, while the latter yields an image showing the interfaces between the different layers of the earth's subsurface. An important difference is that in the case of medical imaging the starting point is better. The body of a woman is known to contain about 55% water and 22 - 30% fat, which allows us to make a good estimate of the velocity of sound inside her body. For the earth's subsurface we do not know velocity-values, but we merely have the rule of thumb that the layered structure of the subsurface leads to much more variation in the vertical direction than in the horizontal direction. And even then we have to keep in mind that oil tends to get trapped in places where this rule is less applicable than elsewhere.

Before any meaningful migration can be attempted, geophysicists first have to make an educated guess of the velocities of sound in the subsurface. The technical term for this educated guess is background or macro model. We assume that a useful macro velocity model is already available based on the rule of thumb mentioned above and a travel time analysis of the reflection measurements; coming up with such a model, is still a research topic on its own.

For purely structural imaging, of which the sound scans discussed above are a typical example, a velocity model is usually enough. The travel times of the reflections, which we will also refer to as their kinematics, can be described completely by a velocity model. But, the ultimate goal of our line of research is inversion for the acoustic properties of the subsurface, and this also requires the analysis of amplitude information, i.e. the dynamics of a wave field. A complete acoustic description of the dynamics also requires a macro model for the mass density, in addition to one for the velocity. The art of constructing density macro models is less developed than that of velocity models, but sources of input are gravity measurements and well logs (a description of the properties of the material dug from wells).

The inversion mentioned above is beyond the scope of this thesis, but to improve the

conditions for inversion we want to undo the effects of wave propagation such that both the kinematics and dynamics of the reflection measurements are treated properly for each point to be imaged. For the kinematics and dynamics there is already a large body of literature and related software implementations that give such treatments (see section 5.2 for a short and far from exhaustive overview). We will give a detailed introduction of our approach in sections 1.3 and 1.8.2, but the general idea is to preserve the dynamics in the process of inverse propagation, that is undoing propagation effects, by observing the law of energy conservation.



1.3 Aim of this thesis

Figure 1.2: Redatuming illustrated.

As part of the process to obtain an image from seismic measurements, exploration geophysicists consider a thought experiment as shown in Figure 1.2 with sources and receivers buried at some particular surface deep in the ground, instead of being positioned at the top surface. An essential step in migration is somehow transforming the data measured at the surface in the real experiment into the data that would be measured with the



Figure 1.3: Complex propagation effects

thought experiment. The technical name for this transformation is redatuming, and more specifically it aims to undo the propagation effects of the overburden between the surface and the buried sources and receivers. In 1979 Berryhill [9] was the first to use the term (re)datuming, but Claerbout¹ [17] had already formulated the principle a few years earlier. A number of authors later on also employed it, and most gave priority to minimizing the computational burden over amplitude preservation, see Tegtmeier et al. [80]. Mulder [66] on the other hand did focus on amplitude preservation, and based his approach on the solution of three inverse problems. In this thesis we discuss an alternative to the latter that is based on solving only one inverse problem, or rather the equivalent thereof; see section 4.5 for a more detailed comparison.

One obvious condition for accurate inverse propagation is that we have an accurate description of the propagation effects. Two basic aspects of wave propagation pose difficulties in meeting this condition. First, most migration algorithms do not take multiple scattering into account. For the situation in Figure 1.3(a) this means that the primary transmission path $SB_1C_1D_1$ is taken into account, but the secondary transmission path $SB_1C_1D_2$ is not, because the reflectivity at the points C_1 and B_2 is neglected. Our

¹Claerbout introduced an alternative term with more visual appeal, *survey sinking*.



Figure 1.4: Undoing propagation effects between the sources of Figure 1.2.

approach accounts for the effect of multiple scattering in the redatuming of primary reflection events. We discuss the theoretical principles and more practical issues in Chapters 5 and 6, respectively. The second problem arises from so-called focal points. In a medium like Figure 1.3(b) where the gray area has a lower velocity than its surroundings, multiple ray-paths are focused in the so-called focal or caustic point F. In the presence of such focal points the calculationg of amplitudes presents a fundamental problem for raytracing, the workhorse technique for modeling seismic wave propagation in the process of migration. After passing through caustic points, wave fronts contain multiple arrivals. With Maslov theory the computation of the wave field at such wave fronts is possible; for example Ten Kroode et al. [56] used this for inversion. However, Maslov theory is unable to compute amplitudes in caustic points such as F in Figure 1.3(b). In principle the Gaussian beam method [67] does have this ability, but this method still has the same practical problems with multiple reflections as ray-based approaches.

Unless stated otherwise, we will use a Finite Difference algorithm in this thesis for wave field modeling to avoid discussions on accuracy. FD algorithms are however much more time consuming than ray methods and still have their limitations.

Similar to redatuming as formulated by Mulder [66], also see section 4.5, we undo propagation in two separate stages: between the receivers of both the real and thought experiment and between their sources. In Figures 1.4(a) and 1.4(b) we have zoomed in on the overburden from Figure 1.2 delimited by the surface and the buried sources/receivers of the thought experiment. Current practice inverse propagation in the context of redatuming amounts to time reversal of the transmission response of the overburden, but neglection of its reflection response, see Figure 1.4(b). This is sufficient for proper removal of the kinematics, but it maltreats the dynamics because the energy carried by the reflection

response, also styled transmission loss in the literature of exploration geophysics, is not accounted for. Esmersoy [24] has demonstrated this fact for arbitrary media.

In the remainder of this chapter we give a brief overview of the mathematical physics used in this thesis and point out the directions we take in later chapters. In section 1.4 we introduce the wave equation and proceed by introducing two basic tools for analysis of the wave equation: generalized functions or distributions in section 1.5 and Fourier transforms in sections 1.6 and 1.7. In section 1.8 we give a short overview of the symmetry and conservation principles used in this thesis. We conclude this chapter with section 1.8.2 in which we use energy conservation to quantify the error resulting from the neglection of transision losses and sketch our solution.

1.4 The coordinate system and fundamental equations

Because the parameters of the subsurface of the earth vary much more rapidly in depth than in the lateral directions, most scattering occurs in the vertical direction. Exploration geophysicists therefore analyze reflection seismics in terms of up and down going waves. The positive vertical direction is taken downward into the earth; down going waves will therefore be labeled with superscript '+', up going waves with a superscript '-' (the precise definition of up and down going waves will be amply discussed in section 2.3 and Chapter 3). Scattering in the direction of propagation (i.e. forward scattering) will be called transmission, whereas scattering in the opposite direction will be called reflection. Because of this emphasis on the vertical direction we will use an alternative expression for the coordinate vector besides the usual one:

$$\mathbf{x} = (x_1, x_2, x_3) \triangleq (\mathbf{x}_H, x_3).$$

This way the horizontal coordinates $\mathbf{x}_H \triangleq (x_1, x_2)$ are separated from the vertical one x_3 . As usual the time will be represented by the symbol t. Analogous to the spatial coordinates, we will use a similar separating notation for any Cartesian vector quantity,

for example

particle velocity :
$$\mathbf{v} = (\mathbf{v}_H, v_3),$$

"nabla"-operator : $\nabla = (\partial_1, \partial_2, \partial_3),$
 $= (\nabla_H, \partial_3),$
wave vector : $\mathbf{k} = (\mathbf{k}_H, k_3),$
etcetera.

Ultimately, the method described in this thesis should be expressed and implemented in terms of elastic wave propagation, but at this stage only acoustic wave propagation will be dealt with. The acoustic pressure $p(\mathbf{x}, t)$ and the particle velocity $\mathbf{v}(\mathbf{x}, t)$ are related by two first order partial differential equations; the first describes translation

$$\nabla p + \rho \partial_t \mathbf{v} = \mathbf{f},\tag{1.1a}$$

the second accounts for expansion and compression,

$$\nabla \cdot \mathbf{v} + \frac{1}{K} \partial_t p = q. \tag{1.1b}$$

Besides the pressure p and particle velocity **v** the other quantities appearing in equation (1.1) are

$$\begin{split} \rho(\mathbf{x}): \text{mass-density}, & K(\mathbf{x}): \text{bulk modulus}, \\ \mathbf{f}(\mathbf{x},t): \text{external force}, & q(\mathbf{x},t): \text{volume-injection rate}. \end{split}$$

Note that we have assumed ρ and K to be time-independent. Although this is not true in general, it is a useful assumption for the duration of a typical seismic experiment, which lasts up to a few weeks.

Besides the system of coupled first order partial differential equation (1.1), one frequently encounters a single, second order partial differential equation in terms of either por \mathbf{v} . To obtain such a relation in terms of p we first take the divergence of equation (1.1a) and differentiate (1.1b) with respect to time. Then we eliminate $\partial_t \nabla \cdot \mathbf{v} = \nabla \cdot \partial_t \mathbf{v}$ from the former with the latter; rearranging terms gives the acoustic wave equation

$$\left[\rho\nabla\cdot\frac{1}{\rho}\nabla-\frac{1}{c^2}\partial_t^2\right]p = -\rho s_p,\tag{1.2}$$

with propagation velocity $c = \sqrt{K/\rho}$ and source-function

$$s_p = \left[\partial_t q - \nabla \cdot \left(\frac{\mathbf{f}}{\rho}\right)\right].$$

Formally equation (1.2) is only valid in fluids, but for a typical seismic experiment it also describes the dominant modes of wave propagation in the solid earth. The first order system of equation (1.1) and the second order equation (1.2), are the analytical fundament of this thesis.

1.5 Generalized functions

The fundamental solution or Green's function to equation (1.2), $g = g(\mathbf{x}, \mathbf{x}_s, t - t_s)$, is defined as the response of a point source (in both space and time)

$$\left[\rho\nabla\cdot\frac{1}{\rho}\nabla-\frac{1}{c^2}\partial_t^2\right]g = -\rho\delta(\mathbf{x}-\mathbf{x}_s)\delta(t-t_s).$$
(1.3)

The source position is represented by the coordinate vector \mathbf{x}_s , while t_s is the time-value at which Green's function source field is nonzero.

The use of the (Dirac) δ -function, appearing on the right hand side of equation (1.3), has a considerable history in physics and mathematics. The δ -function can be traced back to the work of Green on electrostatics in 1828 [39]; in this work he already constructed a point source solution for the Poisson-equation, but did not consider the corresponding source function itself. Kirchhoff [55] and Volterra [86] stated the defining expression of the δ -function in 1881, but the first to note that this could not be a regular function, was Dirac [22] in 1927. It was only with the work of Sobolev [77] and Schwartz [75] that generalized functions and in particular δ -functions, were formally defined and founded. A rigorous definition requires a solid background in mathematics, but for understanding this thesis a working knowledge is sufficient.

Often $\delta(x)$ is defined as the limit of some function $\delta_a(x)$

$$\delta(x) = \lim_{a \downarrow 0} \delta_a(x). \tag{1.4}$$



Figure 1.5: Example realizations of $\delta_a(x)$.

The function $\delta_a(x)$ can have various realizations, see Fig 1.5, but in all cases its limit $\delta(x)$ must obey

$$\int_{-\infty}^{b} \delta(x - x_s) f(x) dx = \begin{cases} 0 & \text{if } b < x_s, \\ f(x_s)/2 & \text{if } b = x_s, \\ f(x_s) & \text{if } b > x_s. \end{cases}$$
(1.5)

Although often appearing as in equation (1.3), its action is only defined in integralexpressions such as (1.5). In addition the function f must satisfy two conditions; (a) it must be infinitely differentiable, i.e. $d^n f/dx^n$ must exist for all $n \in \mathbb{N}$, and (b) it must have compact support, i.e. it should vanish outside some finite domain. Symbolically these requirements are usually summarized as $f \in C_0^{\infty}$. After one of the founding fathers of the theory of generalized functions (also known as distributions) [60, 75], the spaces of functions obeying these conditions are called Schwartz spaces.

The three-dimensional δ -function is defined by $\delta(\mathbf{x}) = \delta(x_1)\delta(x_2)\delta(x_3)$. The main result of the theory of Green's functions is that the general solution p of equation (1.2) is constructed by

$$p(\mathbf{x},t) = \int_{\mathbb{R}} \left[\int_{\mathbb{R}^3} g(\mathbf{x}, \mathbf{x}_s, t - t_s) s_p(\mathbf{x}_s, t_s) d^3 \mathbf{x}_s \right] dt_s,$$
(1.6)

where p and g obey the same boundary conditions.

Another important property is that solutions to equations involving generalized functions, like equation (1.3), are themselves generalized functions; analogous to the δ -function, the action of the Green's function g should always be understood in the sense of equation (1.6), i.e. in an integral expression. Unlike ordinary functions they can be solutions to differential equations with discontinuous coefficients. Farassat [25] provides a highly readable and application-oriented introduction to the subject.

1.6 The Fourier transform

Arguably one of the most widely used tools for quantitative description and analysis is the Fourier transform. It yields trigonometric expansions of square integrable functions.

The development of trigonometric expansions has a long history, in which Joseph Fourier was neither the first to employ them nor did he give the final, rigorous basis for their use. Their first employment was probably due to Leonhard Euler in 1739. Others arrived at or proposed a similar solution before Fourier in his major work on heat transfer; Jean d'Alembert did so in astronomy, while Daniel Bernoulli and Joseph-Louis Lagrange used the wave equation to describe vibrating strings and propagation of sound, respectively.

Fourier's major contribution was to abstract the idea behind these particular solutions and prove that any periodical function could be represented by an infinite series of sines and cosines. This technique nowadays goes by the name of Fourier analysis. Fourier also conjectured that in the limit of infinite periods the method could also be applied to nonperiodic functions; this is still a popular way to introduce the Fourier transform.

A function $f(\mathbf{u}), \mathbf{u} \in \mathbb{R}^n$ is square integrable if

$$\int_{\mathbb{R}^n} |f(\mathbf{u})|^2 d^n \mathbf{u} < \infty;$$

the symbolic abbreviation of this requirement is $f \in L_2$. Of course the subset of square integrable functions is only a small part of the collection of arbitrary functions, but virtually all physical phenomena involving fluctuations allow the use of Fourier transformation; hence its wide range of applicability. Bracewell [13] gives a popular account of the Fourier transform, (almost) free of formulas; the same author [12] also gives a detailed technical description.

But there are more reasons for its widespread use. One is that application of the

Fourier transform to a discrete signal turns out to be surprisingly efficient. If the number of samples N can be factorized into small primes (typically 2,3,5, and 7), then the number of floating point operations involved is essentially proportional to $N \log N$, see for example Press et al. [69]; algorithms exploiting this feature go by the name Fast Fourier Transform, or FFT. Although gaining popular knowledge only in the mid 1960's by the work of Cooley and Tukey [18], this efficient use of the Fourier transform was employed before; in for example geophysical signal processing, Deffeyes [21], and as early as 1805 by Gauss, see Brigham [14]. But only since the work of Cooley and Tukey a vast collection of implementations has been developed.

The explanation of the other reasons of the widespread use of the Fourier transform (i.e. relevant to this thesis), requires some formal notation and definitions:

- this thesis will use $j = \sqrt{-1}$, for the imaginary unit number.
- vectors \mathbf{u}, \mathbf{w} are both coordinates in \mathbb{R}^n ,
- the functions $f = f(\mathbf{u})$ and $\tilde{f} = \tilde{f}(\mathbf{w})$ are both complex-valued.

The Fourier transform $\hat{\mathcal{F}}$ and its inverse $\hat{\mathcal{F}}^{-1}$ are defined by

$$\hat{\mathcal{F}}[f](\mathbf{w}) = \tilde{f}(\mathbf{w}) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} f(\mathbf{u}) e^{\pm j\mathbf{u}\cdot\mathbf{w}} d^n \mathbf{u}, \qquad (1.7a)$$

$$\hat{\mathcal{F}}^{-1}[\tilde{f}](\mathbf{u}) = f(\mathbf{u}) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \tilde{f}(\mathbf{w}) e^{\pm j\mathbf{u}\cdot\mathbf{w}} d^n \mathbf{w},$$
(1.7b)

where $\mathbf{u} \cdot \mathbf{w} = \sum_{i=1}^{n} u_i w_i$. There is still an ambiguity in equation (1.7), but once a sign has been chosen in equation (1.7a), the opposite must be taken in equation (1.7b) or vice versa.

The important properties of the Fourier transform used in this thesis will be given next.

1. Using equation (1.7b) it is clear that the Fourier transform of the gradient of f is

$$\hat{\mathcal{F}}[\nabla_{\mathbf{u}}f](\mathbf{w}) = \mp j\mathbf{w}\tilde{f}(\mathbf{w}).$$
(1.8)

The relation expressed by (1.8) is another reason for the widespread use of the Fourier transform. It allows a differential operator to be "reduced" to multiplication by a complex variable, a property that will be used in section 1.7 and appendix A.1.

2. If in addition to $f = f(\mathbf{u})$ there is a function $g = g(\mathbf{u})$, then their convolution is defined by

$$[f \otimes g](\mathbf{u}) \triangleq (2\pi)^{-n/2} \int_{\mathbb{R}^{n}} f(\mathbf{u}')g(\mathbf{u} - \mathbf{u}')d^{n}\mathbf{u}'.$$
(1.9)

This convolution is symmetric in the sense that $f \otimes g = g \otimes f$. The Fourier transform of a convolution happens to be the algebraic product of the Fourier transforms of its constituents

$$\hat{\mathcal{F}}[f \otimes g](\mathbf{w}) = \tilde{f}(\mathbf{w})\tilde{g}(\mathbf{w}).$$
(1.10)

Conversely, Fourier-domain convolutions become algebraic products in the original domain,

$$f(\mathbf{u})g(\mathbf{u}) = \hat{\mathcal{F}}^{-1}[\tilde{f} \otimes \tilde{g}](\mathbf{u}), \tag{1.11}$$

because of the symmetry (up to a sign) of the forward and backward Fourier transform.

3. An operation closely related to convolution, is correlation. First make the replacement $f(\mathbf{u}) \rightarrow f(-\mathbf{u})$ in equation (1.9) and subsequently substitute $\mathbf{u}' = -\mathbf{u}''$ in the integrand. Correlation of f and g is thus defined as

$$[f * g](\mathbf{u}) \triangleq (2\pi)^{-n/2} \int_{\mathbb{R}^n} f(\mathbf{u}'') g(\mathbf{u} + \mathbf{u}'') d^n \mathbf{u}'', \qquad (1.12)$$

with the Fourier domain equivalent

$$\hat{\mathcal{F}}[f * g](\mathbf{w}) = \tilde{f}^*(\mathbf{w})\tilde{g}(\mathbf{w}).$$
(1.13)

Loosely speaking correlation is related to convolution like $f(t) * g(t) = f(-t) \otimes g(t)$. Convolution is associated with advancing wave fields in time, correlation with reversing time. The latter serves as the basis for undoing propagation effects.

4. Less heavily used but nonetheless crucial for this thesis, is the Fourier transform of the δ -function. Though not formally correct (see for example Vladimirov [85]),



Figure 1.6: Cosine interference at u = 0 for periods $2a, 4a, \ldots, 12a$.

treating the δ -function as an ordinary function does yield the correct transform

$$\hat{\mathcal{F}}[\delta(\mathbf{u}-\mathbf{u}')] = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \delta(\mathbf{u}-\mathbf{u}') e^{\pm j\mathbf{u}\cdot\mathbf{w}} d^n \mathbf{u} = (2\pi)^{-n/2} e^{\pm j\mathbf{u}'\cdot\mathbf{w}}.$$
 (1.14)

The inverse Fourier transform of equation (1.14) for $\mathbf{u}' = 0$, i.e.

$$\delta(\mathbf{u}) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{\mp j \mathbf{u} \cdot \mathbf{w}} d^n \mathbf{w}$$
$$= (2\pi)^{-n} \int_{\mathbb{R}^n} \cos(\mathbf{u} \cdot \mathbf{w}) d^n \mathbf{w}, \qquad (1.15)$$

offers an alternative to construct numerical approximations of the delta function to those illustrated in Fig 1.5, that is more useful when working in the Fourier Domain. In 1D the sum

$$\delta_{a,M}(u) = \frac{1}{Ma} \Big[1 + 2\sum_{m=1}^{M} \cos\left(\frac{2\pi}{Ma}mu\right) \Big],$$
(1.16)

converges to equation (1.15) if $M \to \infty$ and $a \downarrow 0$. Under these two conditions there will be constructive interference only at u = 0, everywhere else the amplitude will tend to zero, see Figure 1.6.

To distinguish between space-time domain quantities and the corresponding Fourier transforms we will adhere to the conventions used in [88]; (a) lower case letters will indicate time-domain quantities, capitals their frequency-domain counterparts, (b) while quantities depending on the horizontal wave vector \mathbf{k}_H will be over lined with a tilde. The signambiguity in the kernels of equations (1.7a) and (1.7b) is resolved by taking a minus-sign in the forward kernel and a plus-sign in the inverse kernel for the temporal transform, and opposite signs for the spatial transform.

Given the frequency ω and horizontal wave number \mathbf{k}_H , a real-valued, time- and space-dependent $f(\mathbf{x}, t)$ is therefore related to its Fourier transforms by

$$F(\mathbf{x},\omega) = (2\pi)^{-1/2} \int_{\mathbb{R}} f(\mathbf{x},t) e^{-j\omega t} dt, \qquad (1.17a)$$

$$f(\mathbf{x},t) = \left(\frac{2}{\pi}\right)^{1/2} \Re \left[\int_{0}^{+\infty} F(\mathbf{x},\omega) e^{j\omega t} d\omega\right],$$
(1.17b)

$$\tilde{F}(\mathbf{k}_H, x_3, \omega) = \frac{1}{2\pi} \int_{\mathbb{R}^2} F(\mathbf{x}_H, x_3, \omega) e^{j\mathbf{k}_H \cdot \mathbf{x}_H} d^2 \mathbf{x}_H, \qquad (1.17c)$$

$$F(\mathbf{x}_H, x_3, \omega) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \tilde{F}(\mathbf{k}_H, x_3, \omega) e^{-j\mathbf{k}_H \cdot \mathbf{x}_H} d^2 \mathbf{k}_H, \qquad (1.17d)$$

where \Re denotes the real part. The reason for omitting negative frequencies is that their inclusion would increase, without benefit, the work needed for derivations involving equation (1.17b) and complicate the resulting expressions. Successive application of equations (1.17a) and (1.17c) transforms f from the space-time domain to the space-frequency domain, and subsequently to the horizontal wavenumber-frequency domain. In the remainder of this thesis we will use the abbreviations

- **x**, *t*-domain for the space-time domain,
- \mathbf{x}, ω -domain for the space-frequency domain,
- $\mathbf{k}_H, x_3, \omega$ -domain for the horizontal wavenumber-frequency domain.

Equations (1.17a) and (1.17c) can be combined into

$$\tilde{F}(\mathbf{k}_H, x_3, \omega) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(\mathbf{x}_H, x_3, t) e^{-j(\omega t - \mathbf{k}_H \cdot \mathbf{x}_H)} d^2 \mathbf{x}_H dt,$$
(1.18a)

the aggregation of equations (1.17b) and (1.17d) yields the corresponding inverse,

$$f(\mathbf{x}_H, x_3, t) = (2\pi^3)^{-1/2} Re \left[\int_0^\infty \int_{\mathbb{R}^2} \tilde{F}(\mathbf{k}_H, x_3, \omega) e^{j(\omega t - \mathbf{k}_H \cdot \mathbf{x}_H)} d^2 \mathbf{k}_H d\omega \right].$$
(1.18b)

If f represents a wave field in a homogeneous medium, then equation (1.18a) represents a decomposition of f into plane waves \tilde{F} , conversely equation (1.18b) represents the composition of plane waves \tilde{F} to f.

In this notation the space-frequency representation of equation (1.6) becomes

$$P(\mathbf{x},\omega) = \int_{\mathbb{R}^3} G(\mathbf{x},\mathbf{x}_s,\omega) S_p(\mathbf{x}_s,\omega) d^3 \mathbf{x}_s.$$
 (1.19)

For notational convenience we will drop the explicit dependence on the angular frequency ω , whenever it is clear from the context.

1.7 The wave equation in the frequency domain

This section serves to introduce notation that turns out to be highly convenient for formulating one-way wave equations (although that will only become completely clear in Chapter 3). The time-independence of ρ and K can be exploited by transforming equation (1.1) to the frequency-domain and using equation (1.8) to eliminate the temporal differential operator ∂_t . To emphasize the vertical variations of the properties of the earth's subsurface we first separate the vertical component of equation (1.1a) from its horizontal components. Because the vertical component of the particle velocity is the only one that will occur separately in this thesis, we will drop the subscript 3, i.e. $V_3 \rightarrow V$. Thus, in the frequency domain equations (1.1a) and (1.1b) can be expressed as

$$\nabla_H P = -j\omega\rho \mathbf{V}_H + \mathbf{F}_H, \qquad (1.20a)$$

$$\partial_3 P = -j\omega\rho V + F_3, \tag{1.20b}$$

$$\partial_3 V = -\frac{j\omega}{K} P - \nabla_H \cdot \mathbf{V}_H + Q. \qquad (1.20c)$$

The term $\nabla_H \cdot \mathbf{V}_H$ is eliminated from equation (1.20c) using the horizontal components given by equation (1.20a). Subsequently, equations (1.20b) and (1.20c) are merged into the first order matrix-vector equation

$$\partial_3 \mathbf{Q} = \hat{\mathbf{A}} \mathbf{Q} + \mathbf{D}, \tag{1.21}$$

with vectors

$$\mathbf{Q} = \begin{pmatrix} P \\ V \end{pmatrix}, \tag{1.22a}$$

$$\mathbf{D} = \begin{pmatrix} F_3 \\ Q - \nabla_H \cdot \left(\frac{1}{j\omega\rho} \mathbf{F}_H\right) \end{pmatrix}, \qquad (1.22b)$$

the two way operator matrix

$$\hat{\mathbf{A}} = \begin{pmatrix} 0 & -j\omega\rho\\ (j\omega\rho)^{-1}\hat{H}_2 & 0 \end{pmatrix}, \qquad (1.22c)$$

and the pseudo Helmholtz-operator

$$\hat{H}_2(\mathbf{x}_H, x_3) = \frac{\omega^2}{c^2} + \rho \nabla_H \cdot \frac{1}{\rho} \nabla_H.$$
(1.23)

The operator character is denoted by the hat $\hat{}$ on top of H_2 . One can of course also introduce this operator by transforming equation (1.2) to the frequency-domain, which allows one to write

$$\rho\partial_3\left(\frac{1}{\rho}\partial_3P\right) + \hat{H}_2P = -\rho S_p. \tag{1.24}$$

The pseudo Helmholtz-operator plays a pivotal part in wave field decomposition, see Chapters 3 and 4 and also Wapenaar et al. [88, 90]. Expressed as equation (1.21) the wave equation is also-called the "two-way" wave equation. This terminology only serves to distinguish equation (1.21) from so-called one-way wave equations, formulated in terms of up and down going waves, which will be introduced in Chapters 2 and 3.7. The adjective "two-way" could mislead the reader into thinking that equation (1.21) is still somehow restricted to up and down going wave fields. This is not the case, they hold for wave fields propagating in arbitrary directions.

1.8 On the symmetries and conservation laws of wave propagation

Now that the Green's function and Fourier transform have been introduced, it is time to give a more technical overview of the contents of the concepts and topics covered in this thesis. This will be done through an overview of some symmetries and conservation laws of seismic wave propagation. The analysis of the symmetries and conservation laws has been, currently is, and will most likely remain the starting point for solving a lot of problems in mathematical physics. Although the analysis does not provide a direct solution, it does highlight the problem's structure and often reveals important aspects of the solution without an actual construction.

The first part of this section will cover symmetry properties frequently encountered in seismic wave propagation. The second part introduces the aim of this thesis, transmission loss correction for the inverse propagation of one-way wave fields.

1.8.1 Symmetries of the wave equation and their use in seismic wave propagation

Wave propagation in homogeneous media exhibits a high degree of symmetry. Along a stepwise increase of variability, this section will indicate which symmetries remain, how they are used in this thesis in particular, and in seismics in general.

First consider a homogeneous medium. In this case the medium parameters K, ρ do not depend on the coordinates x and t, which implies that the general solution to equation (1.3) is shift-invariant in (a combination of) each of these coordinates, i.e.

$$g(\mathbf{x}, \mathbf{x}_s, t) = g(\mathbf{x} - \mathbf{x}_s, 0, t).$$

For the same reason this Green's solution must also be symmetrical in all three spatial coordinates; sign reversal of one or more of the axes does not affect the wave equation (1.3) for homogeneous media, that is for constant ρ and K. Taken together these mirror symmetries in the spatial directions imply that the spatial axes can be rotated over any angle around the origin, without affecting the solution. Therefore g does not depend on the vector $\mathbf{x} - \mathbf{x}_s$ but merely on its scalar length $|\mathbf{x} - \mathbf{x}_s|$.

In section 1.4 we already assumed ρ and K to be time-independent, which resulted in a Green's function that only depends on the time-difference $t - t_s$, instead of on the two variables t and t_s . In homogeneous media the Green's function effectively depends on just two variables instead of all eight variables $\mathbf{x}, \mathbf{x}_s, t$, and t_s , that is

$$g = g(|\mathbf{x} - \mathbf{x}_s|, t - t_s),$$
where $|\mathbf{r}| = (r_1^2 + r_2^2 + r_3^2)^{1/2}$. Setting $t_s = 0$ it is therefore clear that

$$g(\mathbf{x}, \mathbf{x}_s, t) = g(\mathbf{x}_s, \mathbf{x}, t).$$
(1.25)

This symmetry-relation remains valid for media that do vary with \mathbf{x} , but the proof relies on the more general reciprocity theorems, see Chapter 4.

Although the differential operator ∂_t^2 is time-symmetric, seismic data are obviously not; to resolve the discrepancy any Green's function describing seismic data should obey causal boundary conditions,

$$g = 0$$
 and $\partial_t g = 0$ if $t < 0$.

Opposite conditions

$$g_a = 0$$
 and $\partial_t g_a = 0$ if $t > 0$,

yield anti-causal solutions. Anti-causal solutions will be the starting point for undoing propagation effects, see section 2.5 and Chapters 5 and 6. Due to the symmetry of second order temporal differentiation the causal and anti-causal Green's functions are related according to

$$g_a(\mathbf{x}, t; \mathbf{x}_s) = g(\mathbf{x}, -t; \mathbf{x}_s).$$
(1.26a)

or in the frequency-domain

$$G_a(\mathbf{x}, \mathbf{x}_s) = G^*(\mathbf{x}, \mathbf{x}_s). \tag{1.26b}$$

From here on the subscript a will not be used anymore, but instead complex conjugation will be used to express the anti-causal Green's function in terms of the causal one.

In horizontally layered media the medium parameters only depend on the depthcoordinate x_3 , reducing the spherical symmetry of the Green's function to a cylindrical symmetry around the x_3 -axis. As already said before the subsurface varies much faster in the vertical than in the lateral direction. Although an oversimplification of the actual situation, wave propagation in horizontally layered media shares many features and concepts with wave propagation in actual media, but cast in much simpler mathematics. Chapter 2 is entirely devoted to wave propagation in horizontally layered media and reviews the quantities and concepts used in the later chapters in comparatively simple terms.

Next in our hierarchy of increasing variability is the case of a line source, parallel to the x_2 -axis, in media whose parameters depend on the x_1 - and x_3 -coordinates. Now the cylindrical symmetry of the Green's function is reduced to a translational invariance and mirror-symmetry in the x_2 -direction. The relative mathematical simplicity of wave propagation in horizontally layered media is now lost, see Chapter 3 and appendix A.1, but computation and visualization remain manageable. All examples and applications in this thesis will be in 2D inhomogeneous media.

The treatment of problems that also depend on the remaining spatial coordinate x_2 will require a slightly different notation, but it does not add fundamentally different mathematical problems. Instead, it does increase the demands on computational resources and raises profound difficulties in visualization. The former issue will be addressed in Chapter 5, but the latter is beyond the scope of this thesis.

Though far from irrelevant, the final step of allowing the medium parameters to vary with time is also beyond the scope of this thesis, since within the time-span of a typical seismic experiment the subsurface is time-independent. Important topics related to time-dependence, such as(a) time-lapse seismics², in connection with reservoir-characterization, and (b) stress-monitoring, in an attempt to provide an early warning system for earth-quakes, will not be covered here.

1.8.2 Transmission loss correction and energy conservation

The first part of this section provided a helicopter view of symmetries and invariants, frequently encountered in (seismic) wave-propagation. The key invariant to this thesis, energy flux conservation, will receive a separate section.

Most inverse propagation methods used in seismics violate the law of energy conservation because they do not account for transmission-losses. The resulting error is most simply illustrated at the hand of a configuration of two homogeneous half-spaces, connected by a flat interface, and a down going plane wave at normal incidence with this interface, see Figure 1.7(a). Assuming an incident wave with a unit amplitude, the amplitudes of the transmission and reflection responses are the transmission and reflection coefficients t^+ and r^+ . The conventional approach to inverse propagation applied to this case comes down to multiplying the transmission response with its complex conjugate $t^{+,*}$; remember equations (1.12) and (1.13). The reconstruction of the incident plane

²In time-lapse seismics the difference between two experiments performed on the same site at different times are studied. Still the earth's parameters are considered to be constant during each of these experiments.



Figure 1.7: Plane wave transmission loss

wave has amplitude $t^{+,*}t^+$, which is evidently smaller than the unit amplitude of the original.

Energy conservation across the interface requires that for flux normalized plane waves these coefficients are related by

$$1 - r^{+,*}r^{+} = t^{+,*}t^{+}.$$

Consequently the inverse transmission coefficient can be expressed as by

$$\{t^+\}^{-1} = (1 - r^{+,*}r^+)^{-1} t^{+,*}.$$
(1.27)

The precise definition of (flux normalized) transmission and reflection coefficients is given in section 2.3. Equation (1.27) illustrates that, if in the situation of Figure 1.7 propagation is undone with just the time-reversed transmission response $\{t^+\}^{-1} \approx t^{+,*}$, then the transmission loss $r^{+,*}r^+$ is neglected, also see sections 2.5 and 2.6.

The simplicity of the transmission loss correction formulated by equation (1.27) stems from the planar shapes of both the interface between the two layers and the incident field. It remains valid for transmission through and reflection by more than two layers. Even non-planar incident fields can be treated after decomposing the incident field into plane waves at different angles by the Fourier transform; equation (1.27) can be applied to each component separately, as will be demonstrated in Chapter 2 up to and including section 2.5. Similar relations hold for the transmission and reflection response of an up going plane wave incident from below, with an equally similar extension to the case of a nonplanar wave, incident on a stack of layers.

Applying a generalized form of equation (1.27) to real data, allowing for media with

non-planar interfaces separating non homogeneous layers, proves to be cumbersome. Implicit in the concepts of transmission and reflection is directional decomposition into up and down going parts (in the literature on wave propagation directional decomposition is also commonly referred to as wave splitting). This is a rather straightforward process in the \mathbf{k}_H , ω -domain in case of horizontally layered media, see sections 2.2 and 2.3. In laterally varying media on the other hand it is far from trivial, see Chapter 3; for this case a pseudo-differential operator, introduced in appendix A, is required. If in addition the interfaces are curved, then we need to work with curvilinear coordinates. Chapter 7 shows how and under which conditions directional decomposition for curved interfaces can be formulated.

Working with flux normalized wave fields will allow up and down going wave propagation to be treated on equal footage. Notably, flux normalized transmission effects have an identical description for up and down going wave fields, which is not the case otherwise, see equation (1.2). As a result, expressions in terms of these flux normalized wave fields are simpler than expressions cast in terms of wave fields normalized otherwise.

Reciprocity theorems will be used for the derivation of transmission loss correction. But in their usual appearance they are not suitable for flux normalized wave fields; these theorems will therefore have to be derived separately for flux normalized wave fields, see Chapters 4 and 5.

Chapter 2

Review of one-way wave theory in horizontally layered media

2.1 Introduction

As already mentioned before, most scattering in the earth takes place in the vertical direction, due to much more rapid and stronger variations of the medium parameters in the vertical direction. Although usually much weaker, the horizontal variations still make the formally correct analysis of (one-way) wave propagation rather complex. This chapter will therefore focus on one-way wave propagation in horizontally layered media. It follows the same course as Chapters 3, 4, and 5, but without the mathematical complexity of wave propagation in laterally variant media.

In horizontally layered media K and ρ are entirely independent of \mathbf{x}_H , so scattering only takes place in the vertical direction. This independence of \mathbf{x}_H (and of course t) can be exploited by transforming equations (1.1a) and (1.1b) from partial differential equations in four independent variables (x_1, x_2, x_3, t) , into ordinary differential equations in which x_3 is the only dependent variable. Compared to one-way wave theory for arbitrary media, one-way wave theory for horizontally layered media is therefore much less involved and much more matured, see for example Frasier [32], Kennett [53], and Ursin [83]. The content of this chapter is therefore by no means new; it purely serves to introduce and outline the concepts and methods used in Chapters 3, 4, and 5. Those chapters will frequently refer to corresponding concepts and formulas from this chapter.

It turns out that the decomposition of wave fields into up and down going wave fields

Quantity	Transmission	Composition
	coefficient	matrix
Pressure norm.	t^{\pm}	L
Flux norm.	t±	L

Table 2.1: Font examples

is an eigenvalue problem, section 2.3. As with any eigenvalue problem the normalization of the eigenvectors is not unique. This thesis describes two particular choices, pressure normalized and flux normalized decomposition. A recurring issue in this thesis is the comparison of one-way wave theory formulated in one and the other normalization. To distinguish between the two, similar quantities under different normalization will be denoted by the same symbol but in different fonts, see for example Table 2.1.

The fundamental difference is that there is more symmetry in the flux normalized formulation. In particular, flux normalized up and down going Green's functions obey reciprocity, while their pressure normalized counterparts do not, section 2.4. This reciprocity between up and down going Green's functions will prove to be crucial for providing a practically feasible method for transmission loss corrected inverse propagation, see section 2.5 of this chapter. The influence of transmission loss correction will be illustrated with some simple redatuming/imaging examples in sec, 2.6.

But this chapter takes off by formally introducing up and down going waves, in homogeneous media.

2.2 One-way wave theory in homogeneous media

For a source free, homogeneous medium the \mathbf{k}_H , ω -representation of equation (1.24) can be expressed as

$$\partial_3^2 \tilde{P} = -\tilde{H}_2 \tilde{P}. \tag{2.1a}$$

Due to the absence of any \mathbf{x}_H -dependencies the \mathbf{k}_H, ω -representation of \hat{H}_2 reduces to a simple algebraic form; with $k = \omega/c$ the Helmholtz "operator" \tilde{H}_2 is expressed as

$$\tilde{H}_2 = k^2 - \mathbf{k}_H \cdot \mathbf{k}_H. \tag{2.1b}$$

Instead of as a single second order differential equation, equation (2.1a) can also be expressed as a couple of two first order differential equations

$$\partial_3 \tilde{P}^{\pm} = \mp j \tilde{H}_1 \tilde{P}^{\pm}. \tag{2.1c}$$

The square root "operator" for homogeneous media is $\tilde{H}_1 = \sqrt{\tilde{H}_2}$. Obviously the fundamental solutions to equation (2.1c) are of the form

$$\tilde{P}^{\pm}(\mathbf{k}_H, x_3) = \tilde{P}_0^{\pm} e^{\mp j \tilde{H}_1 x_3}.$$
(2.2)

For the interpretation of equation (2.2) bear in mind the definition of the Fourier transform, section 1.6, and the fact that the positive vertical direction points downward. Then clearly $\tilde{P}^+(\mathbf{k}_H, x_3)$ represents a down going plane wave, propagating in the direction $\mathbf{k} = (\mathbf{k}_H, \tilde{H}_1)$, while $\tilde{P}^-(\mathbf{k}_H, x_3)$ represents an up going plane wave, propagating in the direction $\mathbf{k} = (\mathbf{k}_H, -\tilde{H}_1)$.

Substituting equation (2.1c) in a Taylor expansion, wave fields at different depths $x_{3,1} > x_{3,0}$ can be related by

$$\tilde{P}^{+}(\mathbf{k}_{H}, x_{3,1}) = \sum_{n=0}^{\infty} \frac{(x_{3,1} - x_{3,0})^{n}}{n!} (-j\tilde{H}_{1})^{n} \tilde{P}^{+}(\mathbf{k}_{H}, x_{3,0})$$
$$= \tilde{w}^{+}(x_{3,1}; x_{3,0}) \tilde{P}^{+}(\mathbf{k}_{H}, x_{3,0})$$
(2.3)

with \tilde{w}^+ the propagator for down going waves in homogeneous media

$$\tilde{w}^+(x_{3,1};x_{3,0}) = e^{-jH_1(x_{3,1}-x_{3,0})}.$$
(2.4)

Similar manipulations for up going wave fields lead to the propagator for up going waves

$$\tilde{w}^{-}(x_{3,0};x_{3,1}) = e^{jH_1(x_{3,0}-x_{3,1})} = \tilde{w}^+(x_{3,1};x_{3,0}).$$

$$\tilde{H}_1 = \sqrt{\omega^2/c^2 - \mathbf{k}_H \cdot \mathbf{k}_H}.$$

Due to the form of this dependence \tilde{H}_1 becomes imaginary if $\omega^2/c^2 < \mathbf{k}_H \cdot \mathbf{k}_H$.

¹In literature one frequently encounters the use of k_3^2 and k_3 instead of \tilde{H}_2 and \tilde{H}_1 , respectively. Although there is a solid connection between \tilde{H}_1 and the vertical wavenumber k_3 , they appear in the same places, and are used much the same as k_3 , they are definitely not the same. The vertical wavenumber is an independent and real-valued Fourier-variable, while \tilde{H}_1 is a function of

If $|\mathbf{k}_H| \leq \omega/c$, then \tilde{H}_1 is real, the exponent of \tilde{w}^{\pm} is imaginary and therefore \tilde{w}^{\pm} represent propagating plane waves. If on the other hand $|\mathbf{k}_H| > \omega/c$ then \tilde{H}_1 is imaginary, the exponents of \tilde{w}^{\pm} real, and \tilde{w}^{\pm} will represents evanescent plane waves (exponentially increasing waves are discarded on physical grounds, so always $\Im{\{\tilde{H}_1\}} < 0$).

Inverse propagation is defined by

$$\tilde{f}^{\pm} \triangleq \{\tilde{w}^{\pm}\}^{-1}.\tag{2.5}$$

Clearly, straightforward application of equation (2.5) would also invert the evanescent waves, turning them into exponentially growing waves. In any practical computation (for a homogeneous medium or an arbitrarily complex one) this must be avoided at all costs, because even small errors in the input could obscure the useful propagating waves. Therefore inverse propagation of plane waves is often done with the approximation

$$\tilde{f}^{\pm} \approx \{\tilde{w}^{\pm}\}^*; \tag{2.6}$$

under the application of equation (2.6) propagating waves are reversed in time, but evanescent ones are not affected; the result is approximate, but remains stable. This concept remains true for arbitrary inhomogeneous media, see section 3.4.

2.3 Decomposition

As will be shown in this section, up and down going waves in vertically variant media are conveniently expressed by two coupled, first order differential equation. The single variable dependencies of $\rho = \rho(x_3)$ and $K = K(x_3)$ are exploited by transforming equation (1.1) to the \mathbf{k}_H, ω -domain. Analogous to (1.20) one can write

$$-j\mathbf{k}_{H}\tilde{P} = -j\omega\rho\tilde{\mathbf{V}}_{H} + \tilde{\mathbf{F}}_{H}, \qquad (2.7a)$$

$$\partial_3 \tilde{P} = -j\omega\rho \tilde{V} + \tilde{F}_3,$$
 (2.7b)

$$\partial_3 \tilde{V} = -\frac{j\omega}{K} \tilde{P} + j\mathbf{k}_H \cdot \tilde{\mathbf{V}}_H + \tilde{Q}.$$
 (2.7c)

Similar to (1.21), the elimination of the horizontal term $j\mathbf{k}_H \cdot \tilde{\mathbf{V}}_H$ allows the combination of equations (2.7b) and (2.7c) into the first order matrix-vector equation

$$\partial_3 \tilde{\mathbf{Q}} = \tilde{\mathbf{A}} \tilde{\mathbf{Q}} + \tilde{\mathbf{D}},\tag{2.8}$$

with vectors and matrix

$$\tilde{\mathbf{Q}} = \begin{pmatrix} \tilde{P} \\ \tilde{V} \end{pmatrix}, \quad \tilde{\mathbf{D}} = \begin{pmatrix} \tilde{F}_3 \\ \tilde{Q} + \frac{1}{\omega\rho} \mathbf{k}_H \cdot \tilde{\mathbf{F}}_H \end{pmatrix}, \quad \tilde{\mathbf{A}} = \begin{pmatrix} 0 & -j\omega\rho \\ \frac{\tilde{H}_2}{j\omega\rho} & 0 \end{pmatrix},$$

respectively. Remember the defining relations (1.20)-(1.23).

An elementary linear algebra exercise shows that any anti-diagonal 2×2 -matrix is diagonalized as

$$\tilde{\mathbf{A}} = \begin{pmatrix} 0 & \tilde{A}_{1,2} \\ \tilde{A}_{2,1} & 0 \end{pmatrix} = \tilde{\mathcal{L}} \tilde{\mathbf{\Lambda}} \tilde{\mathcal{L}}^{-1},$$
(2.9)

with

$$\tilde{\mathcal{L}} = \begin{pmatrix} \tilde{Y} & \tilde{Y} \\ \tilde{Z} & -\tilde{Z} \end{pmatrix}, \quad \tilde{\Lambda} = \begin{pmatrix} -\tilde{\Lambda} & 0 \\ 0 & \tilde{\Lambda} \end{pmatrix}, \quad \tilde{\mathcal{L}}^{-1} = \frac{1}{2} \begin{pmatrix} \tilde{Y}^{-1} & \tilde{Z}^{-1} \\ \tilde{Y}^{-1} & -\tilde{Z}^{-1} \end{pmatrix}.$$

Repeating this exercise for $\tilde{A}_{1,2} = -j\omega\rho$ and $\tilde{A}_{2,1} = \tilde{H}_2/(j\omega\rho)$ shows that the matrix \tilde{A} has eigenvalues $\Lambda = \mp j\tilde{H}_1$. It is easy to see that this diagonalization actually realizes directional decomposition into up and down going wave fields in a homogeneous layer: first set the source vector \tilde{D} equal to zero in equation (2.8) and substitute equation (2.9), then multiply both sides with $\tilde{\mathcal{L}}^{-1}$,

$$\partial_3 \begin{pmatrix} \tilde{\mathcal{P}}^+ \\ \tilde{\mathcal{P}}^- \end{pmatrix} = \begin{pmatrix} -j\tilde{H}_1 & 0 \\ 0 & j\tilde{H}_1 \end{pmatrix} \begin{pmatrix} \tilde{\mathcal{P}}^+ \\ \tilde{\mathcal{P}}^- \end{pmatrix} \quad \text{where} \quad \begin{pmatrix} \tilde{\mathcal{P}}^+ \\ \tilde{\mathcal{P}}^- \end{pmatrix} = \tilde{\mathcal{L}}^{-1}\tilde{\mathbf{Q}}$$

Obviously this is equation (2.1c) in matrix form. So for any wave field in a homogeneous layer, equation (2.9) realizes decomposition into up and down going waves. From here on until the end of this chapter, we will allow the medium to be depth-dependent. i.e. $K = K(x_3)$ and $\rho = \rho(x_3)$.

