

First MaPhySto Workshop on Inverse Problems:

# Inverse Problems in Stratified Media

Centre for Mathematical Physics and Stochastics — MaPhySto

Department of Mathematical Sciences, University of Aarhus

22-24 April, 1999

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## 1 Introduction

This workshop was the first in a series to be organized by MaPhySto. The workshop brought together researchers with varied backgrounds, with a common interest in inverse problems relating to stratified media. There were series of lectures on both theory and applications.

In this leaflet we have gathered the (extended) abstracts of the talks given and the posters presented. Furthermore, at the end, the list of participants is reproduced.

The organizing committee for the workshop consisted of:

- Jean-Claude Guillot (Université Paris-Nord)
- Jens Ledet Jensen (Aarhus)
- Arne Jensen, (Aalborg)
- Bo Holm-Jacobsen (Aarhus)

## 2 Workshop Program

Thursday April 22 (in Auditorium D2, building 531)

09.00-9.45 REGISTRATION AND COFFEE/TEA

9.45-10.00 WELCOME BY OLE E. BARNDORFF-NIELSEN

**Chairman: Jean-Claude Guillot**

10.00-11.00 **M. Thompson:** *Helioseismology: inferring the structure and dynamics of the inside of the Sun I.*

COFFEE/TEA

11.15-12.15 **V. Enss:** *The Schrödinger Equation – Non-relativistic and Relativistic.*

12.30-14.00 LUNCH

**Chairman: Bo Holm-Jacobsen**

14.00-15.00 **M. Thompson:** *Helioseismology: inferring the structure and dynamics of the inside of the Sun II.*

15.10-16.10 **V. Enss/W. Jung:** *The Klein-Gordon Equation.*

COFFEE/TEA

16.40-17.40 **Poster Presentation by:** *J. M. Jensen, I. Møller, L. Engell-Sørensen, I. Gonzalez Hernandez.*

**Friday April 23 (in Auditorium D2, building 531)**

**Chairman: Volker Enss**

9.30-10.30 **J. Ralston:** *Inverse scattering problems in stratified media.*

COFFEE/TEA

11.00-12.00 **E. Clévéde:** *Global scale seismic tomography I.*

12.30-14.00 LUNCH

**Chairman: Adrian Nachman**

14.00-15.00 **J. Ralston:** *Solving Forward Problems with Gaussian Beams.*

15.10-16.10 **E. Clévéde:** *Global scale seismic tomography II.*

COFFEE/TEA

16.40-17.40 **P. Weidelt:** *The 1D-inverse problem of magnetotellurics:  
A training site for mathematical physicists.*

18.00-19.00 DISCUSSION

19.00-22.00 CONFERENCE DINNER

**Saturday April 24 (in Auditorium D2, building 531)**

**Chairman: Peter Weidelt**

9.00-10.00 **D. Sinoquet:** *Seismic reflection tomography for 3D complex geologic  
structures I.*

COFFEE/TEA

10.30-11.30 **A. Nachman:** *The Dirichlet-to-Neumann map and its connections to  
Inverse Scattering and Inverse Spectral problems.*

12.00-13.00 LUNCH

**Chairman: James Ralston**

13.00-14.00 **P. Weidelt:** *Construction of bounds for spatial averages of electrical  
conductivity.*

14.10-15.10 **A. Nachman:** *An exact, non-iterative inversion method.*

COFFEE/TEA

15.40-16.40 **D. Sinoquet:** *Seismic reflection tomography for 3D complex geologic  
structures II.*

### 3 Abstracts

**Éric Clévéde (Département de Sismologie, Paris):**

*Global Scale Seismic Tomography.*

ABSTRACT: Understanding the physical nature and dynamic of the Earth constitutes a challenge, by the size and uniqueness of this object. If the surface and, in some cases, the first few kilometers below, can be directly observed and sampled, the main part of the Earth's body is unreachable, and only seismology can provide tools to probe the planet. The Earth can be viewed, in a first order approximation, as a layered, one-dimensionally stratified, chemically differentiated planet, composed of crust, mantle and core. However, surface tectonic provides a clue that below the surface matter is in motion. It appears that convection occurs, involving the whole mantle at various spatial scales. The resulting lateral variations in composition and temperature are reflected on the elastic properties of the media, allowing seismology to provide snapshots of the Earth dynamic.

Probing the whole Earth body with seismic waves, the “global scale seismic tomography”, implies several relevant problems. Huge amount of energy is required, provided by the Earth itself through the world wide seismic activity. An inherent problem is thus the spatial repartition of the seismic sources together with the seismometers distribution, linked to the ocean-continent distribution at the Earth's surface. This practical problem influences the choice of data within the seismic signal. The useful seismic signal (in terms of global scale tomography) covers a wide frequency band, ranging from around 1 Hz to 30 mHz for the body waves, 30mHz to 3mHz for the surface waves, and 3mHz to 0.3 mHz for the Earth free oscillations. These different types of data have different resolving power (both spatially and in term of the amplitude spectrum of the structure), depending on their wavelength. The amount of data necessary and the quantity of physical parameters to determine lead to a cumbersome numerical problem, usually treated as a quasi-linear problem. Different approaches have been used to allow this problem to be solved, both in the theoretical aspect (e.g. geometrical optic approximation) and the physical a priori aspect (e.g. neglecting anisotropy). However, with the improvement of computation capability, more complete approaches are in development.

In this presentation the geodynamical context will be first introduced. In a second part, the main tomographic approaches will be described, together with the resulting models. As a conclusion the new prospects in global tomography will be presented.

# Geometrical Approach to Inverse Scattering

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## Abstract

We present a *geometrical* approach to the inverse scattering problem for the Schrödinger and Klein-Gordon equations. For given scattering operator  $S$  we show uniqueness of the potential, we give explicit limits of the high-energy behavior of the scattering operator, and we give reconstruction formulas for the potential.

Our mathematical proofs closely follow physical intuition. A key observation is that at high energies the translation of wave packets dominates over spreading during the interaction time.

## 1 Introduction, the Schrödinger Equation

The **Schrödinger equation** is a linear evolution equation for a function of time  $t \in \mathbb{R}$  with values in a state space (phase space)  $\mathcal{H}$  which is a Hilbert space:

$$\Psi(\cdot) : \mathbb{R} \rightarrow \mathcal{H}.$$

The initial value problem reads

$$i \frac{d}{dt} \Psi(t) = H \Psi(t), \quad \Psi(0) = \Psi, \tag{1.1}$$

with a linear operator  $H$  acting on  $\mathcal{H}$ . This type of equation includes as special cases non-relativistic and relativistic quantum mechanics, the Dirac equation, the linear wave equation (with the usual method to transform a second order equation into a first order system), and other evolution equations. In the models mentioned above the operator  $H$  is self-adjoint on a suitably chosen domain  $\mathcal{D}(H)$ . Then  $\exp\{-itH\}$  is a well defined unitary operator for all  $t \in \mathbb{R}$  and the unique global solution of the initial value problem (1.1) is

$$\Psi(t) = e^{-itH} \Psi. \tag{1.2}$$

We describe our geometrical approach to the inverse problem for the Schrödinger equation as an equation which describes the motion of particles according to the laws of quantum mechanics and for the Klein-Gordon equation. The time scales for interaction and for spreading of wave functions differ at high energies. This implies the simplicity of the leading behavior of the scattering operator because only the translational part of the time evolution matters as long as the interaction is strong. We obtain explicit formulas for the high energy scattering operator which can be used to reconstruct the potential uniquely. We want to explain *why* the statements are true and how physical intuition and mathematical proofs are closely analogous.

## 2 Particles in Quantum Mechanics

We describe the state of a quantum mechanical particle in  $\nu$ -dimensional space by a normalized vector  $\Psi \in \mathcal{H}$ . The vector can be represented by a square integrable function  $\psi(\cdot) \in L^2(\mathbb{R}^\nu, dx)$  with volume measure  $dx$  as a function depending on the *position*  $\mathbf{x} \in \mathbb{R}^\nu$ , or one can use its Fourier transform

$$\hat{\psi}(\cdot) \in L^2(\mathbb{R}^\nu, dp), \quad \hat{\psi}(\mathbf{p}) := (2\pi)^{-\nu/2} \int dx e^{-i\mathbf{p}\mathbf{x}} \psi(\mathbf{x}) \quad (2.1)$$

depending on the *momentum variable*  $\mathbf{p} \in \mathbb{R}^\nu$ . We always assume the normalization

$$\|\Psi\|^2 = \int dx |\psi(\mathbf{x})|^2 = \int dp |\hat{\psi}(\mathbf{p})|^2 = 1.$$

We use for the abstract state vector a capital letter  $\Psi$ , for its representation as a function of position  $\psi(\mathbf{x})$ , or its momentum space wave function  $\hat{\psi}(\mathbf{p})$ , respectively, and write

$$\begin{aligned} \mathcal{H} &\longleftrightarrow L^2(\mathbb{R}^\nu, dx) \longleftrightarrow L^2(\mathbb{R}^\nu, dp) \\ \Psi &\longleftrightarrow \psi(\mathbf{x}) \longleftrightarrow \hat{\psi}(\mathbf{p}) \end{aligned} \quad (2.2)$$

to indicate the switching between representations.

For a given state  $\Psi$  the probability measures  $\mu_{\mathbf{x}}$  on configuration space and  $\mu_{\mathbf{p}}$  on momentum space, respectively,

$$\mu_{\mathbf{x}}(A) = \int_A dx |\psi(\mathbf{x})|^2 \quad \text{and} \quad \mu_{\mathbf{p}}(B) = \int_B dp |\hat{\psi}(\mathbf{p})|^2 \quad (2.3)$$

describe the probabilities to find the particle in  $A \subset \mathbb{R}^\nu$  in configuration space or in  $B \subset \mathbb{R}^\nu$  in momentum space. One may visualize such a state as a cloud of very many particles where  $\mu_{\mathbf{x}}(A)$  describes the fraction of them which have their position in  $A$  and, similarly,  $\mu_{\mathbf{p}}(B)$  is the fraction with momentum in  $B$ . Such a state is also called a *wave packet*.

We extend the triple of representations of state vectors to the linear operators acting on them. The Fourier transformation (2.1) interchanges differentiation and multiplication of a function with its argument. Thus we obtain for the position and momentum operators, respectively,

$$\mathbf{x} \longleftrightarrow \mathbf{x} \longleftrightarrow i\nabla_{\mathbf{p}}, \quad (2.4)$$

$$\mathbf{p} \longleftrightarrow -i\nabla_{\mathbf{x}} \longleftrightarrow \mathbf{p}. \quad (2.5)$$

If the forces acting on the particle are described as the negative gradient of a potential function  $V(\mathbf{x})$  (conservative mechanical system) then the generator  $H$  of the time evolution, the *Hamiltonian* or *Schrödinger operator*, is the energy operator

$$H = H_0 + V(\mathbf{x}) \quad (2.6)$$

which is a sum of the kinetic energy operator  $H_0$  – responsible for the kinematics – and the real valued potential energy which determines the dynamics.

### 3 Kinematics

The kinetic energy operator or *free Hamiltonian*  $H_0$  usually is a function  $H_0(\mathbf{p})$  of the momentum of the particle. We will study two typical cases, nonrelativistic (NR) and relativistic (Rel) kinematics. In the first case

$$\text{NR: } H_0(\mathbf{p}) = \frac{1}{2m}\mathbf{p}^2. \quad (3.1)$$

It acts as a multiplication operator on  $\hat{\phi}$  and as a differential operator on  $\phi$ :

$$H_0 \Phi \longleftrightarrow (H_0 \phi)(\mathbf{x}) = -\frac{1}{2m}(\Delta\phi)(\mathbf{x}) \longleftrightarrow H_0(\mathbf{p}) \hat{\phi}(\mathbf{p}) = \frac{1}{2m}\mathbf{p}^2 \hat{\phi}(\mathbf{p}).$$

Generally, the *velocity operator* is the change of position in time:

$$\mathbf{v}(\mathbf{p}) = \frac{d}{dt} e^{itH_0} \mathbf{x} e^{-itH_0} \Big|_{t=0} = i[H_0, \mathbf{x}] = \nabla_{\mathbf{p}} H_0(\mathbf{p}), \quad (3.2)$$

a function of the momentum operator. In the nonrelativistic case it is unbounded:

$$\text{NR: } \mathbf{v}(\mathbf{p}) = \frac{\mathbf{p}}{m}. \quad (3.3)$$

Let us now turn to the scalar relativistic case:

$$\text{Rel: } H_0(\mathbf{p}) = \sqrt{\mathbf{p}^2 c^2 + m^2 c^4} = \sqrt{\mathbf{p}^2 + m^2} \quad (\text{speed of light } c = 1). \quad (3.4)$$

Here the velocity operator is bounded:

$$\text{Rel: } \mathbf{v}(\mathbf{p}) = \nabla_{\mathbf{p}} H_0(\mathbf{p}) = c \frac{\mathbf{p}c}{\sqrt{\mathbf{p}^2 c^2 + m^2 c^4}} = \frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2}}. \quad (3.5)$$

The **free time evolution** operator is a simple multiplication operator in momentum space

$$e^{-itH_0} \Phi \longleftrightarrow (e^{-itH_0} \phi)(\mathbf{x}) \longleftrightarrow e^{-itH_0(\mathbf{p})} \hat{\phi}(\mathbf{p}). \quad (3.6)$$

While for short times the free classical and quantum time evolutions differ considerably they behave similarly for large times. Asymptotically, the distribution in configuration space of a quantum state is in good approximation the same as that of the corresponding cloud of free classical particles, of the “classical wave packet”. For later applications we study a particular family of states  $\Phi_{\bar{\mathbf{p}}}$  with compact momentum support around a very **large “average” momentum**  $\bar{\mathbf{p}} \in \mathbb{R}^\nu$ . The unitary operator  $\exp(i\bar{\mathbf{p}}\mathbf{x})$ , a function of the position operator  $\mathbf{x}$ , shifts a state in momentum space by  $\bar{\mathbf{p}}$ :

$$\Phi_0 \longleftrightarrow \phi_0(\cdot) \longleftrightarrow \hat{\phi}_0(\cdot) \in C_0^\infty(\mathbb{R}^\nu) \quad (3.7)$$

$$\Phi_{\bar{\mathbf{p}}} = e^{i\bar{\mathbf{p}}\mathbf{x}} \Phi_0 \longleftrightarrow \phi_{\bar{\mathbf{p}}}(\mathbf{x}) = e^{i\bar{\mathbf{p}}\mathbf{x}} \phi_0(\mathbf{x}) \longleftrightarrow \hat{\phi}_{\bar{\mathbf{p}}}(\mathbf{p}) = \hat{\phi}_0(\mathbf{p} - \bar{\mathbf{p}}). \quad (3.8)$$

Since  $\phi_0(\cdot) \in \mathcal{S}(\mathbb{R}^\nu)$ , the Schwartz space of rapidly decreasing functions, these states are well localized in configuration space, too, uniformly in  $\bar{\mathbf{p}}$ . They have average velocities around  $\mathbf{v}(\bar{\mathbf{p}}) \in \mathbb{R}^\nu$ , where

$$\mathbf{v}(\bar{\mathbf{p}}) = \nabla H_0(\bar{\mathbf{p}}) =: v(\bar{\mathbf{p}}) \boldsymbol{\omega} = \begin{cases} \bar{\mathbf{p}}/m & \text{NR,} \\ \bar{\mathbf{p}}/\sqrt{\bar{\mathbf{p}}^2 + m^2} & \text{Rel,} \end{cases} \quad \boldsymbol{\omega} = \frac{\mathbf{v}(\bar{\mathbf{p}})}{|\mathbf{v}(\bar{\mathbf{p}})|} \parallel \bar{\mathbf{p}}. \quad (3.9)$$

In our context we have to control the localization in configuration space of freely evolving wave packets. This depends mainly on the support of the state in velocity (momentum) space. Therefore, we have chosen compactly supported momentum space wave functions. Then in configuration space the states cannot have compact support as well but rapid falloff is sufficient there. A special case of such **non-propagation properties** of quantum wave packets for long times is

$$\int_{|\mathbf{x}| < t v(\bar{\mathbf{p}})/2} dx |(e^{-itH_0} \phi_{\bar{\mathbf{p}}})(\mathbf{x})|^2 < \frac{\text{const}(\Phi_0, n)}{(1 + |t v(\bar{\mathbf{p}})|)^n} \quad (3.10)$$

for any  $n \in \mathbb{N}$  *uniformly* for large  $\bar{\mathbf{p}}$ . A classical free particle which starts at time 0 from the origin and has momentum  $\mathbf{p} \in \text{supp } \hat{\phi}_{\bar{\mathbf{p}}}$  will be localized at time  $t$  in the region

$$\mathbf{x}(t) \in \left\{ \mathbf{x} = t \mathbf{v}(\mathbf{p}) \mid \mathbf{p} \in \text{supp } \hat{\phi}_{\bar{\mathbf{p}}} \right\} \subset \{ \mathbf{x} \mid |\mathbf{x} - t \mathbf{v}(\bar{\mathbf{p}})| < v(\bar{\mathbf{p}})/3 \}. \quad (3.11)$$

The ‘‘classically forbidden’’ region  $|\mathbf{x}| < t v(\bar{\mathbf{p}})/2$  is separated from the ‘‘allowed region’’ by at least  $t v(\bar{\mathbf{p}})/6$ . The state mainly propagates within the classically allowed region which moves away from the origin with a positive minimal speed. The ‘‘quantum tails’’ of the wave packet in the classically forbidden region do not vanish, nevertheless, they decay very fast in time, both in the future and past. This is physically and mathematically in close analogy to rays versus waves in optics. While the shadow behind an obstacle is not totally black due to diffraction it is, nevertheless, quite dark away from the region which can be reached by straight rays (the role of the increasing separation  $t v(\bar{\mathbf{p}})/6$ ).

## 4 Dynamics

The interacting (perturbed) time evolution is generated by the Hamiltonian  $H$ ,

$$e^{-itH} \Psi, \quad H = H_0 + V(\mathbf{x}). \quad (4.1)$$

We will consider here *short-range* potentials  $V(\mathbf{x})$  which are roughly those which decrease at least like  $|\mathbf{x}|^{-(1+\varepsilon)}$ ,  $\varepsilon > 0$ , as  $|\mathbf{x}| \rightarrow \infty$ . More precisely, the set of short-range potentials is

$$\mathcal{V}^s = \left\{ V \mid \int_0^\infty \sup_{|\mathbf{x}| \geq R} |V(\mathbf{x})| dR < \infty \right\}. \quad (4.2)$$

For simplicity of presentation we will restrict ourselves in this paper to bounded potentials. Singular and long-range potentials can be included using standard techniques.

In the present context a short-range potential behaves similarly to a compactly supported one. Depending on the required accuracy it is essentially concentrated in a ball of some radius  $R$  around the origin.

