Maslov asymptotic extension of Generalized Radon Transform inversion in anisotropic elastic media: a Least-Squares approach

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Abstract. Linearized asymptotic inversion of seismic data is carried out in general anisotropic media. In an anisotropic medium, even if it is homogeneous, the shear waves form (instantaneous) caustics. In the absence of caustics, we formulated the seimic inverse scattering problem via the Generalized Radon Transform (GRT). In the presence of caustics, which are associated with multi pathing, we have to rederive the inversion procedure which is now based on the weak formulation of the inverse problem. The key ingredients are the Maslov canonical operators describing the transmission from the image point to the sources and the receivers, and delicate high-dimensional stationary phase analyses. The importance of caustics in practical applications becomes apparent in the analysis of mode converted wave constituents in sedimentary basins.

1. Introduction

For wave propagation in media that are non-trivially heterogeneous and elastic, the formation of caustics is quite common. Due to the heterogeneity, multi-pathing in the set of characteristics or geometrical rays might occur, while due to anisotropic elasticity the quasi-shear-wave fronts might 'fold'. Both phenomena truly coexist in geophysical applications, and may be hard to separate.

In these lecture notes, we will focus on the construction of an asymptotic inversion formula in the presence of multi-pathed and multi-mode wave propagation. The asymptotic inversion of remote scattering data is based on a separation of medium components: a smooth component – typically represented by spline functions – that is *known* and defines the *background* medium, and a singular component – typically step-function like – that is *unknown* and defines the medium *contrast*.

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Caustics are supposed to form in the background medium. The medium contrast is supposed to be represented by a superposition of conormal functions, i.e., functions that are singular across surfaces. Asymptotic inversion carries out a mapping from the singular support of the scattering data (wave front) to the singular support of the medium contrast (interfaces). Underlying the inversion are the assumptions that: the (incident) wave field in the background medium can be evaluated with Maslov asymptotics (the background is sufficiently smooth), and the scattered field can be evaluated in the Born approximation (the contrast is sufficiently localized and small).

The success of the construction presented in these notes relies on the choice of parametrization of the scattering data. Our parametrization is the one of the Generalized Radon Transform (GRT) and originates at each point where the contrast is to be reconstructed. The conventional parametrization, the one of the Kirchhoff diffraction stack, simply uses the coordinates of observation. The GRT parametrization 'unfolds' the scattering data, unlike the Kirchhoff parametrization.

The simplest form of an asymptotic inversion procedure can be found in Norton and Linzer [1]. The scalar GRT was introduced and analyzed by Beylkin [2, 3, 4, 5] and Miller *et al.* [6, 7]. The relation between the GRT and inversion of spherical averages was highlighted by Fawcett [8]. GRT-style inversion formulas for the *linearized* elastic inverse problem have been developed by Beylkin and Burridge [9] for the *isotropic* case and by De Hoop *et al.* [10, 11], Spencer and De Hoop [12] and Burridge *et al.* [13] for the *anisotropic* case. De Hoop and Bleistein [14] developed a GRT formalism exploiting a conormal representation of the medium contrast, following the original work of Bleistein [15]. All these formulas were strictly valid for the case of single pathing. The inclusion of *multi-pathing* in the (anisotropic) elastic asymptotic inversion formulas is the subject of these lecture notes. A summary can be found in De Hoop [16].

The outline of these notes is as follows. In the following section the basic equations for anisotropic elastic wave scattering are given. Our inverse scattering problem, including multi-pathing and multi-modes, is formulated as a *Least-Squares* (LS) minimum solution. In Section 3 Maslov asymptotic theory in anisotropic elastic media is summarized. In Section 4 we introduce the high-frequency-Born approximation to the scattering problem, and analyze the associated direct scattering operator and its properties. Also, using a reciprocity argument, we introduce the *adjoint* of the direct scattering operator. The adjoint operator represents the process of *imaging*, i.e., (re)constructing the singular support of the medium contrast. In Section 5, upon composing the adjoint with the orginal direct scattering operators, we construct the *normal* operator. In this Section we discuss conditions under which imaging is possible. Then we extract from the normal operator a pseudo-differential constituent. In Section 6 we finally construct the inversion formula from the normal and the adjoint operators and obtain the Maslov extension of GRT inversion; using a stationary-phase analysis, we recover a LS-GRT inversion. Finally, in Section 7 we reduce the LS-GRT inversion of

Section 6 to the *direct* GRT inversion.

2. The basic equations

We consider a configuration, in which we illuminate a remote scattering domain $\mathcal{D} \subset \mathbb{R}^3$ with elastic waves generated by point body forces at $\boldsymbol{s} \in \partial S \sim S^2$ and observed by multi-component point receivers at $\boldsymbol{r} \in \partial R \sim S^2$ for times $t \in \mathbb{R}_{\geq 0}$.

We assume that ∂S and ∂R do not intersect $\mathcal{D}$, but ∂S and ∂R may have points in common. We denote the manifold on which experiments are carried out by $\mathcal{Q} = \partial S \times \partial R \times \mathbb{R}_{\geq 0}$. Experiments are sections of a vector bundle with base $\mathcal{Q}$ and fibres containing the polarizations. To enhance consistency in notation, we denote the scattering domain also by $\mathcal{X} = \mathcal{D}$. We will analyze the scattered field due to a singular medium perturbation with support contained in $\mathcal{X}$, on top of a smoothly varying elastic background occupying $\mathbb{R}^3$. The medium perturbation can be viewed as the section of a vector bundle with base $\mathcal{X}$ and fibres containing scalar density combined with the rank four stiffness tensor.

The inverse problem concerns (re)constructing the singular medium perturbation from the information on the singular support (wave front) of the scattered field measurements. We assume that we can measure the arrival time of and amplitude on the wave front of the scattered field, as well as the polarization and the moveout tangent direction. We will restrict our analysis to body waves.

2.1. Notation

First, we introduce some basic notation. We choose Cartesian coordinates in the configuration, and let $\boldsymbol{s} = (s_1, s_2, s_3)$ denote the source position vector, $\boldsymbol{r} = (r_1, r_2, r_3)$ the receiver position vector, $\boldsymbol{x} = (x_1, x_2, x_3)$ and $\boldsymbol{y} = (y_1, y_2, y_3)$ the scattering and image point position vectors, and t the time. The medium is described by $\rho(\boldsymbol{x})$, the scalar density of mass, and $c_{ijk\ell}(\boldsymbol{x})$, the elastic stiffness tensor. The wavefield is represented by the three-component displacement vector $\boldsymbol{u}(\boldsymbol{x}, t) = (u_1(\boldsymbol{x}, t), u_2(\boldsymbol{x}, t), u_3(\boldsymbol{x}, t))$ and is generated by a source distribution given by the body-force source density $\boldsymbol{f}(\boldsymbol{x}, t) = (f_1(\boldsymbol{x}, t), f_2(\boldsymbol{x}, t), f_3(\boldsymbol{x}, t))$. In the following, we will employ the summation convention.

2.2. Governing wave equation

The displacement in a heterogeneous anisotropic elastic medium satisfies the wave equation

$$\rho\, \partial_t^2 u_i - \partial_j (c_{ijk\ell} \partial_\ell u_k) = f_i \ . \tag{1}$$

Let

$$\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{x}', t) = (G_{ip}(\boldsymbol{x}, \boldsymbol{x}', t)) \tag{2}$$

be the causal Green's tensor, which – in the time domain – satisfies (cf. equation (1))

$$\rho\, \partial_t^2 G_{ip} - \partial_j (c_{ijk\ell} \partial_\ell G_{kp}) = \delta_{ip} \delta(\boldsymbol{x} - \boldsymbol{x}') \delta(t) \ , \ \ G_{ip} = 0 \ \text{ for } \ t < 0 \ . \tag{3}$$

In the frequency domain, $\partial_t \to -i\omega$, and we get †

$$\rho\, \omega^2 G_{ip} + \partial_j (c_{ijk\ell} \partial_\ell G_{kp}) = -\delta_{ip} \delta(\boldsymbol{x} - \boldsymbol{x}') \ , \tag{4}$$

where, for $\omega \in \mathbb{R}$, the sense of causality is lost. In the following, we will consider ω to be a large parameter.

3. Maslov asymptotics

Here, we summarize the formulation of Maslov asymptotic theory [17] in anisotropic media with emphasis on the evaluation of the Green's tensor defined in equation (4). For a more detailed discussion, we refer the reader to Kendall and Thomson [18]. For a discussion on acoustic Maslov theory in a geophysical context, see Chapman and Drummond [19].

3.1. Ray geometry, travel time

Let $\tau(\boldsymbol{x}; \boldsymbol{x}')$ denote the travel time along a ray connecting $\boldsymbol{x}$ with $\boldsymbol{x}'$. The wave front is given by $\Sigma(\boldsymbol{x}', t) = \{\boldsymbol{x} \mid \tau(\boldsymbol{x}; \boldsymbol{x}') = t\}$ and the propagation cone by $\{(\boldsymbol{x}, t) \mid \tau(\boldsymbol{x}; \boldsymbol{x}') - t = 0\}$. The travel time satisfies the first-order partial differential equation (cf. equation (1))

$$\det[\rho\, \delta_{ik} - c_{ijk\ell} (\partial_\ell \tau)(\partial_j \tau)] = 0 \ . \tag{5}$$

Let

$$\boldsymbol{\gamma}_{\boldsymbol{x}} = \nabla_{\boldsymbol{x}} \tau(\boldsymbol{x}; \boldsymbol{x}') \tag{6}$$

denote the slowness vector, which is normal to the wave front $\Sigma(\boldsymbol{x}', t)$ at $\boldsymbol{x}$. The slowness vector lies on a sextic surface, $\mathsf{A}(\boldsymbol{x})$, consisting of three ovoid sheets, $\mathsf{A}^{(N)}(\boldsymbol{x})$, $N = 1, 2, 3$, each surrounding the origin. To see this, we define the phase velocity V,

$$V = \frac{1}{|\boldsymbol{\gamma}|} \ , \qquad \boldsymbol{\gamma}_{\boldsymbol{x}} = \frac{\boldsymbol{\alpha}_{\boldsymbol{x}}}{V(\boldsymbol{x}, \boldsymbol{\alpha}_{\boldsymbol{x}})} \ , \tag{7}$$

so that $\boldsymbol{\alpha}_{\boldsymbol{x}}$ is the unit vector in the direction of $\boldsymbol{\gamma}_{\boldsymbol{x}}$. Substituting equation (7) into equation (5) we recognize that ρV^2 are the eigenvalues of a positive symmetric matrix with $_{ik}$ entries $c_{ijk\ell} \alpha_\ell \alpha_j$. Thus at each $\boldsymbol{x}$, for each direction $\boldsymbol{\alpha}_{\boldsymbol{x}}$, there are three positive values $V^{(N)}(\boldsymbol{x}, \boldsymbol{\alpha}_{\boldsymbol{x}})$, $N = 1, 2, 3$, of V. Then, as $\boldsymbol{\alpha}_{\boldsymbol{x}}$ sweeps the unit sphere, each

$$\boldsymbol{\gamma}_{\boldsymbol{x}}^{(N)} = \frac{\boldsymbol{\alpha}_{\boldsymbol{x}}}{V^{(N)}(\boldsymbol{x}, \boldsymbol{\alpha}_{\boldsymbol{x}})} \tag{8}$$

sweeps a closed sheet, $\mathsf{A}^{(N)}(\boldsymbol{x})$, of $\mathsf{A}(\boldsymbol{x})$.

† In our convention, the Fourier transform is given by $\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{x}', t) = (2\pi)^{-1} \int_{-\infty}^{\infty} \boldsymbol{G}(\boldsymbol{x}, \boldsymbol{x}', \omega) \exp(-i\omega t)\, \mathrm{d}\omega$.

For *general* $\boldsymbol{\gamma}$ not necessarily on A, let $\mathcal{V}^{(N)}(\boldsymbol{x},\boldsymbol{\gamma})$ be defined by

$$\det[\rho(\boldsymbol{x})(\mathcal{V}^{(N)})^2\delta_{ik} - c_{ijk\ell}(\boldsymbol{x})\gamma_\ell\gamma_j] = 0 \ . \tag{9}$$

The functions $\mathcal{V}^{(N)}$ are positive homogeneous of degree one in $\boldsymbol{\gamma}$; in view of equation (8) the surface $\mathsf{A}^{(N)}(\boldsymbol{x})$ is given by

$$\mathcal{V}^{(N)}(\boldsymbol{x},\boldsymbol{\gamma}) = 1 \ . \tag{10}$$

For waves in mode N we may then write equation (5) in the form

$$\mathcal{V}^{(N)}(\boldsymbol{x},\nabla_{\boldsymbol{x}}\tau) = 1 \ . \tag{11}$$

It is standard practice to solve equation (11) by the method of characteristics. The characteristic curves follow from the equalities

$$\frac{\mathrm{d}x_i}{\partial_{\gamma_i}\mathcal{V}^{(N)}} = \frac{\mathrm{d}\tau}{\gamma_i\partial_{\gamma_i}\mathcal{V}^{(N)}} = -\frac{\mathrm{d}\gamma_i}{\partial_{x_i}\mathcal{V}^{(N)}} \ . \tag{12}$$

By the homogeneity of $\mathcal{V}^{(N)}$ in $\boldsymbol{\gamma}$ and Euler's relation, we have

$$\gamma_i\partial_{\gamma_i}\mathcal{V}^{(N)} = \mathcal{V}^{(N)} = 1 \ . \tag{13}$$

With this relation, equation (12) implies the Hamilton system

$$\frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \partial_{\gamma_i}\mathcal{V}^{(N)} \ , \qquad \frac{\mathrm{d}\gamma_i}{\mathrm{d}\tau} = -\partial_{x_i}\mathcal{V}^{(N)} \ , \tag{14}$$

subject to the constraint (10), the general solutions of which are the *bi*characteristics $(\boldsymbol{x}^{(N)}(\tau),\boldsymbol{\gamma}_{\boldsymbol{x}}^{(N)}(\tau))$ in phase $(\boldsymbol{x}\boldsymbol{\gamma})$-space. The traces of $\boldsymbol{x}^{(N)}(\tau)$ are the rays in ordinary space. Adding to the Hamilton system an initial condition, the one associated with the Green's tensor (cf. equation (3))

$$\boldsymbol{x}^{(N)}(\tau=0) = \boldsymbol{x}' \ , \quad \boldsymbol{\gamma}^{(N)}(\tau=0) = \frac{\boldsymbol{\alpha}_{\boldsymbol{x}'}}{V^{(N)}(\boldsymbol{x}',\boldsymbol{\alpha}_{\boldsymbol{x}'})} \ , \quad \boldsymbol{\alpha}_{\boldsymbol{x}'} \in S^2_{\boldsymbol{x}'} \subset S^2 \tag{15}$$

for example, the bicharacteristics form a three-dimensional manifold embedded in $\mathbb{R}^6$. Particular coordinates on this manifold follow from equation (6). ($S^2_{\boldsymbol{x}'}$ denotes a subset of the unit sphere; for later use, we introduce coordinates (q_1,q_2) on this sphere.)

Consider the Hamiltonian

$$\mathcal{H}^{(N)} = \mathcal{V}^{(N)} - 1 \ .$$

Via the *inverse* Legendre transformation, this Hamiltonian can be mapped into a Lagrangian, homogeneous of degree one in

$$v_i = \frac{\mathrm{d}x_i}{\mathrm{d}\tau} = \partial_{\gamma_i}\mathcal{V}^{(N)} = \partial_{\gamma_i}\mathcal{H}^{(N)} \ . \tag{16}$$

This relation induces a mapping from the slowness vector $\boldsymbol{\gamma}$ to the group velocity $\boldsymbol{v}$ at each $\boldsymbol{x}$. In view of equation (13) these vectors are each other's polar reciprocals, i.e. $\gamma_i v_i = 1$, which reflects the fact that $\boldsymbol{v}$ represents the coordinates of a tangent vector while $\boldsymbol{\gamma}$ represents the coordinates of the corresponding cotangent vector. In accordance with this observation, we introduce the mapping from the group velocity to the slowness vector $\boldsymbol{\gamma} = \boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{v})$. The Lagrangian then follows as (Epstein and Śniatycki [20])

$$L^{(N)}(\boldsymbol{x}, \boldsymbol{v}) = \gamma_i(\boldsymbol{x}, \boldsymbol{v})\, v_i - \mathcal{H}^{(N)}(\boldsymbol{x}, \boldsymbol{\gamma}(\boldsymbol{x}, \boldsymbol{v})) = \gamma_i(\boldsymbol{x}, \boldsymbol{v})\, v_i \;, \tag{17}$$

in view of constraint (10). In fact, with τ parametrizing the bicharacteristics, $L^{(N)}(\boldsymbol{x}, \boldsymbol{v}) = 1$ (equation (13)); we find that along the bicharacteristics

$$\mathrm{d}\tau^{(N)} = \gamma_i^{(N)} \mathrm{d}x_i^{(N)} \;. \tag{18}$$

If there are multiple rays connecting $\boldsymbol{x}$ with $\boldsymbol{x}'$, we employ the more careful notation $\tau(\boldsymbol{x}; \boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'})$, or $\tau(\boldsymbol{x}; \boldsymbol{\alpha}_{\boldsymbol{x}'})$ in shorthand, to identify each individual ray. This way, the geometry of the bicharacteristics with initial conditions (15) will be represented by $(\boldsymbol{x}^{(N)}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}), \boldsymbol{\gamma}_{\boldsymbol{x}}^{(N)}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}))$. We will omit the superscript $^{(N)}$ in subsections where it is irrelevant which the mode under consideration is.

The form $\gamma_i \mathrm{d}x_i$ is denoted as the fundamental symplectic one form. Taking its exterior derivative, leads to the standard symplectic form in phase space; it is given by $\mathrm{d}\gamma_i \wedge \mathrm{d}x_i$. The restriction of this form to the manifold of bicharacteristics vanishes, because

$$\mathrm{d}(\partial_i \tau) \wedge \mathrm{d}x_i = (\partial_j \partial_i \tau)\, \mathrm{d}x_j \wedge \mathrm{d}x_i$$

$$= \textstyle\sum_i \mathrm{d}(\partial_i^2 \tau)\, \mathrm{d}x_i \wedge \mathrm{d}x_i + \sum_{j \neq i} (\partial_j \partial_i \tau)\, [\mathrm{d}x_j \wedge \mathrm{d}x_i + \mathrm{d}x_i \wedge \mathrm{d}x_j] = 0.$$

This is the generic property of so-called *Lagrangian* manifolds.

3.2. The partial Legendre transformation

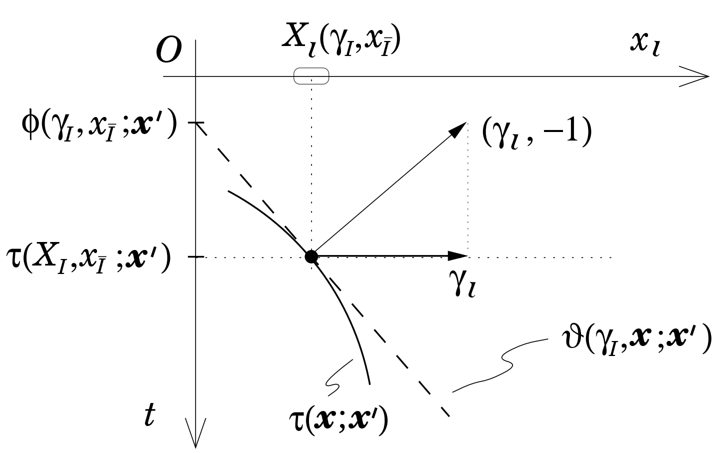

Figure 1. The Legendre transformation and the Maslov phase function.

Applying the *integrated* partial Legendre transformation to the travel time function comprises the following procedure. Let the subsets $I \cup \bar{I} = \{1, 2, 3\}$ induce a partitioning of subscripts: $\imath \in I$ labels at most two out of three coordinates and $\bar{\imath} \in \bar{I}$ the remaining one(s), so that $(\gamma_I, x_{\bar{I}})$ constitute proper coordinates on the Lagrangian manifold over a region Ω_I. We will denote a point in this manifold by $\boldsymbol{\lambda}$; if $\boldsymbol{\lambda} \in \Omega_I$, it has a neighborhood admitting a diffeomorphic projection onto the $(\gamma_I, x_{\bar{I}})$-domain. Let X_I denote the point in the plane $x_{\bar{I}}$ = constant where the wave front has (projected) slowness γ_I; the mapping $\gamma_I \to X_I$ represents a change of coordinates on the Lagrangian manifold.

The Legendre transform ϕ of τ is then given by

$$\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') = \tau(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}; \boldsymbol{x}') - \gamma_\imath X_\imath(\gamma_I, x_{\bar{I}}) \ . \tag{19}$$

Differentiating expression (19) with respect to γ_I, since $\partial_{X_I}\tau = \gamma_I$, it follows that

$$\partial_{\gamma_I}\phi = -X_I \ \text{ for } \ x_{\bar{I}} \ \text{ fixed} \quad (\partial_{x_{\bar{I}}}\phi = \gamma_{\bar{I}} \ \text{ for } \ \gamma_I \ \text{ fixed}) \ . \tag{20}$$

From equations (19)-(20) it also follows that

$$\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') - \gamma_\imath(\partial_{\gamma_\imath}\phi)(\gamma_I, x_{\bar{I}}) = \tau(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}; \boldsymbol{x}') \ . \tag{21}$$

The function ϕ in turn defines a hypersurface $\{(\gamma_I, x_{\bar{I}}, t) \mid t - \phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') = 0\}$. The Legendre transformation can be reapplied to ϕ to yield

$$\tau(X_I, x_{\bar{I}}; \boldsymbol{x}') = \phi(\gamma_I(X_I, x_{\bar{I}}), x_{\bar{I}}; \boldsymbol{x}') + X_\imath\gamma_\imath(X_I, x_{\bar{I}}) \ ,$$

and we recover the original travel time function. Now, in view of equation (20), it follows that

$$\partial_{X_I}\tau = \quad \gamma_I \ \text{ for } \ x_{\bar{I}} \ \text{ fixed} \quad (\partial_{x_{\bar{I}}}\tau = \gamma_{\bar{I}} \ \text{ for } \ x_I \ \text{ fixed}) \ . \tag{22}$$

Note that ϕ satisfies a pseudo-differential equation of the type (11), viz.

$$\mathcal{V}^{(N)}(-\partial_{\gamma_I}\phi, x_{\bar{I}}, \gamma_I, \partial_{x_{\bar{I}}}\phi) = 1 \ . \tag{23}$$

From equation (19) we construct the phase function (see figure 1)

$$\begin{aligned} \vartheta(\gamma_I, \boldsymbol{x}; \boldsymbol{x}') &= \phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') + \gamma_\imath x_\imath \\ &= \tau(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}; \boldsymbol{x}') + \gamma_\imath(x_\imath - X_\imath(\gamma_I, x_{\bar{I}})) \ . \end{aligned} \tag{24}$$

This is the arrival time at x_I of a 'constant $\boldsymbol{\gamma}$ wave' reaching X_I at time $\tau(X_I, x_{\bar{I}}; \boldsymbol{x}')$, see figure 2. At $x_I = X_I(\gamma_I, x_{\bar{I}})$ this phase is stationary, i.e.

$$(\partial_{\gamma_I}\vartheta)(\gamma_I, \boldsymbol{x}; \boldsymbol{x}') = x_I - X_I(\gamma_I, x_{\bar{I}}) = 0 \quad \text{when} \quad \boldsymbol{\gamma} = \boldsymbol{\gamma}_{\boldsymbol{x}}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}) \tag{25}$$

is associated with the geometrical ray connecting $\boldsymbol{x}'$ with $\boldsymbol{x}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'})$. The stationary phase argument leads to

$$\vartheta((\gamma_{\boldsymbol{x}})_I, \boldsymbol{x}; \boldsymbol{x}') = \tau(\boldsymbol{x}; \boldsymbol{x}') \ , \tag{26}$$

on the bicharacteristics, while

$$\nabla_{\boldsymbol{x}}\vartheta((\gamma_{\boldsymbol{x}})_I, \boldsymbol{x}; \boldsymbol{x}') = \boldsymbol{\gamma}_{\boldsymbol{x}} \ . \tag{27}$$

The partial Legendre transformation is illustrated in the $(tx_I$-)domain, in figure 1.