Evaluation of the original eigenvalue-problem $\tilde{\mathbf{A}}\tilde{\mathcal{L}} = \tilde{\mathcal{L}}\tilde{\mathbf{\Lambda}}$ shows that \tilde{Y} and \tilde{Z} are related by $\tilde{Z}/\tilde{Y} = \tilde{H}_1/\omega\rho$. For our purpose the two choices of interest to fix this remaining degree of freedom are (1) pressure normalization and (2) flux normalization. The building blocks of these two choices are introduced as

$$\hat{l} = \hat{H}_1 / (\omega \rho), \qquad (2.10a)$$

$$\tilde{l} = \sqrt{\tilde{H}_1/(\omega\rho)},$$
 (2.10b)

respectively, obviously related by

$$\tilde{l} = \sqrt{\tilde{l}}.$$
 (2.10c)

Pressure normalized (de)composition uses the obvious scaling choice $\tilde{Y} = 1$ and $\tilde{Z} = \tilde{I}$

 $\tilde{\mathit{l}}.$ Replacing $\tilde{\mathbf{\mathcal{L}}} \rightarrow \tilde{\mathbf{L}},$ the corresponding matrices become:

$$\tilde{\mathbf{L}} = \begin{pmatrix} 1 & 1\\ \tilde{l} & -\tilde{l} \end{pmatrix}, \quad \tilde{\mathbf{L}}^{-1} = \frac{1}{2} \begin{pmatrix} 1 & \tilde{l}^{-1}\\ 1 & -\tilde{l}^{-1} \end{pmatrix}.$$

The wave field and source decomposition now read

$$\tilde{\mathbf{Q}} = \tilde{\mathbf{L}}\tilde{\mathbf{P}}, \quad \tilde{\mathbf{P}} = \begin{pmatrix} \tilde{P}^+\\ \tilde{P}^- \end{pmatrix}, \qquad (2.11)$$
$$\tilde{\mathbf{D}} = \tilde{\mathbf{L}}\tilde{\mathbf{S}}, \quad \tilde{\mathbf{S}} = \begin{pmatrix} \tilde{S}^+\\ \tilde{S}^- \end{pmatrix}.$$

With these expressions the "two-way" wave equation (2.8) can be transformed into the pressure normalized one-way wave equation

$$\partial_3 \tilde{\mathbf{P}} = \tilde{\mathbf{B}} \tilde{\mathbf{P}} + \tilde{\mathbf{S}},\tag{2.12}$$

where $\tilde{\mathbf{B}} = \tilde{\mathbf{\Lambda}} - \tilde{\mathbf{L}}^{-1} \partial_3 \tilde{\mathbf{L}}$. The term $\tilde{\mathbf{L}}^{-1} \partial_3 \tilde{\mathbf{L}}$ arises, whenever $\partial_3 c \neq 0$ or $\partial_3 \rho \neq 0$, it describes vertical scattering. The name "pressure normalization" refers to the fact that $\tilde{P} = \tilde{P}^+ + \tilde{P}^-$, remember equation (2.11). This decomposition is used by many authors.

Flux normalized (de)composition uses the scaling $\tilde{Y} = \tilde{l}^{-1}/\sqrt{2}$ and $\tilde{Z} = \tilde{l}/\sqrt{2}$. The (de)composition matrices for flux normalization read

$$\tilde{\mathbf{L}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \tilde{\mathbf{l}}^{-1} & \tilde{\mathbf{l}}^{-1} \\ \tilde{\mathbf{l}} & -\tilde{\mathbf{l}} \end{pmatrix}, \quad \tilde{\mathbf{L}}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \tilde{\mathbf{l}} & \tilde{\mathbf{l}}^{-1} \\ \tilde{\mathbf{l}} & -\tilde{\mathbf{l}}^{-1} \end{pmatrix}.$$

and

The corresponding wave field decompositions are

$$\begin{split} \tilde{\mathbf{Q}} &= \tilde{\mathbf{L}}\tilde{\mathbf{P}}, \quad \tilde{\mathbf{P}} = \begin{pmatrix} \tilde{\mathbf{P}}^+ \\ \tilde{\mathbf{P}}^- \end{pmatrix}, \\ \tilde{\mathbf{D}} &= \tilde{\mathbf{L}}\tilde{\mathbf{S}}, \quad \tilde{\mathbf{S}} = \begin{pmatrix} \tilde{\mathbf{S}}^+ \\ \tilde{\mathbf{S}}^- \end{pmatrix}. \end{split}$$
(2.13)

From the above relations it is clear that the flux normalized one-way wave equation is structurally identical to (2.12)

$$\partial_3 \tilde{\mathbf{P}} = \tilde{\mathbf{B}} \tilde{\mathbf{P}} + \tilde{\mathbf{S}},\tag{2.14}$$

with $\tilde{B} = \tilde{\Lambda} - \tilde{L}^{-1}\partial_3\tilde{L}$. Similar to the pressure normalized case the term $\tilde{L}^{-1}\partial_3\tilde{L}$ describes vertical scattering. Explaining the name flux normalization is slightly more involved than in the pressure normalized case; let

$$\mathbf{J} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } \mathbf{K} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

For $|\mathbf{k}_H| < \omega/c$ the power-flux through a particular x_3 -level is conserved under the transformation $\tilde{\mathbf{L}}$,

$$\tilde{\mathbf{P}}^{+,*}\tilde{\mathbf{P}}^{+} - \tilde{\mathbf{P}}^{-,*}\tilde{\mathbf{P}}^{-} = \tilde{\mathbf{P}}^{\dagger}\mathbf{J}\tilde{\mathbf{P}} = \tilde{\mathbf{Q}}^{\dagger}\{\tilde{\mathbf{L}}^{-1}\}^{t}\mathbf{J}\tilde{\mathbf{L}}^{-1}\tilde{\mathbf{Q}}$$
$$= \tilde{\mathbf{Q}}^{\dagger}\mathbf{K}\tilde{\mathbf{Q}} = \tilde{P}^{*}\tilde{V} + \tilde{V}^{*}\tilde{P}.$$
(2.15)

Here the superscripts t and \dagger denote transposition and taking the adjoint, respectively. Note that the right hand side of equation (2.15) is proportional to the power flux in the x_3 -dimension. Hence the name flux normalized (de)composition.

Cast in terms of up and down going wave fields equation (2.12) and (2.14) are called oneway wave equations, as opposed to the "two-way" wave equation (2.8).

The matrices $\tilde{\mathbf{L}}$ and $\tilde{\mathbf{L}}$ will be called composition matrices, while $\tilde{\mathbf{L}}^{-1}$ and $\tilde{\mathbf{L}}^{-1}$ will be called decomposition matrices. Pressure and flux normalized decomposed wave fields are related to each other by

$$\tilde{\mathsf{P}}^{\pm} = \sqrt{2}\,\tilde{\mathsf{l}}\tilde{P}^{\pm}.\tag{2.16}$$

The difference in scaling between \tilde{P}^{\pm} in equation (2.12) and \tilde{P}^{\pm} in equation (2.14) manifests itself in the transmission coefficients; we will show below that pressure normalized



Figure 2.1: Reflection and transmission at a horizontal interface

up and down going transmission coefficients are not equal, but that their flux normalized counterparts are equal to each other.

To define these coefficients we consider an interface at depth $x_{3,i}$ separating two halfspaces, where the upper one is characterized by parameters ρ_i and c_i and the lower one by parameters ρ_{i+1} and c_{i+1} . The coefficients are defined as ratios of the wave fields at depths $x_{3,u} = x_{3,i} - \epsilon$ and $x_{3,l} = x_{3,i} + \epsilon$, also see Figure 2.1. Given the wave fields \tilde{P}_u^{\pm} at $x_{3,u}$ and \tilde{P}_l^{\pm} at $x_{3,l}$ the transmission- and reflection-coefficients of the horizontal interface at $x_{3,i}$ are customarily defined in the scattering matrix \mathbf{s}_{scat}

$$\begin{pmatrix} \tilde{P}_l^+\\ \tilde{P}_u^- \end{pmatrix} = \mathbf{s}_{scat} \begin{pmatrix} \tilde{P}_u^+\\ \tilde{P}_l^- \end{pmatrix} = \begin{pmatrix} \tilde{t}^+ & \tilde{r}^-\\ \tilde{r}^+ & \tilde{t}^- \end{pmatrix} \begin{pmatrix} \tilde{P}_u^+\\ \tilde{P}_l^- \end{pmatrix}.$$
 (2.17)

The pressure \tilde{P} and vertical velocity \tilde{V} are continuous across the interface. Hence for $\epsilon \to 0$ pressure normalized decomposed wave fields are related

$$\tilde{\mathbf{L}}_u \tilde{\mathbf{P}}_u = \tilde{\mathbf{L}}_l \tilde{\mathbf{P}}_l. \tag{2.18}$$

In case of a source free lower layer, i.e. $\tilde{P}_l^- = 0$, or a source free upper layer, i.e. $\tilde{P}_u^+ = 0$, substitution of the left hand side of equation (2.17) into the continuity condition (2.18) can be written to

$$\begin{pmatrix} (\tilde{t}^+)^{-1} \\ \tilde{r}^+(\tilde{t}^+)^{-1} \end{pmatrix} = \tilde{\mathbf{L}}_u^{-1} \tilde{\mathbf{L}}_l \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \tilde{r}^-(\tilde{t}^-)^{-1} \\ (\tilde{t}^-)^{-1} \end{pmatrix} = \tilde{\mathbf{L}}_l^{-1} \tilde{\mathbf{L}}_u \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad (2.19)$$

respectively. From equation (2.19) the transmission and reflection coefficients can be expressed in terms of $L_{l,u}$ as

$$\tilde{t}^{+} = \frac{2\tilde{l}_{u}}{\tilde{l}_{u} + \tilde{l}_{l}} = 1 + \tilde{r}, \qquad \tilde{r}^{-} = \frac{\tilde{l}_{l} - \tilde{l}_{u}}{\tilde{l}_{l} + \tilde{l}_{u}} = -\tilde{r},$$

$$\tilde{r}^{+} = \frac{\tilde{l}_{u} - \tilde{l}_{l}}{\tilde{l}_{u} + \tilde{l}_{l}} = \tilde{r}, \qquad \tilde{t}^{-} = \frac{2\tilde{l}_{l}}{\tilde{l}_{l} + \tilde{l}_{u}} = 1 - \tilde{r}.$$
(2.20)

Clearly pressure normalized up and down going transmission coefficients are not equal.

For flux normalized wave fields a scattering matrix and continuity condition similar to equations (2.17) and (2.18) can be defined. The flux normalized counterparts of equation (2.19) yield

$$\begin{split} \tilde{t}^{+} &= \frac{2\tilde{l}_{u}\tilde{l}_{l}}{\tilde{l}_{u}^{2} + \tilde{l}_{l}^{2}} = \sqrt{1 - \tilde{r}^{2}}, \quad \tilde{r}^{-} = \frac{\tilde{l}_{l}^{2} - \tilde{l}_{u}^{2}}{\tilde{l}_{l}^{2} + \tilde{l}_{u}^{2}} = -\tilde{r}, \\ \tilde{r}^{+} &= \frac{\tilde{l}_{u}^{2} - \tilde{l}_{l}^{2}}{\tilde{l}_{u}^{2} + \tilde{l}_{l}^{2}} = \tilde{r}, \qquad \tilde{t}^{-} = \frac{2\tilde{l}_{l}\tilde{l}_{u}}{\tilde{l}_{l}^{2} + \tilde{l}_{u}^{2}} = \sqrt{1 - \tilde{r}^{2}}. \end{split}$$
(2.21)

Clearly flux normalized up and down going transmission coefficients *are equal*. Section 2.4 will show that this equality lies at the heart of the reciprocity between flux normalized propagation of up and down going wave fields in horizontally layered media.

2.4 The generalized primary representation

For wave propagation in horizontally layered media, Hubral et al. [48] introduced the term generalized primary, which indicates incorporation of multiple scattering to the description of propagation and reflection, in addition to the more usual approach of only considering primary propagation and reflection. To obtain a recursive expression for the generalized primary representation of reflection data, we analyze scattering by a stack of nflat, homogeneous layers, sandwiched between two homogeneous half spaces, see Figure 2.2. The homogeneous layer between depths $x_{3,n-1}$ and $x_{3,n}$ has parameters ρ_n, c_n . At depth $x_{3,0}$ it is assumed that $\rho_0 = \rho_1$ and $c_0 = c_1$, and therefore $\tilde{t}_0^{\pm} = 1$ and $\tilde{r}_0^{\pm} = 0$, which is indicated in Figure 2.2 by the dotted line at depth $x_{3,0}$ and a lack of distinction between $\tilde{P}_{u,0}^{\pm}$ and $\tilde{P}_{l,0}^{\pm}$. This situation corresponds to that of seismic data without freesurface multiples.

Plane waves incident on and scattered by the stack of interfaces between $x_{3,0}$ and $x_{3,n} + \epsilon$, are related by a scattering matrix analogous to equation (2.17); also compare



Figure 2.2: Scattering configuration

Figures 2.1 and 2.2. This scattering matrix and its constituent transmission/reflection coefficients will be represented by upper case symbols,

$$\begin{pmatrix} \tilde{P}_{l,n}^+\\ \tilde{P}_0^- \end{pmatrix} = \mathbf{S}_{scat} \begin{pmatrix} \tilde{P}_0^+\\ \tilde{P}_{l,n}^- \end{pmatrix} = \begin{pmatrix} \tilde{T}_n^+ & \tilde{R}_n^-\\ \tilde{R}_n^+ & \tilde{T}_n^- \end{pmatrix} \begin{pmatrix} \tilde{P}_0^+\\ \tilde{P}_{l,n}^- \end{pmatrix}.$$
 (2.22)

The upper case symbols in equation (2.22) related to the response of a *stack of layers* will be called global, as opposed to the lower case symbols of equation (2.17) related to *single interface*-responses, which will be called local. A recursive definition of the global coefficients \tilde{T}_n^{\pm} and \tilde{R}_n^{\pm} will be constructed from

- *T*[±]_{n-1} and *R*[±]_{n-1}, the global coefficients of the medium above and including x_{3,n-1}, see Figure 2.3,
- 2. the propagation properties of the homogeneous layer between the interfaces at depths $x_{3,n-1}$ and $x_{3,n}$, \tilde{w}_n^{\pm} , see Figure 2.4,
- 3. the local scattering properties \tilde{t}_n^{\pm} and \tilde{r}_n^{\pm} of the interface at depth $x_{3,n}$, see Figure 2.5,
- 4. and finally the initial conditions $\tilde{T}_0^{\pm} = \tilde{t}_0^{\pm} = 1$ and $\tilde{R}_0^{\pm} = \tilde{r}_0^{\pm} = 0$.



Figure 2.3: Global scattering coefficients for n-1 interfaces



Figure 2.4: Global scattering coefficients for n-1 interfaces *plus* propagation effects up to new interface



Figure 2.5: Global scattering coefficients for n interfaces

This approach provides a convenient way to include internal multiples. The quantities \tilde{W}_n^{\pm} and \tilde{E}_n depicted in Figure 2.4 represent intermediate stages; they include the propagation effects of the added layer between $x_{3,n-1}$ and $x_{3,n}$, but do not contain the scattering effects of the interface at $x_{3,n}$. They are therefore better suited to describe propagation between depths $x_{3,0}$ and $x_{3,n}$; the down going propagator is given by

$$\tilde{W}_n^+ \triangleq \tilde{w}_n^+ \tilde{T}_{n-1}^+, \tag{2.23}$$

and the up going propagator

$$\tilde{W}_n^- \triangleq \tilde{T}_{n-1}^- \tilde{w}_n^-. \tag{2.24}$$

Similarly we use the homogeneous propagators \tilde{w}_n^{\pm} to extrapolate the up going reflection down to the level $x_{3,n} - \epsilon$

$$\tilde{E}_n \triangleq \tilde{w}_n^+ \tilde{R}_{n-1}^- \tilde{w}_n^-.$$
(2.25)

The quantity \tilde{E}_n is responsible for generating the internal multiples. The key notion in the recursive construction is that the internal multiples related to interface n arise from the down going $\tilde{P}_{u,n}^+$ fed back into the scattering medium by the interface n, see Figure 2.2; in the derivations below this notion emerges as a frequent use of (expressions in) the quantities $\tilde{P}_{u,n}^-$ and \tilde{E}_n .

Again, the methods and results presented in this chapter are by no means new. The recursive expressions obtained in this section can be traced back to Kennett [52] in the seismic context, but for the optical case Stokes [78] already derived similar expressions in 1862. This recursive construction is actually a simple example of the general technique called *invariant imbedding*. It is used in a wide range of physics disciplines, all having a focus on wave propagation and/or transport phenomena, also see Bellman and Wing [5]. The scattering matrix approach and additional notation used here are more elaborate than is strictly necessary to construct the recursive definitions mentioned above. The reason for nonetheless doing so, is that it also allows us to derive a generalized primary representation for redatuming in section 2.6.

First we focus on relating \tilde{R}_n^- to \tilde{R}_{n-1}^- by assuming a source-free upper half-space, i.e. $\tilde{P}_0^+ = 0$. Given the reflection response of n-1 interfaces \tilde{R}_{n-1}^- , we use equation (2.3) to extrapolate sources and receivers down to depth $x_{3,n} - \epsilon$; with the help of equation (2.25)

$$\tilde{P}_{l,n-1}^{+} = \tilde{R}_{n-1}\tilde{P}_{l,n-1}^{-},$$

becomes

$$\tilde{P}_{u,n}^+ = \tilde{E}_n \tilde{P}_{u,n}^-. \tag{2.26}$$

Because we chose $\tilde{P}_0^+ = 0$, the upper row of equation (2.22) reads $\tilde{P}_{l,n}^+ = \tilde{R}_n \tilde{P}_{l,n}^-$. Inserting this together with equation (2.26) into the local scattering matrix equation (2.17) for $x_{3,n}$ yields

$$\begin{pmatrix} \tilde{R}_n^- \tilde{P}_{l,n}^-\\ \tilde{P}_{u,n}^- \end{pmatrix} = \begin{pmatrix} \tilde{t}_n^+ & \tilde{r}_n^-\\ \tilde{r}_n^+ & \tilde{t}_n^- \end{pmatrix} \begin{pmatrix} \tilde{E}_n \tilde{P}_{u,n}^-\\ \tilde{P}_{l,n}^- \end{pmatrix},$$
(2.27)

also see Figure 2.6; the feedback-mechanism mentioned earlier this section is clear in equation (2.27). After using the lower row of equation (2.27) to eliminate $\tilde{P}_{u,n}^{-}$ from the upper row, the global down going reflection response can be expressed as

$$\tilde{R}_{n}^{-} = \tilde{r}_{n}^{-} + \tilde{t}_{n}^{+} \tilde{E}_{n} [1 - \tilde{r}_{n}^{+} \tilde{E}_{n}]^{-1} \tilde{t}_{n}^{-};$$
(2.28)

replacing the factor $[1 - \tilde{r}_n^+ \tilde{E}_n]^{-1}$ by a Neumann expansion in $\tilde{r}_n^+ \tilde{E}_n$ will make the internal multiples more explicit.

An analogous course can be taken to relate the global up going transmission coefficients \tilde{T}_{n-1}^- and \tilde{T}_n^- . For a medium of n-1 flat interfaces the condition $\tilde{P}_0^+ = 0$ implies that $\tilde{P}_0^- = \tilde{T}_{n-1}^- \tilde{P}_{l,n-1}^-$. Combining this with equations (2.3) and (2.24) gives

$$\tilde{P}_0^- = \tilde{W}_n^- \tilde{P}_{u,n}^-.$$
(2.29)

The relation (2.29) remains valid, if we add an interface at depth $x_{3,n}$, but what changes are the meanings of \tilde{P}_0^- and $\tilde{P}_{u,n}^-$. From being an unspecified up going wave field directly above $x_{3,n}$, the latter now begets the meaning it had before, in equation (2.27). We are therefore allowed to eliminate $\tilde{P}_{u,n}^-$ from equation (2.29) with the lower row of (2.27). We still have a source free upper half-space, i.e. $\tilde{P}_0^+ = 0$, so now comparison of equation (2.29) with the upper row equation (2.22) yields

$$\tilde{T}_{n}^{-} = \tilde{W}_{n}^{-} \left[1 - \tilde{r}_{n}^{+} \tilde{E}_{n} \right]^{-1} \tilde{t}_{n}^{-}.$$
(2.30)

To obtain expressions for \tilde{R}_n^+ and \tilde{T}_n^+ the treatment of equations (2.26)-(2.30) is basically repeated for a source-free lower half-space, i.e. $\tilde{P}_{l,n}^- = 0$. But now both the initiating transmission response $\tilde{W}_n^+ \tilde{P}_0^+$ and the feedback $\tilde{E}_n \tilde{P}_{u,n}^-$ come in from above



Figure 2.6: Up going source-wave field $\tilde{P}_{l,n}^{-}$ (thick arrow), incident on the bottom interface at $x_{3,n}$, and resulting response.



Figure 2.7: Down going source-wave field \tilde{P}_0^+ (thick arrow), incident on the top interface at $x_{3,0}$, and resulting responses.

on the interface n; therefore the local scattering matrix at $x_{3,n}$ now reads

$$\begin{pmatrix} \tilde{T}_{n}^{+}\tilde{P}_{0}^{+} \\ \tilde{P}_{u,n}^{-} \end{pmatrix} = \begin{pmatrix} \tilde{t}_{n}^{+} & \tilde{r}_{n}^{-} \\ \tilde{r}_{n}^{+} & \tilde{t}_{n}^{-} \end{pmatrix} \begin{pmatrix} \tilde{W}_{n}^{+}\tilde{P}_{0}^{+} + \tilde{E}_{n}\tilde{P}_{u,n}^{-} \\ 0 \end{pmatrix},$$
(2.31)

also see Figure 2.7. Again we eliminate $\tilde{P}_{u,n}^-$ from the upper row with the lower row,

$$\tilde{T}_{n}^{+} = \tilde{t}_{n}^{+} \tilde{W}_{n}^{+} + \tilde{t}_{n}^{+} \tilde{E}_{n} \Big[1 - \tilde{r}_{n}^{+} \tilde{E}_{n} \Big]^{-1} \tilde{r}_{n}^{+} \tilde{W}_{n}^{+},
= \tilde{t}_{n}^{+} \Big[1 - \tilde{E}_{n} \tilde{r}_{n}^{+} \Big]^{-1} \tilde{W}_{n}^{+}.$$
(2.32)

In the last step the two terms on the right hand side were merged into a single term using a Neumann-expansion. A recursive expression for the global up going reflection \tilde{R}_n^+ is based on the (n-1)-analog of the lower row of the global scattering matrix (2.22) in the medium with all n interfaces. Its lower row reads,

$$\tilde{P}_{0}^{-} = \tilde{R}_{n-1}^{+} \tilde{P}_{0}^{+} + \tilde{T}_{n-1}^{-} \tilde{P}_{l,n-1}^{-},$$

$$= \tilde{R}_{n-1}^{+} \tilde{P}_{0}^{+} + \tilde{W}_{n}^{-} \tilde{P}_{u,n}^{-}.$$
(2.33)

For the second step we subsequently substituted equations (2.3) and (2.24). Because we still work with a source free lower half space, i.e. $\tilde{P}_{l,n}^{-} = 0$, we can reuse the lower row of equation (2.31) to eliminate $\tilde{P}_{u,n}^{-}$ from equation (2.33). Matching the elimination result

to the lower row of equation (2.22) yields

$$\tilde{R}_{n}^{+} = \tilde{R}_{n-1}^{+} + \tilde{W}_{n}^{-} \tilde{r}_{n}^{+} \left[1 - \tilde{E}_{n} \tilde{r}_{n}^{+} \right]^{-1} \tilde{W}_{n}^{+},$$

$$= \sum_{i=1}^{n} \tilde{W}_{i}^{-} \tilde{r}_{i}^{+} \left[1 - \tilde{E}_{i} \tilde{r}_{i}^{+} \right]^{-1} \tilde{W}_{i}^{+}.$$
(2.34)

Equation (2.34) supplemented with (2.25), (2.24), (2.23), and recurrent expressions (2.28), (2.30), and (2.32), constitutes the generalized primary representation. A closely related representation is Berkhout's WRW-formulation 2 .

The reflection- and transmission-responses of media with velocity/density profiles continually varying with depth are described by nonlinear differential equations, see for example Bellman and Wing [5]; this explicit nonlinearity limits their usefulness. Therefore they are left out here, but the interested reader can find them in the reference mentioned.

The flux normalized counterparts of the definitions given by equations (2.22), (2.25), (2.24), and (2.23) are structurally identical. Hence, the succeeding manipulations yield structurally identical expressions for the flux normalized counterparts of equations (2.28), (2.30), (2.32) and (2.34). The only sources of difference with the pressure normalized case, are the differences in the local transmission coefficients, see equations (2.20) and (2.21). These differences manifest themselves in the reciprocity of global up and down going transmission response. The quotient of global up and down going transmission

$$\tilde{\mathcal{R}}_n^+ = \sum_{i=1}^n \tilde{\mathcal{W}}_i^- \tilde{r}_i^+ \tilde{\mathcal{W}}_i^+, \qquad (2.35)$$

where \tilde{W}_i^{\pm} are the up/down going primary propagators, and $\tilde{\mathcal{R}}_n^{\pm}$ is the sum of all primary reflections resulting from the interfaces $i = 1, \ldots, n$. This single scattering approach neglects internal multiples. Equation (2.34) on the other hand properly includes the internal multiples. The generalized primary representation equation (2.34) can be recast in a form analogous to equation (2.35), but then the up and down going propagators \tilde{W}_i^{\pm} incorporate transmission and reflection differently, and hence lack reciprocity or will have only partial incorporation of transmission/reflection properties of an interface. Consider for example the choices

$$\tilde{\mathcal{W}}_i^- = \tilde{\mathcal{W}}_i^-, \text{ and } \tilde{\mathcal{W}}_i^+ = \left[1 - \tilde{E}_i \tilde{r}_i^+\right]^{-1} \tilde{\mathcal{W}}_i^+,$$
$$\tilde{\mathcal{W}}_i^- = \tilde{\mathcal{W}}_i^- \left[1 - \tilde{r}_i^+ \tilde{E}_i\right]^{-1/2}, \text{ and } \tilde{\mathcal{W}}_i^+ = \left[1 - \tilde{E}_i \tilde{r}_i^+\right]^{-1/2} \tilde{\mathcal{W}}_i^+.$$

Note the asymmetry between \tilde{W}_i^+ and \tilde{W}_i^- Hence the reason for using the notation of equation (2.34) instead of Berkhout's notation of equation (2.35).

²Berkhout [6] introduced the WRW-formulation,

responses is easily seen to yield

$$\tilde{T}_{n}^{+}/\tilde{T}_{n}^{-} = \prod_{i=1}^{n} \tilde{t}_{i}^{+}/\tilde{t}_{i}^{-}, \qquad (2.36)$$

since each occurrence of the inverse $[1 - \tilde{r}_i^+ \tilde{E}_i]^{-1}$ in \tilde{T}_n^+ is matched in \tilde{T}_n^- , as are the homogeneous propagators. Using the expression for pressure normalized local transmission (2.20), the quotient can be reduced further to

$$\tilde{T}_{n}^{+}/\tilde{T}_{n}^{-} = \prod_{i=1}^{n} \tilde{l}_{i}/\tilde{l}_{i+1} = \tilde{l}_{1}/\tilde{l}_{n+1} \triangleq g_{1,n+1}, \qquad (2.37)$$

with

$$g_{l,m} = \frac{H_{1,l}}{\rho_l} \frac{\rho_m}{\tilde{H}_{1,m}}.$$
 (2.38)

After substitution of equations (2.24), (2.23) and $w_n^+ = w_n^-$, into the left hand side of equation (2.37), it becomes

$$\tilde{W}_{n+1}^{+} = g_{1,n+1}\tilde{W}_{n+1}^{-}.$$
(2.39)

Keeping in mind that $\tilde{t}_i^+ = \tilde{t}_i^-$, it is straightforward to see that the flux normalized counterpart of the quotient (2.36) is equal to 1, so that

$$\tilde{\mathsf{T}}_n^+ = \tilde{\mathsf{T}}_n^- \quad \text{and} \quad \tilde{W}_n^+ = \tilde{W}_n^-.$$
 (2.40)

The reciprocity between up and down going propagators implies reciprocity between up and down going inverse propagators, $\tilde{F}_n^+ = \tilde{F}_n^-$. This will be exploited in the next section.

2.5 Inverse propagation

Usually inverse propagation through inhomogeneous media is achieved by making the approximation

$$\tilde{F}_n^{\pm} \approx \tilde{W}_n^{\mp,*}.$$
(2.41)

This is called the matched filter approach. In case of a two-layer medium (n = 2, also



Figure 2.8: two-layer medium

see Figure 2.8), the error in this approximation is revealed by subsequent substitution of equations (2.41), (2.23), (2.24), and (2.20), in the definition of inverse propagation,

$$\tilde{F}_2^+ \tilde{W}_2^+ \approx \tilde{W}_2^{-,*} \tilde{W}_2^+ = \tilde{t}_1^- \tilde{t}_1^+ = 1 - \tilde{r}_1^2.$$
(2.42)

The flux normalized propagators and inverse propagators obey an identical relation, also see Wapenaar [92]. Clearly the transmission loss is not recovered. Like before this analysis holds for propagating waves only.

The starting point for obtaining the correct inverse of propagator \tilde{W}_n^+ , is the powerflux balance between depths $x_{3,0}$ and $x_{3,n} - \epsilon$. In a medium that is non-scattering and source-free below $x_{3,n} - \epsilon$, the balance reads

$$\tilde{P}_0 \tilde{V}_0^* + \tilde{P}_0^* \tilde{V}_0 = \tilde{P}_{u,n} \tilde{V}_{u,n}^* + \tilde{P}_{u,n}^* \tilde{V}_{u,n}, \qquad (2.43)$$

$$\tilde{P}_{0}^{+}\tilde{P}_{0}^{+,*} - \tilde{P}_{0}^{-}\tilde{P}_{0}^{-,*} = \tilde{P}_{u,n}^{+}\tilde{P}_{u,n}^{+,*}.$$
(2.44)

The flux balance equation (2.44) holds for propagating waves only, but it fully includes transmission losses and internal multiples. We rewrite the balance by first making the substitutions $\tilde{P}_0^- = \tilde{R}_{n-1}^+ \tilde{P}_0^+$ and $\tilde{P}_{u,n}^+ = \tilde{W}_n^+ \tilde{P}_0^+$, and secondly dividing by the source flux $\tilde{P}_0^+ \tilde{P}_0^{+,*}$. This gives

$$1 - \tilde{\mathsf{R}}_{n-1}^{+,*} \tilde{\mathsf{R}}_{n-1}^{+} = \tilde{W}_{n}^{+,*} \tilde{W}_{n}^{+}.$$
(2.45)

Matching equation (2.45) to the defining relation $\tilde{F}_n^+ \tilde{W}_n^+ = 1$, yields

$$\tilde{\mathsf{F}}_{n}^{+} = [1 - \tilde{\mathsf{R}}_{n-1}^{+,*} \tilde{\mathsf{R}}_{n-1}^{+}]^{-1} \tilde{\mathsf{W}}_{n}^{+,*},$$
$$= \sum_{k=0}^{\infty} (\tilde{\mathsf{R}}_{n-1}^{+,*} \tilde{\mathsf{R}}_{n-1}^{+})^{k} \tilde{\mathsf{W}}_{n}^{+,*}.$$
(2.46a)

In practical computations only a finite number of correction terms is used, the terms for k > K will be neglected. This will be indicated by adding a superscript K to \tilde{F}_n^+

$$\tilde{\mathsf{F}}_{n}^{+,(K)} = \sum_{k=0}^{K} (\tilde{\mathsf{R}}_{n-1}^{+,*} \tilde{\mathsf{R}}_{n-1}^{+})^{k} \tilde{W}_{n}^{+,*}.$$
(2.46b)

The series expansion equation (2.46a) shows that the flux normalized counterpart of equation (2.41) is a zero order approximation of equation (2.46b), which works for low to moderate reflectivity, but otherwise significant amplitude defects arise.

The flux-balance (2.43) can of course also be expressed in terms of pressure normalized reflection and transmission responses by means of equation (2.11). For propagating waves we have

$$\tilde{P}\tilde{V}^* + \tilde{P}^*\tilde{V} = \tilde{\mathbf{Q}}^{\dagger}\mathbf{K}\tilde{\mathbf{Q}} = \tilde{\mathbf{P}}^{\dagger}\tilde{\mathbf{L}}^t\mathbf{K}\tilde{\mathbf{L}}\tilde{\mathbf{P}},$$
$$= 2\tilde{l}\,\tilde{\mathbf{P}}^{\dagger}\mathbf{J}\tilde{\mathbf{P}};$$

substitution into both sides of equation (2.43) yields

$$\frac{\tilde{H}_{1,1}}{\rho_1} [1 - \tilde{R}_{n-1}^{+,*} \tilde{R}_{n-1}^+] = \frac{\tilde{H}_{1,n}}{\rho_n} \tilde{W}_n^{+,*} \tilde{W}_n^+;$$
(2.47)

matching equation (2.47) to the identity relation $\tilde{F}_n^+ \tilde{W}_n^+ = 1$ results in a transmission loss correction similar to equation (2.46a),

$$\tilde{F}_n^+ = [1 - \tilde{R}_{n-1}^{+,*} \tilde{R}_{n-1}^+]^{-1} g_{1,n}^{-1} \tilde{W}_n^{+,*}]$$
$$= [1 - \tilde{R}_{n-1}^{+,*} \tilde{R}_{n-1}^+]^{-1} \tilde{W}_n^{-,*}.$$

Using (a selection of) the surface data \tilde{R}_{n-1}^+ or \tilde{R}_{n-1}^+ it is therefore possible to obtain a transmission loss correction for inverse propagation of down-going waves. Inverse prop-

agation of flux normalized up going waves, is achieved by reciprocity, equation (2.40),

$$\tilde{\mathsf{F}}_n^- = \tilde{\mathsf{F}}_n^+. \tag{2.49}$$

Equation (2.39) can be used to obtain \tilde{F}_n^- from \tilde{F}_n^+ , i.e.

$$\tilde{F}_n^- = g_{1,n+1}\tilde{F}_n^+.$$
(2.50)

For laterally varying media equation (2.50), is obviously more cumbersome to implement equation (2.49).

2.6 Redatuming

This section will demonstrate how the results of sections 2.4 and 2.5 facilitate redatuming, the basis for a number of processing steps in seismic practice. After the introduction of redatuming for one-way wave fields, the second part of this section will illustrate the significance of correction for transmission loss in redatuming by estimating the angledependence of the reflection coefficient of a horizontal interface located below another horizontal interface.

As mentioned in Chapter 1 redatuming relates two experiments, the actual surface measurements and a thought experiment with sources and receivers buried at some depth in the subsurface, also see Figure 2.9 (the quantity $\tilde{R}_{n,N}^+$ and $x_{3,N}$, will be discussed in the next paragraph). The data resulting from the thought experiment would be perfect for obtaining an image of the reflecting interface at that depth in the subsurface (inevitably called imaging), or even an estimate of the local reflectivity and its angle-dependence (Amplitude Versus Angle or AVA-analysis) and other post-processing steps such as velocity replacement.

The effects of redatuming will be described in terms of global quantities. The first step will be to express the response of the thought experiment in terms of global reflection responses. This is actually the ideal outcome of redatuming. The second step will be to relate the actual surface measurements to the thought experiment. In the third and final step we will invert this relation, i.e. relate the thought experiment to the surface measurements. This final expression will yield the definition of redatuming and will at once show in which way the redatuming result deviates from the thought experiment response.

Let us consider redatuming to depth $x_{3,n}$ in a medium with a deepest interface at depth $x_{3,N} > x_{3,n}$. If the down going reflection response of the interfaces i = n, ..., N equals





Figure 2.9: Thought experiment at depth $x_{3,m} - \epsilon$

Figure 2.10: Quantities involved in scattering matrix approach to relate surface measurements and thought experiment

 $\tilde{\mathsf{R}}_{n,N}^+$, then the total wave field $(\tilde{\mathsf{P}}_{u,n}^+, \tilde{\mathsf{P}}_{u,n}^-)^t$ at depth $x_{3,n} - \epsilon$ due to a down going source $\tilde{\mathsf{S}}_{u,n}^+$ at the same level satisfies

$$\begin{pmatrix} \tilde{\mathsf{P}}_{u,n}^+ \\ \tilde{\mathsf{P}}_{u,n}^- \end{pmatrix} = \begin{pmatrix} \tilde{\mathsf{S}}_{u,n}^+ \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & \tilde{\mathsf{E}}_n \\ \tilde{\mathsf{R}}_{n,N}^+ & 0 \end{pmatrix} \begin{pmatrix} \tilde{\mathsf{P}}_{u,n}^+ \\ \tilde{\mathsf{P}}_{u,n}^- \end{pmatrix}.$$
 (2.51)

The same feedback-mechanism that featured in section 2.4 is also present in equation (2.51); after eliminating the down going wave field $\tilde{P}^+_{u,n}$, the up going response $\tilde{P}^-_{u,n}$ of the thought experiment can be expressed as

$$\tilde{\mathsf{P}}_{u,n}^{-} = [1 - \tilde{\mathsf{R}}_{n,N}^{+} \tilde{\mathsf{E}}_{n}]^{-1} \tilde{\mathsf{R}}_{n,N}^{+} \tilde{\mathsf{S}}_{u,n}^{+}.$$

$$\triangleq \tilde{\mathsf{R}}_{thght,n} \tilde{\mathsf{S}}_{u,n}^{+}.$$
(2.52)

A pictorial way to represent the transformation of the thought experiment to the surface measurements, is moving sources and receivers from $x_{3,n} - \epsilon$ to $x_{3,0}$. The latter transformation of moving up the receivers is simply accomplished by multiplying the response of the thought experiment with with the up going propagator \tilde{W}_n^- , i.e.

$$W_n^- R_{thght,n}$$
.

The former transformation of moving up the sources is less straightforward. At first sight it just comes down to multiplication by \tilde{W}_n^+ . But then we are missing something.

To express the surface measurements in terms of the thought experiment, we again

take the scattering matrix approach of section 2.4, but now for the wave fields at $x_{3,0}$ and $x_{3,n} - \epsilon$ in the medium with N interfaces in the interval $[x_{3,1}, x_{3,N}]$. See Figure 2.10 for an overview of the quantities involved.

If the only source field is the down going \tilde{S}_0^+ at $x_{3,0}$, then the up going response at $x_{3,0}$ is necessarily $\tilde{R}_N^+ \tilde{S}_0^+$. Although there is no direct up going source at $x_{3,n} - \epsilon$, there is a secondary source field due the reflection response of the interfaces at $x_3 \ge x_{3,n}$. The down going field at depth $x_{3,n} - \epsilon$ is $\tilde{P}_{u,n}^+$. This is different from $\tilde{P}_{u,n}^+$ in equation (2.51), but it represents a down going wave field at the same depth, and therefore undergoes the same scattering; the up going wave field at the same level is

$$\tilde{\mathsf{P}}_{u,n}^{-} = \tilde{\mathsf{P}}_{u,n}^{+} \tilde{\mathsf{R}}_{n,N}^{+}.$$

The scattering matrix for this configuration

$$\begin{pmatrix} \tilde{W}_n^+ & \tilde{\mathsf{E}}_n \\ \tilde{\mathsf{R}}_{n-1}^+ & \tilde{W}_n^- \end{pmatrix}$$

and the wave fields described above are related by

$$\begin{pmatrix} \tilde{\mathsf{P}}_{u,n}^+ \\ \tilde{\mathsf{R}}_N^+ \tilde{\mathsf{S}}_0^+ \end{pmatrix} = \begin{pmatrix} \tilde{\mathsf{W}}_n^+ & \tilde{\mathsf{E}}_n \\ \tilde{\mathsf{R}}_{n-1}^+ & \tilde{\mathsf{W}}_n^- \end{pmatrix} \begin{pmatrix} \tilde{\mathsf{S}}_0^+ \\ \tilde{\mathsf{R}}_{n,N}^+ \tilde{\mathsf{P}}_{u,n}^+ \end{pmatrix}.$$
 (2.53)

Similar to the elimination of $\tilde{P}_{u,n}^+$ from equation (2.51), the elimination of $\tilde{P}_{u,n}^+$ from equation (2.53) allows \tilde{R}_N^+ to be expressed as

$$\tilde{\mathsf{R}}_{N}^{+} = \tilde{\mathsf{R}}_{n-1}^{+} + \tilde{W}_{n}^{-} \tilde{\mathsf{R}}_{thght,n} \tilde{W}_{n}^{+}.$$
(2.54)

Given that the procedure of redatuming aims at recovering the thought experiment response $\tilde{R}_{thght,n}$ from the surface measurements \tilde{R}_N^+ , the structure of equation (2.54) indicates that left and right multiplication by the inverse propagators \tilde{F}_n^- and \tilde{F}_n^+ must be part of the procedure. Redatuming is defined as

$$\tilde{\mathsf{R}}_{dat,n} \triangleq \tilde{\mathsf{F}}_n^- \tilde{\mathsf{R}}_N^+ \tilde{\mathsf{F}}_n^+.$$
(2.55a)

Ideally the reflection response \tilde{R}^+_{n-1} should also be removed, but unless it can modeled separately this is a nontrivial task. Hence besides the thought experiment, redatuming also results in artifacts

$$\tilde{\mathsf{R}}_{dat,n} = \tilde{\mathsf{F}}_n^- \tilde{\mathsf{R}}_{n-1}^+ \tilde{\mathsf{F}}_n^+ + \tilde{\mathsf{R}}_{thght,n}.$$
(2.55b)

A more detailed analysis of the artifacts $\tilde{F}_n^- \tilde{R}_{n-1}^+ \tilde{F}_n^+$ will be given in section 6.2. There we will show that although these artifacts disturb the ideal result $\tilde{R}_{thght,n}$, they also present a possibility to estimate \tilde{R}_{n-1}^+ in a data-driven fashion from \tilde{R}_N^+ , and thereby removing the requirement of separate modeling.

This chapter concludes with an illustration of redatuming in a simple medium and subsequent estimation of the reflection coefficient of the bottom interface. After redatuming, the conventional approach to structural imaging is to transform equation (2.55) back to the x_H, ω -domain and sum all frequency components³ for zero offset. This approach ignores the angle dependence of reflectivity and would render the extra work of transmission loss corrected redatuming useless. Analysis and further processing in the angle-domain is more useful. In the seismic literature, angle dependence in 3D is commonly analyzed in terms of the horizontal slowness or ray parameter

$$\mathbf{p}_{H} = \begin{pmatrix} p_{1} \\ p_{2} \end{pmatrix} = \frac{1}{\omega} \begin{pmatrix} k_{1} \\ k_{2} \end{pmatrix} = \frac{1}{c_{n}} \begin{pmatrix} \cos\beta\sin\alpha \\ \sin\beta\sin\alpha \end{pmatrix}$$

where α is the angle of incidence and β is the azimuth angle (i.e. the angle of the in line direction with some reference direction). De Bruin et al. [15] described how to recover the angle-dependence of \tilde{r}_n^+ from equation (2.35), by summing the frequency components of (the WRW-counterpart of) equation (2.55) along lines of constant horizontal slowness. They used the matched filter approach for redatuming and demonstrated their method on weak to moderately reflecting horizontally layered media. Using the transmission loss correction, it will be demonstrated in Chapters 5 and 6 that their approach can also be applied to laterally varying, high contrast media.

As demonstrated at the beginning of section 2.5, the matched filter approach does not account for transmission losses. At a first glance one might expect that this will just cause the estimate of the reflection coefficient to differ by an overall factor from the expected result, but that its angle-dependence will be recovered correctly in a qualitative sense. However, this first glance is wrong even in horizontally layered media. We will prove

³Summing all frequency components comes down to transforming to the time-domain and evaluating the result at time t = 0.

Layer	Velocity	Density
	(m/s)	(kg/m ³
1	1400	1400
2	2250	2250
3	1500	1500

Table 2.2: Redatuming example medium parameters

this with an AVA-analysis in a 2D medium consisting of a horizontal high velocity layer sandwiched by two low velocity half-spaces, i.e. n = 2.

Take the medium parameters shown in table 2.2. In the p_1, ω -domain the flux normalized primary reflection response at $x_{3,0}$ from the interface at $x_{3,2}$ is

$$\tilde{\mathsf{R}}_2(p_1, x_{3,0}, \omega) \approx \tilde{\mathsf{W}}^-(p_1, x_{3,0}, \omega; x_{3,2})\tilde{\mathsf{r}}_2^+(p_1)\tilde{\mathsf{W}}^+(p_1, x_{3,2}, \omega; x_{3,0});$$
 (2.56)

here the $x_{3,1}$ -primary and internal multiples due to the interface at $x_{3,2}$ have been neglected, see Figure 2.11(a). Redatuming \tilde{R}_2 to interface 2 with the matched filter approach involves left and right multiplication of equation (2.56) with $\{\tilde{W}_2^-\}^*$ and $\{\tilde{W}_2^+\}^*$ respectively, see Figure 2.11(b). With conventional redatuming the reflection coefficient of the bottom interface is estimated as

$$\tilde{\mathbf{r}}_{2,est} = \tilde{W}^{-,*} \tilde{\mathsf{R}}_2 \tilde{W}^{+,*}, \qquad (2.57)$$

The procedure described by equation (2.57) handles the phase correctly, see Figure 2.11(c), but let us analyze the amplitudes. The absolute values of the propagators are

$$|W^-| = |\tilde{\mathfrak{t}}_1^-|,$$

and

$$|\tilde{\mathcal{W}}^+| = |\tilde{\mathfrak{t}}_1^+| = |\tilde{\mathfrak{t}}_1^-| \triangleq |\tilde{\mathfrak{t}}_1|.$$

Therefore the absolute value of $\tilde{r}_{2,est}$ is

$$|\tilde{\mathbf{r}}_{2,est}| = |\tilde{\mathbf{t}}_1|^2 |\tilde{\mathbf{r}}_2| |\tilde{\mathbf{t}}_1|^2.$$
(2.58)

We plotted equation $|\tilde{r}_2|$, $|\tilde{t}_1|$, and $|\tilde{r}_{2,est}|$ as a function of p_1 , see Figure 2.11(d). The difference between the estimated reflection coefficient and the actual one are clear; the abso-



(a) Primary response due to interface at $x_{3,2},$ presented in the $p_1,\tau\text{-domain}.$



(c) Redatuming response, presented in the p_1, τ -domain.



(b) Propagator from $x_{3,0}$ to $x_{3,2}$, presented in the p_1, τ -domain.



(d) Example of primary of redatuming in the p_1, ω -domain without transmission loss correction



Figure 2.11: Example of primary of redatuming in the p_1, ω -domain with transmission loss correction to orders K = 1 (dotted line) and K = 4 (dashed line). The solid line represents the absolute value of the true reflection coefficient.

lute value of the estimate is not just smaller over the whole p_1 -range, the p_1 -dependence is not even recovered correct in a qualitative sense. Instead of rising from a minimum at $p_1 = 0$ to a maximum at the critical angle, it has an approximately constant value for sub-critical values of p_1 and goes to zero at the critical angle. With transmission loss correction as given by equation (2.46b), the estimated reflection coefficient resembles the actual one closer, see Figure 2.11 for correction to order K = 1 and K = 4.

This example illustrates the usefulness of transmission loss correction for redatuming (and subsequent steps) in high-contrast media. The continuum and laterally varying analog of equations (2.46a) and (2.55) will be derived and applied to some simple examples in Chapter 5 and applied to real data in Chapter 6. But in order to do so the concepts of wave field decomposition and data representation have to be extended to media, varying continually in the vertical and horizontal directions. This will be done in Chapters 3 and 4, respectively.