The influence on the particle by the force  $-\nabla V(\mathbf{x})$  is relevant only as long as the particle is essentially localized in the interaction region, i.e. where the potential is strong. We study the scattering states which form the *continuous* spectral subspace  $\mathcal{H}^{\text{cont}}(H) = \{\text{eigenvectors of } H\}^\perp$ , they leave the interaction region for large times.

## 5 Scattering

For short-range potentials the asymptotic motion of scattering states is an essentially free motion: For any scattering state  $\Psi \in \mathcal{H}^{\text{cont}}(H)$  there exist free asymptotic configurations  $\Phi^\pm \in \mathcal{H}$  such that

$$\|e^{-it[H_0+V]} \Psi - e^{-itH_0} \Phi^\pm\| \rightarrow 0 \quad \text{as } t \rightarrow \pm\infty. \quad (5.1)$$

This is usually called asymptotic completeness of the wave operators. Similarly, for any *incoming* configuration  $\Phi^-$  or *outgoing*  $\Phi^+$  there is a corresponding state  $\Psi \in \mathcal{H}^{\text{cont}}(H)$  such that (5.1) holds (existence of wave operators).

A convenient tool to describe scattering is the scattering operator  $S$  which maps an incoming configuration  $\Phi^-$  to the corresponding outgoing configuration  $\Phi^+$  of the same state  $\Psi$ . For given  $\Phi^-$  let

$$\begin{aligned} \Psi &= \lim_{t_- \rightarrow -\infty} e^{it_-[H_0+V]} e^{-it_-H_0} \Phi^- \quad \text{and} \\ \Phi^+ &= \lim_{t_+ \rightarrow \infty} e^{it_+H_0} e^{-it_+[H_0+V]} \Psi. \end{aligned}$$

Then

$$S(t_+, t_-) := e^{it_+H_0} e^{-it_+[H_0+V]} e^{it_-[H_0+V]} e^{-it_-H_0}, \quad (5.2)$$

$$S := \underset{\substack{t_+ \rightarrow \infty \\ t_- \rightarrow -\infty}}{\text{s-lim}} S(t_+, t_-), \quad \text{satisfies } S \Phi^- = \Phi^+. \quad (5.3)$$

For microscopic particles for which quantum mechanics is an adequate description one cannot really observe more details of the scattering process than those encoded in the scattering operator. We denote the mapping

$$\mathcal{V}^s \rightarrow L(\mathcal{H}), \quad V \mapsto S = S(V) \quad (5.4)$$

as the *scattering map* from short-range potentials to bounded (unitary) scattering operators on the Hilbert space of asymptotic configurations.

The **direct** problem of scattering theory is to determine for a given potential  $V$  the scattering operator while the **inverse** problem is to determine the potential(s) if the scattering operator or part of it is known.

## 6 Uniqueness of the Potential

We denote by  $F(H_0 \geq E)$  the multiplication operator in momentum space with the characteristic function of the set  $\{\mathbf{p} \in \mathbb{R}^\nu \mid H_0(\mathbf{p}) \geq E\}$ , i.e. the spectral projection of the kinetic energy operator to energies above  $E$ . The main results about uniqueness are of the following form. They are a corollary of the asymptotic behavior of the scattering operator shown below.

**Theorem 6.1** *The scattering map  $S: \mathcal{V}^s \rightarrow L(\mathcal{H})$  is injective. Actually, the high-energy part of the scattering operator alone:  $S F(H_0 \geq E)$ ,  $E$  arbitrarily large, determines the short-range potential uniquely.*

## 7 Time Scales and Length Scales for Interaction and Spreading

For high energy states as constructed in (3.8) scattering theory becomes simple because two time scales, an interaction time  $T_I(\bar{\mathbf{p}})$  and a kinematical time of spreading  $T_{Sp}(\bar{\mathbf{p}})$  satisfy  $T_I(\bar{\mathbf{p}})/T_{Sp}(\bar{\mathbf{p}}) \rightarrow 0$  as  $|\bar{\mathbf{p}}| \rightarrow \infty$ . For a potential which is essentially supported in a ball of radius  $R$  the **interaction time** is of the order  $T_I(\bar{\mathbf{p}}) = R/v(\bar{\mathbf{p}})$ . More precisely, for  $\Phi_{\bar{\mathbf{p}}}$ ,  $\Phi'_{\bar{\mathbf{p}}}$  as in (3.8) and any  $\varepsilon > 0$  there is a radius  $\rho(\varepsilon)$  such that uniformly for large  $|\bar{\mathbf{p}}|$

$$|(\Phi'_{\bar{\mathbf{p}}}, [S - S(t_+, t_-)] \Phi_{\bar{\mathbf{p}}})| < \frac{\varepsilon}{v(\bar{\mathbf{p}})} \quad \text{if} \quad \pm t_{\pm} > \rho(\varepsilon)/v(\bar{\mathbf{p}}) \approx T_I(\bar{\mathbf{p}}). \quad (7.1)$$

$\rho(\varepsilon)$  is the length scale  $L_I$  of interaction which is independent of  $\bar{\mathbf{p}}$ . Intuitively, the radius of the interaction region and the extension in configuration space of the states up to effects of size  $\varepsilon$  sum up to  $\rho(\varepsilon)$ . The interaction time (and consequently the interaction strength) decreases with  $|\bar{\mathbf{p}}| \rightarrow \infty$  in the nonrelativistic case and remains fixed and positive for relativistic kinematics.

The kinematical **time scale of spreading**  $T_{Sp}(\bar{\mathbf{p}})$  denotes the time after which spreading of wave packets becomes relevant in the time evolution. As

$$H_0(\mathbf{p}) \Psi_{\bar{\mathbf{p}}} = H_0(\mathbf{p}) e^{i\bar{\mathbf{p}}\mathbf{x}} \Psi_0 = e^{i\bar{\mathbf{p}}\mathbf{x}} H_0(\bar{\mathbf{p}} + \mathbf{p}) \Psi_0$$

we will expand the kinetic energy function around  $\bar{\mathbf{p}}$

$$H_0(\bar{\mathbf{p}} + \mathbf{p}) =: H_0(\bar{\mathbf{p}}) + \nabla H_0(\bar{\mathbf{p}}) \cdot \mathbf{p} + H_2(\bar{\mathbf{p}}, \mathbf{p}). \quad (7.2)$$

The first summand is a number giving an irrelevant phase, the second equals  $\mathbf{v}(\bar{\mathbf{p}}) \cdot \mathbf{p}$  by (3.9). It is the dominant term which – as a multiple of the momentum operator – generates a translation of the wave packet *without changing its shape*. Only the third term  $H_2$  (which is defined by (7.2)) is responsible for the spreading of the wave packet. In our examples of “power like” Hamiltonians this part of the Hamiltonian is weak compared to the translational component: On a compact subset of momentum space like  $\mathbf{p} \in \text{supp } \hat{\phi}_0$

$$\frac{T_I(\bar{\mathbf{p}})}{T_{Sp}(\bar{\mathbf{p}})} \sim \frac{|H_2(\bar{\mathbf{p}}, \mathbf{p})|}{v(\bar{\mathbf{p}})} \leq \frac{\text{const}}{|\bar{\mathbf{p}}|} \xrightarrow{|\bar{\mathbf{p}}| \rightarrow \infty} 0. \quad (7.3)$$

Therefore, the time  $T_{Sp}(\bar{\mathbf{p}})$  is by a factor proportional to  $|\bar{\mathbf{p}}|$  longer than  $T_I(\bar{\mathbf{p}})$ , *independent* of the kinematics. For large  $|\bar{\mathbf{p}}|$  we may choose times when the scattering due to the potential is over but the spreading has not yet really started. Alternatively, the time  $T_{Sp}(\bar{\mathbf{p}})$  translates into a length scale  $L_{Sp}(\bar{\mathbf{p}}) = v(\bar{\mathbf{p}}) T_{Sp}(\bar{\mathbf{p}})$ . A particle has to travel at least that far until spreading may become visible.  $L_{Sp}(\bar{\mathbf{p}})$  increases proportional to  $|\bar{\mathbf{p}}|$  for both kinematics. Again, the ratio  $L_I/L_{Sp} = T_I/T_{Sp} \sim 1/|\bar{\mathbf{p}}| \rightarrow 0$  for any precision  $\varepsilon$ .

Usually, an interacting time evolution is complicated because the translation of a wave packet, its spreading, and the influence of the potential all occur at the same time and in the same region. In the high-energy limit it is sufficient for the calculation of the scattering operator to treat translation of wave packets rather than their correct free evolution. Since in this limit spreading occurs only when and where the interaction is negligible, i.e. when the free and interacting time evolutions are almost the same, the effect of spreading is canceled (becomes invisible) in the scattering operator. Thus, high energy scattering is simple and it can be inverted simply!

## 8 High Energy Scattering

The crucial uniformity of the estimate (7.1) enables us to interchange the limits  $\pm t_{\pm} \rightarrow \infty$  and  $|\bar{\mathbf{p}}| \rightarrow \infty$ . This simplifies the remaining discussion very much. Actually, not the time but the separation from the region of a strong potential determines the quality of approximation. With correspondingly chosen variables  $r_{\pm} := t_{\pm} v(\bar{\mathbf{p}})$  we get

$$\begin{aligned}
\lim_{|\bar{\mathbf{p}}| \rightarrow \infty} (\Phi'_{\bar{\mathbf{p}}}, S \Phi_{\bar{\mathbf{p}}}) &= \lim_{|\bar{\mathbf{p}}| \rightarrow \infty} \lim_{\pm t_{\pm} \rightarrow \infty} (\Phi'_{\bar{\mathbf{p}}}, S(t_{+}, t_{-}) \Phi_{\bar{\mathbf{p}}}) \\
&= \lim_{|\bar{\mathbf{p}}| \rightarrow \infty} \lim_{\pm r_{\pm} \rightarrow \infty} \left( \Phi'_{\bar{\mathbf{p}}}, S \left( \frac{r_{+}}{v(\bar{\mathbf{p}})}, \frac{r_{-}}{v(\bar{\mathbf{p}})} \right) \Phi_{\bar{\mathbf{p}}} \right) \\
&= \lim_{\pm r_{\pm} \rightarrow \infty} \lim_{|\bar{\mathbf{p}}| \rightarrow \infty} \left( \Phi'_{\bar{\mathbf{p}}}, S \left( \frac{r_{+}}{v(\bar{\mathbf{p}})}, \frac{r_{-}}{v(\bar{\mathbf{p}})} \right) \Phi_{\bar{\mathbf{p}}} \right). \tag{8.1}
\end{aligned}$$

As seen in (7.1) the asymptotic equality (8.1) remains true even after multiplication with  $v(\bar{\mathbf{p}})$  which is a much stronger statement in the nonrelativistic case. To determine

$$(\Phi'_{\bar{\mathbf{p}}}, S(t_{+}, t_{-}) \Phi_{\bar{\mathbf{p}}}) = (\Phi'_{\mathbf{0}}, e^{-i\bar{\mathbf{p}}\mathbf{x}} S(t_{+}, t_{-}) e^{i\bar{\mathbf{p}}\mathbf{x}} \Phi_{\mathbf{0}}) \tag{8.2}$$

for large finite times and  $\bar{\mathbf{p}}$  consider e.g. the second pair of factors in (5.2).

$$\begin{aligned}
&e^{-i\bar{\mathbf{p}}\mathbf{x}} e^{it_{-}[H_0+V]} e^{-it_{-}H_0} e^{i\bar{\mathbf{p}}\mathbf{x}} \\
&= e^{it_{-}[H_0(\mathbf{p}+\bar{\mathbf{p}})+V(\mathbf{x})]} e^{-it_{-}H_0(\mathbf{p}+\bar{\mathbf{p}})} \\
&= e^{it_{-}[H_0(\bar{\mathbf{p}})+\mathbf{v}(\bar{\mathbf{p}})\cdot\mathbf{p}+H_2(\bar{\mathbf{p}},\mathbf{p})+V(\mathbf{x})]} e^{-it_{-}[H_0(\bar{\mathbf{p}})+\mathbf{v}(\bar{\mathbf{p}})\cdot\mathbf{p}+H_2(\bar{\mathbf{p}},\mathbf{p})]} \\
&= e^{it_{-}[\mathbf{v}(\bar{\mathbf{p}})\cdot\mathbf{p}+H_2(\bar{\mathbf{p}},\mathbf{p})+V(\mathbf{x})]} e^{-it_{-}[\mathbf{v}(\bar{\mathbf{p}})\cdot\mathbf{p}+H_2(\bar{\mathbf{p}},\mathbf{p})]} \\
&= e^{ir_{-}[\boldsymbol{\omega}\cdot\mathbf{p}+\{H_2(\bar{\mathbf{p}},\mathbf{p})/v(\bar{\mathbf{p}})\}+\{V(\mathbf{x})/v(\bar{\mathbf{p}})\}]} e^{-ir_{-}[\boldsymbol{\omega}\cdot\mathbf{p}+\{H_2(\bar{\mathbf{p}},\mathbf{p})/v(\bar{\mathbf{p}})\}]} \tag{8.3}
\end{aligned}$$

using again  $t_{\pm} = r_{\pm}/v(\bar{\mathbf{p}})$  and the direction  $\boldsymbol{\omega} = \mathbf{v}(\bar{\mathbf{p}})/v(\bar{\mathbf{p}})$  as in (3.9). Due to (7.3) the functions of the momentum operator

$$[\boldsymbol{\omega} \cdot \mathbf{p} + \{H_2(\bar{\mathbf{p}}, \mathbf{p})/v(\bar{\mathbf{p}})\}] \xrightarrow{|\bar{\mathbf{p}}| \rightarrow \infty} \boldsymbol{\omega} \cdot \mathbf{p} \tag{8.4}$$

converge in strong resolvent sense and similarly for the other exponent. Therefore, for fixed  $r_{-}$  and large  $|\bar{\mathbf{p}}|$  the following approximation is good:

$$\begin{aligned}
&e^{ir_{-}[\boldsymbol{\omega}\cdot\mathbf{p}+\{H_2(\bar{\mathbf{p}},\mathbf{p})/v(\bar{\mathbf{p}})\}+\{V(\mathbf{x})/v(\bar{\mathbf{p}})\}]} e^{-ir_{-}[\boldsymbol{\omega}\cdot\mathbf{p}+\{H_2(\bar{\mathbf{p}},\mathbf{p})/v(\bar{\mathbf{p}})\}]} \\
&\approx e^{ir_{-}[\boldsymbol{\omega}\cdot\mathbf{p}+\{V(\mathbf{x})/v(\bar{\mathbf{p}})\}]} e^{-ir_{-}\boldsymbol{\omega}\cdot\mathbf{p}} \tag{8.5}
\end{aligned}$$

$$= \exp \left\{ \frac{-i}{v(\bar{\mathbf{p}})} \int_{r_{-}}^0 dr V(\mathbf{x} + \boldsymbol{\omega} r) \right\}. \tag{8.6}$$

The approximation (8.5) is the only approximation we have to make! If  $\{H_2(\bar{\mathbf{p}}, \mathbf{p})/v(\bar{\mathbf{p}})\}$  would commute with  $\{V(\mathbf{x})/v(\bar{\mathbf{p}})\}$  then we would have exact cancellation and (8.5) would be an equality as well. A careful estimate of the correction terms can be given for all Hamiltonians considered here. It is uniform in  $r_{-}$  and when compared to  $\{V(\mathbf{x})/v(\bar{\mathbf{p}})\}$  it has additional falloff like  $1/|\bar{\mathbf{p}}|$  for  $\bar{\mathbf{p}} \rightarrow \infty$  due to (7.3).

Combining (8.6) with the corresponding term for positive times we obtain for large  $|\bar{\mathbf{p}}|$

$$(\Phi'_{\bar{\mathbf{p}}}, S \Phi_{\bar{\mathbf{p}}}) \approx \left( \Phi'_0, \exp \left\{ \frac{-i}{v(\bar{\mathbf{p}})} \int_{-\infty}^{\infty} dr V(\mathbf{x} + \boldsymbol{\omega}r) \right\} \Phi_0 \right). \quad (8.7)$$

## 9 High Energy Limits of the Scattering Operator

Next we give the limiting behavior of the scattering operator in simple cases,  $\Phi_{\bar{\mathbf{p}}}$ ,  $\Phi'_{\bar{\mathbf{p}}}$ , and  $\bar{\mathbf{p}} \in \mathbb{R}^\nu$  as given in (3.8). The strong influence of the kinematics is clearly visible. For an overview of many further results see [5] and the references.

### Theorem 9.1 (scalar relativistic, short-range, [15])

For the scalar relativistic Hamiltonian

$$H = \sqrt{\mathbf{p}^2 + m^2} + V(\mathbf{x})$$

with  $v(\bar{\mathbf{p}}) \rightarrow 1$  one obtains

$$(\Phi'_{\bar{\mathbf{p}}}, S \Phi_{\bar{\mathbf{p}}}) \xrightarrow{|\bar{\mathbf{p}}| \rightarrow \infty} \left( \Phi'_0, \exp \left\{ -i \int dr V(\mathbf{x} + \boldsymbol{\omega}r) \right\} \Phi_0 \right). \quad (9.1)$$

If, however,  $v(\bar{\mathbf{p}}) \rightarrow \infty$  we can expand the exponential in (8.7)

$$\begin{aligned} & \exp \left\{ -\frac{i}{v(\bar{\mathbf{p}})} \int dr V(\mathbf{x} + \boldsymbol{\omega}r) \right\} \\ & \approx 1 - \frac{i}{v(\bar{\mathbf{p}})} \int dr V(\mathbf{x} + \boldsymbol{\omega}r) + \dots \end{aligned} \quad (9.2)$$

which explains the following nonrelativistic result. The leading behavior of the scattering operator is the identity operator (no scattering). The next order correction depends on the potential.

### Theorem 9.2 (nonrelativistic, short-range, [10], [4], [18], [6], [8])

For the Hamiltonian

$$H = \frac{1}{2m} \mathbf{p}^2 + V(\mathbf{x})$$

$$v(\bar{\mathbf{p}}) (\Phi'_{\bar{\mathbf{p}}}, i(S - \mathbf{1}) \Phi_{\bar{\mathbf{p}}}) \xrightarrow{|\bar{\mathbf{p}}| \rightarrow \infty} \int dr (\Phi'_0, V(\mathbf{x} + \boldsymbol{\omega}r) \Phi_0). \quad (9.3)$$

In the quotations we have included similar results obtained by other methods, sometimes under more restrictive assumptions. This result is to be expected from the Born approximation. It holds also under the given weaker assumptions on the falloff of the potential where the validity of the Born approximation is not established.

The estimate (7.1) and the remark following (8.6) justify that multiplication with  $v(\bar{\mathbf{p}}) \sim |\bar{\mathbf{p}}|$  is permitted. The terms omitted in the approximation are smaller than those involving  $V/v(\bar{\mathbf{p}})$ .