3.3. The Maslov canonical operator

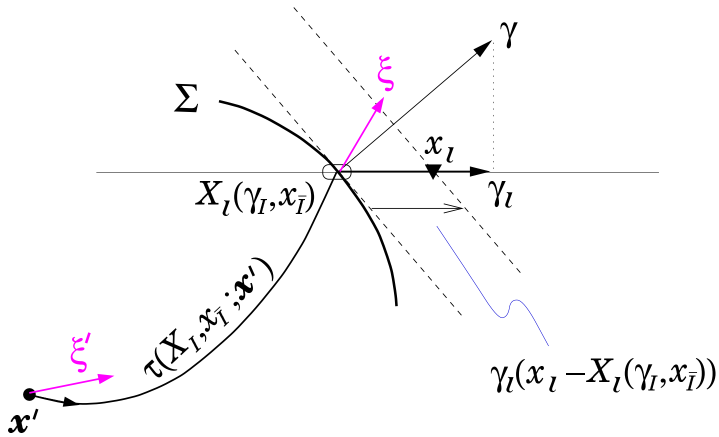

Figure 2. Contributions from neighboring rays at the point of observation with coordinates $x_\imath$.

In the high-frequency approximation†, the Green's tensor decomposes into three uncoupled modes $N \in \{1, 2, 3\}$, associated with qP, qS1 and qS2 polarized wave constituents. The ('one-way') Maslov asymptotic representation for each mode on a given region, Ω_I, of the Lagrangian manifold is given by

$$G_{ip}^{(N)}(\boldsymbol{x}, \boldsymbol{x}', \omega) \sim \left(\frac{i\omega}{2\pi}\right)^{|I|/2} \times$$
$$\int B^{(N)}(\gamma_I, x_{\bar I}; \boldsymbol{x}')\, \xi_i^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I}) \xi_p^{(N)}(\boldsymbol{x}')\ \exp[i\omega\, \vartheta^{(N)}(\gamma_I, \boldsymbol{x}; \boldsymbol{x}')]\, \mathrm{d}\gamma_I \tag{28}$$

(see figures 2 and 3). Note that the Legendre transformation of travel time generates a term $\gamma_\imath(x_\imath - X_\imath(\gamma_I, x_{\bar I}))$ in the Maslov phase function (24), which implies that the integrand in equation (28) is a (high-frequency) representation of the Green's tensor in the spatial Fourier ($\omega\gamma_I$-)domain. The entire amplitude tensor appearing in the oscillatory integral of equation (28) is yet to be determined. As before, we will freely omit the superscripts $^{(N)}$.

In the stationary phase analysis (cf. equations (25)-(27)) of equation (28) we encounter the $|I| \times |I|$ Hessian

$$\frac{\partial^2 \vartheta}{\partial \gamma_I^2} = -\frac{\partial X_I}{\partial \gamma_I} \text{ for } x_{\bar I} \text{ fixed}, \tag{29}$$

using equation (24). Carrying out this stationary phase analysis of the Maslov representation‡,

† Away from conical points, in the absence of kiss or intersection singularities (for a treatment of those see Coates and Chapman [21]).

‡ Thom's theorem can be employed to prescribe a normal form of the Maslov phase function [22]; this form can be used to evaluate the slowness integral representation *at* a caustic [23].

away from caustics, yields the mapping from $B^{(N)}$ to the geometrical ray amplitude $A^{(N)}$,

$$A(X_I(\gamma_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}), x_{\bar{I}}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'})), x_{\bar{I}}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}); \boldsymbol{x}') = \frac{B(\gamma_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}), x_{\bar{I}}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}); \boldsymbol{x}')}{\sqrt{|\det[\mathsf{h}_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'})]|}} \exp\left[i\tfrac{1}{2}\pi \mathrm{sgn}(\omega)\ \mathrm{inerdex}\, \mathsf{h}_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'})\right] , \tag{30}$$

with

$$\mathsf{h}_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}) \equiv \left(\frac{\partial^2 \vartheta}{\partial \gamma_I^2}\right)\Bigg|_{(\gamma_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}), \boldsymbol{x}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}); \boldsymbol{x}')} , \tag{31}$$

which, with the aid of expression (29), can be rewritten as

$$\mathsf{h}_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}) = -\left(\frac{\partial X_I}{\partial \gamma_I}\right)\Bigg|_{(\gamma_I(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}), x_{\bar{I}}(\boldsymbol{x}', \boldsymbol{\alpha}_{\boldsymbol{x}'}))} , \tag{32}$$

and

$$\mathrm{inerdex}\, \mathsf{h}_I \equiv \tfrac{1}{2}\left(\mathrm{sgn}\, \mathsf{h}_I + |I|\right) = \tfrac{1}{2}\left(-\mathrm{sgn}\left(\frac{\partial X_I}{\partial \gamma_I}\right) + |I|\right) \equiv -\mathrm{inerdex}\left(\frac{\partial X_I}{\partial \gamma_I}\right), \tag{33}$$

the inertial index of h_I (its number of positive eigenvalues). The Jacobian in the right-hand

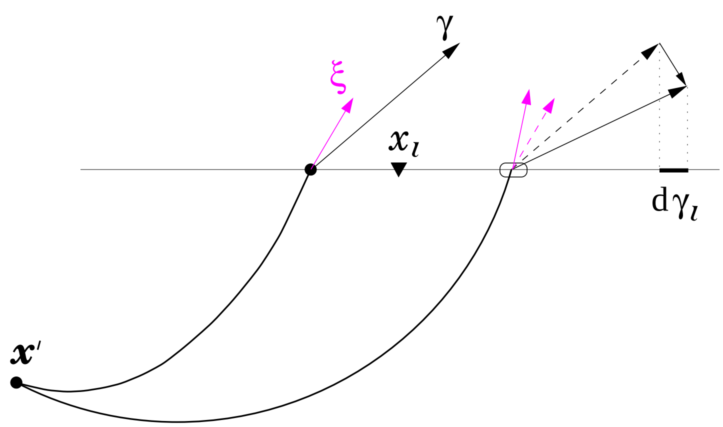

Figure 3. The Maslov integral.

side of equation (32) is related to the geometrical spreading, see figure 4.

Let us now analyze and compare representations of the type (28), and their stationary phase approximations, at *different* points, $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$ say, on a curve, ℓ say, contained in Ω_I (see Mishchenko *et al.* [24]). Assuming that B is well defined everywhere on Ω_I, but allowing the occurrence of a singular point† associated with a caustic (in the $\boldsymbol{x}$-domain) on the curve, the

† A point $\boldsymbol{\lambda}$ in the Lagrangian manifold is said to be *non*-singular if it has a neighborhood admitting a diffeomorphic projection onto the $\boldsymbol{x}$-domain.

path index is introduced as

$$\mathrm{ind}\,\ell[\boldsymbol{\lambda},\boldsymbol{\lambda}'] = -\mathrm{inerdex}\,\left(\frac{\partial X_I}{\partial \gamma_I}\right)\bigg|_{\boldsymbol{\lambda}} + \mathrm{inerdex}\,\left(\frac{\partial X_I}{\partial \gamma_I}\right)\bigg|_{\boldsymbol{\lambda}'} \,. \tag{34}$$

The index counts the number of changes of sign in the curvatures of the wave front between (the projections of) the non-singular points $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}$. A ray lifts to a curve on the Lagrangian manifold that can be broken up into segments $\ell \subset \Omega_I$. The accumulation of the indices $\mathrm{ind}\,\ell$ along the curve is the so-called KMAH index σ: in the presence of caustics, the amplitude A connecting $\boldsymbol{x}$ with $\boldsymbol{x}'$ becomes complex with phase factor $\exp[i\frac{1}{2}\pi\mathrm{sgn}(\omega)\;\sigma(\boldsymbol{x}(\boldsymbol{x}',\boldsymbol{\alpha}_{\boldsymbol{x}'}))]$ [25, 26].

On the other hand, representations (28) on overlapping regions $\Omega_I \cap \Omega_J$ say – where Ω_J admits coordinates $(\gamma_J, x_{\bar{J}})$ – should 'match' asymptotically at a *common* point. A special case of such a match was discussed in equations (30)-(33) where $J = \emptyset$ and $\bar{J} = \{1,2,3\}$. In general, let us introduce the set notation

$$\bar{\jmath}_I \in I \cap \bar{J} \quad \text{and} \quad \jmath_{\bar{I}} \in \bar{I} \cap J \,.$$

Then we have to apply the cascade of (inverse) Fourier transforms,

$$\left(\frac{-i\omega}{2\pi}\right)^{|\bar{I}\cap J|/2} \int \left(\frac{i\omega}{2\pi}\right)^{|I\cap\bar{J}|/2} \int \exp[i\omega\,(\gamma_{\bar{\jmath}_I} x_{\bar{\jmath}_I} - \gamma_{\jmath_{\bar{I}}} x_{\jmath_{\bar{I}}})] \cdots \mathrm{d}\gamma_{I\cap\bar{J}}\,\mathrm{d}x_{\bar{I}\cap J} \,,$$

to the integrand of the integral in equation (28)

$$B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\,\xi_i^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\xi_p^{(N)}(\boldsymbol{x}')\;\exp[i\omega\,\phi^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')]$$

to obtain the integrand in a representation of the type

$$\left(\frac{i\omega}{2\pi}\right)^{|J|/2} \int \cdots \exp[i\omega\,\gamma_\jmath x_\jmath]\,\mathrm{d}\gamma_J \,,$$

which resembles representation (28) on the region Ω_J (cf. equation (24)). The factor in front of the Fourier transforms can be rewritten as (with $(-1) = \exp[-i\pi]$)

$$\left(\frac{-i\omega}{2\pi}\right)^{|\bar{I}\cap J|/2} \left(\frac{i\omega}{2\pi}\right)^{|I\cap\bar{J}|/2} = (-1)^{|\bar{I}\cap J|/2} \left(\frac{i\omega}{2\pi}\right)^{(|I\cap\bar{J}|+|\bar{I}\cap J|)/2} \,.$$

The phase of this cascade of Fourier transforms, $\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') + \gamma_{\bar{\jmath}_I} x_{\bar{\jmath}_I} - \gamma_{\jmath_{\bar{I}}} x_{\jmath_{\bar{I}}}$, is *stationary* (compare equation (25)) if

$$\left\{ \begin{array}{rcccl} x_{\bar{\jmath}_I} & = & -\partial_{\gamma_{\bar{\jmath}_I}}\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') & = & X_{\bar{\jmath}_I}(\gamma_I, x_{\bar{I}}) \,, \\ \\ \gamma_{\jmath_{\bar{I}}} & = & \partial_{x_{\jmath_{\bar{I}}}}\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') & = & \gamma_{\jmath_{\bar{I}}}(\gamma_I, x_{\bar{I}}) \end{array} \right. \tag{35}$$

(using equation (20)). This system of equations represents the transformation of coordinates $(\gamma_I, x_{\bar{I}})$ to $(\gamma_J, x_{\bar{J}})$: $x_{\jmath_{\bar{I}}} \to \gamma_{\jmath_{\bar{I}}}$, $\gamma_{\bar{\jmath}_I} \to x_{\bar{\jmath}_I}$ on $\Omega_I \cap \Omega_J$.

Carrying out the stationary phase analysis of the cascade of Fourier transforms, we encounter the Hessian of $\phi(\gamma_I, x_{\bar I}; \boldsymbol{x}')$ with respect to the coordinates $(x_{\jmath_{\bar I}}, \gamma_{\bar\jmath_I})$, which with the aid of equation (35) can be written as the $(|I \cap \bar J| + |\bar I \cap J|) \times (|I \cap \bar J| + |\bar I \cap J|)$ Jacobian

$$\mathsf{j}_{I\to J}(\gamma_I, x_{\bar I}) = \frac{\partial(\gamma_{\jmath_{\bar I}}, -x_{\bar\jmath_I})}{\partial(x_{\jmath_{\bar I}}, \gamma_{\bar\jmath_I})} \ . \tag{36}$$

Then the phase factor associated with the stationary phase analysis is given by

$$\exp\left[i\ \left(\tfrac{1}{2}\pi \mathrm{sgn}(\omega)\, \mathrm{inerdex}\, \mathsf{j}_{I\to J} + \omega\left\{\phi(\gamma_I, x_{\bar I}; \boldsymbol{x}') + \gamma_{\bar\jmath_I} x_{\bar\jmath_I} - \gamma_{\jmath_{\bar I}} x_{\jmath_{\bar I}}\right\}\right)\right] \ ,$$

evaluated at the stationary point set (cf. equation (35)), with

$$\mathrm{inerdex}\, \mathsf{j}_{I\to J} = \tfrac{1}{2}\left(\mathrm{sgn}\, \mathsf{j}_{I\to J} + |I \cap \bar J| + |\bar I \cap J|\right) \ . \tag{37}$$

Hence, the transformation of representation (28) on Ω_I to the associated representation on Ω_J amounts to a multiplication by the phase factor (Mishchenko *et al.* [24, 4.1.2]),

$$\exp[i\ (\tfrac{1}{2}\pi \mathrm{sgn}(\omega)\, \mathsf{c}_{IJ} + \omega\, \mathsf{d}_{IJ})] \ ,$$

with

$$\mathsf{c}_{IJ} = \mathrm{inerdex}\, \mathsf{j}_{I\to J} - |\bar I \cap J| \ , \tag{38}$$

$$\mathsf{d}_{IJ} = \phi(\gamma_I, x_{\bar I}; \boldsymbol{x}') - \phi(\gamma_J, x_{\bar J}; \boldsymbol{x}') + \gamma_{\bar\jmath_I} x_{\bar\jmath_I} - \gamma_{\jmath_{\bar I}} x_{\jmath_{\bar I}} \tag{39}$$

(representing the difference in partial Legendre transformations: $\gamma_{\bar\jmath_I} x_{\bar\jmath_I} - \gamma_{\jmath_{\bar I}} x_{\jmath_{\bar I}} = \gamma_\imath x_\imath - \gamma_\jmath x_\jmath$), and a division of the kind

$$B(\gamma_J, x_{\bar J}; \boldsymbol{x}') = \frac{B(\gamma_I, x_{\bar I}; \boldsymbol{x}')}{\sqrt{|\det[\mathsf{j}_{I\to J}]|}} \ , \tag{40}$$

in accordance with the coordinate transformation given by equation (35). It can be shown that d_{IJ} is a real-valued constant ($\mathrm{d}\,\mathsf{d}_{IJ} = 0$) whereas c_{IJ} is an integer to be considered $\bmod 4$.

Away from caustics in the $\boldsymbol{x}$-domain, in the case where $J = \emptyset$ and $\bar J = \{1, 2, 3\}$ (hence $\bar I \cap J = \emptyset$ also) we find the identification $\mathsf{j}_{I\to J} \to \mathsf{h}_I$ (cf. equation (36)). Equation (35) then reduces to equation (25), i.e., $x_I = X_I(\gamma_I, x_{\bar I})$ while $\mathsf{d}_{IJ} = 0$. Upon applying the analysis of equation (30) to representations (28) on Ω_I and on Ω_J, and matching the results, leads to the observation that the index c_{IJ} of the pair (Ω_I, Ω_J) can directly be related to the ray geometry according to

$$\mathsf{c}_{IJ} = -\mathrm{inerdex}\ \left.\left(\frac{\partial X_I}{\partial \gamma_I}\right)\right|_{\boldsymbol{\lambda}} + \mathrm{inerdex}\ \left.\left(\frac{\partial X_J}{\partial \gamma_J}\right)\right|_{\boldsymbol{\lambda}} \tag{41}$$

(compare equation (34)). It can be shown that the difference in equation (41) is constant ($\bmod 4$) on the set of all non-singular points $\boldsymbol{\lambda} \in \Omega_I \cap \Omega_J$ (Maslov and Fedoriuk [17, Lemma 6.4]). As a consequence, the index $\mathrm{ind}\,\ell$ in equation (34) along a curve ℓ contained in $\Omega_I \cap \Omega_J$, does not depend on the choice of coordinates.

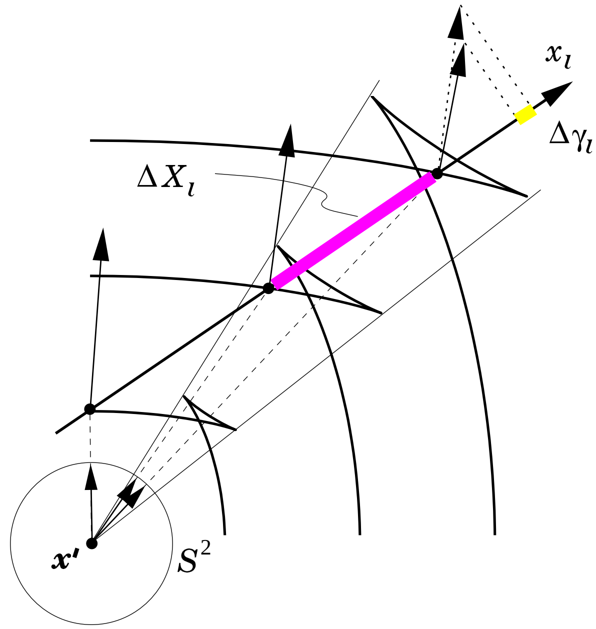

Figure 4. Illustration of the geometrical spreading – of a qSV wave – in the $x_\imath$ direction. In gray are depicted the differences $\Delta X_\imath$ and $\Delta\gamma_\imath$; on S^2 is shown the difference in group direction associated with $\Delta X_\imath$.

3.4. The transport equation

We will now discuss the equations that $\boldsymbol{\xi}$ and B, appearing in the integrand of equation (28), should satisfy. To this end, implicitly, we will develop a 'commutation formula' for the elastic wave operator defined by equation (3) and the Maslov integral given in equation (28), see Maslov and Fedoriuk [17, §8.3].

While substituting representation (28) into equation (4), we will make use of the following derivatives: from equation (24) we obtain

$$\partial_{x_\imath}\vartheta = \gamma_\imath \ , \tag{42}$$

whereas from equation (24) with equation (20) we obtain

$$\partial_{x_{\bar\imath}}\vartheta = \partial_{x_{\bar\imath}}\phi = \gamma_{\bar\imath} \ \text{ for } \ \gamma_I \ \text{ fixed} \ , \tag{43}$$

where, implicitly, $\gamma_{\bar\imath} = \gamma_{\bar\imath}(\gamma_I, x_{\bar I})$.

Carrying out the substitution into equation (4), and collecting terms $\mathcal{O}(\omega^n)$, $n = 2, 1, 0$, yields ($n = 2 - m$; m increases with smoothness)

$$\sum_{m=0}^{2}\left(\frac{i\omega}{2\pi}\right)^{|I|/2}(i\omega)^{2-m}\rho(\boldsymbol{x}) \int \mathcal{I}_{ip}^{(2-m)}(\boldsymbol{x},\boldsymbol{\gamma};\boldsymbol{x}') \ \exp[i\omega\,\vartheta^{(N)}(\gamma_I,\boldsymbol{x};\boldsymbol{x}')]\,\mathrm{d}\gamma_I = 0 \ , \tag{44}$$

where, with $c_{ijk\ell} = \rho\, \hat{c}_{ijk\ell}$,

$$\mathcal{I}^{(2)}_{ip}(\boldsymbol{x},\boldsymbol{\gamma};\boldsymbol{x'}) =$$

$$[\delta_{ik} - \hat{c}_{i\imath k\imath'}(\boldsymbol{x})\gamma_\imath\gamma_{\imath'} - \hat{c}_{i\bar{\imath}k\imath'}(\boldsymbol{x})\gamma_{\bar{\imath}}\gamma_{\imath'} - \hat{c}_{i\imath k\bar{\imath}'}(\boldsymbol{x})\gamma_\imath\gamma_{\bar{\imath}'} - \hat{c}_{i\bar{\imath}k\bar{\imath}'}(\boldsymbol{x})\gamma_{\bar{\imath}}\gamma_{\bar{\imath}'}] \tag{45}$$

$$B^{(N)}(\gamma_I, x_{\bar{I}};\boldsymbol{x'})\,\xi^{(N)}_k(X_I(\gamma_I,x_{\bar{I}}),x_{\bar{I}})\xi^{(N)}_p(\boldsymbol{x'})\ ,$$

in which $\imath,\imath' \in I$ and $\bar{\imath},\bar{\imath}' \in \bar{I}$, and (since $\partial_{x_\imath}\{B^{(N)}\,\xi^{(N)}_k\xi^{(N)}_p\} = 0$)

$$\mathcal{I}^{(1)}_{ip}(\boldsymbol{x},\boldsymbol{\gamma};\boldsymbol{x'}) = -[\rho(\boldsymbol{x})]^{-1}$$

$$[(\partial_{x_\imath}c_{i\imath k\imath'})(\boldsymbol{x})\,\gamma_{\imath'} + (\partial_{x_{\bar{\imath}}}c_{i\bar{\imath}k\imath'})(\boldsymbol{x})\,\gamma_{\imath'} + (\partial_{x_\imath}c_{i\imath k\bar{\imath}'})(\boldsymbol{x})\,\gamma_{\bar{\imath}'} + (\partial_{x_{\bar{\imath}}}c_{i\bar{\imath}k\bar{\imath}'})(\boldsymbol{x})\,\gamma_{\bar{\imath}'}]$$

$$B^{(N)}(\gamma_I, x_{\bar{I}};\boldsymbol{x'})\,\xi^{(N)}_k(X_I(\gamma_I,x_{\bar{I}}),x_{\bar{I}})\xi^{(N)}_p(\boldsymbol{x'})$$

$$-[\hat{c}_{i\imath k\bar{\imath}'}(\boldsymbol{x})\gamma_\imath\,\partial_{x_{\bar{\imath}'}} + \hat{c}_{i\bar{\imath}k\imath'}(\boldsymbol{x})\gamma_{\imath'}\,\partial_{x_{\bar{\imath}}} + \hat{c}_{i\bar{\imath}k\bar{\imath}'}(\boldsymbol{x})\gamma_{\bar{\imath}}\,\partial_{x_{\bar{\imath}'}} \tag{46}$$

$$+\hat{c}_{i\bar{\imath}k\bar{\imath}'}(\boldsymbol{x})\gamma_{\bar{\imath}'}\,\partial_{x_{\bar{\imath}}} + \hat{c}_{i\bar{\imath}k\bar{\imath}'}(\boldsymbol{x})(\partial_{x_{\bar{\imath}}}\gamma_{\bar{\imath}'})]$$

$$B^{(N)}(\gamma_I, x_{\bar{I}};\boldsymbol{x'})\xi^{(N)}_k(X_I(\gamma_I,x_{\bar{I}}),x_{\bar{I}})\xi^{(N)}_p(\boldsymbol{x'})\ ,$$

and so on. Here, partial derivatives of medium parameters enclosed in parentheses, $(\partial_{x_{\bar{\imath}}}c_{i\bar{\imath}k\imath'})$ for instance, are taken under the assumption that $\{x_I, x_{\bar{I}}\}$ are the independent variables, i.e., such derivatives relate simply to the arguments. In expressions (45)-(46), $\boldsymbol{x} = (x_I, x_{\bar{I}})$ and γ_I are not necessarily connected through the mapping $x_I = X_I(\gamma_I, x_{\bar{I}})$ via a point on a bicharacteristic. Also, note that $\mathcal{I}^{(n)}_{ip}$ depends on x_I through the medium parameters (scalar density and stiffness tensor) only. Let us now expand $\mathcal{I}^{(n)}_{ip}$ as a function of x_I in a Taylor series about $x_I = X_I$:

$$\mathcal{I}^{(n)}_{ip}(\boldsymbol{x},\boldsymbol{\gamma};\boldsymbol{x'}) = \mathcal{I}^{(n)}_{ip}(X_I, x_{\bar{I}},\boldsymbol{\gamma};\boldsymbol{x'}) + (x_\imath - X_\imath)\,\mathcal{R}^{(n)}_{\imath ip}(X_I,\boldsymbol{x},\boldsymbol{\gamma};\boldsymbol{x'})\ . \tag{47}$$

Since $\mathcal{R}^{(n)}_{\imath ip}$ represents the higher-order terms in a Taylor series, its dependence on x_I is via a polynomial in $x_I - X_I$. In view of equation (25), we have

$$(i\omega)^{-1}\partial_{\gamma_\imath}\exp[i\omega\,\vartheta^{(N)}(\gamma_I,\boldsymbol{x};\boldsymbol{x'})] = [x_\imath - X_\imath(\gamma_I,x_{\bar{I}})]\exp[i\omega\,\vartheta^{(N)}(\gamma_I,\boldsymbol{x};\boldsymbol{x'})]$$

so that the second term in equation (47) induces a contribution to the integral in equation (44) of the type

$$\int (x_\imath - X_\imath)\, \mathcal{R}^{(n)}_{\imath ip}(X_I, \boldsymbol{x}, \boldsymbol{\gamma}; \boldsymbol{x}')\, \exp[i\omega\, \vartheta^{(N)}(\gamma_I, \boldsymbol{x}; \boldsymbol{x}')]\, \mathrm{d}\gamma_I$$

$$= (i\omega)^{-1} \int \partial_{\gamma_\imath} \left\{ \mathcal{R}^{(n)}_{\imath ip}(X_I(\gamma_I, x_{\bar{I}}), \boldsymbol{x}, \boldsymbol{\gamma}; \boldsymbol{x}')\, \exp[i\omega\, \vartheta^{(N)}(\gamma_I, \boldsymbol{x}; \boldsymbol{x}')] \right\} \mathrm{d}\gamma_I \tag{48}$$

$$-(i\omega)^{-1} \int \left\{ \partial_{\gamma_\imath} \mathcal{R}^{(n)}_{\imath ip}(X_I(\gamma_I, x_{\bar{I}}), \boldsymbol{x}, \boldsymbol{\gamma}; \boldsymbol{x}') \right\} \exp[i\omega\, \vartheta^{(N)}(\gamma_I, \boldsymbol{x}; \boldsymbol{x}')]\, \mathrm{d}\gamma_I\ .$$

With the aid of Gauss' divergence theorem, it can be shown that the first term on the right-hand side of this equation yields a boundary contribution that can be eliminated; the second term transfers into $\mathcal{I}^{(n-1)}_{ip}$. We will focus on the leading-order terms ($n = 2$).