Chapter 3

Wave field Decomposition

3.1 Introduction

Decomposition into up and down going wave fields along the lines described in section 2.3, is still possible for more complex media, where the compressibility and density depend on all three spatial coordinates. But due to these more general dependencies, the differential operators do not reduce to straightforward algebraic multiplications in the wavenumber-frequency domain but become convolutions instead. Defining the various fractional powers of the Helmholtz operator as in section 2.3 becomes less obvious.

However, there is a transformation that does for the more general dependencies what Fourier transformation did for media only varying with depth: transform the Helmholtz operator to an ordinary variable and thereby allowing for fractional powers. In linear algebra terms this transformation "diagonalizes" the Helmholtz-operator.

The vast body of mathematics defining such a transformation revolves around objects called pseudo-differential operators. Much of the associated concepts are actually derived from linear algebra; transposition, complex conjugation, inversion. Contrary to their much more involved formal definitions, they are used essentially the same as in linear algebra; see appendices A.1 and A.2 on pseudo-differential operators (abbreviated to Ψ DO in this thesis) and kernels. Eigenvalues, eigenvectors, and matrix diagonalization also have their analogs in Ψ DO-theory. Without mentioning it, Chapter 2 was already based on these analogs; \tilde{H}_2 and Fourier transformation make up the spectrum and corresponding basis of eigenfunctions of the pseudo Helmholtz-operator in case the density and compression modulus are only functions of depth.

For media that vary also in the lateral directions, the "diagonalization" or rather modal

decomposition of the Helmholtz operator is closely related to the "diagonalization" of the Hamiltonian from quantum physics¹. Section 3.2 will explain how to relate the (pseudo) Helmholtz operator to the Hamiltonian, which allows us to rely on the well developed theory of non-relativistic quantum physics. Section 3.3 will introduce the operator-equivalent of matrix diagonalization, allowing for the formal definition of fractional powers of the Helmholtz operator in section 3.4.

A problem of notation arises due to the fact that in general the spectrum of the Helmholtz operator has a discrete part in addition to the continuum spectrum of the horizontally layered case, see section 3.3. It is possible to double the number of algebraic expressions from Chapter 2, by adding discrete counterparts to the already existing expressions for the continuous part of the spectrum. However, here we choose to work in the space domain instead of the wavenumber domain of Chapter 2. Now extending the expressions of section 2.3 to laterally varying media, comes down to repeating the derivation for non-commuting quantities. This is done in sections 3.5 and 3.6.

Section 3.7 gives a detailed discussion on the numerical implementation of the modal decomposition. Finally, section 3.8 concludes this chapter with some examples of up/down decomposition of wave fields generated by a Finite Difference algorithm.

3.2 The two-way wave equation in complex media

Although not approaching it that way, Claerbout [16] realized that the foundation for a formally correct solution to extending equation (2.1c) to laterally varying media, was a Ψ DO called \hat{H}_1 , implicitly defined by

$$\hat{H}_2 = \hat{H}_1 \hat{H}_1;$$
 (3.1)

after the homogeneous case he baptized this the "square root" operator (note that Claerbout used a different notation). Consider up or down going wave fields propagating in a source free, vertically homogeneous, medium. Without vertical variations to change their direction, wave fields propagating upward keep on doing so; the same holds for down

¹In the first part of the twentieth century physicists started to gain the ability to observe and experiment with natural phenomena on atomic scales. Their most startling observation was that the outcomes of their measurements did not vary continuously, but discretely; the resulting new field called quantum physics would set the course for a wide range of scientific and technical developments. Eigenvalues and eigenfunctions (the continuum analogs of eigenvectors) became the tools for the theoretical study of this field. And although these concepts had been used in the preceding centuries, quantum physics accelerated their development and made its impression on the nomenclature; for example the collection of eigenvalues is commonly referred to as spectrum.

going wave fields. In this situation, equation (1.24) extends to

$$\partial_3^2 P^{\pm}(\mathbf{x}_H, x_3) = -\hat{H}_2 P^{\pm}(\mathbf{x}_H, x_3) = (j\hat{H}_1)^2 P^{\pm}(\mathbf{x}_H, x_3),$$

$$\partial_3 P^{\pm}(\mathbf{x}_H, x_3) = \mp j\hat{H}_1 P^{\pm}(\mathbf{x}_H, x_3).$$

The sign was chosen in accordance with the completely homogeneous situation.

Unlike Claerbout, Fishman and McCoy [27] did take a formal approach employing symbol-calculus, see appendix A.1; they based their solution on that of the closely related mathematical problem, the solution of the non-relativistic Schrödinger equation. See Fishman et al. [28] for an extensive list on numerical and theoretical aspects.

Wapenaar and Grimbergen [90] also exploited the quantum mechanics connection. The pseudo Helmholtz-operator can be cast in the form of a non-relativistic Hamiltonian operator by the transformation

$$\hat{\mathsf{H}}_2 = \rho^{-1/2} \hat{H}_2 \rho^{1/2}, \tag{3.2a}$$

$$=k^{2}(\mathbf{x})+\nabla_{H}\cdot\nabla_{H},$$
(3.2b)

where

$$k^{2}(\mathbf{x}) = \left(\frac{\omega}{c}\right)^{2} - \frac{3(\nabla_{H}\rho)^{2}}{4\rho^{2}} + \frac{\nabla_{H}\cdot\nabla_{H}\rho}{2\rho}.$$
(3.2c)

The transformation described by equation (3.2a) allows a straightforward map of the wellknown properties of the quantum mechanical Hamiltonian operator $\hat{\mathcal{H}}$ to the Helmholtz operator $\hat{\mathcal{H}}_2$;

$$\hat{\mathcal{H}} = -\nabla_H \cdot \nabla_H + V(\mathbf{x}_H),
\hat{\mathcal{H}}_2 = k_0^2(x_3) - [\{k_0^2(x_3) - k^2(\mathbf{x}_H, x_3)\} - \nabla_H \cdot \nabla_H],
= k_0^2(x_3) - \hat{\mathcal{H}}.$$
(3.3)

We assume that at x_3 the medium is laterally homogeneous outside some finite range of x_H ; the wavenumber for this homogeneous embedding is

$$k_0(x_3) = \omega/c_0$$

with velocity c_0 . The "potential" $V(\mathbf{x}_H) = k_0^2(x_3) - k^2(\mathbf{x}_H, x_3)$ therefore has compact support, i.e. is zero outside some finite range and can be seen as a perturbation of the



Figure 3.1: Operator spectra for homogeneous media

Laplacian operator $-\nabla_H \cdot \nabla_H$. In the literature of mathematical physics, the study of spectra of these kinds of operators falls under *Scattering theory*.

The operator-character of $\hat{\mathcal{H}}_2$ is exclusively \mathbf{x}_H -based. Therefore the homogeneous embedding term $k_0^2(x_3)$ in equation (3.3) does not affect the modal decomposition, so the Hamiltonian $\hat{\mathcal{H}}_2$ and the Helmholtz-operator $\hat{\mathcal{H}}_2$ have identical eigenfunctions. To emphasize this \mathbf{x}_H -based operator-character, the x_3 -dependencies will be suppressed in this chapter to reappear again afterward.

Applying the spectral (or modal) decomposition of the Hamiltonian to the Helmholtzoperator \hat{H}_2 , Wapenaar and Grimbergen [90] essentially extended the plane wave decomposition for horizontally layered media, equations (2.9)-(2.16), to laterally varying media. The modal decomposition not only facilitates the definition and construction of fractional powers of the Helmholtz operator, it is also used to prove their symmetry. This is crucial for the extension to complex media of the reciprocity properties of the flux normalized one-way wave equation for horizontally layered media.

3.3 Modal decomposition of the Helmholtz operator

Actually we have already used the modal decomposition of the Helmholtz operator implicitly, for homogeneous media in section 2.2. In a more explicit notation than was used in that section, we can now say that the operator

$$\hat{\mathsf{H}}_{2,0} = k_0^2 + \nabla_H \cdot \nabla_H,$$

has eigenvectors

$$\phi_0(\mathbf{x}_H; \mathbf{k}_H) = \exp\left(j\mathbf{k}_H \cdot \mathbf{x}_H\right),$$

remember the definition of the spatial Fourier transform, equation (1.17c), while the corresponding eigenvalues are

$$\lambda_0(\mathbf{k}_H) = k_0^2 - \mathbf{k}_H \cdot \mathbf{k}_H.$$

The eigenvalue problem of the homogeneous Helmholtz operator is essentially the same as that of the Laplacian which has a real, negative spectrum $-\mathbf{k}_H \cdot \mathbf{k}_H$, also see Figure 3.1(a). Adding a constant k_0^2 to the operator does not affect the eigenvectors, it merely shifts the part of the spectrum onto the positive real axis, see Figure 3.1(b).

We return to the Hamiltonian operator $\hat{\mathcal{H}}$. It is self-adjoint and therefore has a real spectrum, see Reed and Simon [72] or Shubin [76]. This feature is the continuum analog of Hermitian matrices having real eigenvalues in linear algebra; see appendices A.2 and A.3 for an elaboration of the analogy between operators and square matrices. The spectrum $\sigma(\hat{\mathcal{H}})$ consists of a discrete part $\mu_i \in \sigma_d(\hat{\mathcal{H}})$, and a continuous part $\mu(\mathbf{k}_H) \in \sigma_{cont}(\hat{\mathcal{H}})$, where $\mathbf{k}_H = (k_1, k_2)$ and

$$\mu(\mathbf{k}_H) = \mathbf{k}_H \cdot \mathbf{k}_H. \tag{3.4}$$

The eigenfunctions $\phi^{(i)}(\mathbf{x}_H)$ and $\phi(\mathbf{x}_H; \mathbf{k}_H)$ correspond to the eigenvalues μ_i and $\mu(\mathbf{k}_H)$, respectively. Analogous to the unitary eigenvector-basis of an Hermitian matrix, the eigenfunctions corresponding to the continuous part of the spectrum obey

$$\phi^*(\mathbf{x}_H; \mathbf{k}_H) = \phi(\mathbf{x}_H; -\mathbf{k}_H), \tag{3.5}$$

Reed and Simon [73]. From equation (3.3) it follows that these eigenfunctions of the Hamiltonian $\hat{\mathcal{H}}$ are also the eigenfunctions of the Helmholtz operator \hat{H}_2 . The eigenvalues of \hat{H}_2 , defined by

$$\hat{\mathsf{H}}_2 \phi^{(i)}(\mathbf{x}_H) = \lambda^{(i)} \phi^{(i)}(\mathbf{x}_H), \tag{3.6a}$$

$$\hat{\mathsf{H}}_2\phi(\mathbf{x}_H;\mathbf{k}_H) = \lambda(\mathbf{k}_H)\phi(\mathbf{x}_H;\mathbf{k}_H), \tag{3.6b}$$



Figure 3.2: 1D square well velocity function

are therefore related to those of $\hat{\mathcal{H}}$ in a way similar to their operators,

$$\lambda^{(i)} = k_0^2(x_3) - \mu^{(i)}, \tag{3.7a}$$

$$\lambda(\mathbf{k}_H) = k_0^2(x_3) - \mu(\mathbf{k}_H),$$

= $k_0^2(x_3) - \mathbf{k}_H \cdot \mathbf{k}_H,$ (3.7b)

again see equation (3.3).

The physics behind the separation of the spectrum into a continuous and discrete part, is most easily illustrated by considering the eigenvalue problem for the Helmholtz operator in a homogeneous medium with a square well velocity perturbation in the lateral x_1 -direction,

$$c(x_1) = egin{cases} c_0 & ext{for } x_1 < x_l, \ c_1 & ext{for } x_l < x_1 < x_r \ c_0 & ext{for } x_r < x_1. \end{cases}$$

Here the velocities c_1 and c_0 obey $0 < c_1 < c_0$, also see Figure 3.2(a). The corresponding perturbed "potential", see equation (3.2c), is

$$k^{2}(x_{1}) = \begin{cases} k_{0}^{2} & \text{if } x_{1} < x_{l}, \\ k_{1}^{2} & \text{if } x_{l} < x_{1} < x_{r}, \\ k_{0}^{2} & \text{if } x_{r} < x_{1}; \end{cases}$$
(3.8)

the "wave numbers" are given by $k_i = \omega/c_i$. Also see Figure 3.2(b).

The eigenvalue problem is a second order differential equation in x_1

$$\partial_1^2 \phi(x_1) + \left[k^2(x_1) - \lambda\right] \phi(x_1) = 0,$$

remember equation (3.2b). The eigenfunctions corresponding to eigenvalues $\lambda < k_0^2$ oscillate, see the gray area of Figure 3.2(c) and the middle line in Figure 3.3. They are called radiating modes and correspond to the homogeneous eigenfunctions ϕ_0 . The eigenvalues in the interval $k_0^2 < \lambda < k_1^2$ have no analogies in the homogeneous case. The eigenfunction is oscillating in the interval $x_l < x_1 < x_r$, and exponentially decaying outside this interval. In the latter case the wave field will be reflected back and forth between the discontinuities at x_l and x_r , see top of Figure 3.3. The resulting interference can only be constructive if the width $|x_r - x_l|$ is an integer multiple of the wavelength, otherwise the interference is destructive and no propagation in the x_1 -direction will occur; hence the discrete eigenvalues. Analogous to Figure 3.1(b) for homogeneous media, the spectrum for the Helmholtz operator of a laterally varying medium is depicted Figure 3.3.

A typical situation for this type of wave fields is in waveguides. Therefore the discrete modes are commonly referred to as guided modes. For the mathematical details of this example the reader should consult an introductory text to quantum physics, such as Gasciorowicz [36], or any book on waveguides.

Together $\phi(\mathbf{x}_H; \mathbf{k}_H)$ and $\phi^{(i)}(\mathbf{x}_H)$ make up an orthonormal basis of \mathbb{R}^2 ; any function F in the Sobolev space $H^2(\mathbb{R}^2)$ can be expanded in terms of these eigenfunctions, see Reed and Simon [73],

$$\mathsf{F}(\mathbf{x}_H) = \int_{\mathbb{R}^2} \phi(\mathbf{x}_H, \mathbf{k}_H) \bar{\mathsf{F}}(\mathbf{k}_H) d^2 \mathbf{k}_H + \sum_{\lambda_i \in \sigma_d} \phi^{(i)}(\mathbf{x}_H) \bar{\mathsf{F}}^{(i)}, \quad (3.9a)$$

and conversely

$$\bar{\mathsf{F}}(\mathbf{k}_{H}) = \int_{\mathbb{R}^{2}} \phi^{*}(\mathbf{x}_{H}^{'}, \mathbf{k}_{H}) \mathsf{F}(\mathbf{x}_{H}^{'}) d^{2}\mathbf{x}_{H}^{'}, \qquad (3.9b)$$

$$\bar{\mathsf{F}}^{(i)} = \int_{\mathbb{R}^{2}} \phi^{(i)}(\mathbf{x}_{H}^{'}) \mathsf{F}(\mathbf{x}_{H}^{'}) d^{2}\mathbf{x}_{H}^{'}.$$
(3.9c)

Modal decomposition will refer to the combination of equations (3.9b) and (3.9c), while modal composition will refer to (3.9a).

In the next section extensive use will be made of the kernel notation. The kernel


Figure 3.3: Dashed gray : guided mode, solid gray : radiating mode, solid black : square well velocity contrast.

notation, see appendix A.2, allows us to express the operator in terms of its eigenfunctions and -values,

$$\hat{\mathsf{H}}_{2}(\mathbf{x}_{H})F(\mathbf{x}_{H}) = \int_{\mathbb{R}^{2}} \mathsf{H}_{2}(\mathbf{x}_{H}; \mathbf{x}_{H}^{'})F(\mathbf{x}_{H}^{'})d^{2}\mathbf{x}_{H}^{'}.$$
(3.10)

Subsequent substitution of equations (3.9a), (3.6), (3.9b), and (3.9c), into the left hand side of equation (3.10), results in

$$H_{2}(\mathbf{x}_{H}; \mathbf{x}_{H}^{'}) = \int_{\mathbb{R}^{2}} \phi(\mathbf{x}_{H}; \mathbf{k}_{H}) \lambda(\mathbf{k}_{H}) \phi^{*}(\mathbf{x}_{H}^{'}; \mathbf{k}_{H}) d^{2}\mathbf{k}_{H}$$
$$+ \sum_{\lambda_{i} \in \sigma_{d}} \phi^{(i)}(\mathbf{x}_{H}) \lambda_{i} \phi^{(i)}(\mathbf{x}_{H}^{'}).$$
(3.11)



Figure 3.4: Spectrum of the operator $k^2(\mathbf{x}) + \nabla_H \cdot \nabla_H$

For future use we note that the identity operator \hat{I} has the kernel representation

$$\delta(\mathbf{x}_{H} - \mathbf{x}_{H}^{'}) = \int_{\mathbb{R}^{2}} \phi(\mathbf{x}_{H}; \mathbf{k}_{H}) \phi^{*}(\mathbf{x}_{H}^{'}; \mathbf{k}_{H}) d^{2} \mathbf{k}_{H}$$
$$+ \sum_{\lambda_{i} \in \sigma_{d}} \phi^{(i)}(\mathbf{x}_{H}) \phi^{(i)}(\mathbf{x}_{H}^{'}).$$
(3.12)

3.4 Fractional powers of the Helmholtz operator

Starting from equation (3.11) one can express the \mathbf{x}_H, ω -domain operator/kernel analogs of the root quantities $\tilde{H}_1^{\pm 1}$, and $\tilde{H}_1^{\pm 1/2}$, that appear in wave field (de)composition in horizontally layered media.

In the formal definition of Helmholtz and the square root operators, equations (1.23), (3.1), and (3.2), the power/order has been lowered to the subscript. Here, contrary to Wapenaar et al. [93, 90], we will continue to use this convention for inverse and/or root operators. Consequently, the symbol \hat{H}_{-1} will be used for the inverse of the square root operator related to the pseudo Helmholtz operator \hat{H}_2 . Similarly, the (inverse) square root operator of the Helmholtz operator \hat{H}_2 will be denoted by $\hat{H}_{\pm 1}$. Flux normalized decomposition will require the fourth root operators, $\hat{H}_{\pm 1/2}$. For the sake of completeness all the implicit definitions are given below,

$$\begin{aligned} \hat{H}_2 &= \hat{H}_1 \hat{H}_1, & \hat{H}_{-1} \triangleq \hat{H}_1^{-1}, \\ \hat{H}_2 &= \hat{H}_1 \hat{H}_1, & \hat{H}_{-1} \triangleq \hat{H}_1^{-1}, \\ \hat{H}_1 &= \hat{H}_{1/2} \hat{H}_{1/2}, & \hat{H}_{-1} = \hat{H}_{-1/2} \hat{H}_{-1/2}, & \text{and} \quad \hat{H}_0 \triangleq \hat{I}. \end{aligned}$$

First we note that equation (3.2a) can extended to

$$\hat{\mathbf{H}}_p = \rho^{-1/2} \hat{H}_p \rho^{1/2}, \qquad p \in \{2, \pm 1\},$$
(3.13)

so the kernel expressions for \hat{H}_p follow straightforwardly from those for \hat{H}_p . The former will therefore not be stated explicitly in this section, which will just show the construction of the kernels

$$H_p(\mathbf{x}_H; \mathbf{x}'_H)$$
 corresponding to the operators $\hat{H}_p(\mathbf{x}_H)$, $p \in \{\pm 1, \pm 1/2\}$.

The relation $\hat{H}_p \hat{H}_p = \hat{H}_{2p}$ has the kernel equivalent

$$\int_{\mathbb{R}^2} \mathsf{H}_p(\mathbf{x}_H; \mathbf{x}'_H) \mathsf{H}_p(\mathbf{x}'_H; \mathbf{x}''_H) d^2 \mathbf{x}'_H = \mathsf{H}_{2p}(\mathbf{x}_H; \mathbf{x}''_H).$$
(3.14)

For p = 1 the left side of equation (3.14) can be replaced by (3.11). Then insertion of the identity kernel expressed by equation (3.12), yields the kernel representation of \hat{H}_1 . Repeating these two steps for p = 1/2 does the same for $\hat{H}_{1/2}$. Therefore the sought after kernel representations are

with sign-choices

$$\begin{split} \Re(\lambda^{p/2}) &\geq 0 \qquad \text{for } \lambda \geq 0 \text{ (propagating wave modes),} \\ \Im(\lambda^{p/2}) &< 0 \qquad \text{for } \lambda < 0 \text{ (evanescent wave modes),} \end{split}$$

the eigenvalues are in accordance with the homogeneous situation. In the complex plane the eigenvalue distributions look like Figures 3.5(a) and 3.5(b).

This section concludes by noting that the kernels $\mathsf{H}_p(\mathbf{x}_H;\mathbf{x}_H^{'})$ are symmetric,

$$\mathsf{H}_p(\mathbf{x}_H; \mathbf{x}'_H) = \mathsf{H}_p(\mathbf{x}'_H; \mathbf{x}_H). \tag{3.16a}$$



Figure 3.5: Spectra of fractional power operators

This symmetry-property arises from the fact that as any self-adjoint operator, the Helmholtz operator has unitary eigenfunctions. Because of equations (3.5) and (3.7b), transforming the integration variable in equation (3.15) like $\mathbf{k}_H = -\mathbf{k}'_H$, leads to equation (3.16a). Obviously a symmetric kernel comes with a symmetric operator

$$\hat{\mathsf{H}}_p = \hat{\mathsf{H}}_p^t, \tag{3.16b}$$

also see appendix A.2. These symmetry relations also hold for the inverse operators, of course provided they exist. In dissipative media the eigenfunctions can no longer be unitary, but still the dissipative square root operators are symmetric, see Wapenaar et al. [93].

3.5 One-way wave equations in complex acoustic media

The rather simple diagonalization of anti-diagonal matrices given by equation (2.9) remains valid for non-commuting entries,

$$\hat{\mathbf{A}} = \begin{pmatrix} \hat{0} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{0} \end{pmatrix} = \hat{\mathcal{L}}\hat{\mathbf{A}}\hat{\mathcal{L}}^{-1}, \qquad (3.17)$$

with

$$\hat{\mathcal{L}} = \begin{pmatrix} \hat{Y} & \hat{Y} \\ \hat{Z} & -\hat{Z} \end{pmatrix}, \quad \hat{\mathbf{\Lambda}} = \begin{pmatrix} -\hat{\Lambda} & 0 \\ 0 & \hat{\Lambda} \end{pmatrix}, \quad \hat{\mathcal{L}}^{-1} = \frac{1}{2} \begin{pmatrix} \hat{Y}^{-1} & \hat{Z}^{-1} \\ \hat{Y}^{-1} & -\hat{Z}^{-1} \end{pmatrix}.$$

This is easily proved by substitution, which yields as an intermediate result that the five matrix-elements are interconnected by the two relations

$$\hat{A}_{12} = \hat{Y}\hat{\Lambda}\hat{Z}^{-1}$$
(3.18a)

$$\hat{A}_{21} = \hat{Z}\hat{\Lambda}\hat{Y}^{-1}.$$
 (3.18b)

Obviously, equation (3.17) expressed in matrices has been reduced to two scalar expressions, relating five scalar operators. This leaves us with three remaining degrees of freedom. In our case two of these are already taken by the entries of the operator matrix $\hat{\mathbf{A}}$, remember equation (3.17). The remaining degree of freedom is the usual eigenvector normalization.

By analogy with section 2.3, equation (2.10) is generalized to laterally varying media;

$$\hat{l} = (\omega \rho)^{-1} \hat{H}_1,$$
 (3.19a)

$$\hat{\mathbf{l}}^t = (\omega \rho)^{-1/2} \hat{\mathbf{H}}_{1/2}.$$
 (3.19b)

Using the symmetry relation equation (3.16) it is clear that $\hat{l} = \hat{H}_{1/2}(\omega\rho)^{-1/2}$. So with the help of equation (3.13), \hat{l}^t and \hat{l} are easily seen to be related by

$$\hat{l} = \hat{l}^t \hat{l}. \tag{3.19c}$$

As in section 2.3 we start with $\hat{Y} = 1$. Then multiplication of equation (3.18) yields $\hat{A}_{12}\hat{A}_{21} = \hat{\Lambda}^2$. Subsequent substitution of the matrix-elements of equation (1.22c), $\hat{A}_{12} = -j\omega\rho$ and $\hat{A}_{21} = (j\omega\rho)^{-1}\hat{H}_2$, results in $\hat{\Lambda} = j\hat{H}_1$, and finally $\hat{Z} = \hat{l}$. After Chapter 2 we denote the conventional pressure normalized diagonalization of the operator matrix \hat{A} by \hat{L} and \hat{L}^{-1} , i.e. $\hat{\mathcal{L}} \to \hat{L}$ in equation (3.17) and corresponding expressions. For pressure normalization the diagonal matrix is

$$\hat{\mathbf{A}}_p = \begin{pmatrix} -j\hat{H}_1 & 0\\ 0 & j\hat{H}_1 \end{pmatrix}.$$
(3.20)

The \mathbf{x}_H, ω -representation of the pressure normalized composition is the operator matrix $\hat{\mathbf{L}}$ acting like

$$\mathbf{Q} = \hat{\mathbf{L}}\mathbf{P},\tag{3.21a}$$

where

$$\hat{\mathbf{L}} = \begin{pmatrix} 1 & 1 \\ \hat{l} & -\hat{l} \end{pmatrix}.$$

Similarly decomposition has the representation

$$\mathbf{P} = \begin{pmatrix} P^+ \\ P^- \end{pmatrix} = \hat{\mathbf{L}}^{-1} \mathbf{Q}, \qquad (3.21b)$$

where

$$\hat{\mathbf{L}}^{-1} = \frac{1}{2} \begin{pmatrix} 1 & \hat{l}^{-1} \\ 1 & -\hat{l}^{-1} \end{pmatrix}.$$

The analogies with horizontally layered media mentioned before, are continued in the definition of flux normalized wave field (de)composition. Using equation (3.19c) the pressure normalized composition and decomposition matrices can be factored into

$$\hat{\mathbf{L}} = \sqrt{2} \ \hat{\mathbf{L}} \ \hat{\mathbf{l}},$$
 and $\hat{\mathbf{L}}^{-1} = \frac{1}{\sqrt{2}} \hat{\mathbf{l}}^{-1} \hat{\mathbf{L}}^{-1},$ (3.22)

respectively, which implicitly defines their flux-normalized counterparts

$$\hat{\mathbf{L}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{l}^{-1} & \hat{l}^{-1} \\ \hat{l}^{t} & -\hat{l}^{t} \end{pmatrix}, \quad \text{and} \quad \hat{\mathbf{L}}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{l} & \hat{l}^{t,-1} \\ \hat{l} & -\hat{l}^{t,-1} \end{pmatrix}.$$
(3.23)

Wapenaar et al. [93, 90, 91] consistently use $\hat{L}_1 = \hat{l}^{-1}$ and $\hat{L}_2 = \hat{l}^t$. The reader could argue that the notation $\hat{l}^{t,-1}$ is ambiguous; does it mean $\{\hat{l}^{-1}\}^t$ or $\{\hat{l}^t\}^{-1}$. However, the definitions of inverse linear operators and transposed linear operators show that there is no such ambiguity, so $\{\hat{l}^{-1}\}^t = \{\hat{l}^t\}^{-1}$.

Equation (3.22) allows one to go from pressure normalized to flux normalized diagonalization:

$$\hat{\mathbf{A}} = \hat{\mathbf{L}}\hat{\mathbf{\Lambda}}_p\hat{\mathbf{L}}^{-1} = \hat{\mathbf{L}}\hat{\mathbf{l}}\hat{\mathbf{\Lambda}}_p\hat{\mathbf{l}}^{-1}\hat{\mathbf{L}}^{-1}.$$

Using equation (3.13) and the symmetry relation (3.16), the product $\hat{l}\hat{H}_1\hat{l}^{-1}$ reduces to

$$\hat{\mathsf{H}}_1 = \hat{\mathsf{l}} \hat{H}_1 \, \hat{\mathsf{l}}^{-1}.$$

Under flux normalization we therefore have the diagonal matrix

$$\hat{\mathbf{\Lambda}}_f = \begin{pmatrix} -j\hat{\mathbf{H}}_1 & 0\\ 0 & j\hat{\mathbf{H}}_1 \end{pmatrix}.$$
(3.24)

Note that in the \mathbf{k}_{H}, ω -domain expressions of Chapter 2 the diagonal matrix $\tilde{\mathbf{\Lambda}}$ was used for both pressure and flux normalization, which is not the case in the x_H, ω -expressions given here. This is reflected in the diagonal matrices by subscripts p and f.

The flux normalized counterpart of equation (3.21a) is

$$\mathbf{Q} = \hat{\mathbf{L}}\mathbf{P}.\tag{3.25}$$

Combining equations (3.21a) and (3.25), obviously leads to $\hat{\mathbf{L}}\mathbf{P} = \hat{\mathbf{L}}\mathbf{P}$. After substitution of equation (3.22) into this identity relation, multiplying both sides with $\hat{\mathbf{L}}^{-1}$ yields the operator equivalent of equation (2.16),

$$\mathsf{P}^{\pm} = \sqrt{2}\,\hat{\mathsf{l}}\,P^{\pm},\tag{3.26}$$

relating pressure and flux normalized wave fields.

Analogous to the one-way wave equations for horizontally layered media from section 2.3, the wave field decompositions discussed above lead to one-way wave equations for laterally varying media:

the pressure normalized one-way wave equation

$$\partial_3 \mathbf{P} = \mathbf{B} \mathbf{P} + \mathbf{S}, \tag{3.27a}$$

~

$$\hat{\mathbf{B}} = \hat{\mathbf{\Lambda}}_p - \hat{\mathbf{\Theta}}_p, \tag{3.27b}$$

the flux normalized one-way wave equation

$$\partial_3 \mathbf{P} = \hat{\mathbf{B}} \mathbf{P} + \mathbf{S}, \qquad (3.28a)$$

$$\hat{\mathbf{B}} = \hat{\mathbf{\Lambda}}_f - \hat{\mathbf{\Theta}}_f. \tag{3.28b}$$

The operator matrices $\hat{\mathbf{B}}$ and $\hat{\mathbf{B}}$ will be called one-way operators. The diagonal propagation matrices $\hat{\mathbf{A}}_p$ and $\hat{\mathbf{A}}_f$ have already been defined, the corresponding matrices for vertical scattering are

$$\hat{\Theta}_p = \hat{\mathbf{L}}^{-1} \partial_3 \hat{\mathbf{L}}$$
 and $\hat{\Theta}_f = \hat{\mathbf{L}}^{-1} \partial_3 \hat{\mathbf{L}};$

they are called scattering operators and will feature in section 3.6.

3.6 Local transmission and reflection

The definition of local transmission and reflection operators is simplified by first focusing on the structure of the scattering operators. By evaluating the product $\hat{\mathbf{L}}^{-1}\partial_3 \hat{\mathbf{L}}$, the pressure normalized scattering operator $\hat{\mathbf{\Theta}}_p$ is easily seen to read

$$\hat{\Theta}_p = \frac{\hat{\theta}}{2} \begin{pmatrix} 1 & -1\\ -1 & 1 \end{pmatrix}, \qquad (3.29)$$

with $\hat{\theta} = \hat{l}^{-1}\partial_3\hat{l}$. The flux normalized formulation takes more work. Evaluation of the product $\hat{L}^{-1}\partial_3\hat{L}$, shows that it is composed of scalar operator products

$$\hat{\eta} \triangleq \hat{\iota} \, \partial_3 \, \hat{\iota}^{-1}$$
 and $\hat{\eta}^t \triangleq \hat{\iota}^{t,-1} \, \partial_3 \, \hat{\iota}^t$

That the products $\hat{l} \partial_3 \hat{l}^{-1}$ and $\hat{l}^{t,-1} \partial_3 \hat{l}^t$ are indeed related by transposition can be confirmed by differentiating the identity-relation $\hat{l} \hat{l}^{-1} = 1$ with respect to x_3 . Then $\hat{\eta}$ can be expressed like

$$-\hat{\eta} = (\partial_3 \hat{\mathfrak{l}})\hat{\mathfrak{l}}^{-1} = [\hat{\mathfrak{l}}^{t,-1}(\partial_3 \hat{\mathfrak{l}})^t]^t = [\hat{\mathfrak{l}}^{t,-1} \partial_3 \hat{\mathfrak{l}}^t]^t,$$
$$= \hat{\eta}_f^t.$$

For the last step we used $(\partial_3 \hat{l})^t = \partial_3 \hat{l}^t$. This is allowed because the operator-character of \hat{l} is exclusively related to ∇_H ; when differentiated with respect to x_3 , such operators behave like functions. Hence the scattering operator can be expressed exclusively in terms of $\hat{\eta}$,

$$\hat{\boldsymbol{\Theta}}_{f} = \frac{1}{2} \begin{pmatrix} \hat{\eta} - \hat{\eta}^{t} & \hat{\eta} + \hat{\eta}^{t} \\ \hat{\eta} + \hat{\eta}^{t} & \hat{\eta} - \hat{\eta}^{t} \end{pmatrix}$$

We define local transmission and reflection operators by

$$\hat{\mathbf{B}} \triangleq \begin{pmatrix} \hat{t}^+ & \hat{r}^- \\ -\hat{r}^+ & -\hat{t}^- \end{pmatrix}, \qquad (3.30)$$

for pressure normalized wave fields that is. Combining equations (3.20), (3.29), and (3.30) shows that

$$\hat{t}^{+} = -j\hat{H}_{1} - \hat{\theta}/2 = -j\hat{H}_{1} - \hat{r}, \qquad \hat{r}^{-} = -\hat{\theta}/2 = -\hat{r},$$

$$\hat{r}^{+} = \hat{\theta}/2 \triangleq \hat{r}, \qquad \qquad \hat{t}^{-} = -j\hat{H}_{1} + \hat{\theta}/2 = -j\hat{H}_{1} + \hat{r}.$$
(3.31)

For the flux normalized case we define the local transmission and reflection operators by

$$\hat{\mathbf{B}} \triangleq \begin{pmatrix} \hat{\mathbf{t}}^+ & \hat{\mathbf{r}}^- \\ -\hat{\mathbf{r}}^+ & -\hat{\mathbf{t}}^- \end{pmatrix}.$$
(3.32)

Similarly combining equations (3.24), (3.28b), and (3.32) shows that

$$\hat{\mathbf{t}}^{+} = -j\hat{\mathbf{H}}_{1} - (\hat{\eta} - \hat{\eta}^{t})/2 \triangleq \hat{\mathbf{t}}, \qquad \hat{\mathbf{r}}^{-} = (\hat{\eta} + \hat{\eta}^{t})/2 = -\hat{\mathbf{r}},
\hat{\mathbf{r}}^{+} = -(\hat{\eta} + \hat{\eta}^{t})/2 \triangleq \hat{\mathbf{r}}, \qquad \hat{\mathbf{t}}^{-} = -j\hat{\mathbf{H}}_{1} + (\hat{\eta} - \hat{\eta}^{t})/2 = \hat{\mathbf{t}}^{t}.$$
(3.33)

Note that by construction local reflection operators for flux normalized wave fields are symmetric and local up and down going transmission operators obey reciprocity. This concludes the discussion of the fundamental theory of acoustic wave field decomposition. The last two sections of this chapter deal with the implementation and related choices.

3.7 Translating the Helmholtz and square root operators to matrices

We start this section by introducing some notation. Second we will discuss the influence of discretization of the differential operators $\partial_{1,2}$ on the accuracy of the diagonalization of \hat{H}_2 . This will be done by comparing pressure normalized wave field composition with independently generated up and down going wave fields.

We will assume N_1 stations (sources and/or receivers) in the x_1 -direction and N_2 in the x_2 -direction, and set $N_2 = 1$ only when dealing with the numerical examples and

applications. The total number of stations amounts to

$$M = N_1 N_2.$$

Then discrete representations of wave field quantities such as P, V, P^{\pm} , and P^{\mp} are column vectors in \mathbb{C}^M . For operators, or rather their corresponding kernels, these representations are square matrices in $\mathbb{R}^{M \times M}$ or $\mathbb{C}^{M \times M}$. Using the notation introduced in detail in appendix A.3, the product $\hat{H}_2(\mathbf{x}_H) f(\mathbf{x}_H)$ is easily seen to have a discrete representation $\mathbf{H}_2\mathbf{F}$, where \mathbf{F} is a column-vector in \mathbb{C}^M and \mathbf{H}_2 a square matrix in $\mathbb{R}^{M \times M}$. With reference to equation (3.2b), the Helmholtz-*matrix* \mathbf{H}_2 , is given by

$$\mathbf{H}_2 = \mathbf{K}_2 + \mathbf{D}_L.$$

The matrix $\mathbf{D}_L \in \mathbb{R}^{M \times M}$ is the discrete approximation of the Laplacian $\nabla_H \cdot \nabla_H$, see appendix C, while the diagonal matrix $\mathbf{K}_2 \in \mathbb{R}^{M \times M}$ corresponds to the laterally varying wavenumber $k^2(\mathbf{x})$. The matrix \mathbf{H}_2 will serve as input for a diagonalization-routine, which yields an orthogonal matrix $\mathbf{\Phi} \in \mathbb{R}^{M \times M}$ holding the eigenvectors and a diagonal matrix $\boldsymbol{\lambda} \in \mathbb{R}^{M \times M}$ containing the eigenvalues of \mathbf{H}_2 . Obviously, these three matrices are interrelated by

$$\mathbf{H}_2 = \mathbf{\Phi} \boldsymbol{\lambda} \mathbf{\Phi}^{-1}. \tag{3.34a}$$

Now the matrices $\mathbf{H}_{\pm 1}$, $\mathbf{H}_{\pm 1/2} \in \mathbb{C}^{M \times M}$ can be constructed in the eigenvector-domain, analogous to equations (3.11) and (3.15);

$$\mathbf{H}_{p} = \mathbf{\Phi} \boldsymbol{\lambda}^{p/2} \mathbf{\Phi}^{-1} \text{ for } p \in \{2, \pm 1, \pm 1/2\}.$$
(3.34b)

A straightforward approach to check the accuracy of the diagonalization would be to do the diagonalization for $k^2(x_1)$ -profiles which can also be solved analytically. Besides the homogeneous case of section 2.2 and the square well profile discussed in section 3.3, one can also use hyperbolic functions, see for example Morse and Feshbach [65]. Although this strategy allows a detailed comparison, the restriction to analytically solvable cases is a severe one. Here we take an approach that allows any horizontal profile to be examined.

In vertically invariant media it is possible to model up and down going pressure and particle velocity wave fields independently and to high accuracy by means of the Finite Difference algorithm. For a purely up going wave field the lower row of equation (3.21a) reduces to

$$V^{-} = -(\omega\rho)^{-1} \hat{H}_1 P^{-}.$$
(3.35)

We will use verification of this identity to assess the accuracy of the numerical construction of H_1 . Although the Finite Difference method is an accurate method, it cannot yield the exact solution. We therefore examine the relative error

$$E_{\hat{H}}(x_1,\omega) = \left| \frac{(\omega\rho)^{-1} \hat{H}_1 P^-}{V^-} + 1 \right|.$$
(3.36)

In the ideal case when equation (3.35) is exactly satisfied, the relative error $E_{\hat{H}}$ equals zero. In our case the involved quantities result from numerical algorithms, so $E_{\hat{H}}$ will deviate from zero. It serves as a measure for the closeness of left and right hand sides of equation (3.35) and in particular of the quality of the H₁-construction, if we take the accuracy of P^- and V^- for granted. In case of a properly functioning diagonalizationroutine², the accuracy of H₁ is determined by that of the input H₂. This in turn depends on the discrete and approximate representations of the ∂_1 - and ∂_2 -operators and the Laplacian $\nabla_H \cdot \nabla_H$, the matrices $\mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_L \in \mathbb{R}^{M \times M}$, respectively. The remainder of this section will deal with this issue.

Given a 1D function g(u) tabulated at equidistant points, first and second order derivatives of a 1D function have straightforward finite difference approximations,

$$g'_{i} = \frac{g_{i+1} - g_{i-1}}{2\Delta u} + O(\Delta u^{2}),$$
 (3.37a)

$$g_i'' = \frac{g_{i+1} - 2g_i + g_{i-1}}{\Delta u^2} + O(\Delta u^2).$$
(3.37b)

The schemes described by equation (3.37) and their higher order relatives, see appendix C.1, should be applied with care for two reasons. First there is the conflict between the facts that *accurate* differentiation demands small sampling, while *fast* and *stable* differentiation demands coarse (enough) sampling, see Press et al. [69]. The second reason is application at borders of the finite aperture. Consider N tabulated values of g and let them be contained in the column vector **G** as $\mathbf{G}^t = [g_1, \ldots, g_N]$. Then the values of the derivatives obtained with equations (3.37) are conveniently expressed by

$$\mathbf{G}^{'} \approx \mathbf{d}^{(1)}\mathbf{G}$$
 and $\mathbf{G}^{''} \approx \mathbf{d}^{(2)}\mathbf{G}$.

²Here the general purpose *ssyev*-subroutine from the LAPACK-library will be used, also see Golub and Van Loan [38].



Figure 3.6: Plots of $E_{\hat{H}}(x_1, \omega)$ for a dipole source, with different $\mathbf{d}^{(2)}$ -approximations. The vertical axis shows the frequency $f = \omega/2\pi$.

Obviously the square matrices $\mathbf{d}^{(1)}, \mathbf{d}^{(2)} \in \mathbb{R}^{N \times N}$ have a Toeplitz-structure, i.e. they are constant along all diagonals (for 2D inhomogeneous media one can identify $\mathbf{D}_L = \mathbf{d}^{(2)}$, but for 3D inhomogeneous media some additional notation is necessary, see appendix A.3).

Using equations (3.37) for the construction of H_2 ensures its hermiticity. On the other hand they lead to erroneous values at the boundaries i = 1 and i = N. Synthesizing g_0 and g_{N+1} by extrapolation from the available samples g_1, \ldots, g_N , would repair the mistreatment but destroys the symmetry of the matrix $d^{(2)}$; this extrapolation therefore introduces complex eigenvalues, and is not an option. Just replacing equations (3.37) by higher order analogs is not a perfect remedy either; now also interior points will contain

erroneous values. Due to the iterative nature of the transmission-loss correction proposed in Chapter 5, amplification of these boundary errors is not unlikely. Also the construction of primary propagators is likely increase the errors and propagate them into the interior of the aperture, see Chapter 6. Three approaches will be used here, each with their drawbacks.

For an illustration of these three approaches that is not obscured by issues related to wave field modeling, we briefly return to a 2D homogeneous medium. Now up and down going wave fields can be generated by analytical expressions based on Hankel functions, see for example Berkhout [7]. The specific configuration used here consists of a dipole source located at depth $x_3 = 400$ m and $x_1 = 0$, while the receivers are placed at $x_3 = 0$ with offsets in the interval [-688 m, 2192m]. The receiver spacing was $\delta x_1 = 8$ m, the time-sampling $\delta t = 0.8$ ms and the velocity was $c_p = 3000$ km/s. The three approaches are listed below and the corresponding contour plots of $E_{\hat{H}}(x_1, \omega)$ for the configuration mentioned are given in Figure 3.6.

- a. Use equation (3.37b) and do not do anything, that is simply accept the boundary inaccuracies. See Figure 3.6a for the corresponding plot of $E_{\hat{H}}$.
- b. Use periodic boundary conditions, i.e. use g_N instead of the non existing g_0 to compute the derivatives at i = 1 with equations (3.37), also see appendix C.2. Spurious effects will remain, now due to wraparound, because the wave fields do not obey periodic boundary conditions. For Figure 3.6b the periodic boundary approximation with highest accuracy was used, i.e. $\mathbf{d}^{(2)}$ was constructed in the wavenumber domain.
- c. Apply some sort of absorbing/radiating boundary condition to equation (3.37b). Here one of the simplest possibilities is used, lateral tapering. Because tapering does not absorb the boundary-effects completely spurious effects will remain. But they are probably weaker because now the boundary conditions of operators and wave fields are more similar. Note a slight improvement in Figure 3.6c compared to Figure 3.6a.

In case of the equation (3.37b)-based approximations used in approaches a and c, $d^{(2)}$ acts as a low pass filter. For a minimum of 10 sampling intervals per wavelength for an accurate discretization of the wave field, the upper limit of the low pass filter is about $f_{max} = 19$ Hz. Up to $f_{max} = 19$ the performance of the three approaches is comparable, but at higher frequencies the accuracy of H_1 based on the wavenumber domain approximation of ∂_1^2 is superior. It is therefore employed in the examples of the next, closing



Figure 3.7: Finite Difference modeled dipole responses in waveguides

sections of this chapter and in those of Chapter 5.

However, the use of Fourier expansions to construct matrix-representations of differential operators acting on non-periodic and non-smooth functions is known to have its limitations, see for example Fornberg [31]; Chebyshev polynomials and wavelets perform better on such functions. For our purpose Chebyshev polynomials are not suitable because the resulting matrix-representation of ∂_i^2 is not symmetric, again see for example Fornberg [31]. On the other hand, Beylkin [10] showed that ∂_i^2 's wavelet-based representation is symmetric.

3.8 Test and examples of wave field composition in laterally varying media

Now that the choice for periodic boundary conditions has been made, the time has come to examine modal decomposition in x-dependent media. To separate the effects of modal decomposition on one hand and vertical scattering due to x_3 -dependence of velocity and density on the other, this section will first focus on wave field composition in laterally varying but vertically constant media. As in the previous section this allows the independent modeling of up and down going wave fields. Therefore the ratio $E_{\hat{H}}$ defined by equation (3.36) remains the tool for examination of the accuracy of H_1 in x_H -dependent (or rather x_1 -dependent) media. The final step of modal decomposition in media that also vary with depth, allows for a less detailed examination, because now the

	min.	step size	max.		min	max
t(s)	0	8e-4	2.912	$c(m.s^{-1})$	1500	3000
$x_1(m)$	0	4	3008	$\rho(kg.m^{-3})$	1500	3000
$x_3(m)$	0	4	200	$freq(s^{-1})$	7	35

Table 3.1: Finite difference parameters

up and down going wave fields cannot be obtained independently. This final example will therefore only be subjected to a simple travel time analysis.

General Ψ DO-literature [23, 50, 57, 98] requires all functions involved in the construction and use of Ψ DO's to be infinitely differentiable. Fortunately, in the particular case of the Hamiltonian/Helmholtz-operator it can be relaxed to $k^2(\mathbf{x})$ being square integrable locally, see Reed and Simon [71] and Shubin [76]. So besides discontinuities, Ψ DOtheory allows $k^2(\mathbf{x})$ to have integrable singularities. On physical grounds its constituent functions phase-velocity c and density ρ , remember equation (3.2), vary discontinuously at most, but are bounded. Because of the way these functions appear in k^2 , the discontinuities in c will merely give rise to discontinuities in k^2 , but discontinuities in ρ can lead to singularities through the first and second order derivatives $\nabla_H \rho$ and $\nabla_H \cdot \nabla_H \rho$, also see equation (3.2c). The latter are not necessarily integrable.

These considerations led us to examine vertically invariant media with in the horizontal direction either an infinitely differentiable Gaussian profile, see the bottom of Figure 3.7(a), or a discontinuous square well profile, see the bottom of Figure 3.7(b). In addition to a dipole source at $x_1 = 0$, the same as in the homogeneous example of section 3.7, a second dipole source was used. Other than a different horizontal location $x_1 = 752$ m to stimulate the guided modes, this second dipole source had the same source signature and was located at the same depth $x_3 = 400$ m as the first. The receiver array was identical to that of the homogeneous examples of section 3.7. The finite difference (FD) algorithm with the parameters listed in Table 3.1 was used to generate wave fields in each of four media described below. For each case a contour plot of $E_{\hat{H}}$ with the same color-scale as in Figure 3.6 is presented in Figures 3.8(a)-3.8(d):

3.8(a): A medium with a smooth, Gaussian velocity profile and constant density.