**Remark**

In all these limits there are **error bounds** for large but finite  $|\bar{\mathbf{p}}|$  which are explicit. E.g. in equation (9.3) we obtain

$$\left| v(\bar{\mathbf{p}}) (\Phi'_{\bar{\mathbf{p}}}, i(S-1)\Phi_{\bar{\mathbf{p}}}) - \int dr (\Phi'_0, V(\mathbf{x} + \boldsymbol{\omega}r)\Phi_0) \right| \leq \frac{\text{const}(\Phi'_0, \Phi_0, V)}{|\bar{\mathbf{p}}|}.$$

## 10 Reconstruction of the Potential

The condition  $\nu \geq 2$  (*multidimensional inverse problem*) enters here to obtain from the above limits reconstruction formulas and uniqueness. For bounded continuous (or more general) functions  $V$  the expression

$$X(\mathbf{x}, \boldsymbol{\omega}) := \int dr V(\mathbf{x} + \boldsymbol{\omega}r) \tag{10.1}$$

is the X-ray transform of  $V$ . In  $\nu = 2$  dimensions lines and hyperplanes are the same. Therefore, (10.1) is the Radon transform as well. The latter is known to be uniquely invertible because the assumption (4.2) implies  $V \in L^2(\mathbb{R}^2)$ , see e.g. Theorem 2.17 in Chapter I of [11]. The inverse Radon transform yields the unique potential. In higher dimensions one fixes e.g.  $x_3, \dots, x_\nu$  and reconstructs the ‘‘slices’’ subsequently. In particular, it is sufficient to vary  $\boldsymbol{\omega}$  in a two dimensional plane. For unbounded or discontinuous potentials the expectation value between states from a dense set of nice vectors (like those which satisfy (3.7)) effectively smoothes the potential. This is enough to reconstruct the potential as a multiplication operator.

## 11 The Klein-Gordon Equation

The Klein-Gordon equation describes the evolution of a wave-packet for a relativistic spin-0 particle of mass  $m > 0$  in  $\mathbb{R}^\nu$ . Setting the velocity of light  $c = 1$ , Planck’s constant  $\hbar = 1$  and the charge  $q = 1$ , we have the free equation

$$\ddot{u} = \Delta u - m^2 u, \quad \text{or} \quad \ddot{u} + [\mathbf{p}^2 + m^2]u = 0 \tag{11.1}$$

with the momentum operator  $\mathbf{p} = -i\nabla$ . For a particle in an electromagnetic field  $\mathbf{E} = -\nabla A_0$ , the corresponding equation reads

$$\begin{aligned} (\partial_t + iA_0(\mathbf{x}))^2 u &= \Delta u - m^2 u, \quad \text{or} \\ \ddot{u} + i2A_0(\mathbf{x})\dot{u} + [\mathbf{p}^2 + m^2 - A_0(\mathbf{x})^2]u &= 0, \end{aligned} \tag{11.2}$$

thus  $A_0 : \mathbb{R}^\nu \rightarrow \mathbb{R}$  influences the evolution of  $u(t) : \mathbb{R}^\nu \rightarrow \mathbb{C}$ . In the direct scattering problem, the large time/large distance asymptotics of solutions of (11.2) are described by a scattering operator  $S$ , that is determined from a suitably decaying potential  $A_0$ . We shall solve the inverse problem: Determine  $A_0$  from  $S$ , thus from data that are in principle measurable

in a scattering experiment. All spin-0 particles in nature are unstable, and the one-particle Klein-Gordon equation has very limited physical applications. We believe that it is interesting nevertheless, since we can compare the results to the Dirac equation (a relativistic wave equation for spin-1/2 particles), and to acoustic scattering.

To obtain a system of first-order equations, we set

$$\tilde{\psi}(\mathbf{x}) = \begin{pmatrix} \tilde{\psi}_1(\mathbf{x}) \\ \tilde{\psi}_2(\mathbf{x}) \end{pmatrix} := \begin{pmatrix} u(\mathbf{x}) \\ \dot{u}(\mathbf{x}) \end{pmatrix}, \quad \text{and} \quad \tilde{\psi}(\mathbf{p}) = \begin{pmatrix} \hat{\psi}_1(\mathbf{p}) \\ \hat{\psi}_2(\mathbf{p}) \end{pmatrix} \quad (11.3)$$

for the momentum representation. The tilde is used because we will soon introduce another representation, where the tilde is omitted. Now (11.1)  $\Leftrightarrow i\dot{\tilde{\Psi}} = \tilde{H}_0 \tilde{\Psi}$

$$\text{with } \tilde{H}_0 = \begin{pmatrix} 0 & i \\ -iB_0^2 & 0 \end{pmatrix} \text{ and } B_0^2 = -\Delta + m^2 = \mathbf{p}^2 + m^2, \text{ and (11.2) } \Leftrightarrow i\dot{\tilde{\Psi}} = \tilde{H}_1 \tilde{\Psi}$$

$$\text{with } \tilde{H}_1 = \begin{pmatrix} 0 & i \\ -iB_1^2 & 2A_0(\mathbf{x}) \end{pmatrix}, \text{ where } B_1^2 = -\Delta + m^2 - A_0(\mathbf{x})^2 = \mathbf{p}^2 + m^2 - A_0(\mathbf{x})^2.$$

We have to specify Hilbert spaces and domains for  $\tilde{H}_0$  and  $\tilde{H}_1$ , such that these operators are well-defined and self-adjoint. The choice of  $\tilde{\mathcal{H}} = L^2(\mathbb{R}^\nu, \mathbb{C}^2)$  is not possible, and before we can define the correct spaces, we shall take a look at  $B_0^2$  and  $B_1^2$  in  $\mathcal{H} = L^2(\mathbb{R}^\nu, \mathbb{C})$ :  $B_0^2$  is self-adjoint and strictly positive on its domain  $H^2(\mathbb{R}^\nu)$  (a Sobolev space), and we assume  $A_0 \in L^\infty(\mathbb{R}^\nu, \mathbb{R})$  with  $\|A_0^2\Phi\|_{L^2} \leq a\|B_0^2\Phi\|_{L^2}$  for some  $a < 1$  and all  $\Phi \in H^2$ . By the Kato-Rellich Theorem,  $B_1^2$  is self-adjoint and strictly positive on  $H^2(\mathbb{R}^\nu)$ . Now  $B_k := \sqrt{B_k^2}$  is a well-defined self-adjoint operator on  $H^1(\mathbb{R}^\nu)$ .  $B_0^2$  and  $B_1^2$  are second-order differential operators, and  $B_0$  is a pseudo-differential operator:  $(\widehat{B_0\Phi})(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2} \hat{\Phi}(\mathbf{p})$ . There is no explicit expression for  $B_1$ . If we define the Hilbert spaces

$$\tilde{\mathcal{H}}_0 := H^1(\mathbb{R}^\nu) \oplus L^2(\mathbb{R}^\nu) \quad \text{with} \quad \|\tilde{\psi}\|_{\tilde{\mathcal{H}}_0}^2 = \|B_0 \tilde{\psi}_1\|_{L^2}^2 + \|\tilde{\psi}_2\|_{L^2}^2 \quad \text{and} \quad (11.4)$$

$$\tilde{\mathcal{H}}_1 := H^1(\mathbb{R}^\nu) \oplus L^2(\mathbb{R}^\nu) \quad \text{with} \quad \|\tilde{\psi}\|_{\tilde{\mathcal{H}}_1}^2 = \|B_1 \tilde{\psi}_1\|_{L^2}^2 + \|\tilde{\psi}_2\|_{L^2}^2, \quad (11.5)$$

then  $\tilde{H}_k$  is self-adjoint in  $\tilde{\mathcal{H}}_k$  with  $D_{\tilde{H}_k} = H^2 \oplus H^1$ . Now  $\tilde{\mathcal{H}}_0$  and  $\tilde{\mathcal{H}}_1$  are equal as sets, they have different but equivalent norms, and the natural identification operator  $J : \tilde{\mathcal{H}}_0 \rightarrow \tilde{\mathcal{H}}_1$  is a linear isomorphism. For the Schrödinger- or Dirac equation, the integrand  $|\psi(\mathbf{x})|^2$  of the squared norm is interpreted as a probability or charge density, and for the Klein-Gordon equation,  $\tilde{\psi}_1^*(\mathbf{x})(-\Delta + m^2 - A_0^2(\mathbf{x}))\tilde{\psi}_1(\mathbf{x}) + |\tilde{\psi}_2(\mathbf{x})|^2$  represents an energy density.

Now  $\tilde{H}_0$  and  $\tilde{H}_1$  act on different Hilbert spaces, and the definition of the wave operators must be modified: The identification operator  $J$  is used to compare the interacting states with free asymptotic configurations.  $e^{-i\tilde{H}_1 t} \tilde{\Psi}_\pm - J e^{-i\tilde{H}_0 t} \tilde{\Psi} \rightarrow 0$  for  $t \rightarrow \pm\infty$  leads to  $\tilde{\Psi}_\pm = \tilde{\Omega}_\pm \tilde{\Psi}$  with the wave operators

$$\tilde{\Omega}_\pm := \text{s-lim}_{t \rightarrow \pm\infty} e^{i\tilde{H}_1 t} J e^{-i\tilde{H}_0 t} : \tilde{\mathcal{H}}_0 \rightarrow \tilde{\mathcal{H}}_1. \quad (11.6)$$

$J$  is not isometric, but the unitary operator  $\tilde{T} = \begin{pmatrix} \frac{1}{B_1} B_0 & 0 \\ 0 & 1 \end{pmatrix}$  “behaves like  $J$  for large  $|\mathbf{x}|$ ”,

thus  $\tilde{\Omega}_\pm = \text{s-lim}_{t \rightarrow \pm\infty} e^{i\tilde{H}_1 t} \tilde{T} e^{-i\tilde{H}_0 t}$ , and it is isometric. On suitable states  $\tilde{\Psi}$  with momentum support bounded away from the origin, we have the representation

$$\tilde{\Omega}_\pm \tilde{\Psi} = \tilde{\Psi} + i \int_0^{\pm\infty} dt e^{i\tilde{H}_1 t} (\tilde{H}_1 J - J \tilde{H}_0) e^{-i\tilde{H}_0 t} \tilde{\Psi} \quad (11.7)$$

as an absolutely convergent Riemann or Bochner integral. It is obtained by writing the RHS of (11.6) as an integral of its derivative.

We shall introduce the Foldy-Wouthuysen representation of  $\tilde{\mathcal{H}}_k$ : For  $\tilde{\Psi} \in \tilde{\mathcal{H}}_0$  or  $\tilde{\Psi} \in \tilde{\mathcal{H}}_1$  set  $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} := \begin{pmatrix} B_0 \tilde{\Psi}_1 \\ \tilde{\Psi}_2 \end{pmatrix}$ . In the FW-momentum representation, we have  $\hat{\psi}(\mathbf{p}) = \begin{pmatrix} \sqrt{\mathbf{p}^2 + m^2} \hat{\psi}_1(\mathbf{p}) \\ \hat{\psi}_2(\mathbf{p}) \end{pmatrix}$ , and the FW-position representation is given by the inverse Fourier transform  $\psi(\mathbf{y})$  of  $\hat{\psi}(\mathbf{p})$ . The Newton-Wigner position operator  $\mathbf{y}$  is defined as multiplication with  $\mathbf{y}$  in the representation  $\psi(\mathbf{y})$ . Now  $\mathcal{H}_0 = L^2(\mathbb{R}^\nu) \oplus L^2(\mathbb{R}^\nu) = \mathcal{H}_1$  as sets, and we keep the notation  $J$  for the natural identification operator. The inner products are given by

$$\|\psi\|_{\mathcal{H}_0}^2 = \|\psi_1\|_{L^2}^2 + \|\psi_2\|_{L^2}^2 \quad \|\psi\|_{\mathcal{H}_1}^2 = \|B_1 \frac{1}{B_0} \psi_1\|_{L^2}^2 + \|\psi_2\|_{L^2}^2. \quad (11.8)$$

( $B_0$  and  $B_1$  are isomorphisms  $L^2 \rightarrow H^1$ , thus  $B_1 1/B_0$  is an isomorphism  $L^2 \rightarrow L^2$ .) The Foldy-Wouthuysen representation of the Hamiltonians is

$$H_0 = \begin{pmatrix} 0 & i\sqrt{\mathbf{p}^2 + m^2} \\ -i\sqrt{\mathbf{p}^2 + m^2} & 0 \end{pmatrix} \quad \text{and} \quad (11.9)$$

$$H_1 = \begin{pmatrix} 0 & i\sqrt{\mathbf{p}^2 + m^2} \\ -i[\mathbf{p}^2 + m^2 - A_0^2(\mathbf{y})] \frac{1}{\sqrt{\mathbf{p}^2 + m^2}} & 2A_0(\mathbf{y}) \end{pmatrix} \quad (11.10)$$

The inner product of  $\mathcal{H}_1$  can be written as  $(\Phi, \Psi)_{\mathcal{H}_1} = (J^{-1}\Phi, g J^{-1}\Psi)_{\mathcal{H}_0}$  for  $\Phi, \Psi \in \mathcal{H}_1$ , where  $g := \begin{pmatrix} 1 - \frac{1}{\sqrt{\mathbf{p}^2 + m^2}} A_0^2(\mathbf{y}) \frac{1}{\sqrt{\mathbf{p}^2 + m^2}} & 0 \\ 0 & 1 \end{pmatrix}$  is a strictly positive, bounded self-adjoint operator on  $\mathcal{H}_0$ . The S-matrix is given by

$$S = \Omega_+^* \Omega_- = (J^{-1}\Omega_+)^* g (J^{-1}\Omega_-). \quad (11.11)$$

In contrast to  $\mathbf{x}$ , the Newton-Wigner position operator  $\mathbf{y}$  is self-adjoint. We have

$H_0 = \sqrt{\mathbf{p}^2 + m^2} \beta$  with the matrix  $\beta = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ . The velocity is given by

$$\mathbf{v} = i[H_0, \mathbf{y}] = \nabla_{\mathbf{p}} H_0 = \frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2}} \beta. \quad (11.12)$$

The eigenspaces  $\beta = \pm 1$  are the spectral subspaces of positive/negative kinetic energy. The negative energy subspace corresponds to anti-particles, here we have

$$\mathbf{v} = -\frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2}}.$$

## 12 Inverse Scattering for the Klein-Gordon Equation

The NW-position operator generates translations in momentum space:

$$\Psi_{\bar{\mathbf{p}}} := e^{i\bar{\mathbf{p}} \cdot \mathbf{y}} \Psi_0 \quad \longleftrightarrow \quad \psi_{\bar{\mathbf{p}}}(\mathbf{y}) = e^{i\bar{\mathbf{p}} \cdot \mathbf{y}} \psi_0(\mathbf{y}) \quad \longleftrightarrow \quad \hat{\psi}_{\bar{\mathbf{p}}}(\mathbf{p}) = \hat{\psi}_0(\mathbf{p} - \bar{\mathbf{p}}) \quad (12.1)$$

with  $\bar{\mathbf{p}} = \bar{p}\boldsymbol{\omega}$ ,  $\boldsymbol{\omega} \in S^{\nu-1}$ ,  $\bar{p} \geq 0$ . We shall consider the high-energy asymptotics of scattering by letting  $\bar{p} \rightarrow \infty$ . Now

$$e^{-i\bar{\mathbf{P}} \cdot \mathbf{y}} \left( S \psi_{\bar{\mathbf{p}}} \right) = \left( e^{-i\bar{\mathbf{P}} \cdot \mathbf{y}} S e^{i\bar{\mathbf{P}} \cdot \mathbf{y}} \right) \Psi_0, \quad (12.2)$$

and we have

**Theorem 12.1** *Suppose that  $\nu \in \mathbb{N}$ ,  $m > 0$  and  $S$  is the scattering operator for a Klein-Gordon particle of mass  $m$  in an electrostatic field  $\mathbf{E} = \nabla A_0$ , where  $A_0 : \mathbb{R}^\nu \rightarrow \mathbb{R}$  is continuous and vanishes at infinity with integrable decay:*

*$\int_0^\infty dR \|\chi(|\mathbf{x}| > R) A_0(\mathbf{x})\|_\infty < \infty$ . Moreover, we make the Kato-Rellich assumption*

*$\|A_0^2 \Psi\| \leq a \|(\mathbf{p}^2 + m^2) \Psi\|$  with  $a < 1$ . Then the high-energy asymptotics of  $S$  are given by*

$$\text{s-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{P}} \mathbf{y}} S e^{i\bar{\mathbf{P}} \mathbf{y}} = \exp \left\{ -i \int_{-\infty}^{\infty} dr A_0(\mathbf{y} + r\boldsymbol{\omega}) \right\}, \quad (12.3)$$

where  $\bar{\mathbf{p}} = \bar{p}\boldsymbol{\omega}$  with  $\boldsymbol{\omega} \in S^{\nu-1}$ . If  $\nu \geq 2$ , then  $A_0$  can be reconstructed uniquely from the scattering operator  $S$ .

Existence of the wave operators and completeness (i.e.  $\text{Ran}(\Omega_-) = \text{Ran}(\Omega_+)$ ) can be shown with standard techniques. By (11.11) we have

$$e^{-i\bar{\mathbf{P}} \mathbf{y}} S e^{i\bar{\mathbf{P}} \mathbf{y}} = \left( e^{-i\bar{\mathbf{P}} \mathbf{y}} (J^{-1} \Omega_+) e^{i\bar{\mathbf{P}} \mathbf{y}} \right)^* \left( e^{-i\bar{\mathbf{P}} \mathbf{y}} g e^{i\bar{\mathbf{P}} \mathbf{y}} \right) \left( e^{-i\bar{\mathbf{P}} \mathbf{y}} (J^{-1} \Omega_-) e^{i\bar{\mathbf{P}} \mathbf{y}} \right).$$

The term in the middle is negligible for  $\bar{p} \rightarrow \infty$  due to the strong convergence

$$e^{-i\bar{\mathbf{P}} \mathbf{y}} g e^{i\bar{\mathbf{P}} \mathbf{y}} = \begin{pmatrix} 1 - \frac{1}{\sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2}} A_0^2(\mathbf{y}) \frac{1}{\sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2}} & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

By Lemma 12.2 below, we have

$$\text{s-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{P}} \mathbf{y}} J^{-1} \Omega_{\pm} e^{i\bar{\mathbf{P}} \mathbf{y}} = \exp \left\{ i \int_0^{\pm\infty} dr W(r) \right\},$$

where  $W(r)$  is the multiplication operator in the Foldy-Wouthuysen position representation  $\psi(\mathbf{y})$  given by

$$\begin{aligned} W(r) &= e^{i\beta \boldsymbol{\omega} \cdot \mathbf{p} r} A_0(\mathbf{y}) e^{-i\beta \boldsymbol{\omega} \cdot \mathbf{p} r} \\ &= e^{i\boldsymbol{\omega} \cdot \mathbf{p} r} \frac{1+\beta}{2} A_0(\mathbf{y}) e^{-i\boldsymbol{\omega} \cdot \mathbf{p} r} + e^{-i\boldsymbol{\omega} \cdot \mathbf{p} r} \frac{1-\beta}{2} A_0(\mathbf{y}) e^{i\boldsymbol{\omega} \cdot \mathbf{p} r} \\ &= \frac{1+\beta}{2} A_0(\mathbf{y} + r\boldsymbol{\omega}) + \frac{1-\beta}{2} A_0(\mathbf{y} - r\boldsymbol{\omega}). \end{aligned} \quad (12.4)$$

Note that positive energy states are translated with the asymptotic velocity  $\boldsymbol{\omega} = c\boldsymbol{\omega}$ , and negative energy states with  $-c\boldsymbol{\omega}$ . Combining the three strong limits yields

$$\begin{aligned} \text{w-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{P}} \mathbf{y}} S e^{i\bar{\mathbf{P}} \mathbf{y}} &= \left( \exp \left\{ i \int_0^\infty dr W(r) \right\} \right)^* \mathbf{1} \exp \left\{ i \int_0^{-\infty} dr W(r) \right\} \\ &= \exp \left\{ -i \int_{-\infty}^\infty dr W(r) \right\}. \end{aligned}$$

Now both  $e^{-i\bar{\mathbf{p}}\mathbf{y}} S e^{i\bar{\mathbf{p}}\mathbf{y}}$  and the weak limit are unitary, thus strong convergence is established. We employ the equation (12.4) for  $W(r)$  and replace  $-r$  by  $r$  in the integral of the second term to obtain (12.3).