Since

$$\mathcal{R}^{(2)}_{\imath ip}(X_I, \boldsymbol{x}, \boldsymbol{\gamma}; \boldsymbol{x}') = (\partial_{x_\imath} \mathcal{I}^{(2)}_{ip})(X_I, x_{\bar{I}}, \boldsymbol{\gamma}; \boldsymbol{x}')$$
$$+ \tfrac{1}{2}(x_{\imath'} - X_{\imath'})\, (\partial_{x'_\imath} \partial_{x_\imath} \mathcal{I}^{(2)}_{ip})(X_I, x_{\bar{I}}, \boldsymbol{\gamma}; \boldsymbol{x}') + \cdots\ ,$$

we find that

$$-\partial_{\gamma_\imath} \mathcal{R}^{(2)}_{\imath ip}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}, \boldsymbol{\gamma}; \boldsymbol{x}')$$
$$= \partial_{\gamma_\imath} \Big\{ (\partial_{x_\imath} \hat{c}_{ijk\ell})(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_j \gamma_\ell$$
$$B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi^{(N)}_k(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) \xi^{(N)}_p(\boldsymbol{x}') \Big\}$$
$$- \tfrac{1}{2}(\partial_{\gamma_\imath} X_{\imath'})(\gamma_I, x_{\bar{I}})\, (\partial_{x_{\imath'}} \partial_{x_\imath} \hat{c}_{ijk\ell})(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_j \gamma_\ell$$
$$B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi^{(N)}_k(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) \xi^{(N)}_p(\boldsymbol{x}') + \cdots \tag{49}$$
$$= (\partial_{x_\imath} \hat{c}_{ijk\ell})(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \partial_{\gamma_\imath} \Big\{ \gamma_j \gamma_\ell$$
$$B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi^{(N)}_k(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) \xi^{(N)}_p(\boldsymbol{x}') \Big\}$$
$$+ \tfrac{1}{2}(\partial_{\gamma_\imath} X_{\imath'})(\gamma_I, x_{\bar{I}})\, (\partial_{x_{\imath'}} \partial_{x_\imath} \hat{c}_{ijk\ell})(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_j \gamma_\ell$$
$$B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi^{(N)}_k(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) \xi^{(N)}_p(\boldsymbol{x}') + \cdots\ ,$$

and so on.

Upon substituting equation (45) and equation (46) together with (49) into equation (44), collecting terms $\mathcal{O}(\omega^2)$, yields an equation for $\boldsymbol{\xi}$: $\mathcal{I}^{(2)}_{ip}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}, \boldsymbol{\gamma}; \boldsymbol{x}') = 0$ or (cf. equation (45))

$$[\delta_{ik} - \hat{c}_{ijk\ell}(X_I, x_{\bar{I}})\gamma_j\gamma_\ell]\,\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) = 0\;, \tag{50}$$

the solutions of which are the *polarization* vectors on bicharacteristics. Collecting all terms $\mathcal{O}(\omega)$, yields an equation for B (cf. equations (46) and (49)). Taking terms in equation (46) together, for instance,

$$\hat{c}_{i\imath k\bar{\imath}'}(X_I, x_{\bar{I}})\gamma_\imath\,\partial_{x_{\bar{\imath}'}} + \hat{c}_{i\bar{\imath}k\bar{\imath}'}(X_I, x_{\bar{I}})\gamma_{\bar{\imath}}\,\partial_{x_{\bar{\imath}'}} = \hat{c}_{ijk\bar{\imath}'}(X_I, x_{\bar{I}})\gamma_j\,\partial_{x_{\bar{\imath}'}}\;,$$

we obtain

$$\begin{aligned}
&[\rho(X_I, x_{\bar{I}})]^{-1}\partial_{x_j}(\rho\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\,\gamma_\ell \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x'})\,\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\xi_p^{(N)}(\boldsymbol{x'}) \\
&+[\hat{c}_{ijk\bar{\imath}'}(X_I, x_{\bar{I}})\gamma_j\,\partial_{x_{\bar{\imath}'}} + \hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\gamma_\ell\,\partial_{x_{\bar{\imath}}} + \hat{c}_{i\bar{\imath}k\bar{\imath}'}(X_I, x_{\bar{I}})\,(\partial_{x_{\bar{\imath}}}\gamma_{\bar{\imath}'})] \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x'})\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\xi_p^{(N)}(\boldsymbol{x'}) \\
&-(\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\,\partial_{\gamma_\imath}\Big\{\gamma_j\gamma_\ell \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x'})\,\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\xi_p^{(N)}(\boldsymbol{x'})\Big\} \\
&-\tfrac{1}{2}(\partial_{\gamma_\imath}X_{\imath'})\,(\partial_{x_{\imath'}}\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\,\gamma_j\gamma_\ell \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x'})\,\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\xi_p^{(N)}(\boldsymbol{x'}) = 0\;.
\end{aligned} \tag{51}$$

Next, we contract this equation with the polarization vector $\xi_i^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})$. In this process we will make use of several identities. First, note that $\partial_{x_{\bar{\imath}}}\gamma_{\imath'} = 0$. Second, exploiting the symmetry of the stiffness tensor, we find the identity associated with the second term,

$$\begin{aligned}
&\xi_i^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\hat{c}_{ijk\bar{\imath}'}(X_I, x_{\bar{I}})\gamma_j\,(\partial_{x_{\bar{\imath}'}}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})) \\
&\qquad+\xi_i^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\gamma_\ell\,(\partial_{x_{\bar{\imath}}}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})) \\
&\qquad+\xi_i^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})(\partial_{x_{\bar{\imath}}}\gamma_\ell)\,\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}}) \\
&\qquad\qquad= \hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\,\partial_{x_{\bar{\imath}}}\Big\{\gamma_\ell\,\xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\Big\}\;.
\end{aligned}$$

Third, in view of the symmetry of the stiffness tensor again, we have

$$\xi_i^{(N)}(X_I, x_{\bar I})\hat c_{ijk\bar\imath'}(X_I, x_{\bar I})\gamma_j\,\xi_k^{(N)}(X_I, x_{\bar I})\partial_{x_{\bar\imath'}}B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')$$

$$+\xi_i^{(N)}(X_I, x_{\bar I})\hat c_{i\bar\imath k\ell}(X_I, x_{\bar I})\gamma_\ell\,\xi_k^{(N)}(X_I, x_{\bar I})\partial_{x_{\bar\imath}}B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')$$

$$= 2\,\xi_i^{(N)}(X_I, x_{\bar I})\hat c_{i\bar\imath k\ell}(X_I, x_{\bar I})\gamma_\ell\,\xi_k^{(N)}(X_I, x_{\bar I})\partial_{x_{\bar\imath}}B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\ .$$

Fourth, associated with the third term,

$$-\xi_i^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})(\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\gamma_j\gamma_\ell\,\partial_{\gamma_\imath}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})$$

$$= -\tfrac{1}{2}(\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\gamma_j\gamma_\ell\,\partial_{\gamma_\imath}\left\{\xi_i^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})\xi_k^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})\right\}\ .$$

The outcome of the contraction, reordering terms, then follows as,

$$\begin{aligned}
&[\rho(X_I, x_{\bar I})]^{-1}\partial_{x_j}(\rho\hat c_{ijk\ell})(X_I, x_{\bar I})\,\xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar I})\,\gamma_\ell B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\\
&+\hat c_{i\bar\imath k\ell}(X_I, x_{\bar I})\,\partial_{x_{\bar\imath}}\left\{\xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})\,\gamma_\ell\right\}\,B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\\
&\qquad+2\hat c_{i\bar\imath k\ell}(X_I, x_{\bar I})\,\xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar I})\,\gamma_\ell\,\partial_{x_{\bar\imath}}\left\{B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\right\}\\
&-\tfrac{1}{2}(\partial_{\gamma_\imath}X_{\imath'})\,(\partial_{x_{\imath'}}\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar I})\,\gamma_j\gamma_\ell\\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\\
&-\tfrac{1}{2}(\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\partial_{\gamma_\imath}\left\{\xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar I}), x_{\bar I})\,\gamma_j\gamma_\ell\right\}\\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\\
&-\tfrac{1}{2}(\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar I})\,\partial_{\gamma_\imath}\left\{\gamma_j\gamma_\ell\right\}\\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\\
&-(\partial_{x_\imath}\hat c_{ijk\ell})(X_I, x_{\bar I})\,\xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar I})\,\gamma_j\gamma_\ell\\
&\qquad\qquad\qquad\qquad\partial_{\gamma_\imath}\left\{B^{(N)}(\gamma_I, x_{\bar I};\boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')\right\} = 0\ .
\end{aligned}\tag{52}$$

We will now employ a fifth identity, associated with the sixth term,

$$
\begin{aligned}
&\tfrac{1}{2}(\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \partial_{\gamma_\imath}\{\gamma_j\gamma_\ell\} \\
&\quad = (\partial_{x_\imath}\hat{c}_{i\imath k\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell \\
&\qquad\qquad + (\partial_{x_\imath}\hat{c}_{i\bar{\imath}k\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, (\partial_{\gamma_\imath}\gamma_{\bar{\imath}})\gamma_\ell \ ,
\end{aligned}
$$

to eliminate $(\partial_{x_\imath}\hat{c}_{i\imath k\ell})$ from the first term in equation (52). This leads to

$$
\begin{aligned}
&[\rho(X_I, x_{\bar{I}})]^{-1}(\partial_{x_j}\rho)\, \hat{c}_{ijk\ell}(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&+ (\partial_{x_{\bar{\imath}}}\hat{c}_{i\bar{\imath}k\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&+ \hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\, \partial_{x_{\bar{\imath}}}\left\{\xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_\ell\right\}\, B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&\qquad + 2\hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell\, \partial_{x_{\bar{\imath}}}\left\{B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')\right\} \\
&- \tfrac{1}{2}(\partial_{\gamma_\imath}X_{\imath'})\, (\partial_{x_{\imath'}}\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_j\gamma_\ell \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&- \tfrac{1}{2}(\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\, \partial_{\gamma_\imath}\left\{\xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_j\gamma_\ell\right\} \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&- (\partial_{x_\imath}\hat{c}_{i\bar{\imath}k\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, (\partial_{\gamma_\imath}\gamma_{\bar{\imath}})\gamma_\ell \\
&\qquad\qquad B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}') \\
&- (\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_j\gamma_\ell \\
&\qquad\qquad\qquad \partial_{\gamma_\imath}\left\{B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')\right\} = 0 \ .
\end{aligned}
\tag{53}
$$

At this stage, we will make use of a sixth identity associated with the seventh term,

$$
\partial_{\gamma_\imath}\gamma_{\bar{\imath}} = \partial_{\gamma_\imath}\partial_{x_{\bar{\imath}}}\phi = \partial_{x_{\bar{\imath}}}\partial_{\gamma_\imath}\phi = -\partial_{x_{\bar{\imath}}}X_\imath
$$

(cf. equations (43) and (20)). Then we rewrite the medium coefficient of the sum of the second and seventh terms as follows,

$$
(\partial_{x_{\bar{\imath}}}\hat{c}_{i\bar{\imath}k\ell})(X_I, x_{\bar{I}}) - (\partial_{x_\imath}\hat{c}_{i\bar{\imath}k\ell})(X_I, x_{\bar{I}})\, (\partial_{\gamma_\imath}\gamma_{\bar{\imath}}) = \partial_{x_{\bar{\imath}}}\left\{\hat{c}_{i\bar{\imath}k\ell}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\right\} \ .
$$

Hence, taking together the second, third and seventh terms, and the fifth and sixth terms, yields

$$
\begin{aligned}
&[\rho(X_I, x_{\bar{I}})]^{-1}(\partial_{x_j}\rho)\, \hat{c}_{ijk\ell}(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell \\
&\qquad\qquad [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2 \\
&+\partial_{x_{\bar{\imath}}}\left\{\hat{c}_{i\bar{\imath}k\ell}(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I, x_{\bar{I}})\, \gamma_\ell\, [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2\right\} \\
&+\partial_{\gamma_\imath}\left\{-\tfrac{1}{2}(\partial_{x_\imath}\hat{c}_{ijk\ell})(X_I, x_{\bar{I}})\, \xi_i^{(N)}\xi_k^{(N)}(X_I(\gamma_I, x_{\bar{I}}), x_{\bar{I}})\, \gamma_j\gamma_\ell\right. \\
&\qquad\qquad \left.[B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2\right\} = 0\ .
\end{aligned}
\tag{54}
$$

In this equation, we recognize the Hamilton system of equation (14): the Hamiltonian $\mathcal{V}^{(N)}$ in equation (9) can be expressed in terms of eigenvectors $\boldsymbol{\xi}^{(N)}$ of the matrix $\hat{c}_{ijk\ell}(\boldsymbol{x})\gamma_\ell\gamma_j$,

$$
[\mathcal{V}^{(N)}(\boldsymbol{x}, \boldsymbol{\gamma})]^2 = \hat{c}_{ijk\ell}(\boldsymbol{x})\, \xi_i^{(N)}\xi_k^{(N)}(\boldsymbol{x}, \boldsymbol{\gamma})\, \gamma_j\gamma_\ell\ . \tag{55}
$$

Hence, *on* the bicharacteristics,

$$
\left\{
\begin{array}{rcll}
\partial_{\gamma_{\bar{\imath}}}\mathcal{V}^{(N)} & = & \hat{c}_{i\bar{\imath}k\ell}\, \xi_i^{(N)}\xi_k^{(N)}\, \gamma_\ell & , \\
-\partial_{x_\imath}\mathcal{V}^{(N)} & = & -\frac{1}{2}(\partial_{x_\imath}\hat{c}_{ijk\ell})\, \xi_i^{(N)}\xi_k^{(N)}\, \gamma_j\gamma_\ell & .
\end{array}
\right.
\tag{56}
$$

Substituting equation (56) into equation (14), and identifying the resulting system with factors in the second and third terms of equation (54), finally yields

$$
\begin{aligned}
&\rho^{-1}(\partial_{x_j}\rho)(X_I, x_{\bar{I}})\, \frac{\mathrm{d}x_j}{\mathrm{d}\tau}\, [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2 \\
&\quad +\partial_{x_{\bar{\imath}}}\left\{\frac{\mathrm{d}x_{\bar{\imath}}}{\mathrm{d}\tau}\ [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2\right\} \\
&\quad +\partial_{\gamma_\imath}\left\{\frac{\mathrm{d}\gamma_\imath}{\mathrm{d}\tau}\ [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2\right\} = 0\ .
\end{aligned}
\tag{57}
$$

Hence,

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}\tau}\ \log\left\{\rho(X_I, x_{\bar{I}})\, [B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\, \xi_p^{(N)}(\boldsymbol{x}')]^2\right\} \\
&\qquad = -\partial_{\gamma_\imath}\left\{\frac{\mathrm{d}\gamma_\imath}{\mathrm{d}\tau}\right\} - \partial_{x_{\bar{\imath}}}\left\{\frac{\mathrm{d}x_{\bar{\imath}}}{\mathrm{d}\tau}\right\},
\end{aligned}
\tag{58}
$$

where, in the right-hand side, we recognize (minus) the divergence of a vector, the 'group' vector, given by the components

$$
\left(\frac{\mathrm{d}\gamma_I}{\mathrm{d}\tau}, \frac{\mathrm{d}x_{\bar{I}}}{\mathrm{d}\tau}\right)\ .
$$

This vector is the *tangent* vector to the bicharacteristic projected onto the $(\gamma_I x_{\bar{I}})$-space. The 'wave front' in this space is determined by an equation of the type $\phi(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') = \varphi$ (equation (19)). The *normal* to this front follows from the gradient of ϕ,

$$\left(\partial_{\gamma_I}\phi, \partial_{x_{\bar{I}}}\phi\right) = (-X_I, \gamma_{\bar{I}})$$

(equation (20)), denoted as the 'phase' vector.

With the aid of Smirnov's lemma [27, p.442], the solution of equation (58) can be written in terms of a Jacobian,

$$\rho(X_I, x_{\bar{I}})\,[B^{(N)}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\,\xi_p^{(N)}(\boldsymbol{x}')]^2 = \frac{[C_I(\boldsymbol{x}')]^2}{\mathrm{M}(\gamma_I, x_{\bar{I}})}$$
$$\text{with} \quad \mathrm{M}(\gamma_I, x_{\bar{I}}) = \left|\,\det\left[\left.\frac{\partial(\gamma_I, x_{\bar{I}})}{\partial(q_1, q_2, \tau)}\right|_{(\gamma_I, x_{\bar{I}})}\right]\right|\,. \tag{59}$$

Here, (q_1, q_2) are coordinates on $S^2_{\boldsymbol{x}'}$ (see equation (15)) and C_I is a constant (independent of $(\gamma_I, x_{\bar{I}})$).

The structure of solution (59) reveals the conservation of power flux. From this structure we now extract an amplitude function $\mathcal{B}$ directly associated with the Lagrangian manifold,

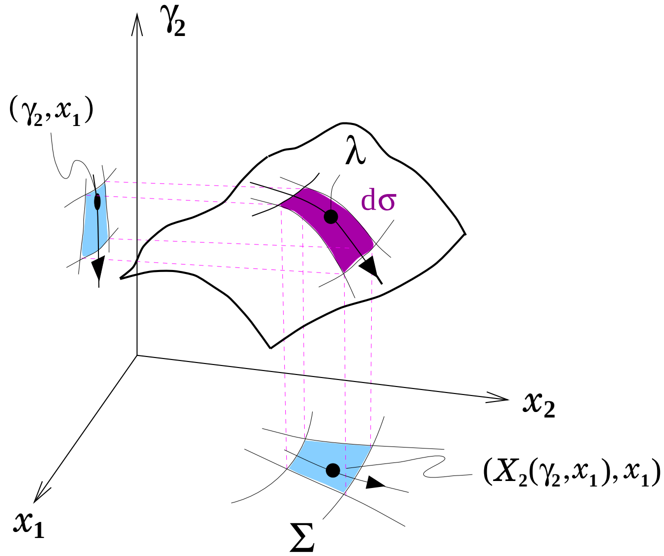

Figure 5. The Lagrangian manifold. Illustration of volume elements.

$$B(\gamma_I, x_{\bar{I}}; \boldsymbol{x}') = \mathcal{B}(\gamma_I, x_{\bar{I}}; \boldsymbol{x}')\sqrt{\left|\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\gamma_I \mathrm{d}x_{\bar{I}}}\right|}\,\exp\left[i\tfrac{1}{2}\arg\left(\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\gamma_I \mathrm{d}x_{\bar{I}}}\right)\right]\,. \tag{60}$$

The expression inside the square-root represents a Radon-Nikodym derivative of measures [28, Section 11.6 – Theorem 23]; $\boldsymbol{\sigma}$ represents the three curvi-linear coordinates on the

Lagrangian manifold generated by the bicharacteristics, while $\mathrm{d}\boldsymbol{\sigma}$ denotes a volume element in this manifold (figure 5).

For the special case where $I = \emptyset$, $\bar{I} = \{1,2,3\}$, B reduces to the geometrical ray amplitude A and equation (60) reduces to

$$A(\boldsymbol{x};\boldsymbol{x}') = \mathcal{A}(\boldsymbol{x};\boldsymbol{x}')\sqrt{\left|\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{x}}\right|}\,\exp\left[i\tfrac{1}{2}\arg\left(\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{x}}\right)\right]\ . \tag{61}$$

In view of equation (30), the mapping from $\mathcal{B}$ to $\mathcal{A}$ on the bicharacteristics is just a multiplication by a phase factor. (Similarly, the mapping (40) becomes a phase multiplication between corresponding $\mathcal{B}$'s.)

Also, in the expression for $A(\boldsymbol{x};\boldsymbol{x}')$ following from equation (59), we can write the Jacobian M in a special form. If the local, orthogonal coordinates associated with $\boldsymbol{x}$ are chosen in a wave-front normal sense, i.e. $\boldsymbol{x} = (\boldsymbol{x}^\Sigma, x^{\boldsymbol{\alpha}})$ where $\boldsymbol{x}^\Sigma$ represents a vector in the wave front $\Sigma(\boldsymbol{x}',\tau)$ while $x^{\boldsymbol{\alpha}}$ is the coordinate normal to the wave front, then

$$\mathrm{M}(\boldsymbol{x}) = |\det\left[\frac{\partial \boldsymbol{x}^\Sigma}{\partial \boldsymbol{\gamma}^{\mathsf{A}'}}\right]|\,\det\left[\frac{\partial(\boldsymbol{\gamma}^{\mathsf{A}'})}{\partial(q_1,q_2)}\right]\,V(\boldsymbol{x})\ , \tag{62}$$

with

$$\det\left[\frac{\partial(\boldsymbol{\gamma}^{\mathsf{A}'})}{\partial(q_1,q_2)}\right] = \frac{|\boldsymbol{v}(\boldsymbol{x}')|}{[V(\boldsymbol{x}')]^3}\ , \tag{63}$$

where $\boldsymbol{\gamma}^{\mathsf{A}'}$ denotes a vector on the slowness surface $\mathsf{A}' = \mathsf{A}(\boldsymbol{x}')$ at $\boldsymbol{x}'$, and $v_i = (\partial_{\gamma_i}\mathcal{V})(\boldsymbol{x}',\boldsymbol{\gamma}^{\mathsf{A}'})$ denotes the associated group velocity vector (cf. equation (16)).

The constant C_I in equation (59) follows from the initial conditions associated with the point body-force sources (see equation (4)). Assuming that the source is contained in a small, homogeneous ball, following Burridge *et al.* [13, Appendix B], we find that

$$C_I(\boldsymbol{x}') = \frac{1}{4\pi[\rho(\boldsymbol{x}')]^{1/2}[V(\boldsymbol{x}')]^{3/2}} \quad \text{if} \quad |I| = 2\ , \tag{64}$$

consistent with the Herglotz-Petrovsky-Leray formula [29, 30] †. A proper *initial* choice of coordinates $(\gamma_I, x_{\bar{I}})$ is guaranteed by the condition $|I| = 2$. However, in a caustic-free environment, C_I is given by equation (64) for any choice of $|I|$. $V(\boldsymbol{x}')$ is evaluated in the direction $\boldsymbol{\alpha}_{\boldsymbol{x}'}$ which defines the ray from which γ_I in the Maslov representation is extracted.