3.8(b): A medium where both density and velocity were a Gaussian profile.

3.8(c): A medium with a square well velocity profile and again a constant density.

3.8(d): A medium where both density and velocity were a square well profile.



(a) Gaussian velocity, homogeneous den- (b) Gaussian velocity, Gaussian density sity



(c) Square well velocity, homogeneous (d) Square well velocity, square well dendensity sity

Figure 3.8: $E_{\hat{H}}(x_1, \omega)$ for laterally varying velocity/density profiles. See Figure 3.6 for a legend of the gray scale used in Figures 3.8(a)-3.8(d).

The tendencies displayed in Figures 3.8(a)-3.8(d) confirm the problems with non differentiability related to Ψ DO-theory. For cases 3.8(a) and 3.8(b) generated with Gaussian profiles $E_{\hat{H}}$ shows an essentially similar pattern as the homogeneous case: small discrepancies directly above the sources which increase slightly further away from the sources, while they increase drastically towards the edges of the receiver-array. But for cases 3.8(c) and 3.8(d) where a discontinuous velocity and/or density was used, the accuracy also deteriorates near the discontinuities; this is particularly so when also the density has discontinuities.

For flux normalized wave fields and depth-dependent medium parameters an accuracy measure like equation (3.36) cannot be formulated, because up and down going wave

fields cannot be obtained without modal decomposition. An amplitude analysis is therefore hard to conduct, but a comparison of events in a seismogram of the two-way quantity p on one hand and seismograms of one-way quantities (p^+ and p^-) on the other, is a useful exercise. First we mention that for the configurations without vertical contrast discussed earlier this section, flux normalized decomposition does not introduce spurious events. The configuration displayed in Figure 3.9(a) is another matter. It consists of a syncline interface intersected by a horizontal line of receivers (dotted line C) and is illuminated from below by an array of dipole sources (dashed line). In Figures 3.9 the intersections of line C and the syncline are marked by the vertical lines A and B. The velocities, densities and sampling-parameters are those from Table 3.1.

The total pressure field at line C as it was calculated by the FD-algorithm is plotted in Figure 3.9(b). The first arrival is obviously the up going wave field, plane at the left and right of lines A and B, respectively, while between A and B the field is being focused, also see Figure 3.9(c). The second arrival is the down going reflection from the horizontal parts of the interface, also see Figure 3.9(d). The third event is the field scattered in the horizontal direction from the 45-degree part of the syncline and therefore shows up in both Figures 3.9(c) and 3.9(d). But the anti causal events in Figures 3.9(c) and 3.9(d), which seemingly originate from the discontinuities at the intersections of A and B with C, do not have counterparts in Figure 3.9(b).

Such anti causal artifacts were not present in the decomposed wave fields resulting from the configurations without contrasts in the vertical directions. The artifacts therefore appear to be related to the vertical variations in the density and velocity.



(c) Up going wave field P⁻, obtained from (d) Down going wave field P⁺, idem Figthe two-way wave field of Figure 3.9(b) ure 3.9(c) by our implementation of flux normalized wave field decomposition.

B

А

0.25

0.5

t[s]

B

А

0.25

0.5

t[s]

Figure 3.9: Syncline medium, all displayed wave fields are obtained by convolved with a Ricker wavelet.

Chapter 4

One-way representations

4.1 Introduction

In 1D media the separate modes, i.e. plane waves propagating at different angles, do not mix when propagated up- or downward. This is because the modal decomposition in horizontally layered media, i.e. the spatial Fourier transform given by equation (1.17c), is identical at all depths. Wave fields at different depths can therefore be related by simple algebraic expressions, see section 2.4. In arbitrary acoustic media on the other hand, the modal decomposition *is* depth-dependent because the lateral velocity/density profiles do change with depth and so the separate modes do mix.

Despite this complication, the extension of the concepts given in Chapter 2, can be continued here. As section 2.3 on wave field decomposition was a stepping stone to section 2.4 on the generalized primary representation, the extension of wave field (de)composition to laterally varying media in Chapter 3, prepares the extension of this representation to laterally varying media. In section 4.2 the previously mentioned concept of *invariant imbedding* is readily expressed in differential equations in terms of the operators associated with the one-way wave equations as defined in section 3.6. By integrating the differential equations, it is possible to relate the in- and out coming wave fields at both sides of a horizontal slab to each other. Some workers have actually taken this approach to model one-way wave fields, see for example Fishman and McCoy [27, 28]. Here we will only use the resulting expressions to arrive at a data representation for redatuming. For wave field modeling in Chapters 5 and 6 we will use a conventional Finite Difference algorithm.

Given the kernel-notation for operators introduced in section A.2, the use of reci-

procity theorems is a natural next step. Reciprocity theorems are particular corollaries of the divergence theorem (also known as Gauss's theorem), which relates the divergence of a vector field integrated over some *domain* to the flux of the vector field integrated over the *boundary* of this domain; also see appendix B. Von Helmholtz [45] introduced what are nowadays called reciprocity theorems to show the source-receiver reciprocity principle for acoustic wave fields ; a signal sent from location A to location B has the same phase and amplitude as when sent from location B to A. Also see Lord Rayleigh [79]. Or stated in more physical terms, reversing the direction of propagation has no influence on the dynamical behavior of acoustic wave fields. Since their introduction, use has spread to elasto-dynamic and electromagnetic wave propagation, but reciprocity theorems can also be applied in diffusion and flow problems, or combinations of all of these areas, Wapenaar and Fokkema [95].

Fokkema and Van den Berg [30] used them as a starting point to derive a number of seismic processing steps. One-way expressions have been derived from them by Wapenaar and Berkhout [88], but as they are formulated in terms of the quantities P and V, the usual reciprocity theorems are not convenient for one-way wave fields, see appendix B. Wapenaar [90] introduced reciprocity theorems for flux normalized one-way wave fields and derived a number of relations useful in imaging and seismic interferometry [87, 93, 94], also see section 4.3.1.

The final section of this chapter will formulate a representation that allows one to define redatuming. The essential tool is one of the fundamental equations of scattering theory, the Lippmann-Schwinger equation. Its prominence first became clear in quantum physics, Lippmann and Schwinger [58] and March [61], but later it also permeated into other disciplines. The Lippmann-Schwinger equation and the closely related T-matrix approach are for example also used in electromagnetic scattering computations [64], for multiple elimination in seismic exploration [96, 97] and shale acoustics [51].

4.2 Invariant imbedding and seismic wave propagation

Berkhout [6] launched his "WRW"-notation in the context of exploration seismics for migration (the Ws denote up and down going propagation, whereas R refers to reflection). Like many good ideas it was "in the air" and a number of workers, in the seismic community as well as in other disciplines, had already proposed similar expressions. In retrospect the common principle underlying their work was called invariant imbedding. All these disciplines, see Bellman and Wing [5], have in common that they analyze some

kind of transport phenomenon, and approach the problem by first dividing the medium in thin slices and accumulating the effects of each slice. Some obvious examples are transmission/reflection problems in wave propagation, and radiative transfer theory, used to analyze the effects of stellar radiation on atmospheres and (inter)stellar clouds. Less obvious examples are perhaps random walks in diffusion-processes and neutron scattering in nuclear fission.

Unlike for example Fishman and McCoy [27, 28], we will not use equation (4.8) as the basis for wave field modeling. Instead it will give us a normalization independent representation of wave field propagation in the WRW-fashion for continously varying media, whereas the derivation by Wapenaar [87] is only valid for flux-normalized wave fields.

Invariant imbedding is used to derive formal expressions for the transmission and/or reflection characteristics of the part of the medium between depths a and b. In section 4.5 we will attach further meaning to these two depths, but for now we will just assume that $a \leq b$. The space \mathbb{R}^3 is partitioned as follows. The upper and lower boundaries of the horizontal slab between a and b are denoted by

$$\partial \mathbb{X}\{a\} = \{\mathbf{x} \in \mathbb{R}^3 \mid x_3 = a\},\tag{4.1a}$$

and

$$\partial \mathbb{X}\{b\} = \{\mathbf{x} \in \mathbb{R}^3 \mid x_3 = b\}.$$
(4.1b)

On occasion the notation $\partial \mathbb{X}\{a, b\}$ will be used to refer to the combination of the two boundaries $\partial \mathbb{X}\{a\} \cup \partial \mathbb{X}\{b\}$. The horizontal slab between depths a and b will occur in two subtly different ways. As an open domain *excluding* the boundaries, the slab will be denoted by

$$\mathbb{X}(a,b) = \{ \mathbf{x} \in \mathbb{R}^3 \, | \, a < x_3 < b \}.$$
(4.1c)

As a closed domain *including* the boundaries, it will instead be denoted by

$$\mathbb{X}[a,b] = \{ \mathbf{x} \in \mathbb{R}^3 \mid a \le x_3 \le b \}.$$
(4.1d)

To isolate the propagation effects between depths a and b this chapter considers a hypothetical medium that is equal to the actual medium between a and b, but is non-scattering in the vertical direction outside this region, i.e. for $x_3 < a$ and $b < x_3$;

also see Figure 4.1. This medium and its properties essential to invariant imbedding, and from now on be referred to by the prefix or subscript "iib". Extending the notation introduced by equation (4.1), the horizontal slab will be denoted by $\mathbb{X}[a, b]$, the upper and lower half-space by $\mathbb{X}(-\infty, a)$, and $\mathbb{X}(b, \infty)$ respectively. For notational convenience the dependence of the lateral coordinates of all quantities will be dropped in this section, but will reappear when dealing with reciprocity theorems and representation theorems based upon them.

The parameters corresponding to the iib-medium will be denoted by $\{\rho, K\}_{iib}$. Their distinguishing property is that

$$\partial_3\{\rho, K\}_{iib} = 0 \text{ for } \mathbf{x} \notin \mathbb{X}[a, b].$$
(4.2)

Equation (4.2) immediately implies that $\hat{H}_p(x_3) = \hat{H}_p(a)$ in the upper half space and $\hat{H}_p(x_3) = \hat{H}_p(b)$ in the lower, that is up and down going wave fields cannot change direction outside the horizontal slab. The transmission and reflection properties of the iibmedium are defined similarly to those of a stack of horizontal layers, remember equation (2.22). A source in the upper half space $\mathbb{X}(-\infty, a)$ of an iib-medium only generates a down going wave field $P^+(a)$ at depth $x_3 = a$, just a source in the lower half space $\mathbb{X}(b,\infty)$ can only generate an up going wave field $P^-(b)$. If the intermediate slab $\mathbb{X}[a, b]$ is source free, then the incoming fields generate outgoing wave fields $P^+(b)$ and $P^-(a)$, see Figure 4.1. Given these incoming and outgoing wave fields are related by the global scattering matrix, whose elements are defined as

$$\begin{pmatrix}
P^+(b) \\
P^-(a)
\end{pmatrix} = \hat{\mathbf{S}}_{scat}(a;b) \begin{pmatrix}
P^+(a) \\
P^-(b)
\end{pmatrix},$$

$$\triangleq \begin{pmatrix}
\hat{T}^+(b;a) & \hat{R}^-(b;b|a) \\
\hat{R}^+(a;a|b) & \hat{T}^-(a;b)
\end{pmatrix} \begin{pmatrix}
P^+(a) \\
P^-(b)
\end{pmatrix};$$
(4.3)

again see Figure 4.1. Note that the elements \hat{T}^{\pm} and \hat{R}^{\pm} of the matrix \hat{S}_{scat} are operators. Therefore \hat{S}_{scat} is called an operator-matrix, see appendix A.2 for a more elaborate definition. Also note that the reflection operators have three arguments, whereas the transmission operators only have two. In both cases the first argument from the left denotes receiver depth and the second denotes source depth. In case of the transmission operators correspond. For the reflection operator both sources and receivers necessarily lie on one side of the medium slab, so the third argument on the right side of the vertical bar is required to indi-



Figure 4.1: Invariant imbedding configuration

cate the other side of the corresponding medium slab.

In order to allow for media that vary continuously with the all three spatial coordinates $\mathbf{x} = (x_1, x_2, x_3)$, we will work with differential equations instead of the discrete approach of section 2.4 leading to recursive expressions. This has three consequences. The representations derived in this chapter do not allow discontinuities in the medium parameters, something to keep in mind with practical applications which inevitably do have discontinuities. Second, there is no need for constructing propagators in vertically constant media, as the propagators for homogeneous media were a prerequisite in section 2.4. The third consequence is that we do not start from a local scattering matrix but instead from the one-way wave equation. In a source-free region both the pressure and flux normalized one-way wave equations (3.27a) and (3.28a) have the form

$$\partial_3 \begin{pmatrix} P^+ \\ P^- \end{pmatrix} = \begin{pmatrix} \hat{t}^+ & \hat{r}^- \\ -\hat{r}^+ & -\hat{t}^- \end{pmatrix} \begin{pmatrix} P^+ \\ P^- \end{pmatrix}.$$
(4.4)

We take the approach of Corones [19] and Davison [20], contrary to earlier work by Redheffer [70]. We first differentiate both sides of equation (4.3) with respect to b,

$$\partial_b \hat{\mathbf{S}}_{scat} \begin{pmatrix} P^+(a) \\ P^-(b) \end{pmatrix} = \begin{pmatrix} \partial_3 P^+(b) \\ 0 \end{pmatrix} - \hat{\mathbf{S}}_{scat} \begin{pmatrix} 0 \\ \partial_3 P^-(b) \end{pmatrix}.$$
(4.5)

Next we eliminate the vertical derivatives $\partial_3 P^{\pm}(b)$ by substituting the upper and lower row of equation (4.4) into the first and second term on the right hand side of equation (4.5), respectively; this yields

$$\partial_{b} \hat{\mathbf{S}}_{scat} \begin{pmatrix} P^{+}(a) \\ P^{-}(b) \end{pmatrix} = \left[\begin{pmatrix} \hat{t}^{+}(b) & \hat{r}^{-}(b) \\ 0 & 0 \end{pmatrix} + \hat{\mathbf{S}}_{scat} \begin{pmatrix} 0 & 0 \\ \hat{r}^{+}(b) & \hat{t}^{-}(b) \end{pmatrix} \right] \begin{pmatrix} P^{+}(b) \\ P^{-}(b) \end{pmatrix}$$
$$= \begin{pmatrix} 1 & \hat{R}^{-} \\ 0 & \hat{T}^{-} \end{pmatrix} \begin{pmatrix} \hat{t}^{+}(b) & \hat{r}^{-}(b) \\ \hat{r}^{+}(b) & \hat{t}^{-}(b) \end{pmatrix} \begin{pmatrix} P^{+}(b) \\ P^{-}(b) \end{pmatrix}.$$
(4.6)

The compression in the last step leading to equation (4.6) was achieved by noting that the elements of the left column of the operator matrix $\hat{\mathbf{S}}_{scat}$ are multiplied by zero. Then substituting the upper row of the scattering matrix for $P^+(b)$ in equation (4.6) allows one to take out the column vector with incoming fields $P^+(a)$ and $P^-(b)$

$$\partial_b \hat{\mathbf{S}}_{scat} = \begin{pmatrix} 1 & \hat{R}^- \\ 0 & \hat{T}^- \end{pmatrix} \begin{pmatrix} \hat{t}^+(b) & \hat{r}^-(b) \\ \hat{r}^+(b) & \hat{t}^-(b) \end{pmatrix} \begin{pmatrix} \hat{T}^+ & \hat{R}^- \\ 0 & 1 \end{pmatrix}.$$
 (4.7)

Evaluation of the right hand side matrix-products of equation (4.7) yields the desired results,

$$\partial_b \hat{R}^- = \hat{r}^-(b) + \hat{t}^+(b)\hat{R}^- + \hat{R}^-\hat{t}^-(b) + \hat{R}^-\hat{r}^+(b)\hat{R}^-, \qquad (4.8a)$$

$$\partial_b \hat{T}^- = \hat{T}^- [\hat{t}^-(b) + \hat{r}^+(b)\hat{R}^-], \qquad (4.8b)$$

$$\partial_b \hat{T}^+ = \left[\hat{t}^+(b) + \hat{R}^- \hat{r}^+(b) \right] \hat{T}^+, \tag{4.8c}$$

$$\partial_b \hat{R}^+ = \hat{T}^- \hat{r}^+ (b) \hat{T}^+.$$
 (4.8d)

Similar to the mathematics of Chapter 3, the manipulations that led to equations (4.8) are strictly speaking only valid if the medium-parameters have smooth x-dependencies. And again similar to Chapter 3, in this chapter and the following we will keep this theoretical restriction in mind, but will not respect it in practical applications.

The WRW-concept follows as a corollary. If we replace b by b' in equation (4.8d) and

integrate over the b'-variable on the interval [a, b], then we have

$$\hat{R}^{+}(a;a|b) = \int_{a}^{b} \partial_{b}^{'} \hat{R}^{+}(a;a|b^{'})db^{'} = \int_{a}^{b} \hat{T}^{-}(a;b^{'})\hat{r}^{+}(b^{'})\hat{T}^{+}(b^{'};a)db^{'}.$$
(4.9)

Contrary to the derivation of equation (4.9) by Wapenaar [87] for *flux normalized* wave fields, the approach taken here is normalization independent. Hence, as in section 2.4, structurally identical expressions hold for pressure normalized wave fields and operators $\{P, \hat{T}, \hat{R}\}^{\pm}$, as well as for their flux normalized wave fields $\{P, \hat{T}, \hat{R}\}^{\pm}$.

Although the form of equation (4.9) bears resemblance to (2.34), their correspondence is not obvious. Equally so is the integration the expressions (4.8a), (4.8b), and (4.8c) and the subsequent steps connecting them to equations (2.28), (2.30), (2.32), respectively. We limit ourselves to stating that the equations derived in section 2.4 coincide with those derived by Fishman and McCoy [27, 28], and that they based their derivations on a discretized version of equation (4.8) for a medium consisting of parallel layers, with properties that do not vary in the vertical direction within each layer. Because equations (2.28), (2.30), (2.32), and (2.34) were derived without using the commutativity of ordinary variables, these relations are entirely equivalent to the expressions of Fishman and McCoy.

In section 2.4 on horizontally layered media, we initialized the recursive expressions by assuming homogeneity at $x_3 = 0$. Equivalent conditions for equations (4.8), are using an iib-domain that is open at $x_3 = a$ and therefore induces initial conditions

$$\hat{T}^{\pm}(a;a) = 1$$
 and $\hat{R}^{\pm}(a;a|a) = 0,$ (4.10)

i.e. no vertical scattering at depth a. Instead working with a domain that is closed at $x_3 = a$, comes down to taking for the differential equation (4.7) the initial condition

$$\hat{T}^{\pm}(a;a) = \hat{t}^{\pm}(a)$$
 and $\hat{R}^{\pm}(a;a|a) = \hat{r}^{\pm}(a),$ (4.11)

i.e. allowing for scattering at depth *a*. For the moment we will not yet make the choice for an open or closed iib-domain. However this decision will have to be made in the sections 4.3 and 5.5 on reciprocity theorems.

	State A	State B
Field	$\mathbf{P}_A(\mathbf{x})$	$\mathbf{P}_B(\mathbf{x})$
One-way operator	$\hat{\mathbf{B}}_A(\mathbf{x})$	$\hat{\mathbf{B}}_B(\mathbf{x})$
Source	${f S}_A({f x})$	${f S}_B({f x})$

Table 4.1: General state table for flux normalized, one-way wave fields

4.3 Kernel representations of global transmission and reflection operators

In this section the Ψ DO's for $\{\hat{T}, \hat{R}\}^{\pm}$ will be expressed as integral operators in terms of the up and down going Green's functions of the one-way wave equations (3.27a) and (3.28a). For both the pressure and flux normalized case the starting point will be reciprocity theorems.

For flux normalized wave fields the reciprocity theorems introduced by Wapenaar and Grimbergen [90] will be used. For pressure normalized one-way wave fields the interaction of up and down going wave fields in the classical Kirchhoff Helmholtz theorem will be analyzed. The derivation of the former is shorter and simpler for two reasons. First because they are not defined for integration domains of arbitrary shape, but specifically for the iib-domain $\mathbb{X}[a, b]$. The second reason is that the two-way wave fields featuring in the Kirchhoff Helmholtz theorem first have to be decomposed into up and down going wave fields, requires $\partial_3 \{\rho, K\} = 0$ at the boundaries $x_3 = a$ and $x_3 = b$. Therefore this section only gives the flux normalized case, while the more lengthy pressure normalized case is deferred to appendix B.

4.3.1 One-way reciprocity theorem of the convolution type for flux normalized wave fields

The interaction quantity

$$U_3 = P_A^+ P_B^- - P_A^- P_B^+, \tag{4.12}$$

cast in terms of the wave fields from table 4.1, is the basis of reciprocity theorems for flux normalized, one-way wave fields. For notational convenience equation (4.12) is expressed as $U_3 = \mathbf{P}_A^t \mathbf{N} \mathbf{P}_B$ where

$$\mathbf{N} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$
, with inverse $\mathbf{N}^{-1} = -\mathbf{N}$,

and **P** defined in equation $(3.25)^1$.

With U_3 as integrand, the integral theorem of Gauss on the volume $\mathbb{X}[a, b]$ reads

$$\int_{\partial \mathbb{X}\{a,b\}} \mathsf{U}_3 n_3 d^2 \mathbf{x}_H = \int_{\mathbb{X}[a,b]} \partial_3 \mathsf{U}_3 d^3 \mathbf{x}, \tag{4.13}$$

where n_3 is the vertical component of the outward pointing normal **n** of the boundary $\partial \mathbb{X}\{a, b\}$, see Figure 4.2. Using the product rule on the right hand side of equation (4.13), allows one to substitute the one-way wave equation (3.28a). Hence, the theorem of Gauss can be expanded as

$$\int_{\partial \mathbb{X}\{a,b\}} \mathbf{P}_{A}^{t} \mathbf{N} \mathbf{P}_{B} n_{3} d^{2} \mathbf{x}_{H} = \int_{\mathbb{X}[a,b]} [\mathbf{P}_{A}^{t} \mathbf{N} \hat{\boldsymbol{\Delta}} \mathbf{P}_{B} + \mathbf{S}_{A}^{t} \mathbf{N} \mathbf{P}_{B} + \mathbf{P}_{A}^{t} \mathbf{N} \mathbf{S}_{B}] d^{3} \mathbf{x}, \quad (4.14)$$

with the contrast operator implicitly defined by

$$\mathbf{N}\hat{\mathbf{\Delta}} = \mathbf{N}\hat{\mathbf{B}}_B + \hat{\mathbf{B}}_A^t\mathbf{N}, \text{ or } \hat{\mathbf{\Delta}} = \hat{\mathbf{B}}_B - \mathbf{N}\hat{\mathbf{B}}_A^t\mathbf{N}.$$

If we combine the definition of the transposed of an operator matrix, i.e. equation (A.17), with the symmetry relations implied by equation (3.33), the contrast operator can be expressed more conveniently as

$$\hat{\mathbf{\Delta}} = \hat{\mathbf{B}}_B - \hat{\mathbf{B}}_A.$$

Now the contrast-term in equation (4.14) vanishes when the medium-parameters are identical, as one would expect intuitively.



Figure 4.2: Integration configuration for one-way flux normalized wave fields

	State A	State B
Field	$\mathbf{G}(\mathbf{x};\mathbf{x}_A)$	$\mathbf{G}(\mathbf{x};\mathbf{x}_B)$
One-way operator	$\hat{\mathbf{B}}_{iib}(\mathbf{x})$	$\hat{\mathbf{B}}_{iib}(\mathbf{x})$
Source	$\mathbf{I}\delta(\mathbf{x}-\mathbf{x}_A)$	$\mathbf{I}\delta(\mathbf{x}-\mathbf{x}_B)$

Table 4.2: States leading to source-receiver reciprocity for flux-normalized one-way wave fields

4.3.2 Source-receiver reciprocity and a representation theorem

The first application of reciprocity theorems is, not surprisingly, proving source-receiver reciprocity. To meet this end, the Green's function of the wave equation (3.28a) will be introduced. Instead of a 2-vector, this is a 2×2 -matrix; the left-column contains the solution for an impulsive *down going* point source, while the right-column contains the solution for an impulsive *up going* point source,

$$\mathbf{G}(\mathbf{x};\mathbf{x}_s) = \begin{pmatrix} \mathsf{G}^{+,+} & \mathsf{G}^{+,-} \\ \mathsf{G}^{-,+} & \mathsf{G}^{-,-} \end{pmatrix} (\mathbf{x};\mathbf{x}_s).$$

¹Note that $\hat{\mathbf{L}}^t \mathbf{N} \hat{\mathbf{L}} = -\mathbf{N}$ and therefore $\mathbf{P}_A^t \mathbf{N} \mathbf{P}_B = -\mathbf{Q}_A^t \mathbf{N} \mathbf{Q}_B = \mathbf{Q}_B^t \mathbf{N} \mathbf{Q}_A$.

	State A	State B
Field	$\mathbf{G}(\mathbf{x};\mathbf{x}^{'})$	$\mathbf{P}(\mathbf{x})$
One-way operator	$\hat{\mathbf{B}}_{iib}(\mathbf{x})$	$\hat{\mathbf{B}}(\mathbf{x})$
Source	$\mathbf{I}\delta(\mathbf{x}-\mathbf{x}^{'})$	$\mathbf{S}(\mathbf{x})$

Table 4.3: States for representation theorems for flux-normalized one-way wave fields

This Green's function matrix satisfies the differential equation

$$[\partial_3 - \hat{\mathbf{B}}_{iib}(\mathbf{x})]\mathbf{G}(\mathbf{x};\mathbf{x}_s) = \mathbf{I}\delta(\mathbf{x} - \mathbf{x}_s)$$

The one-way operator $\hat{\mathbf{B}}_{iib}(\mathbf{x})$ describes the iib-medium, which does not scatter in the vertical direction outside the region $\mathbb{X}[a, b]$, see Figure 4.1.

Consider the states from table 4.2. For the iib-medium, the inward propagating fields at the boundary $\partial \mathbb{X}\{a, b\}$ are zero if the source is located at $\mathbf{x}_s \in \mathbb{X}(a, b)$. So given the states from table 4.2 both the boundary and contrast terms of equation (4.14) vanish if $\mathbf{x}_{A,B} \in \mathbb{X}(a, b)$, only the last integral containing the source terms remains. After resolving the δ -functions, left multiplication with \mathbf{N}^{-1} yields

$$\mathbf{G}(\mathbf{x}_A;\mathbf{x}_B) = \mathbf{N}\mathbf{G}^t(\mathbf{x}_B;\mathbf{x}_A)\mathbf{N},\tag{4.15a}$$

or resolving the matrix-matrix products

$$\begin{pmatrix} G^{+,+} & G^{+,-} \\ G^{-,+} & G^{-,-} \end{pmatrix} (\mathbf{x}_A; \mathbf{x}_B) = \begin{pmatrix} -G^{-,-} & G^{+,-} \\ G^{-,+} & -G^{+,+} \end{pmatrix} (\mathbf{x}_B; \mathbf{x}_A).$$
(4.15b)

In particular the diagonal part of equation (4.15b) reads

$$\mathsf{G}^{+,+}(\mathbf{x}_A;\mathbf{x}_B) = -\mathsf{G}^{-,-}(\mathbf{x}_B;\mathbf{x}_A). \tag{4.15c}$$

The second application is deriving a representation theorem. To derive one-way representation theorems a third medium is required, besides the actual medium and the iibmedium. Given the states in table 4.3, the right hand side of equation (4.14) reduces to $NP(\mathbf{x}')$ when two conditions are met:

- I. $\mathbf{S}(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{X}[a, \infty)$,
- II. The Green's source coordinate is $\mathbf{x}' \in \mathbb{X}(a, b)$,

Left multiplication by N^{-1} and subsequent use of equation (4.15a) leads to the one-way representation theorem

$$\mathbf{P}(\mathbf{x}') = -\int_{\partial \mathbb{X}\{a,b\}} \mathbf{G}(\mathbf{x}';\mathbf{x})\mathbf{P}(\mathbf{x})n_3(\mathbf{x})d^2\mathbf{x}_H.$$
(4.16)

The flux normalized representation theorem equation (4.16) (and similarly its pressure normalized equivalent) is expressed in integrals over the boundaries $\partial X\{a\}$ and $\partial X\{b\}$. The integrals over these boundaries will be indicated by the integration-variables a_H and b_H , which are the horizontal parts of the 3-vectors

$$\mathbf{a} = (\mathbf{a}_H, a)$$
 and $\mathbf{b} = (\mathbf{b}_H, b)$.

Note that the vertical components of a and b have no subscript 3. With this convention a scalar surface-integral over $\partial \mathbb{X}\{a\}$ will be expressed as

$$\int_{\partial \mathbb{X}\{a\}} f(\mathbf{x}_H, a) d^2 \mathbf{x}_H \to \int f(\mathbf{a}) d^2 \mathbf{a}_H$$

a similar convention is also used for $\partial \mathbb{X}\{b\}$. Often the depth components of both arguments of the kernel will have the same value. Then the horizontal coordinates and the full 3-vectors will be distinguished by one or more primes, i.e. $\mathbf{a} = (\mathbf{a}_H, a)$ v.s. $\mathbf{a}' = (\mathbf{a}_H', a)$.

In the iib-medium wave fields emitted from point sources located on the boundary $\partial X\{a, b\}$ only reach interior points when propagating inward, see Figures 4.1 and 4.2. Removing the zero-valued outward propagating Green's functions from equation (4.16), and using $n_3(a) = -1$ and $n_3(b) = 1$ leads to

$$\begin{pmatrix} \mathsf{P}^{+} \\ \mathsf{P}^{-} \end{pmatrix}(\mathbf{x}^{'}) = \int \begin{pmatrix} \mathsf{G}^{+,+} \\ \mathsf{G}^{-,+} \end{pmatrix}(\mathbf{x}^{'};\mathbf{a})\mathsf{P}^{+}(\mathbf{a})d^{2}\mathbf{a}_{H} - \int \begin{pmatrix} \mathsf{G}^{+,-} \\ \mathsf{G}^{-,-} \end{pmatrix}(\mathbf{x}^{'};\mathbf{b})\mathsf{P}^{-}(\mathbf{b})d^{2}\mathbf{b}_{H}.$$
(4.17)

The pressure normalized equivalent of equation (4.17) is given by equation (B.15).

The second part of this section will relate the kernel equivalents of the global transmission and reflection operators of section 4.2 to representations of the type of equations (4.17) and (B.15). A principal obstacle stems from the conflict between the requirement of \mathbf{x}' lying *inside* $\mathbb{X}(a, b)$, and the wave fields on the left hand side of equation (4.3) being taken *outside* $\mathbb{X}(a, b)$, on $\partial \mathbb{X}\{a, b\}$. Equations (4.16) and (B.15) can therefore only be matched to (4.3) in a limiting sense; as

$$a_{+} = \lim_{\epsilon \to 0} a + \epsilon$$
 and $b'_{-} = \lim_{\epsilon \to 0} b - \epsilon$,

or

$$\mathbf{a}_+ = (\mathbf{a}_H, a_+)$$
 and $\mathbf{b}_- = (\mathbf{b}_H, b_-).$

A short look at equation (4.3) shows that isolating the expressions

$$P^+(b) = \hat{T}^+(b;a)P^+(a)$$
 and $P^-(a) = \hat{R}^+(a;a|b)P^+(a)$

requires $P^{-}(b) = 0$. This can only be assured if the domain $\mathbb{X}[b, \infty)$ is source free. In the limiting sense given above the kernels in integrand in the left term of equation (4.17) are equal to the kernels of T^+ and R^+ , i.e.

$$G^{+,+}(\mathbf{b}_{-};\mathbf{a}) \to T^{+}(\mathbf{b};\mathbf{a}),$$
 (4.18a)

$$\mathsf{G}^{-,+}(\mathbf{a}_{+}^{'};\mathbf{a}) \to \mathsf{R}^{+}(\mathbf{a}^{'};\mathbf{a}|b). \tag{4.18b}$$

Note that this effectively amounts to using the non scattering boundary conditions given by equation (4.10).

Similarly, isolating the expressions

$$P^{-}(a) = \hat{T}^{-}(a,b)P^{-}(b)$$
 and $P^{+}(b) = \hat{R}^{-}(b,b|a)P^{-}(b)$

from equation (4.3) requires $P^+(a) = 0$, which in turn requires the domain $\mathbb{X}(-\infty, a]$ to be source free. In the same limiting sense the kernels in the integrand of the right term of

equation (4.17) are equal to the kernels of R^- and T^-

$$-\mathbf{G}^{-,-}(\mathbf{a}_{+};\mathbf{b}) \to \mathbf{T}^{-}(\mathbf{a};\mathbf{b}), \tag{4.19a}$$

$$\mathbf{G}^{+,-}(\mathbf{b}_{-}^{'};\mathbf{b}) \to \mathbf{R}^{-}(\mathbf{b}^{'};\mathbf{b}|a). \tag{4.19b}$$

A consequence of the fact that Green's functions only match to operator-kernels in the limit $\epsilon \rightarrow 0$, is that the Green's functions have to depend continuously on their source and receiver coordinates. This is the case if the medium-parameters depend continuously on **x**, a restriction we already imposed in section 4.2.

When we ignore the fact that the extrapolation levels are separated by infinitesimal distances from the receiver-levels, we can see that the equations (4.15c), (4.18a), and (4.19a) immediately give rise to

$$\mathsf{T}^{-}(\mathbf{a};\mathbf{b}) = \mathsf{T}^{+}(\mathbf{b};\mathbf{a}),\tag{4.20a}$$

or in operator notation

$$\hat{\mathsf{T}}^{-}(a;b) = \{\hat{\mathsf{T}}^{+}(b;a)\}^{t},$$
(4.20b)

Their pressure normalized counterparts lack such a symmetry relation, which can be traced back to the differences between the local pressure and flux normalized transmission operators, remember equations (3.31) and (3.33).

4.4 From pressure normalized Green's functions to flux normalized operators

Expressions in terms of flux normalized operators are more symmetric and simpler, and therefore more amenable to abstract manipulation. However, measurements and established modeling algorithms, for example the Finite difference algorithm we use in Chapters 3 and 5, yield pressure normalized Green's functions. Hence the former need to be expressed in the latter. To do so we return to the operator-notation of section 4.2, suppressing the lateral dependencies and integrals inherent to kernel-notation.

Substitute equation (3.26) into $P^+(b) = \hat{T}^+(b;a)P^+(a)$ and match it to

$$\mathsf{P}^{+}(b) = \hat{\mathsf{T}}^{+}(b;a)\mathsf{P}^{+}(a). \tag{4.21}$$

This yields

$$\hat{\mathsf{T}}^{+}(b;a) = \hat{\mathsf{l}}(b)\hat{T}^{+}(b;a)\hat{\mathsf{l}}^{-1}(a).$$
(4.22)

Casting equation (B.16b) in operator-notation, takes a little more work. First note that if x'_3 approaches b, then the up going wave field G^- on the right hand side of equation (B.14) goes to zero, so

$$G^{-}(\mathbf{a};\mathbf{b}) = G^{+}(\mathbf{b};\mathbf{a}),$$

or $\hat{G}^+(b;a) = \hat{G}^{-,t}(a;b)$ in operator-notation. This allows one to write

$$\partial_3 \hat{G}^+(b;x_3)|_{x_3=a} = \{\partial_3 \hat{G}^-(x_3;b)\}^t|_{x_3=a}.$$

Although ∂_3 is an operator, it is not affected by the operator-transposition, which is exclusively related to ∇_H , not to ∂_3 . Combined with the fact that the medium does not scatter in the vertical direction at depth *a*, this allows one to rewrite

$$\partial_a \hat{G}^+(b;a) = \{j\hat{H}_1(a)\hat{G}^-(a;b)\}^t = j\hat{G}^+(b;a)\hat{H}_1^t(a).$$

With the help of equation (3.19a) one can therefore express the operator equivalent of equation (B.16b) as

$$\hat{T}^{+}(b;a) = 2j\omega\,\hat{G}^{+}(b;a)\,\hat{l}(a).$$
 (4.23)

After substitution of equation (4.23) into (4.22), equation (3.19c) can be used to resolve to

$$\hat{\mathsf{T}}^{+}(b;a) = 2j\omega\,\hat{\mathsf{l}}(b)\,\hat{G}^{+}(b;a)\,\hat{\mathsf{l}}^{t}(a).$$
(4.24)

Similar considerations let the up going transmission and reflection operators be expressed as

$$\begin{split} \hat{\mathsf{T}}^{-}(a;b) =& 2j\omega\,\hat{\mathsf{l}}(a)\,\hat{G}^{-}(a;b)\,\hat{\mathsf{l}}^{t}(b),\\ \hat{\mathsf{R}}^{+}(a;a|b) =& 2j\omega\,\hat{\mathsf{l}}(a)\,\hat{G}^{-}(a;a|b)\,\hat{\mathsf{l}}^{t}(a),\\ \hat{\mathsf{R}}^{-}(b;b|a) =& 2j\omega\,\hat{\mathsf{l}}(b)\,\hat{G}^{+}(b;b|a)\,\hat{\mathsf{l}}^{t}(b). \end{split}$$



Figure 4.3: Configurations for Redatuming representation.

Independent of the source-receiver reciprocity resulting from flux normalized reciprocity theorems, the construction of \hat{T}^{\pm} laid down in this section also guarantees the reciprocity of global up and down going transmission due to the source-receiver reciprocity of the conventional Green's function, equation (B.4).

4.5 A redatuming representation based on the Lippmann-Schwinger equation

Here we divert from the track laid out in Chapter 2. In that chapter, section 2.4 on the generalized primary presentation was followed by section 2.5 on inverse propagation with transmission loss correction. The latter subject will be covered extensively for 3D inhomogeneous media in Chapter 5. Here we first present a data representation that is more suitable for redatuming, that is we extend the first part of section 2.6 to 3D inhomogeneous media. To do so, we start this section by discussing the configuration and corresponding boundary conditions.

In the previous sections of this chapter we focused on wave propagation between depths a and b but did not attach a specific meaning to them other than that a < b. But from now on we will take a to be the surface of the earth and b the redatuming depth; the corresponding domain boundaries are renamed to

$$\partial \mathbb{S} = \partial \mathbb{X}\{a\}$$
 and $\partial \mathbb{D} = \partial \mathbb{X}\{b\},\$

respectively. The upper half space of the actual medium, $\mathbb{X}(-\infty, a]$, is taken to be homogeneous; we assume that data does not contain free surface multiples. The subsurface containing the geology is denoted by

$$\mathbb{G} = \mathbb{X}(a, \infty). \tag{4.25}$$

Also see Figure 4.3(a). Note that the surface boundary $\partial \mathbb{S}$ is not included in the geology, which reflects our assumption that the down going reflection response $\hat{R}^+_{\mathbb{G}}$ does not contain free surface multiples². The geology \mathbb{G} is further subdivided into an overburden \mathbb{O} and lower half space \mathbb{L} , which are defined in iib-terms as

$$\mathbb{O} = \mathbb{X}(a, b), \tag{4.26a}$$

$$\mathbb{L} = \mathbb{X}[b, \infty), \tag{4.26b}$$

respectively, also see Figure 4.3(b). Note that the boundary $\partial \mathbb{D}$ is included in \mathbb{L} .

Let us consider two different reflection experiments, similar to those of section 2.6:

- 1. The actual experiment at depth *a* with sources emitting down going wave fields and receivers measuring up going wave fields, also see Figure 4.3(a). This specification implies that surface waves and free surface multiple reflections need to have been removed.
- A thought experiment at depth b in the subsurface, again with sources emitting down going wave fields and receivers measuring up going wave fields, also see Figures 4.3(b) and 2.9.

The final goal of this section is to interrelate the two reflection experiments mentioned above. This involves a significant amount of manipulating different reflection and transmission operators. These manipulations will appear more complex than strictly necessary, if we use the explicit depth-dependencies for each operator. Therefore we introduce a more compact notation for this section only. Together with their section 2.6-correspondences the relevant reflection-characteristics of the half spaces \mathbb{G} and \mathbb{L} are

$$\begin{split} \hat{R}^+_{\mathbb{G}} &= \hat{R}^+(a;a|\infty), & \qquad \hat{R}^+_{\mathbb{L}} &= \hat{R}^+(b;b|\infty), \\ \uparrow & \uparrow & \uparrow \\ \tilde{R}^+_N, & \qquad \tilde{R}^+_{n,N}, \end{split}$$

²In section 2.4 we represented this assumption by the condition $\tilde{r}^+ = 0$ at $x_{3,0}$.

respectively. The reflection-characteristics of the overburden $\mathbb O$ are

$$\begin{split} \hat{R}_{\mathbb{O}}^{-} &= \hat{R}^{-}(b;b|a), & \qquad \hat{R}_{\mathbb{O}}^{+} &= \hat{R}^{+}(a;a|b), \\ & \uparrow & \qquad \uparrow \\ & \tilde{\mathsf{E}}_{n}, & \qquad \tilde{\mathsf{R}}_{n-1}^{+}, \end{split}$$

In addition the transmission characteristics of the overburden are

$$\begin{split} \hat{T}^+_{\mathbb{O}} &= \hat{T}^-(b;a), & \qquad \hat{T}^-_{\mathbb{O}} &= \hat{T}^+(a;b), \\ & \uparrow & & \uparrow \\ & \tilde{W}^+_n, & \qquad \tilde{W}^-_n. \end{split}$$

Similar to \tilde{E}_n in Chapter 2, $\hat{R}_{\mathbb{O}}^-$ is the reflection response of the overburden \mathbb{O} due to an up going source at the redatuming depth, but it does not include the reflectivity of the redatuming level (also remember equation (4.26a)). The last mathematical manipulations of this chapter are algebraically identical to those contained in equations (2.51)-(2.54), because we derived those expressions without using commutativity.

To obtain a redatuming representation the response of the actual experiment must be related to that of the thought experiment. The latter is the up going wave field at depth b due to down going source-field $S^+(b)$ at the same depth. The total wave field at depth b satisfies

$$\begin{pmatrix} P^+(b) \\ P^-(b) \end{pmatrix} = \begin{pmatrix} S^+(b) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & \hat{R}_{\mathbb{D}}^- \\ \hat{R}_{\mathbb{L}}^+ & 0 \end{pmatrix} \begin{pmatrix} P^+(b) \\ P^-(b) \end{pmatrix}.$$
 (4.27)

Multiply both sides of the upper row of equation (4.27) with $\hat{R}^+_{\mathbb{L}}$. Because the lower row of equation (4.27) reads $P^-(b) = \hat{R}^+_{\mathbb{L}}P^+(b)$, elimination of $P^+(b)$ leads to the Lippmann-Schwinger equation³

$$P^{-}(b) = \hat{R}_{\mathbb{L}}^{+} S^{+}(b) + \hat{R}_{\mathbb{L}}^{+} \hat{R}_{\mathbb{O}}^{-} P^{-}(b).$$
(4.28)

³Strictly speaking the Lippmann-Schwinger equation has the structure

$$\hat{R}_{tot}^{+} = \hat{R}_{\mathbb{L}}^{+} + \hat{R}_{\mathbb{L}}^{+} \hat{R}_{\mathbb{O}}^{-} \hat{R}_{tot}^{+}.$$

But assuming that $S^+(b)$ corresponds to a point source with coordinates in the same aperture as the receiver coordinate, the conversion of equation (4.28) to this format is straightforward.
Equation (4.28) in turn allows the total up going field $P^{-}(b)$ of the thought experiment to be expressed as

$$P^{-}(b) = \left[1 - \hat{R}_{\mathbb{L}}^{+} \hat{R}_{\mathbb{D}}^{-}\right]^{-1} \hat{R}_{\mathbb{L}}^{+} S^{+}(b),$$

$$= \hat{R}_{\mathbb{L}}^{+} S^{+}(b) + \hat{R}_{\mathbb{L}}^{+} \hat{R}_{\mathbb{D}}^{-} \hat{R}_{\mathbb{L}}^{+} S^{+}(b) + \dots,$$

$$\triangleq \hat{R}_{thght}(b; b) S^{+}(b).$$
(4.29)

In section 2.6 we used the scattering matrix approach to relate the response of an actual experiment \tilde{R}_N^+ to that of a thought experiment $\tilde{R}_{thght,n}$. This approach can be applied similarly to the laterally varying case treated here. A down going source-field $P^+(a) = S^+(a)$ at the surface generates an up going wave field $\hat{R}_{\mathbb{G}}^+S^+(a)$ at $x_3 = a$ and a down going wave field $P^+(b)$ at $x_3 = b$. This down going response is reflected upward by the geology in the lower half space \mathbb{L} , giving rise to an up going incident wave field $P^-(b) = \hat{R}_{\mathbb{L}}^+P^+(b)$ at $x_3 = b$. Note that although the wave fields $P^+(b)$ and $P^-(b)$ are not equal to their appearances in equations (4.27)-(4.29), they are related in the same manner. After equation (4.3) the scattering matrix for the overburden \mathbb{O} relates the wave fields resulting from the source field $S^+(a)$ like

$$\begin{pmatrix} P^+(b)\\ \hat{R}^+_{\mathbb{G}}S^+(a) \end{pmatrix} = \begin{pmatrix} \hat{T}^+_{\mathbb{O}} & \hat{R}^-_{\mathbb{O}}\\ \hat{R}^+_{\mathbb{O}} & \hat{T}^-_{\mathbb{O}} \end{pmatrix} \begin{pmatrix} S^+(a)\\ \hat{R}^+_{\mathbb{L}}P^+(b) \end{pmatrix}.$$
(4.30)

Similar to the horizontally layered case discussed in section 2.6, the transmission and reflection operator of the overburden \mathbb{O} do not include the scattering properties of depths $x_3 = a$ and $x_3 = b$, but just those of the medium in between.

After eliminating $P^+(b)$ from the lower row of equation (4.30) with the upper, it is clear that the reflection operators $\hat{R}^+_{\mathbb{G}}$ and \hat{R}^+_{thght} are related by

$$\hat{R}^+_{\mathbb{G}} = \hat{R}^+_{\mathbb{O}} + \hat{T}^-_{\mathbb{O}} \hat{R}_{thght} \hat{T}^+_{\mathbb{O}}.$$

$$(4.31)$$

To undo the transmission effects of the overburden, Chapter 5 deals with the construction of the inverse operators $\hat{F}_{\mathbb{O}}^{-} \triangleq \{\hat{T}_{\mathbb{O}}^{-}\}^{-1}$ and $\hat{F}_{\mathbb{O}}^{+} \triangleq \{\hat{T}_{\mathbb{O}}^{+}\}^{-1}$ for up and down going propagation, respectively (only for flux normalized wave fields). Given these operators we define redatuming as left multiplication of equation (4.31) by $\hat{F}_{\mathbb{O}}^{-}$ and right multiplication by $\hat{F}^+_{\mathbb{O}}$

$$\hat{R}_{dat}(b;b) \triangleq \hat{F}_{\mathbb{O}}^{-} \hat{R}_{\mathbb{G}}^{+} \hat{F}_{\mathbb{O}}^{+},$$

$$= \hat{F}_{\mathbb{O}}^{-} \hat{R}_{\mathbb{O}}^{+} \hat{F}_{\mathbb{O}}^{+} + \hat{R}_{thght}(b;b).$$
(4.32)

We note that besides the sought after response of the thought experiment, redatuming defined by equation (4.32) also yields artifacts in the form of the product $\hat{F}_{\mathbb{O}}^-\hat{R}_{\mathbb{O}}^+\hat{F}_{\mathbb{O}}^+$. Suppose we already had the exact inverse propagators $\hat{F}_{\mathbb{O}}^\pm$. Then the artifacts would be a pure nuisance. However, to construct the inverse propagator $\hat{F}_{\mathbb{O}}^+$ corrected for transmission loss we need $\hat{R}_{\mathbb{O}}^+$ in addition to $\hat{T}_{\mathbb{O}}^+$; see section 5.5 for a detailed derivation. In Chapter 6 we will therefore propose a data driven method to estimate $\hat{R}_{\mathbb{O}}^+$ from these artifacts.