The exponent in (12.3) contains the X-ray transform of the electrostatic potential

$X(\mathbf{y}, \boldsymbol{\omega}) = \int_{-\infty}^{\infty} dr A_0(\mathbf{y} + r\boldsymbol{\omega})$ .  $X$  is continuous and vanishes for  $|\mathbf{y}| \rightarrow \infty$  orthogonal to  $\boldsymbol{\omega}$ , thus it can be obtained uniquely from its exponential, and the potential  $A_0$  is recovered as explained in Section 10.

**Lemma 12.2** *Under the assumptions of Theorem 12.1 we have the limit*

$$\text{s-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{p}}\mathbf{y}} J^{-1} \Omega_{\pm} e^{i\bar{\mathbf{p}}\mathbf{y}} = \exp \left\{ i \int_0^{\pm\infty} dr W(r) \right\}, \quad (12.5)$$

where  $W(r)$  is given by (12.4).

To prove (12.5), we show first that it is sufficient to consider a finite time interval. We employ the dense subspace  $\mathcal{D} := \{\Psi \in \mathcal{H}_0 \mid \hat{\psi} \in C_0^\infty(\mathbb{R}^\nu)\}$ . For  $\Psi \in \mathcal{D}$ , we have the Bochner integral

$$\begin{aligned} & e^{-i\bar{\mathbf{p}}\mathbf{y}} (J^{-1} \Omega_{\pm}) e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi - e^{-i\bar{\mathbf{p}}\mathbf{y}} J^{-1} e^{iH_1 t} J e^{-iH_0 t} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \\ &= i \int_t^{\pm\infty} ds e^{-i\bar{\mathbf{p}}\mathbf{y}} J^{-1} e^{iH_1 s} (H_1 J - J H_0) e^{-iH_0 s} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi, \end{aligned} \quad (12.6)$$

and the integrand is bounded by an integrable function  $h(s)$ , which is independent of  $\bar{p} \geq \bar{p}_0$ .  
Setting

$$V := J^{-1} H_1 J - H_0 = \begin{pmatrix} 0 & 0 \\ iA_0^2(\mathbf{y}) \frac{1}{\sqrt{\mathbf{p}^2 + m^2}} & 2A_0(\mathbf{y}) \end{pmatrix}, \quad (12.7)$$

$h(s)$  is obtained from the decomposition

$$\begin{aligned} & \left\| V e^{-iH_0 s} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \right\| \\ & \leq \left\| V F(|\mathbf{y}| \leq \frac{s}{2}) e^{-iH_0 s} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \right\| + \left\| V F(|\mathbf{y}| \geq \frac{s}{2}) e^{-iH_0 s} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \right\| \\ & \leq \left\| V \right\| \cdot \left\| F(|\mathbf{y}| \leq \frac{s}{2}) e^{-iH_0 s} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \right\| + \left\| V F(|\mathbf{y}| \geq \frac{s}{2}) \right\| \cdot \left\| \Psi \right\|, \end{aligned}$$

where  $F(\dots)$  is the multiplication with the characteristic function of the indicated region. Now the first term is bounded by  $\frac{\text{const}}{(1+s)^2}$  from a non-propagation property analogous to (3.10), and the second term is integrable by the decay properties of  $A_0$ .  $\frac{s}{2}$  should be read as  $\frac{cs}{2}$ , where  $c$  is the velocity of light: For large  $\bar{p}$  the velocity support of  $\Psi_{\bar{\mathbf{p}}}$  is contained in

$|\mathbf{v}| > c/2$ . Now the LHS of (12.6) is bounded by  $\pm \int_t^{\pm\infty} ds h(s)$  uniformly for  $\bar{p} \geq \bar{p}_0$ , and

by an  $\varepsilon/3$ -trick we may interchange the limits  $t \rightarrow \pm\infty$  and  $\bar{p} \rightarrow \infty$ . Thus it is sufficient to show

$$\lim_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{p}}\mathbf{y}} J^{-1} e^{iH_1 t} J e^{-iH_0 t} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi = \exp \left\{ i \int_0^t dr W(r) \right\} \Psi. \quad (12.8)$$

We employ the Dyson-expansion

$$\begin{aligned} & e^{-i\bar{\mathbf{p}}\mathbf{y}} J^{-1} e^{iH_1 t} J e^{-iH_0 t} e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \\ &= \sum_{n=0}^{\infty} i^n \int_0^t dt_n \int_{t_n}^t dt_{n-1} \cdots \int_{t_3}^t dt_2 \int_{t_2}^t dt_1 e^{-i\bar{\mathbf{p}}\mathbf{y}} V(t_n) V(t_{n-1}) \cdots V(t_2) V(t_1) e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \end{aligned}$$

with  $V(t) := e^{iH_0 t} V e^{-iH_0 t}$ , where  $V$  is given by (12.7). The  $n$ -th term is bounded by  $(|t| \|V\|_{\mathcal{L}(\mathcal{H}_0)})^n \|\Psi\|/n!$  independently of  $\bar{p}$ , thus the limit  $\bar{p} \rightarrow \infty$  can be taken term-wise.

Now (12.8) follows from

$$\begin{aligned} & \lim_{\bar{p} \rightarrow \infty} \int_0^t dt_n \int_{t_n}^t dt_{n-1} \cdots \int_{t_3}^t dt_2 \int_{t_2}^t dt_1 e^{-i\bar{\mathbf{p}}\mathbf{y}} V(t_n) V(t_{n-1}) \cdots V(t_2) V(t_1) e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi \\ &= \int_0^t dt_n \int_{t_n}^t dt_{n-1} \cdots \int_{t_3}^t dt_2 \int_{t_2}^t dt_1 W(t_n) W(t_{n-1}) \cdots W(t_2) W(t_1) \Psi \\ &= \frac{1}{n!} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_2 \int_0^{t_2} dt_1 W(t_n) W(t_{n-1}) \cdots W(t_2) W(t_1) \Psi \\ &= \frac{1}{n!} \left( \int_0^t dr W(r) \right)^n \Psi. \end{aligned}$$

This is proved in [16], and here we shall sketch the proof for  $n = 1$ :

$$\lim_{\bar{p} \rightarrow \infty} \int_0^t dr e^{-i\bar{\mathbf{p}}\mathbf{y}} V(r) e^{i\bar{\mathbf{p}}\mathbf{y}} \Psi = \int_0^t dr W(r) \Psi. \quad (12.9)$$

The integrand can be written as a product

$$\left( e^{-i\bar{\mathbf{p}}\mathbf{y}} e^{iH_0 r} e^{i\bar{\mathbf{p}}\mathbf{y}} \right) \left( e^{-i\bar{\mathbf{p}}\mathbf{y}} V e^{i\bar{\mathbf{p}}\mathbf{y}} \right) \left( e^{-i\bar{\mathbf{p}}\mathbf{y}} e^{-iH_0 r} e^{i\bar{\mathbf{p}}\mathbf{y}} \right) \Psi \text{ with}$$

$$e^{-i\bar{\mathbf{p}}\mathbf{y}} e^{\pm iH_0 r} e^{i\bar{\mathbf{p}}\mathbf{y}} = e^{\pm i\beta \sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2} r}. \text{ We have}$$

$\sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2} - (\bar{p} + \boldsymbol{\omega} \cdot \mathbf{p}) \rightarrow 0$  for  $\bar{p} \rightarrow \infty$  and  $\mathbf{p} \in \mathbb{R}^\nu$ . Thus

$$\begin{aligned} & \left( e^{i\beta \sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2} t} - e^{i\beta (\bar{p} + \boldsymbol{\omega} \cdot \mathbf{p}) t} \right) \Psi \\ &= e^{i\beta (\bar{p} + \boldsymbol{\omega} \cdot \mathbf{p}) t} \left( e^{i\beta (\sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2} - \bar{p} - \boldsymbol{\omega} \cdot \mathbf{p}) t} - 1 \right) \Psi \rightarrow 0 \end{aligned} \quad (12.10)$$

for all  $\Psi \in \mathcal{H}_0$  (by the dominated convergence theorem applied to  $\int d^\nu p |\dots \hat{\psi}(\mathbf{p})|^2$ ). This equation shows that in the high-energy limit, the spreading of a wave packet is negligible compared to the translation. We have

$$e^{-i\bar{\mathbf{p}}\mathbf{y}} V e^{i\bar{\mathbf{p}}\mathbf{y}} = \begin{pmatrix} 0 & 0 \\ iA_0^2 \frac{1}{\sqrt{(\mathbf{p} + \bar{\mathbf{p}})^2 + m^2}} & 2A_0(\mathbf{y}) \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & 2A_0(\mathbf{y}) \end{pmatrix}, \quad (12.11)$$

and thus the integral on the LHS of (12.9) is asymptotically

$$\begin{aligned} & \int_0^t dr e^{i\beta(\bar{\mathbf{p}} + \boldsymbol{\omega} \cdot \mathbf{p})r} \begin{pmatrix} 0 & 0 \\ 0 & 2A_0 \end{pmatrix} e^{-i\beta(\bar{\mathbf{p}} + \boldsymbol{\omega} \cdot \mathbf{p})r} \Psi \\ &= \int_0^t dr e^{i\beta 2\bar{\mathbf{p}}r} e^{i\beta \boldsymbol{\omega} \cdot \mathbf{p}r} \begin{pmatrix} -A_0 & 0 \\ 0 & A_0 \end{pmatrix} e^{-i\beta \boldsymbol{\omega} \cdot \mathbf{p}r} \Psi \\ &+ \int_0^t dr e^{i\beta \boldsymbol{\omega} \cdot \mathbf{p}r} \begin{pmatrix} A_0 & 0 \\ 0 & A_0 \end{pmatrix} e^{-i\beta \boldsymbol{\omega} \cdot \mathbf{p}r} \Psi, \end{aligned}$$

since the second matrix commutes with  $\beta$ , while the first is anti-commuting with  $\beta$ . Now the Riemann-Lebesgue Lemma is valid for the Bochner integral, thus the integral of the first term vanishes for  $\bar{p} \rightarrow \infty$ , due to cancellations by rapid oscillations. The second integral yields the RHS of (12.9).

This completes our sketch of the proof of Lemma 12.2, and thus of Theorem 12.1. It can be generalized to include an electromagnetic field  $(A_0, \mathbf{A})$ : Then the Klein-Gordon equation reads

$$\ddot{u} + i2A_0 \dot{u} + [(\mathbf{p} - \mathbf{A})^2 + m^2 - A_0^2]u = 0,$$

and the operators and Hilbert spaces are defined in a similar way, where  $B_1^2$  is changed to  $B_1^2 = (\mathbf{p} - \mathbf{A}(\mathbf{x}))^2 + m^2 - A_0(\mathbf{x})^2$ . We have

**Theorem 12.3** *Suppose that  $\nu \in \mathbb{N}$ ,  $m > 0$  and  $S$  is the scattering operator for a Klein-Gordon particle of mass  $m$  in an electromagnetic field  $(A_0, \mathbf{A})$ , which is bounded and decays integrably: For  $A \in \{A_0, \mathbf{A}, \operatorname{div} \mathbf{A}\}$  we have  $A \in L^\infty(\mathbb{R}^\nu)$  and*

*$\int_0^\infty dR \|\chi(|\mathbf{x}| > R) A(\mathbf{x})\|_\infty < \infty$ . Moreover, we make the Kato-Rellich assumption*

*$\|(B_1^2 - B_0^2)\Psi\| \leq a\|B_0^2\Psi\|$  with  $a < 1$ . Then the high-energy asymptotics of  $S$  are given by*

$$\operatorname{s-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{p}}\mathbf{y}} S e^{i\bar{\mathbf{p}}\mathbf{y}} = \exp \left\{ -i \int_{-\infty}^{\infty} dr \begin{pmatrix} A_0 & -i\boldsymbol{\omega} \cdot \mathbf{A} \\ i\boldsymbol{\omega} \cdot \mathbf{A} & A_0 \end{pmatrix} (\mathbf{y} + r\boldsymbol{\omega}) \right\}, \quad (12.12)$$

where  $\bar{\mathbf{p}} = \bar{p}\boldsymbol{\omega}$  with  $\boldsymbol{\omega} \in S^{\nu-1}$ . Denoting the restriction of  $S$  onto the subspace of positive/negative energy by  $S_\pm$ , we obtain

$$\operatorname{s-lim}_{\bar{p} \rightarrow \infty} e^{-i\bar{\mathbf{p}}\mathbf{y}} S_\pm e^{i\bar{\mathbf{p}}\mathbf{y}} = \exp \left\{ -i \int_{-\infty}^{\infty} dr \left( A_0 \mp \boldsymbol{\omega} \cdot \mathbf{A} \right) (\mathbf{y} + r\boldsymbol{\omega}) \right\}. \quad (12.13)$$

If  $\nu \geq 2$  and  $A_0, \mathbf{A}$  are continuous, then  $A_0$  and  $\mathbf{B} = \operatorname{rot} \mathbf{A} \in \mathcal{S}'$  can be reconstructed uniquely from  $S$  or  $S_+$  (we need an additional technical assumption on  $\mathbf{A}$ , e.g.  $\mathbf{A} \in L^2$  is sufficient).

This theorem was announced in [15], and a complete proof will be given in [16]. Note that equation (12.13) is the same for the Dirac equation, which was treated in [15] by a similar approach, where the decay assumptions on the potentials are the same, but the Kato-Rellich condition looks less restrictive. The inverse scattering problem for the Dirac equation was solved by stationary methods in [13] and [12] under stronger assumptions on the potentials, and the geometrical, time-dependent method of [15] was extended in [14] to cover time-dependent electromagnetic fields. In [1], the inverse scattering problem for the Schrödinger equation with electric and magnetic potentials was solved with the geometrical method.

Acoustic waves in an inhomogeneous medium are described by  $\ddot{u} = c^2 \rho \nabla_{\rho}^{\perp} \nabla u$ . If  $c(\mathbf{x}) \rightarrow 1$  and  $\rho(\mathbf{x}) \rightarrow 1$  for  $|\mathbf{x}| \rightarrow \infty$  suitably, there is a scattering theory with the corresponding free equation given by  $\ddot{u} = \Delta u$ . The high-energy asymptotics will be described by the eikonal equation and are not easily obtained from our time-dependent approach. If we consider the special case of  $c \equiv 1$ , thus  $\ddot{u} = \Delta u - \frac{1}{\rho} \nabla \rho \cdot \nabla u$ , the high-energy limit is calculated in the same way as for the Klein-Gordon equation with magnetic field, and  $\left(\frac{1}{\rho} \boldsymbol{\omega} \cdot \nabla \rho\right)(\mathbf{y} + \boldsymbol{\omega} r) = \frac{\partial}{\partial r} \log \rho(\mathbf{y} + \boldsymbol{\omega} r)$  yields  $e^{-i\bar{\mathbf{P}}\mathbf{y}} \Omega_{\pm} e^{i\bar{\mathbf{P}}\mathbf{y}} \rightarrow \rho^{1/2}$ . Together with  $e^{-i\bar{\mathbf{P}}\mathbf{y}} g e^{i\bar{\mathbf{P}}\mathbf{y}} \rightarrow \rho^{-1}$ , the limit  $e^{-i\bar{\mathbf{P}}\mathbf{y}} S e^{i\bar{\mathbf{P}}\mathbf{y}} \rightarrow 1$  is obtained. See [16] for details.

The books [17] and [19] give the background on mathematical scattering theory for Schrödinger and Dirac operators. The paper [5] introduces the method in an elementary way for non-specialists and gives many references.

The papers [1], [2], [5]-[9], and [15] (preprint versions) can be downloaded via our homepages <http://www.iram.rwth-aachen.de/~enss> and [.../~jung](http://www.iram.rwth-aachen.de/~jung) or by FTP from <ftp://iram.rwth-aachen.de/pub/papers/...> or from [mp\\_arc](mailto:mp_arc).

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## **Jesper Munk Jensen (Aarhus) <sup>1</sup>:**

### *Forward and inverse modelling in an acoustic sun.*

ABSTRACT: Helioseismology is an area where geophysical methods have found application in solar physics and enabled investigation of the solar interior. In helioseismology the traditional approach has been to consider global oscillation modes of the entire sun, but in the last few years a new approach, called Time-Distance helioseismology, has emerged, where one considers local wave propagation on the sun. It has become possible to measure the traveltime between two points on the solar surface as a cross correlation function and thus produce solar seismograms which are very much like the seismogram considered in terrestrial seismology. From these data it is possible to do a tomographic imaging of local structures in the outer part of the sun (Kosovichev and Duvall 1997). This approach is very close to traditional terrestrial seismology and we have used methods from this field to investigate properties of both the forward and inverse problem.

Using a Finite-Difference code, we have modelled the wave propagation in an acoustic media with properties reminiscent to those of the sun. Thus we have produced artificial data to use in the inverse procedure. For the inversion we have used a method that is based on a MultiChannel Deconvolution (MCD) algorithm (Jacobsen et al. 1998) that speeds up the calculations by doing the computational work in the Fourier domain. This means that inversions can be done in a matter of seconds, even for high volume data sets. Solving the inverse problem in this way require knowledge of the correct Fréchet kernels. We have tested two different approaches to the calculation of the Fréchet kernels. One is the well known ray approximation, but as this is a high frequency approximation we have problems with the low frequency wave propagation on the sun. The other approach takes the whole first Fresnel zone into account and is better suited to investigation of low frequency phenomena.