3.5. *Source and receiver Green's functions*

From the Green's tensor introduced so far we can generate the 'two-way' scattering process – from the source at $\boldsymbol{s}$ in mode N via the scattering point at $\boldsymbol{x}$ to the receiver at $\boldsymbol{r}$ in mode

† Inside the homogeneous ball containing the source at $\boldsymbol{x}'$, for $I = \{1,2\}$, $\bar{I} = \{3\}$ ($|I| = 2$), the Legendre transform is given by $\phi(\gamma_1,\gamma_2,x_3;\boldsymbol{x}') = \gamma_3(\gamma_1,\gamma_2)(x_3 - x_3') - \gamma_1 x_1' - \gamma_2 x_2'$. Here, $\gamma_3(\gamma_1,\gamma_2)$ is the (implicit) solution of equation (10) at $\boldsymbol{x}'$. In analogy with equations (62)-(63), we employ the following relations

$$\mathrm{M}(\gamma_1,\gamma_2,x_3) = |\det\left[\frac{\partial(\gamma_1,\gamma_2)}{\partial(\boldsymbol{\gamma}^{\mathsf{A}'})}\right]|\det\left[\frac{\partial(\boldsymbol{\gamma}^{\mathsf{A}'})}{\partial(q_1,q_2)}\right]|v_3| \text{ and } |\det\left[\frac{\partial(\gamma_1,\gamma_2)}{\partial(\boldsymbol{\gamma}^{\mathsf{A}'})}\right]| = \frac{|v_3|}{|\boldsymbol{v}|}.$$

M – that takes place in the subsurface, see figure 6. For this, we will have to convolve, in the time domain, the Green's tensor originating at the source and observed at the scattering point with the Green's tensor originating at the scattering point and observed at the receiver. The associated substitutions to be made in the Green's tensor of Subsections 2.2 and 3.3 are given in Table 1. In the remainder of these notes we will follow a particular example of the Maslov

original	substitution	interpretation
$\boldsymbol{x}'$	$\boldsymbol{x}$ or $\boldsymbol{y}$	scattering or image point
$\boldsymbol{x}$	$\boldsymbol{s}$ or $\boldsymbol{r}$	source or receiver point

Table 1. Change of arguments in equation (28).

representation, the others being easily obtained from this example. Thus, we will consider (cf. equation (28))

$$G_{ip}^{(N)}(\boldsymbol{x},\boldsymbol{x}',\omega) \sim \left(\frac{i\omega}{2\pi}\right)^{1/2} \int B^{(N)}(\gamma_1, x_{2,3}; \boldsymbol{x}')$$

$$\xi_i^{(N)}(X_1(\gamma_1, x_{2,3}), x_{2,3})\xi_p^{(N)}(\boldsymbol{x}') \, \exp[i\omega\,\vartheta^{(N)}(\gamma_1, \boldsymbol{x}; \boldsymbol{x}')] \, \mathrm{d}\gamma_1 \; .$$

Following the substitutions of Table 1 we then introduce the Green's tensors originating at the source and the scattering points,

$$\tilde{G}_{kq}^{(N)}(\boldsymbol{x},\omega) = G_{kq}^{(N)}(\boldsymbol{x},\boldsymbol{s},\omega) \; , \qquad \hat{G}_{pi}^{(M)}(\boldsymbol{x},\omega) = G_{pi}^{(M)}(\boldsymbol{r},\boldsymbol{x},\omega) \; , \tag{65}$$

respectively. Using reciprocity, we have

$$\tilde{G}_{kq}^{(N)}(\boldsymbol{x},\omega) = G_{qk}^{(N)}(\boldsymbol{s},\boldsymbol{x},\omega) \; . \tag{66}$$

To distinguish the source and the receiver Maslov integrals, we then introduce the notation

$$\tilde{G}_{kq}^{(N)}(\boldsymbol{x},\omega) \sim \left(\frac{i\omega}{2\pi}\right)^{1/2} \int \tilde{B}^{(N)}(\tilde{\gamma}_1, s_{2,3}; \boldsymbol{x})$$
$$\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1, s_{2,3}), s_{2,3})\tilde{\xi}_k^{(N)}(\boldsymbol{x}) \, \exp[i\omega\,\tilde{\vartheta}^{(N)}(\tilde{\gamma}_1, \boldsymbol{s}; \boldsymbol{x})] \, \mathrm{d}\tilde{\gamma}_1 \; , \tag{67}$$

while

$$\hat{G}_{pi}^{(M)}(\boldsymbol{x},\omega) \sim \left(\frac{i\omega}{2\pi}\right)^{1/2} \int \hat{B}^{(M)}(\hat{\gamma}_1, r_{2,3}; \boldsymbol{x})$$
$$\hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1, r_{2,3}), r_{2,3})\hat{\xi}_i^{(M)}(\boldsymbol{x}) \, \exp[i\omega\,\hat{\vartheta}^{(M)}(\hat{\gamma}_1, \boldsymbol{r}; \boldsymbol{x})] \, \mathrm{d}\hat{\gamma}_1 \; . \tag{68}$$

The time-domain convolution of these Green's tensors corresponds with a multiplication of their frequency-domain counterparts. In this process, the amplitudes multiply, viz.

$$B^{(NM)}(\hat{\gamma}_1, r_{2,3}, \boldsymbol{x}, \tilde{\gamma}_1, s_{2,3}) = \rho(\boldsymbol{x}) \, \tilde{B}^{(N)}(\tilde{\gamma}_1, s_{2,3}; \boldsymbol{x})\hat{B}^{(M)}(\hat{\gamma}_1, r_{2,3}; \boldsymbol{x}) \; , \tag{69}$$

introducing the two-way Maslov amplitude scaled by density of mass, and the phases add up, viz.

$$\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) = \tilde{\vartheta}^{(N)}(\tilde{\gamma}_1, \boldsymbol{s}; \boldsymbol{x}) + \hat{\vartheta}^{(M)}(\hat{\gamma}_1, \boldsymbol{r}; \boldsymbol{x}) \ , \tag{70}$$

introducing the two-way Maslov phase. Including the inverse Fourier transform from ω to t in our two-way scattered-field Maslov representation yields a total *phase function*

$$\Phi(\boldsymbol{q}, \boldsymbol{x}, \boldsymbol{\zeta}) = \omega \left[\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) - t\right] \ ; \tag{71}$$

in Table 2 the relevant variables are grouped appropriately.

variables	domain	role
$\boldsymbol{q} = (\boldsymbol{s}, \boldsymbol{r}, t)$	$\mathcal{Q} = \partial S \times \partial R \times \mathbb{R}_{\geq 0}$	acquisition
$\boldsymbol{x}$	$\mathcal{X} = \mathcal{D}$	subsurface
$\boldsymbol{\zeta} = (\tilde{\gamma}_1, \hat{\gamma}_1, \omega)$	$\mathcal{Z} = \tilde{\mathcal{O}} \times \hat{\mathcal{O}} \times \mathbb{R}$	integration

Table 2. Variables in the scattering process. (Here, $\tilde{\mathcal{O}}, \hat{\mathcal{O}} \subset \mathbb{R}$, open.)

The phase Φ is *stationary* if

$$\nabla_{\boldsymbol{\zeta}} \Phi = 0 \, , \text{i.e. if} \begin{cases} \partial_{\tilde{\gamma}_1} \tilde{\vartheta}^{(N)} = 0 \ , \\ \partial_{\hat{\gamma}_1} \hat{\vartheta}^{(M)} = 0 \ , \\ \vartheta^{(NM)} - t = 0 \ . \end{cases} \tag{72}$$

In accordance with equation (25) we find the solution set

$$\begin{cases} (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tilde{\gamma}_1(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \ , \\ (\boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \hat{\gamma}_1(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \ , \\ t = \tau^{(N)}(\boldsymbol{s}; \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) + \tau^{(M)}(\boldsymbol{r}; \boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ , \end{cases} \tag{73}$$

the (multiple) characteristics connecting $\boldsymbol{r}$ with $\boldsymbol{s}$ via $\boldsymbol{x}$, for $\boldsymbol{x} \in \mathcal{D}$. Here, the initial phase directions – at the scattering point $\boldsymbol{x}$ – of the geometrical rays to the source and the receiver positions have been denoted as

$$\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} \in \widetilde{S^2_{\boldsymbol{x}}} \subset S^2 \quad \text{and} \quad \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}} \in \widehat{S^2_{\boldsymbol{x}}} \subset S^2 \ . \tag{74}$$

They uniquely determine the rays. Not all the rays that leave $\boldsymbol{x}$ will intersect ∂S or ∂R hence the introduction of *partial* spheres $\widetilde{S^2_{\boldsymbol{x}}}$ and $\widehat{S^2_{\boldsymbol{x}}}$. In fact, the stationary points associated with equation (73) are parametrized by $(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}; \omega) \in \mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R}$ according to the

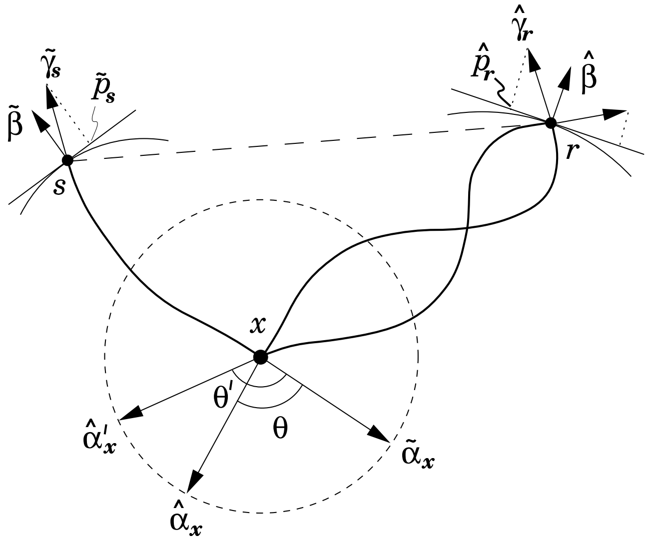

Figure 6. Parametrization of the stationary point set.

mapping (figure 6)

$$(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}; \omega) \to (\boldsymbol{q}, \boldsymbol{x}, \boldsymbol{\zeta}) =$$
$$(\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \boldsymbol{x}, \tilde{\gamma}_1(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \hat{\gamma}_1(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \omega) \ . \tag{75}$$

This mapping (not necessarily one-to-one) defines the 'stationary point set' $S_\Phi \subset \mathcal{Q} \times \mathcal{X} \times \mathcal{Z}$. We have introduced the two-way travel time

$$\tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}) = \tau^{(N)}(\boldsymbol{s}; \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) + \tau^{(M)}(\boldsymbol{r}; \boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ . \tag{76}$$

Let us review the level surfaces associated with the phase function. For 'one-way' propagation we had

$$\{\boldsymbol{x} \mid \vartheta^{(N)}(\gamma_1, \boldsymbol{x}; \boldsymbol{x}') - t = 0\}$$

which reduces to the *wave front* $\Sigma(\boldsymbol{x}', t)$ on the stationary point set. The associated slowness vector is $\nabla_{\boldsymbol{x}} \vartheta^{(N)}$. For two-way propagation we distinguish two level surfaces, one where $\boldsymbol{q} = (\boldsymbol{s}, \boldsymbol{r}, t)$ is fixed,

$$\{\boldsymbol{x} \mid \omega\,[\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) - t] = 0\} = \{\boldsymbol{x} \mid \Phi(\boldsymbol{q}, \boldsymbol{x}, \boldsymbol{\zeta}) = 0\} \tag{77}$$

parametrized by $\boldsymbol{\zeta}$, which reduces to the *isochrone surface* on the stationary point set (cf. equation (73)). The associated 'wave vector' is

$$\nabla_{\boldsymbol{x}} \Phi = \omega\, \nabla_{\boldsymbol{x}} \vartheta^{(NM)} = \omega\,[\nabla_{\boldsymbol{x}} \tilde{\vartheta}^{(N)} + \nabla_{\boldsymbol{x}} \hat{\vartheta}^{(M)}] \tag{78}$$

from which – at stationarity – the 'slowness vector', $\boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)}$, is obtained upon division by ω (see figure 7 for an illustration of equation (78); see figure 8 for an illustration of isochrones). The second two-way level surface is obtained by keeping $\boldsymbol{x}$ is fixed,

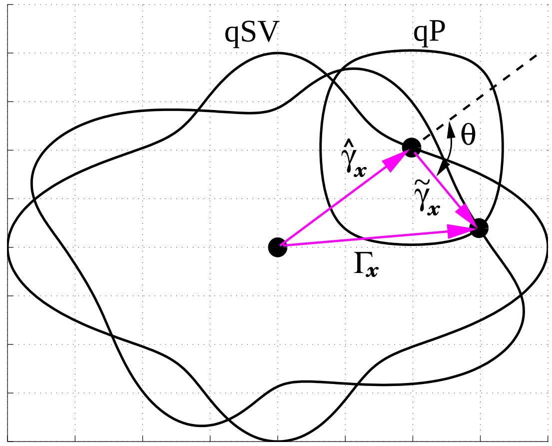

Figure 7. A two-way slowness vector $\boldsymbol{\Gamma_x}$, with $\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}\cdot\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}} = \cos\theta$ fixed, for qP-qSV conversion on the stationary point set. (Construction of the anisotropic analogue of the Ewald sphere [31].)

$$\{(\boldsymbol{s},\boldsymbol{r},t)\,|\,\omega\,[\vartheta^{(NM)}(\hat{\gamma}_1,\boldsymbol{r},\boldsymbol{x},\tilde{\gamma}_1,\boldsymbol{s})-t]=0\}=\{\boldsymbol{q}\,|\,\Phi(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta})=0\} \tag{79}$$

parametrized by $\boldsymbol{\zeta}$, which reduces to the *diffraction surface* on the stationary point set (cf. equation (73)). Let $\tilde{\boldsymbol{\beta}}(\boldsymbol{s})$ denote the unit outward normal to ∂S at $\boldsymbol{s}$ then we define the directional derivative in ∂S as

$$D_{\boldsymbol{s}}\cdot=\nabla_{\boldsymbol{s}}\cdot-\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\,(\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\cdot\nabla_{\boldsymbol{s}}\cdot) \tag{80}$$

and likewise let $\hat{\boldsymbol{\beta}}(\boldsymbol{r})$ denote the unit outward normal to ∂R at $\boldsymbol{r}$ then we define the directional derivative in ∂R as

$$D_{\boldsymbol{r}}\cdot=\nabla_{\boldsymbol{r}}\cdot-\hat{\boldsymbol{\beta}}(\boldsymbol{r})\,(\hat{\boldsymbol{\beta}}(\boldsymbol{r})\cdot\nabla_{\boldsymbol{r}}\cdot)\;. \tag{81}$$

The ‘wave vector’ associated with the second two-way level surface is then given by

$$\nabla_{\boldsymbol{q}}\Phi=(D_{\boldsymbol{s}},D_{\boldsymbol{r}},\partial_t)\,\Phi=(\omega\,\tilde{\boldsymbol{p}},\omega\,\hat{\boldsymbol{p}},-\omega) \tag{82}$$

with

$$\left\{\begin{array}{l}\tilde{\boldsymbol{p}}=D_{\boldsymbol{s}}\tilde{\vartheta}^{(N)}\;=\tilde{\boldsymbol{\gamma}}-(\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\cdot\tilde{\boldsymbol{\gamma}})\,\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\;,\\[2ex] \hat{\boldsymbol{p}}=D_{\boldsymbol{r}}\hat{\vartheta}^{(M)}=\hat{\boldsymbol{\gamma}}-(\hat{\boldsymbol{\beta}}(\boldsymbol{r})\cdot\hat{\boldsymbol{\gamma}})\,\hat{\boldsymbol{\beta}}(\boldsymbol{r})\;,\end{array}\right. \tag{83}$$

where (cf. equations (42)-(43))

$$\tilde{\boldsymbol{\gamma}}=(\tilde{\gamma}_1,\tilde{\gamma}_{2,3}(\tilde{\gamma}_1,s_{2,3}))\;,\qquad\hat{\boldsymbol{\gamma}}=(\hat{\gamma}_1,\hat{\gamma}_{2,3}(\hat{\gamma}_1,r_{2,3}))\;.$$

From equation (82) – at stationarity – the ‘slowness vector’, $\boldsymbol{\Upsilon}_{\boldsymbol{q}}^{(NM)}$, is obtained upon division by ω. On the stationary point set, we find

$$\begin{cases} \tilde{\boldsymbol{p}} = \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) = D_{\boldsymbol{s}} \tau^{(N)}(\boldsymbol{s}; \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ , \\ \hat{\boldsymbol{p}} = \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) = D_{\boldsymbol{r}} \tau^{(M)}(\boldsymbol{r}; \boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ , \end{cases} \tag{84}$$

see figure 6. Note that $\boldsymbol{\Upsilon}_{\boldsymbol{q}}^{(NM)} = (\tilde{\boldsymbol{p}}_{\boldsymbol{s}}, \hat{\boldsymbol{p}}_{\boldsymbol{r}}, -1)$.

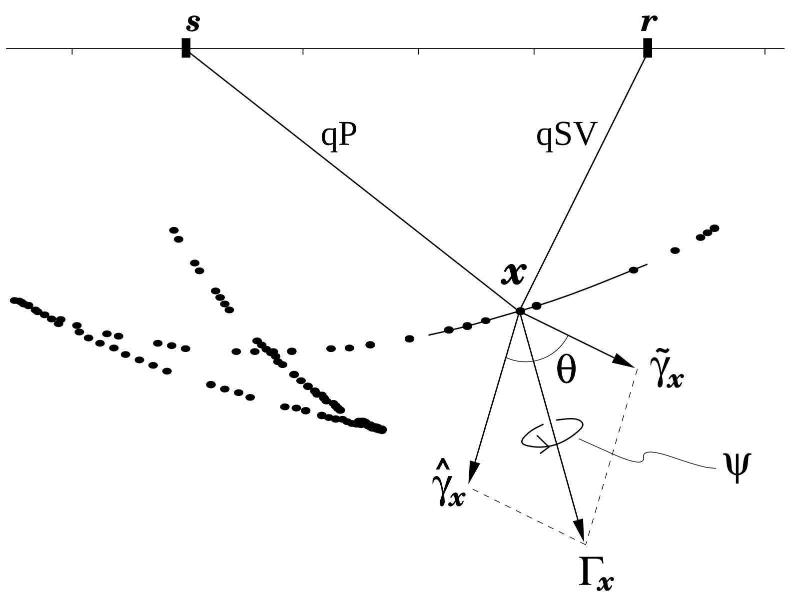

Figure 8. An isochrone surface for qP-qSV conversion. The dots indicate points on the isochrone from numerical computations. The relation between the one-way and two-way slowness vectors is shown.

4. The single scattering approximation

*4.1. The direct scattering (*modeling*) operator*

We begin the analysis with the volume-scattering representation of the Maslov-Born approximation for the *scattered* displacement field (for the geometrical ray-Born approximation analogue, see De Hoop *et al.* [11, (22)-(23)]) $\boldsymbol{u}^{(1)}$ for the (NM) conversion due to a contrast in density, $\rho^{(1)}$, and contrast in stiffness, $c^{(1)}_{ijk\ell}$, on $\mathcal{X} = \mathcal{D}$. We represent the relative medium contrast or perturbation by

$$\mathbf{c}^{(1)} = \left\{ \frac{\rho^{(1)}}{\rho}, \frac{c^{(1)}_{ijk\ell}}{\rho\, V_\circ^{(M)} V_\circ^{(N)}} \right\} \ , \tag{85}$$

which is a tensor-valued distribution in $\mathcal{X}$. The *embedding* or background medium does not carry any superscripts. We have introduced $V_\circ^{(N,M)}$, the (local) phase velocity of mode N, M

in the background medium averaged over all phase directions. The notation $_\circ$ is meant to emphasize that the quantity is angle independent, which is important for retaining the actual medium perturbation from $\mathbf{c}^{(1)}$.

The p-component displacement at $\boldsymbol{r}$ due to a q-component point body force at $\boldsymbol{s}$ is a tensor-valued distribution in $\mathcal{Q}$, follows from the linearized reciprocity theorem of the time-convolution type (see Burridge *et al.* [13, (2.21)]), and is given by (cf. equations (67)-(68))

$$u_{pq}^{(1)}(\boldsymbol{r},\boldsymbol{s},t) \sim (\boldsymbol{L}\mathbf{c}^{(1)})(\boldsymbol{r},\boldsymbol{s},t) =$$

$$\frac{1}{2\pi i}\int_{\mathbb{R}} \mathrm{d}\omega\ \omega^2 \left(\frac{\omega}{2\pi}\right) \int \mathrm{d}\hat{\gamma}_1 \int \mathrm{d}\tilde{\gamma}_1 \int_{\mathcal{D}} \hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1,r_{2,3}),r_{2,3})\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1,s_{2,3}),s_{2,3})$$
$$B^{(NM)}(\hat{\gamma}_1,r_{2,3},\boldsymbol{x},\tilde{\gamma}_1,s_{2,3}) \tag{86}$$
$$(\mathbf{w}^{(NM)}(\hat{\gamma}_1,\boldsymbol{r},\boldsymbol{x},\tilde{\gamma}_1,\boldsymbol{s}))^T\mathbf{c}^{(1)}(\boldsymbol{x})\ \exp[i\omega(\vartheta^{(NM)}(\hat{\gamma}_1,\boldsymbol{r},\boldsymbol{x},\tilde{\gamma}_1,\boldsymbol{s})-t)]\,\mathrm{d}\boldsymbol{x}\ ,$$

where

$$\mathbf{w}^{(NM)} = \left\{\hat{\xi}_m^{(M)}\tilde{\xi}_m^{(N)}, V_\circ^{(M)}V_\circ^{(N)}\left[\hat{\xi}_i^{(M)}(\nabla_{\boldsymbol{x}}\hat{\vartheta}^{(M)})_j\tilde{\xi}_k^{(N)}(\nabla_{\boldsymbol{x}}\tilde{\vartheta}^{(N)})_\ell\right]\right\}, \tag{87}$$

describes the contrast-source radiation patterns. The operator $\boldsymbol{L}$ defines a linear mapping from the relative medium contrast defined on $\mathcal{X}$ to the displacement observed on $\mathcal{Q}$. The first three integrals in equation (86) can be grouped together with the notation of Table 2, viz.

$$\int_{\mathbb{R}} \mathrm{d}\omega \int \mathrm{d}\hat{\gamma}_1 \int \mathrm{d}\tilde{\gamma}_1 = \int_{\mathcal{Z}} \mathrm{d}\boldsymbol{\zeta}\ . \tag{88}$$

Observe that here $\dim\mathcal{Z} = 3$. We recognize the phase in the integral on the right-hand side of equation (86) to be Φ. We introduce the 'amplitude tensor' $\boldsymbol{a}_{pq}$ as

$$\boldsymbol{a}_{pq}(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta}) \equiv \frac{1}{2\pi i}\left(\frac{\omega}{2\pi}\right)\ \hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1,r_{2,3}),r_{2,3})\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1,s_{2,3}),s_{2,3})$$
$$B^{(NM)}(\hat{\gamma}_1,r_{2,3},\boldsymbol{x},\tilde{\gamma}_1,s_{2,3})(\mathbf{w}^{(NM)}(\hat{\gamma}_1,\boldsymbol{r},\boldsymbol{x},\tilde{\gamma}_1,\boldsymbol{s}))^T\ . \tag{89}$$

4.2. *Analysis of the phase of the direct scattering operator*

Let us introduce the wave numbers

$$\tilde{k}_1 = \omega\tilde{\gamma}_1\ ,\ \hat{k}_1 = \omega\hat{\gamma}_1 \quad \text{and} \quad \boldsymbol{\zeta}_\omega = (\tilde{k}_1,\hat{k}_1,\omega)\ . \tag{90}$$

This change of variables induces the change in volume forms $\mathrm{d}\boldsymbol{\zeta} = \omega^{-2}\mathrm{d}\boldsymbol{\zeta}_\omega$. The phase Φ (cf. equation (71)) can be written as a function of $\boldsymbol{\zeta}_\omega$, viz.

$$\Phi_\omega(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta}_\omega) = \Phi(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta}_\omega/\omega) = \omega\,[\vartheta^{(NM)}(\hat{k}_1/\omega,\boldsymbol{r},\boldsymbol{x},\tilde{k}_1/\omega,\boldsymbol{s})-t]\ ,$$

and since

$$\Phi_\omega(\boldsymbol{q},\boldsymbol{x},\epsilon\boldsymbol{\zeta}_\omega) = \epsilon\Phi_\omega(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta}_\omega)\ ,$$

Φ_ω is *homogeneous of degree one* in $\boldsymbol{\zeta}_\omega$.