For the construction of the inverse propagator for up going wave fields $\hat{F}_{\mathbb{O}}^-$, we would need to make a similar estimate of $\hat{R}_{\mathbb{O}}^-$, the reflection of the overburden with sources and receivers buried at depth $x_3 = b$. To avoid this requirement we will work with flux normalized wave fields. Similar to flux normalized forward propagators, the corresponding inverse propagators obey source receiver reciprocity

$$\hat{\mathsf{F}}_{\mathbb{O}}^{-} = \hat{\mathsf{F}}_{\mathbb{O}}^{+,t}; \tag{4.33}$$

remember equation (B.4).

For the total pressure wave field Mulder [66] formulated an approach to acoustic redatuming analogous to ours, amounting to three inverse problems. If we take equation (4.31) as a starting point, then the first of these inverse problems, source redatuming, is equivalent to evaluating

$$\hat{R}_{src,dat} \triangleq (\hat{R}_{\mathbb{G}}^+ - \hat{R}_{\mathbb{O}}^+)\hat{F}_{\mathbb{O}}^+.$$

Mulder gave the name receiver redatuming to the combined effect of solving the second and third inverse problems. This is equivalent to extracting $\hat{R}^+_{\mathbb{L}}$ from $\hat{T}^-_{\mathbb{O}}\hat{R}_{thght}$ (remember equation (4.29)). To reduce the computational burden, he did not solve the second. Taking into account the approximation, the solution of the final inverse problem is equivalent to

$$\hat{R}_{thght} = \hat{F}_{\mathbb{O}}^{-} \hat{R}_{src,dat}.$$

There are two differences between Mulders approach and ours. First our approach requires the extra computational burden of flux normalization. However, we only construct the inverse propagator \hat{F}_{\square}^+ ; that is we solve just one inverse problem. Due to flux normalization we can obtain the other inverse propagator by $\hat{F}_{\mathbb{O}}^{-} = \hat{F}_{\mathbb{O}}^{+,t}$. The second difference is the solution method. Mulder employs a singular value decomposition, while we construct the inverse through a Neumann expansion, see Chapter 5.

From here on we resume indicating depth-dependencies in favor of subscripting operators with \mathbb{G}, \mathbb{O} , and \mathbb{L} ;

 $\hat{\mathsf{T}}^+_{\mathbb{O}} \to \hat{\mathsf{T}}^+(a;b),$ etcetera.

Chapter 5

Theory of inverse one-way propagation

5.1 Introduction

It is well-known that if the inverse propagation step in Kirchhoff migration only uses the first arrivals of the Green's functions, significant artifacts can arise in the migration output for complex velocity models [37]. These artifacts are caused by the negligence of the later arrivals of multivalued Green's functions, with stronger amplitudes than the first arrivals. Using all arrivals yields the best result that Kirchhoff migration can possibly give. However, it is a common misconception that this best result is the correct one. We do not refer to the fact that ray-traced Green's functions, single- or multivalued, are high frequency approximations of the exact Green's functions, nor do we refer to the negligence of evanescent wave fields. We refer instead to the negligence of transmission loss as illustrated on horizontally layered media in section 2.5. Application of the exact Kirchhoff-Helmholtz integral with exact Green's functions suffers from the same defect and may give rise to amplitude errors of the same order of magnitude as those caused by the negligence of later arrivals. In section 5.3 we illustrate the defects mentioned above and to avoid discussions on inaccurate modeling we use a Finite Difference algorithm to generate the wave fields.

But first we discuss the basics of inverse propagation and the interpretation of its application to redatuming in section 5.2. The conclusion is that for flux normalized wave

fields the point spread filters¹ for inverse propagation of up and down going wave fields are each other's transposed, where the up going case allows a more convenient interpretation. In section 5.3 we therefore leave out the down going case.

Deriving and constructing a data driven correction for transmission loss, is however more straightforward for down going fields. Up going wave fields will therefore play a minor role in sections 5.4-5.7 on the construction and implementation of the transmission loss correction.

In section 5.8 we present some numerical examples of transmission loss corrected inverse propagation and discuss limitations on the applicability. We conclude this chapter with an example of redatuming in section 5.9. Again all wave fields used in the examples are generated with a Finite Difference algorithm.

5.2 Inverse propagation in relation to redatuming of oneway wave fields

In Chapter 4 we adopted the convention a < b. Moreover, in section 4.5 we identified a with the surface of the earth and b with the redatuming depth. Integrals over flat planes at these depths will be represented with integration variables

$$\mathbf{a} = (\mathbf{a}_H, a)$$
 and $\mathbf{b} = (\mathbf{b}_H, b)$.

With equation (4.32) we defined redatuming as left multiplication by \hat{F}^- and right multiplication by \hat{F}^+ . The annihilation of the transmission operators \hat{T}^{\pm} between equations (4.31) and (4.32) therefore reads

$$\hat{\mathsf{F}}^-(b;a)\hat{\mathsf{T}}^-(a;b) = \hat{\mathsf{I}}$$
 and $\hat{\mathsf{T}}^+(b;a)\hat{\mathsf{F}}^+(a;b) = \hat{\mathsf{I}};$

their kernel equivalents are

$$\int_{\partial S} \mathsf{F}^{-}(\mathbf{b}; \mathbf{a}) \mathsf{T}^{-}(\mathbf{a}; \mathbf{b}') d^{2} \mathbf{a}_{H} = \delta(\mathbf{b}_{H} - \mathbf{b}_{H}'), \tag{5.1a}$$

$$\int_{\partial S} \mathsf{T}^{+}(\mathbf{b}; \mathbf{a}) \mathsf{F}^{+}(\mathbf{a}; \mathbf{b}') d^{2} \mathbf{a}_{H} = \delta(\mathbf{b}_{H} - \mathbf{b}_{H}'), \tag{5.1b}$$

¹The terms resolution filter or function also circulate in the seismic community. But the precise meanings tend to vary, so we avoid their use.

for up and down going waves, respectively. The interpretation of equation (5.1a) is straightforward. Given an up going wave field $P^{-}(b)$ at the redatuming depth *b*, we can reconstruct this wave field from its up going response at the surface, $P^{-}(a) = \hat{T}^{-}(a;b)P^{-}(b)$, by left multiplication with $\hat{F}^{-}(b;a)$.

We cannot use the same interpretation for equation (5.1b), which amounts to reconstructing a down going source field at the surface, from its down going response at the redatuming depth. Instead equation (5.1b) should be interpreted as the inverse propagation of a down going wave field from b to a, after which the down going propagation effects are again applied. However, for an examination of the accuracy of inverse down going propagation we do not need to bother with this interpretation; due to flux normalization equations (5.1a) and (5.1b), together with their discrete representations, obey a simple relation.

Let the square matrices $\mathbf{T}^+(b; a)$ and $\mathbf{T}^-(a; b)$ be the discrete, finite aperture representations of the transmission operators $\hat{\mathbf{T}}^+(b; a)$ and $\hat{\mathbf{T}}^-(a; b)$, respectively; in section A.3 we give the mapping of operators and kernels to square matrices. Similarly the inverse propagators $\hat{\mathbf{F}}^+(a; b)$ and $\hat{\mathbf{F}}^-(b; a)$ have discrete representations $\mathbf{F}^+(a; b)$ and $\mathbf{F}^-(b; a)$. Ideally these matrices are related by the discrete equivalents of equations (5.1), $\mathbf{F}^-\mathbf{T}^- = \mathbf{I}$ and $\mathbf{T}^+\mathbf{F}^+ = \mathbf{I}$. In the less than ideal practical situation we will deal with the point spread filters for up and down going wave fields

$$\mathbf{M}^{-}(b;b|a) = \mathbf{F}^{-}(b;a)\mathbf{T}_{w}\mathbf{T}^{-}(a;b),$$
(5.2a)

$$\mathbf{M}^{+}(b;b|a) = \mathbf{T}^{+}(b;a)\mathbf{T}_{w}\mathbf{F}^{+}(a;b),$$
(5.2b)

respectively. T_w is a real, diagonal matrix to suppress finite aperture artifacts.

Because we choose to work with flux normalized wave fields, the point spread filters obey a simple relation. The up and down going transmission operators are each other's transposed and equivalently the corresponding kernels obey reciprocity, remember section 4.3.2. An immediate consequence is that the inverse operators are also each other's transposed and that the corresponding kernels also obey reciprocity,

$$\hat{\mathsf{F}}^{-}(b;a) = \{\hat{\mathsf{F}}^{+}(a;b)\}^{t},$$
(5.3a)

and

$$\mathsf{F}^{-}(\mathbf{b};\mathbf{a}) = \mathsf{F}^{+}(\mathbf{a};\mathbf{b}),\tag{5.3b}$$

respectively. In our numerical schemes we exploit these source-receiver reciprocityrelations to avoid the explicit construction of the matrices $\mathbf{T}^{-}(a; b)$ and $\mathbf{F}^{-}(b; a)$. Hence the up and down going point spread filters obey

$$\mathbf{M}^{-} = \{\mathbf{M}^{+}\}^{t}.\tag{5.4}$$

Although we will actually construct $\mathbf{F}^+(a; b)$ instead of $\mathbf{F}^-(b; a)$, the relations (5.3) and (5.4) allow us to test the accuracy of $\mathbf{F}^+(a; b)$ on inverse propagation of up going wave fields. The example applications in sections 5.3 and 5.8, will therefore only focus on inverse propagation of up going wave fields.

5.3 Overview of common one-way inverse propagation methods



Figure 5.1: Example configuration for inverse propagation of an up going wave field. The wave field is emitted at $\partial \mathbb{D}$ from the array of diamonds to $\partial \mathbb{S}$, and inverse propagated to $\partial \mathbb{D}$. The arrows represent the rays for propagation from $\partial \mathbb{D}$ to $\partial \mathbb{S}$. The boundary planes $\partial \mathbb{S}$ and $\partial \mathbb{D}$ lie at depths a = 0.08 km and b = 0.6 km.

Geophysicists have devised a number of methods to construct/approximate F^{\pm} . To a varying degree these take into account amplitude effects, but transmission loss is neglected by all. A number of common methods will be illustrated by inverse propagation of the response of an up going plane wave source in the configuration of Figure 5.1, a setup which has been used before for inverse wave propagation by Wapenaar et al. [89]. The methods illustrated here work for pressure normalized wave fields, so the corresponding point spread filters for up and down going wave fields do not obey equation (5.4). However, we do not pursue a thorough analysis of their amplitude behavior, but merely wish to illustrate the effect of ignoring transmission loss. This overview has been presented before at the 2003 EAGE meeting, [34].

The combination of the syncline shape of the interface in Figure 5.1 and the high contrast between top and bottom half-space,

$$c_1 = 1.5 * 10^3 \text{ m/s}, \qquad \rho_1 = 1.5 * 10^3 \text{ kg/m}^3,$$

$$c_2 = 2c_1, \qquad \qquad \rho_2 = 2\rho_1, \qquad (5.5)$$

cause the interface to exhibit strong (de)focusing effects; note that multiple up going ray paths leaving from (0, 600) arrive at the same receiver location. To avoid discussions on the modeling of multi arrivals, all wave fields are generated on a staggered grid by a finite difference algorithm with 2nd order accuracy in time and 4th order accuracy in space. We sample the medium depicted by Figure 5.1 with $\delta x_1 = \delta x_3 = 4$ m, and the time domain with $\delta t = 8 * 10^{-4}$ s. In the frequency domain we focus on the band [10 Hz, 35 Hz]. At depth a = 0.08 km we measure the response of a plane wave source of half the receiver aperture positioned at depth b = 0.6 km centered at $x_1 = 0$ km to put an emphasis on the focusing effects of the syncline. The transmission response at ∂S is inverse propagated by four types of inverse propagators.

- First we apply the matched filter approach, as defined by equation (B.27a). This
 is essentially the transmitted Green's function response corresponding to sources
 and receivers at ∂D and ∂S, respectively; see Figure 5.3 for the case of a point
 source right below the syncline and note that the triplications are included. Using
 its adjoint to reconstruct the plane wave source from the transmission response of
 Figure 5.2 results in Figure 5.5. Kinematically the source wave field is properly
 reconstructed, but its amplitude-behavior is not; see Figure 5.7. Note that in correspondence with equation (2.42) and the values of the medium parameters as given
 by equation (5.5) the amplitude error is ca. 36 percent.
- 2. For the second case the first arrivals of the Green's function are used, see Figure 5.4. Instead of a standard raytracing package, we generated this inverse propagator by aligning all first arrivals at t = 0, transformed to the wavenumber-frequency domain and just selected (a small band around) the $k_1 = 0$ component. Now the amplitude-discrepancy deteriorates, again see Figure 5.7, and even the recovery of the kinematics of the source field becomes erroneous, see Figure 5.6, both in particular below the syncline.
- 3. The plane wave reconstruction delivered by reverse time extrapolation as described by McMechan [63] is identical to that of the matched filter approach illustrated by



Figure 5.2: Up going transmission response at ∂S in Figure 5.1 due to a plane wave source at $\partial \mathbb{D}$.



Figure 5.4: First arrival of Green's function transmission response at ∂S in Figure 5.1.



Figure 5.6: Reconstruction of the up going plane wave source at $\partial \mathbb{D}$ in Figure 5.1 with first arrivals of Green's function transmission response; also see Figure 5.4.



Figure 5.3: Green's function transmission response at ∂S in Figure 5.1 due to a point-source at (0, 600).



Figure 5.5: Reconstruction of the up going plane wave source at $\partial \mathbb{D}$ in Figure 5.1 with full Green's function transmission response, i.e. the matched filter approach; also see Figure 5.3.



Figure 5.7: Amplitude comparison of the plane wave reconstructions of Figures 5.5 (solid black), 5.6 (dashed) vs. the original source-function (solid gray).

Figure 5.5, see Figures 5.8 and 5.10. This was to be expected, because the two methods are entirely equivalent [24].

4. The commonly used recursive depth extrapolation algorithm [47, 81] also properly recovers the kinematics of the source field, see Figure 5.9, but its estimate of the amplitude is poorer than that of reverse time extrapolation, again see Figure 5.10. Since it is essentially a phase shift operator, no amplitude correction is applied at all. In a horizontally layered medium with the parameters given by equation (5.5), the recovered amplitude would have been the transmission coefficient, i.e. 40 per cent of the proper value.





Figure 5.8: Reconstruction of the up going plane wave source in Figure 5.1 with reverse time extrapolation.

Figure 5.9: Reconstruction of the up going plane wave source in Figure 5.1 with recursive explicit depth extrapolation.



Figure 5.10: Amplitude comparison of plane wave reconstructions of Fig's 5.9 (dashed), 5.8 (solid black) and the original source-function (solid gray).

Wapenaar and Berkhout [88] formulated inverse propagators for pressure normalized wave fields with a transmission loss correction that was essentially similar to the correction proposed in the next section. But it was not yet suitable for application, because

it required the up going reflection $R^{-}(\mathbf{b}; \mathbf{b}|a)$ for inverse propagation of up going wave fields. The flux normalized approach discussed in the next section we circumvent this drawback, by exploiting the source receiver reciprocity implied by equation (5.3).

5.4 One-way reciprocity theorem of the correlation type for flux normalized wave fields

One obvious conclusion to be drawn from the examples of section 5.3 is that the adjoint transmission operator, i.e. the complex conjugate and transposed of the transmission operator, properly removes the kinematic effects of propagation. Notwithstanding its erroneous treatment of the amplitudes, the adjoint transmission operator is an essential part of inverse propagation. We therefore start our search for kernel representations of inverse propagators, by considering a reciprocity theorem based on the interaction quantity that contains the adjoint,

$$\mathbf{U}_{3} = \{\mathbf{P}_{A}^{+}\}^{*}\mathbf{P}_{B}^{+} - \{\mathbf{P}_{A}^{-}\}^{*}\mathbf{P}_{B}^{-} = \mathbf{P}_{A}^{\dagger}\mathbf{J}\mathbf{P}_{B};$$
(5.6)

the states $\mathbf{P}_{A,B}$ are taken from Table 4.1 and the 2 \times 2 matrix **J** is given by

$$\mathbf{J} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
, with the inverse $\mathbf{J}^{-1} = \mathbf{J}$.

The resulting reciprocity theorem is often said to be of the correlation type, since a product of one function and the complex conjugate of another in the frequency domain, corresponds to a correlation of their time-domain counterparts.

Similar to the convolution type reciprocity theorem discussed in section 4.3.1, the correlation type reciprocity theorem results from an evaluation of the integral theorem of Gauss, equation (4.13), for the case of equation (5.6). Again we substitute the one-way wave equation (3.28a) for states A and B in the volume-integral and obtain

$$\int_{\partial \mathbb{X}\{a,b\}} \mathbf{P}_{A}^{\dagger} \mathbf{J} \mathbf{P}_{B} n_{3} d^{2} \mathbf{x}_{H} = \int_{\mathbb{X}[a,b]} [\mathbf{P}_{A}^{\dagger} \mathbf{J} \hat{\mathbf{\Gamma}} \mathbf{P}_{B} + \mathbf{S}_{A}^{\dagger} \mathbf{J} \mathbf{P}_{B} + \mathbf{P}_{A}^{\dagger} \mathbf{J} \mathbf{S}_{B}] d^{3} \mathbf{x};$$
(5.7)

the correlation type contrast operator is defined by

$$\mathbf{J}\hat{\mathbf{\Gamma}} = \mathbf{J}\hat{\mathbf{B}}_B + \hat{\mathbf{B}}_A^{\dagger}\mathbf{J}, \quad \text{or} \quad \hat{\mathbf{\Gamma}} = \hat{\mathbf{B}}_B + \mathbf{J}\hat{\mathbf{B}}_A^{\dagger}\mathbf{J}.$$
(5.8)

Another name, used by Fokkema and Van den Berg [30], is power reciprocity theorem. This name is inspired by the surface-integral on the left hand side of equation (5.7). For identical states A and B it represents the net power flux across the boundaries $\partial X\{a\}$ and $\partial X\{b\}$.

Similar to the convolution type reciprocity theorem one would intuitively expect the contrast-operator $\hat{\Gamma}$ to vanish for identical media. But here intuition is not entirely correct. After setting $\hat{B}_B = \hat{B}_A = \hat{B}$ in equation (5.8), evaluation of the matrix product $J\hat{B}^{\dagger}J$ shows that $\hat{\Gamma}$ would only vanish if the square root operator would be self-adjoint, $\hat{H}_1 = \hat{H}_1^{\dagger}$. However, due to the nonzero imaginary part of its spectrum, \hat{H}_1 is not self-adjoint; it can only be made so by neglecting its evanescent modes. Besides making the contrast-operator $\hat{\Gamma}$ vanish approximately for identical media, neglecting evanescent modes also helps making numerical implementations stable; inverse evanescent wave fields are exponential so they will obscure all propagating wave fields. In the following we will retain the equal sign = if neglecting evanescent modes is the only approximation.

5.5 Transmission loss correction for inverse propagation of flux normalized, one-way wave fields

Wapenaar and Berkhout [88] proposed an iterative method for transmission loss correction, based on equation (B.26) describing inverse propagation for up and down going wave fields. Due to the asymmetry between up and down going transmission the correction had to be constructed separately for both directions, or one had to be constructed from the other through a generalization of equations (2.38) and (2.50) to laterally varying media. By equation (5.3) we showed that flux normalized up and down going inverse propagation only differ by a transposition.

Here the careful reader could make the point that there is little difference in analytical and computational complexity between transforming pressure normalized data and operators to flux normalized ones on one hand, and extending equation (2.50) to laterally varying media on the other; both approaches require the construction of roots of the Helmholtz operator, the fourth root in the former case and the square root in the latter. However, our preference for flux normalized wave fields stems from the source receiver reciprocity between up and down transmission; once the root operators have been constructed, this reciprocity does limit the computational complexity, remember section 5.2.

After Wapenaar [87] we use the states of Table 5.1 to rewrite equation (5.7) into a balance relation for laterally varying media similar to equation (2.45) for horizontally

	State A	State B
Field	$\mathbf{G}(\mathbf{x};\mathbf{x}^{'} b)$	$\mathbf{G}(\mathbf{x};\mathbf{x}^{''} b)$
One-way operator	$\hat{\mathbf{B}}_{iib}(\mathbf{x})$	$\hat{\mathbf{B}}_{iib}(\mathbf{x})$
Source	$\mathbf{I}\delta(\mathbf{x}-\mathbf{x}^{'})$	$\mathbf{I}\delta(\mathbf{x}-\mathbf{x}^{''})$

Table 5.1: States for obtaining transmission loss correction to inverse propagation

layered media. Now we run into an obstacle closely related to the one we met before in section 4.4, where we matched Green's functions to the kernels corresponding to transmission and reflection operators. For transmission loss corrected inverse propagation of down going wave fields, we would like to have the sources and receivers of $R^+(\mathbf{a}; \mathbf{a}|b)$ at the same depth, i.e. $x_3 = a$, but this puts the source points of the Green's functions \mathbf{x}' and \mathbf{x}'' exactly at the integration boundary $\partial \mathbb{X}\{a\}$, leading to an awkward contribution of the δ -functions to the integral.

To avoid this we problem take the same approach as in section 4.4; instead of keeping the upper boundary of the integration-volume and hence the receivers at depth $x_3 = a$, we lower them to

$$a_+ = a + \epsilon$$
, with $\epsilon > 0$,

a vanishing positive constant. We also take $x_3 = a_+$ as the depth above which there is no vertical scattering. Then at depths a_+ and b the Green's matrices of state Table 5.1 have nonzero structures

$$\mathbf{G}(\mathbf{a}_{+};\mathbf{a}^{'}|b) = \begin{pmatrix} \mathbf{G}^{+,+} & 0\\ \mathbf{G}^{-,+} & 0 \end{pmatrix} (\mathbf{a}_{+};\mathbf{a}^{'}|b), \text{ and } \mathbf{G}(\mathbf{b};\mathbf{a}^{'}|b) = \begin{pmatrix} \mathbf{G}^{+,+} & 0\\ 0 & 0 \end{pmatrix} (\mathbf{b};\mathbf{a}^{'}|b),$$

respectively, where $\mathbf{a}_{+} = (\mathbf{a}_{H}, a_{+})$ and $\mathbf{a}' = (\mathbf{a}'_{H}, a)$. As in section 4.4 we let $\epsilon \to 0$ and obtain equation (4.18), repeated her for convenience

$$\mathbf{G}^{-,+}(\mathbf{a}_+;\mathbf{a}'|b) \to \mathbf{R}^+(\mathbf{a};\mathbf{a}'|b), \tag{5.9a}$$

$$\mathbf{G}^{+,+}(\mathbf{b};\mathbf{a}'|b) \to \mathbf{T}^{+}(\mathbf{b};\mathbf{a}'). \tag{5.9b}$$

Note that at $x_3 = a$ we again used the non-scattering boundary conditions given by equation (4.10), and we can therefore also say that

$$\mathbf{G}^{+,+}(\mathbf{a}_{+};\mathbf{a}'|b) \to \delta(\mathbf{a}_{H}-\mathbf{a}_{H}').$$
(5.9c)

With the limits given by equations (5.9) the power reciprocity theorem (5.7) reduces to balance relation

$$\delta(\mathbf{a}'_{H} - \mathbf{a}''_{H}) - C(\mathbf{a}'; \mathbf{a}''|b) = \int \mathsf{T}^{+,\dagger}(\mathbf{b}; \mathbf{a}') \mathsf{T}^{+}(\mathbf{b}; \mathbf{a}'') d^{2}\mathbf{b}_{H},$$
(5.10)

where

$$C(\mathbf{a}';\mathbf{a}''|b) = \int R^{+,\dagger}(\mathbf{a};\mathbf{a}'|b)R^{+}(\mathbf{a};\mathbf{a}''|b)d^{2}\mathbf{a}_{H}.$$
 (5.11)

Note that for $\mathbf{a}' = \mathbf{a}''$ equation (5.10) states energy conservation for propagating wave fields.

For point sources at $a_1'' = 0$ on $\partial \mathbb{S}$ in the configuration of Figure 5.1 the space-time



(a) Reflection response $R^+(a_1, 80; 0, 80|b)$ (b) Cross correlation $C(a_1', 80; 0, 80|b)$

Figure 5.11: Reflection response and cross-correlation for the configuration of Figure 5.1. Both are convolved with a Ricker wavelet in the time-domain.

plots of R^+ and C are given by Figures 5.11(a) and 5.11(b). For the sake of clarity we used an example that does not generate intra bed multiples, but our method does deal with them; see section 5.8 and in particular Figures 5.17(b) and 5.17(d).

The flux balance expressed by equation (5.10) and the subsidiary expression (5.11) represent the extension to laterally varying media of the flux balance given by equation (2.45). The extraction of an expression for the kernel of the inverse propagator for down

going wave fields, $F^+(\mathbf{a}; \mathbf{b})$, is not a direct extension to laterally varying of the steps leading towards equation (2.46b), but still the final result can surely be interpreted as such. First we add $C(\mathbf{a}'; \mathbf{a}''|b)$ to both sides of equation (5.10), and then we multiply with $F^+(\mathbf{a}''; \mathbf{b})$. If we integrate the result over \mathbf{a}''_H , we are allowed to substitute the identity relation (5.1b) and obtain a Fredholm integral equation of the second kind for $F^+(\mathbf{a}; \mathbf{b})$,

$$F^{+}(\mathbf{a}';\mathbf{b}) = T^{+,\dagger}(\mathbf{b};\mathbf{a}') + \int C(\mathbf{a}';\mathbf{a}''|b)F^{+}(\mathbf{a}'';\mathbf{b})d^{2}\mathbf{a}''_{H}.$$
 (5.12)

The standard approach to solving this kind of equation, is iterating

$$\mathsf{F}^{+,(k)}(\mathbf{a}';\mathbf{b}) = \mathsf{F}^{+,(0)}(\mathbf{a}';\mathbf{b}) + \int \mathsf{C}(\mathbf{a}';\mathbf{a}''|b)\mathsf{F}^{+,(k-1)}(\mathbf{a}'';\mathbf{b})d^{2}\mathbf{a}''_{H}.$$
 (5.13a)

initialized by

$$\mathsf{F}^{+,(0)}(\mathbf{a}';\mathbf{b}) = \mathsf{T}^{+,\dagger}(\mathbf{b};\mathbf{a}'). \tag{5.13b}$$

Note that the zero order version given by equation (5.13b) is just the conventional matched filter approach to inverse propagation, i.e. take the adjoint of the transmission operator. We expand $F^{+,(k-1)}(\mathbf{a}''; \mathbf{b})$ in equation (5.13) by repeated back substitution into equation (5.13) itself, until we reach k = 0. This yields an extension of equation (2.46b) to laterally varying media, an expression that we will use as the basis for numerical implementation.

5.6 Discretization

The results of implementing a simple discretization of equation (5.13) will contain severe artifacts due to the fact that any integral over an infinite domain has to be replaced by one over a finite domain². To suppress these artifacts we use the taper weight function introduced in section A.3, or rather its discrete matrix representation T_w which we already encountered in section 5.2. The discrete, finite aperture representations of the continuous, infinite aperture integral expressions (5.11) and (5.13) are the matrix-expressions

$$\mathbf{C}_0(a;a|b) = \mathbf{R}^{+,\dagger}(a;a|b)\mathbf{T}_w\mathbf{R}^+(a;a|b),$$
(5.14)

²In signal analysis literature these artifacts are called finite aperture artifacts.

$$\mathbf{F}^{+,(k)}(a;b) = \mathbf{F}^{+,(0)}(a;b) + \mathbf{C}_0(a;a|b)\mathbf{T}_w\mathbf{F}^{+,(k-1)}(a;b),$$
(5.15a)

with

$$\mathbf{F}^{+,(0)}(a;b) = \mathbf{T}^{+,\dagger}(b;a).$$
(5.15b)

For the final step of redatuming we omit the intermediate step of converting the operator expression (4.32) to an integral expression in terms of the corresponding kernels and just state that we implement redatuming based on the expression

$$\mathbf{R}_{dat}^{(k)}(b;b) = \mathbf{F}^{-,(k)}(b;a)\mathbf{R}^{+}(a;a|\infty)\mathbf{F}^{+,(k)}(a;b).$$
(5.16)

All matrices appearing in equations (5.14)-(5.16) are square and have $N = N_1N_2$ rows and columns, where the aperture is discretized with N_1 cells in the x_1 -direction and with N_2 cells in the x_2 -direction. We conclude this section by listing the matrices involved in equation (5.15) and properties that can be exploited for the reduction of memory use and the computational burden.

- The real-valued, diagonal matrix \mathbf{T}_w is the discrete representation of the taper weight function, remember equation (A.26).
- The complex-valued matrix R⁺(a; a|∞) is the discrete representation of the kernel R⁺_G(a; a'|∞), i.e. the reflection response of the complete geology, and is symmetric on account of source-receiver reciprocity.
- The complex-valued matrix $\mathbf{R}^+(a; a|b)$ is the discrete representation of the kernel $\mathsf{R}^+(\mathbf{a}; \mathbf{a}'|b)$, i.e. the reflection response of the overburden, and is similarly symmetric on account of source-receiver reciprocity.
- The matrix $C_0(a; a|b)$ corresponds to $C(\mathbf{a}'; \mathbf{a}''|b)$ and is complex Hermitian by construction, remember equation (5.14). The reason for adding the subscript 0 will be given later in this section.
- The matrices F^{±,(k)} correspond to the kernels F^{±,(k)}. They are complex-valued and interrelated by a straightforward transposition, F^{-,(k)}(b; a) = {F^{+,(k)}(a; b)}^t.
- The complex-valued matrix $\mathbf{R}_{dat}(b; b)$ is the discrete representation of the kernel $\mathsf{R}_{dat}(\mathbf{b}; \mathbf{b}')$ and is symmetric by construction, remember equation (5.16).



Figure 5.12: Data reordering

5.7 Optimization

In Chapter 1 we stated the goal of this thesis to be undoing propagations effects as accurately as possible. In Chapters 3, 4, and sections 5.2-5.5 of this chapter, we laid down the framework of mathematical physics that facilitates this goal. The resulting equations (3.34) and (5.14)-(5.16) are the basis for our algorithms. In this section we will discuss their implementation with an emphasis on minimizing memory use and number of Flops (Floating point Operations).

Memory use is a potential bottle-neck for seismic processing in general, and in particular for the algorithm proposed here; it is "survey"-based rather than "shot record"-based. So even on modern computers, limiting memory-use to its bare minimum is a necessary condition for practical application. To fulfill this requirement we exploit the well known fact that algorithms based on the frequency domain expressions (3.34) and (5.14)-(5.16) can be applied to each single frequency component independently, so the others need not be kept in memory. Given the standard ordering of a seismic data cube in common shot gathers, this exploitation requires a two stage transposition to common frequency gathers, see Figure 5.12. Given a limited amount of memory this is a nontrivial operation. For our implementations we assume that the amount of memory available, is big enough to hold at least one $x_r - \omega$ -gather, and once the data are properly ordered, all workspace required for the evaluation of equations (3.34) and (5.14)-(5.16) of one frequency-component.

We will pay more attention to minimizing the number of Flop's. Iterative expressions of the form of equation (5.15) frequently appear in scientific computation and therefore the form got its own name, Horner's scheme³; also see Golub and Van Loan [38]. Straightforward iteration of equation (5.15) to order K clearly takes K matrix multiplications of $O(N^3)$ Flop's each. Efficiency is therefore to be gained from reducing (a) the computational burden per matrix multiplication and (b) reducing the total number of these multiplications.

Although the self-adjoint nature of $C_0(a; a|b)$ allows its construction from $\mathbf{R}^+(a; a|b)$ in half the number of Flop's required for a full matrix multiplication, the form of equation (5.15) does not allow further the exploitation of this property. But the introduction of two additional matrices changes this situation and also opens up extra possibilities,

$$\mathbf{T}_{sq} = \sqrt{\mathbf{T}_w}$$
 and $\mathbf{C} = \mathbf{T}_{sq} \mathbf{C}_0 \mathbf{T}_{sq}$

The matrix **C** inherits the hermiticity of the original cross-correlation matrix C_0 , but the way it features in equation (5.15) does allow its hermiticity to be exploited. After multiplying both sides of equation (5.15) with T_{sq} , it can be expanded into

$$\mathbf{T}_{sq}\mathbf{F}^{+,(K)} = \mathbf{T}_{sq}\sum_{k=0}^{K} (\mathbf{C}_0\mathbf{T}_w)^k \{\mathbf{T}^+\}^\dagger = \mathbf{S}^{(K)}\mathbf{T}_{sq}\{\mathbf{T}^+\}^\dagger,$$

with

$$\mathbf{S}^{(K)} = \sum_{k=0}^{K} \mathbf{C}^k.$$
(5.17)

First note that because C is self-adjoint, so are C^k and $S^{(K)}$; this allows the cost of the construction and storage of $S^{(K)}$ to be reduced by a factor 2. The polynomial structure of equation (5.17) suggests two ways for further reduction:

1. Paterson's scheme: reduce the number of matrix multiplications $K \to 2\sqrt{K}$, see Paterson et al. [68] or Golub and Van Loan [38]. Paterson's scheme is based on the fact that if $K = L^2$, then $\mathbf{C}^K = {\{\mathbf{C}^L\}}^L$. This principle can be made to work for

³In computer science one also encounters the name Horner's rule.



Figure 5.13: Computation time comparison for constructing $\mathbf{P}^{+,(K)}(a) = \mathbf{F}^{+,(K)}\mathbf{P}^{+}(b)$ with Horner's scheme, Paterson's scheme, and diagonalization. The measurements were done for 75 frequency components and a configuration with 189 sources/receivers.

all $K \in \mathbb{N}$, see Van Loan [59], but here only the optimal cases with $L \in \mathbb{N}$ will be considered. Introducing

$$\mathbf{Q}^{(l)} = \mathbf{C}^l, \quad \text{for} \quad l = 0, 1, \dots, L,$$

allows equation (5.17) to be expressed alternatively as

$$\mathbf{S}^{(K)} = \sum_{k=0}^{K} \mathbf{C}^{k} = \{\mathbf{Q}^{(L)}\}^{L} + \mathbf{S}^{(L-1)} \sum_{q=0}^{L-1} \{\mathbf{Q}^{(L)}\}^{l}.$$
 (5.18)

An iterative scheme for evaluating equation (5.18) is an aggregation of two *L*-order Horner's schemes. The first can be summarized as

$$\left. \begin{array}{ll} \mathbf{Q}^{(l+1)} = & \mathbf{C}\mathbf{Q}^{(l)} \\ \mathbf{S}^{(l)} = & \mathbf{S}^{(l-1)} + \mathbf{Q}^{(l)} \end{array} \right\} \qquad \text{for } l = 1, \dots, L-1,$$

with $\mathbf{S}^{(0)} = \mathbf{I}$ and $\mathbf{Q}^{(1)} = \mathbf{C}$. The second Horner scheme is

$$\mathbf{S}^{(lL)} = \mathbf{Q}^{(L)} \mathbf{S}^{([l-1]L)} + \mathbf{S}^{(L-1)}, \quad \text{for } l = 1, \dots, L.$$

The matrices C and S^(K) have the same set of eigenvectors. Let these eigenvectors be collected in the orthonormal matrix V and let the corresponding eigenvalues be contained in the real, diagonal matrix Λ. Then C is diagonalized by

$$\mathbf{C} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{\dagger},$$

and similarly \mathbf{C}^k and $\mathbf{S}^{(K)}$ are diagonalized by $\mathbf{C}^k = \mathbf{V} \mathbf{\Lambda}^k \mathbf{V}^\dagger$ and

$$\mathbf{S}^{(K)} = \mathbf{V} \sum_{k=0}^{K} \mathbf{\Lambda}^{k} \mathbf{V}^{\dagger}, \qquad (5.19)$$

respectively. In the eigenvector domain equation (5.17) can be evaluated in O(KN)Flop's instead of $O(KN^3)$. Of course the diagonalization of C and back transformation do not come for free. Typically a few full matrix multiplications are necessary.

How do the different approaches for constructing $\mathbf{F}^{+,(K)}$ compare ?

First the issue of intermediate iteration results. Horner's scheme delivers them without additional effort, while the two alternatives proposed above do require additional effort. Diagonalization can offer expansion up to any order at the cost of (effectively) one matrix multiplication. If all intermediate results are required this amounts to K full matrix multiplications in addition to the diagonalization cost. Paterson's scheme can only deliver intermediate results for $k = 0, L, ..., (L - 1)L, L^2$, when expanding to order $K = L^2$, and also here each intermediate results requires one extra matrix multiplication. When (a lot of) intermediate results of the expansion are required, Horner's scheme is still most convenient.

When only the final result is important, Paterson's scheme and diagonalization clearly beat Horner's scheme, see Figure 5.13. Although the performance of the diagonalization approach is K-independent, the overhead resulting from the diagonalization itself can be significant. This overhead of course depends on the particular algorithm⁴. The break even point in the benchmark-test presented in this Figure is K = 16.

But even for K > 16, an important advantage of Paterson's scheme over diagonalization is that the former is exactly equal to the original Horner's scheme while the latter has its own inherent inaccuracies. In the example applications of section 5.8 and others later this thesis we will therefore use either Horner's or Paterson's scheme without making further distinction between the two.

⁴We used *cheev*-subroutine from the LAPACK-library for the results of Figure 5.13

5.8 Applications of inverse propagation corrected for transmission loss

In the previous sections we developed the inverse propagator for down going wave fields, because we need the surface measurements to construct the transmission loss correction. As argued in section 5.2 inverse propagation of up going wave fields is however more convenient for an accuracy analysis.

For our first set of examples we return to the configuration of Figure 5.1 in section 5.3, repeated here in the form of Figure 5.14(a). In that earlier section we dealt with inverse propagation from a low velocity, upper half space back to a bottom half space with a high velocity, separated by a single syncline interface. We continue with examples of the same simplicity by (a) changing the syncline shape of the interface to anticline and (b) interchanging the velocities of the upper and lower half space. For these sets of examples we perform all forward modeling (Green's function and plane wave transmission responses) with the same Finite Difference algorithm and necessary input parameters as in section 5.3. The subsequent wave field decomposition and flux normalization is performed according to sections 3.5 and 4.4. Our final example of this section deals with the more complex SEG salt model [2].

The matched filter approach to inverse propagation essentially yields the same result for pressure and flux normalized wave fields: a proper reconstruction of the kinematical aspects of the plane wave source field, see Figures 5.5 and 5.14(b), but the amplitudes are underestimated, see the difference between gray and black lines in Figures 5.7 and 5.14(c). With correction for transmission loss the amplitude mismatch can be removed almost completely. However, inverse propagation from the surface ∂S to the redatuming depth ∂D does not fully require all the mathematics of inverse propagation we developed in the previous chapters; the lack of lateral variations at ∂S and ∂D still allows the straightforward modal decomposition of the Helmholtz operator \hat{H}_2 from Chapter 2.

We return to the configuration displayed in Figure 3.9(a), where we did wave field decomposition on the response of the same plane wave source in the same medium we use here. We performed the decomposition at depth $x_3 = 360$ m, indicated by the horizontal line C, or $\partial \mathbb{D}'$ in Figure 5.14(a). Obviously the medium properties do vary laterally at this depth. Instead of the plane wave source, we now use the up going wave field displayed in Figure 3.9(c) as a reference, see Figures 5.14(d) and 5.14(e). Obviously there is no need for correction between the vertical lines A and B, because there the up going wave field already passed the interface. However, left from A and right from B the up going wave



(a) Configuration, $\partial \mathbb{S}$ at $x_3 = 80$ m, $\partial \mathbb{D}$ at $x_3 = 600$ m, and $\partial \mathbb{D}'$ at $x_3 = 360$ m.



(b) Reconstruction of up going plane wave source at $\partial \mathbb{D}$ without transmission loss correction.



(d) Reconstruction of up going plane wave response at $\partial \mathbb{D}^{'}$ without transmission loss correction.



(c) Amplitude comparisons of plane wave reconstruction at $\partial \mathbb{D}$ for transmission loss correction to order K = 0, 2, 10.



(e) Amplitude comparison of inverse propagation to $\partial \mathbb{D}'$ for transmission loss correction to order K = 0, 10. Note that for K = 10 the inverse propagation and reference almost overlay each other except close to A and B.

Figure 5.14: Inverse propagation in Figure 5.14(a) of a flux normalized wave field, from $\partial \mathbb{S}$ to $\partial \mathbb{D}$. Transmission loss corrections to order K = 0, 10 are displayed by the solid, dashed and dotted lines, respectively. Solid gray represents the "true" result.

field has yet to pass the interface, so there inverse propagation from ∂S back to $\partial D'$ does require transmission loss correction. Except in the vicinities of A and B, the correction property meets those differing needs. The erroneous amplitudes near A and B are unavoidable because the modal decomposition of \hat{H}_2 is less accurate in and around lateral discontinuities, remember section 3.8.

Our second set of examples starts with inverse propagation in the configuration of Figure 5.15(a), an anticline interface separating an upper and lower half space with again the medium parameters given by equations (5.5). The kinematic reconstruction of the plane wave source field is just as good as in the syncline case, and Figure 5.15(b) shows that the improvement of amplitude recovery is even more significant than in the syncline configuration of Figure 5.14(a). Despite the difference in shape between the interfaces in



(a) Configuration focusing up going wave fields, the boundary planes $\partial\mathbb{S}$ and $\partial\mathbb{D}$ lie at depths a = 0.2 km and b = 0.72 km.



5.15(a).

Figure 5.15: In the anticline configuration of Figure 5.15(a) the velocity contrast causes up going wave fields to focus, see the rays emitted from $\partial \mathbb{D}$ to $\partial \mathbb{S}$. Similar to earlier amplitude comparisons, the results of transmission loss correction to order K = 0, 2, 10in Figure 5.15(b) are represented by solid, dotted and dashed lines, respectively. Solid gray represents the original plane wave source.

the configurations of Figures 5.1/5.14(a) on the one hand and 5.15(a) on the other, both

focus the up going wave fields due to the higher velocity in the bottom half space; see the ray fans in both configurations. For point sources away from the aperture limits, the transmission responses end up largely in the same part of the aperture. Not withstanding their high contrast and significant lateral variations, transmission loss corrected inverse propagation performs well in these configurations.

Unfortunately, this performance is not guaranteed. To see how and why, we take the configuration of Figure 5.15(a), but interchange the velocity-values of the top and bottom half space, resulting in Figure 5.16(a). In this configuration up going wave fields experience severe defocusing, in particular for sources below the part of the anticline with a slope of ca 45 degrees. Not only does the transmission response spread over the entire aperture, nearly vertical rays also hit the interface at super-critical angles (for the velocity values given by equation (5.5) the critical angle is only 30 degrees) and do therefore not contribute to the transmission at all. As a result the matched filter approach is therefore not able to give a proper kinematic reconstruction of the source field to begin with, see Figure 5.16(b). Since our transmission loss correction does not affect the kinematics of primary events, it cannot improve the matched filter result where it is most needed, see Figure 5.16(c). This is an important reason why *sub salt* imaging is such a daunting task. The energy incident from above is greatly reduced under downward propagation through a salt body due to the high contrast with their surroundings. If this energy reduction were the only problem, transmission loss correction would be the solution. But under upward propagation, there is also the erratic critical reflection illustrated in Figure 5.16(a).

This is an issue we have to keep in mind when dealing with more complex cases such as the SEG salt model [2]. The velocity-ratio of the salt-body and its surroundings, and hence also the critical angle, is the same as for the examples discussed above, and at numerous places the surface of the bottom of the salt body makes an angle of more than 30 degrees with the horizontal axis; the range $-3 \text{ km} < x_1 < 0 \text{ km}$ does so in particular, see Figure 5.17(a). In addition to setting

$$c_p(x_1, x_3) = c_p(x_1, b),$$

below $\partial \mathbb{D}$, we therefore limit our modeling and inverse propagation efforts to the part of the medium where $x_1 > 0$ km.

Because we used a constant density $\rho = 1500 \text{ kg/m}^3$, the amplitude errors in the matched filter approach are less pronounced than in the previous examples, see Figure 5.17(c). But contrary to the examples of Figures 5.14-5.16, the multiple interfaces in the overburden cause intra bed multiples. In turn the multiples lead to significant artefact in



(a) Configuration defocusing up going wave fields, the boundary planes ∂S and ∂D lie at depths a = 0.2 km and b = 0.72 km.





(b) Reconstruction of up going plane wave source in Figure 5.16(a) without transmission loss correction.

(c) Amplitude comparison for K = 0, 2.

Figure 5.16: In this configuration the velocity contrast causes up going wave fields to diverge, see the rays emitted from $\partial \mathbb{D}$ to $\partial \mathbb{S}$. Due to the low critical angle the plane wave source is poorly reconstructed, both in the kinematic and dynamic sense.

the matched filter reconstruction of the plane wave source, displayed by Figure 5.17(b). Transmission loss correction to order K = 4 selectively suppresses these artefacts and amplifies the reconstruction of the plane wave source, see Figure 5.17(d). But around $x_1 = 1$ km, directly below a steeply dipping part of the salt base, the errors are as severe as in Figure 5.16. As shown by Figure 5.17(e) they remain so even with transmission loss correction to orders as high as K = 25, for the reasons illustrated by Figure 5.16.

5.9 A first example of redatuming

In section 5.8 we argued that sub salt imaging is difficult due to erratic critical reflection related to up going propagation. However, for *salt base* imaging this is not an issue, because we need not consider wave fields propagated below the salt base. As an illustration we repeat the exercise presented earlier in [33] and Figure 2.11 in this thesis, of



(a) Configuration and velocity model. The density was kept constant at $\rho = 1500 \text{ kg/m}^3$.



(b) Inverse propagation from ∂S back to $\partial \mathbb{D}$ without transmission loss correction.



(d) Inverse propagation from ∂S back to ∂D with transmission loss correction to order K = 4.



(c) Amplitude comparison for correction to order K = 0, 1, 4, represented by the solid, dashed, and dotted black lines, respectively.



(e) Amplitude comparison for correction to order K = 10, 25, represented by the solid, and dashed black lines, respectively.

Figure 5.17: Inverse propagation in the SEG salt model. Like before, the gray lines in Figures 5.17(c) and 5.17(e) represent the source field to be reconstructed. In Figures 5.17(b) and 5.17(d) the amplitudes are clipped to 40% of the plane wave source field.

estimating the reflection coefficient of a flat and horizontal interface, which is separated from the sources and receivers at the surface by a second interface. But instead of a flat upper interface we now take an anticline structure, see Figure 5.18(a) for the configuration and Table 5.2 for the medium parameters, and estimate the operator below the top of the anticline at the point A with coordinates (0, 700) in the redatuming plane $\partial \mathbb{D}$.