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## **Ingelise Møller (Aarhus):**

### *Inversion of 2D geoelectrical data by iterative use of a 1D Fréchet derivative.*

ABSTRACT: Geoelectrical methods have many applications in environmental geophysics. The development of fast data acquisition systems (e.g. Sørensen 1996) that can collect 10 - 15 profile kilometres during one day have made DC-resistivity methods practicable in large scale mapping. Data collected at every one metre in 8 electrode configurations result in about 100 000 data values per day in the field. Interpretation of such amounts of data is a computational heavy task, where shortcuts in the inversion procedures are useful.

The geoelectrical data are nonlinear functions of the ground resistivity. Therefore the inverse problem is usually solved iteratively using a linearized Gauss Newton method (e.g., Sasaki, 1989) where the Jacobian matrix (the partial derivatives of the forward solution with respect to the model parameters) has to be calculated at each iteration. When large data volumes are to be inverted this procedure becomes very time consuming because partial derivatives must be calculated and large linear systems must be solved. The computations can be reduced avoiding calculations of the Jacobian matrix (e.g., Li and Oldenburg 1994, Loke and Barker 1996). Sasaki (1994) has used the partial derivative of the homogeneous halfspace, which is given analytically, as the Jacobian matrix.

A 2D inversion algorithm is presented that uses the partial derivatives of the homogeneous halfspace as Jacobian matrix. Because the partial derivative of the homogeneous halfspace is translational invariant, the inversion at each iteration can be solved as a multichannel deconvolution (Møller et al. 1998). A multichannel deconvolution formulation leads to an inverse solution in the wave number domain, where the 2D problem decouples into many 1D problems. The regularization follows a pragmatic stochastic approach.

A profile of 512 m with data sampled every one metres in 8 electrode configurations results in 4096 data values. The model is parameterized into 7680 model cells. One inversion with 8 iterations takes 48 cpu minutes on a pentium PC. More than 99% of the calculation time is spent on the forward modelling.

Model estimates obtained by the algorithm have been compared with model estimates from a rigorous 2D inversion program. Models with equal rms misfit are not significantly different.

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## **Lisbeth Engell-Sørensen (Bergen):**

### *Micro-Seismicity for Passive Monitoring of Rock-Masses.*

ABSTRACT: The main objectives of the project is to investigate the information potential of micro seismic events recorded by passive geophone monitoring within the subsurface. The Ekofisk area serve as a test area and especially the recordings obtained through the acquisition campaign early 1997 in Central Ekofisk field. The following sub-objectives are explicitly investigated for the present application:

- a) Source relocation in a stratified reservoir model.
- b) Source mechanism determination, which includes the determination for composite sources.
- c) Simultaneous inversion for layered velocity structure and location to refine the position of sources. All three objectives consider the presence of observations obtained in one or more boreholes.

In order to be able to include anisotropy in the reservoir model, a recently completed raytracing computer code has been chosen for modelling arrival times and waveforms of P, SV and SH waves in a three-dimensional model on three-component sensors. In order to spend the least computer time, the computer code has been adobted for the present purpose: tracing rays from many sources to few receivers, and not visa versa. The location problem has been solved by grid search and linear interpolation between grid points, where the object function is a weighted sum of P and P-minus-S wave traveltme residuals and P-wave polarity residuals. The source mechanism problem has been solved by linear inversion (the least-squares solution) of first arriving P, SV, and SH waveforms. The relocation shows clustering of events along planes, whereas the source mechanism study give more distributed slip directions.

Based on the experiments so far, the micro-seismicity in the Ekofisk chalk reservoir may turn out to deliver valuable information for production monitoring, drilling/completion, and structural geology.

**Irene Gonzalez Hernandez (Queen Mary and Westfield College):**

*Ring diagram analysis: A local helioseismology technique.*

ABSTRACT: Meridional (north-south) flows and differential rotation beneath the surface of the Sun are studied using ring-diagram analysis. The technique is based on the construction and analysis of the 3-dimensional power spectrum of acoustic waves of medium-high horizontal wavenumber. The “traditional” helioseismic analyses, using the frequencies of the Sun’s global resonant modes of oscillation, produce only longitudinal averages of the solar interior. By contrast, ring-diagram analysis allows the study of the structure beneath relatively small ( $\sim 15^\circ \times 15^\circ$ ) patches of the Sun’s surface. The existence of horizontal velocity fields in the region where the waves propagate produces a shift in their frequencies. By fitting the observations to a model of this frequency shift, and performing inversions in the radial direction beneath each patch, we reconstruct the depth dependence of the Sun’s subsurface velocity field.

Here we show the results of applying this technique to 120 patches over the solar surface, covering a total surface extension of  $360^\circ$  in longitude and about  $75^\circ$  in latitude. The data, which are from the Michelson Doppler Imager (MDI) instrument on board the Solar and Heliospheric Observatory (SoHO) satellite, are full-disc dopplergrams taken every minute during the first MDI *Dynamics Program* and span an entire solar rotation.

## **Adrian I. Nachman (Rochester):**

*The Dirichlet-to-Neumann map and its connection to Inverse Scattering and Inverse Spectral problems.*

*An exact, noniterative inversion method.*

### EXTENDED ABSTRACT

These lectures followed the lively group discussion at the workshop between practitioners and theoreticians working on Inverse Problems. My aim was to show that new bridges between the two groups are being built: significant recent progress in the analytical understanding of multi-dimensional inverse problems has made it possible for an increasing number of mathematicians to begin to address some of the difficult issues arising in practical inversion.

In addition to proofs of uniqueness for a number of classical multidimensional problems which had been open for a long time, we now have exact reconstruction methods, stability estimates and (at least) an indirect characterization of admissible data for inversion. On other issues raised at the workshop, such as nonlinear resolution analysis and what can be inferred from finite sets of data, answers are beginning to emerge in one dimensional problems. (See, for example, the nonlinear version of the Shannon Sampling Theorem in [24] and the error estimates on determination from partial data in [5].) Other problems mentioned during the discussion, such as an explicit characterization of the data, simple examples of exact multidimensional inversion and fast reconstruction algorithms, require further research. By analogy to the history of the Fourier transform, one could say that we have just found (for a number of problems) the nonlinear analogue of the Fourier Inversion Theorem. More time will be needed for (what I would call) a FIST (Fast Inverse Scattering (or Inverse Spectral) Transform) to emerge.

Central to many of the new developments has been the work on the electric impedance tomography problem. The basic question it poses is whether it is possible to determine the (variable) electric conductivity inside a body from voltage and current measurements made on its surface. This question appears to have been motivated originally by geophysical applications ([9]); it is also of great interest in medical imaging ([6]). Mathematically, the problem can be formulated as follows. Let  $\Omega$  be a bounded region in  $\mathbb{R}^n$ ,  $n \geq 2$ , (the cases of interest in applications are  $n = 2$  and  $n = 3$ ) with a smooth (or at least Lipschitz) boundary  $\partial\Omega$ . Application of a voltage potential  $f$  (to electrodes) on the boundary  $\partial\Omega$  induces a potential  $u(x)$  inside  $\Omega$ . If the conductivity is assumed isotropic (the anisotropic problem will be discussed below) then it is represented by a function  $\gamma(x)$ , which we assume bounded and with a positive lower bound. The vector of current flow is then  $\gamma(x)\nabla u(x)$ , by Ohm's law. If there are no current sources or sinks inside  $\Omega$ , then the divergence of the current is zero, and this yields the second order elliptic equation satisfied by  $u(x)$ :

$$\nabla \cdot (\gamma(x)\nabla u(x)) = 0 \text{ in } \Omega$$

with Dirichlet boundary condition  $u(x) = f(x)$  for  $x$  on  $\partial\Omega$ . For any voltage  $f(x)$  on  $\partial\Omega$  we can measure the corresponding normal component of the current flux across the boundary  $\partial\Omega$ . This defines a linear operator  $\Lambda_\gamma$  on  $\partial\Omega$ , the Dirichlet-to-Neumann (voltage-to-current) map:

$$\Lambda_\gamma f(x) = \nu(x) \cdot \gamma(x)\nabla u(x) \quad , \quad x \in \partial\Omega \quad ,$$

with  $u$  the unique solution of the Dirichlet problem described above. The inverse problem is to determine the conductivity  $\gamma(x)$  inside  $\bar{\Omega}$  from knowledge of  $\Lambda_\gamma$  on the boundary. It was first formulated at this level of generality by Calderón ([4]), whose paper has sparked a considerable amount of research on this and a variety of related problems. The reader interested in the corresponding question for the Maxwell equations (where the data consists of the map taking the tangential component of the electric field on the boundary to the tangential component of the resulting magnetic field) is referred to [11,12,18,19,20] For the analogous problem in elasticity, see [17].

Note that, while the operator  $\Lambda$  on  $\partial\Omega$  is linear, its dependence on  $\gamma$  is nonlinear, hence so is the inverse problem. A formal variable count shows that in dimension  $n$  the data depends on  $2(n-1)$  variables, while  $\gamma(x)$  is a function of  $n$  variables; thus, the problem is overdetermined if  $n \geq 3$  and formally determined when  $n = 2$ . Uniqueness was proved in [23] for  $n \geq 3$  and [14] for  $n = 2$ . The paper [14] gives a method to calculate  $\gamma$  from  $\Lambda_\gamma$ . The method is, in principle, exact (no linearizing approximations are introduced) and direct (i.e. does not require multiple solutions of the forward problem through updated guesses of the medium). An intermediate object, the scattering transform  $t(k)$  of  $\gamma(x)$  is calculated from  $\Lambda_\gamma$  by solving certain linear integral equations on the boundary  $\partial\Omega$ ;  $\gamma(x)$  is then obtained from  $t(k)$  by solving linear integral equations in the complex domain. The introduction in [14] explains the main steps in this reconstruction procedure.

In joint work with my graduate student, L. Liu ([10]), we proved that this method yields the following stability estimate in dimension 2 (similar to the ones obtained in [1,2] for dimensions  $n \geq 3$ ): Assume that there is an a priori bound on the  $L^p$  norm of the derivatives up to order 2 of the conductivities  $\gamma_1, \gamma_2 : \|\gamma_j\|_{W^{2,p}(\Omega)} \leq M$  for some  $p > 1$ , and  $\gamma_j(x) \geq 1/M$ ,  $j = 1, 2$ . Then for any  $\delta < 2(p-1)/p$ , there is a constant  $C_M$  such that

$$\|\gamma_1 - \gamma_2\|_{L^\infty(\Omega)} \leq C_M |\log \|\Lambda_1 - \Lambda_2\|^{-\delta},$$

where  $\|\Lambda_1 - \Lambda_2\|$  is the distance in the operator norm (from  $H^{1/2}(\partial\Omega)$  to  $H^{-1/2}(\partial\Omega)$ ) between the corresponding Dirichlet-to-Neumann maps.

The inversion method of [14] was applied in [7] to the inverse scattering problem at fixed frequency (with data measured in the far field or the near field – see also [13]), as well as to the recovery of an inhomogeneous nonlinear medium, where the equation is of the form

$$-\Delta u + a(x, u) = 0.$$

For the nonlinear conductivity equation, see [21].

Inversion from the Dirichlet-to-Neumann map can also be used for solving certain multidimensional inverse spectral problems. In [16] we showed that for the Schrödinger operator  $-\Delta + q$ , knowledge of the Dirichlet eigenvalues in the domain  $\Omega \subset \mathbb{R}^n$ ,  $n \geq 2$ , as well as of the normal derivatives on the boundary  $\partial\Omega$  of the corresponding orthonormal eigenfunctions determines the appropriate Dirichlet-to-Neumann map and thereby the potential  $q$ . This boundary spectral data in fact determines the boundary data at all frequencies, and so can be treated by time-domain methods (quite different from the fixed frequency methods discussed in these lectures) as well. See, for instance, [3,8] for some far reaching generalizations.

When the conductivity is anisotropic, it is represented by a symmetric positive definite matrix-

valued function  $\gamma = (\gamma^{ij}(x))$  and the equation for the potential  $u$  inside  $\Omega$  becomes

$$\sum_{i,j=1}^n \frac{\partial}{\partial x_i} \left( \gamma^{ij}(x) \frac{\partial u}{\partial x_j} \right) = 0 \text{ in } \Omega, \quad u = f \text{ on } \partial\Omega .$$

The corresponding Dirichlet-to-Neumann map, defined by

$$\Lambda_\gamma f = \sum_{i,j=1}^n \nu^i \gamma^{ij} \frac{\partial u}{\partial x_j} \Big|_{\partial\Omega} ,$$

no longer determines  $\gamma$  in this case: any diffeomorphism  $\Phi$  of  $\Omega$  which equals the identity on the boundary gives rise to a conductivity

$$\gamma_* = \frac{(D\Phi)^T \gamma (D\Phi)}{\det(D\Phi)} \circ \Phi^{-1}$$

with  $\Lambda_{\gamma_*} = \Lambda_\gamma$ . Nevertheless, in joint work with P. Ola [15], we investigated precisely what can be reconstructed from knowledge of  $\Lambda_\gamma$  in dimension two. In particular, given  $\Lambda_\gamma$ , is it possible to determine whether there exists an isotropic conductivity  $\tilde{\gamma}$  in  $\Omega$  yielding the same boundary measurements  $\Lambda_{\tilde{\gamma}} = \Lambda_\gamma$ ? Assume, for simplicity, that  $\gamma = 1$ , the identity matrix, near  $\partial\Omega$  and extend  $\gamma$  to be  $= 1$  outside  $\Omega$ . There is (see [22]) a unique diffeomorphism  $\Phi$  of  $\mathbb{R}^2$  which tends to the identity at infinity such that the corresponding  $\gamma_*$  (as defined above) is isotropic. We are thus relying on the presence of the isothermic coordinates in two dimensions. Given  $\Omega$  with an anisotropic conductivity  $\gamma$ , we can think of the forward problem as yielding the Dirichlet-to-Neumann map  $\Lambda_\gamma$  on  $\partial\Omega$  as well as the diffeomorphism  $\Phi$ , the corresponding isotropic  $\gamma_*$  and the domain  $\Omega_* = \Phi(\Omega)$ . In the inverse problem we are given  $\Lambda_\gamma$  on  $\partial\Omega$ , and our result is that one can reconstruct  $\Omega_*$ ,  $\gamma_*$  on  $\Omega_*$  and  $\Phi$  outside  $\Omega$  (but not  $\Phi$  inside  $\Omega$ ). In particular we are able to determine that the measurements  $\Lambda_\gamma$  are compatible with an isotropic conductivity  $\tilde{\gamma}$  (i.e.  $\Lambda_\gamma = \Lambda_{\tilde{\gamma}}$ ) if and only if the function  $\Phi|_{\partial\Omega}$  (which we can calculate from  $\Lambda_\gamma$ ) is the identity on  $\partial\Omega$ . In general, if two conductivities  $\gamma_1$  and  $\gamma_2$  with corresponding  $\Phi_1, \Phi_2$  have the same Dirichlet-to-Neumann map, then  $\Phi_1$  and  $\Phi_2$  agree on  $\partial\Omega$  and  $\gamma_2$  can be obtained from  $\gamma_1$  via the diffeomorphism  $\Phi_2^{-1} \circ \Phi_1$  which equals the identity on the boundary.

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## James Ralston (UCLA):

### *Inverse scattering problems in stratified media.*

#### EXTENDED ABSTRACT

This talk was on inverse scattering at fixed energy for the acoustic wave equation in a layered medium, and it was based on [GR]. The layered medium problem is typical of a class of inverse problems in which the scattering amplitude is given, and one wishes to recover coefficients in the wave equation. One can introduce the scattering amplitude for these problems in the following way. Assume that the motion of an idealized, “unperturbed” medium is governed by a wave equation

$$u_{tt} + L_0 u = 0, \quad (1)$$

where  $L_0$  is a nonnegative, self-adjoint differential operator. Assuming further that  $L_0$  has a spectral representation in terms of generalized eigenfunctions  $\psi_0$ , i.e.  $L_0 \psi_0 = k^2 \psi_0$ , we can construct time-harmonic solutions,  $u = \exp(-ikt) \psi_0$ ,  $k > 0$ , of (1). In simple cases these will be travelling plane waves. Next we suppose that the motion of a more realistic medium is governed by the “perturbed” wave equation

$$u_{tt} + L u = 0, \quad (2)$$

where  $L$  is also self-adjoint and  $L - L_0$  is strongly localized in space – either it vanishes outside a bounded set or its coefficients tend rapidly to zero as  $|x| \rightarrow \infty$ . In this situation one expects that there should be time-harmonic solutions of (2) which are superpositions of  $\exp(-ikt) \psi_0$  and a scattered wave propagating away from the perturbation. One way to get such solutions is to imagine that the perturbation is turned on at time  $t = 0$ , and consider the solution  $u(x, t) = \exp(-ikt) \psi_0(x) + v(x, t)$  to (2) in  $t > 0$  with

$$v_{tt} + L v = e^{-ikt} (L_0 - L) \psi_0, \quad v(x, 0) = v_t(x, 0) = 0. \quad (3)$$