Next, we will show that the phase function Φ is *nondegenerate*, i.e., we will show that

$$\nabla_{(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta})}\,\partial_{\zeta_J}\Phi\ ,\qquad J=1,2,3\quad\text{with}\quad \nabla_{(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta})}=(D_{\boldsymbol{s}},D_{\boldsymbol{r}},\partial_t,\nabla_{\boldsymbol{x}},\nabla_{\boldsymbol{\zeta}})$$

(cf. equation (82)) are linearly independent for $(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta})\in S_\Phi$. Equivalently, we must show that the rank of the matrix $\nabla_{(\boldsymbol{q},\boldsymbol{x},\boldsymbol{\zeta})}\nabla_{\boldsymbol{\zeta}}\Phi\Big|_{S_\Phi}$ is three. Alternatively, since

$$\partial_{\zeta_1}\Phi=\omega\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)}\ ,\ \ \partial_{\zeta_2}\Phi=\omega\partial_{\hat\gamma_1}\hat\vartheta^{(M)}\ ,\ \ \partial_{\zeta_3}\Phi=\vartheta^{(NM)}-t\ ,$$

upon regrouping the derivatives, we will have to show that

$$\operatorname{rank}\left[\begin{array}{cc|c} (D_{\boldsymbol{s}},\partial_{\tilde\gamma_1})(\omega\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)}) & 0 & (D_{\boldsymbol{s}},\partial_{\tilde\gamma_1})\tilde\vartheta^{(N)} \\ 0 & (D_{\boldsymbol{r}},\partial_{\hat\gamma_1})(\omega\partial_{\hat\gamma_1}\hat\vartheta^{(M)}) & (D_{\boldsymbol{r}},\partial_{\hat\gamma_1})\hat\vartheta^{(M)} \\ \nabla_{\boldsymbol{x}}(\omega\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)}) & \nabla_{\boldsymbol{x}}(\omega\partial_{\hat\gamma_1}\hat\vartheta^{(M)}) & \nabla_{\boldsymbol{x}}\vartheta^{(NM)} \\ \hline 0 & 0 & -1 \\ \partial_{\tilde\gamma_1}\tilde\vartheta^{(N)} & \partial_{\hat\gamma_1}\hat\vartheta^{(M)} & 0 \end{array}\right]=3. \tag{91}$$

From the structure of this matrix, however, we observe that the third column must be linearly independent of the first two columns. Also note that on the stationary point set $\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)}=\partial_{\hat\gamma_1}\hat\vartheta^{(M)}=0$ (cf. equation (25)). Hence, it remains to be shown that the first two columns of the upper left submatrix are linearly independent. Consider the first column, in particular its combined first entry, which is the 3×1 matrix

$$(D_{\boldsymbol{s}},\partial_{\tilde\gamma_1})(\omega\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)})=\omega\begin{bmatrix} D_{\boldsymbol{s}}\partial_{\tilde\gamma_1}\tilde\vartheta^{(N)} \\ \partial^2_{\tilde\gamma_1}\tilde\vartheta^{(N)}\end{bmatrix}\ .$$

In case this column matrix reduces to the zero column matrix (its rank is no longer 1), the first two columns in the matrix of equation (91) will *not* be linearly independent. We will investigate that particular case. In view of equation (29) we have $\partial^2_{\tilde\gamma_1}\tilde\vartheta^{(N)}=-\partial_{\tilde\gamma_1}S_1$, showing that this second-order derivative vanishes at a caustic with normal that is aligned with the s_1-axis. Now observe that using equation (24) and then equation (19),

$$\partial_{s_2}\tilde\vartheta^{(N)}(\tilde\gamma_1,\boldsymbol{s};\boldsymbol{x})=\partial_{s_2}\phi^{(N)}(\tilde\gamma_1,s_2,s_3;\boldsymbol{x})=(\partial_{s_2}\tau^{(N)})(S_1(\tilde\gamma_1,s_2,s_3),s_2,s_3;\boldsymbol{x}),$$

hence

$$\partial_{\tilde\gamma_1}\partial_{s_2}\tilde\vartheta^{(N)}(\tilde\gamma_1,\boldsymbol{s};\boldsymbol{x})=(\partial_{s_1}\partial_{s_2}\tau^{(N)})(S_1(\tilde\gamma_1,s_2,s_3),s_2,s_3;\boldsymbol{x})\ (\partial_{\tilde\gamma_1}S_1)(\tilde\gamma_1,s_2,s_3),$$

which vanishes precisely at a caustic for which $\partial^2_{\tilde\gamma_1}\tilde\vartheta^{(N)}=0$. The same is true for $\partial_{\tilde\gamma_1}\partial_{s_3}\tilde\vartheta^{(N)}$. With this observation and using equation (42), at such a caustic upon substituting equation (80),

$$D_{\boldsymbol{s}}\partial_{\tilde{\gamma}_1}\tilde{\vartheta}^{(N)} = \nabla_{\boldsymbol{s}}\partial_{\tilde{\gamma}_1}\tilde{\vartheta}^{(N)} - \tilde{\boldsymbol{\beta}}(\boldsymbol{s})\,(\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\cdot\nabla_{\boldsymbol{s}}\partial_{\tilde{\gamma}_1}\tilde{\vartheta}^{(N)})$$

$$= \partial_{\tilde{\gamma}_1}\nabla_{\boldsymbol{s}}\tilde{\vartheta}^{(N)} - \tilde{\boldsymbol{\beta}}(\boldsymbol{s})\,(\tilde{\boldsymbol{\beta}}(\boldsymbol{s})\cdot\partial_{\tilde{\gamma}_1}\nabla_{\boldsymbol{s}}\tilde{\vartheta}^{(N)}) = \mathbf{e}_1 - \tilde{\boldsymbol{\beta}}(\boldsymbol{s})\,\tilde{\beta}_1(\boldsymbol{s}) \ ,$$

which equals the first column of the matrix representation of the orthogonal projection onto the tangent plane to ∂S at $\boldsymbol{s}$. Here $\mathbf{e}_1 = (1,0,0)^T$. If this column vanishes (as well as $\partial^2_{\tilde{\gamma}_1}\tilde{\vartheta}^{(N)}$), we find that $|\tilde{\beta}_1| = 1$ i.e. $\tilde{\boldsymbol{\beta}} \parallel \mathbf{e}_1$. Thus, the column matrix $(D_{\boldsymbol{s}}, \partial_{\tilde{\gamma}_1})(\omega\partial_{\tilde{\gamma}_1}\tilde{\vartheta}^{(N)})$ does *not* reduce to the zero column matrix if we exclude the occurrence of ‘grazing caustics’, i.e. caustics at a source the normals to which align with the normal of the tangent plane to the source manifold (see figure 9). For a similar reason, we exclude the occurrence of caustics at a receiver the normals to which align with the normal of the tangent plane to the receiver manifold. In conclusion, the linear independence condition will be satisfied if we exclude the occurrence of ‘grazing caustics’ associated with either the source or receiver manifolds.

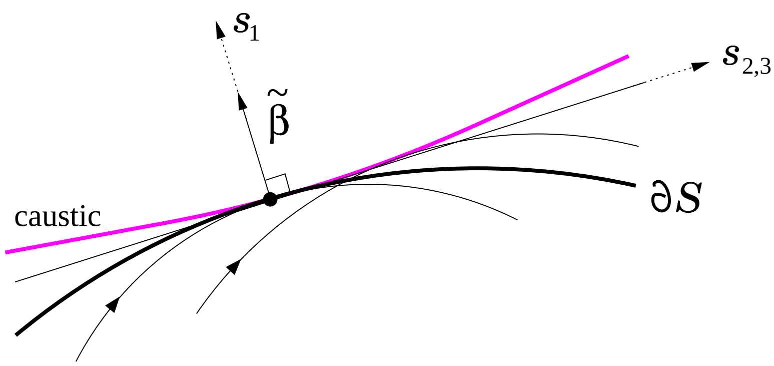

Figure 9. Illustration of degeneration of the phase Φ due to a caustic aligned with the source manifold.

With the aid of the phase function Φ, we can now extend mapping (75) to an imbedding of the type

$$S_\Phi \ni (\boldsymbol{q}, \boldsymbol{x}, \boldsymbol{\zeta}) =$$

$$(\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \boldsymbol{x}, \tilde{\gamma}_1(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \hat{\gamma}_1(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \omega)$$

$$\to (\boldsymbol{q}, \nabla_{\boldsymbol{q}}\Phi; \boldsymbol{x}, \nabla_{\boldsymbol{x}}\Phi) = \tag{92}$$

$$(\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \omega\tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \omega\hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), -\omega;$$

$$\boldsymbol{x}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \in T^*\mathcal{Q} \times T^*\mathcal{X} \ ,$$

where $T^*\mathcal{Q}$ denotes the cotangent bundle over $\mathcal{Q}$ and $T^*\mathcal{X}$ denotes the cotangent bundle over $\mathcal{X}$. Equation (92) pairs the (medium related) isochrone cotangent bundle $T^*\mathcal{X}$ with the (measurement related) diffraction cotangent bundle $T^*\mathcal{Q}$ into a wave front relation for $(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}; \omega) \in \mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R}$. The exclusion of the bicharacteristics associated with $|\tilde{\boldsymbol{p}}_{\boldsymbol{s}}| = 0$ and $|\hat{\boldsymbol{p}}_{\boldsymbol{r}}| = 0$ (i.e. grazing rays) and the exclusion of the ones associated with $|\boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)}| = 0$ (i.e. $\theta = \pi$) enforces that the mapping in equation (92), in fact, induces an embedding into $(T^*\mathcal{Q}\backslash 0) \times (T^*\mathcal{X}\backslash 0)$. We denote the image of S_Φ, constrained appropriately, under this embedding by Λ_Φ. The exclusion of grazing rays implies the exclusion of grazing caustics.

Note that $\tilde{\boldsymbol{p}}_{\boldsymbol{s}}$ and $\hat{\boldsymbol{p}}_{\boldsymbol{r}}$ (contained in an analysis of Riabinkin [32]) can be directly estimated from $u_{pq}^{(1)}$ as a function of $\boldsymbol{s}$ and $\boldsymbol{r}$ on the diffraction surface, a process familiar in stereotomography (Billette *et al.* [33]). Such an estimate determines a cotangent vector in $T^*\mathcal{Q}$, and one would hope that this cotangent vector would uniquely determine the ray and bicharacteristic geometry, in particular a cotangent vector in $T^*\mathcal{X}$. This is unfortunately not always the case. However, zooming in to a piece $\langle\Lambda_\Phi\rangle$ of Λ_Φ sufficiently small, we can re-establish a relation between $T^*\mathcal{Q}\backslash 0$ and $T^*\mathcal{X}\backslash 0$: let $\pi_{\mathcal{Q}} : (T^*\mathcal{Q}\backslash 0) \times (T^*\mathcal{X}\backslash 0) \to (T^*\mathcal{Q}\backslash 0)$ denote the natural projection; then there exists a smooth mapping $b_{\langle\Lambda_\Phi\rangle}$ such that

$$\begin{array}{ccccc} & \langle\Lambda_\Phi\rangle & \subset & \Lambda_\Phi & \\ & \pi_{\mathcal{Q}} \downarrow & & & \\ (T^*\mathcal{Q}\backslash 0) \supset & \lambda_\Phi & \overset{b_{\langle\Lambda_\Phi\rangle}}{\hookrightarrow} & (T^*\mathcal{X}\backslash 0) & \end{array} \tag{93}$$

We can carry out this construction for a sufficiently small neighborhood of any point in Λ_Φ, making use of the local immersion theorem [45, p.16] and Appendix A. We will make sure that λ_Φ is open, hence is a submanifold. Note that $b_{\langle\Lambda_\Phi\rangle}$ can be viewed as a local conic symplectomorphism [43, VIII.6]. A neighborhood or piece $\langle\Lambda_\Phi\rangle$ is controlled by a range of values for $(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$.

Applying the analysis of Duistermaat [34, Section 2.4], it follows that our operator $\boldsymbol{L}$ is a local Fourier integral operator. This result is an extension from isotropic acoustics to anisotropic elasticity of a theorem due to Rakesh [35]. The order of the operator is (Duistermaat [34, (2.4.22)])

$$\mu + \tfrac{1}{2}\mathrm{dim}\mathcal{Z} - \tfrac{1}{4}(\mathrm{dim}\mathcal{X} + \mathrm{dim}\mathcal{Q}) = 1 + \tfrac{3}{2} - 2 = \tfrac{1}{2}\,, \tag{94}$$

with $\mu = 1$ denoting the degree of homogeneity of $\boldsymbol{a}_{pq}$ (equation (89)) as a function of $\boldsymbol{\zeta}_\omega$ (equation (90)).

*4.3. The adjoint scattering (*imaging*) operator*

The linearized reciprocity theorem of the time-correlation type (De Hoop and De Hoop [36, (5.12)-(5.13)]) leads to a natural introduction of the adjoint $\boldsymbol{L}^\dagger$ of the direct scattering operator

$\boldsymbol{L}$, viz.

$$(\boldsymbol{L}^{\dagger}u^{(1)})(\boldsymbol{y}) =$$

$$-\frac{1}{2\pi i}\int_{\mathrm{I\!R}}\mathrm{d}\omega'\,(\omega')^2\left(\frac{\omega'}{2\pi}\right)\int\mathrm{d}\hat{\gamma}'_1\int\mathrm{d}\tilde{\gamma}'_1\int_{\partial S\times\partial R}\int_{\mathrm{I\!R}_{\geq 0}}[B^{(NM)}(\hat{\gamma}'_1,r_{2,3},\boldsymbol{y},\tilde{\gamma}'_1,s_{2,3})]^* \tag{95}$$

$$\mathbf{w}^{(NM)}(\hat{\gamma}'_1,\boldsymbol{r},\boldsymbol{y},\tilde{\gamma}'_1,\boldsymbol{s})\,\hat{\xi}^{(M)}_p(R_1(\hat{\gamma}'_1,r_{2,3}),r_{2,3})u^{(1)}_{pq}(\boldsymbol{r},\boldsymbol{s},t)\tilde{\xi}^{(N)}_q(S_1(\tilde{\gamma}'_1,s_{2,3}),s_{2,3})$$

$$\exp[-i\omega'(\vartheta^{(NM)}(\hat{\gamma}'_1,\boldsymbol{r},\boldsymbol{y},\tilde{\gamma}'_1,\boldsymbol{s})-t)]\,\mathrm{d}t\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{s}\ ,$$

which maps a tensor-valued distribution in $\mathcal{Q}$ into a tensor-valued distribution in $\mathcal{X}'$, $\mathcal{X}'$ being a copy of $\mathcal{X}$. The wave front relation of this operator, $\Lambda^{\dagger}_{\Phi'}$, is the same as the one of Eq.(86) but with $\mathcal{Q}$ and $\mathcal{X}$ interchanged. For a discussion on the geometrical-ray adjoint analogue in the case of isotropic acoustics in the absence of caustics, we refer the reader to Fomel [37]. The adjoint operator produces an 'image' of $\mathbf{c}^{(1)}$.

Expression (95) is in fact the Maslov extension of the 'Kirchhoff diffraction stack' [38]. The Maslov integrals do not necessarily align with (the tangent planes to) ∂S or ∂R (see figure 10). If they do, in view of the terms

$$\tilde{\gamma}'_1 s_1 + \hat{\gamma}'_1 r_1$$

contained in the Maslov phase function $\vartheta^{(NM)}$, the integration over $\boldsymbol{q}$ induces a (local) Fourier transform of the scattered field. (Focussing on the receiver Fourier transform, we find similarities with the work of Akbar *et al.* [39, 40].)

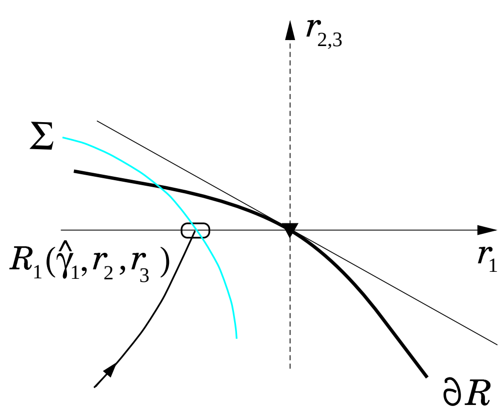

Figure 10. Illustration of the Maslov integration relative to the receiver manifold.

4.4. 'Stack' versus 'superposition'

Let us write

$$u^{(1)}_{pq}(\boldsymbol{r},\boldsymbol{s},t) = \int\int\int u^{(1)}_{p'q'}(\boldsymbol{r}',\boldsymbol{s}',t')\ \delta_{q'q}\delta_{p'p}\,\delta(\boldsymbol{s}-\boldsymbol{s}')\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')\ \mathrm{d}t'\mathrm{d}\boldsymbol{r}'\mathrm{d}\boldsymbol{s}'\ .$$

Then, upon extracting a particular sample, $\delta(\boldsymbol{s}-\boldsymbol{s}')\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$, out of the scattered field, we introduce

$$\boldsymbol{L}^{\dagger}_{G;p'q'}(\boldsymbol{r}',\boldsymbol{y},\boldsymbol{s}',t') =$$

$$-\frac{1}{2\pi i}\int_{\mathbb{R}}\mathrm{d}\omega'\ (\omega')^2\left(\frac{\omega'}{2\pi}\right)\ \int\mathrm{d}\hat{\gamma}_1'\int\mathrm{d}\tilde{\gamma}_1'\ [B^{(NM)}(\hat{\gamma}_1',r_{2,3}',\boldsymbol{y},\tilde{\gamma}_1',s_{2,3}')]^*$$

$$\mathbf{w}^{(NM)}(\hat{\gamma}_1',\boldsymbol{r}',\boldsymbol{y},\tilde{\gamma}_1',\boldsymbol{s}')\ \hat{\xi}^{(M)}_p(R_1(\hat{\gamma}_1',r_{2,3}'),r_{2,3}')\tilde{\xi}^{(N)}_q(S_1(\tilde{\gamma}_1',s_{2,3}'),s_{2,3}')$$

$$\exp[-i\omega'(\vartheta^{(NM)}(\hat{\gamma}_1',\boldsymbol{r}',\boldsymbol{y},\tilde{\gamma}_1',\boldsymbol{s}')-t')]\ .$$

The wave front in $\boldsymbol{y}\in\mathcal{X}'$ of this distribution is exactly the isochrone surface at time t' for the source-receiver pair $(\boldsymbol{s}',\boldsymbol{r}')$. The adjoint operator can then be written in the form of a superposition, viz.

$$(\boldsymbol{L}^{\dagger}u^{(1)})(\boldsymbol{y}) = \int_{\partial S\times\partial R}\int_{\mathbb{R}_{\geq 0}}\boldsymbol{L}^{\dagger}_{G;p'q'}(\boldsymbol{r}',\boldsymbol{y},\boldsymbol{s}',t')\ u^{(1)}_{p'q'}(\boldsymbol{r}',\boldsymbol{s}',t')\ \mathrm{d}t'\mathrm{d}\boldsymbol{r}'\mathrm{d}\boldsymbol{s}'\ . \quad (96)$$

Thus the wave front, i.e. the singular support, of the image can be viewed as an *envelope* of isochrone surfaces.

5. The normal operator

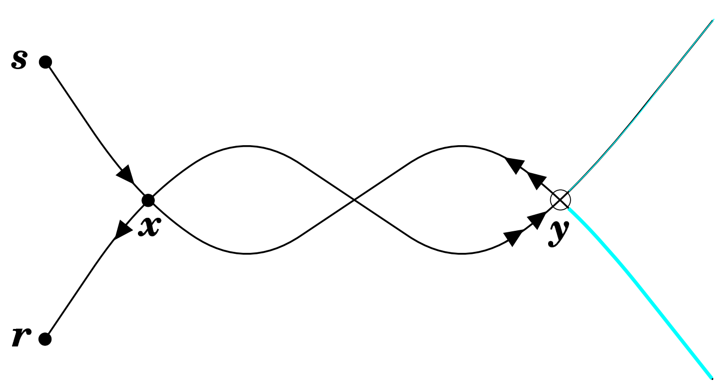

Figure 11. Illustration of a pair of non-reciprocal paths associated with *different* two-way travel times.

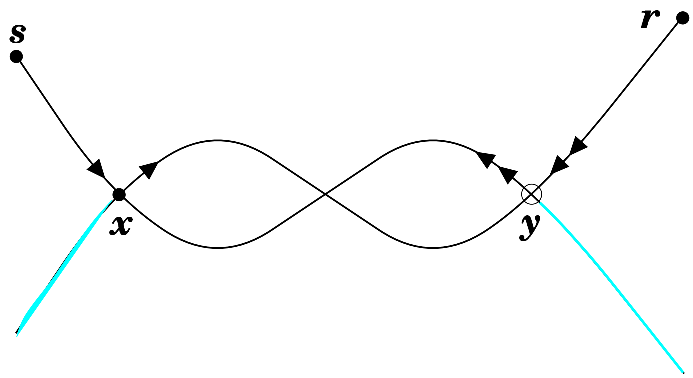

Figure 12. Illustration of a pair of non-reciprocal paths ($\boldsymbol{y} \neq \boldsymbol{x}$ but $(\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}) = (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$) associated with the *same* vector out of the diffraction cotangent bundle.

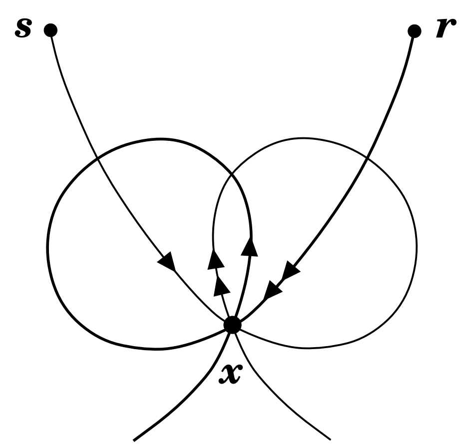

Figure 13. Illustration of a pair of non-reciprocal paths ($\boldsymbol{y} = \boldsymbol{x}$ but $(\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}) \neq (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$) associated with the *same* vector out of the diffraction cotangent bundle.

In the spirit of Least-Squares migration-imaging [41, 42], in preparation of the weak linearized inversion, we compose the direct scattering (modeling) operator with its adjoint (imaging) to form the so-called normal operator. To analyze this operator, we will employ the calculus of Fourier integral operators [43, VIII.5].

The normal operator will map a medium contrast into its image. For the image to be representative of the medium contrast, we will require that the singular support of the image is contained in the singular support of the medium contrast (the ‘pseudolocality’ property). In the process of composing the imaging operator with the modeling operator, we will encounter the complication that we may construct pairs of *non*-reciprocal paths which define the *same* cotangent vector in $T^*\mathcal{Q}$ (compare figure 11 with figures 12 and 13). One path out of the pair could then be associated with the modeling operator while the other path could be associated with the imaging operator leaving the composition of the two to become a stationary path for the normal operator. In the phase analysis of the normal operator, we will have to distinguish non-reciprocal from reciprocal paths contributions. In fact, we will need a refinement of properties of phase functions, from 'nondegenerate' to 'clean'.

The normal operator will 'compose' the wave front relations of the imaging and modeling operators:

$$\Lambda^{\dagger}_{\Phi'} \circ \Lambda_{\Phi} = \Big\{ (\boldsymbol{y}, \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}); \boldsymbol{x}, \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \mid \exists_{(\boldsymbol{s}, \boldsymbol{r}, \tau^{(NM)}, \omega\tilde{\boldsymbol{p}}_{\boldsymbol{s}}, \omega\hat{\boldsymbol{p}}_{\boldsymbol{r}}, -\omega)}$$
$$(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}; \omega) \overset{(75),(92)}{\rightarrow} (\boldsymbol{s}, \boldsymbol{r}, \tau^{(NM)}, \omega\tilde{\boldsymbol{p}}_{\boldsymbol{s}}, \omega\hat{\boldsymbol{p}}_{\boldsymbol{r}}, -\omega) \tag{97}$$
$$\wedge\ (\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}; \omega) \overset{(75),(92)}{\rightarrow} (\boldsymbol{s}, \boldsymbol{r}, \tau^{(NM)}, \omega\tilde{\boldsymbol{p}}_{\boldsymbol{s}}, \omega\hat{\boldsymbol{p}}_{\boldsymbol{r}}, -\omega) \Big\} .$$

If we replace the direct scattering operator by actual scattered field measurements, the normal operator reveals whether or not a 'phantom' image could be generated by applying the imaging operator to the measurements, which would violate the pseudolocality property.