Figure 5.18(b) shows the result of redatuming the up going reflections at the surface $\partial \mathbb{S}$ down to $\partial \mathbb{D}$ for the source point *A*. No transmission loss correction is applied. The event at t = 0 s and $x_1 = 0$ m is the reflection response of the down going source field of the thought experiment, it corresponds to the $\hat{R}_{\mathbb{L}}^+S^+(b)$ -term in equation (4.29). The anti causal triplication is the anticline reflection whose kinematic propagation effects have been over compensated, it corresponds to the redatuming artefact $\hat{F}_{\mathbb{O}}^-\hat{R}_{\mathbb{O}}^+\hat{F}_{\mathbb{O}}^+$ in equation (4.32). The much weaker causal triplication is the tertiary reflection response of the thought experiment represented by the term $\hat{R}_{\mathbb{L}}^+\hat{R}_{\mathbb{O}}^-\hat{R}_{\mathbb{L}}^+S^+(b)$ in equation (4.29). It is first reflected in the upward direction by the flat interface at $\partial \mathbb{D}$, then down by the anticline, and finally reflected upward once again by the flat interface.

To asses the amplitude behavior we follow De Bruin et al. [15]. After transformation to the horizontal slowness domain of $R_{dat}(b_1, 700; 0, 700)$, we estimate the reflection operator by integrating over all frequencies. Figure 5.18(c) shows the absolute values for various estimates of this reflection operator compared to the true one, represented by the gray line. Without transmission loss correction, the black line, the operator is underestimated and does not reproduce the trend of higher reflection amplitude for higher angles but rather remains constant as a function of p_1 . Transmission loss correction to orders K = 1, 4 removes most of these discrepancies. The remaining discrepancy can only be removed by increasing the aperture.

With this proof of the principle of transmission loss corrected redatuming, we conclude Chapter 5. But a number of issues have to be dealt with before practical application can be considered. Problems common to all amplitude preserving methods are obtaining velocity and density models of the overburden, or source wavelet estimation for deconvolution. Although important for our objective, we will not discuss these two subjects in this thesis, as they are research topics on their own. Two others, related to the specific nature of our method, will receive attention in Chapters 6 and 7.

The redatuming example presented earlier this section aimed at estimating the reflection coefficient corresponding to a flat interface; the choice for this example was motivated by the flat boundaries of the reciprocity theorems underlying the our transmission loss correction, remember equations (4.14) and (5.7). In Chapter 7 we will show how to rewrite the matrix-vector formulation of the wave equation, that is the expressions (1.20a)-(1.23),



(a) Idealized "salt base" configuration, with medium parameters given by Table 5.2. The redatuming plane $\partial \mathbb{D}$ lies at depth $x_3 = 700$ m. $\frac{p_1[\text{s/km}]}{0}$





-0.5

1

 $|\tilde{r}_A^+|$

(b) Redatuming result from Figure 5.18(a) for the source point A. No transmission loss correction was applied.

(c) Absolute value of reflection operator in point A, true (gray) and estimated with transmission loss correction to order K =0 (solid black), K = 1 (dashed) and K =4 (dotted).

0.5

Figure 5.18: Redatuming to the base of a simplified "salt-body".

Layer	Velocity	Density
	(m/s)	(kg/m ³
1	2500	1000
2	4500	1500
3	2300	1500

Table 5.2: Redatuming example medium parameters

such that the theory developed in Chapters 3-5 can also be applied to curved boundaries. But first we will introduce in Chapter 6 a method for estimating the reflection response of the overburden from the full reflection data.

Chapter 6

Toward data-driven redatuming with correction for transmission loss

6.1 Introduction

We went to great lengths to account for internal multiples in our transmission loss correction for inverse propagation through an overburden, that is the medium between the surface and redatuming depth. However modeling useful multiples requires the kind of detailed information we were looking for in the first place. Data-driven approaches for obtaining the transmission and reflection response of the overburden are therefore preferable.

For the (inverse) transmission response possibilities have been raised. These are based on flux/energy balance relations of the type used in section 2.5 and Chapter 5, and as a result they also require the overburden reflection response as input. Herman [46] and Massier et al. [62] proposed a method to estimate the inverse transmission operator by solving a linear system with a Toeplitz structure. More recently Thorbecke and Wapenaar [82] have shown how to obtain the transmission coda of the overburden of a horizontally layered medium through matrix diagonalization. A straightforward multiplication with the primary propagator yields the full transmission response of such an overburden. However, these two methods have not yet matured into readily applicable procedures.

Contrary to the transmission response, the geophysical literature does not yet describe

Layer	Velocity	Density	interface
	(km/s)	(10^3 kg/m^3)	depth (km)
Surface			x _{3,0} =0
1	1	1	
			x _{3,1} =0.2
2	4	1	
			$x_{3,2}=0.4$
3	2	1	0.6
4	1	1	x _{3,3} =0.6
4	1	1	
Redatuming depth			x _{3,4} =0.8
5	3	1	
			$x_{3,5}=1$
6	2	1	
			$x_{3,5}=1.2$
7	1	1	

Table 6.1: Redatuming example medium parameters

a method to obtain the reflection response of the overburden, so we have to develop one here. Manually identifying and separating this subset of reflection measurements is not a realistic option, so we need an automatic procedure. To this end we exploit the fact that the primary reflection response of the overburden plus its lower order multiples are made anti causal by redatuming to depths below the overburden. Of course we cannot use the inverse generalized primary propagators of Chapter 5 for redatuming, because we need the reflection of overburden in the first place to correct for transmission loss. We therefore perform redatuming with inverse primary propagators to make the event mentioned anti causal, because primary propagators are both easier to construct and invert. In the spirit of Chapter 2 we will first present a derivation for a stack of horizontal and homogeneous layers in section 6.2, illustrated with examples based on the layered medium described by Table 6.1. The actual experiment is done with sources and receivers on top of layer 1, the thought experiment has its sources and receivers in layer 4 just above layer 5. In section 6.3 we extend the principle to a stack of layers whose parameters are now allowed to vary in the lateral directions, but still do not vary in the vertical direction inside each layer. This is a reasonable assumption for sufficiently small layer thickness. We will illustrate

the method on configurations similar to the one we used in section 5.9.

In section 6.5 we will estimate the overburden response from a real data set and make a suggestion how to extend the implementations developed sofar for 2D media to 3D media. Section 6.4 serves as a preliminary to this suggestion for the likely case that we need to work with the transmission response based on a macro model. Using a macro model rules out the generation of short period internal multiples due to fine layering.

6.2 Estimation of the overburden reflection response by primary redatuming in a horizontally layered medium

We return to equation (2.55), but in a slightly different formulation; we will now make explicit use of the symmetry between up and down going propagation of flux normalized wave fields by dropping the \pm -superscripts on transmission coefficients and (inverse) propagators;

$$\begin{split} \tilde{\mathfrak{t}}_n &\triangleq \tilde{\mathfrak{t}}_n^{\pm}, \qquad \tilde{w}_n \triangleq \tilde{w}_n^{\pm}, \\ \tilde{W}_n &\triangleq \tilde{W}_n^{\pm}, \qquad \tilde{\mathsf{F}}_n \triangleq \tilde{\mathsf{F}}_n^{\pm}, \end{split}$$

Therefore equation (2.55) now reads

$$\tilde{\mathsf{R}}_{dat,n} = \tilde{\mathsf{F}}_n \tilde{\mathsf{R}}_N^+ \tilde{\mathsf{F}}_n = \tilde{\mathsf{A}}_n + \tilde{\mathsf{R}}_{thght,n}, \qquad (6.1)$$

where

$$\tilde{\mathsf{A}}_n = \tilde{\mathsf{F}}_n \tilde{\mathsf{R}}_{n-1}^+ \tilde{\mathsf{F}}_n$$
 and $\tilde{\mathsf{R}}_{thght,n} = [1 - \tilde{\mathsf{R}}_{n,N}^+ \tilde{\mathsf{E}}_n]^{-1} \tilde{\mathsf{R}}_{n,N}^+$

Redatuming of the total reflection response \tilde{R}_N^+ yields the response of the thought experiment with sources and receivers buried at depth, $\tilde{R}_{thght,n}$, plus artifacts contained in the term \tilde{A}_n . These artifacts present both good and bad news, which is illuminated by a causality analysis of $\tilde{R}_{dat,n}$. This analysis will again be illustrated by redatuming in the medium specified by Table 6.1, so for this situation n in equation (6.1) reads n = 4. Therefore the transmission losses we consider, correspond to the reflection response of the interfaces between the surface and depth $x_{3,4}$.

We start the causality analysis by using equation (2.34) to rewrite equation (6.1) as the



Figure 6.1: Gray line : redatuming artifacts $\tilde{A}_4(\mathbf{k}_H = 0, \tau)$. Black line : thought experiment $\tilde{R}_{thght,4}(\mathbf{k}_H = 0, \tau)$. Both with parameters from table 6.1. The anti causal "travel times" $\{\tau_i\}$ are defined by equation (6.6).

sum of *partial* redatuming results $\tilde{D}_{n,i}$,

$$\tilde{\mathsf{R}}_{dat,n} \triangleq \sum_{i=1}^{N} \tilde{\mathsf{D}}_{n,i},\tag{6.2a}$$

with

$$\tilde{\mathsf{D}}_{n,i} \triangleq \tilde{\mathsf{F}}_n \tilde{W}_i \tilde{\mathsf{r}}_i^+ (1 - \tilde{\mathsf{E}}_i \tilde{\mathsf{r}}_i^+)^{-1} \tilde{W}_i \tilde{\mathsf{F}}_n.$$
(6.2b)

Equation (6.2a) allows the artifacts and thought experiment response to be rewritten as

$$\tilde{A}_n = \sum_{i=1}^{n-1} \tilde{D}_{n,i}$$
 and $\tilde{R}_{thght,n} = \sum_{i=n}^{N} \tilde{D}_{n,i}$

respectively. $\tilde{R}_{thght,n}$ is causal because both constituting components $\tilde{R}_{n,N}^+$ and \tilde{E}_n are, also see Figure 6.1. Determining the temporal behavior of the redatuming artifacts \tilde{A}_n requires more effort, again see Figure 6.1. Although in each term $\tilde{D}_{n,i}$ the product

$$\tilde{\mathfrak{r}}_i^+(1-\tilde{\mathsf{E}}_i\tilde{\mathfrak{r}}_i^+)^{-1}$$

is obviously causal, the temporal behavior of the product $\tilde{F}_n \tilde{W}_i$ is less obvious. This can be resolved by making the definitions in section 2.4 of the generalized primary propagators more explicit. With repeated substitution of the recursive expression (2.32), the



Figure 6.2: Black : $\tilde{F}_4(\mathbf{k}_H = 0, \tau)$. Gray : $\tilde{W}_4(\mathbf{k}_H = 0, \tau)$. Again see table 6.1 for medium parameters.

definition of generalized down going propagation by equation (2.23) can be replaced with

$$\tilde{\mathcal{M}}_{j} \triangleq \tilde{\mathfrak{t}}_{j} \left(1 - \tilde{\mathsf{E}}_{j} \tilde{\mathfrak{r}}_{j}^{+}\right)^{-1}, \quad \text{and} \quad \tilde{\mathcal{W}}_{n} = \tilde{w}_{n} \prod_{j=1}^{n-1} \tilde{\mathcal{M}}_{j} \tilde{w}_{j}.$$
 (6.3a)

See Figure 6.2 for $\tilde{W}_4(\mathbf{k}_H = 0, \tau)$ constructed with the parameters of table 6.1. The factor \tilde{M}_j represents the intra bed multiples related to the interface at depth $x_{3,j}$ and is related to the coda, but is not its equal. The inverse generalized primary propagator for down going wave fields can be factorized in the same fashion

$$\tilde{\mathsf{M}}_{j}^{-1} \triangleq \left(1 - \tilde{\mathsf{E}}_{j}\tilde{\mathsf{r}}_{j}^{+}\right)\tilde{\mathsf{t}}_{j}^{-1} \quad \text{and} \quad \tilde{\mathsf{F}}_{n} = \prod_{j=1}^{n-1} \left[\tilde{w}_{j}^{*}\tilde{\mathsf{M}}_{j}^{-1}\right]\tilde{w}_{n}^{*}, \quad (6.3b)$$

also see Figure 6.2 for $\tilde{F}_4(\mathbf{k}_H = 0, \tau)$. As was the case throughout Chapter 2, equation (6.3b) is only valid for propagating waves. In equation (6.2b) for i < n, equations (6.3a) and (6.3b) let the products of forward and inverse propagators reduce to

$$\tilde{\mathsf{F}}_n \tilde{\mathsf{W}}_i = \tilde{\mathsf{W}}_i \tilde{\mathsf{F}}_n = \prod_{j=i}^{n-1} \tilde{\mathsf{M}}_j^{-1} \tilde{\mathsf{w}}_{j+1}^*.$$

The partial redatuming result $\tilde{D}_{n,n-1}$ now reads

$$\tilde{\mathsf{D}}_{n,n-1} = \left(1 - \tilde{\mathsf{E}}_{n-1}\tilde{\mathsf{r}}_{n-1}^+\right)\tilde{\mathsf{r}}_{n-1}^+\tilde{\mathsf{t}}_{n-1}^{-2}(\tilde{w}_n^*)^2.$$
(6.4)

The homogeneous propagator \tilde{w}_n is causal, and implies a shift

$$\delta \tau_{n-1} = c_n / (x_{3,n} - x_{3,n-1}) > 0$$

to positive time. Its complex conjugate \tilde{w}_n^* in equation (6.4) is necessarily anti causal, and implies a shift $-\delta \tau_{n-1}$ back in time. After redatuming, the event corresponding to the primary reflection from the interface at depth $x_{3,n-1}$, the event corresponding to the first term for $\mathbf{k}_H = 0$ in equation (6.4), is therefore shifted to $\tau = -2\delta \tau_{n-1}$. The events corresponding to the second, multiple related term are in the interval $(-2\delta \tau_{n-1}, \infty)$ and are therefore mixed with the response of the causal thought experiment. However, being intra bed multiples of increasing order, their amplitudes decrease with time.

In case i < n - 1 the partial redatuming result $D_{n,i}$ reads

$$\tilde{\mathsf{D}}_{n,i} = \left(1 - \tilde{\mathsf{E}}_i \tilde{\mathsf{r}}_i^+\right) \tilde{\mathsf{r}}_i^+ \tilde{\mathsf{t}}_i^{-2} \left[\tilde{w}_{i+1}^* \prod_{j=i+1}^{n-1} \tilde{\mathsf{M}}_j^{-1} \tilde{w}_{j+1}^*\right]^2.$$
(6.5)

Similar to equation (6.4) for the (i = n - 1)-case, it is the purpose of this rather lengthy expression to point out that in the (i < n - 1)-case the event corresponding to the $x_{3,i}$ -primary is shifted to

$$\tau_i = -2\sum_{j=i}^{n-1} \delta \tau_j < 0, \tag{6.6}$$

while the events corresponding to the remaining, multiple related terms are shifted to the interval (τ_i, ∞) , see Figure 6.1. The conclusion is that when redatuming to depth $x_{3,n}$ all primary reflections from the interfaces above $x_{3,i}$, become completely anti causal in the time domain, whereas the primary reflections from depth $x_{3,n}$ and below remain causal. Furthermore the lower order multiples also become anti causal, although the extent to which decreases with increasing $x_{3,i}$; the higher order multiples remain causal and are mixed with $\tilde{R}_{thght,n}$.

The bad news mentioned earlier this section is that the \tilde{R}_{n-1}^+ -multiples still extend to causal times after redatuming and can therefore not be distinguished from $\tilde{R}_{thght,n}$ in $\tilde{R}_{dat,n}$ by a causality analysis. The closely related good news is that all events in $\tilde{R}_{dat,n}$



Figure 6.3: Gray line : directly modeled $-\tilde{R}_3^+(\mathbf{k}_H = 0, \tau)$. Black line : estimate $\tilde{R}_{est,3}^+(\mathbf{k}_H = 0, \tau)$ based on primary redatuming. See table 6.1 for medium parameters.

corresponding to \tilde{R}_{n-1}^+ -primaries are anti-causal, and that the anti-causal times only harbor \tilde{R}_{n-1}^+ -related events; the events corresponding to reflections from below $x_{3,n}$ are exclusively causal. After muting the causal events in the time-domain representation of $\tilde{R}_{dat,n}$, we can therefore isolate the primary events in \tilde{R}_{n-1}^+ , by restoring the propagation effects.

If one would need the inverse generalized primary propagators to make the primary reflections in \tilde{R}_{n-1}^+ anti causal, this property would not be useful for estimating \tilde{R}_{n-1}^+ because then \tilde{R}_{n-1}^+ would be needed to estimate itself. Fortunately the same effect can also be achieved by primary redatuming, that is by replacing \tilde{F}_n in equation (6.2) by the inverse *primary* propagators $\tilde{F}_{p,n}$, defined by

$$\tilde{W}_{p,n} = \prod_{k=1}^{n} \tilde{w}_k,
= \tilde{w}_n \tilde{W}_{p,n-1},$$
(6.7)

$$\tilde{\mathsf{F}}_{p,n} \triangleq \tilde{W}_{p,n}^{-1} = \prod_{k=1}^{n} \tilde{w}_{k}^{*}$$
 again for $|\mathbf{k}_{H}| \le \omega/c.$ (6.8)

The laterally varying analogs of $\tilde{W}_{p,n}$ are easier to construct and invert, than the analogs of the generalized primary propagator \tilde{W}_n .

In equation (6.3b), (6.5), and intermediate steps, a transition from inverse generalized primary propagation to inverse primary propagation comes down to letting $\tilde{M}_i^{-1} \rightarrow 1$.
Thus estimating \tilde{R}_{n-1}^+ from \tilde{R}_N^+ by primary redatuming can be expressed by the following three consecutive steps. The first one is primary redatuming

$$\tilde{R}_{dat,p} \triangleq \tilde{\mathsf{F}}_{p,n} \tilde{\mathsf{R}}_N^+ \tilde{\mathsf{F}}_{p,n}.$$
(6.9a)

The second step is represented by

$$B(\tau) \triangleq \hat{\mathcal{F}}^{-1} \big[\tilde{\mathbf{s}}_{Rick} \tilde{R}_{dat,p} \big] (\tau) h(-\tau), \tag{6.9b}$$

where $\hat{\mathcal{F}}$ is the temporal Fourier transform, $\tilde{s}_{Rick} = \tilde{s}_{Rick}(\omega)$ the Fourier transform of a Ricker wavelet and $h(\tau)$ is (a smooth approximation of) the Heaviside step function, Abramowitz and Stegun [1]. Then multiplication by $h(-\tau)$, which equals 0 for positive τ and 1 for negative τ , clearly mutes causal events. This muting operation should not be applied directly, because band-limited approximations of delta-functions have a rather long extent in time; even if the peak of an event occurs at negative times it can still extend to positive times. The preceding convolution with the Ricker wavelet serves to narrow down the extent in time of events. Finally, transformation back to the frequency-domain and subsequent deconvolution for the Ricker wavelet results in the estimated overburden response

$$\tilde{\mathsf{R}}_{est,n-1}^{+} \triangleq \tilde{W}_{p,n} \tilde{s}_{Rick}^{-1} \hat{\mathcal{F}}[B](\omega) \tilde{W}_{p,n}.$$
(6.9c)

Just as equation (6.8), equation (6.9) is only valid for subcritical events. In Figure 6.3 we compare the time domain representations of $-\tilde{R}_3^+$ and $\tilde{R}_{est,3}^+$.

6.3 Estimation of the overburden reflection response by primary redatuming in a laterally varying medium

In this section we extend the application of equation (6.9) to a stack of horizontal layers, whose parameters are now allowed to vary in the lateral direction. First we are going to construct the primary propagators for such a medium. Then we discuss under which conditions the conclusions of the causality analysis in section 6.2 remain valid for laterally varying media and illustrate these conditions with some simple examples.

The continuum representation of Chapter 4 is not suitable for the type of causality analysis presented in section 6.2. We will therefore use the fact that Fishman and McCoy

[28] have derived expressions of the same form as equations (2.28), (2.30), (2.32), and (2.34), but then for layers whose characteristics only need to be independent of depth. For such a layer the flux normalized one-way operator defined by equation (3.28b) reduces to $\hat{\mathbf{B}} = \hat{\mathbf{A}}_f$. Hence, the one-way wave equation (3.28a) reduces to

$$\partial_3 \mathsf{P}^{\pm}(x_3) = \mp j \hat{\mathsf{H}}_1(x_3) \mathsf{P}^{\pm}(x_3).$$

After the completely homogeneous case described in section 2.2, we denote by \hat{w}^{\pm} propagators in the vertical direction for layers whose characteristics do not vary depth with depth in the interval $x_{3,0} < x_{3,1}$. Given the initial condition $\hat{w}^+(x_{3,0}; x_{3,0}) = I$, a Taylor expansion of $\hat{w}^+(x_{3,1}; x_{3,0})$ in terms of the difference $(x_{3,1} - x_{3,0})$ can thus be expressed as

$$\hat{w}^{+}(x_{3,1};x_{3,0}) = \sum_{k=0}^{\infty} \frac{(x_{3,1} - x_{3,0})^k}{k!} [-j\hat{H}_1(x_{3,0})]^k.$$
(6.10a)

After Grimbergen [41] we express equation (6.10a) symbolically as

$$\hat{w}^+(x_{3,1};x_{3,0}) \triangleq \exp[-j(x_{3,1}-x_{3,0})\hat{H}_1(x_{3,0})].$$
 (6.10b)

Expressions similar to (6.10) can be derived for the up going $\hat{w}^{-}(a; b)$, which is equal to the transposed $\{\hat{w}^{+}(b; a)\}^{t}$ on account of section 4.3.2.

To describe primary propagation in an overburden with both vertical and lateral variations, we assume that we can represent the overburden by a stack of horizontal layers, with lateral variations but none in the depth-direction, separated by interfaces at depths $x_{3,1} < \ldots < x_{3,n-1}$. If we restrict ourselves to the usual rectangular coordinates, this assumption can limit the applicability; both equations (6.11) and the expressions derived by Fishman and McCoy are based on Ψ DO's, which can only be constructed accurately if the lateral variations in the medium parameters are smooth, also see section 3.8. There are two possible approaches to avoid the distortions resulting from discontinuous variations:

- I apply a smoothing operator to the medium parameters before diagonalizing \hat{H}_2 ,
- II or use a discontinuity aligned, curvilinear coordinate system of the kind discussed in section 7.3.

For the examples in this thesis we take approach I.

After equation (6.7) we define the operators for up and down going primary propaga-



(b) Absolute value of reflection operator in point A, for the dashed line the anticline reflection response estimated by primary redatuming in a *discontinuous* medium was used.

0.5

0

(c) Absolute value of reflection operator in point A, for the dashed line the anti-

in point A, for the dashed line the anticline reflection response estimated by primary redatuming in a *smoothed* medium was used.

Figure 6.4: In Figures 6.4(b) and 6.4(c) the gray line corresponds to the true reflection coefficient, dotted and dashed lines to redatuming with fourth-order transmission loss correction, the black lines to redatuming without transmission loss correction. The dotted lines in both Figures are the same and used the FD-modeled anticline reflection response for the correction, see the captions of Figures 6.4(b) and 6.4(c) for the meanings of the dashed lines.

tion between depths $x_{3,0} < x_{3,1}$ and $x_{3,n} > x_{3,n-1}$ by the recursive expressions

$$\hat{W}_{p}^{-}(x_{3,0};x_{3,j}) = \hat{W}_{p}^{-}(x_{3,0};x_{3,j-1})\hat{w}^{-}(x_{3,j-1};x_{3,j}),$$
(6.11a)

and
$$\hat{W}_{p}^{+}(x_{3,j};x_{3,0}) = \hat{w}^{+}(x_{3,j};x_{3,j-1})\hat{W}_{p}^{+}(x_{3,j-1};x_{3,0}),$$
 (6.11b)

with $j \leq n$. Note that by construction the primary propagators \hat{W}_p^{\pm} inherit the source receiver reciprocity of the single layer propagators \hat{w}^{\pm} . To estimate reflection response of the overburden we will exploit the fact that if we neglect the evanescent modes of the square root operator \hat{H}_1 , then the primary propagators defined by equations (6.11b) and (6.11a) have inverses

$$\hat{\mathsf{F}}_{p}^{+}(x_{3,0};x_{3,j}) \approx \{\hat{W}_{p}^{+}(x_{3,j};x_{3,0})\}^{\dagger}$$
 (6.12a)

and
$$\hat{\mathsf{F}}_{p}^{-}(x_{3,j};x_{3,0}) \approx \{\hat{W}_{p}^{-}(x_{3,0};x_{3,j})\}^{\dagger}.$$
 (6.12b)

As a first example we take the medium shown in Figure 6.4(a). The medium parameters are those of Table 5.2, but the slope of the "anticline" is much less than in Figure 5.18(a). We perform primary redatuming according to section 6.2, and use the resulting estimate of the reflection response of the overburden for subsequent (full wave field) redatuming with transmission loss correction. We constructed two primary propagators: for the first the square root operators were constructed via a modal decomposition based on the discontinuous medium parameters, and for the second the modal decomposition was based on smoothed medium parameters.

We used both to estimate the overburden reflection response and used both redatuming to $\partial \mathbb{D}$ with fourth order transmission loss correction. To verify accuracy, we estimated the reflection coefficient of point A at $\partial \mathbb{D}$ from these redatuming results and plotted the absolute values as the dashed lines in Figures 6.4(b) and 6.4(c). The dashed line in Figure 6.4(b) corresponds to transmission loss correction with the overburden reflection response estimated through primary redatuming in the medium between $\partial \mathbb{D}$ and ∂S . A smoothed version of the same medium was used to estimate the overburden reflection response used for transmission loss correction in 6.4(c). Clearly both estimates display the right trend. However transmission loss correction based on the smoothed medium performs slightly better than the one based the discontinuous medium.

As a second example of isolating the primary reflection response of the overburden by primary redatuming from the reflection data, we reconsider the redatuming example discussed in section 5.9. The redatuming result obtained with transmission loss correction based on the overburden response estimated by primary redatuming, is shown in Figure





(a) For the dashed line the anticline reflection response estimated by primary redatuming in *discontinuous* medium was used.

(b) For the dashed line the anticline reflection response estimated by primary redatuming in *smoothed* medium was used.

6.5(a). Although angle dependence of the reflection coefficient is recovered in a qualitative way, it is severely underestimated for all angles; for normal incidence it is hardly affected by transision loss correction. Besides violating the smoothness condition for Ψ DO's, this underestimation is also due to neglection of multiple scattering by applying equation (6.10a). This multiple scattering occurs despite the fact that the overburden in Figure 5.18(a) only consists of a single anticline interface.

For example the reflection ray-path SCC' corresponds to transmission ray-path SBCA'; although the former is a primary reflection, the latter arrives at the redatuming level $\partial \mathbb{D}$ through multiple scattering via transmission at B and subsequent reflection at C. If we represent the medium by a stack of thin layers slicing through the anticline interface and model primary propagation by equations (6.11) to a depth below point C, say A', then the ray path SBCA' will not be included. In case of an overburden with high dipping angles in general and syncline/anticline interfaces in particular, the primary propagators constructed from equations (6.10)-(6.12) should therefore be applied with caution.

Figure 6.5: In Figures 6.5(a) and 6.5(b) the gray line corresponds to the true reflection coefficient in point A of Figure 6.6(a), dotted and dashed lines to estimates based on redatuming with fourth-order transmission loss correction, the black lines to redatuming without transmission loss correction. The dotted lines in both Figures are the same and used the FD-modeled anticline reflection response for the correction, see the captions of Figures 6.5(a) and 6.5(b) for the dashed lines.



(a) Ray-paths of single interface multiple scattering, for $c_1 = 2.5$ km/s and $c_2 = 4.5$ km/s.



(b) Anticline reflection response due to a point source at *S*, modeled with Finite difference.



(c) Anticline reflection response due to a source at S, estimated via primary redatuming.

Figure 6.6: Single interface multiple scattering and its effect on primary redatuming, illustrated on an anticline configuration.

6.4 Transmission loss correction on an inverse propagator without internal multiples

In sections 6.2 and 6.3 we proposed a data-driven method for estimating the overburden reflection response to avoid the requirement of detailed velocity and density models in order to obtain useful internal multiples. Ideally we employ an equally data-driven method to construct the transmission response of the overburden. Unfortunately the methods mentioned in the introduction to this chapter were not (yet) ready for our approach to redatuming when this thesis was nearing completion. This section therefore considers the following question. Suppose we just have a macro model, without the fine layering necessary to generate (all) the multiples, and use it to construct the transmission response of the overburden. Then what will be the effect of transmission loss correction with a reflection response containing the multiples ?

We return to the horizontally layered medium with redatuming configuration defined by Table 6.1 and take the primary event in \tilde{W}_4 as the transmission response resulting from a "macro" model of this configuration. To this end we focus on the product $\tilde{I} = \tilde{F}_4 \tilde{W}_4$ in equation (6.2b), or rather on the convergence behavior of its approximation $\tilde{I}^{(K)} = \tilde{F}_4^{(K)} \tilde{W}_4$, employing equation (2.46a) for $\tilde{F}_4^{(K)}$. The correlations of \tilde{W}_4 and \tilde{R}_3^+ ,

$$\tilde{C} = \tilde{R}_3^{+,*}\tilde{R}_3^+$$
 and $\tilde{I}^{(0)} = \tilde{W}_4^*\tilde{W}_4$,

allow a recursive expression of $\tilde{I}^{(K)}$

$$\tilde{\mathbf{I}}^{(K)} = \tilde{\mathbf{C}}\tilde{\mathbf{I}}^{(K-1)} + \tilde{\mathbf{I}}^{(0)}, \text{ for } K \ge 1.$$

The time-domain representation of $\tilde{I}^{(K)}$ converges to a single pulse of height 1 at $\tau = 0$, that is the gray traces displayed in Figures 6.7(a)-6.7(d). The corresponding black traces arise from a closely related series in which we neglect the multiples in the generalized primary propagator, that is $\tilde{M}_j \rightarrow \tilde{t}_j$ in (6.3a). Note that we can only make this neglection in the modeled propagator, not in the data. Instead of $\tilde{I}^{(0)}$, we now initiate the sequence with

$$\widetilde{\mathrm{I}}_{p}^{(0)} = (\widetilde{\mathrm{t}}_{1}\widetilde{\mathrm{t}}_{2}\widetilde{\mathrm{t}}_{3}\widetilde{W}_{p,4})^{*}\widetilde{W}_{4},$$



Figure 6.7: Source pulse reconstructions. Black line : \tilde{I}_p^k without multiples in inverse propagator, gray line : $-\tilde{I}^k$ with multiples in inverse propagator.

so that the gray traces in Figures 6.7(a)-6.7(d) are the time domain representation of the iterates

$$\tilde{\mathbf{I}}_{p}^{(K)} = \tilde{C}\tilde{\mathbf{I}}_{p}^{(K-1)} + \tilde{\mathbf{I}}_{p}^{0}.$$
(6.13)

Equation (6.13) describes the effect of transmission loss correction applied to an inverse propagator with erroneously missing internal multiples but with the correct primary amplitude. For $K \to \infty$, $\tilde{I}_p^{(K)}$ converges to a single pulse of height 1 at $\tau = 0$, although the multiples do not converge to zero, see the black traces in Figures 6.7(a)-6.7(d). This means that the amplitude behavior of a target reflector, is the same with or without the multiples in the inverse propagator, as long as the primary amplitude is correct. In section 6.5 we will use this observation as a possible criterion for amplitude balancing.

6.5 Toward data-driven redatuming with correction for transmission loss

Before a real data set can undergo the one-way redatuming processes described in this thesis, either with the inverse of primary propagators of the sections 6.2 and 6.3 or the inverse of the generalized primary propagators of Chapters 4 and 5, a number of processing steps has to be applied. The two major ones are interpolation or regularization to a square grid of equidistant sources and receivers and removal of free surface multiples. Berkhout and Verschuur [8] describe a theoretical description of the removal procedure, while Verschuur and Prein [84] discuss a few case studies.

We need to apply this removal to make a useful estimate of the overburden response, because in section 5.5 we did not include free surface multiples in the flux-balance underlying our transmission loss correction. The iterative transmission loss correction derived from this balance, will otherwise diverge due to the spurious multiple energy still present in the cross-correlation C.

Layer	Velocity	interface
	(km/s)	depth (km)
		0
1	1.47	
		1.25
2	1.45	
		1.35
3	1.82	1.55
	0.1	1.55
4	2.1	1 71
	2.2	1./1
5	2.3	

By courtesy of the former Saga Petroleum A.S., now part of Norsk Hydro, we ob-

Table 6.2: Macro velocity model

tained a 2D marine data set from the Voring area in the North Sea. After the free surface multiples were removed (many thanks to Eric Verschuur !), we estimated a horizontally layered macro velocity model with Dix' equation. The resulting velocities and interface depths are listed in Table 6.2. From the full data set we selected a fixed spread geometry with sources and receivers in the interval 5 km $\leq x_1 \leq 9.6$ km; Figure 6.8 shows the shot record for the source-position $x_1 = 7.5$ km. Using the velocities of Table 6.2 we performed primary redatuming to depth $x_3 = 1.7$ km, see Figure 6.9. After muting the

causal parts we restored the primary propagation effects so that at $x_1 = 7.5$ km we obtain the overburden response represented by Figure 6.10. The kinematic behavior of the events in Figure 6.10 clearly matches that of the corresponding events in Figure 6.8. For an amplitude comparison in Figure 6.11 we took the zero offset traces from both shot records and laid the estimated overburden response (dotted black) on top of the full original (solid gray). Up to t = 2.3 s the amplitudes are identical, afterward the response from below the overburden is reduced to low noise levels. Due to the pre-mute convolution with the Ricker wavelet, remember equation (6.9b), the reflections from directly below the overburden also partly transform into anti causal events in Figure 6.9 so, they are still present as a small residue in the estimated overburden response in Figure 6.10.

For 3D reflection data it need not be necessary to construct 3D primary propagators, because one can still use 2D primary propagators to estimate the overburden reflection response and still preserve the amplitudes, while avoiding the computational burden of applying and constructing 3D primary propagators. Although inverse 2D primary propagators cannot properly undo the dynamics of 3D data, we mute events based only on their kinematic properties. Afterward we apply the 2D primary propagators and this precisely undoes the effects of redatuming for the still remaining events. In the terminology of section 4.5 we have estimated $\hat{R}^+(0;0|b = 1.7 \text{ km})$ from $\hat{R}^+(0;0|\infty)$. In Figure 6.12 we show a space-time panel corresponding to a single column of the cross correlation $\hat{C}(0;0|b = 1.7 \text{ km}) = \hat{R}^{+,\dagger}\hat{R}^+$ based on this estimate. This cross correlation should be used to construct the inverse propagators

$$\{\hat{\mathsf{F}}^+(b;0)\}^t = \hat{\mathsf{F}}^+(0;b) = (\hat{\mathsf{I}} - \hat{\mathsf{C}})^{-1}\{\hat{\mathsf{T}}^+(b;0)\}^\dagger \quad (\text{with } b = 1.7 \text{ km}), \tag{6.14}$$

through a Neumann expansion of the correction factor $(\hat{I} - \hat{C})^{-1}$. Unlike primary redatuming, full wave redatuming of real 3D data requires both the kinematic and dynamic 3D propagation effects in the data need to be undone. So for a meaningful assessment of the amplitude behavior of the redatuming result, we need 3D propagation effects in the transmission response $\hat{T}^+(b = 1.7 \text{ km}; 0)$ in equation (6.14). This raises two related questions.

To model \hat{T}^+ we should ideally use a data driven method, like one of those mentioned in the introductory section 6.1. For want of those we will have to work with a macro model based transmission response, which lacks internal multiples. In section 6.4 we showed that in principle it is possible to preserve amplitude information in the redatuming result for t = 0, provided that the primary amplitudes of the modeled transmission response are correct. Of course one cannot expect correct amplitudes from modeling the transmission response in a macro model. One possible solution is scaling the modeled transmission response such that together with the estimated reflection response of the overburden, it satisfies the balance relation (5.10). A second possibility is to look for the maximum scaling such that the sequence resulting from the iterative expression (5.15a),

 $\hat{\mathsf{F}}^{+,(0)}, \hat{\mathsf{F}}^{+,(1)}, \dots, \hat{\mathsf{F}}^{+,(k)},$

still converges. Such tests need not be done for each frequency, a small subset should be sufficient. Actually performing the tests is left as future work.



Figure 6.8: Single shot from Voring area in the North Sea for a source at $x_1 = 7.5$ km. Free surface multiples removed, and flux normalized.



Figure 6.9: Voring data primary redatumed to depth $x_3 = 1.7$ km, again for a source at $x_1 = 7.5$ km.



Figure 6.10: Voring overburden reflection for a source at $x_1 = 7.5$ km, estimated by zeroing causal part of the primary redatuming result and (primary) propagated back to the surface.



Figure 6.11: Amplitude comparison of zero offset traces in full data from Figure 6.8 (gray), and overburden reflection estimated by primary redatuming from Figure 6.10 (dashed).

Figure 6.12: Cross correlation of the estimated overburden reflection for source at $x_1 = 7.5$ km.

8

Chapter 7

Directional decomposition in the direction normal to a curved interface

7.1 Introduction

Haines et al. [42, 43, 44, 49] have developed a framework¹ for accurate one-way wave field modeling, which does not employ the standard Cartesian coordinate system, but rather a coordinate system in which one of the coordinates is constant along the major discontinuities in the medium parameters. Such coordinate systems are called curvilinear and were first used in solid mechanics, for the description of deformation of solids under stress. Later, the mathematics developed for this application was also for used general relativity theory and fluid dynamics. We use Fung [35] as a reference to curvilinear coordinates and the closely related tensor-calculus, but other books can serve as a reference equally well, for example the more recent work by Farrashkhalvat and Miles [26].

This chapter will show how to make acoustic one-way wave fields resulting from algorithms suitable for the one-way reciprocity theorems of the type defined in sections 4.3.1 and 5.4. This is a nontrivial task because curvilinear coordinates require one to work with base vectors whose length and direction must be allowed to vary with position. In section 7.2 we therefore give a short review of aspects of curvilinear coordinates and tensor

¹Implementations exist for acoustic and elastic wave propagation, but sofar only the isotropic case has been dealt. Nonetheless anisotropic and even poroelastic wave propagation can be modeled along the same lines.

analysis. This review does provide a rigorous introduction, but aims to familiarize the unacquainted reader with the concepts and manipulations deployed in sections 7.3 and 7.4. In section 7.3 we introduce two particular types of curvilinear coordinates: first the one used by Haines et al. [43, 44, 49] and second the socal led semi-orthogonal curvilinear coordinates, used recently by Sava and Fomel [74] in the context of Riemannian wave field extrapolation. The former is necessary for a generalization of invariant imbedding to media with curved interfaces. However, it cannot produce explicit expressions for wave field decomposition and resulting reciprocity theorems suitable for implementation on a computer. The underlying problem is essentially the same as for elastic wave field decomposition: for the curvilinear coordinates chosen by Haines et al, the analog of the matrix \hat{A} in equation (3.17) has nonzero diagonal elements.

In sections 7.4 and 7.5 we show that (a) in terms of semi-orthogonal coordinates the anti-diagonal structure of \hat{A} is conserved, and that (b) one element is proportional to the density while the other is a self-adjoint, Helmholtz-type operator. These conditions do allow expressions suitable for computer-implementation, and the concepts and ideas introduced in Chapters 4, 5, and 6 can thus be extended to curved boundaries.

7.2 An overview of curvilinear coordinates and tensor analysis

In section 3.8 we illustrated that Ψ DO's behave poorly, if the functions from which they are constructed, depend discontinuously on the lateral coordinates. One can avoid these discontinuous dependencies in a curvilinear coordinate system, where one coordinate is taken constant along discontinuities in the medium parameters. But the use of such coordinates requires tensor analysis and its intrinsic complexity.

The metric tensor, one of the cornerstones of tensor-calculus, is a 3×3 unit matrix in the standard Cartesian coordinate system for three-dimensional space. This trivial structure of the metric tensor is responsible for the relatively simple Cartesian representations of the gradient- and divergence operators. For example the gradient of the pressure P and the divergence of the particle velocity \mathbf{V} are

$$\nabla P = \mathbf{i}_k \partial_k P, \tag{7.1a}$$

$$\nabla \cdot \mathbf{V} = \partial_k V_k. \tag{7.1b}$$

We denote Cartesian unit vectors by $\{i_k\}$ for k = 1, 2, 3 and sum over the repeated index k, unless the contrary is stated explicitly. A combination of the divergence and gradient is the Laplacian; its action on the pressure is given by

$$\nabla \cdot \nabla p = \partial_k \partial_k p. \tag{7.1c}$$

On several occasions we just consider the lateral indices 1, 2, which we will indicate by the use of Greek indices α , β instead. For these Greek indices we will also use the summation convention introduced above, again unless the contrary is stated explicitly.

Each of the three terms on the right hand side of the expressions (7.1) corresponds to a nonzero component of the metric tensor for Cartesian coordinates. For general curvilinear coordinates all components become position dependent, so the diagonal components of the metric tensor deviate from unity and the off-diagonal components can also deviate from zero. Just as in the Cartesian case described by equations (7.1), the differential operators for curvilinear coordinates contain one term for each nonzero component of the corresponding metric tensor, which can amount to $3 \times 3 = 9$ in the most general case; see Fung [35] for a detailed description. In the remainder of this section we will just describe the elements of tensor-analysis relevant for our application.

We consider a volume \mathbb{V} with the usual Cartesian coordinates $\mathbf{x} = (x_1, x_2, x_3)$ assigned to each point in \mathbb{V} . In addition to \mathbf{x} we will also consider an alternative set of curvilinear coordinates $\{y_1, y_2, y_3\}$. We assume there is a one-to-one and reversible mapping between these coordinates,

$$y_j = y_j(x_1, x_2, x_3)$$
 and $x_i = x_i(y_1, y_2, y_3)$, for $i, j = \{1, 2, 3\}$.
(7.2)

These assumptions are fulfilled if the mappings are single-valued, continuous, have continuous first partial derivatives and if finally the determinant of the matrix of partial derivatives, also-called the Jacobian matrix, is nonzero² everywhere in \mathbb{V} . The explicit statement of this last condition is that for the Jacobian matrix

$$\frac{\partial \mathbf{x}}{\partial \mathbf{y}} \triangleq (\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3), \quad \text{with column-vectors} \quad \mathbf{g}_i = \frac{\partial x_k}{\partial y_i} \mathbf{i}_k, \quad (7.3)$$

²A transformation to ray-coordinates is an example of a mapping that does not meet these requirements. In caustic points two distinct triplets of ray coordinates can be mapped to a single point (x_1, x_2, x_3) , while socal led shadow zones are not covered at all by ray-coordinates.

the determinant obeys $det(\partial \mathbf{x}/\partial \mathbf{y}) \neq 0$ everywhere in \mathbb{V} . For a geometric interpretation of equation (7.3) keep two of the curvilinear coordinates constant and only vary the remaining curvilinear coordinate. In case of fixed y_2 and y_3 , the left column of $\partial \mathbf{x}/\partial \mathbf{y}$ is the tangential direction of the curve parameterized by y_1 ; the other two columns have similar interpretations. Any spatial direction can be represented by a linear combination of the three vectors \mathbf{g}_i . They can therefore be used as base vectors, although they are not mutually orthogonal in general. It follows from the geometric interpretation of \mathbf{g}_i that the direction normal to surfaces of constant y_3 is parallel to the cross-product

$$\mathbf{n} = \mathbf{g}_1 \times \mathbf{g}_2. \tag{7.4}$$

In the remainder of this chapter this direction **n** will play the same part as the 3-direction did in the other chapters.

The total wave field is completely determined by the pressure and the particle velocity in this normal direction **n**. The latter is proportional to

$$V^n \triangleq \mathbf{n}^t \mathbf{V}; \tag{7.5}$$

note that V^n differs from the particle velocity in the normal direction by a factor $|\mathbf{n}|$, the length of the normal vector \mathbf{n} . It turns out that V^n is a more convenient quantity for the definition of reciprocity theorems for flux normalized wave fields, than the actual particle velocity in the direction of \mathbf{n} . This definition is based on integrals of the acoustic Poynting vector $P\mathbf{V}$ over a surface of constant y_3 ; these are given by

$$\int_{y_3=a} P\mathbf{V} \cdot d^2 \mathbf{S} = \int_{y_3=a} P\mathbf{V} \cdot (\mathbf{g}_1 \times \mathbf{g}_2) dy_1 dy_2 = \int_{y_3=a} PV^n dy_1 dy_2.$$
(7.6)

We will also work with the inverse Jacobian matrix,

$$\begin{aligned} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} &\triangleq \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)^{-1}, \\ &= (\mathbf{g}^1, \mathbf{g}^2, \mathbf{g}^3)^t, \qquad \text{with column-vectors} \qquad \mathbf{g}^j = \frac{\partial y_j}{\partial x_k} \mathbf{i}^k. \end{aligned} (7.7)$$

where $\mathbf{i}^k \triangleq \mathbf{i}_k$. The vectors \mathbf{g}^j can also be used as base vectors, and they are neither mutually orthogonal in general. Their geometrical interpretation is closely related to that

of the columns of the Jacobian $\partial \mathbf{x} / \partial \mathbf{y}$, yet not the same. If one expands the identity

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \ \frac{\partial \mathbf{x}}{\partial \mathbf{y}} = \mathbf{I}$$

through equations (7.3) and (7.7), then it is straightforward to see that

$$\mathbf{g}^j \cdot \mathbf{g}_i = \delta_{ji}.\tag{7.8}$$

Clearly \mathbf{g}^3 is orthogonal to \mathbf{g}_1 and \mathbf{g}_2 , and similar orthogonality relations hold for the other rows of $\partial \mathbf{y} / \partial \mathbf{x}$ and columns of $\partial \mathbf{x} / \partial \mathbf{y}$. The normal direction \mathbf{n} is therefore parallel to \mathbf{g}^3 . However, in the light of equation (7.6), \mathbf{n} is more convenient than \mathbf{g}^3 to extend the wave equation in the form of (1.21) to curvilinear coordinates.

The conventions to distinguish between the two sets of base vectors, differ from one field to another. Here we will use the one from experimental physics and engineering; \mathbf{g}_i derived from equation (7.3) are simply called base-vectors, while \mathbf{g}^j derived from (7.7) are called reciprocal base vectors. In the special cases that the base-vectors are mutually orthogonal at all points in \mathbb{V} , the pairs \mathbf{g}_i and \mathbf{g}^j become parallel, so that distinction between the two types becomes unnecessary. Although less generally applicable, the analytical importance of these special cases earns them their own name : orthogonal coordinates³. Nontrivial examples are cylindrical and spherical coordinates. In this chapter we will consider socal led semi-orthogonal coordinates; the 3-direction is orthogonal to the 1, 2-directions, although the latter two need not be mutually orthogonal.

The matrix $\partial \mathbf{x} / \partial \mathbf{y}$ relates the differential vectors $d\mathbf{x} = (dx_1, dx_2, dx_3)$ and $d\mathbf{y} = (dy_1, dy_2, dy_3)$ in the two coordinate systems by $d\mathbf{x} = (\partial \mathbf{x} / \partial \mathbf{y}) d\mathbf{y}$. Via the squared length of $d\mathbf{x}$ we introduce the metric tensor \mathbf{g} ;

$$ds^{2} = d\mathbf{x}^{t} d\mathbf{x} = d\mathbf{y}^{t} (\partial \mathbf{x} / \partial \mathbf{y})^{t} \partial \mathbf{x} / \partial \mathbf{y} d\mathbf{y},$$
$$= d\mathbf{y}^{t} \mathbf{g} d\mathbf{y} \ge 0,$$
where $\mathbf{g} \triangleq (\partial \mathbf{x} / \partial \mathbf{y})^{t} \partial \mathbf{x} / \partial \mathbf{y}.$ (7.9a)

 $^{^{3}}$ Most graduate level text books usually only treat orthogonal coordinates if they treat curvilinear coordinates at all.