In many cases the “Limiting Amplitude Principle” (see [LP], Chpt. V.4) shows that  $v$  does tend to  $\exp(-ikt) w(x)$  as  $t \rightarrow \infty$  so that

$$w_\epsilon(x) = \epsilon \int_0^\infty e^{(ik - \epsilon)t} v(x, t) dt$$

converges to  $w$  as  $\epsilon \rightarrow 0_+$ . However, in the mathematical literature  $w_\epsilon$  is more often introduced as the square-integrable solution to

$$(L - (k + i\epsilon)^2) w_\epsilon = (L_0 - L) \psi_0.$$

Then one recovers  $w$  by showing that the resolvent  $(L - (k + i\epsilon)^2 I)^{-1}$  converges in suitable norms as  $\epsilon \rightarrow 0_+$  (the “Limiting Absorption Principle”). However one introduces the scattered wave  $w$  associated with  $\psi_0$ , it is the asymptotics of  $w$  as  $|x| \rightarrow \infty$  that determine the scattering amplitude. In the simplest case, i.e.  $L_0 = -\Delta$ ,  $L = -c^2 \Delta$  with  $c(x) = 1$  for  $|x|$  large, and  $\psi_0(x) = \exp(ik\omega \cdot x)$ ,  $|\omega| = 1$ , one finds that  $\exp(-ikt) w(x)$  is asymptotically an outgoing spherical wave: in  $n$  space dimensions

$$w(x) = e^{ik|x|} / |x|^{(n-1)/2} (a(x/|x|, \omega) + O(1/|x|)),$$

and the scattering amplitude at energy  $k^2$  is the function  $a(\theta, \omega)$ . There are constraints on what one can hope to recover from the scattering amplitude. To see how these arise (and introduce an equation that I will need shortly) let  $h$  be the Fourier transform of  $(\Delta + k^2)w$  in the example above. Then  $h$  is a solution of the singular integral equation

$$h(\xi, k\omega) + \lim_{\epsilon \rightarrow 0_+} (2\pi)^{-n} \int_{R^n} \hat{q}(\xi - \eta) \frac{h(\eta, k\omega)}{|\eta|^2 - k^2 - i\epsilon} d\eta = -\hat{q}(\xi - k\omega), \quad (4)$$

where  $q = k^2(c^{-2} - 1)$  and  $\hat{f}$  denotes the Fourier transform. One can show by fairly standard asymptotic analysis that  $h$  is related to the scattering amplitude by

$$h(k\theta, k\omega) = c(n, k)a(\theta, \omega), \quad (5)$$

where  $c$  is a constant:  $c(3, k) = (4\pi)^{-1}$ . If one considers the variational (Frechet) derivative of  $h$  with respect to  $\hat{q}$ , and evaluates this at  $\hat{q} = 0$ , it follows from (4) and (5) that

$$c(n, k)\delta a(\theta, \omega) = -\delta \hat{q}(k(\theta - \omega)).$$

In other words, infinitesimally close to the zero perturbation, the scattering amplitude at energy  $k^2$  only determines that Fourier transform of the perturbation on the ball of radius  $2k$ . This suggests that one can only hope to recover the perturbation exactly from the scattering amplitude at finite energies when its Fourier transform on a ball determines the Fourier transform on all space. This is true when the perturbation decays at an exponential rate – so that its Fourier transform is real analytic – and we shall assume that here. The preceding is based on an observation of Roman Novikov, and one should see [N2] for further discussion of its implications in potential scattering. The equation (4) is a starting point for recovering the perturbation from the scattering amplitude. To proceed one first connects the scattering amplitude with a nonphysical scattering amplitude depending on a real parameter  $\sigma$  and a unit vector  $\nu$ , using ideas of Faddeev [F]. Then one performs an unlikely analytic continuation from [ER] which is made possible by the exponential decay of the perturbation. At the end of this reasoning one concludes that, if one can solve

$$h_\nu(\xi) + (2\pi)^{-n} \int_{R^n} \hat{q}(\xi - \eta) \frac{h_\nu(\eta)}{(\eta + i\tau\nu)^2 - k^2} d\eta = -\hat{q}(\xi - \zeta)$$

for  $h_\nu(\xi; \zeta, i\tau)$  for  $\tau$  sufficiently large, then the scattering amplitude determines the restriction of  $h_\nu$  to the (complex) manifold determined by

$$(\xi + i\tau\nu)^2 = (\zeta + i\tau\nu)^2 = k^2 \quad (7)$$

for  $|\text{Im}\{\xi\}|$  and  $|\text{Im}\{\zeta\}|$  sufficiently small. Then one shows that the norm of the integral operator in (6) goes to zero as  $\tau$  goes to infinity (when the dimension  $n$  greater than 2), establishing the existence of the solution for  $\tau$  sufficiently large. Taking limits in (6) along suitable curves  $(\xi(s), \zeta(s), \tau(s))$  lying in (7) with  $\tau(s) \rightarrow \infty$ , one shows that the scattering amplitude determines the restriction of  $\hat{q}(\xi)$  to  $|\xi| < 2k$ . When the wave equation in a layered medium is the unperturbed problem – as opposed to the homogeneous medium in the example above – the unperturbed operator  $L_0$  no longer has a spectral representation in terms of the Fourier transform. In [GR] the unperturbed operator is  $L_0 = -c_0^2(x_n)\Delta$  in  $R^n$ ,  $n \geq 3$ , where  $c_0(s)$  takes positive

constant values  $c_+$  for  $s > s_+$  and  $c_-$  for  $s < s_-$  with  $c_- < c_+$ , but for  $s_- \leq s \leq s_+$   $c(s)$  can be any positive measurable function such that  $c$  and  $1/c$  are bounded. This complicates the structure of the resolvent  $(L_0 - \lambda I)^{-1}$ , and the integral equations (4) and (6). However, the limiting absorption principle holds for this problem (and more general ones: see [dBP], [BdMM]), and, using the representation of  $(L_0 - \lambda I)^{-1}$  in terms of the Fourier transform in the variables other than  $x_n$  and a Green's function in  $x_n$ , one can carry out the argument outlined in the preceding paragraph. The scattering amplitude itself is considerably more complicated because of the total reflection of waves with incident directions  $\theta = (\theta_1, \dots, \theta_n)$ ,  $|\theta| = 1$ ,  $0 < \theta_n < \sqrt{1 - (c_-/c_+)^2}$ , and the possibility of guided waves which have zero asymptotics in all directions with  $\theta_n \neq 0$ . One needs to include the asymptotics of all these waves in the scattering amplitude to link the physical scattering amplitude with the Faddeev-type scattering amplitude. Thus, in addition to requiring an analytic continuation which cannot be done numerically, this method of recovering the perturbation makes use of the full scattering data at energy  $k^2$  which could be very difficult to collect. It is not proposed as a practical method of recovering the physical sound speed  $c(x)$ . Instead I offer it as an example of what can be shown to be theoretically possible. The part of the inverse scattering literature that is closest in spirit to what I have discussed here deals with perturbations which decay exponentially in space (in dimensions three and greater). In quantum scattering R. Novikov [N1] showed that the scattering amplitude at fixed energy determined the potential in this case. This was followed by [ER] which obtained the same result for both a potential and a magnetic field. Isozaki [I] treated perturbations of a simple layered medium, using the analytic continuation introduced in [ER]. His results are generalized in [W] and [GR]. When one considers perturbations of the homogeneous medium which are localized in a bounded domain  $D$  – or any perturbed equation which reduces to  $\Delta$  outside  $D$  – knowing the scattering amplitude at energy  $k^2$  is equivalent to knowing the Dirichlet-to-Neumann map for  $L - k^2$  for the boundary of  $D$ . Thus these problems can be attacked by the methods described by Professor Nachman in his lectures. In fact the solution of (6) is related to the construction of the exponentially growing solutions. For the Schrödinger equation with magnetic potential a construction of such solutions based on (6) has been carried out by Ziqi Sun [S]. I will not attempt to survey the literature on inverse problems where one is given the Dirichlet-to-Neumann map. However, since the acoustic layered medium is in a sense a prototype for the elastic layered medium, I should point out that Nakamura and Uhlmann [NU] have shown that the parameters of an elastic medium are determined by its Dirichlet-to-Neumann data.

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## James Ralston (UCLA):

### *Solving Forward Problems with Gaussian Beams.*

#### EXTENDED ABSTRACT

Gaussian beams are high frequency asymptotic solutions to linear partial differential equations. Over the past thirty years they have been useful in a variety of problems in mathematical physics and the theory of partial differential equations ([2]-[8]), and they have been used to model lasers in electrical engineering ([1]). In this talk I gave a short description of how they are constructed. They may be useful in solving forward problems efficiently when caustics are present, and they could be used to refine ray tracing methods if one wished to determine more than the travel time. In essence Gaussian beams are geometric optics approximations restricted to follow a single ray path. One begins with the Ansatz

$$u(x, t, k) = e^{ik\phi(x,t)} a(x, t, k), \quad a(x, t, k) = a_0(x, t) + k^{-1}a_1(x, t) + \cdots + k^{-S}a_S(x, t),$$

where the amplitude  $a(x, t, k)$  is vector-valued when one is solving a system of equations. In geometric optics one uses precisely this Ansatz, and assumes that the phase function  $\phi$  is real-valued. One can localize  $u$  to a small bundle of ray paths by choosing the amplitude correctly, but the asymptotic solution will usually develop caustics as it evolves, and then the solution cannot be continued in the form given in the Ansatz. In the construction of Gaussian beams the phase has a nonnegative imaginary part which is strictly positive off a single ray path. More precisely,  $\phi$  will be constructed so that the imaginary part of its Hessian is strictly positive on vectors orthogonal to the ray path in space-time. In this case caustics do not develop. The localization to a single ray path makes the beam construction simpler than geometric optics. If one applies any  $k$ -independent linear partial differential operator to  $u$ , the result will be an expression of the form

$$\sum_{m=-S}^M k^m b_m(x, t) e^{ik\phi(x,t)}. \quad (1)$$

If  $b$  vanishes to order  $r$  on the ray path  $(x(t), t)$ , the positive imaginary part of  $\phi$  makes

$$|b(x, t) e^{ik\phi(x,t)}| \leq C |x - x(t)|^r e^{-c|x-x(t)|^2} = O(k^{-r/2}),$$

uniformly in  $t$ . Thus we can solve the equation up to any prescribed order (say  $k^{-S+M}$ ) simply by making the coefficients  $b_m$  vanish to sufficiently high order on the ray path. This can be done by solving ordinary differential equations along the ray path. On any fixed interval in time the difference between the true solution and the Gaussian beam with the same initial data will then be of the order of  $k^{-S+M}$ . The key observations in the Gaussian beam construction enter when one solves the equation  $b_M(x, t) = 0$  to eliminate the highest power of  $k$  in (1). For scalar equations the requirement  $b_M(x, t) = 0$  is equivalent to the eichonal equation. For systems it is homogeneous system of linear equations which must have a nontrivial solution. In isotropic elasticity this system has nontrivial solutions if and only if the phase satisfies either of the equations

$$i) (\phi_t)^2 = (\lambda(x) + 2\mu(x)) |\nabla_x \phi|^2 \text{ ("compression waves")} \text{ or}$$

$$ii) (\phi_t)^2 = \mu(x)|\nabla_x \phi|^2 \text{ ("shear waves")},$$

i.e. one has an eichonal equation for each wave speed. Setting  $z = (x, t)$ , we can write these equations compactly as  $P(z, \phi_z) = 0$ , where  $\phi_z$  denotes the gradient in  $(x, t)$ , and  $P(z, \zeta)$  is a polynomial in  $\zeta$ . The ray paths are the projections onto  $z$  of the solutions of the system

$$\dot{z} = P_\zeta(z, \zeta), \quad \dot{\zeta} = -P_z(z, \zeta), \quad (2)$$

such that  $P(z(s), \zeta(s)) = 0$ . For the Gaussian beam construction we want  $P(z, \phi_z)$  to vanish to high order on a ray path  $z(s)$ . If we set  $\phi_z(z(s)) = \zeta(s)$ , then the gradient of  $P(z, \phi_z(z))$  evaluated on  $z = z(s)$ ,

$$P_{z_i}(z(s), \phi_z(z(s))) + P_{\zeta_j}(z(s), \phi_z(z(s)))\phi_{z_j z_i}(z(s))$$

vanishes by (2). Requiring that the Hessian of  $P(z, \phi_z(z))$  vanish on  $z = z(s)$  leads to the matrix equation

$$\dot{M} + A + BM + MB^t + MCM = 0, \quad (3)$$

where

$$A(s) = P_{zz}(z(s), \zeta(s)), \quad B(s) = P_{z\zeta}(z(s), \zeta(s)), \quad C(s) = P_{\zeta\zeta}(z(s), \zeta(s)) \text{ and}$$

$$M(s) = \phi_{zz}(z(s)).$$

This is a matrix Riccati equation, and one can solve it by taking  $M = NY^{-1}$ , where  $(Y, N)$  is a matrix solution to the linearization of (2) along  $(z(s), \zeta(s))$

$$\dot{y} = B^t y + C\eta, \quad \dot{\eta} = -Ay - B\eta. \quad (4).$$

The forms (symplectic and complex symplectic)

$$\langle (y^1, \eta^1), (y^2, \eta^2) \rangle = y^1 \cdot \eta^2 - y^2 \cdot \eta^1, \text{ and}$$

$$\langle (y^1, \eta^1), (y^2, \eta^2) \rangle_C = \overline{y^1} \cdot \eta^2 - y^2 \cdot \overline{\eta^1}$$

are constant on pairs of solutions of (4). Making use of this, elementary arguments show that any matrix solution  $(Y(s), N(s))$  of (4) with initial data  $(Y(0), N(0)) = (I, M_0)$ , where  $M_0 \dot{z}(0) = \dot{\zeta}(0)$  and  $\text{Im}\{M_0\}$  is positive on vectors orthogonal to  $\dot{z}(0)$ , will have  $Y(s)$  invertible for all  $s$ . This leads to the absence of caustics in Gaussian beams. Then one can go on verify the following: Given any ray path on which time is strictly increasing, and the corresponding curve  $(z(s), \zeta(s))$ , for every choice of the initial Hessian  $\phi_{xx}(z(0))$  such that  $\text{Im}\{\phi_{xx}(z(0))\} > 0$  one can construct a complex phase  $\phi$  such that

$$\phi(z(s)) = \int_0^s \zeta(r) \cdot \dot{z}(r) dr,$$

$\phi_z(z(s)) = \zeta(s)$ ,  $\phi_{zz}(z(s))$  satisfies (3) and  $\text{Im}\{\phi_{zz}(z(s))\}$  is strictly positive on vectors orthogonal to the ray path. This gives us the Taylor series of the phase along the ray path up to order 2. The equations for the higher order terms in the Taylor series of the phase are linear systems of ordinary differential equations along  $z(s)$ , as are the equations for the Taylor series of the amplitudes  $a_j$ . Thus the remainder of the construction can be carried out quite easily. A

Gaussian beam is essentially zero outside a tube of radius  $O(k^{-1/2})$  around its ray path. To get solutions with larger support one can take linear superpositions via integration with respect to the parameters in the initial data. This will produce solutions following a bundle of ray paths which can develop caustics. Since the solutions are uniformly accurate with respect to the parameters, the superposition will give an accurate asymptotic solution near caustics. I concluded with one explicit example. For the acoustic wave equation

$$u_{tt} = \Delta u$$

and the ray path  $(x_1(s), x_2(s), t(s)) = (0, s, s)$  one has the Gaussian beam

$$u(x_1, x_2, t) = a(x_1, x_2, t)e^{ik\phi(x_1, x_2, t)},$$

$$\phi = \frac{x_2 - t}{2} + \frac{a^2 t x_1^2}{1 + 4a^2 t^2} + i\left(\frac{ax_1^2}{2 + 8a^2 t^2} + \frac{b(x_2 - t)^2}{2}\right) \text{ and } a(0, t, t) = (1 + 2ait)^{-1/2}.$$

Note that the phase is shifted by  $\pi/2$  as one would expect at a caustic, but here the shift takes place continuously as one goes from  $t = -\infty$  to  $t = \infty$ .

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## **Delphine Sinoquet (Institut Francais du Petrole):**

### *Seismic reflection tomography for 3D complex geologic structures.*

ABSTRACT: Seismic reflection tomography allows the determination of the velocity and of the reflector geometries of the subsurface from the traveltimes of the seismic waves. The solution of the inverse problem is the model that minimizes the misfits between observed traveltimes and traveltimes computed by ray tracing (the forward problem).

In the inverse problem, the introduction of a priori geological information is crucial to well pose the mathematical problem, more especially to remove the indetermination linked to the depth-velocity ambiguity inherent in traveltime inversion.

An other difficulty comes from the complexity of the traveltime curves to be inverted. The geological structures we are interested in, often generate multi-valued traveltimes (several traveltimes for one couple source-receiver). These data are very precious to well determine the earth model but they require an adequate formulation of the forward and inverse problems.

In this talk, I will address these different issues and illustrate them with applications in oil exploration.

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**Michael J. Thompson (Queen Mary and Westfield College):**

*Helioseismology: inferring the structure and dynamics of the inside of the Sun.*

EXTENDED ABSTRACT

## **1. Introduction; the Sun, a star**

Helioseismology is the study of the internal structure and dynamics of the Sun using ‘sunquakes’. To be more precise, the Sun is oscillating simultaneously in many thousands of global normal modes. These oscillations, which are far too small to be seen with the naked eye, are excited by turbulent convection just below the visible surface and manifest themselves in minute brightness variations and displacements over the Sun’s surface. The frequencies of the normal modes are determined by conditions inside the Sun: the helioseismic inversion problem is to use these frequencies to make inferences about the structure and dynamics of the solar interior. A good starting point for learning about helioseismology is the collection of articles in the 31 May 1996 issue of *Science* (*Science* **272**, 1281 – 1309). Another is the review paper by Gough & Toomre (1991).

## **2. Global resonant oscillations of the Sun**

The Sun is a self-gravitating fluid body, held up by pressure against collapsing under its own gravity. As such its structure is described by the equations of fluid dynamics, together with details of the microphysics (nuclear reaction rates, equation of state of the fluid, opacity of the material to radiation). The starting point for helioseismic investigations is usually a spherically symmetric, non-rotating model of the Sun, obtained by solving the fluid equations numerically. For a good up-to-date discussion of the modelling, see Christensen-Dalsgaard *et al.* (1996); for an extensive discussion of the modelling of stars see *e.g.* the books by Kippenhahn & Weigert (1990) and Hansen & Kawaler (1994).

The normal-mode oscillations that we study can be well approximated by linear adiabatic perturbations of the equilibrium model. (Strictly speaking, at this stage, these are oscillations of the non-rotating star: we introduce rotation in the next section.) The linear approximation is a good one, since the mode amplitudes are only up to a few metres, compared with the radius of the Sun which is  $7 \times 10^8$  metres. The adiabatic approximation is that the fluid elements do not exchange heat with their surroundings during the oscillation: this is an excellent approximation throughout most of the solar interior, where the timescale for heat exchange is very much longer than the periods of the oscillations. Together with appropriate boundary conditions at the centre and surface of the solar model, the oscillation equations constitute a self-adjoint eigenvalue problem, the eigenvalues being the squared frequencies of the normal modes. Given an equilibrium model of the Sun (see above), this eigenvalue problem is solved numerically to obtain the

frequency spectrum and associated eigenfunctions as functions of position through the solar interior. See for example Christensen-Dalsgaard (1982) or Christensen-Dalsgaard & Berthomieu (1991), or the books by Unno *et al.* (1989) and Cox (1980). The outcome of these calculations is that *e.g.* the radial displacement of a given mode is

$$\mathcal{R} [\xi_{nl}(r)Y_l^m(\theta, \phi)e^{i\omega t}]$$

where  $(r, \theta, \phi)$  are spherical polar coordinates centred on the centre of the Sun,  $(n, l, m)$  are three integers labelling the mode – usually called the radial order ( $n$ ), the degree ( $l$ ) and the azimuthal order ( $m$ );  $\omega$  is the frequency of the mode;  $t$  is time; and  $\mathcal{R}[\dots]$  denotes the real part. Also  $Y_l^m$  is a spherical harmonic or degree  $l$  and order  $m$ , and the radially dependent functions  $\xi_{nl}$  are obtained from the numerical calculation. Of course at the surface of the Sun the temporal and horizontal dependencies can be observed, but not directly the radial dependence. In the case of the spherically symmetric model, the frequencies depend only on  $n$  and  $l$ , not on  $m$ . Since the azimuthal order  $m$  runs over all integer values from  $-l$  to  $+l$ , this means that each frequency of the spherically symmetric model has a  $(2l + 1)$ -fold degeneracy. This degeneracy is lifted by rotation or other departures from spherical symmetry.