5.1. Composition of the direct scattering operator and its adjoint

Composing equations (95) with (86) yields

$$(\boldsymbol{L}^{\dagger}\boldsymbol{L}\mathbf{c}^{(1)})(\boldsymbol{y}) =$$
$$\frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega'\ (\omega')^2 \left(\frac{\omega'}{2\pi}\right) \int \mathrm{d}\hat{\gamma}'_1 \int \mathrm{d}\tilde{\gamma}'_1\ \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega\ \omega^2 \left(\frac{\omega}{2\pi}\right) \int \mathrm{d}\hat{\gamma}_1 \int \mathrm{d}\tilde{\gamma}_1 \int_{\partial S\times\partial R} \int_{\mathbb{R}_{\geq 0}} \int_{\mathcal{D}}$$
$$\hat{\xi}^{(M)}_p(R_1(\hat{\gamma}'_1, r_{2,3}), r_{2,3}) \hat{\xi}^{(M)}_p(R_1(\hat{\gamma}_1, r_{2,3}), r_{2,3})$$
$$\tilde{\xi}^{(N)}_q(S_1(\tilde{\gamma}'_1, s_{2,3}), s_{2,3}) \tilde{\xi}^{(N)}_q(S_1(\tilde{\gamma}_1, s_{2,3}), s_{2,3}) \tag{98}$$
$$[B^{(NM)}(\hat{\gamma}'_1, r_{2,3}, \boldsymbol{y}, \tilde{\gamma}'_1, s_{2,3})]^* B^{(NM)}(\hat{\gamma}_1, r_{2,3}, \boldsymbol{x}, \tilde{\gamma}_1, s_{2,3})$$
$$\mathbf{w}^{(NM)}(\hat{\gamma}'_1, \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}'_1, \boldsymbol{s})\ (\mathbf{w}^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}))^T \mathbf{c}^{(1)}(\boldsymbol{x})$$
$$\exp[i\ (\omega(\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) - t) - \omega'(\vartheta^{(NM)}(\hat{\gamma}'_1, \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}'_1, \boldsymbol{s}) - t))]\, \mathrm{d}\boldsymbol{x}\ \mathrm{d}t\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{s}\ .$$

The integration over t generates a Dirac distribution, $2\pi\delta(\omega' - \omega)$; the integration over ω' then yields

$$
\begin{aligned}
(\boldsymbol{L}^\dagger \boldsymbol{L}\mathbf{c}^{(1)})(\boldsymbol{y}) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega\, \omega^4 \left(\frac{\omega}{2\pi}\right)^2 \int \mathrm{d}\hat{\gamma}_1' \int \mathrm{d}\tilde{\gamma}_1' \int \mathrm{d}\hat{\gamma}_1 \int \mathrm{d}\tilde{\gamma}_1 \int_{\partial S \times \partial R} \int_{\mathcal{D}} \\
\hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1', r_{2,3}), r_{2,3}) \hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1, r_{2,3}), r_{2,3}) \\
\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1', s_{2,3}), s_{2,3}) \tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1, s_{2,3}), s_{2,3}) \\
[B^{(NM)}(\hat{\gamma}_1', r_{2,3}, \boldsymbol{y}, \tilde{\gamma}_1', s_{2,3})]^* B^{(NM)}(\hat{\gamma}_1, r_{2,3}, \boldsymbol{x}, \tilde{\gamma}_1, s_{2,3}) \\
\mathbf{w}^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}_1', \boldsymbol{s}) \, (\mathbf{w}^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}))^T \mathbf{c}^{(1)}(\boldsymbol{x}) \\
\exp[i\omega\, (\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) - \vartheta^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}_1', \boldsymbol{s}))]\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{s} \, .
\end{aligned}
\tag{99}
$$

Hidden in this high-dimensional integral are the contributions from all pairs of reciprocal and pairs of non-reciprocal paths. Also, observe that the dyadic product in the fifth line generates a 22×22 matrix.

In analogy with equations (70)-(71) we introduce the phase Ψ of the normal operator,

$$
\Psi(\boldsymbol{y}, \boldsymbol{x}, \ddot{\boldsymbol{\zeta}}, \boldsymbol{q}) = \omega\, (\vartheta^{(NM)}(\hat{\gamma}_1, \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1, \boldsymbol{s}) - \vartheta^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}_1', \boldsymbol{s}))\, , \tag{100}
$$

where (see table 2)

$$
\ddot{\boldsymbol{\zeta}} = (\tilde{\gamma}_1', \hat{\gamma}_1', \tilde{\gamma}_1, \hat{\gamma}_1, \omega) \in \ddot{\mathcal{Z}} = \tilde{\mathcal{O}}' \times \hat{\mathcal{O}}' \times \tilde{\mathcal{O}} \times \hat{\mathcal{O}} \times \mathbb{R}\, , \tag{101}
$$

where $\tilde{\mathcal{O}}'$ is a copy of $\tilde{\mathcal{O}}$ and $\hat{\mathcal{O}}'$ is a copy of $\hat{\mathcal{O}}$; observe that $\dim \ddot{\mathcal{Z}} = 5$. In view of the simplification going from equation (98) to equation (99) the phase Ψ does not depend on t. We will denote the normal operator by $\boldsymbol{N}$.

5.2. *Stationary phase analysis: pairs of reciprocal and pairs of non-reciprocal paths*

In this subsection, we will investigate the phase Ψ with a view to the properties of the normal operator. First, we will establish under what conditions the normal operator is a Fourier integral operator, using the clean intersection calculus (Trèves [43, pp.457-461]). Second, we will unravel this Fourier integral operator into constituent operators, the stationary point sets of which can be identified with pairs of reciprocal paths (‘the reciprocal constituent’) and with pairs of non-reciprocal paths (‘the non-reciprocal constituent’) respectively. We will show under what conditions the non-reciprocal constituent operator is a Fourier integral operator of lower order then the reciprocal constituent operator. Third, we will show that the reciprocal constituent operator is in fact an elliptic pseudo-differential operator. We will derive an explicit representation of this elliptic pseudo-differential operator.

The normal phase Ψ given by equation (100) can be written as the difference

$$\Psi = \Phi - \Phi' \quad \text{at} \quad \omega' = \omega \ ,$$

where $\Phi = \Phi(\boldsymbol{q}, \boldsymbol{x}, \boldsymbol{\zeta})$ is given by equation (71) while

$$\Phi' \equiv \Phi(\boldsymbol{q}, \boldsymbol{y}, \boldsymbol{\zeta}') \quad \text{with} \quad \boldsymbol{\zeta}' = (\tilde{\gamma}_1', \hat{\gamma}_1', \omega') \ .$$

The phase Ψ in equation (98) is *stationary* (in analogy with equation (72)) if

$$\nabla_{(\ddot{\zeta}, \boldsymbol{q})} \Psi = 0 \, , \text{i.e. if} \left\{ \begin{array}{rcl} \nabla_{\boldsymbol{\zeta}'} \Phi' & = & 0 \, , \\ \nabla_{\boldsymbol{\zeta}} \Phi & = & 0 \, , \\ \nabla_{\boldsymbol{q}} \Phi & = & \nabla_{\boldsymbol{q}} \Phi' \ . \end{array} \right. \tag{102}$$

With the aid of equation (92) we find that the solution or stationary point set $S_\Psi \subset \mathcal{X}' \times \mathcal{X} \times \ddot{\mathcal{Z}} \times \mathcal{Q}$ is parametrized by $(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}'; \omega)$ and can be imbedded into

$$\mathcal{M} \equiv (T^* \mathcal{X}' \backslash 0) \times \Delta_{\mathcal{Q}}^* \times (T^* \mathcal{X} \backslash 0)$$

in accordance with

$$\left\{ \begin{array}{l} (\boldsymbol{q}, \nabla_{\boldsymbol{q}} \Phi'; \boldsymbol{y}, \nabla_{\boldsymbol{y}} \Phi') = \\ (\boldsymbol{s}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \boldsymbol{r}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}'}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \boldsymbol{s}), \omega \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \omega \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), -\omega; \\ \qquad \boldsymbol{y}, \omega \boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}')) \ , \\ (\boldsymbol{q}, \nabla_{\boldsymbol{q}} \Phi; \boldsymbol{x}, \nabla_{\boldsymbol{x}} \Phi) = \\ (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \omega \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \omega \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), -\omega; \\ \qquad \boldsymbol{x}, \omega \boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \ , \\ (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \omega \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \omega \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), -\omega) = \\ (\boldsymbol{s}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \boldsymbol{r}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}'}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \boldsymbol{s}), \omega \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), \omega \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}'), -\omega) \quad , \end{array} \right. \tag{103}$$

where $\Delta_{\mathcal{Q}}^*$ denotes the diagonal in $(T^* \mathcal{Q} \backslash 0) \times (T^* \mathcal{Q} \backslash 0)$. These equations define a pair of two-way paths that 'match' in $(T^* \mathcal{Q} \backslash 0)$. A pair of paths in S_Ψ is reciprocal iff $(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}') = (\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$. A pair of paths in S_Ψ is non-reciprocal if either $\boldsymbol{y} \neq \boldsymbol{x}$, see figure 12, or $(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}', \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}') \neq (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$, see figure 13.

Let the first equality in equation (103) generate $\Lambda_\Phi \subset (T^* \mathcal{Q} \backslash 0) \times (T^* \mathcal{X} \backslash 0)$ as in equation (92), and let the second equality generate $\Lambda_{\Phi'} \subset (T^* \mathcal{Q} \backslash 0) \times (T^* \mathcal{X}' \backslash 0)$ – upon interchanging $\mathcal{Q}$ and $\mathcal{X}'$, we obtain $\Lambda^{\dagger}_{\Phi'} \subset (T^*\mathcal{X}'\backslash 0) \times (T^*\mathcal{Q}\backslash 0)$ – and let us introduce the product

$$\mathcal{L} \equiv \Lambda^{\dagger}_{\Phi'} \times \Lambda_{\Phi} \ .$$

Then Λ_Ψ associated with the stationary point set S_Ψ, generated by $(\boldsymbol{y}, \nabla_{\boldsymbol{y}}\Psi; \boldsymbol{x}, \nabla_{\boldsymbol{x}}\Psi)$ in accordance with equation (103), is represented by equation (97), but is also determined by the intersection

$$\mathcal{L} \cap \mathcal{M}$$

through the natural projection $\mathcal{L} \cap \mathcal{M} \to \Lambda^{\dagger}_{\Phi'} \circ \Lambda_{\Phi} = \Lambda_\Psi$. Λ_Ψ pairs the isochrone cotangent vectors associated with the medium with the isochrone cotangent vectors associated with the image.

In accordance with Theorem 5.3 (Trèves [43, Section VIII.5]), the normal operator is a (global) Fourier integral operator if $\mathcal{L}$ and $\mathcal{M}$ intersect *cleanly*, i.e.

$$\mathcal{L} \cap \mathcal{M} \text{ is a manifold,} \quad T_{\cdot}(\mathcal{L} \cap \mathcal{M}) = T_{\cdot}\mathcal{L} \cap T_{\cdot}\mathcal{M} \ \text{ pointwise in } \mathcal{L} \cap \mathcal{M}.$$

The latter condition requires that $\dim T_{\cdot}\mathcal{L} \cap T_{\cdot}\mathcal{M} = \dim \mathcal{L} \cap \mathcal{M}$ *independent of* the point in $\mathcal{L} \cap \mathcal{M}$. Following Ten Kroode *et al.* [44] below, we will break this condition into conditions that guarantee clean intersection for our reciprocal and non-reciprocal constituent operators separately.

Let the dimension of the fibers in the projection $\mathcal{L} \cap \mathcal{M} \to \Lambda^{\dagger}_{\Phi'} \circ \Lambda_{\Phi}$, described by (equation (111)) $\to$ (equation (97)), be e; then $\dim \mathcal{L} \cap \mathcal{M} = \dim \Lambda_\Psi + e$. We refer to e as the *excess*. If $\mathcal{L}$ and $\mathcal{M}$ intersect cleanly with excess e, then [43, p.458]

$$\dim T_{\cdot}\mathcal{L} \cap T_{\cdot}\Delta^*_{\mathcal{Q}} = e$$

at any point in $\mathcal{L} \cap \mathcal{M}$.

To relate the clean intersection condition to the phase Ψ, we make the following observation. To every $(\boldsymbol{y}, \boldsymbol{x}, \ddot{\boldsymbol{\zeta}}, \boldsymbol{q}) \in S_\Psi$ can be assigned an element $(\boldsymbol{y}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}; \boldsymbol{q}, \omega\boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}, \boldsymbol{q}, \omega\boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}; \boldsymbol{x}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}) \in \mathcal{L} \cap \mathcal{M}$ by taking the appropriate gradients of Ψ (equation (103)); on the other hand, in $\mathcal{L} \cap \mathcal{M}$, to $(\boldsymbol{q}, \omega\boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}})$ can be assigned a value of $(\ddot{\boldsymbol{\zeta}}, \boldsymbol{q})$ by constructing $\tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}}$ and $\hat{\boldsymbol{\gamma}}_{\boldsymbol{r}}$ from the values of $\tilde{\boldsymbol{p}}_{\boldsymbol{s}}$ and $\hat{\boldsymbol{p}}_{\boldsymbol{r}}$ using the eikonal equation (11) at $\boldsymbol{s}$ and $\boldsymbol{r}$. Thus, the projection $\mathcal{L} \cap \mathcal{M} \to \Lambda^{\dagger}_{\Phi'} \circ \Lambda_{\Phi}$ can be viewed as a mapping

$$S_\Psi \ni (\boldsymbol{y}, \boldsymbol{x}, \ddot{\boldsymbol{\zeta}}, \boldsymbol{q}) \to (\boldsymbol{y}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}; \boldsymbol{x}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}) \in \Lambda_\Psi \ ,$$

evaluated by taking the appropriate gradients of Ψ (cf. equation (78)). For interpretational convenience, let us compose this mapping with the permutation of $\omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}$ and $\boldsymbol{x}$. The resulting mapping, Π say,

$$S_\Psi \ni (\boldsymbol{y}, \boldsymbol{x}, \ddot{\boldsymbol{\zeta}}, \boldsymbol{q}) \overset{\Pi}{\to} (\boldsymbol{y}, \boldsymbol{x}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}, \omega\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}) \ , \quad \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}} = \omega^{-1}\nabla_{\boldsymbol{y}}\Psi \ , \quad \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}} = \omega^{-1}\nabla_{\boldsymbol{x}}\Psi \ ,$$

has smooth fibers of dimension equal to the dimension of the null space $\mathcal{N}_{D\Pi}$ of the Jacobian $D\Pi$ of Π at any point in S_Ψ, with

$$D\Pi_{.} = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ \nabla_{\boldsymbol{y}}\nabla_{\boldsymbol{y}}\Psi & \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{y}}\Psi & \nabla_{\ddot{\boldsymbol{\zeta}}}\nabla_{\boldsymbol{y}}\Psi & \nabla_{\boldsymbol{q}}\nabla_{\boldsymbol{y}}\Psi \\ \nabla_{\boldsymbol{y}}\nabla_{\boldsymbol{x}}\Psi & \nabla_{\boldsymbol{x}}\nabla_{\boldsymbol{x}}\Psi & \nabla_{\ddot{\boldsymbol{\zeta}}}\nabla_{\boldsymbol{x}}\Psi & \nabla_{\boldsymbol{q}}\nabla_{\boldsymbol{x}}\Psi \end{bmatrix} .$$

Let $[W_{\boldsymbol{y}}, W_{\boldsymbol{x}}, W_{\ddot{\boldsymbol{\zeta}}}, W_{\boldsymbol{q}}]^T = [W_{(\boldsymbol{y},\boldsymbol{x})}, W_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}]^T$ represent the components of a vector W in the tangent space $T_{.}S_\Psi$ and let us determine the null space of $D\Pi_{.}$. From the explicit form of $D\Pi_{.}$ it follows that $W \in \mathcal{N}_{D\Pi}$ if

$$W_{(\boldsymbol{y},\boldsymbol{x})} = \boldsymbol{0} \ , \quad W_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K}\, \partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K} \nabla_{(\boldsymbol{y},\boldsymbol{x})}\Psi = \boldsymbol{0} \ . \tag{104}$$

On the other hand, note that $S_\Psi = \cap_{J=1,\cdots,10}\{(\boldsymbol{y},\boldsymbol{x},\ddot{\boldsymbol{\zeta}},\boldsymbol{q}) \mid \partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_J}\Psi = 0\}$, viewing $\partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_J}\Psi$ as functions. Since a vector in $T_{.}S_\Psi$ must be orthogonal to the normals to any of the zero-level sets contained in this intersection, $[\boldsymbol{0}, W_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}]^T \in T_{.}S_\Psi$ if

$$W_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K}\, \partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K} \partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_J}\Psi = 0 \ , \quad J = 1,\cdots,10 \ . \tag{105}$$

Combining the equations (104)-(105) for W leads to

$$(\nabla_{(\boldsymbol{y},\boldsymbol{x},\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}\partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K}\Psi)\, W_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K} = \boldsymbol{0} \ .$$

Introducing the span of gradients of $\partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K}\Psi$ appearing in this equation,

$$\mathcal{G} \equiv \mathrm{span}\{\nabla_{(\boldsymbol{y},\boldsymbol{x},\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}\partial_{(\ddot{\boldsymbol{\zeta}},\boldsymbol{q})_K}\Psi\}_{K=1,\cdots,10} \ ,$$

we conclude that

$$\mathcal{N}_{D\Pi} \subset \mathcal{G}^\perp \ , \tag{106}$$

where $\mathcal{G}^\perp$ denotes the *orthogonal* to the span of gradients $\mathcal{G}$. The dimension of $\mathcal{N}_{D\Pi}$ is precisely the excess e; thus, with the mapping Π, we have

$$\dim S_\Psi = 2\dim \mathcal{X} + e \ . \tag{107}$$

Through equation (102) the span of gradients allows the partitioning $\mathcal{G} = \mathcal{G}_{\mathcal{L}} + \mathcal{G}_{\mathcal{M}}$ with

$$\mathcal{G}_{\mathcal{L}} = \mathrm{span}\{\nabla_{(\boldsymbol{y},\boldsymbol{x},\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}\partial_{\ddot{\boldsymbol{\zeta}}_K}\Psi\}_{K=1,\cdots,5} \ , \quad \mathcal{G}_{\mathcal{M}} = \mathrm{span}\{\nabla_{(\boldsymbol{y},\boldsymbol{x},\ddot{\boldsymbol{\zeta}},\boldsymbol{q})}\partial_{\boldsymbol{q}_K}\Psi\}_{K=1,\cdots,5} \ .$$

Observe that $\mathcal{G}_{\mathcal{L}}^\perp$ can be associated with $T_{.}\mathcal{L}$, whereas $\mathcal{G}_{\mathcal{M}}^\perp$ can be associated with $T_{.}\mathcal{M}$. If $\mathcal{L}$ and $\mathcal{M}$ intersect *cleanly*, the phase Ψ will be *clean* as well, i.e., in an open conic subset of $\mathcal{X}' \times \mathcal{X} \times \ddot{\mathcal{Z}} \times \mathcal{Q}$ we have

$$T_{.}S_\Psi = \mathcal{G}^\perp \quad \text{at every one of its points;} \quad \mathcal{G}^\perp = \mathcal{G}_{\mathcal{L}}^\perp \cap \mathcal{G}_{\mathcal{M}}^\perp \ . \tag{108}$$

Then, with $\dim T_{\cdot} S_{\Psi}$ given by equation (107), upon taking the codimension of equality (108), we find that the span $\mathcal{G}$ has dimension [43, p.417]

$$\dim \mathcal{G} = 2 \dim \mathcal{X} + \dim \ddot{\mathcal{Z}} + \dim \mathcal{Q} - \dim T_{\cdot} S_{\Psi} = \dim \ddot{\mathcal{Z}} + \dim \mathcal{Q} - e. \tag{109}$$

With equations (106), (107) and (109), a requirement for Ψ to be clean is that $\dim \mathcal{G} = \dim \ddot{\mathcal{Z}} + \dim \mathcal{Q} - \dim \mathcal{N}_{D\Pi}$. Here, $\dim \mathcal{G} = \operatorname{rank} \nabla_{(\boldsymbol{y},\boldsymbol{x},\ddot{\zeta},\boldsymbol{q})} \nabla_{(\ddot{\zeta},\boldsymbol{q})} \Psi$, whereas (cf. equation (104)) $\dim \mathcal{N}_{D\Pi} = \operatorname{nullity} \nabla_{(\boldsymbol{y},\boldsymbol{x})} \nabla_{(\ddot{\zeta},\boldsymbol{q})} \Psi$. Observe that if the excess $e = 0$ that then the phase Ψ is nondegenerate.

With excess e, the order of the normal (Fourier integral) operator is given by (cf. equation (94))

$$2 \left[\mu + \tfrac{1}{2} \mathrm{dim} \mathcal{Z} - \tfrac{1}{4} (\mathrm{dim} \mathcal{X} + \mathrm{dim} \mathcal{Q})\right] + \tfrac{1}{2} e = 2 \left[1 + \tfrac{3}{2} - 2\right] + \tfrac{1}{2} e = 1 + \tfrac{1}{2} e \; . \tag{110}$$

The intersection viewed in the diffraction cotangent bundle

Let us introduce for every point in Λ_Φ a neighborhood $\langle \Lambda_\Phi \rangle$ (as in equation (93)) and for every point in $\Lambda_{\Phi'}$ a neighborhood $\langle \Lambda_{\Phi'} \rangle$, with associated (stereotomographic) mappings $b_{\langle \Lambda_\Phi \rangle}$ and $b_{\langle \Lambda_{\Phi'} \rangle}$ that determine the ray geometries uniquely from any vector in $\lambda_\Phi = \pi_{\mathcal{Q}} \langle \Lambda_\Phi \rangle$ or $\lambda_{\Phi'} = \pi_{\mathcal{Q}} \langle \Lambda'_\Phi \rangle$ in $T^* \mathcal{Q} \backslash 0$, respectively. Then, with equation (103), the intersection $\mathcal{L} \cap \mathcal{M}$ can be written as (cf. equations (78) and (82))

$$\begin{aligned} &\Big\{ (\boldsymbol{y}, \omega \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}; \boldsymbol{q}, \omega \boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}, \boldsymbol{q}, \omega \boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}; \boldsymbol{x}, \omega \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}) \mid \\ &\quad (\boldsymbol{q}, \omega \boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}) \in \lambda_{\Phi'} \cap \lambda_\Phi \; , \; (\boldsymbol{y}, \omega \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}) = b_{\langle \Lambda_{\Phi'} \rangle} (\boldsymbol{q}, \omega \boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}) \; , \\ &\qquad\qquad (\boldsymbol{x}, \omega \boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{x}}) = b_{\langle \Lambda_\Phi \rangle} (\boldsymbol{q}, \omega \boldsymbol{\Upsilon}^{(NM)}_{\boldsymbol{q}}) \Big\}. \end{aligned} \tag{111}$$

This set is the union of (subsets of) pairs of neighborhoods $\langle \Lambda^\dagger_{\Phi'} \rangle \times \langle \Lambda_\Phi \rangle$ with $\lambda_{\Phi'} \cap \lambda_\Phi \neq \emptyset$. The key, here, is that the properties of the intersection $\mathcal{L} \cap \mathcal{M}$ follow from the properties of the intersection $\lambda_{\Phi'} \cap \lambda_\Phi$ in the *measurement related* diffraction cotangent bundle.