Clearly g is symmetric and in the case of orthogonal coordinates diagonal. To express the gradient and divergence in partial derivative operators $\partial/\partial y_j$ we will need the inverse and determinant of g,

$$\mathbf{g}^{-1} = \begin{pmatrix} g^{11} & g^{12} & g^{13} \\ g^{21} & g^{22} & g^{23} \\ g^{31} & g^{32} & g^{33} \end{pmatrix}$$
(7.9b)

and

$$g = \det \mathbf{g} = (\det \partial \mathbf{x} / \partial \mathbf{y})^2 > 0, \tag{7.9c}$$

respectively. We conclude this resume by relating scalar-quantities, such as the pressure P, and components of vectors-quantities, like the particle velocity V, in Cartesian coordinates to curvilinear coordinates. If we adopt the convention attach a prime '-superscript to functions of the latter, then we have for the pressure that

$$P(x_1, x_2, x_3) = P'(y_1, y_2, y_3).$$
 (7.10a)

For vector-quantities such a relation requires some extra consideration. The Cartesian components and curvilinear base vector components are obviously related by

$$\mathbf{V} = V^k \mathbf{i}_k = V^{'i} \mathbf{g}_i. \tag{7.10b}$$

From the preceding discussion it should be clear that in general

$$V^{'k}(y_1, y_2, y_3) \neq V^k(x_1, x_2, x_3).$$

But if we substitute equation (7.3) into equation (7.10b) and match the results on the left and right hand sides, then the components V^k and V'^i are related by

$$\begin{pmatrix} V^{1} \\ V^{2} \\ V^{3} \end{pmatrix} (x_{1}, x_{2}, x_{3}) = \frac{\partial \mathbf{x}}{\partial \mathbf{y}} \begin{pmatrix} V^{'1} \\ V^{'2} \\ V^{'3} \end{pmatrix} (y_{1}, y_{2}, y_{3}).$$
(7.10c)

7.3 Two types of coordinate transformation mapping interfaces to depth-like coordinates

For our application two different types of curvilinear coordinates are important. The first has been employed by Haines et al. [43, 44, 49] for modeling of one-way wave fields, and all off-diagonal elements of its metric tensor are nonzero. In section 7.4 we show that these nonzero off-diagonal elements make it unsuitable for directional wave field decomposition in a similar way as in Chapter 3. The second type makes use of socal led semi-orthogonal coordinates. These have been employed recently by Sava and Fomel [74] for wave field extrapolation. Semi-orthogonal coordinates are characterized by the fact that one of the coordinates is orthogonal to the other two, so that the corresponding metric tensor is block-diagonal. This feature does allow directional wave field after Chapter 3-5. To distinguish the two particular coordinate systems from the general curvilinear coordinates y we will make the transitions $y \to \xi$ and $y \to \overline{\xi}$, for the wave modeling and the semi-orthogonal coordinate systems, respectively. Similarly we will write γ and $\overline{\gamma}$ instead of g for the metric tensors, while we will denote the components of the particle velocity by Υ^i and $\overline{\Upsilon^i}$ instead of V'^i .

Haines et al. [43, 44, 49] model one-way wave fields with an extension to 3D laterally varying media of the invariant imbedding principle. One of the central ideas behind this extension is to replace the depth-coordinate x_3 by a depth-like coordinate that is constant at surfaces representing major discontinuities. We denote this coordinate system by $y \rightarrow \xi$, and it is of the form

$$x_1 = \xi_1, \qquad x_2 = \xi_2, \qquad x_3 = z(\boldsymbol{\xi}_H, \xi_3).$$
 (7.11a)

where constant values of ξ_3 are attached to a single interface. The corresponding Jacobian matrix and determinant are given by

$$\frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}} = \begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & 0\\ \partial_{\xi_1} z & \partial_{\xi_2} z & \partial_{\xi_3} z \end{pmatrix} \quad \text{and} \quad \det\left(\frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}}\right) = \partial_{\xi_3} z, \quad (7.11b)$$

respectively. We will denote the denote the corresponding metric tensor by γ and its determinant by γ . The determinant equals

$$\gamma = (\partial_{\xi_3} z)^2, \tag{7.11c}$$

in the light of equations (7.9c) and (7.11b). The direction normal to the interfaces n and the particle velocity in this direction V^n , are conveniently expressed in the coordinate system (7.11a). The normal direction n can be expressed in ξ -coordinates as

$$\mathbf{n} = \left(-\partial_{\xi_1} z, -\partial_{\xi_2} z, 1\right)^t; \tag{7.12}$$

to arrive at equation (7.12), we combined equations (7.4) and (7.11b). We will not attempt to obtain a explicit representation of the $\bar{\xi}$ -coordinates of the form of equation (7.2), but just make some general requirements. So even in the context of $\bar{\xi}$ -coordinates we will use equation (7.12) as a representation for **n**.

As simple as ξ -coordinates and their Jacobian matrix may look at first sight, all elements of the metric tensor γ are nonzero. As a result the ξ -equivalent of the matrix $\hat{\mathbf{A}}$ in the matrix-vector wave equation (1.21) loses its anti-diagonal structure, and thereby the straightforward diagonalization given by equation (3.17).

Therefore we introduce a second coordinate system, denoted by $y \to \overline{\xi}$, for which we require that it retains the discontinuity-alignment of equation (7.11a) for the accurate construction of Ψ DO's, that is

$$\frac{\partial \bar{\xi}_3 / \partial x_1}{\partial \xi_3 / \partial x_1} = \frac{\partial \bar{\xi}_3 / \partial x_2}{\partial \xi_3 / \partial x_2} = \frac{\partial \bar{\xi}_3 / \partial x_3}{\partial \xi_3 / \partial x_3},\tag{7.13a}$$

and that the metric tensor and its inverse are block-diagonal,

$$\bar{\gamma}^{-1} = \begin{pmatrix} \bar{\gamma}^{11} & \bar{\gamma}^{12} & 0\\ \bar{\gamma}^{21} & \bar{\gamma}^{22} & 0\\ 0 & 0 & \bar{\gamma}^{33} \end{pmatrix}.$$
 (7.13b)

The purpose of requiring the block diagonal structure stated by equation (7.13b), will become clear at the end of section 7.4. For now we note that equation (7.13b) implies that in the $\bar{\xi}$ -coordinate system both "lateral" $\bar{\xi}_1$ - and $\bar{\xi}_2$ -directions are orthogonal to the $\bar{\xi}_3$ direction normal to the interfaces, although the $\bar{\xi}_1$ - and $\bar{\xi}_2$ -directions need not be orthogonal to each other. Reserving the connotation semi-orthogonal for this kind of coordinate systems, can lead to ambiguity; it is equally appropriate for coordinate systems where either the $\bar{\xi}_1$ - or $\bar{\xi}_2$ -coordinate is orthogonal to the other two. Nonetheless we use the term semi-orthogonal exclusively for coordinate systems where the $\bar{\xi}_3$ -direction is orthogonal to the other two.

Equations (7.13) do not determine the base vectors of $\bar{\xi}$ -coordinates uniquely. An obvious implication of the requirements stated above is that the $\bar{\xi}_3$ -direction is parallel to n, but we are still free to choose its length. We can therefore simply take n itself as a base vector for this direction. Of the two remaining base vectors we only require that they are orthogonal to n and not parallel to each other. Other than that, their lengths and directions can be chosen for convenience. The leading convenience here will be to obtain a tight connection between V^n in both coordinate systems.

Bearing in mind that **n** was constructed from equation (7.4), convenient choices are the vectors represented by the left and middle column of $\partial \mathbf{x} / \partial \boldsymbol{\xi}$. We therefore have that for $\bar{\boldsymbol{\xi}}$ -coordinates the Jacobian matrix and determinant

$$\frac{\partial \mathbf{x}}{\partial \bar{\boldsymbol{\xi}}} = \begin{pmatrix} 1 & 0 & -\partial_{\xi_1} z \\ 0 & 1 & -\partial_{\xi_2} z \\ \partial_{\xi_1} z & \partial_{\xi_2} z & 1 \end{pmatrix} \quad \text{and} \quad \det\left(\frac{\partial \mathbf{x}}{\partial \bar{\boldsymbol{\xi}}}\right) = |\mathbf{n}|^2,$$

respectively. By construction the metric tensor

$$\bar{\boldsymbol{\gamma}} \triangleq \left(\frac{\partial \mathbf{x}}{\partial \bar{\boldsymbol{\xi}}}\right)^t \frac{\partial \mathbf{x}}{\partial \bar{\boldsymbol{\xi}}}$$

has the block-diagonal structure indicated by equation (7.13b). For later convenience we note that $\bar{\gamma}^{33} = {\bar{\gamma}_{33}}^{-1} = |\mathbf{n}|^{-2}$, and that the determinant equals $\bar{\gamma} = |\mathbf{n}|^4$. The remaining requirement expressed by equation (7.13a) is also satisfied; it is straightforward to verify that the elements of the lower rows of the inverse Jacobian matrices $\partial \boldsymbol{\xi} / \partial \mathbf{x}$ and $\partial \bar{\boldsymbol{\xi}} \partial \mathbf{x}$ correspond to the columns

$$\boldsymbol{\gamma}^{3} = (\partial_{\xi_{3}} z)^{-1} \begin{pmatrix} -\partial_{\xi_{1}} z \\ -\partial_{\xi_{2}} z \\ 1 \end{pmatrix} \quad \text{and} \quad \bar{\boldsymbol{\gamma}}^{3} = |\mathbf{n}|^{-2} \begin{pmatrix} -\partial_{\xi_{1}} z \\ -\partial_{\xi_{2}} z \\ 1 \end{pmatrix},$$

respectively. The concluding expressions of this section will express V^n in ξ - and $\overline{\xi}$ coordinates. To this end we substitute specializations of equation (7.10c) to both ξ - and $\bar{\xi}$ -coordinates into equation (7.5):

$$V^{n} = \mathbf{n}^{t} \mathbf{V} = \mathbf{n}^{t} \frac{\partial \mathbf{x}}{\partial \bar{\boldsymbol{\xi}}} \begin{pmatrix} \bar{\boldsymbol{\Upsilon}}^{1} \\ \bar{\boldsymbol{\Upsilon}}^{2} \\ \bar{\boldsymbol{\Upsilon}}^{3} \end{pmatrix} = |\mathbf{n}|^{2} \bar{\boldsymbol{\Upsilon}}^{3} = \bar{\gamma}^{1/2} \bar{\boldsymbol{\Upsilon}}^{3},$$
(7.14a)

$$= \mathbf{n}^{t} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\xi}} \begin{pmatrix} \Upsilon^{1} \\ \Upsilon^{2} \\ \Upsilon^{3} \end{pmatrix} = (\partial_{\xi_{3}} z) \Upsilon^{3} = \gamma^{1/2} \Upsilon^{3}.$$
(7.14b)

Equations (7.14) allow us to connect the "vertical" particle velocity Υ^3 in ξ -coordinates to $\overline{\Upsilon}^3$ in $\overline{\xi}$ -coordinates. The former can be the result of the generalized invariant imbedding approach proposed and implemented by Haines et al. [43, 44, 49]. In sections 7.4 and 7.5 we will show that the latter is a suitable starting point for the formulation of reciprocity theorems for one-way wave fields. Note that the particle velocity in the normal direction **n** has similar representations in both ξ - and $\overline{\xi}$ -coordinates. In section 7.4 we will exploit this similarity to obtain similar forms of the matrix-vector wave equation.

7.4 The wave equation in curvilinear coordinates

If we want to express the wave equation in the unspecified curvilinear coordinates (y_1, y_2, y_3) , then a consistent application of the convention introduced by equations (7.10) would lead us to attach prime '-superscripts to all involved quantities. For notational convenience we drop that convention in this section. Therefore equations (1.20a)-(1.20b) expressed in terms of general curvilinear coordinates y read

$$g^{ij}\frac{\partial P}{\partial y_j} = -j\omega\rho V^i + F^i, \qquad (7.15a)$$

while equation (1.20c) expressed in the same form reads

$$g^{-1/2}\frac{\partial(g^{1/2}V^i)}{\partial y_i} = -\frac{j\omega}{K}P + Q.$$
(7.15b)

For a derivation of equations (7.15a) and (7.15b) we refer the interested reader to Fung [35] or Farrashkhalvat and Miles [26]. In the light of equations (7.14) we want to retain $V^n = \sqrt{g}V^3$. We therefore rewrite equation (7.15b) as

$$\frac{\partial V^n}{\partial y_3} + \frac{\partial (\sqrt{g}V^\beta)}{\partial y_\beta} = -\frac{j\omega\sqrt{g}}{K}P + \sqrt{g}Q.$$
(7.15c)

In orthogonal coordinates the off-diagonal elements g^{ij} of the metric tensor **g** are zero, so that we can eliminate V^1 and V^2 in the same way as in section 1.7. But the nonzero off-diagonal elements of **g** in case of more general coordinate transforms prevent such a straightforward repetition.

After Haines et al. [43] we will show that the system of equations (7.15a) and (7.15c) can be cast in the form

$$\frac{\partial}{\partial y_3} \begin{pmatrix} -P\\V^n \end{pmatrix} + \hat{\mathbf{A}} \begin{pmatrix} -P\\V^n \end{pmatrix} = \mathbf{D}.$$

The exact form of the two-vector source **D** is not relevant here, except that it contains all references to the source-terms Q and F^r . For the remaining analysis in this section we will therefore take Q = 0 and $F^1 = F^2 = F^3 = 0$. Relevant here is that, analogous to the previous chapters, the operator-character of the matrix $\hat{\mathbf{A}}$ is based exclusively on $\partial/\partial y_1$ and $\partial/\partial y_2$. But similar to the elastic, anisotropic wave equation the diagonal elements of $\hat{\mathbf{A}}$ will not be zero anymore.

From the i = 3-component of equation (7.15a) we obtain that

$$\frac{\partial(-P)}{\partial y_3} + \frac{g^{3\alpha}}{g^{33}}\frac{\partial(-P)}{\partial y_\alpha} - \frac{j\omega\rho}{\sqrt{g}\,g^{33}}V^n = 0.$$
(7.16a)

so that

$$\hat{A}_{11} = \frac{g^{3\alpha}}{g^{33}} \frac{\partial}{\partial y_{\alpha}},\tag{7.16b}$$

and
$$\hat{A}_{12} = -\frac{j\omega\rho}{\sqrt{g}\,g^{33}}.$$
 (7.16c)

Note the nonzero diagonal element \hat{A}_{11} . The next step is to eliminate V^1 and V^2 from equation (7.15c). In comparison to the similar elimination-procedure described earlier in section 1.7 a complication arises: due to the (in general) nonzero functions g^{13} and g^{23} in equation (7.15a), we must allow V^1 and V^2 to depend also on a term proportional to

 $\partial P/\partial \xi_3$. We will eliminate these terms with equation (7.16a), at the cost of making the diagonal element \hat{A}_{22} also nonzero. After evaluating these steps we arrive at

$$\hat{A}_{22} = -\hat{A}_{11}^t, \tag{7.17a}$$

$$\hat{A}_{21} = -\frac{j\omega\sqrt{g}}{K} + \frac{1}{j\omega}\frac{\partial}{\partial y_{\beta}}\left[\frac{\sqrt{g}}{\rho}\left(g^{\beta\alpha} - \frac{g^{\beta3}g^{3\alpha}}{g^{33}}\right)\frac{\partial}{\partial y_{\alpha}}\cdot\right],\tag{7.17b}$$

where the superscript t denotes the transposed, see appendix A.2. Haines et al. [43] noted that in addition to relation (7.17a) between the diagonal elements, the off-diagonal elements are both symmetric; collectively these properties are indicated by stating that $\hat{\mathbf{A}}$ satisfies the symplectic property,

$$\hat{\mathbf{A}}^t \mathbf{N} = -\mathbf{N}\hat{\mathbf{A}}.\tag{7.18}$$

Similar to elastic wave propagation [87], a diagonalization of $\hat{\mathbf{A}}$ similar to equation (3.17) is severely complicated by the fact that its diagonal elements \hat{A}_{11} and \hat{A}_{22} are non-zero. For this reason we restrict ourselves to semi-orthogonal coordinate systems; if the inverse metric tensor satisfies equation (7.13b), then $\hat{A}_{11} = \hat{A}_{22} = 0$ and hence diagonalization in the form of equation (3.17) becomes possibles again. In section 7.5 we will show that the lower left operator \hat{A}_{21} can be expressed in a modal decomposition similar to \hat{H}_2 .

7.5 Helmholtz-type operators in semi-orthogonal curvilinear coordinates

In the semi-orthogonal coordinates $\bar{\xi}$ the diagonal elements \hat{A}_{11} and \hat{A}_{22} of the operator matrix \hat{A} are zero as argued above, while the operator \hat{A}_{21} reads

$$\hat{A}_{21} = -\frac{j\omega\sqrt{\bar{\gamma}}}{K} + \frac{1}{j\omega}\frac{\partial}{\partial\bar{\xi}_{\beta}} \left[\frac{\bar{\gamma}^{\beta\alpha}\sqrt{\bar{\gamma}}}{\rho}\frac{\partial}{\partial\bar{\xi}_{\alpha}}\cdot\right].$$
(7.19)

To achieve the goal stated at the end of section 7.4 we only need to establish that there is a couple of Helmholtz-type operators \hat{A}_P and \hat{A}_F , similar to the pseudo-Helmholtz operator \hat{H}_2 and the Helmholtz-operator \hat{H}_2 respectively. We define these Helmholtztype operators as $\hat{A}_P = -\hat{A}_{12}\hat{A}_{21}$, and

$$\hat{A}_{F} = -\hat{A}_{12}^{1/2}\hat{A}_{21}\hat{A}_{12}^{1/2},$$

$$= \frac{\omega^{2}|\mathbf{n}|^{2}\rho}{K} + \rho^{1/2}\frac{\partial}{\partial\bar{\xi}_{\beta}}\left[\frac{\bar{\gamma}^{\beta\alpha}|\mathbf{n}|^{2}}{\rho}\frac{\partial}{\partial\bar{\xi}_{\alpha}}(\rho^{1/2}\cdot)\right].$$
(7.20)

To arrive at equation (7.20) we have used that $\bar{\gamma}^{33}\sqrt{\bar{\gamma}} = 1$ and $\sqrt{\bar{\gamma}} = |\mathbf{n}|^2$. The two operators \hat{A}_P and \hat{A}_F are obviously interrelated by an expression similar to equation (3.2a),

$$\hat{A}_F = \hat{A}_{12}^{-1/2} \hat{A}_P \hat{A}_{12}^{1/2}.$$
(7.21)

If we can establish that \hat{A}_F is self-adjoint like \hat{H}_2 , then all proofs and constructions based on the self-adjoint nature of \hat{H}_2 proceed along the same lines and have similar results for \hat{A}_F ; from the symmetry of \hat{A}_F and its root operators, via the definition of directional decomposition, and finally to the vanishing of flux normalized one-way operators for identical media in reciprocity theorems with curved boundaries.

To make this establishment we use definitions (A.12) and (A.14) of adjoint and selfadjoint operators. Obviously the left term on the right hand side of equation (7.20), that is the real valued wavenumber-term, is a trivial self-adjoint operator. To deal with the remaining second order differential operator, we need to formulate the action of the adjoint of the first order differential operator $\partial/\partial \bar{\xi}^{\alpha}$. If it operates on functions f, h in the Sobolev space, then partial integration shows that

$$\langle \partial f / \partial \bar{\xi}_{\alpha}, h \rangle_s = - \langle f, \partial h / \partial \bar{\xi}_{\alpha} \rangle_s.$$

Now the action of the adjoint of the second order differential operator on the left hand side of equation (7.20) is conveniently expressed as

$$\left\langle \left(\hat{A}_{F} - \frac{\omega^{2}\rho}{\bar{\gamma}^{33}K}\right)f,h\right\rangle_{s} = \left\langle \rho^{1/2}\frac{\partial}{\partial\bar{\xi}_{\beta}}\left[\frac{\bar{\gamma}^{\beta\alpha}\sqrt{\bar{\gamma}}}{\rho}\frac{\partial}{\partial\bar{\xi}_{\alpha}}(\rho^{1/2}f)\right],h\right\rangle_{s},$$
$$= -\left\langle \frac{\bar{\gamma}^{\beta\alpha}\sqrt{\bar{\gamma}}}{\rho}\frac{\partial}{\partial\bar{\xi}_{\alpha}}(\rho^{1/2}f),\frac{\partial}{\partial\bar{\xi}_{\beta}}(\rho^{1/2}h)\right\rangle_{s},$$
$$= \left\langle f,\rho^{1/2}\frac{\partial}{\partial\bar{\xi}_{\alpha}}\left[\frac{\bar{\gamma}^{\beta\alpha}\sqrt{\bar{\gamma}}}{\rho}\frac{\partial}{\partial\bar{\xi}_{\beta}}(\rho^{1/2}h)\right]\right\rangle_{s}.$$
(7.22)

Since $\bar{\gamma}^{\beta\alpha} = \bar{\gamma}^{\alpha\beta}$, equation (7.22) establishes that $\hat{A}_F^{\dagger} = \hat{A}_F$. In semi-orthogonal coordinates we can therefore construct fractional powers of \hat{A}_F , so that we can formulate flux normalized wave field decomposition along curved surfaces and therefore also reciprocity theorems with curved boundaries after Chapters 3-5. With output of an acoustic modeling algorithm as formulated by Haines and De Hoop [43], it is therefore possible to extend redatuming with transmission loss correction to non flat interfaces described by coordinate transformations like equation (7.11a).

The analoguous formulation of the mathematics presented in this chapter for the elastic wave equation, suffers from the same problem as diagonalizing $\hat{\mathbf{A}}$ for general curvilinear coordinates: the (block-)diagonal elements of the elastic analog of $\hat{\mathbf{A}}$ become nonzero. In terms of For arbitrary anisotropic media this problem remains as tough as it already was for Cartesian coordinates, but for transversely isotropic media a transformation to anti diagonal form is again possible in terms of semi-orthogonal coordinates.

Chapter 8

Summary, conclusions, and possibilities for future work

Standard formulations of seismic migration algorithms are based on low contrast media. These approaches can be sufficient to analyze and process the kinematics of seismic reflection measurements, but in case of high contrast media they are likely to fall short with respect to the dynamics. We focused on the ability of redatuming to preserve the dynamical information in reflection measurements. To improve this for high contrast media, we proposed a correction for transmission losses in the inverse propagation step that aims to satisfy the law of energy conservation.

This idea can be expressed and implemented in a straightforward manner if the medium properties vary only with depth, see Chapter 2. The central theme of this thesis was to derive and implement for media varying also in other directions, acoustic redatuming with transmission loss correction to preserve amplitude information (we are aware of the fact that processing elastic wave fields as if they are acoustic can result in severe amplitude distortions). The central motivation behind the different aspects of our approach is to account for the symmetries and conservation laws of wave propagation as much as possible, in the redatuming procedure itself as well as in preparatory processing steps.

Chapter 3 dealt with two processing steps required by our approach to redatuming: directional decomposition of the wave fields into up and down going components, and flux normalization to induce source receiver reciprocity between up and down going wave fields. In particular we focused on the root operators of the Helmholtz operator in terms of which these two steps are formulated and the symmetries of these operators. We constructed the root operators from a so-called modal decomposition of the Helmholtz operator. In computational practice this came down to a diagonalization of a discrete matrix representation of the Helmholtz operator, for which we used Fourier expansions of the differential operators. Due to this choice of basis functions we obtained high accuracy in smooth media with periodic boundary conditions, but lower accuracy at and close to discontinuities, see section 3.8 for some examples¹. We see two possibilities to overcome this problem.

- 1 Use wavelets for basis functions; Beylkin [10] showed that wavelet-based representations of differential operators can be constructed with the same symmetry properties as Fourier expansions, while wavelets are more suitable to deal with discontinuities than sines and cosines.
- 2 Discontinuities in properties of the subsurface of the earth primarily occur at the boundaries between layers. Haines et al. [42, 43, 44, 49] have proposed and developed a one-way wave modeling algorithm that works with a curvilinear coordinate transformation defined in such a way that one of the curvilinear coordinates is constant at the non-flat layer boundaries. In Chapter 7 we have proposed a closely related coordinate transformation. Based on this second transformation we extended the definitions of Chapter 3 of wave field decomposition and flux normalization, such that the direction of decomposition was the direction normal to the non-flat layer boundaries.

Possibly the combined application of options 1 and 2 is most fruitful. An additional advantage of using option 2 for full wave modeling is that its evolution parameter is depth, whereas this is time for FD methods. In prestack migration depth extrapolation allows a straightforward reuse of the modeling efforts for previous depths, while this is more difficult for FD methods. The results discussed sofar are not just relevant for redatuming, but also for other applications of one-way wave fields and their appearance in reciprocity theorems, see for example Wapenaar et al. [94]. The remaining discussion deals specifically with inverse propagation and redatuming.

In section 5.5 we used a correlation type reciprocity theorem to express a balance between flux normalized, global transmission and reflection operators, a balance relation that incorporates energy conservation for propagating wave fields. In Chapter 5 we

¹In Chapters 5 and 6 we avoided problems with discontinuities for the time being, and we focused mainly on inverse propagation and redatuming examples with (at most) smooth variations at the surface and redatuming depths. However, between those two depths we did allow for discontinuous variations of the medium parameters in both the horizontal and vertical directions.

demonstrated that for inverse propagation across a single syncline interface, a multivalued inverse propagator alone is not enough to restore both the kinematics and dynamics of a source wave field. But with correction for transmission loss, it is possible to construct an inverse propagator that also restores the dynamics. In a similar experiment we analyzed media that defocus up going wave fields, an issue occurring with redatuming to depths below salt bodies. In such a situation it is a realistic possibility that events in the overburden response do not have counterparts in the transmission response in the same finite aperture, or the other way around. As a result the aforementioned balance relation cannot be satisfied, and thus the performance of transmission loss correction will not be optimal, see section 5.8. On the other hand we could recover the reflection coefficient of the "salt base" in the simplified configuration considered in section 5.9; the overburden corresponding to this salt base does focus wave fields in the up going direction. So redatuming to salt bases is a possible application for transmission loss correction.

In the examples of Chapter 5 we modeled the transmission and reflection response of the overburden concurrently. In realistic applications this is not an option; models with already enough detail to produce useful multiples will be hard to improve with results from transmission loss corrected redatuming. In Chapter 6 we therefore proposed a datadriven method to separate the reflection response of the overburden from the response of the deeper subsurface and applied it to a real data set. Of course a similarly data-driven approach is required for the transmission response of the overburden. Although principles exist for doing this, the corresponding implementations are not available yet. We therefore concluded Chapter 6 with a suggestions for balancing the amplitudes of the transmission response based on a macro model.

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Appendix A

Pseudo-differential operators and kernels

A.1 An introduction of pseudo-differential operators

For constant k^2 the Fourier transform of equation (3.2b) is a simple algebraic expression (remember (2.1a)),

$$\tilde{\mathsf{H}}_2 \tilde{f} = (k^2 - \mathbf{k}_H \cdot \mathbf{k}_H) \tilde{f}.$$

The operator \hat{H}_2 reduces to a simple scalar number and equally so does its square root $\tilde{H}_1 = \tilde{H}_2^{1/2}$; see section 2.2. For laterally varying $k^2(\mathbf{x}_H)$ this simplification of \hat{H}_2 and \hat{H}_2 in the \mathbf{k}_H, ω -domain does not occur. Since the operators \hat{H}_1 and \hat{H}_1 cannot be expressed as polynomials in $\partial_{1,2}$ they are called pseudo-differential operators (abbreviated to Ψ DO in this thesis). Together with section A.2 the remainder of this one will introduce Ψ DO's and (some of) their properties.

Any linear partial differential equation can be represented as a linear operator \hat{P} acting on a function f

$$\hat{P}(\mathbf{u})f(\mathbf{u}) = S(\mathbf{u}), \qquad \mathbf{u} \in \mathbb{R}^n.$$
 (A.1)

Formally, the solution f can be represented as $f(\mathbf{u}) = \hat{P}^{-1}(\mathbf{u})S(\mathbf{u})$. In the early 1960s attempts were made at actually constructing the operator \hat{P}^{-1} (the particular approximation resulting from these attempts is called a parametrix). It turned out that the formalism

for generalizing linear partial differential operators to Ψ DO's, is not just valid for \hat{P}^{-1} but can be extended to \hat{P}^m , $m \in \mathbb{R}$, see for example Grigis and Sjöstrand [40]; that includes the fractional powers required here. The completion of the rigorous foundation and finding the limits of the applicability of this theory are both still subjects of active research, see Egorov and Schulze [23].

Like section 1.5 on generalized functions, this section will try to develop a working knowledge, instead of going into the details of their formal definition. See Hörmander [50] or Kumano-go [57] for rigorous and comprehensive treatments. Egorov and Schulze [23], Grigis and Sjöstrand [40], and Wong [98] also cover the topic but sacrificed completeness for accessibility.

Fourier transformation and generalized functions are essential elements of Ψ DOtheory; not just for their formal definition, also for their proper use. But before trying to illuminate this, we introduce multi-index notation, which allows any linear differential equation to be cast in a compact notation. A multi-index α maps the vector w to a scalar

$$\mathbf{w}^{\boldsymbol{\alpha}} = w_1^{\alpha_1} \dots w_n^{\alpha_n}, \qquad \boldsymbol{\alpha} \in \mathbb{N}^n, \, \mathbf{w} \in \mathbb{R}^n.$$
(A.2)

The multi-index has a norm $|\alpha| = \alpha_1 + \ldots + \alpha_n$. For partial differentiation with respect to $\mathbf{u} \in \mathbb{R}^n$, the $\nabla_{\mathbf{u}}$ -operator is disguised as $\mathbf{D}_{\mathbf{u}} = j \nabla_{\mathbf{u}}$. Using the fact

$$(j\partial/\partial u_i)^{\alpha_i} e^{-j\mathbf{u}\cdot\mathbf{w}} = w_i^{\alpha_i} e^{-j\mathbf{u}\cdot\mathbf{w}},$$

multi-index notation can be used for compact expression of arbitrary combinations of partial differential operators of order $|\alpha|$ as

$$\mathbf{D}_{\mathbf{u}}^{\boldsymbol{\alpha}} e^{-j\mathbf{u}\cdot\mathbf{w}} = (j\partial/\partial u_1)^{\alpha_1} \dots (j\partial/\partial u_n)^{\alpha_n} e^{-j\mathbf{u}\cdot\mathbf{w}} = \mathbf{w}^{\boldsymbol{\alpha}} e^{-j\mathbf{u}\cdot\mathbf{w}}.$$
 (A.3)

The linear differential operator \hat{P} from equation (A.1) can be written as a power series in $\mathbf{D}_{\mathbf{u}}$ with corresponding coefficients $a_{\boldsymbol{\alpha}}(\mathbf{u})$

$$\hat{P} = \sum_{|\boldsymbol{\alpha}| \le s} a_{\boldsymbol{\alpha}}(\mathbf{u}) \mathbf{D}_{\mathbf{u}}^{\boldsymbol{\alpha}}.$$
(A.4)

In the particular case of the 2D Helmholtz operator $\hat{H}_2(\mathbf{x}_H) = k^2(\mathbf{x}_H) + \nabla_H^2$, the nonzero coefficients have multi-indices $\boldsymbol{\alpha} = (0,0), (2,0), \text{ and } (0,2)$. The pseudo Helmholtz operator \hat{H}_2 , remember equation (1.23), has two additional nonzero coefficients, i.e. the first order ones with multi-indices $\boldsymbol{\alpha} = (1,0)$ and (0,1).

A symbol of order s is polynomial p in \mathbf{u} and \mathbf{w} ,

$$p(\mathbf{u};\mathbf{w}) = \sum_{|\boldsymbol{\alpha}| \le s} a_{\boldsymbol{\alpha}}(\mathbf{u}) \mathbf{w}^{\boldsymbol{\alpha}};$$

the symbol corresponding to \hat{H}_2 is $h_2(\mathbf{x}_H, \mathbf{y}_H) = k^2(\mathbf{x}_H) + y_1^2 + y_2^2$. Lets evaluate the product of a symbol and the Fourier kernel. The term wise use of the relation (A.3) allows one to make the identification

$$p(\mathbf{u}; \mathbf{w})e^{-j\mathbf{u}\cdot\mathbf{w}} = p(\mathbf{u}; \mathbf{D}_{\mathbf{u}})e^{-j\mathbf{u}\cdot\mathbf{w}}.$$
(A.5)

Now the action of an *s*-order linear differential operator $\hat{P}(\mathbf{u}) = p(\mathbf{u}; \mathbf{D}_{\mathbf{u}})$ on a function f can be expressed in the Fourier domain¹ like

$$\hat{P}(\mathbf{u})f(\mathbf{u}) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} p(\mathbf{u}; \mathbf{w}) \tilde{f}(\mathbf{w}) e^{-j\mathbf{u}\cdot\mathbf{w}} d^n \mathbf{w}.$$
(A.6)

Summarizing one can say that the action of Ψ DO's is a generalization of the action of regular, linear differential operators. One of the basic results of Ψ DO-theory is that it is possible to define symbols whose order is *not restricted to natural numbers* but *extended to real numbers*. For natural order these symbols reduce to polynomials.

A.2 From pseudo-differential operators to kernels

The basic result of Ψ DO-theory essential to this thesis, is that Ψ DO's can also be represented by so-called Schwartz kernels (the prefix Schwartz will be dropped in this thesis). Equation (A.6) can also be expressed as

$$\hat{P}(\mathbf{u})f(\mathbf{u}) = \int_{\mathbb{R}^{n}} P(\mathbf{u};\mathbf{u}')f(\mathbf{u}')d^{n}\mathbf{u}', \qquad (A.7)$$

where the function P, is expressed in terms of the symbol p by

$$P(\mathbf{u};\mathbf{u}') = (2\pi)^{-n} \int_{\mathbb{R}^n} p(\mathbf{u};\mathbf{w}) e^{-j(\mathbf{u}-\mathbf{u}')\cdot\mathbf{w}} d^n \mathbf{w}.$$
 (A.8)

¹Note that in accordance with Chapter 2 we choose the sign-convention for spatial Fourier transformation. On the other hand, Hörmander [50], Kumano-go [57], Egorov and Schulze [23] and Wong [98], use the temporal sign-convention, because it reduces the number of minus-signs.

Kernels can also be introduced as the action of the operator on the δ -function

$$\hat{P}(\mathbf{u})\delta(\mathbf{u}-\mathbf{u}') = P(\mathbf{u};\mathbf{u}').$$
(A.9)

Clearly P is a generalized function; see section 1.5 and note that Green's functions are also kernels.

The combined actions of generalized functions and the Fourier transformation restrict the applicability of Ψ DO's to functions from so-called Sobolev spaces $H^s(\mathbb{R}^n)$. Loosely speaking, these are the spaces of continuously differentiable functions with compact support that are square integrable and whose *s*-order derivatives are also square integrable.

The product \hat{C} of two Ψ DO's \hat{A}, \hat{B} is again a Ψ DO². Repeated substitution of equation (A.7) shows that the corresponding kernels are related as

$$\hat{C}(\mathbf{u})f(\mathbf{u}) = \hat{A}(\mathbf{u})\hat{B}(\mathbf{u})f(\mathbf{u}) = \int_{\mathbb{R}^{n}} A(\mathbf{u};\mathbf{u}'') \left[\int_{\mathbb{R}^{n}} B(\mathbf{u}'';\mathbf{u}')f(\mathbf{u}')d^{n}\mathbf{u}' \right] d^{n}\mathbf{u}'',$$
$$= \int_{\mathbb{R}^{n}} C(\mathbf{u};\mathbf{u}')f(\mathbf{u}')d^{n}\mathbf{u}',$$
(A.10)

where

$$C(\mathbf{u};\mathbf{u}^{'}) = \int_{\mathbb{R}^{n}} A(\mathbf{u};\mathbf{u}^{''})B(\mathbf{u}^{''};\mathbf{u}^{'})d^{n}\mathbf{u}^{''}.$$

Usually the product of two Ψ DO's is studied in terms of symbols, see Fishman et al. [28] for an example in the context of wave propagation. Here the kernel-formulation will be used because it allows a natural connection to linear algebra; identifying kernels with matrices, functions with vectors, and integral signs with summations, equation (A.10) is the continuum analog of a matrix-vector product $g_i = \sum_j P_{ij} f_j$. The concepts of matrixtransposition and -conjugation have straightforward analogs in the language of integral operators and kernels.

For any two functions $f, g \in H^{s}(\mathbb{R}^{n})$ the inner products from linear algebra have

²The case of interest is the Helmholtz operator and its square root operator, $\hat{H}_2 = \hat{H}_1 \hat{H}_1$.

continuum analogs in the bilinear and sesquilinear forms

$$\langle f, g \rangle_b = \int_{\mathbb{D}_n} f(\mathbf{u}) g(\mathbf{u}) d^n \mathbf{u},$$
 (A.11)

$$\langle f, g \rangle_s = \int_{\mathbb{D}_n}^{\infty} f^*(\mathbf{u}) g(\mathbf{u}) d^n \mathbf{u},$$
 (A.12)

respectively. The domain \mathbb{D}_n can be any sub domain of \mathbb{R}^n , but unless explicitly stated otherwise, \mathbb{D}_n should be identified with \mathbb{R}^n . The transposed and adjoint of an operator $\hat{P}(\mathbf{u})$ are introduced by

$$\langle f, \hat{P}^t g \rangle_b = \langle \hat{P}f, g \rangle_b,$$
 (A.13)

$$\langle f, \hat{P}^{\dagger}g \rangle_s = \langle \hat{P}f, g \rangle_s,$$
 (A.14)

respectively; equivalent to definition (A.13) is to say that the transposed of an operator works to the left. Also note that like for matrices $\hat{P}^{\dagger} = {\{\hat{P}^t\}}^*$. Special types of operator frequently encountered in wave propagation are

symmetric operators:
$$\hat{P}^t = \hat{P}$$
,
self-adjoint operators: $\hat{P}^{\dagger} = \hat{P}$,
skew-symmetric operators: $\hat{P}^t = -\hat{P}$.

The rules for transposition/adjoining products of operators are identical to those for matrices. Let $\hat{R} = \hat{P}\hat{Q}$. Then repeated use of the definitions (A.13) and (A.14) leads to $\hat{R}^t = \hat{Q}^t \hat{P}^t$ and $\hat{R}^\dagger = \hat{Q}^\dagger \hat{P}^\dagger$, respectively.

The rules and definitions for transposed and adjoint kernels are similar to those of operators.

- The transposed of a kernel is $\{P(\mathbf{u}; \mathbf{u}')\}^t = P(\mathbf{u}'; \mathbf{u}).$
- The conjugate of a kernel is $\{P(\mathbf{u};\mathbf{u}')\}^{\dagger} = \{P^*(\mathbf{u};\mathbf{u}')\}^t$,
- A kernel is symmetric if it obeys $P(\mathbf{u}; \mathbf{u}') = P(\mathbf{u}'; \mathbf{u})$.
- A kernel is self-adjoint if $P^*(\mathbf{u}'; \mathbf{u}) = P(\mathbf{u}; \mathbf{u}')$.
- A kernel is skew-symmetric if it obeys $P(\mathbf{u}; \mathbf{u}') = -P(\mathbf{u}'; \mathbf{u})$.

Section A.3 describes in detail how to connect the *continuous* kernels to *discrete* matrices. Two vector functions $\mathbf{f}(\mathbf{u}), \mathbf{g}(\mathbf{u})$ with all components $\{f_i, g_i\} \in H^s(\mathbb{R}^n)$, have associated inner products analogous to equations (A.11) and (A.12)

$$\langle \mathbf{f}, \mathbf{g} \rangle_b = \int_{\mathbb{D}_n} \mathbf{f}^t(\mathbf{u}) \mathbf{g}(\mathbf{u}) d^n \mathbf{u},$$
 (A.15)

$$\langle \mathbf{f}, \mathbf{g} \rangle_s = \int_{\mathbb{D}_n} \mathbf{f}^{\dagger}(\mathbf{u}) \mathbf{g}(\mathbf{u}) d^n \mathbf{u}.$$
 (A.16)

An operator matrix

$$\hat{\mathbf{M}} = \hat{\mathbf{M}}(\mathbf{u}, \nabla_{\mathbf{u}}) = \begin{pmatrix} \hat{M}_{11} & \hat{M}_{12} \\ \hat{M}_{21} & \hat{M}_{22} \end{pmatrix},$$

has associated transposed and adjoint operators

$$\langle \hat{\mathbf{M}} \mathbf{f}, \mathbf{g} \rangle_b = \langle \mathbf{f}, \hat{\mathbf{M}}^t \mathbf{g} \rangle_b, \qquad \hat{\mathbf{M}}^t = \begin{pmatrix} \hat{M}_{11}^t & \hat{M}_{21}^t \\ \hat{M}_{12}^t & \hat{M}_{22}^t \end{pmatrix}, \qquad (A.17)$$

$$\langle \hat{\mathbf{M}} \mathbf{f}, \mathbf{g} \rangle_s = \langle \mathbf{f}, \hat{\mathbf{M}}^{\dagger} \mathbf{g} \rangle_s \qquad \hat{\mathbf{M}}^{\dagger} = \begin{pmatrix} \hat{M}_{11}^{\dagger} & \hat{M}_{21}^{\dagger} \\ \hat{M}_{12}^{\dagger} & \hat{M}_{22}^{\dagger} \end{pmatrix},$$
(A.18)

respectively. Similar to scalar operators,

- adjoint and transposed matrix-operators are related by $\hat{\mathbf{M}}^{\dagger} = {\{\hat{\mathbf{M}}^t\}^*}$,
- symmetric matrix-operators obey $\hat{\mathbf{M}}^t = \hat{\mathbf{M}}$,
- self-adjoint matrix-operators obey $\hat{\mathbf{M}}^{\dagger} = \hat{\mathbf{M}}$,
- skew-symmetric matrix-operators obey $\hat{\mathbf{M}}^t = -\hat{\mathbf{M}}$.

A.3 Matrices as discrete approximations of kernels

The discrete approximations of kernels/ Ψ DO's are square matrices with real or complex entries. The sets of real and complex square matrices will be denoted by $\mathbb{R}^{m \times m}$ and $\mathbb{C}^{m \times m}$, respectively.

The discrete representation of kernels/operators will be introduced in two phases. First, 1D kernels/operators will be discretized, because that is more simple and it is used in the examples and applications of this thesis. Then, along the same lines, kernels with 2-dimensional coordinates \mathbf{u} will be considered. An extension to *n*-dimensional coordi-



Figure A.1: Discretization of the 1D do-Figure A.2: Taper weights as a function main \mathbb{D} . of u.

nates is straightforward, but the notation becomes rather involved and is therefore omitted here.

A.3.1 Discretization of kernels with 1D arguments

For notational convenience we will write u instead of u_1 in this subsection. Let \mathbb{D}_1 be the finite domain $\mathbb{D}_1 = \{u \in \mathbb{R} | u_L \leq u \leq u_R\}$. The range $[u_L, u_R]$ is subdivided in Ncells centered at

$$u_j = u_L + (j + 1/2)\Delta u_j$$

with sampling-rate $\Delta u = (u_R - u_L)/N$, also see fig. A.1. At the nodes $\{u_j\}$ the functions f = f(u) and g = g(u) have values $f_j = f(u_j)$ and $g_j = g(u_j)$, which are collected in column-vectors $\mathbf{F}, \mathbf{G} \in \mathbb{C}^N$

$$\mathbf{F}^{t} = [f_{1}, \dots, f_{N}] \text{ and } \mathbf{G}^{t} = [g_{1}, \dots, g_{N}].$$

Similarly the kernel P = P(u, u') has nodal values

$$[\mathbf{P}]_{j,k} = P(u_j, u_k); \tag{A.19}$$

these can be collected in the matrix $\mathbf{P} \in \mathbb{C}^{N \times N}$.

If at least one of the two functions f, g vanishes outside \mathbb{D}_1 , then the (n = 1)-versions of equations (A.11) and (A.12) can be approximated as

$$\langle f, g \rangle_b \approx \Delta u \sum_{j=1}^N f_j g_j = \Delta u \mathbf{F}^t \mathbf{G},$$
 (A.20a)

$$\langle f,g \rangle_s \approx \Delta u \sum_{j=1}^N f_j^* g_j = \Delta u \mathbf{F}^{\dagger} \mathbf{G},$$
 (A.20b)

respectively. However, in practical computations neither f or g vanishes outside \mathbb{D}_1 , but rather tend to zero for $u \to \pm \infty$. Approximating an integral over $[-\infty, \infty]$ by one over the finite interval $[u_L, u_R]$ should be done with care. The measure taken here is tapering and is specifically suited to oscillating integrands that tend to zero for $u \to \pm \infty$. The integrand is multiplied by a real-valued weight function, that is equal to 1 everywhere, except close to the limits on the intervals

$$[u_L, u_L + \Delta u_{tap}]$$
 and $[u_R - \Delta u_{tap}, u_R].$

On those intervals the value of the weight function must be between 0 and 1. It must provide a smooth connection between the weights 0 and 1. In Figure A.2 (and all applications) we used for example the weight function

$$t_w(u) = \begin{cases} 0 & \text{if } u < u_L, \\ \sin^2 \left(\frac{\pi(u - u_L)}{2\Delta u_{tap}} \right) & \text{if } 0 \le u - u_L < \Delta u_{tap}, \\ 1 & \text{if } u_L + \Delta u_{tap} \le u \le u_R - \Delta u_{tap}, \\ \sin^2 \left(\frac{\pi(u_R - u)}{2\Delta u_{tap}} \right) & \text{if } 0 < u_R - u \le \Delta u_{tap}, \\ 0 & \text{if } u_R < u. \end{cases}$$

For the discrete representation of the taper weight function t_w we take the diagonal matrix \mathbf{T}_w with entries

$$[\mathbf{T}_w]_{i,i} = t_w(u_i).$$

Instead of the equations (A.20), we approximate the linear forms (A.11) and (A.12) by

$$\langle f, g \rangle_b \approx \int_{\mathbb{D}_1} f(u) t_w(u) g(u) du \approx \Delta u \mathbf{F}^t \mathbf{T}_w \mathbf{G},$$
 (A.21a)

$$\langle f,g \rangle_s \approx \int_{\mathbb{D}_1} f^*(u) t_w(u) g(u) du \approx \Delta u \mathbf{F}^{\dagger} \mathbf{T}_w \mathbf{G},$$
 (A.21b)

Similarly multiplication by the linear operator \hat{P} with kernel P(u', u) is discretized by

$$(\hat{P}f)(u_{j}^{'}) \approx \int_{\mathbb{D}_{1}} P(u_{j}^{'}; u) t_{w}(u) f(u) du \approx \Delta u [\mathbf{PT}_{w}\mathbf{F}]_{j}.$$
 (A.22)

A.3.2 Discretization of kernels with 2-dimensional arguments

The discretization of kernels with *n*-dimensional arguments is essentially similar to the one for 1-dimensional arguments, but the notation required for proper indexing makes live more complicated even for the 2-dimensional case. The index *i* will range over the 2 dimensions, i.e. i = 1, 2.