### 3. Effect of rotation on the oscillations

The observed modes have periods in the region of 5 minutes. The rotation period of the Sun is much longer, about one month. Therefore the effects of rotation on the observed modes can be treated as a small perturbation. The leading-order effect of rotation is to shift the frequencies of  $m \neq 0$  modes, so that the frequency of a mode with quantum numbers  $(n, l, m)$  differs from the frequency of a corresponding mode with  $m = 0$  by an amount

$$\omega_{nlm} - \omega_{nl0} = m \int K_{nlm}(r, \theta)\Omega(r, \theta)r \, dr \, d\theta ,$$

a weighted integral of the internal rotation  $\Omega(r, \theta)$  inside the Sun. Here the integral is over the whole of the interior of the Sun, and the kernels  $K_{nlm}(r, \theta)$  are presumed known functions which are calculated from a spherically symmetric non-rotating model and its eigenfunctions. I note in passing that the symmetry properties of the kernels means that at this order the observable frequency splitting  $\omega_{nlm} - \omega_{nl0}$  is an odd function of  $m$  that depends only on a North-South symmetric, longitudinally averaged measure of the internal rotation rate. However, the kernels do have different dependencies on radius  $r$  and colatitude  $\theta$  according to the values of  $(n, l, m)$ , which enables us to resolve the internal rotation in the Sun as a function of  $r$  and  $\theta$ . Details of the kernels and some of the inversion methods are given by *e.g.* Schou *et al.* (1994). The inversion problem is then to make inferences about  $\Omega$  given the observational data (the frequency splittings) and given the kernels  $K_{nlm}$ .

### 4. The inversion problem & techniques

The above inversion problem can be written schematically as

$$d_i = \int K_i(\mathbf{r})\Omega(\mathbf{r}) \, d\mathbf{r} + \epsilon_i \quad (i = 1, \dots, M)$$

Given a finite number of  $M$  data  $d_i$ , and known functions  $K_i(r)$ , we wish to make inferences about the function  $\Omega(r)$ . I have explicitly shown here that the data contain errors (noise)  $\epsilon_i$ . This is a linear inversion problem for which various approaches are possible. Two techniques which are commonly used in helioseismology are data fitting with the Regularized Least Squares method (Tikhonov regularization) and construction of averages with the Optimally Localized Averages (Backus-Gilbert) method. These and other techniques as they are applied in helioseismology are discussed in the papers by Christensen-Dalsgaard *et al.* (1990), Pijpers & Thompson (1992, 1994), Thompson (1995); not so current, but still interesting, is the paper by Gough (1985).

## 5. Results on the Sun's internal rotation

Recent results on the solar internal rotation as inferred by helioseismology may be found in Schou *et al.* (1998), Thompson *et al.* (1996), Chaplin *et al.* (1999) and Elsworth *et al.* (1995). There have been many surprises, basically because our understanding of angular momentum transport under stellar conditions is still rather poor. It has long been known that at its surface the Sun rotates differentially, with the equatorial regions completing one rotation in about 25 days, and the higher solar latitudes rotating rather more slowly. Prior to helioseismology, numerical simulations of the rotation in the Sun's convective envelope (the outer 30 per cent of the Sun by radius) suggested that the surfaces of constant rotation rate would be essentially cylinders centred on the rotation axis: in fact it seems that the rotation is more nearly constant with depth, at any given latitude, so that the surface rotation profile persists through the convection zone. There are departures from this, however, including a local maximum in the rotation rate which occurs in the equatorial region and at a depth corresponding to about 7 per cent of the Sun's total radius. There is also a shear layer immediately beneath the visible surface, at least at low- and mid-latitudes. Beneath the convective envelope, there is a transition to a latitudinally-independent rotation rate, the transition occurring in a thin layer which has been named the 'tachocline'. The tachocline width seems to be smaller than the inversion resolution at those depths, but it has been estimated (by assuming the transition is a simple step with a characteristic width) that its width is of the order of 4 per cent of the solar radius (Charbonneau *et al.* 1999; cf. Antia *et al.* 1998, Kosovichev 1996). Inferences about the deep interior, especially the inner 20 per cent, remain very difficult because of the relatively few modes that penetrate there and because of the predominant influence on the modes of the outer part of the star. As best we can tell, the rotation of the inner 60 per cent is consistent with rigid-body rotation, and certainly some earlier models which predicted a very rapidly rotating core (a relic of the young Sun, which probably did rotate much more rapidly than the Sun does today) can be firmly ruled out.

## 6. Results on the Sun's internal structure and physics

The inferences about rotation utilise the splitting between modes of different azimuthal order within the same multiplet of  $2l+1$  modes ( $m = -l, \dots, l$ ). The mean frequency of the multiplet is used to make inferences about the radially symmetric structure of the solar interior, and about the physics that governs the structure. The most accessible quantity is the adiabatic sound speed. Early inferences were made using an Abel inversion of an asymptotic formula based on a WKB representation of the modes (Christensen-Dalsgaard *et al.* 1985). Most recent work though has

been based upon linearizing about a known reference model, utilizing a variational principle for the frequencies (*e.g.*, Dziembowski *et al.* 1990, Basu *et al.* 1996, 1997). For further results, see the paper by Gough *et al.* (1996). A comprehensive study of the effect of choices of values of trade-off parameters in such structure inversions has been made by Rabello-Soares *et al.* (1999). Although the sound speed is the most accessible aspect of structure, it is also possible for example to estimate the density stratification, which also directly affects the modes. More indirectly, one can study other secondary quantities, for instance by calculating the dependence of the frequencies on these quantities, and then inverting for them (*e.g.*, parametrising the opacity of the solar interior to radiation, then calculating the effect of opacity changes on the frequencies, and inverting the frequencies to make inferences about the opacity: Korzennik & Ulrich 1989, Tripathy *et al.* 1998). Among the inferences from helioseismology are that the depth of the Sun's convective envelope is about 29 per cent of the total radius (Christensen-Dalsgaard *et al.* 1991) and that the helium abundance in the convective envelope is about 25 per cent by mass (*e.g.*, Vorontsov *et al.* 1991, Richard *et al.* 1998). The latter is an interesting result, since it is about 3 per cent lower than the initial solar helium abundance necessary to produce models of the present solar age that have the observed solar luminosity: together with evidence from the run of sound speed with depth – Christensen-Dalsgaard *et al.* (1993) – it provides rather compelling evidence that the helium and other elements heavier than hydrogen have gradually settled under the influence of gravity over the lifetime of the Sun. The observed modes are also sensitive to relatively small changes in the equation of state, and helioseismology has been able to guide theoretical development of equations of state under stellar conditions (Christensen-Dalsgaard & Däppen 1992).

The study of departures from spherical symmetry is much less well developed than the study of the symmetric structure. Such asymmetries could arise from magnetic fields and from large convective cells, for example. For some intriguing inversion results, see the paper by Gough *et al.* (1996).

## 7. Local helioseismology techniques

Recently, helioseismologists have also begun to develop and exploit local techniques which depend on observations of wave fields on patches of the surface. These techniques may well provide a better way to study departures from spherical symmetry in the Sun, at least in the outer part of the solar interior. Here I shall do no more than list some of the techniques and give some references to them. The ring-diagram analysis decomposes the wave field observed in a patch of surface of the Sun by Fourier-analysing it in two horizontal spatial directions and in time, hence producing 3-D power spectra. The technique is so named because slices through such spectra at fixed temporal frequency produce rings of power, showing how the dispersion relation varies as a function of horizontal wavenumber. The technique is described, together with some solar results, in the papers by Patrón *et al.* (1995), González Hernández *et al.* (1998), Thompson *et al.* (1996), Haber *et al.* (1998) and Schou & Bogart (1998).

A quite different technique, but one which shows considerable promise, is time-distance helioseismology. The idea is that one measures travel times along rays between observed points at the surface of the Sun. In fact, what is done is to correlate the wave displacement at some point with points in an annulus about it, and to infer a travel time from the time-lag. For details, see Duvall *et al.* (1993, 1997) and Kosovichev & Duvall (1997); also Jensen *et al.* (1998).

Other techniques include helioseismic holography (Braun *et al.* 1998), and the study of variations of spatial phase over the solar surface (Julien *et al.* 1995).

Some if not all of these local techniques will add valuable information to what has been and will be learned from the global techniques, particularly in terms of structures and flows near sunspots and other magnetic features and the structure of the turbulent convection in the subsurface layers of the Sun.

I thank the organisers for a nice meeting and for inviting me to give these two lectures on helioseismology and helioseismic inversion. I am also very grateful to the Theoretical Astrophysics Center, Aarhus, for their hospitality and financial support for my visit during March and April of 1999.

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## Peter Weidelt (TU Braunschweig):

*The inverse problem of magnetotellurics: A training site for the mathematical geophysicist.*

EXTENDED ABSTRACT

### 1. Introduction

Magnetotellurics is a geophysical method, which tries to infer the electrical conductivity distribution inside the Earth from determinations of the frequency dependence of the electromagnetic surface impedance, which is the ratio of orthogonal horizontal electric and magnetic field components. These fields are either excited by controlled sources or induced by time-varying magnetic fields of ionospheric or magnetospheric origin. Generally, the frequencies are so low that displacement currents can safely be neglected and diffusion dominates over wave propagation.

The electromagnetic skin effect is the physical basis behind the fact that the frequency dependence of the surface impedance contains differential information about the variability of electrical conductivity with depth: Low frequency electromagnetic fields penetrate deeper into the Earth than high frequency fields. Therefore the highest frequencies reveal the conductivity at the shallowest levels, lower frequencies contain *in addition* information about deeper levels, although with poorer resolution.

Here we shall consider magnetotellurics only for a layered Earth and *quasi-uniform* inducing fields such that the electrical conductivity  $\sigma$  and the electric and magnetic field depend on depth  $z$  only,  $0 \leq z < \infty$ . We assume a horizontal inducing magnetic field excited in  $z \leq 0$  and polarized in  $y$ -direction with harmonic time variation  $\exp(i\omega t)$ , where  $\omega$  is the angular frequency. Then the density of induced currents is  $J_x(z, \omega) = \sigma(z)E_x(z, \omega)$ . Electric field  $E_x$  and magnetic field  $H_y$  are connected via Ørsted's and Faraday's law by

$$H_y'(z, \omega) = -\sigma(z)E_x(z, \omega), \quad E_x'(z, \omega) = -i\omega\mu_0 H_y(z, \omega), \quad (1)$$

leading after elimination of  $H_y$  to the ordinary differential equation

$$\boxed{E_x''(z, \omega) = i\omega\mu_0\sigma(z)E_x(z, \omega), \quad 0 \leq z < \infty} \quad (2)$$

where the primes denote differentiation with respect to  $z$  and  $\mu_0 = 4\pi \cdot 10^{-7}$  Vs/(Am) is the induction constant. Eq. (2) is a one-dimensional diffusion equation in the frequency domain. Of interest are fields diffusing into the conductor such that  $E_x'(z, \omega) \rightarrow 0$  for  $z \rightarrow \infty$ . The data is the surface impedance

$$Z(\omega) := \frac{E_x(0, \omega)}{H_y(0, \omega)} = -\frac{i\omega\mu_0 E_x(0, \omega)}{E_x'(0, \omega)}. \quad (3)$$

In the sequel it is more convenient to use instead of  $Z(\omega)$  the derived transfer function

$$\boxed{c(\omega) = \frac{Z(\omega)}{i\omega\mu_0} = -\frac{E_x(0, \omega)}{E_x'(0, \omega)}} \quad (4)$$

which has the dimension of a length. (Later it will be seen that the depth  $\Re(c)$  is the ‘center of gravity’ of the induced currents). The inverse problem of 1D magnetotellurics consists in making inferences about the coefficient  $\sigma(z)$  in the differential equation (2) from the boundary values  $c(\omega)$ , which in practice are available only as an incomplete, inaccurate and inconsistent data set. Because of its simple structure, this inverse problem is one of the best studied inverse problems in geophysics with a great variety of approaches.

## 2. The data $c(\omega)$

Without proof we will enumerate some important properties of the theoretical data  $c(\omega)$ .

### a) Analytical properties

$c(\omega)$  is a holomorphic function in the whole  $\omega$ -plane, except on the positive imaginary axis, where it has either an infinite number of poles or a branch point and a finite number (which can be nil) of poles according whether the integral

$$\int_0^{z_m} \sqrt{\sigma(z)} dz$$

is finite or not. Here  $z_m$  is the maximum thickness of the conductor, which is either infinity or the depth to a possibly existing perfect conductor (be excluded in the integral).

### b) Spectral representation

$c(\omega)$  admits the spectral representation

$$\boxed{c(\omega) = a_0 + \int_0^\infty \frac{a(\lambda) d\lambda}{\lambda + i\omega}, \quad a_0 \geq 0, \quad a(\lambda) \geq 0} \quad (5)$$

where  $a(\lambda)$  is a generalized function to include both the continuous and discrete part of the spectrum (alternatively Steltjes integral notation would be appropriate). - As an example, the uniform halfspace with conductivity  $\sigma$  yields

$$c(\omega) = \frac{1}{\sqrt{i\omega\mu_0\sigma}} = \frac{1}{\pi} \int_0^\infty \frac{d\lambda}{\sqrt{\mu_0\sigma\lambda(\lambda + i\omega)}}.$$

### c) Existence

For the (pairwise different)  $M$  frequencies  $\omega_j$  are given the data  $c_j := c(\omega_j)$ ,  $j = 1, \dots, M$ . Then form the  $k$ -dimensional Hermitian determinants

$$D_k := \det \left\{ \frac{i(c_m - c_n^*)}{\omega_m + \omega_n} \right\}, \quad \bar{D}_k := \det \left\{ \frac{i(\omega c_m + \omega_n c_n^*)}{\omega_m + \omega_n} \right\}, \quad m, n = 1, \dots, k.$$

For the existence of a 1D conductivity model it is necessary and sufficient that the  $2M$  determinants

$$D_k, \quad \bar{D}_k, \quad k = 1, \dots, M$$

are positive. - As an example take  $M = 2$  and let  $c_j = g_j - ih_j$ . Then the four conditions to be satisfied are

$$\begin{aligned} k = 1 & : h_1/\omega_1 > 0, \quad g_1 > 0 \\ k = 2 & : \left| \frac{c_2 - c_1}{\omega_2 - \omega_1} \right|^2 < \frac{h_1 h_2}{\omega_1 \omega_2}, \quad \left| \frac{\omega_2 c_2 - \omega_1 c_1}{\omega_2 - \omega_1} \right|^2 < g_1 g_2 \end{aligned}$$

The two conditions for  $k = 1$  grant the existence of a model for  $c_1$ , the additional conditions for  $k = 2$  ensure that a model exists which fits both  $c_1$  and  $c_2$ . The conditions for  $k > 1$  define in the complex  $c$ -plane lens-shaped compatibility regions of decreasing size bounded by circular arcs.

d)  $\Re c$  as ‘center of gravity’ of induced currents

$g(\omega) := \Re c(\omega)$  admits a simple physical interpretation as

$$g(\omega) = \int_0^\infty z \Re[J_x(z, \omega)] dz / \int_0^\infty \Re[J_x(z, \omega)] dz,$$

which in analogy to mechanics can be interpreted ‘center of gravity’ of the induced in-phase current system. From (5) follows that

$$g(\omega) = \int_0^\infty \frac{\lambda a(\lambda) d\lambda}{\lambda^2 + \omega^2}$$

decreases monotonously with frequency, in accordance with the fact that the distribution of fields with depth is controlled by the skin effect.

e) **Earth flattening transformation**

For a radially symmetric conductivity distribution  $\sigma(r)$  and an inducing spherical harmonic of degree  $n$  the basic equation is instead of (1)

$$w_n''(r, \omega) = \left\{ \frac{n(n+1)}{r^2} + i\omega\mu_0\sigma(r) \right\} w_n(r, \omega). \quad (6)$$

Let  $a$  be the radius of the Earth and let  $\varrho := r/a$  and  $f(\varrho) := [(n+1)\varrho^{-n} + n\varrho^{n+1}]/(2n+1)$ . Then (6) is transformed via

$$\tilde{z} := a \frac{\varrho^{-n} - \varrho^{n+1}}{(2n+1)f(\varrho)}, \quad \tilde{w}(\tilde{z}, \omega) := \frac{w_n(r, \omega)}{f(\varrho)}, \quad \tilde{\sigma}(\tilde{z}) := \sigma(r) \cdot f^4(\varrho)$$

into a differential equation of type (1), i.e.

$$\tilde{w}''(\tilde{z}, \omega) = i\omega\mu_0\tilde{\sigma}(\tilde{z})\tilde{w}(\tilde{z}, \omega),$$

without changing the data,

$$c(\omega) = + \frac{w_n(a, \omega)}{w_n'(a, \omega)} = - \frac{\tilde{w}(0, \omega)}{\tilde{w}'(0, \omega)}.$$

Therefore spherical data can first be interpreted by a flat Earth and a uniform field and the resulting profile  $\tilde{\sigma}(\tilde{z})$  is then transformed into the true profile by

$$\sigma(r) = f^{-4}(\varrho) \cdot \tilde{\sigma} \left( a \frac{\varrho^{-n} - \varrho^{n+1}}{(2n+1)f(\varrho)} \right).$$

Such a transformation is possible only if  $c(0) \leq a/(n+1)$ .

f) **Dispersion relations**

Since  $c(\omega)$  is analytical in the lower frequency plane, real and imaginary part of  $c$  are related by Hilbert transforms (dispersion relations). In addition, the spectral presentation (5) shows that  $c(\omega)$  has no zeroes there. Hence  $\log c(\omega)$  is analytical in  $\Im\omega < 0$  and dispersion relations exist also between  $\log |c(\omega)|$  and the phase of  $c(\omega)$ .

Suitable references for this section are Nussenzweig (1972), Parker (1980, 1994), Weidelt (1972, 1986), and Yee & Paulson (1988a,b).

### 3. Inversion methods

Tikhonov (1965) has shown that the 1D magnetotelluric inverse problem has in principle a unique solution. Because of the analyticity of  $c(\omega)$ , in theory a small frequency interval contains already all information to recover the whole conductivity profile. In practice, however, incomplete, inaccurate and inconsistent data yield in general very non-unique results.