A tangent vector in a manifold is generated by a parametrized curve on that manifold (see, for example, Guilleman and Pollack [45]). With this representation, it becomes clear that $T_{\cdot}(\mathcal{L} \cap \mathcal{M}) \subset T_{\cdot}\mathcal{L} \cap T_{\cdot}\mathcal{M}$ (a curve on $\mathcal{L} \cap \mathcal{M}$ is a curve on $\mathcal{L}$ and on $\mathcal{M}$ simultaneously). On the other hand, consider curves on $\mathcal{L}$ and $\mathcal{M}$ independently. In the following diagrams we trace these curves down to the diffraction cotangent bundle,

$$
\begin{array}{ccc}
 & \Lambda^{\dagger}_{\Phi'} \times \Lambda_{\Phi} & \\
 \swarrow & & \searrow \\
\Lambda_{\Phi'} & & \Lambda_{\Phi} \\
\downarrow & \pi_{\mathcal{Q}} & \downarrow \\
\lambda_{\Phi'} & & \lambda_{\Phi}
\end{array}
\qquad
\begin{array}{ccc}
 & (T^*\mathcal{X}'\backslash 0) \times \Delta^*_{\mathcal{Q}} \times (T^*\mathcal{X}\backslash 0) & \\
 \swarrow & & \searrow \\
(T^*\mathcal{X}'\backslash 0) \times (T^*\mathcal{Q}\backslash 0) & & (T^*\mathcal{Q}\backslash 0) \times (T^*\mathcal{X}\backslash 0) \\
\downarrow & \pi_{\mathcal{Q}} & \downarrow \\
(T^*\mathcal{Q}\backslash 0) & \leftrightarrow & (T^*\mathcal{Q}\backslash 0)
\end{array}
$$

In the right-hand diagram, the curves must coincide in the diffraction cotangent bundle. Thus, on the one hand a curve on $\mathcal{L}$ that generates a tangent vector in $T_{\cdot}\mathcal{L}$ can be traced to a pair of curves, one on $\lambda_{\Phi'}$ and one on λ_{Φ}. For this tangent vector to be contained in $T_{\cdot}\mathcal{M}$ as well, the curves in the pair must coincide, and be contained in $\lambda_{\Phi'} \cap \lambda_{\Phi}$. Now, through the local stereotomographic mappings, we can reverse the diagrams above from the bottom up. Thus, a curve on $\lambda_{\Phi'} \cap \lambda_{\Phi}$ lifts to a curve on $\mathcal{L}$ (left diagram) and a curve on $\mathcal{M}$ (right diagram) simultaneously. Such curve generates a tangent vector in $T_{\cdot}(\mathcal{L} \cap \mathcal{M})$. We conclude that $T_{\cdot}\mathcal{L} \cap T_{\cdot}\mathcal{M} \subset T_{\cdot}(\mathcal{L} \cap \mathcal{M})$. Hence, the existence of the local stereotomographic mappings guarantees that

$$T_{\cdot}\mathcal{L} \cap T_{\cdot}\mathcal{M} = T_{\cdot}(\mathcal{L} \cap \mathcal{M}) \, ,$$

and that *if* $\lambda_{\Phi'} \cap \lambda_{\Phi}$ *is a manifold*, the intersection $\mathcal{L} \cap \mathcal{M}$ must be clean.

Combining the analysis of the previous sections, we find the sequence of mappings

$$\mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} \stackrel{(75)}{\to} S_{\Phi} \stackrel{(92)}{\to} \Lambda_{\Phi} \stackrel{(93)}{\to} \lambda_{\Phi} \hookrightarrow T^*\mathcal{Q} \, . \tag{112}$$

Hence

$$\dim \lambda_{\Phi} = \dim \mathcal{X} + \dim \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} = \dim \lambda_{\Phi'} \, ,$$

while

$$\dim \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} = \dim \mathcal{Q} \, .$$

We will also make use of the fact that $\dim T^*\mathcal{Q} = 2 \dim \mathcal{Q}$.

The non-reciprocal constituent: $\langle \Lambda_{\Phi'} \rangle \cap \langle \Lambda_{\Phi} \rangle = \emptyset$

For the non-reciprocal pairs, we invoke the **transversal intersection condition**: i.e. we will assume that the background medium is such that there are *no* points $(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}) \neq (\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})$ such that (omitting the trivial equality involving the frequency in bottom line of equation (103), yielding 9 equations for the 14 variables)

$$
\begin{aligned}
&(\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \boldsymbol{r}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}, \boldsymbol{s}), \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \\
&\quad = (\boldsymbol{s}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}), \boldsymbol{r}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}), \tau^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}'}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}, \boldsymbol{s}), \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}), \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{y}, \hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}))
\end{aligned}
$$

and the rank of the matrix,

$$\operatorname{rank}\left[\begin{array}{ccc|ccc} \nabla_{\boldsymbol{x}}\boldsymbol{s} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{s} & \mathbf{0} & \nabla_{\boldsymbol{y}}\boldsymbol{s} & \nabla_{\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\boldsymbol{s} & \mathbf{0} \\ \nabla_{\boldsymbol{x}}\boldsymbol{r} & \mathbf{0} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{r} & \nabla_{\boldsymbol{y}}\boldsymbol{r} & \mathbf{0} & \nabla_{\hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\boldsymbol{r} \\ \nabla_{\boldsymbol{x}}\mathcal{T}^{(NM)} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\mathcal{T}^{(NM)} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\mathcal{T}^{(NM)} & \nabla_{\boldsymbol{y}}\mathcal{T}^{(NM)} & \nabla_{\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\mathcal{T}^{(NM)} & \nabla_{\hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\mathcal{T}^{(NM)} \\ \nabla_{\boldsymbol{x}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \mathbf{0} & \nabla_{\boldsymbol{y}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \nabla_{\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \mathbf{0} \\ \nabla_{\boldsymbol{x}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} & \mathbf{0} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} & \nabla_{\boldsymbol{y}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} & \mathbf{0} & \nabla_{\hat{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} \end{array}\right] < 9. \tag{113}$$

In this equation, for example, $\nabla_{\boldsymbol{y}}\boldsymbol{s}$ should be interpreted as $\nabla_{\boldsymbol{x}}\boldsymbol{s}|_{\boldsymbol{y}}$, and $\nabla_{\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}\boldsymbol{s}$ should be interpreted as $\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{s}|_{\tilde{\boldsymbol{\alpha}}'_{\boldsymbol{y}}}$, etc. Equation (113) is a condition on the geometry of the bicharacteristics at the sources and receivers. This condition can be reformulated in terms of derivatives of a mapping from $\boldsymbol{y}$ to $\boldsymbol{x}$ along a pair of different bicharacteristics (see Stolk [46, Section 3]). It guarantees that $\lambda_{\Phi'}$ and λ_{Φ} intersect transversally in the diffraction cotangent vector $(\boldsymbol{q}, \omega\boldsymbol{\Upsilon}_{\boldsymbol{q}}^{(NM)})$, i.e.

$$T_{.}\lambda_{\Phi'} + T_{.}\lambda_{\Phi} = T_{.}T^{*}\mathcal{Q} \ .$$

In this respect, notice that the Jacobian of the sequence of mappings (112) at frozen ω, generates the left-half submatrix in equation (113) the columns of which span $T_{.}\lambda_{\Phi}$. A similar reasoning leads to a geometrical interpretation of the right-half submatrix in equation (113).

Since $\lambda_{\Phi'}$ and λ_{Φ} intersect transversally in $T^{*}\mathcal{Q}$, we have

$$\operatorname{codim}\lambda_{\Phi'} \cap \lambda_{\Phi} = \operatorname{codim}\lambda_{\Phi'} + \operatorname{codim}\lambda_{\Phi} \ ,$$

i.e.

$$\dim\lambda_{\Phi'} \cap \lambda_{\Phi} = \dim\lambda_{\Phi'} + \dim\lambda_{\Phi} - \dim T^{*}\mathcal{Q} = 2\dim\mathcal{X} \ ;$$

then also, locally, $\dim\mathcal{L}\cap\mathcal{M} = 2\dim\mathcal{X}$ is the dimension of S_{Ψ}.

Since, with the transversal intersection condition, $\lambda_{\Phi'} \cap \lambda_{\Phi}$ is a manifold, the intersection $\mathcal{L}\cap\mathcal{M}$ is clean. With equation (107), the excess is

$$e = \dim S_{\Psi} - 2\dim\mathcal{X} = 0 \ ,$$

independent of the intersection point in $\mathcal{L}\cap\mathcal{M}$. It follows that $\mathcal{L}$ and $\mathcal{M}$ intersect cleanly with zero excess [43, p.458].

As a consequence, the phase Ψ is clean with zero excess, hence is non-degenerate. Then – by virtue of the tranversal intersection condition – the order of the associated constituent Fourier integral operator is 1 (cf. equation (110)); we will denote this operator by $\boldsymbol{N}^{\not\leftrightarrow}$.

The reciprocal constituent: $\langle\Lambda_{\Phi'}\rangle \cap \langle\Lambda_\Phi\rangle \neq \emptyset$

For the *reciprocal* constituent, we find that $\lambda_{\Phi'} \cap \lambda_\Phi$ is naturally a manifold. Since now $b_{\langle\Lambda_{\Phi'}\rangle}$ and $b_{\langle\Lambda_\Phi\rangle}$ must coincide on $\lambda_{\Phi'} \cap \lambda_\Phi$, this intersection is diffeomorphic to $\langle\Lambda_{\Phi'}\rangle \cap \langle\Lambda_\Phi\rangle$ with dimension,

$$\dim \lambda_{\Phi'} \cap \lambda_\Phi = \dim \langle\Lambda_\Phi\rangle = \dim \Lambda_\Phi = \dim \lambda_\Phi = \dim \mathcal{X} + \dim \mathcal{Q} \ ;$$

then also, locally, $\dim \mathcal{L} \cap \mathcal{M} = \dim \mathcal{X} + \dim \mathcal{Q}$ is the dimension of S_Ψ.

Since $\lambda_{\Phi'} \cap \lambda_\Phi$ is a manifold, the intersection $\mathcal{L} \cap \mathcal{M}$ is clean. With equation (107), the excess is

$$e = \dim S_\Psi - 2 \dim \mathcal{X} = \dim \mathcal{Q} - \dim \mathcal{X} \ ,$$

independent of the intersection point in $\mathcal{L} \cap \mathcal{M}$. It follows that $\mathcal{L}$ and $\mathcal{M}$ intersect cleanly with excess $e = \dim \mathcal{Q} - \dim \mathcal{X} = 5 - 3 = 2$.

As a consequence, the phase Ψ is clean with excess 2. Then the order of the associated constituent Fourier integral operator is 2 (cf. equation (110)), which, by virtue of the transversal intersection condition, is larger by $\frac{1}{2}e = 1$ then the order of the non-reciprocal constituent; we will denote this operator by $\boldsymbol{N}^{\leftrightarrow}$.

Observe that, once again since $b_{\langle\Lambda_{\Phi'}\rangle}$ and $b_{\langle\Lambda_\Phi\rangle}$ must coincide on $\lambda_{\Phi'} \cap \lambda_\Phi$, $\langle\Lambda^\dagger_{\Phi'}\rangle \times \langle\Lambda_\Phi\rangle\Big|_{\langle\Lambda_{\Phi'}\rangle\cap\langle\Lambda_\Phi\rangle}$ is the graph of the identity of $T^*\mathcal{X}\backslash 0$. It follows that the reciprocal constituent is in fact a pseudo-differential operator [47]. We will analyze this pseudo-differential operator in greater detail in the remainder of this Section.

Carrying out the stationary phase analysis of equation (99) in the slowness vectors for the reciprocal constituent, with the aid of equation (30) leads to

$$(\boldsymbol{N}^{\leftrightarrow}\mathbf{c}^{(1)})(\boldsymbol{y}) \sim \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega\ \omega^4 \int_{\partial S\times\partial R}\int_{\mathcal{D}} |A^{(NM)}(\boldsymbol{r},\boldsymbol{y},\boldsymbol{s})|^2$$
$$\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\,(\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T\mathbf{c}^{(1)}(\boldsymbol{x}) \tag{114}$$
$$\exp[i\omega\ (\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}) - \tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}))]\,\mathrm{d}\boldsymbol{x}\ \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{s}\ ,$$

up to leading order (where the sum over multiple reciprocal paths has been suppressed) since (see equation (70))

$$\vartheta^{(NM)}(\hat{\gamma}_1(\boldsymbol{x},\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}),\boldsymbol{r}(\boldsymbol{x},\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}),\boldsymbol{x},\tilde{\gamma}_1(\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}),\boldsymbol{s}(\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})) =$$
$$\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}},\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}},\boldsymbol{s})\ ,$$
$$\vartheta^{(NM)}(\hat{\gamma}_1(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{y},\tilde{\gamma}_1(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})) = \tag{115}$$
$$\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})\ ,$$

while we have introduced the simplified notation

$$\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) := \\ \mathbf{w}^{(NM)}(\hat{\gamma}_1(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{y},\tilde{\gamma}_1(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}))\ . \tag{116}$$

In equation (114), $\mathrm{d}\boldsymbol{r} = \mathrm{d}\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})$ and $\mathrm{d}\boldsymbol{s} = \mathrm{d}\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})$, hence the integration over $\partial S \times \partial R$ could be viewed as a Stieltjes integral in the absence of caustics.

5.3. Integration over phase directions

In equation (114), as in De Hoop *et al.* [10, 11], we change variables of integration (see figure 6)

$$\partial S \times \partial R \leftarrow \widetilde{S^2} \times \widehat{S^2}\ :\ (\boldsymbol{s},\boldsymbol{r}) \leftarrow (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\ , \quad \text{given } \boldsymbol{y}.$$

In the presence of caustics, this mapping is *multi-valued*. On the other hand, this change of variables unfolds the multi pathing. The associated Jacobian,

$$\frac{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{s},\boldsymbol{r})} = \frac{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{s})}\,\frac{\partial(\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{r})}\ , \tag{117}$$

is directly related to dynamic ray theory. In general, the factors can be expressed in terms of the dynamic ray amplitudes since, like the amplitudes, they follow from a variation of the anisotropic ray tracing equations. Introducing wave-front normal coordinates $(\boldsymbol{s}^{\Sigma}, s^{\boldsymbol{\alpha}})$ at the source in $\boldsymbol{s}$, we get

$$\frac{\partial(\boldsymbol{s}^{\Sigma})}{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})} = \frac{1}{16\pi^2\rho(\boldsymbol{s})\rho(\boldsymbol{y})\,\tilde{V}^{(N)}(\boldsymbol{s})(\tilde{V}^{(N)}(\boldsymbol{y}))^3\,|\tilde{A}^{(N)}(\boldsymbol{s};\boldsymbol{y})|^2}\ . \tag{118}$$

If ∂S in the neighborhood of $\boldsymbol{s}$ does not coincide with the wave front $\Sigma(\boldsymbol{y},\tau^{(N)}(\boldsymbol{s};\boldsymbol{y}))$ originating at $\boldsymbol{y}$, we have to correct for the ratio of the area on ∂S to the area on the wave front at $\boldsymbol{s}$ onto which it is mapped by projection along the rays. It amounts to dividing the previous Jacobian by the Jacobian

$$\frac{\partial(\boldsymbol{s}^{\Sigma})}{\partial(\boldsymbol{s})} = (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{s}}\boldsymbol{\cdot}\tilde{\boldsymbol{\beta}}(\boldsymbol{s}))\ .$$

Note that $\tilde{\boldsymbol{\alpha}}_{\boldsymbol{s}}$ is the normal to the wave front at $\boldsymbol{s}$. Similar expressions hold for the receiver side.

Combining equations (117) and (118), with a view to the first line of equation (114), leads us to introduce

$$\jmath^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}) = |A^{(NM)}(\boldsymbol{r},\boldsymbol{y},\boldsymbol{s})|^2\,\frac{\partial(\boldsymbol{s},\boldsymbol{r})}{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}$$

$$= \frac{1}{16\pi^2\rho(\boldsymbol{s})\rho(\boldsymbol{y})\,\tilde{V}^{(N)}(\boldsymbol{s})(\tilde{V}^{(N)}(\boldsymbol{y}))^3\;16\pi^2\rho(\boldsymbol{r})\rho(\boldsymbol{y})\,\hat{V}^{(M)}(\boldsymbol{r})(\hat{V}^{(M)}(\boldsymbol{y}))^3} \tag{119}$$

$$\frac{1}{(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{s}}\cdot\tilde{\boldsymbol{\beta}}(\boldsymbol{s}))\;(\hat{\boldsymbol{\alpha}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{\beta}}(\boldsymbol{r}))}\;,$$

a function that remains finite and smooth in the vicinity of caustics. For $\jmath^{(NM)}$ to remain finite in general, we have to exclude grazing rays at the source and at the receiver as we did already:

$$\tilde{\boldsymbol{\alpha}}_{\boldsymbol{s}}\cdot\tilde{\boldsymbol{\beta}}(\boldsymbol{s}) \neq 0\;, \qquad \hat{\boldsymbol{\alpha}}_{\boldsymbol{r}}\cdot\hat{\boldsymbol{\beta}}(\boldsymbol{r}) \neq 0\;. \tag{120}$$

Carrying out the change of integration variables then yields

$$(\boldsymbol{N}^{\leftrightarrow}\mathbf{c}^{(1)})(\boldsymbol{y}) \sim \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\omega\;\omega^4\int_{\widetilde{S^2}\times\widehat{S^2}}\int_{\mathcal{D}}\jmath^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})$$

$$\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\,(\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T\mathbf{c}^{(1)}(\boldsymbol{x}) \tag{121}$$

$$\exp[i\omega\,(\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}) - \tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}))]\,\mathrm{d}\boldsymbol{x}\;\mathrm{d}\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\mathrm{d}\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\;.$$

Since the phase is stationary for $(\boldsymbol{x},\boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)})$ near $(\boldsymbol{y},\boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)})$, we can restrict the integration over $\mathcal{D}$ to a small neighborhood of $\boldsymbol{y}$ (see also Beylkin [4]). On this neighborhood, we have

$$\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}) - \tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})$$

$$\sim \boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\cdot(\boldsymbol{x}-\boldsymbol{y})\;. \tag{122}$$

Upon substituting equation (122) into equation (121), the integration over $\boldsymbol{x}$ becomes a Fourier transform of the medium contrast, that appears also in diffraction tomography [48]. The normal operator takes the explicit form of a pseudo-differential operator. In equation (122), $\boldsymbol{s} = \boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \in \partial S$ and $\boldsymbol{r} = \boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \in \partial R$.

To be able to introduce an integration over the orientation $\boldsymbol{\nu}_{\boldsymbol{y}}$ of the gradient $\boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)}$ of two-way travel time $\tau^{(NM)}$, we have to exclude scattering over $\theta = \pi$: then

$$\boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)} \neq \mathbf{0}\;. \tag{123}$$

With $\boldsymbol{\nu}_{\boldsymbol{y}} = |\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}|^{-1}\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}$, together with the homogeneity in ω, we get

$$(\boldsymbol{N}^{\leftrightarrow}\mathbf{c}^{(1)})(\boldsymbol{y}) \sim \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega\ \omega^4 \int_{\widetilde{S^2}\times\widehat{S^2}} \int_{\mathcal{D}} \mu_{\mathrm{LS}}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{s})$$
$$\mathbf{w}^{(NM)}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\, (\mathbf{w}^{(NM)}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T \mathbf{c}^{(1)}(\boldsymbol{x}) \tag{124}$$
$$\exp[i\omega\ \boldsymbol{\nu}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\cdot(\boldsymbol{x}-\boldsymbol{y})]\, \mathrm{d}\boldsymbol{x}\ \mathrm{d}\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\mathrm{d}\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\ ,$$

where

$$\mu_{\mathrm{LS}}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{s}) \equiv \frac{\jmath^{(NM)}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{s})}{|\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})|^5}\ . \tag{125}$$

5.4. The principal symbol matrix

Following De Hoop *et al.* [10, 11], we change the variables of integration, $(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})$, to dip $\boldsymbol{\nu}$, scattering angle θ and azimuth ψ (see figure 8)

$$\widetilde{S^2}\times\widehat{S^2} \to E_{\boldsymbol{\nu}} \times (E_\theta(\boldsymbol{\nu}) \times E_\psi(\theta,\boldsymbol{\nu}))\ :\ (\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \to (\boldsymbol{\nu}_{\boldsymbol{y}}, \theta_{\boldsymbol{y}}, \psi_{\boldsymbol{y}})\ , \tag{126}$$

in which (Burridge *et al.* [13, Appendix D])

$$\begin{cases} \boldsymbol{\nu}_{\boldsymbol{y}} = \dfrac{\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{|\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})|} \in S^2\ , \\[2ex] \cos\theta_{\boldsymbol{y}} = \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\cdot\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\ , \qquad \theta \in [0,\pi)\ , \\[2ex] \psi_{\boldsymbol{y}} = \dfrac{1}{\sin\theta_{\boldsymbol{y}}}\,(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}} \wedge \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \wedge \boldsymbol{\nu}_{\boldsymbol{y}} = \dfrac{(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\cdot\boldsymbol{\nu}_{\boldsymbol{y}})\,\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}} - (\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\cdot\boldsymbol{\nu}_{\boldsymbol{y}})\,\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}}{\sin\theta_{\boldsymbol{y}}} \in S^1\ . \end{cases} \tag{127}$$

Then equation (124) takes the form

$$(\boldsymbol{N}^{\leftrightarrow}\mathbf{c}^{(1)})(\boldsymbol{y}) \sim \frac{1}{2\pi}\int_{\mathbb{R}} \mathrm{d}\omega\ \omega^4 \int_{E_{\boldsymbol{\nu}}} \int_{\mathcal{D}} \Big\{ \int_{E_\theta\times E_\psi} \mu_{\mathrm{LS}}(\boldsymbol{r}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \boldsymbol{s})$$
$$\mathbf{w}^{(NM)}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\, (\mathbf{w}^{(NM)}(\boldsymbol{y}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T \frac{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{\nu}_{\boldsymbol{y}}, \theta_{\boldsymbol{y}}, \psi_{\boldsymbol{y}})}\, \mathrm{d}\theta_{\boldsymbol{y}}\mathrm{d}\psi_{\boldsymbol{y}} \Big\} \tag{128}$$
$$\mathbf{c}^{(1)}(\boldsymbol{x})\ \exp[i\omega\ \boldsymbol{\nu}_{\boldsymbol{y}}\cdot(\boldsymbol{y}-\boldsymbol{x})]\, \mathrm{d}\boldsymbol{x}\ \mathrm{d}\boldsymbol{\nu}_{\boldsymbol{y}}\ .$$

In this equation, $\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}} = \tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}(\boldsymbol{\nu}_{\boldsymbol{y}}, \theta_{\boldsymbol{y}}, \psi_{\boldsymbol{y}}) \in \widetilde{S^2_{\boldsymbol{y}}}$ and $\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}} = \hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}(\boldsymbol{\nu}_{\boldsymbol{y}}, \theta_{\boldsymbol{y}}, \psi_{\boldsymbol{y}}) \in \widehat{S^2_{\boldsymbol{y}}}$. From the integrand in between the braces, we extract a point-symmetrized matrix in the form of an angular average

$$\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y}) \equiv \int_{E_\theta\times E_\psi} \mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\,(\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T$$
$$\tfrac{1}{2}\mu_{\rm LS}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})\;\frac{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{\nu_y},\theta_{\boldsymbol{y}},\psi_{\boldsymbol{y}})}\,\mathrm{d}\theta_{\boldsymbol{y}}\mathrm{d}\psi_{\boldsymbol{y}} + (\cdots)(\boldsymbol{y},-\boldsymbol{\nu_y})\ . \tag{129}$$

The Jacobian inside this integral can be found in Burridge *et al.* [13, Appendix D]. The matrix in equation (129) is positive whence the operator is elliptic. We then obtain

$$(\boldsymbol{N}^{\leftrightarrow}\mathbf{c}^{(1)})(\boldsymbol{y}) \sim \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}_{\geq 0}} \omega^2\mathrm{d}\omega\;\omega^2 \int_{E_{\boldsymbol{\nu}}} 8\pi^2\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y})\int_{\mathcal{D}}$$
$$\mathbf{c}^{(1)}(\boldsymbol{x})\;\exp[i\omega\;\boldsymbol{\nu_y}\boldsymbol{\cdot}(\boldsymbol{y}-\boldsymbol{x})]\,\mathrm{d}\boldsymbol{x}\;\mathrm{d}\boldsymbol{\nu_y}\ . \tag{130}$$

Upon combining $\omega^2\mathrm{d}\omega$ with $\mathrm{d}\boldsymbol{\nu_y}$, we recognize $\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y})$ as the principal symbol matrix associated with the reciprocal constituent of the normal operator. The condition number of the principal symbol matrix can be small; in fact, the principal symbol matrix may not have full rank, see De Hoop and Spencer [49]. We observe that the order of the operator is 2 indeed.

6. *Least-Squares* inversion

6.1. *The parametrix of the normal operator*

The leading-order matrix kernel $\mathcal{P}$ of the 'parametrix' $\boldsymbol{P}$ of the normal operator in Eq.(130) is given by

$$\mathcal{P}(\boldsymbol{y},\boldsymbol{x}) \sim \left(\frac{1}{2\pi}\right)^3 \int_{\mathbb{R}_{\geq 0}} \omega^2\mathrm{d}\omega\;\omega^{-2}\int_{E_{\boldsymbol{\nu}}} \mathrm{d}\boldsymbol{\nu_y}\;\langle 8\pi^2\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y})\rangle^{-1}\;\exp[i\omega\;\boldsymbol{\nu_y}\boldsymbol{\cdot}(\boldsymbol{x}-\boldsymbol{y})]\ . \tag{131}$$

In view of the possibility of $\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y})$ having a small condition number, we introduce its *pseudo-inverse* indicated by the angular brackets [50, 51].