Let \mathbb{D}_2 be the finite domain

$$\mathbb{D}_2 = \{ \mathbf{u} \in \mathbb{R}^2, i = 1, 2 | u_{i,L} \le u_i \le u_{i,R} \}.$$

Each range $[u_{i,L}, u_{i,R}]$ is subdivided into N_i cells centered around

$$u_{1,\alpha} = u_{1,L} + (\alpha - 1/2)\Delta u_1$$
 and $u_{1,\beta} = u_{2,L} + (\beta - 1/2)\Delta u_2$,

where $\Delta u_i = (u_{i,R} - u_{i,L})/N_i$ are sampling-rates and α and β the coordinate-indices; in total we have $M = N_1 N_2$ sampling points. We will not add an extra index for the second dimension, leading to coordinate-matrices and corresponding function-matrices. Similar to the 1D case we will work with coordinate and function vectors and reserve the matrix-notation for kernels. However, this requires the pair (α, β) to be mapped to mapped to a single index,

$$i = \alpha + (\beta - 1)N_1. \tag{A.23}$$

The reader familiar with programming will recognize equation (A.23) as the way to access a 2D array, actually stored as a 1D array. With this index map the two functions $f = f(\mathbf{u}_H)$ and $g = g(\mathbf{u}_H)$ are given discrete representations

$$\mathbf{F}^{t} = [f_{1}, \dots, f_{M}] \quad \text{where} \quad f_{\alpha+(\beta-1)N_{1}} \triangleq f(u_{1,\alpha}, u_{2,\beta}), \tag{A.24}$$

and
$$\mathbf{G}^{t} = [g_{1}, \dots, g_{M}] \quad \text{where} \quad g_{\alpha+(\beta-1)N_{1}} \triangleq g(u_{1,\alpha}, u_{2,\beta}),$$

respectively. Now that we have chosen a specific ordering for discrete values into vectors, the moment has come to introduce the corresponding ordering for matrices and to connect them to the matrices for the 1D case discussed previously. Given two square matrices $\mathbf{A} \in \mathbb{C}^{N_2 \times N_2}$ and $\mathbf{B} \in \mathbb{C}^{N_1 \times N_1}$, the Kronecker or matrix direct product $\mathbf{A} \otimes \mathbf{B} \in \mathbb{C}^{M \times M}$

is given by

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} A_{11}\mathbf{B} & \dots & A_{1N_2}\mathbf{B} \\ \vdots & \ddots & \vdots \\ A_{N_21}\mathbf{B} & \dots & A_{N_2N_2}\mathbf{B}. \end{pmatrix}.$$
 (A.25)

The first example of the Kronecker product used here is the discrete representation of the taper weight function (see section C.3 for other examples). Let $t_{w,1}(u_1)$ and $t_{w,2}(u_2)$ be the taper weight functions for the coordinates u_1 and u_2 , respectively. If the vector-entries are ordered as dictated by equation (A.23), then the corresponding taper weight matrices $\mathbf{T}_{w,1}$ and $\mathbf{T}_{w,2}$ can be combined into a the discrete representation of the 2D taper weight function

$$t_w(\mathbf{u}_H) = t_{w,1}(u_1)t_{w,2}(u_2)$$

like

$$\mathbf{T}_w = \mathbf{T}_{w,2} \otimes \mathbf{T}_{w,1}. \tag{A.26}$$

Note that due to diagonal structure of its building blocks $\mathbf{T}_{w,1}$ and $\mathbf{T}_{w,2}$, the matrix \mathbf{T}_w is also diagonal. With the definitions introduced by equations (A.23)-(A.26), the (n = 2)-versions of equations (A.11) and (A.12) can be approximated by

$$\langle f, g \rangle_b \approx \int_{\mathbb{D}_2} f(\mathbf{u}_H) t_{w,1}(u_1) t_{w,2}(u_2) g(\mathbf{u}_H) d^2 \mathbf{u}_H,$$

$$\approx \Delta U \sum_{\beta=1}^{N_2} \sum_{\alpha=1}^{N_1} f_{\alpha+(\beta-1)N_1} [\mathbf{T}_{w,1}]_{\alpha,\alpha} [\mathbf{T}_{w,2}]_{\beta,\beta} g_{\alpha+(\beta-1)N_1},$$

$$= \Delta U \mathbf{F}^t \mathbf{T}_w \mathbf{G},$$

$$\langle f, g \rangle_s \approx \Delta U \mathbf{F}^\dagger \mathbf{T}_w \mathbf{G},$$

$$(A.27)$$

where ΔU is redefined to $\Delta U = \Delta u_1 \Delta u_2$.

Analogous to the discrete representation of the function f by equation (A.24), we give a kernel with 2-dimensional arguments the discrete matrix representation

$$P(u_{1,\alpha'}, u_{2,\beta'}; u_{1,\alpha}, u_{2,\beta}) = [\mathbf{P}]_{\alpha' + (\beta' - 1)N_1, \alpha + (\beta - 1)N_1},$$
(A.29)

where $\mathbf{P} \in \mathbb{C}^{M \times M}$ and the factor ΔU has been absorbed in **P**. Similar to the 1D case, the discrete representation of equation (A.7) now reads

$$\hat{P}(u_{1,\alpha'}, u_{2,\beta'})f(u_{1,\alpha'}, u_{2,\beta'}) \approx \int_{\mathbb{D}_2} P(u_{1,\alpha'}, u_{2,\beta'}; \mathbf{u}_H)t_w(\mathbf{u}_H)f(\mathbf{u}_H)d^2\mathbf{u}_H,$$
$$\approx \Delta U[\mathbf{PT}_w\mathbf{F}]_{\alpha'+(\beta'-1)N_1}.$$
(A.30)

This discrete approximation of equation (A.11) and (A.12) also works in case of periodic f, g, assuming all periods lie within the boundaries of the domain \mathbb{D}_n . In case of non-periodicity or non-vanishing integrands outside \mathbb{D}_n , one has to accept finite aperture artifacts and/or try to suppress them. Also see section 3.7.

Appendix B

Pressure normalized reciprocity theorems

B.1 Outline

Besides the normalization of the wave fields involved, the reciprocity theorems used in this thesis can be categorized according to their time-domain appearance. In *convolution* type reciprocity theorems the wave field states involved occur in pairs $P_A P_B$, which becomes a convolution in the time-domain. These theorems are the basis for datarepresentations and a number of seismic processing steps, see Fokkema and Van den Berg [30]. *Correlation* type reciprocity theorems are based on the products $P_A^* P_B$, implying a reversed time-axis for state A. In the time-domain this product becomes a correlation. Correlation type reciprocity theorems are starting points of inversion algorithms.

This appendix will formulate a reciprocity theorem for wave fields, i.e. the one obtained by Lord Rayleigh [79]. For one-way pressure normalized wave fields none has been formulated yet. Although perfectly possible, the derivation is complicated by the fact that local up and down going transmission behaves differently (remember sections 2.3 and 3.6).

Analogous to section 4.3.1 the general form of the convolution type theorem will be introduced, and then as a first application source-receiver reciprocity will deduced. Again the second application is stating a representation theorem, connecting the wave field on a closed surface to the same wave field at some interior point of the volume enclosed by the surface. Then the similarity with section 4.3.1 disappears, and the interactions of up and

down going wave fields will be analyzed.

Correlation type reciprocity theorems for pressure normalized wave fields are almost identical to their convolution type counterparts, aside from the time-reversal in the Green's functions. Only when one-way wave fields are introduced into them, the analysis starts to deviate a little.

B.2 The Rayleigh integral

Helmholtz derived reciprocity theorems independent of the coordinate-system and the shape of the domain. Let P_A and P_B be solutions to equation (1.2) for medium-parameters $\{\rho_A, K_A\}$ and $\{\rho_B, K_B\}$ and source-functions S_A and S_B , respectively; also see table B.1. His physical and mathematical brilliance led Helmholtz to analyze the vector

$$\mathbf{U} = P_A \frac{1}{\rho_B} \nabla P_B - P_B \frac{1}{\rho_A} \nabla P_A. \tag{B.1}$$

Given a volume \mathbb{V} and its corresponding closed surface $\partial \mathbb{V}$ with outward pointing normal **n**, the integral theorem of Gauss states that the outgoing flux through $\partial \mathbb{V}$ and divergence $\nabla \cdot \mathbf{U}$ are related by

$$\oint_{\partial \mathbb{V}} \mathbf{U} \cdot \mathbf{n} d^2 \boldsymbol{\sigma} = \int_{\mathbb{V}} \nabla \cdot \mathbf{U} d^3 \mathbf{x}.$$
(B.2)

The infinitesimal surface-element $d^2 \sigma$ of $\partial \mathbb{V}$ is equal to $d^2 \mathbf{x}_H$ if $\partial \mathbb{V}$ equals $\partial \mathbb{X}\{a, b\}$. After using the frequency-domain version of equation (1.2) to rewrite $\nabla \cdot \mathbf{U}$, equation

	State A	State B
Field	$P_A(\mathbf{x})$	$P_B(\mathbf{x})$
Medium	$\{\rho_A, K_A\}(\mathbf{x})$	$\{\rho_B, K_B\}(\mathbf{x})$
Source	$S_A(\mathbf{x})$	$S_B(\mathbf{x})$

Table B.1: General state table

(B.2) can be expanded into

$$\oint_{\partial \mathbb{V}} \left[P_A \frac{1}{\rho_B} \nabla P_B - P_B \frac{1}{\rho_A} \nabla P_A \right] \cdot \mathbf{n} d^2 \boldsymbol{\sigma} = \int_{\mathbb{V}} \left[P_B S_A - P_A S_B + \omega^2 \left(\frac{1}{K_A} - \frac{1}{K_B} \right) P_A P_B + \left(\frac{1}{\rho_A} - \frac{1}{\rho_B} \right) (\nabla P_A) \cdot (\nabla P_B) \right] d^3 \mathbf{x},$$
(B.3)

which is known as Rayleigh's reciprocity theorem.

Once equation (B.3) is recast in one-way wave fields it would be possible to follow the same approach as for flux normalized wave fields. But Rayleigh derived sourcereceiver reciprocity with less restrictions on the media and the shape of the integrationvolume/surface. To see how, use the states from table B.2. The wave fields are Green's functions for two identical, but otherwise arbitrary media. The point sources need to lie in the interior of \mathbb{V} , that is they are not allowed to lie on the edge $\partial \mathbb{V}$. Shorthand notation for this requirement is to say that the positions $\mathbf{x}_{A,B}$ must obey

$$\mathbf{x}_{A,B} \in \mathbb{V}/\{\partial \mathbb{V}\}.$$

For both states we take $t_s = 0$ (remember equation (1.3)).

Provided the left hand side integral over the boundary $\partial \mathbb{V}$ vanishes, these choices reduce equation (B.3) to

$$G(\mathbf{x}_A; \mathbf{x}_B) = G(\mathbf{x}_B; \mathbf{x}_A). \tag{B.4}$$

Two straightforward, sufficient conditions that make the boundary-integral vanish, are that $\partial \mathbb{V}$ is either free to move or completely rigid; then

$$G(\mathbf{x}; \mathbf{x}_A) = G(\mathbf{x}; \mathbf{x}_B) = 0 \text{ or } \mathbf{n} \cdot \nabla G(\mathbf{x}; \mathbf{x}_A) = \mathbf{n} \cdot \nabla G(\mathbf{x}; \mathbf{x}_B) = 0,$$

on $\partial \mathbb{V}$, respectively.

A third, more general, possibility arises when the configuration obeys *Sommerfeld's* radiation condition for unbounded media, see Bleistein et al. [11]. For the special case that the medium is homogeneous outside a sphere with a finite radius, also containing x_A and x_B , this condition can be translated as follows. On a spherical surface S_{∞} with a radius extending to infinity, the wavefronts of $G_{A,B}$ are locally plane and propagating

	State A	State B
Field	$G(\mathbf{x};\mathbf{x}_A)$	$G(\mathbf{x};\mathbf{x}_B)$
Medium	$\{\rho,K\}(\mathbf{x})$	$\{\rho,K\}(\mathbf{x})$
Source	$\delta(\mathbf{x}-\mathbf{x}_A)$	$\delta(\mathbf{x}-\mathbf{x}_B)$

Table B.2: States for demonstrating source-receiver reciprocity.

both in the direction n, so

$$\mathbf{n} \cdot \nabla G_{A,B} = -jkG_{A,B}.$$

Then again the left hand side of equation (B.3) vanishes, resulting in equation (B.4).

B.3 Pressure normalized representation theorems

	State A	State B
Field	$G(\mathbf{x};\mathbf{x}^{'})$	$P(\mathbf{x})$
Medium	$\{\rho,K\}(\mathbf{x})$	$\{\rho,K\}(\mathbf{x})$
Source	$\delta(\mathbf{x}-\mathbf{x}^{'})$	$S(\mathbf{x})$

Table B.3: States for Kirchhoff Helmholtz integral theorem theorem

The states from table B.3 corresponding to two identical, but again arbitrary media, are plugged into equation (B.3). If \mathbf{x}' lies in $\mathbb{V}/\{\partial\mathbb{V}\}$ and the source-function S is only



Figure B.1: Kirchhoff-Helmholtz configuration

nonzero outside \mathbb{V} , this leads to

$$P(\mathbf{x}') = \oint_{\partial \mathbb{V}} \frac{1}{\rho(\mathbf{x})} \left[G(\mathbf{x}; \mathbf{x}') \nabla P(\mathbf{x}) - P(\mathbf{x}) \nabla G(\mathbf{x}; \mathbf{x}') \right] \cdot \mathbf{n} d^2 \boldsymbol{\sigma}.$$
(B.5)

Equation (B.5) is known as the Kirchhoff Helmholtz integral theorem, also see Figure B.1.

To match the arbitrary volume \mathbb{V} to the slab $\mathbb{X}[a, b]$ the approach of Wapenaar and Berkhout [88] is taken. Let \mathbb{V} have the shape of a cylinder, whose axis goes through \mathbf{x}' and is parallel to the x_3 -axis. The boundary surface of this cylindrical volume is described by

$$\mathbb{V} = \partial \mathbb{V}_a \cup \partial \mathbb{V}_b \cup \partial \mathbb{V}_r$$

where

$$\begin{split} \partial \mathbb{V}_{a} = & \{ \mathbf{x} \in \mathbb{R}^{3} | x_{3} = a, \qquad |\mathbf{x}_{H} - \mathbf{x}_{H}^{'}| < r \}, \\ \partial \mathbb{V}_{b} = & \{ \mathbf{x} \in \mathbb{R}^{3} | x_{3} = b, \qquad |\mathbf{x}_{H} - \mathbf{x}_{H}^{'}| < r \}, \\ \partial \mathbb{V}_{r} = & \{ \mathbf{x} \in \mathbb{R}^{3} | a \le x_{3} \le b, |\mathbf{x}_{H} - \mathbf{x}_{H}^{'}| = r \}; \end{split}$$

also see Figure B.2. To analyze the part of the integral equation (B.5) over $\partial \mathbb{V}_r$,



Figure B.2: Cross-section of the cylindrical integration volume in the parallel to x_1, x_3 -plane, going through \mathbf{x}' .

$$P_{r}(\mathbf{x}') = \int_{\partial \mathbb{V}_{r}} \frac{1}{\rho(\mathbf{x})} \left[G(\mathbf{x}; \mathbf{x}') \nabla P(\mathbf{x}) - P(\mathbf{x}) \nabla G(\mathbf{x}; \mathbf{x}') \right] \cdot \mathbf{n} d^{2} \boldsymbol{\sigma},$$

it is assumed that P is the response of a monopole source at \mathbf{x}'' above or below \mathbb{V} , close to the cylinder-axis, i.e. $|\mathbf{x}''_H - \mathbf{x}'_H| \ll r$. Then the integrand is proportional to r^{-2} at $\partial \mathbb{V}_r$. As the surface-area of $\partial \mathbb{V}_r$ is proportional to r, P_r vanishes if $r \to \infty$. Another consequence of $r \to \infty$ is that $\partial \mathbb{V}_a \to \partial \mathbb{X}\{a\}$ and $\partial \mathbb{V}_b \to \partial \mathbb{X}\{b\}$. Hence for the iib-configuration equation (B.5) reads

$$P(\mathbf{x}') = P_a(\mathbf{x}') - P_b(\mathbf{x}'),$$
(B.6)

where

$$P_{a}(\mathbf{x}') = \int_{\partial \mathbb{X}\{a\}} \frac{1}{\rho} \bigg[G(\mathbf{a}; \mathbf{x}') \partial_{a} P(\mathbf{a}) - P(\mathbf{a}) \partial_{a} G(\mathbf{a}; \mathbf{x}') \bigg] d^{2} \mathbf{a}_{H},$$

and a similar expression for $P_b(\mathbf{x}')$.

Equation (B.6) for pressure normalized two-way wave fields has a form similar to equation (4.16) for flux normalized wave fields. But to arrive at a representation theorem for pressure normalized one-way wave fields it turns out we need an additional constraint:

the medium is not allowed to scatter in the vertical direction, or in mathematical terms

$$\partial_3\{\rho, K\} = 0 \quad \text{at} \quad x_3 = a, b.$$
 (B.7)

This ensures that the up and down going wave fields do not interact at the boundaries $\partial \mathbb{X}\{a, b\}$, so that the pressure normalized one-way wave equation (3.27a) decouples into two independent differential equations for up and down going wave fields; that is at $x_3 = a$ and $x_3 = b$ equation (3.27a) reduces to

$$\partial_3 P^{\pm} = \mp j \hat{H}_1 P^{\pm} = \mp j \rho^{1/2} \hat{H}_1 \rho^{-1/2} P^{\pm};$$
 (B.8)

in the second step equation (3.13) was substituted. If we set $P_s^{\pm} = P^{\pm}/\sqrt{\rho}$, then the absence of vertical scattering formulated by equation (B.7) allows us to rewrite equation (B.8) as

$$\partial_3 P_s^{\pm} = \mp j \hat{\mathsf{H}}_1 P_s^{\pm},\tag{B.9}$$

The same goes for the up and down going parts of the Green's function, $\partial_3 G_s^{\pm} = \pm j \hat{H}_1 G_s^{\pm}$, where similarly $G_s^{\pm} = G^{\pm}/\sqrt{\rho}$. Hence in equation (B.6) $P_a(\mathbf{x}')$ and $P_b(\mathbf{x}')$ can be expanded as

$$P_{c}(\mathbf{x}') = \int_{\partial \mathbb{X}\{c\}} \left[(G_{s}^{+} + G_{s}^{-})\partial_{3}(P_{s}^{+} + P_{s}^{-}) - (P_{s}^{+} + P_{s}^{-})\partial_{3}(G_{s}^{+} + G_{s}^{-}) \right] d^{2}\mathbf{x}_{H},$$
(B.10)

with c = a, b. A further expansion in equation (B.10) of products of sums into a sum of products leads to eight individual products. We will now demonstrate that only products of wave fields propagating in opposite directions contribute. Subsequent use of equation (B.9), and the symmetry of \hat{H}_1 as explained in section 3.4 and equation (3.16), allows us to rewrite

$$P_s^{\pm}\partial_3 G_s^{\pm} = \pm j P_s^{\pm} \hat{\mathsf{H}}_1^t G_s^{\pm}. \tag{B.11}$$

Because we only use these products in an integral expression, we are also allowed to use

the definition of a transposed operator equation (A.13) to reverse the order and say

$$\int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \partial_3 G_s^{\pm} d^2 \mathbf{x}_H = \mp j \int_{\partial \mathbb{X}\{c\}} G_s^{\pm} \hat{H}_1 P_s^{\pm} d^2 \mathbf{x}_H,$$
$$= \int_{\partial \mathbb{X}\{c\}} G_s^{\pm} \partial_3 P_s^{\pm} d^2 \mathbf{x}_H.$$
(B.12a)

Hence in equation (B.10) all products of wave fields propagating in the same direction cancel. However, the same arguments that lead us to equation (B.12a) allow us to relate the cross-terms in (B.10) by

$$\int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \partial_3 G_s^{\mp} d^2 \mathbf{x}_H = -\int_{\partial \mathbb{X}\{c\}} G_s^{\mp} \partial_3 P_s^{\pm} d^2 \mathbf{x}_H.$$
(B.12b)

Clearly the cross-terms in equation (B.10) do not cancel. If in addition there is no vertical scattering in $\mathbb{X}(-\infty, a]$, a point-source in $\mathbb{X}(a, b)$ only produces an outward propagating, up going response at $\partial \mathbb{X}\{a\}$, i.e. $G^+ = 0$ at depth a. Similarly, the same point-source produces only a down going response at $\partial \mathbb{X}\{b\}$ if there is also no vertical scattering in $\mathbb{X}[b,\infty)$, amounting to $G^- = 0$ at depth b. These are exactly the properties of the iibmedium, remember section 4.2, and they allow us to reduce $P_a(\mathbf{x}')$ and $P_b(\mathbf{x}')$ to

$$P_{a}(\mathbf{x}') = -\int \frac{2}{\rho} P^{+}(\mathbf{a}) \partial_{a} G^{-}(\mathbf{a}_{H}, a; \mathbf{x}') d^{2} \mathbf{a}_{H}, \qquad (B.13a)$$

and

$$P_{b}(\mathbf{x}') = -\int \frac{2}{\rho} P^{-}(\mathbf{b}) \partial_{b} G^{+}(\mathbf{b}_{H}, b; \mathbf{x}') d^{2} \mathbf{b}_{H}, \qquad (B.13b)$$

respectively. Note that equation (B.13) only contains products of wave fields propagating in opposite directions. The notation involving integration over \mathbf{a}_H and \mathbf{b}_H was first used on page 86.

Similar to deriving equation (4.17) the main ingredient of the last step toward its pressure normalized equivalent is using source-receiver reciprocity. Invoking reciprocity for receivers at depth *a* means

$$G^{-}(\mathbf{a};\mathbf{x}') = G^{+}(\mathbf{x}';\mathbf{a}) + G^{-}(\mathbf{x}';\mathbf{a}).$$
 (B.14)



Figure B.3: Up and down going parts of $G(\mathbf{x}'; \mathbf{a})$.

The factor P^+ on the right hand side of equation (B.13a) acts as purely a down going source at depth a, so the up and down going parts of equation (B.14) are directly related to the up and down going parts of the left hand side of equation (B.13a), respectively, also see Figure B.3. $G^+(\mathbf{x}'; \mathbf{a})$ corresponds to the transmission response of the domain $\mathbb{X}(a, x_3')$, while $G^-(\mathbf{x}'; \mathbf{a})$ contains the reflection response of the domain $\mathbb{X}[x_3', b)$. Together with a similar argument for $P_b(\mathbf{x}')$ the wave field at \mathbf{x}' is therefore decomposed into the up and down going parts

$$P^{\pm}(\mathbf{x}') = \int \frac{2}{\rho(\mathbf{a})} \frac{\partial G^{\pm}(\mathbf{x}'; \mathbf{a}_H, a)}{\partial a} P^{+}(\mathbf{a}) d^2 \mathbf{a}_H$$
$$-\int \frac{2}{\rho(\mathbf{b})} \frac{\partial G^{\pm}(\mathbf{x}'; \mathbf{b}_H, b)}{\partial b} P^{-}(\mathbf{b}) d^2 \mathbf{b}_H.$$
(B.15)

If $x_3^{'} \rightarrow b$ and $P^-(\mathbf{b}) = 0$ then equation (B.15) splits into

$$P^{+}(\mathbf{b}) = \int T^{+}(\mathbf{b}; \mathbf{a}) P^{+}(\mathbf{a}) d^{2} \mathbf{a}_{H}$$
(B.16a)

where

$$T^{+}(\mathbf{b}; \mathbf{a}) = \frac{2}{\rho(\mathbf{a})} \frac{\partial G^{+}(\mathbf{b}; \mathbf{a}_{H}, a)}{\partial a},$$
 (B.16b)

and

$$P^{-}(\mathbf{a}) = \int R^{+}(\mathbf{a}'; \mathbf{a}|b)P^{+}(\mathbf{a})d^{2}\mathbf{a}_{H},$$
(B.16c)

where

$$R^{+}(\mathbf{a}';\mathbf{a}|b) = \frac{2}{\rho(\mathbf{a})} \frac{\partial G^{-}(\mathbf{a}';\mathbf{a}_{H},a|b)}{\partial a}.$$
 (B.16d)

Similarly the conditions $x'_3 \to a$ and $P^+(\mathbf{a}) = 0$ lead to expressions for the up going transmission and reflection kernels

$$T^{-}(\mathbf{a}; \mathbf{b}) = \frac{-2}{\rho(\mathbf{b})} \frac{\partial G^{-}(\mathbf{a}; \mathbf{b}_{H}, b)}{\partial b},$$
(B.17)

$$R^{-}(\mathbf{b}';\mathbf{b}|a) = \frac{2}{\rho(\mathbf{b})} \frac{\partial G^{+}(\mathbf{b}';\mathbf{b}_{H},b|a)}{\partial b},$$
(B.18)

B.4 Correlation type representation theorem

Earlier this appendix we decided to derive representation theorems for pressure normalized, one-way wave fields from the two-way Kirchhoff-Helmholtz reciprocity theorem. This decision already forced us to move away from our approach of treating pressure and flux normalized wave fields on equal terms. This is true even more for defining pressure normalized inverse propagation with transmission loss correction. Instead of emulating the steps taken in section 5.5, we follow Wapenaar and Berkhout [88]. They arrived at the extension of equation(s) (2.48) to laterally varying media through a correlation type representation theorem similar to equation (B.15) based on the Kirchhoff-Helmholtz reciprocity theorem.

The derivation of the correlation-type representation theorem is similar to that of its convolution counterpart, but there are some subtle differences. Given the states of table B.1 consider the correlation interaction quantity

$$\mathbf{U} = P_A^* \frac{1}{\rho_B} \nabla P_B - P_B \frac{1}{\rho_A} \{ \nabla P_A \}^*;$$
(B.19)

see section 5.3 of Fokkema and Van den Berg [30] for the reason of this choice. Tracing the effects of inserting equation (B.19) instead of (B.1) into the theorem of Gauss, equation (B.2), to the representation theorem equation (B.5), shows that its correlation type counterpart reads

$$P(\mathbf{x}) = \oint_{\partial \mathbb{V}} \frac{1}{\rho(\mathbf{x})} \left[G^*(\mathbf{x}'; \mathbf{x}) \nabla P(\mathbf{x}') - P(\mathbf{x}') \{ \nabla G(\mathbf{x}'; \mathbf{x}) \}^* \right] \cdot \mathbf{n} d^2 \boldsymbol{\sigma}'.$$
(B.20)



Figure B.4: Time reversed Kirchoff-Helmholtz configuration

Also see Figure B.4. The transition $\mathbb{V} \to \mathbb{X}[a, b]$ does not interfere with the analysis leading to equation (B.6), so its correlation type counterpart reads

$$P(\mathbf{x}) = \bar{P}_b(\mathbf{x}) - \bar{P}_a(\mathbf{x}), \tag{B.21}$$

where

$$\bar{P}_{c}(\mathbf{x}') = \int_{\partial \mathbb{X}\{c\}} \frac{1}{\rho} \bigg[G^{*} \partial_{3} P - P\{\partial_{3} G\}^{*} \bigg] d^{2} \mathbf{x}'_{H},$$

for c = a, b. Besides the switch of primes, the other differences between equations (B.6) and (B.21),

 $G \to G^*$, and $\partial_3 G \to \{\partial_3 G\}^*$,

although seemingly minor, become more profound when analyzing the interactions of up and down going wave fields. In equation (B.11) it is perfectly possible to make the transition $G^{\pm} \rightarrow \{G^{\pm}\}^*$, so that

$$\int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \partial_3 \{G_s^{\pm}\}^* d^2 \mathbf{x}_H = \mp j \int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \{\hat{\mathsf{H}}_1 G_s^{\pm}\}^* d^2 \mathbf{x}_H,$$
$$= \pm j \int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \hat{\mathsf{H}}_1^{\dagger} \{G_s^{\pm}\}^* d^2 \mathbf{x}_H.$$
(B.22)

Because also these products only appear in an integral, using equation (A.13) defining the transposed of an operator to reverse the order is allowed once again. However, the result of this last step is not exactly what we want because

$$\partial_3 P_s^{\pm} \neq \mp j \hat{\mathsf{H}}_1^* P_s^{\pm};$$

substitution of equation (B.9) does therefore not produce a useful result. But neglecting evanescent wave fields allows $\hat{H}_1^* \approx \hat{H}_1$, so we can obtain the (approximate) correlation counterparts of equation (B.12)

$$\int_{\partial \mathbb{X}\{c\}} \{G_s^{\pm}\}^* \partial_3 P_s^{\pm} d^2 \mathbf{x}_H \approx -\int_{\partial \mathbb{X}\{c\}} P_s^{\pm} \{\partial_3 G^{\pm}\}^* d^2 \mathbf{x}_H$$
(B.23a)

and

$$\int_{\partial \mathbb{X}\{c\}} \{G_s^{\pm}\}^* \partial_3 P_s^{\mp} d^2 \mathbf{x}_H \approx \int_{\partial \mathbb{X}\{c\}} P_s^{\mp} \partial_3 \{G_s^{\pm}\}^* d^2 \mathbf{x}_H.$$
(B.23b)

The approximation-sign \approx in equation (B.23) and expressions derived from it will be replaced by an equal-sign = as long as negligence of evanescent wave fields is the only approximation.

Just as in the flux normalized case this approximation is a blessing in disguise; as a result the useful propagating wave fields will not be obscured by time reversed evanescent wave fields turning into exponentially growing. Due to the change of sign in equation (B.23) compared to (B.12), neglecting evanescent wave fields allows the reduction of equation (B.21) to

$$P(\mathbf{x}) \approx \int \frac{2}{\rho(\mathbf{a})} \left[\frac{\partial G^{-}(\mathbf{a}; \mathbf{x})}{\partial a} \right]^{*} P^{-}(\mathbf{a}) d^{2} \mathbf{a}_{H} - \int \frac{2}{\rho(\mathbf{b})} \left[\frac{\partial G^{+}(\mathbf{b}; \mathbf{x})}{\partial b} \right]^{*} P^{+}(\mathbf{b}) d^{2} \mathbf{b}_{H}.$$
(B.24)

As in equation (B.13) the fact was used that only the outward propagating Green's functions at $\partial \mathbb{X}\{a, b\}$ are nonzero, if G^{\pm} corresponds to an iib-medium. Another similarity is that only wave fields propagating in different directions do not cancel. The decomposition of the left hand side of equation (B.24) into up and down going parts will lead to expressions less compact than equation (B.15), because reconstructing the up or down going source field at \mathbf{x}' requires both the transmission and reflection response. But it uses much the same ideas.

Similar to equation (B.14) the up going Green's function $G^{-}(\mathbf{a}; \mathbf{x})$ is the sum of two parts,

$$G^{-}(\mathbf{a}; \mathbf{x}) = G_r^{-}(\mathbf{a}; \mathbf{x}) + G_d^{-}(\mathbf{a}; \mathbf{x}).$$
(B.25a)

 $G_r^-(\mathbf{a}; \mathbf{x})$ is due to the down going part of the source field scattered upward, while $G_d^-(\mathbf{a}; \mathbf{x})$ is due to the up going part of the source field and going directly from \mathbf{x} to \mathbf{a} , also see Figure B.5. The down going Green's function allows a decomposition analogous to equation (B.25a),

$$G^{+}(\mathbf{b};\mathbf{x}) = G_{r}^{+}(\mathbf{b};\mathbf{x}) + G_{d}^{+}(\mathbf{b};\mathbf{x}).$$
(B.25b)

Here $G_r^+(\mathbf{b}; \mathbf{x})$ is due to the up going part of the source field scattered downward, and $G_d^+(\mathbf{b}; \mathbf{x})$ is due to the down going part of the source field and going directly from \mathbf{x}' to **b**. Hence, equation (B.25) permits the separation of (B.24) in up and down going parts



Figure B.5: Up going response at $\partial \mathbb{X}(a)$ due to down going source field (left) and up going source field (right).

like

$$P^{-}(\mathbf{x}) = \int \frac{2}{\rho(\mathbf{a})} \left[\frac{\partial G_{d}^{-}(\mathbf{a}; \mathbf{x})}{\partial a} \right]^{*} P^{-}(\mathbf{a}) d^{2} \mathbf{a}_{H}$$
$$- \int \frac{2}{\rho(\mathbf{b})} \left[\frac{\partial G_{r}^{+}(\mathbf{b}; \mathbf{x})}{\partial b} \right]^{*} P^{+}(\mathbf{b}) d^{2} \mathbf{b}_{H}, \qquad (B.26a)$$

$$P^{+}(\mathbf{x}) = \int \frac{2}{\rho(\mathbf{a})} \left[\frac{\partial G_{r}^{-}(\mathbf{a};\mathbf{x})}{\partial a} \right]^{*} P^{-}(\mathbf{a}) d^{2} \mathbf{a}_{H}$$
$$- \int \frac{2}{\rho(\mathbf{b})} \left[\frac{\partial G_{d}^{+}(\mathbf{b};\mathbf{x})}{\partial b} \right]^{*} P^{+}(\mathbf{b}) d^{2} \mathbf{b}_{H}.$$
(B.26b)

For inverse propagation of up going, pressure normalized wave fields, we assume that the source S is zero in the upper halfspace $\mathbb{X}(-\infty, b]$ and we take $x_3 \to b$ in equation (B.26a). Note that for this limit $P^+(\mathbf{b})$ becomes a pure reflection, which we indicate by attaching a subscript r, and the reflected Green's function becomes the up going reflection response of horizontal slab between depths a and b,

$$G_r^+(\mathbf{b}; \mathbf{x}) \longrightarrow R^-(\mathbf{b}; \mathbf{b}').$$

Also see equation (B.18). For the up going case we take $x_3 \to a$ in equation (B.26b), and assume that the source S is zero in the half space $\mathbb{X}[a, \infty)$. The conventional approach is to assume $G_r^{\pm} = 0$, leading to the so-called matched filter approach; take for the kernels of the inverse up and down going transmission operators

$$F^{-}(\mathbf{b}; \mathbf{a}) \approx \frac{2}{\rho(\mathbf{a})} \left[\frac{\partial G_d^{-}(\mathbf{a}; \mathbf{b})}{\partial a} \right]^*$$
 (B.27a)

and

$$F^{+}(\mathbf{a}, \mathbf{b}) \approx \frac{2}{\rho(\mathbf{b})} \left[\frac{\partial G_d^{+}(\mathbf{b}; \mathbf{a})}{\partial b} \right]^*,$$
 (B.27b)

respectively. Bearing in mind the horizontally layered case, equation (2.42), we state that the error is proportional to the squared reflection response. For weak to moderate contrasts this error is therefore small. But for stronger contrasts the amplitude errors become significant.

After substitution of equation (B.16c) for the up going reflection kernel into (B.26b), Wapenaar and Berkhout [88] arrived at an expression of essentially the same form as equation (5.12) for inverse propagation of down going, flux normalized wave fields.

Appendix C

Numerical differentiation

C.1 Numerical differentiation and polynomial interpolation

Given a function g tabulated at points N + 1 points (or nodes) $u_0 < u_1 < \ldots < u_N$. The function can be approximated by interpolation through the Lagrange form

$$g(u) \approx \sum_{i=0}^{N} g(u_i) l_i(u) + \frac{g^{(n+1)}(\xi_u)}{(n+1)!} w(u),$$
(C.1)

where the cardinal functions l_i are given by

$$l_i(u) = \prod_{\substack{j=0\\j\neq i}}^N \frac{u - u_j}{u_i - u_j}.$$
 (C.2)

See Kincaid [54]. First and second order derivatives of the cardinal functions are given by

$$l_{i}^{'}(u) = C_{i} \sum_{\substack{k=0\\k\neq i}}^{N} \prod_{\substack{j=0\\k\neq i,k}}^{N} (u-u_{j}), \text{ and } l_{i}^{''}(u) = C_{i} \sum_{\substack{k=0\\k\neq i}}^{N} \sum_{\substack{l=0\\k\neq i,k}}^{N} \prod_{\substack{j=0\\j\neq i,k,l}}^{N} (u-u_{j}),$$

where

$$C_i = \prod_{\substack{j=0\\ j \neq i}}^{N} (u_i - u_j)^{-1}.$$

Here N is taken even, m = N/2, and the equidistant nodes are chosen symmetric around $u_i = u_0 + (i - m) * \Delta u$. Now C_i reads

$$C_i = \Delta u^{-N} \prod_{\substack{j=0\\j \neq i}}^{N} (i-j)^{-1}.$$

At the central node u_m the derivatives of the cardinal functions read

$$l_{i}^{'}(u_{m}) = C_{i}\Delta u^{N-1} \sum_{\substack{k=0\\k\neq i}}^{N} \prod_{\substack{j=0\\j\neq i,k}}^{N} (m-j),$$
(C.3)
$$l_{i}^{''}(u_{m}) = C_{i}\Delta u^{N-2} \sum_{\substack{k=0\\k\neq i}}^{N} \sum_{\substack{l=0\\k\neq i}}^{N} \prod_{\substack{j=0\\j\neq i,k,l}}^{N} (m-j).$$
(C.4)

For N = 2 one obtains the expressions

$$g_{0}^{'} = \frac{g_{1} - g_{-1}}{2\Delta u} + O(\Delta u^{2}) \quad \text{and} \quad g_{0}^{''} = \frac{g_{1} - 2g_{0} + g_{-1}}{\Delta u^{2}} + O(\Delta u^{2}).$$

Note that all indices were lowered by an amount of m/2 for notational convenience. More accurate approximations can be obtained for N = 4,

$$\begin{split} g_{0}^{'} &- O(\Delta u^{4}) = \frac{-g_{a,2} + 8g_{a,1}}{12\Delta u}, \\ g_{0}^{''} &- O(\Delta u^{4}) = \frac{-g_{s,2} + 16g_{s,1} - 30g_{0}}{12\Delta u^{2}}, \end{split}$$

or even N = 6,

$$\begin{split} g_{0}^{'} &- O(\Delta u^{6}) = \frac{3g_{a,3} - 27g_{a,2} + 135g_{a,1}}{180\Delta u}, \\ g_{0}^{''} &- O(\Delta u^{6}) = \frac{2g_{s,3} - 27g_{s,2} + 270g_{s,1} - 490g_{0}}{180\Delta u^{2}}, \end{split}$$

respectively, where $g_{s,i} = g_i + g_{-i}$ and $g_{a,i} = g_i - g_{-i}$. These expressions were obtained using the Ginac C++-library for symbolic computation.

C.2 Numerical differentiation in the Fourier domain

Under periodic boundary conditions another approach is available; multiplication with the frequency/wavenumber in the Fourier domain, remember equation (1.8). If periodic boundary conditions are used while applying the polynomial expressions of section C.1, the resulting operators are equal to those generated by Fourier domain multiplication. This will not be proven here.

To construct the matrix representations of first and second order differentiation in the Fourier domain, go back to the formal definition of Ψ DO's in appendix A.1, and use equations (A.7) and (A.8). Setting $\hat{P} = \partial_u^m$ and $p(u, w) = (jw)^m$ in equations (A.7) and (A.8), respectively, leads to

$$\partial_{u}^{m}g(u) = \frac{1}{2\pi} \int_{\mathbb{R}} \left[\int_{\mathbb{R}} (jw)^{m} e^{jw(u-u')} g(u') du' \right] dw.$$
(C.5)

After first reversing the order of integration and then using the fact that anti-symmetric integrands vanish, the first and second order derivatives have kernel representations

$$\partial_{u}g(u) = \int_{\mathbb{R}} d^{(1)}(u, u^{'})g(u^{'})du^{'}, \quad \text{and} \quad \partial_{u}^{2}g(u) = \int_{\mathbb{R}} d^{(2)}(u, u^{'})g(u^{'})du^{'},$$

where

$$d^{(1)}(u, u') = \frac{-1}{2\pi} \int_{\mathbb{R}} w \sin(w(u - u')) dw, \qquad (C.6a)$$

$$d^{(2)}(u, u') = \frac{-1}{2\pi} \int_{\mathbb{R}} w^2 \cos(w(u - u')) dw.$$
 (C.6b)

Equation (C.5) implies

$$d^{(2)}(u, u^{''}) = \int_{\mathbb{R}} d^{(1)}(u, u^{'}) d^{(1)}(u^{'}, u^{''}) du^{'}.$$
 (C.6c)

Instead of the usual expressions of the type of equations (3.37), the discrete finite aperture approximations $d^{(1)}$ and $d^{(2)}$ of (C.6a) and (C.6b) are obtained with standard discrete Fourier transformation,

$$d_{pq}^{(1)} = -\frac{1}{N} \sum_{s} \sin\left(\frac{2\pi s(q-p)}{N}\right) w_s,$$

$$d_{pq}^{(2)} = -\frac{1}{N} \sum_{s} \cos\left(\frac{2\pi s(q-p)}{N}\right) w_s^2.$$

Applying periodic boundary conditions to functions not obeying them of course also mistreats differentiation at the boundaries, introducing the spurious wrap around effects commonly encountered in the use of discrete Fourier transform.

C.3 The discrete representation of two dimensional differential operators

For the purpose of this thesis we could stop here. But for future application to 2D media some additional notation is given, based on the notation introduced in section A.3. Let $\mathbf{I}_{1,2}$ be unit matrices $\mathbf{I}_1 \in \mathbb{R}^{N_1 \times N_1}$ and $\mathbf{I}_2 \in \mathbb{R}^{N_2 \times N_2}$. Given 1D approximate matrix representations $\mathbf{d}_1^{(1)} \in \mathbb{R}^{N_1 \times N_1}$ and $\mathbf{d}_2^{(1)} \in \mathbb{R}^{N_2 \times N_2}$ of the differential operators ∂_1 and ∂_2 respectively, the full 2D approximations are expressed as Kronecker products,

$$\mathbf{D}_1 = \mathbf{I}_2 \otimes \mathbf{d}_1^{(1)} \quad \text{and} \quad \mathbf{D}_2 = \mathbf{d}_2^{(1)} \otimes \mathbf{I}_1. \tag{C.7}$$

With 1D approximate matrix representations $\mathbf{d}_1^{(2)} \in \mathbb{R}^{N_1 \times N_1}$ and $\mathbf{d}_2^{(2)} \in \mathbb{R}^{N_2 \times N_2}$ of the differential operators ∂_1^2 and ∂_2^2 , respectively, the approximate matrix representation of the Laplacian $\nabla_H \cdot \nabla_H$ is

$$\mathbf{D}_L = \mathbf{I}_2 \otimes \mathbf{d}_1^{(2)} + \mathbf{d}_2^{(2)} \otimes \mathbf{I}_1.$$
(C.8)

Abstract

Seismic redatuming with transmission loss correction in complex media

In the years 1920-1930 men that we would nowadays call exploration geophysicists, started using seismic reflections to explore the subsurface of the earth for oil. A decade later they first employend migration algorithms to construct images of the subsurface.

Traditionally migration and redatuming algorithms focus primarily on the kinematic information in seismic reflections, that is traveltimes. They disregard amplitude information, that is reflection strength, because processing amplitude information requires more measurements and much more computing resources. In this thesis we describe and develop an algorithm for redatuming that aims to preserve amplitude information, by observing the symmetries and conservation laws of acoustic wave propagation. In particular we want to observe energy conservation while undoing the propagation effects between the actual sources and receivers on the surface, the original datum, and the sources and receivers buried in the subsurface, the new datum.

Conventional redatuming amounts to correlation of the reflection data with the up and down going transmission responses of the overburden, the part of the medium between the surface datum on the one hand and the datum buried in the subsurface on the other. Even if the exact Green's functions are used, conventional redatuming fails to preserve amplitude information. This is particularly true for high contrast media because the energy lost in transmission, that is the energy carried by the reflections of the overburden, is not accounted for. Starting from reciprocity theorems for flux normalized one-way wave fields, Wapenaar derived a correction for these transmission losses, which holds for multiply scattered wave fields in laterally varying 2D and 3D media.

For 1D media, Chapter 2 of this thesis gives a review of the one-way wave field the-

ory used in the later Chapters. Chapters 3, 4 and the first part of Chapter 5 extend the theoretical review of Chapter 2 to laterally varying media. We conclude Chapter 5 by discussing an optimized implementation of media of transmission loss corrected redatuming. In Chapter 6 we show how to estimate the reflection response of the overburden from the measured data. In Chapter 7 we show how to extend the one-way wave field of Chapters 3-6 to curvilinear. This allows amongst others redatuming to a non-flat datum in the subsurface, for example a curved reflector.

Samenvatting

Seismisch redatumen met correctie voor transmissieverliezen in complexe media

In de periode 1920-1930 begonnen lieden die we nu exploratie-geofysici zouden noemen, seismische reflecties te gebruiken om naar olie te zoeken. Een decenium later gebruikten ze voor het eerst migratie-algoritmes om afbeeldingen te maken van de ondergrond.

Van oudsher zijn migratie- en redatum-algoritmes in de eerste plaats gericht op de kinematische informatie in de seismische reflecties, dat wil zeggen de reistijden. Ze verstoren de amplitude informatie, dat wil zeggen reflectie-sterkte, omdat het correct verwerken hiervan meer metingen en veel meer rekenkracht vergt. In dit proefschrift beschrijven en ontwikkelen we een algoritme dat poogt de amplitude informatie wel te behouden, door de symmetriëen en behoudswetten van geluidsvoortplanting in acht nemen. In het bijzonder richten we ons op energiebehoud tijdens het verwijderen van de propagatie-effecten tussen de daadwerkelijke bronnen en ontvangers aan het oppervlak, het originele datumvlak, en de hypothetische bronnen en ontvangers gelegen op het nieuwe datum-vlak in de ondergrond.

Reguliere redatum-algoritmes komen neer op correlatie van de reflectie-data met de op- en neergaande transmissie responsies van de deklagen, het gedeelte van de ondergrond tussen het oppervlakte datum-vlak en het datum-vlak in de ondergrond. Ook als hiervoor de exacte Greense functies worden gebruikt, dan nog zal regulier redatumen de amplitude informatie verstoren. Dit geldt in het bijzonder voor deklagen met grote onderlinge contrasten omdat de transmissie-verliezen, dat wil zeggen de energie van de reflecties van de deklagen, verwaarloosd worden. Op basis van reciprociteit-stellingen voor fluxgenormalizeerde éénweg golfvelden heeft Wapenaar een correctie voor deze transmissieverliezen opgesteld. Deze correctie is geldig voor meervoudig verstrooide golfvelden in 2D en 3D media met laterale variaties.

Voor 2D media recapituleert Hoofdstuk 2 van dit proefschrift de theorie voor éénweg golfvelden, waarna Hoofdstukken 3, 4 en het eerste deel van Hoofdstuk 5 de recapitulatie verder uitwerken voor media met laterale variaties. We sluiten Hoofdstuk 5 af met het bespreken van een geoptimalizeerde implementatie van correctie voor transmissieverliezen. Vervolgens bespreken we in Hoofdstuk 6 een methode om de reflectie respons van de deklagen te schatten uit de gemeten reflecties. In Hoofdstuk 7 laten we zien hoe flux-genormalizeerde golfveld decompositie uitgebreid kan worden naar curvilineaire coordinaten. Dit maakt het onder andere mogelijk om met gekromde datum-vlakken te werken.
About the author

Martijn Frijlink was born on the 20th of July 1975 in Zwolle, but moved to Eindhoven on his first anniversary. Upon acquiring his gymnasium diploma in 1993, he moved to Amsterdam to join the physics department of the University of Amsterdam. Here, the omnipresent Ajax-fans brought to live an hitherto latent adherence to PSV.

After some initial doubts and changes of direction, Martijn finally ended up in computational physics, between the two traditional branches of experimental and theoretical physics. In the year 2000 he earned his M.Sc.-degree for radiation pressure computations on interstellar dust-particles.

Upon completion he turned his sights 180 degrees, and joined the Geotechnologydepartment of the faculty of Civil Engineering and Geosciences (CiTG). In the section of Applied Geophysics and Petrophysics he started his Ph.D. research under the supervision of Prof. dr. ir. Wapenaar on True Amplitude migration.

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