The 1D magnetotelluric inverse problem has been approached from different directions (e.g., Whittall & Oldenburg, 1992). We will not consider unspecific iterative methods like the Marquardt-Levenberg algorithm, genetic algorithms or stochastic approaches and will mention only a few methods, which are more or less specific for the magnetotelluric problem.

a) **Gel'fand-Levitan/Marchenko method**

The magnetotelluric inverse problem is an inverse scattering problem, to which we can adapt after suitable transformations and shortcuts the Gel'fand-Levitan/Marchenko formalism (Weidelt, 1972, Whittall & Oldenburg, 1986). The results are not very encouraging, because high quality data are required. The difficult step in the solution is the analytical continuation of the data measured on the real frequency axis in direction to the sources (poles and branch cut) on the positive-imaginary frequency axis. More stable alternative methods are discussed by Whittall & Oldenburg (1986).

b) **The  $D^+$ -method of Parker (1980)**

This popular method determines the best fitting 1D model to a set of imperfect real data by first fitting to the data a spectral representation of type (5). For  $M$  given frequencies  $\omega_j$ , data  $c_j$  and estimated standard deviations  $s_j$ ,  $j = 1, \dots, M$  he minimizes the quadratic functional

$$Q(a_0, a_1, \dots, a_N) := \sum_{j=1}^M \frac{1}{s_j^2} \left| a_0 + \sum_{n=1}^N \frac{a_n}{\lambda_n + i\omega_j} - c_j \right|^2$$

subject to the non-negativity constraints

$$a_n \geq 0, \quad n = 0, \dots, N.$$

The (fine) partition  $\lambda_n$  is prescribed and oriented at the given frequency range. This quadratic programming problem is efficiently solved by the algorithm NNLS of Lawson & Hanson (1974).

The resulting 'cleaned data'

$$\tilde{c}_j = a_0 + \sum_{n=1}^N \frac{a_n}{\lambda_n + i\omega_j}, \quad a_n \geq 0, \quad n = 0, \dots, N,$$

give the best fitting 1D model. This model belongs to a degenerate conductivity profile consisting of insulating layers and thin highly conducting layers with the conductance  $\tau_k$  (= product of thickness and conductivity) at  $z = h_k$ ,  $k = 1, \dots, K$  with  $K < N$ ,

$$\sigma(z) = \sum_{k=1}^K \tau_k \delta(z - h_k).$$

A stable algorithm for the determination of  $(\tau_k, h_k)$  from  $(a_n, \lambda_n)$  is given by Parker & Whaler (1981). This method is of appeal because it determines a unique lower bound on the misfit, such that all other competing models will show a fit, which is equal or worse.

**c) A simple approximate inversion**

Rather than applying sophisticated algorithms, a first guess on the underlying conductivity structure can be obtained without ease (Schmucker, 1970) by using each frequency separately. Let again  $c(\omega) = g(\omega) - ih(\omega)$ . Then an estimate for  $\sigma(z)$  at the ‘center of gravity’ of induced currents,  $z = g(\omega)$ , is

$$\hat{\sigma} = \frac{1}{2\omega\mu_0 h^2(\omega)}, \quad g(\omega) \geq h(\omega),$$

$$\hat{\sigma} = \frac{2g^2(\omega)}{\omega\mu_0 |c(\omega)|^4}, \quad g(\omega) \leq h(\omega).$$

These guesses are obtained by interpreting the complex datum  $c$  by simple two-parameter models, consisting in the first case of an insulating layer over a halfspace and in the second case of a thin sheet over a halfspace. Determined is then the conductivity  $\hat{\sigma}$  of the halfspace. Under the given conditions, the second parameter (thickness of the insulating layer or conductance of the surface sheet) is non-negative and negative else. The approximations are excellent if the conductivity increases with depth.

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## Peter Weidelt (TU Braunschweig):

### *Construction of bounds on spatial averages of electrical conductivity.*

EXTENDED ABSTRACT

#### 1. Introduction

All methods of geophysical inversion, which try to interpret *real* data, are methods of optimization. Whereas traditional approaches search for the model, which minimizes the misfit between measured and modelled data, more recent approaches pre-assign the misfit and place emphasis on the construction of the model, that extremizes a model property of geophysical interest. Prominent representatives of the latter strategy are the minimum structure models (e.g. Constable et al. 1987, Smith & Booker 1988) or the models leading to maximum depth rules (e.g. Smith 1959, 1960, Parker 1974, 1975). The actual structure of the extremal models is in general of subordinate interest. What is learnt from the inversion is the extremal value of the model property under investigation, because this number is a bound, which all other competing - and possibly more realistic - models have to satisfy.

This contribution considers the simplest problem of magnetotellurics, where the electrical conductivity  $\sigma$  depends on depth  $z$  only. For any finite set of even accurate data, point estimates of the electrical conductivity become meaningless, since at a specified depth level one may introduce either a thin highly conducting sheet or a thin insulating layer without changing the fit to the data. Therefore at the specified depth the conductivity may range between zero and infinity. Of geophysical interest, however, are estimates of the conductivity in a given depth *range* rather than point estimates. If the assigned depth range is sufficiently extended and shallow, the observed penetration of the longer periods may not allow to fill it completely with the highest conducting material, or - on the other hand - the observed damping may be inconsistent with an extended poorly conducting layer. Therefore the average conductivity in the depth range may be constrained by the data. The possibility of putting constraints on linear averages of the conductivity is in accord with the fact that the inverse problem for the conductance (= integrated conductivity) is well-posed (Berdichevskiy & Dmitriev 1992, p. 198-201).

For a given set of  $M$  frequency dependent surface impedances we construct those extremal models, which maximize or minimize the arithmetic average of  $\sigma$  in the given depth range  $z_1 \leq z \leq z_2$ . Moreover,  $\sigma$  may be subjected to the *a priori* constraints  $\sigma_- \leq \sigma(z) \leq \sigma_+$  with  $\sigma_-$  and  $\sigma_+$  prescribed.

Problems of this kind have been treated previously by Oldenburg (1983) and Dosso & Oldenburg (1989). After discretizing the conductivity structure, these authors reduce the problem of determining the bounds to a problem in non-linear programming. Starting with an initial guess and linearizing the functional, which maps the conductivity on the data, the problem is solved iteratively by a sequence of linear programming problems.

The special problem of extremizing the conductivity integrated between the surface  $z_1 = 0$  and the level  $z_2$  for the unconstrained case  $\sigma_- = 0, \sigma_+ = \infty$  has been considered by Weidelt (1985) by exploring in a fully non-linear treatment the exact structure of the extremal models for a small number of data. The present contribution extends these results by assuming a depth range  $z_1 \leq z \leq z_2$  and finite *a priori* bounds  $\sigma_- \geq 0$  and  $\sigma_+ \leq \infty$ . A simple structure is obtained only in the one-frequency case, where  $\sigma(z)$  is found to flip between the extremes  $\sigma_-$  and  $\sigma_+$ . For  $M > 1$ , in addition transitional continuous conductivity variations may occur.

The methods of Oldenburg (1983) and Dosso & Oldenburg (1989) on one side and those the present contribution on the other side are complementary: The former approximate approach is robust, computationally efficient, flexible, and suitable for a big data set, the latter exact approach is computationally awkward in the case of many frequencies, but sheds a clearer light on the nature of the underlying problem.

## 2. Basic equations and necessary extremal conditions

Attention is confined to a one-dimensional conductivity profile  $\sigma(z)$ ,  $z$  positive downwards, and a uniform inducing magnetic field in  $y$ -direction. Assuming a time factor  $e^{i\omega t}$ ,  $\omega > 0$ , throughout, the field equations in the quasi-static limit are

$$E'_x(z, \omega) = -i\omega\mu_0 H_y(z, \omega), \quad H'_y(z, \omega) = -\sigma(z)E_x(z, \omega),$$

where the prime denotes differentiation with respect to  $z$ . They lead to the differential equation

$$f''(z, \omega) = i\omega\mu_0\sigma(z)f(z, \omega) \quad (1)$$

with

$$f(z, \omega) := -E_x(z, \omega)/E'_x(0^-, \omega),$$

where the discontinuity of  $E'_x$  due to a possible thin conducting surface sheet has been taken into account. The boundary conditions imposed on  $f(z)$  are

$$f'(0^-) = -1, \quad f'(\infty) = 0. \quad (2)$$

In the sequel we use Schmucker's response function (Schmucker 1970, p.69)

$$c(\omega) := \frac{E_x(0, \omega)}{i\omega\mu_0 H_y(0^-, \omega)} = f(0, \omega),$$

with  $c = g - ih$  and  $g, h > 0$ .

A set of  $M$  frequencies  $\omega_j$ ,  $j \in [1, M]$  is considered, with the measured responses  $c_j := c(\omega_j)$  being either exact or corrupted by noise with the standard deviations  $s_j$ . In addition, let  $c_j[\sigma] = f(0, \omega_j)$  be the data functional, i.e. the result of solving (1) with the boundary conditions (2) for the conductivity profile  $\sigma(z)$  and the frequency  $\omega_j$ . Then  $\sigma(z)$  is an acceptable model if in the case of exact data

$$c_j = c_j[\sigma], \quad j = 1, \dots, M, \quad (3)$$

or if in the case of noisy data the soft  $\chi^2$ -bound

$$\sum_{j=1}^M |c_j - c_j[\sigma]|^2 / s_j^2 \leq B \quad (4)$$

is satisfied, where  $B := \chi_{2M; \alpha}^2$  is the threshold, which for  $2M$  degrees of freedom is exceeded with probability  $\alpha$ .

Apart from degenerate data, e.g.

$$c_j = \frac{a}{b + i\omega_j}, \quad a > 0, b \geq 0,$$

for which in the case of exact data and  $M > 1$  only a single conductivity model exists, there will be a whole family of acceptable conductivity profiles. After pre-assigning a depth range  $z_1 \leq z \leq z_2$  and an a-priori conductivity range

$$\sigma_- \leq \sigma(z) \leq \sigma_+, \quad 0 \leq z < \infty, \quad (5)$$

we will try to find that model, which minimizes or maximizes

$$\bar{\sigma}(z_1, z_2) := \frac{1}{\Delta} \int_{z_1}^{z_2} \sigma(z) dz, \quad \Delta := z_2 - z_1,$$

subject to the constraints (3) [or (4)] and (5). The extremal averages are  $\bar{\sigma}_{min}(z_1, z_2)$  and  $\bar{\sigma}_{max}(z_1, z_2)$ . Hence the objective function to be minimized is

$$Q[\sigma] = \int_0^\infty w(z)\sigma(z) dz$$

with the weight function

$$w(z) = \begin{cases} 0, & z \notin (z_1, z_2) \\ +1/\Delta, & z \in (z_1, z_2), \quad Q \rightarrow +\bar{\sigma}_{min}(z_1, z_2) \\ -1/\Delta, & z \in (z_1, z_2), \quad Q \rightarrow -\bar{\sigma}_{max}(z_1, z_2) \end{cases} \quad (6)$$

The constraints (3) to (5) are taken into account by Lagrangian multipliers, see e.g. Avriel (1976) for a concise treatment. In the case of exact data (3) the Lagrange function is

$$L[\sigma] = Q[\sigma] + \Re \sum_{j=1}^M \lambda_j \{c_j[\sigma] - c_j\} + \int_0^\infty [\mu_+(z)\{\sigma(z) - \sigma_+\} + \mu_-(z)\{\sigma_- - \sigma(z)\}] dz, \quad (7)$$

where  $\Re$  denotes the real part. In the case of noisy data (4) the second RHS term is replaced by

$$\Lambda \left\{ \sum_{j=1}^M |c_j[\sigma] - c_j|^2 / s_j^2 - B \right\}. \quad (8)$$

Real and imaginary part of the complex ordinary Lagrangian multipliers  $\lambda_j$ , enforcing equality constraints, are unrestricted in sign, whereas the generalized Lagrangian multipliers  $\Lambda$  and  $\mu_\pm(z)$ , accounting for inequality constraints, are sign-restricted and non-negative in the present definitions. In particular these multipliers are zero, whenever the constraints are inactive and non-negative if the constraints are binding. Therefore the expressions (8) and

$$\mu_\pm(z)[\sigma(z) - \sigma_\pm], \quad 0 \leq z < \infty$$

always vanish. The Lagrangian multipliers  $\lambda_j$  and  $\Lambda$  are closely related to the sensitivity of the minimum value  $Q_0$  of  $Q[\sigma]$  to changes in the data. Let  $c_j =: g_j - ih_j$ . Then

$$\Re \lambda_j = -\frac{\partial Q_0}{\partial g_j}, \quad \Im \lambda_j = -\frac{\partial Q_0}{\partial h_j}, \quad \Lambda = -\frac{\partial Q_0}{\partial B}, \quad (9)$$

where  $\Im$  denotes the imaginary part. The last equation expresses the obvious fact that an increase of the active  $\chi^2$ -bound leads to a further decrease of  $Q_0$ . The functions  $\mu_\pm(z)$  describe

the sensitivity of  $Q_0$  to local changes of the conductivity bounds  $\sigma_{\pm}$  at position  $z$ : If in a small range  $\delta z$  around  $z$  the bounds  $\sigma_{\pm}$  are increased to  $\sigma_{\pm} + \sigma_0$ , then with  $\delta\tau_{\pm}(z) := \sigma_0\delta z$  one obtains in the limit  $\delta z \rightarrow 0$

$$\mu_{\pm}(z) = \mp \frac{\partial Q_0}{\partial \tau_{\pm}(z)}, \quad (10)$$

i.e, if  $\sigma(z) = \sigma_-$ , implying  $\mu_-(z) \geq 0$ , an increase of  $\sigma_-$  will not lead to a deeper minimum  $Q_0$ , whereas for  $\sigma(z) > \sigma_-$ , implying  $\mu_-(z) = 0$ , the change of an inactive bound does not affect  $Q_0$ . A similar interpretation holds for  $\mu_+(z)$  and  $\sigma_+$ . The sensitivity of  $Q_0$  to a global change of  $\sigma_{\pm}$  is given by

$$\int_0^{\infty} \mu_{\pm}(z) dz = \mp \frac{\partial Q_0}{\partial \sigma_{\pm}}.$$

As a necessary extremal condition the first variation of the Lagrangian  $L[\sigma]$  with respect to  $\sigma(z)$  has to vanish. Whereas the first and third RHS term of (7) are linear in  $\sigma$  and pose no problems, the first variation of the non-linear data functional  $c_j[\sigma]$  has to be expressed in terms of its Fréchet derivative  $F_j(z)$  defined by

$$\delta c_j[\sigma] = \int_0^{\infty} F_j(z) \delta \sigma(z) dz \quad (11)$$

with

$$F_j(z) = -i\omega_j \mu_0 f_j^2(z), \quad (12)$$

where  $f_j(z) := f(z, \omega_j)$  is the solution of (1) with the boundary conditions (2) [e.g. Parker 1977]. Hence  $\delta L[\sigma] = 0$  implies for the exact data case (3)

$$w(z) + \Re \sum_{j=1}^M \lambda_j F_j(z) + \mu_+(z) - \mu_-(z) = 0. \quad (13)$$

In the case of noisy data,  $\lambda_j$  in (13) is replaced by

$$\tilde{\lambda}_j := 2\Lambda(c_j[\sigma] - c_j)^*/s_j^2, \quad (14)$$

where \* marks the complex conjugate.

In the sequel the necessary condition (13) is used to define the control function

$$D(z) := w(z) + \Re \sum_{j=1}^M \lambda_j F_j(z) = \mu_-(z) - \mu_+(z), \quad (15)$$

which states that

$$\begin{aligned} D(z) &\geq 0, \text{ where } \sigma(z) = \sigma_- \\ D(z) &= 0, \text{ where } \sigma_- < \sigma(z) < \sigma_+ \\ D(z) &\leq 0, \text{ where } \sigma(z) = \sigma_+. \end{aligned} \quad (16)$$

It is stressed that - in exceptional situations - only the weak condition  $D(z) = 0$  rather than strict positivity or negativity can be achieved in some depth interval, where a conductivity constraint is active.

The process of model construction therefore consists in selecting a model within the class of models satisfying the data in the sense of (3) or (4), for which there exists a linear combination  $D(z)$  of its Fréchet derivatives, which according to (16) is non-negative (non-positive), where  $\sigma(z)$  attains its lower (upper) bound.

The problems with this prescription are at least three-fold:

- a) It does not lead to an immediate model construction, since in general  $\sigma(z)$  has to be determined iteratively on the basis of the information on  $\sigma(z)$  obtained from the sign changes of  $D(z)$ .
- b) There might be more models satisfying this necessary condition. In order to single out the extremal model one has to be sure to know all these admissible models.
- c) The structure of possible extremal models is not known at the outset: Does it consist only of discrete layers or do in addition continuous conductivity variations occur? How many layers are required?

Despite these complications, satisfactory model constructions are possible in many cases, since it turns out that in most instances the conductivity only flips between the extremes  $\sigma_-$  and  $\sigma_+$ . This particularly holds for the modest one-frequency case. Moreover, it is often easy to find the pertinent extremal model for small  $z_1$  and  $z_2$ . By gradually deforming this solution and monitoring the change of  $D(z)$ , it is possible to decide for which parameter combination  $(z_1, z_2)$  the type of the model has to change, e.g. where a conducting layer at the surface or at  $z_1$  emerges or disappears, where two conducting layers coalesce, or where a continuous conductivity variation is required in some section of the model. These changes, of course, reflect the full non-linearity, which we take into account.

Rather than presenting detailed results, we shall show only the kind of reasoning which can be applied. We shall prove that one-frequency extremal models have the property that  $\sigma(z)$  only attains the values  $\sigma_-$  and  $\sigma_+$  (provided that  $\sigma_-$  and  $\sigma_+$  are suitably chosen such that feasible models exist at all). This is proved by contradiction on assuming that there exists a depth interval  $(a, b)$  completely inside or outside  $(z_1, z_2)$  such that  $\sigma_- < \sigma(z) < \sigma_+$  for  $z \in (a, b)$ . Then, according to (16),  $D(z)$  and all its derivatives vanish identically for  $z \in (a, b)$ . Dropping in the case  $M = 1$  consistently the subscript  $j$  identifying the frequency and using the fact that  $w(z)$  is piecewise constant, the first and second derivative of  $D(z)$  yield with reference to (15)

$$\Re[\lambda F'(z)] = 0, \quad \Re[\lambda F''(z)] = 0.$$

These two homogeneous linear equations for  $\lambda$  have to satisfy the compatibility condition

$$\Im[F''(z)/F'(z)] = 0.$$

However, from (12) and (1) follows that

$$\Im[F''(z)/F'(z)] = -\Im[i\omega\mu_0\sigma(z)c(z) + 1/c(z)] = -[\omega\mu_0\sigma(z)g(z) + h(z)/|c(z)|^2] < 0,$$

since  $g(z)$  and  $h(z)$  are positive as real part and negative imaginary part of the response function  $c$  at level  $z$ ,

$$c(z) = -f(z)/f'(z) = g(z) - ih(z).$$

Hence the compatibility condition cannot be satisfied and no continuous conductivity section exists.

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