Composing the parametrix associated with the reciprocal constituent of the normal operator with the full normal operator yields the resolution operator. Since

$$\boldsymbol{P}\,\boldsymbol{N} = \boldsymbol{P}\,[\boldsymbol{N}^{\leftrightarrow} + \boldsymbol{N}^{\not\leftrightarrow}] \sim \boldsymbol{P}\boldsymbol{N}^{\leftrightarrow}$$

up to leading order, to obtain the leading-order asymptotic inverse scattering operator, it suffices to incorporate the reciprocal constituent only in the parametrix construction.

6.2. *Maslov-Fourier representation*

While composing the parametrix $\boldsymbol{P}$ of the normal operator with the adjoint scattering operator $\boldsymbol{L}^\dagger$ in equation (95), we apply the following changes: in equation (95) we replace $\boldsymbol{y}$ by $\boldsymbol{x}$; we observe then that the entire integrand in the composition transforms into its complex conjugate upon mapping $(\omega', \boldsymbol{\nu_y}) \to (-\omega', -\boldsymbol{\nu_y})$. Thus, the integration over ω' is made one-sided and we obtain the inverse scattering operator

$$(\boldsymbol{PL}^\dagger u^{(1)})(\boldsymbol{y}) =$$

$$\frac{1}{\pi}\mathrm{Re}\ \frac{i}{(2\pi)^3}\int_{\mathbb{R}_{\geq 0}}\mathrm{d}\omega\ \int_{E_{\boldsymbol{\nu}}}\mathrm{d}\boldsymbol{\nu_y}\int_{\mathcal{D}}\mathrm{d}\boldsymbol{x}\ \int_{\mathbb{R}_{\geq 0}}\mathrm{d}\omega'\ (\omega')^2\left(\frac{\omega'}{2\pi}\right)\ \int\mathrm{d}\hat{\gamma}_1'\int\mathrm{d}\tilde{\gamma}_1'\ \int_{\partial S\times\partial R}$$

$$\langle 8\pi^2\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu_y})\rangle^{-1}\,[B^{(NM)}(\hat{\gamma}_1', r_{2,3}, \boldsymbol{x}, \tilde{\gamma}_1', s_{2,3})]^* \tag{132}$$

$$\mathbf{w}^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1', \boldsymbol{s})\ \hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1', r_{2,3}), r_{2,3})u_{pq}^{(1)}(\boldsymbol{r},\boldsymbol{s},\omega')\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1', s_{2,3}), s_{2,3})$$

$$\exp[i\omega\boldsymbol{\nu_y}\cdot(\boldsymbol{x}-\boldsymbol{y}) - i\omega'\vartheta^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1', \boldsymbol{s})]\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{s}\ .$$

Then we expand $\vartheta^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1', \boldsymbol{s})$ in a Taylor series about $\boldsymbol{y}$. The integration in $\boldsymbol{x}$ can now be carried out to yield

$$(2\pi)^3\delta(\omega\boldsymbol{\nu_y} - \omega'\nabla_{\boldsymbol{y}}\vartheta^{(NM)}) = (2\pi)^3\delta(\omega\boldsymbol{\nu_y} - \omega'|\nabla_{\boldsymbol{y}}\vartheta^{(NM)}|\,\boldsymbol{\nu}_{\boldsymbol{y}}^{\mathrm{M}})$$

with

$$\boldsymbol{\nu}_{\boldsymbol{y}}^{\mathrm{M}} \equiv |\nabla_{\boldsymbol{y}}\vartheta^{(NM)}|^{-1}\nabla_{\boldsymbol{y}}\vartheta^{(NM)} \tag{133}$$

representing the 'Maslov dip'. Considering $\omega\boldsymbol{\nu_y}$ and $\omega'|\nabla_{\boldsymbol{y}}\vartheta^{(NM)}|\boldsymbol{\nu}_{\boldsymbol{y}}^{\mathrm{M}}$ as (intermediate) wave vectors, we carry out the integration over ω' and $\boldsymbol{\nu_y}$. We obtain

$$(\boldsymbol{PL}^\dagger u^{(1)})(\boldsymbol{y}) =$$

$$\frac{1}{\pi}\mathrm{Re}\ \frac{1}{8\pi^2}\int_{\mathbb{R}_{\geq 0}}\mathrm{d}\omega\ i\left(\frac{\omega}{2\pi}\right)^3\ \int\mathrm{d}\hat{\gamma}_1'\int\mathrm{d}\tilde{\gamma}_1'\ \int_{\partial S\times\partial R}\frac{1}{|(\nabla_{\boldsymbol{y}}\vartheta^{(NM)})(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}_1', \boldsymbol{s})|^2}$$

$$\langle\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu}_{\boldsymbol{y}}^{\mathrm{M}})\rangle^{-1}\,[B^{(NM)}(\hat{\gamma}_1', r_{2,3}, \boldsymbol{x}, \tilde{\gamma}_1', s_{2,3})]^* \tag{134}$$

$$\mathbf{w}^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{x}, \tilde{\gamma}_1', \boldsymbol{s})\ \hat{\xi}_p^{(M)}(R_1(\hat{\gamma}_1', r_{2,3}), r_{2,3})u_{pq}^{(1)}(\boldsymbol{r},\boldsymbol{s},\omega)\tilde{\xi}_q^{(N)}(S_1(\tilde{\gamma}_1', s_{2,3}), s_{2,3})$$

$$\exp[-i\omega\vartheta^{(NM)}(\hat{\gamma}_1', \boldsymbol{r}, \boldsymbol{y}, \tilde{\gamma}_1', \boldsymbol{s})]\,\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{s}\ .$$

This formula represents the Maslov-GRT inversion and is perhaps the most stable procedure for linearized inverse scattering in the vicinity of caustics.

6.3. Stationary phase analysis: GRT representation

A stationary phase analysis of Eq.(134) over the slowness vectors, and a transformation from source/receiver coordinates to phase directions, as in equation (124) finally yields the GRT-style inversion

$$
\begin{aligned}
&(\boldsymbol{P}\boldsymbol{L}^{\dagger}u^{(1)})(\boldsymbol{y}) = \\
&\frac{1}{\pi}\mathrm{Re}\int_{\mathbb{R}_{\geq 0}} \mathrm{d}\omega\ \frac{1}{8\pi^2}\int_{\widetilde{S}^2\times\widehat{S}^2} \chi_{\{A^{-1}\neq 0\}}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\ \mu_{\mathrm{LS}}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s}) \\
&\qquad \langle\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu}_{\boldsymbol{y}})\rangle^{-1}\frac{|\boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})|^3}{A^{(NM)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{y},\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}))}\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \\
&\qquad \hat{\xi}_p^{(M)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))u_{pq}^{(1)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\omega)\tilde{\xi}_q^{(N)}(\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})) \\
&\qquad\qquad \exp[-i\omega\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})]\,\mathrm{d}\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\mathrm{d}\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\ ,
\end{aligned}
\tag{135}
$$

where, through the characteristic function χ, we smoothly taper away caustics at the source or the receiver. Observe that this would happen abruptly in view of the amplitude factor in the third line of equation (135).

The action of $\langle\Lambda^{(NM)}(\boldsymbol{y},\boldsymbol{\nu}_{\boldsymbol{y}})\rangle^{-1}$ combined with the premultiplication by $\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})$ for fixed dip $\boldsymbol{\nu}_{\boldsymbol{y}}$ generates what is known as A(mplitude) V(ersus scattering) A(ngles) inversion at the image point $\boldsymbol{y}$.

The time-domain *diffraction stack* is found upon carrying out the one-sided inverse Fourier transform,

$$
\begin{aligned}
&\frac{1}{\pi}\int_{\mathbb{R}_{\geq 0}} \mathrm{d}\omega\ \exp[-i\omega t]\,u_{pq}^{(1)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\omega) \\
&\qquad = u_{pq}^{(1)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),t) + i\mathrm{H}u_{pq}^{(1)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),t)
\end{aligned}
\tag{136}
$$

at $t = \tau^{(NM)}$. Here, H denotes the Hilbert transform. The right-hand side of equation (136) represents the ‘analytic trace’ associated with the scattered field. The stack is over the phase directions $\tilde{\boldsymbol{\alpha}}, \hat{\boldsymbol{\alpha}}$ attached to the image point $\boldsymbol{y}$.

7. Reduction to *direct* GRT inversion

In equation (135), observe that the factor $|\boldsymbol{\Gamma}_{\boldsymbol{y}}^{(NM)}|^3$ induces a natural taper attenuating contributions over increasingly large scattering angles. This tapering is counteracted by the factor μ_{LS} given by equation (125). To restore the natural tapering action, in the stationary phase approximation, we replace μ_{LS} by 1. We then recover the original GRT formulation [10, 11] with

$$\Lambda^{(NM)}_{\mathrm{GRT}}(\boldsymbol{y},\boldsymbol{\nu}_{\boldsymbol{y}}) \equiv \tfrac{1}{2}\int_{E_\theta\times E_\psi} \mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})\,(\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))^T \frac{\partial(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})}{\partial(\boldsymbol{\nu}_{\boldsymbol{y}},\theta_{\boldsymbol{y}},\psi_{\boldsymbol{y}})}\,\mathrm{d}\theta_{\boldsymbol{y}}\mathrm{d}\psi_{\boldsymbol{y}} + (\cdots)(\boldsymbol{y},-\boldsymbol{\nu}_{\boldsymbol{y}})\ ; \tag{137}$$

then the GRT inverse is given by

$$(\boldsymbol{P}\boldsymbol{L}^{\dagger}u^{(1)})_{\mathrm{GRT}}(\boldsymbol{y}) = \frac{1}{\pi}\mathrm{Re}\int_{\mathbb{R}_{\geq 0}}\mathrm{d}\omega\ \frac{1}{8\pi^2}\int_{\widetilde{S}^2\times\widehat{S}^2}\chi_{\{A^{-1}\neq 0\}}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \langle\Lambda^{(NM)}_{\mathrm{GRT}}(\boldsymbol{y},\boldsymbol{\nu}_{\boldsymbol{y}})\rangle^{-1}\frac{|\boldsymbol{\Gamma}^{(NM)}_{\boldsymbol{y}}(\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}})|^3}{A^{(NM)}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{y},\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}))}\mathbf{w}^{(NM)}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}) \hat{\xi}^{(M)}_p(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}))u^{(1)}_{pq}(\boldsymbol{r}(\boldsymbol{y},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}),\omega)\tilde{\xi}^{(N)}_q(\boldsymbol{s}(\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}})) \exp[-i\omega\tau^{(NM)}(\boldsymbol{r},\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{y},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}},\boldsymbol{s})]\,\mathrm{d}\tilde{\boldsymbol{\alpha}}_{\boldsymbol{y}}\mathrm{d}\hat{\boldsymbol{\alpha}}_{\boldsymbol{y}}\ . \tag{138}$$

This formula in itself is a generalization of the formulation of Schleicher *et al.* [52], who developed a first step towards allowing for caustics, via the inclusion of the KMAH index, in the diffraction stack for the case of isotropic acoustics.

8. Discussion

We have developed a Maslov asymptotic extension of the Generalized Radon Transform (GRT) inversion for elastic parameters in anisotropic media. The extension naturally allows for the occurrence of caustics, either ‘macroscopic’ ones in either polarization due to heterogeneity or ‘instantaneous’ ones in the shear polarizations due to anisotropy.

Starting with the Maslov representation for elastic one-way propagation between image point and source or receiver, we have derived a Maslov extension of the GRT describing elastic two-way scattering, or modeling, in the distorted Born approximation. From this two-way scattering representation we have derived the Maslov extension of the adjoint GRT for imaging. (The Gaussian beam counterpart of the imaging operator for scalar, isotropic acoustics was developed by Hill [53].) Composing the imaging with the modeling operators we found the normal operator, which pairs two two-way scattering processes. Imposing a transversal intersection condition associated with the bicharacteristic geometry in the background medium, for anisotropic elasticity, we selected the most singular contribution to the normal operator and, with the aid of a stationary phase approximation, constructed its parametrix – as in the analysis of GRTs. Inversion is accomplished upon composing the parametrix with the imaging operator. A key ingredient in the analysis is the concept of *microlocalization*, i.e., localization in the cotangent bundles associated with the isochrones and the diffraction surfaces.

To prevent that information in the scattered field – measured with finite resolution – gets lost in the vicinity of caustics, we proposed to evaluate the inversion operator *with* the Maslov representation in the imaging component. When applying a stationary phase analysis to this inversion operator, we recovered the GRT inversion formula.

For the inversion procedure to be well defined, it is key to use *all* the data, i.e., open sets of source and receiver locations. Aspects of an inversion procedure using all the data, in the case of isotropic acoustics in the absence of caustics, were addressed by Oristaglio [54]. The complications arising from *partial* acquisition geometries, in the case of isotropic acoustics, were analyzed by Nolan and Symes [55].

For the numerical implementation of the Maslov amplitudes, we suggest the use of the work of Červený [56]. For the discretization of the imaging and inversion operators, we refer to De Hoop and Spencer [57].

In the framework of the local optimization approach to inverse scattering, our adjoint operator provides the 'gradient' while the parametrix can be employed as a 'preconditioner', see Sevink and Herman [58].

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Appendix A. Local stereotomographic duality

A mapping between manifolds is called an immersion if its *derivative* (Jacobian) is *one-to-one* at every point of its domain. It tells us about the *local* behavior of the mapping, and does not imply that the mapping *itself* is one-to-one (Guilleman and Pollack [45]).

'one-way' immersion

Here, we will show that the 'one-way' mapping

$$\widetilde{S^2_{\boldsymbol{x}}} \ni \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} \to (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \tag{A1}$$

(see text below equation (18)) is an immersion. With the eikonal equation (11), this mapping can be extended to the equivalent mapping

$$\widetilde{S^2_{\boldsymbol{x}}} \ni \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} \to (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \ . \tag{A2}$$

It follows immediately from the fact that bicharacteristics, solving the Hamilton system (14) with initial conditions, cannot intersect on the Lagrangian manifold, that

$$\operatorname{rank}\begin{bmatrix} \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \boldsymbol{s} \\ \\ \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}} \end{bmatrix} = 2\,, \tag{A3}$$

whence the mapping (A1) is an immersion.
(The mapping $\widehat{S^2_{\boldsymbol{x}}} \ni \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}} \to (\boldsymbol{r}(\boldsymbol{x},\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \hat{\boldsymbol{p}}_{\boldsymbol{r}}(\boldsymbol{x},\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}))$ is an immersion as well.)

'two-way' immersion

With the result of the first subsection (equation (A1) is an immersion), it follows immediately that the 'two-way' mapping

$$\mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} \overset{(75)}{\to} S_\Phi \overset{(92)}{\to} \Lambda_\Phi \tag{A4}$$

is an immersion also.

stereotomographic duality

Let us consider mapping (112)

$$\mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} \overset{(75)}{\to} S_\Phi \overset{(92)}{\to} \Lambda_\Phi \overset{(93)}{\to} \lambda_\Phi \tag{A5}$$

and denote it by P_Φ, and let us introduce its Jacobian $(DP_\Phi)_.$:

$$(DP_\Phi)_. = \begin{bmatrix} \nabla_{\boldsymbol{x}}\boldsymbol{s} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{s} & \boldsymbol{0} & \boldsymbol{0} \\ \nabla_{\boldsymbol{x}}\boldsymbol{r} & \boldsymbol{0} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{r} & \boldsymbol{0} \\ \nabla_{\boldsymbol{x}}\tau^{(NM)} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(NM)} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(NM)} & \boldsymbol{0} \\ \nabla_{\boldsymbol{x}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} & \boldsymbol{0} & \boldsymbol{0} \\ \nabla_{\boldsymbol{x}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} & \boldsymbol{0} & \nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} & \boldsymbol{0} \\ 0 & 0 & 0 & -1 \end{bmatrix},$$

which corresponds with the left submatrix in equation (113). To evaluate the null space of this Jacobian, let

$$U = [U_{\boldsymbol{x}}, U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}, U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}, U_\omega]^T$$

represent the components of a vector in $T_{\cdot}(\mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R})$. Then, $(DP_\Phi)_{\cdot} U = 0$ implies that on the bicharacteristics,

$$
\begin{aligned}
&U_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{s} && + \; U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{s} && && = \boldsymbol{0}, \quad \text{(i)}\\
&U_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{r} && && + \; U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\boldsymbol{r} && = \boldsymbol{0}, \quad \text{(ii)}\\
&U_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{x}}\tau^{(NM)} && + \; U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(N)} && + \; U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(M)} && = 0, \quad \text{(iii)}\\
&U_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{x}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} && + \; U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tilde{\boldsymbol{p}}_{\boldsymbol{s}} && && = \boldsymbol{0}, \quad \text{(iv)}\\
&U_{\boldsymbol{x}}\cdot\nabla_{\boldsymbol{x}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} && && + \; U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\hat{\boldsymbol{p}}_{\boldsymbol{r}} && = \boldsymbol{0}, \quad \text{(v)}\\
& && && \qquad\qquad - \; U_\omega && = 0. \quad \text{(vi)}
\end{aligned}
$$

We contract (i) with $\partial_{s_i}\tilde{\vartheta}^{(N)}$, and obtain

$$U_{\boldsymbol{x}}\cdot(\nabla_{\boldsymbol{x}} s_i)\,\partial_{s_i}\tilde{\vartheta}^{(N)} + U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot(\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} s_i)\,\partial_{s_i}\tilde{\vartheta}^{(N)} = 0\;. \tag{A6}$$

In view of equation (26), with $\boldsymbol{s} \in \partial S$ we have

$$\tau^{(N)}(\boldsymbol{s};\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) = \tilde{\vartheta}^{(N)}((\tilde{\gamma}_{\boldsymbol{s}}(\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}))_1, \boldsymbol{s}(\boldsymbol{x},\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}});\boldsymbol{x})\;. \tag{A7}$$

Differentiating this equality with respect to $\boldsymbol{x}$, since $\partial_{\tilde{\gamma}_1}\vartheta^{(N)} = 0$, leads to

$$\nabla_{\boldsymbol{x}}\tau^{(N)} = \nabla_{\boldsymbol{x}}\tilde{\vartheta}^{(N)} + (\nabla_{\boldsymbol{x}} s_i)\,\partial_{s_i}\tilde{\vartheta}^{(N)}\;, \tag{A8}$$

where the left-hand side derivative is a total derivative †, whereas

$$\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(N)} = (\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} s_i)\,\partial_{s_i}\tilde{\vartheta}^{(N)}\;, \tag{A9}$$

where the left-hand side derivative is a total derivative again. Equation (A8) can be written in the form

$$(\nabla_{\boldsymbol{x}} s_i)\,\partial_{s_i}\tilde{\vartheta}^{(N)} = \nabla_{\boldsymbol{x}}\tau^{(N)} - \nabla_{\boldsymbol{x}}\tilde{\vartheta}^{(N)}\;. \tag{A10}$$

Substituting equations (A10), (A9) into equation (A6) yields

$$U_{\boldsymbol{x}}\cdot(\nabla_{\boldsymbol{x}}\tau^{(N)} - \nabla_{\boldsymbol{x}}\tilde{\vartheta}^{(N)}) + U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(N)} = 0\;. \tag{A11}$$

Similarly, contracting (ii) with $\partial_{r_i}\hat{\vartheta}^{(M)}$, we obtain

$$U_{\boldsymbol{x}}\cdot(\nabla_{\boldsymbol{x}}\tau^{(M)} - \nabla_{\boldsymbol{x}}\hat{\vartheta}^{(M)}) + U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(M)} = 0\;. \tag{A12}$$

Adding equations (A11) and (A12) together, yields

$$U_{\boldsymbol{x}}\cdot(\nabla_{\boldsymbol{x}}\tau^{(NM)} - \nabla_{\boldsymbol{x}}\vartheta^{(NM)}) + U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(N)} + U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\cdot\nabla_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}}\tau^{(M)} = 0\;. \tag{A13}$$

† In the present analysis, the mappings for $\boldsymbol{s}$ and $\boldsymbol{r}$ must be substituted in the two-way travel time $\tau^{(NM)}$.

Substracting equation (A13) from (iii) then results in

$$U_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{x}} \vartheta^{(NM)} = 0 \ ,$$

which on the stationary point set reduces to (cf. equation (78))

$$U_{\boldsymbol{x}} \cdot \boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)} = 0 \ , \tag{A14}$$

which states that $U_{\boldsymbol{x}}$ must be perpendicular to the migration dip (note that $\boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)} \neq \mathbf{0}$, having excluded scattering over π in the main text).

The left-hand side of (i) generates the perturbation of initial conditions,

$$\boldsymbol{s}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}) = \boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) + \epsilon \{ U_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{x}} \boldsymbol{s} + U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \cdot \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \boldsymbol{s} \} + .. \tag{A15}$$

If $(U_{\boldsymbol{x}}, U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}})$ is a solution of (i), equation (A15) implies that

$$\boldsymbol{s}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}) = \boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ . \tag{A16}$$

With (iv), applying a similar analysis to $\tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}})$, we find that

$$\tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}) = \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ . \tag{A17}$$

With the aid of the eikonal equation (11), we find that equation (A17) must hold for all the components of the slowness vector $\tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}}$, and hence (i) and (iv) imply that

$$(\boldsymbol{s}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}}), \tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}}(\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} + \epsilon U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}})) = (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tilde{\boldsymbol{\gamma}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})) \ . \tag{A18}$$

From the fact that bicharacteristics, solving the Hamilton system (14) with initial conditions, cannot intersect on the Lagrangian manifold, we conclude that $\boldsymbol{x} + \epsilon U_{\boldsymbol{x}}$ lies on the characteristic with initial values $(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}})$. Hence,

$$U_{\boldsymbol{x}} \parallel \boldsymbol{v}^{(N)}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ , \tag{A19}$$

cf. equation (16). Starting from (ii) and (v), we also find that

$$U_{\boldsymbol{x}} \parallel \boldsymbol{v}^{(M)}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \ . \tag{A20}$$

If both N and M are the qP constituent, equations (A14), (A19) and (A20) combined, imply that $\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}} = -\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}$, which case we have excluded already. For the other combinations of N and M, we will now also exclude rays for which

$$\boldsymbol{v}^{(N)}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \parallel \boldsymbol{v}^{(M)}(\boldsymbol{x}, \hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}) \perp \boldsymbol{\Gamma}_{\boldsymbol{x}}^{(NM)} \ .$$

Then the only solution to equations (A14), (A19) and (A20) is $U_{\boldsymbol{x}} = \mathbf{0}$. Substituting this into (i) and (iv) yields

$$\begin{aligned} U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \cdot \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \boldsymbol{s} &= \mathbf{0}, \\ U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \cdot \nabla_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} \tilde{\boldsymbol{p}}_{\boldsymbol{s}} &= \mathbf{0}. \end{aligned} \tag{A21}$$

Since, as we showed in the first subsection of this Appendix, the 'one-way' mapping $\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}} \to (\boldsymbol{s}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}), \tilde{\boldsymbol{p}}_{\boldsymbol{s}}(\boldsymbol{x}, \tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}))$ is an immersion, we find that $U_{\tilde{\boldsymbol{\alpha}}_{\boldsymbol{x}}} = \boldsymbol{0}$. Then also $U_{\hat{\boldsymbol{\alpha}}_{\boldsymbol{x}}} = \boldsymbol{0}$. Finally, (vi) implies that $U_\omega = 0$, and we conclude that with the appropriate exclusion of particular rays, the mapping P_Φ is an immersion.

Returning to equation (A5), from the fact that P_Φ is an immersion and the fact that the 'two-way' mapping

$$\mathcal{X} \times \widetilde{S^2} \times \widehat{S^2} \times \mathbb{R} \overset{(75)}{\to} S_\Phi \overset{(92)}{\to} \Lambda_\Phi$$

is an immersion as well (second subsection of this Appendix), it follows that $\pi_{\mathcal{Q}}$ in equation (93), the right-most leg of the sequence in equation (A5), is an immersion. The latter immersion establishes the microlocal duality between the isochrone and diffraction cotangent bundles. In the absence of caustics, this duality is global and, in the case of scalar acoustics, has been analyzed by Tygel *et al.* [59].

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