On the Continuum Limit of a Discrete Inverse Spectral Problem on Optimal Finite Difference Grids

LILIANA BORCEA
Computational and Applied Mathematics
Rice University

VLADIMIR DRUSKIN
Schlumberger–Doll Research Center

AND

LEONID KNIZHNERMAN
Central Geophysical Expedition

Abstract

We consider finite difference approximations of solutions of inverse Sturm-Liouville problems in bounded intervals. Using three-point finite difference schemes, we discretize the equations on so-called optimal grids constructed as follows: For a staggered grid with $2k$ points, we ask that the finite difference operator (a $k \times k$ Jacobi matrix) and the Sturm-Liouville differential operator share the k lowest eigenvalues and the values of the orthonormal eigenfunctions at one end of the interval. This requirement determines uniquely the entries in the Jacobi matrix, which are grid cell averages of the coefficients in the continuum problem. If these coefficients are known, we can find the grid, which we call optimal because it gives, by design, a finite difference operator with a prescribed spectral measure. We focus attention on the inverse problem, where neither the coefficients nor the grid are known.

A key question in inversion is how to parametrize the coefficients, i.e., how to choose the grid. It is clear that, to be successful, this grid must be close to the optimal one, which is unknown. Fortunately, as we show here, the grid dependence on the unknown coefficients is weak, so the inversion can be done on a precomputed grid for an a priori guess of the unknown coefficients. This observation leads to a simple yet efficient inversion algorithm, which gives coefficients that converge pointwise to the true solution as the number k of data points tends to infinity. The cornerstone of our convergence proof is showing that optimal grids provide an implicit, natural regularization of the inverse problem, by giving reconstructions with uniformly bounded total variation. The analysis is based on a novel, explicit perturbation analysis of Lanczos recursions and on a discrete Gel′fand-Levitan formulation. © 2004 Wiley Periodicals, Inc.

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1 Introduction

We consider a two-point boundary value problem for the Sturm-Liouville equation

$$\begin{aligned} \frac{d}{dz}\left[\sigma(z)\frac{du(z)}{dz}\right] - \lambda\sigma(z)u(z) = 0 \quad \text{for } 0 < z < 1, \\ -\sigma(0)\frac{du(0)}{dz} = 1, \\ u(1) = 0, \end{aligned} \tag{1.1}$$

where λ is a complex spectral parameter satisfying

$$\lambda \in \mathbb{C} \setminus (-\infty, 0) \tag{1.2}$$

and $\sigma(z)$ is a bounded, strictly positive function in $[0, 1]$ obeying some suitable smoothness conditions, including continuity at 0, where we suppose, without any loss of generality, that

$$\sigma(0) = 1. \tag{1.3}$$

We are interested in the inverse problem of finding the coefficient $\sigma(z)$ in the unit interval, given measurements of the Neumann-to-Dirichlet map

$$F^{\sigma}(\lambda) = u(0). \tag{1.4}$$

Sturm-Liouville equations of the form (1.1) arise in applications such as oscillatory motions of strings, electrical conduction, and wave propagation and scattering in layered media. Equations (1.1) can also be obtained from more general Sturm-Liouville equations by means of well-known Liouville transformations [15, 57, 62]. The inverse problem for (1.1) has been studied extensively and it is well understood, at least from the theoretical point of view [9, 11, 12, 15, 26, 35, 43, 55, 56, 57, 61, 63, 65, 77, 79]. The novelty of this paper consists in addressing the question of convergence of discrete, finite difference solutions of the inverse problem to the true coefficient $\sigma(z)$ without using constraints such as artificial regularization in the inversion scheme.

We discretize problem (1.1) with a finite difference approach and, given finitely many, say $2k$ measurements of $F^\sigma(\lambda)$, we wish to reconstruct $\sigma(z)$ at $2k$ points in the unit interval. So far the standard method has been to discretize the equations on arbitrary, usually equidistant grids and to reconstruct $\sigma(z)$ by solving an inverse, discrete eigenvalue problem. Unfortunately, the results are usually not close to the true coefficient and, more importantly, the reconstructions do not improve if we add more data. The reason for this is well-known: the finite difference operator in the discrete problem and the differential operator in (1.1) have different spectral measures. While the low-frequency part of the spectrum can be approximated well by adding more grid points, the large eigenvalues in the discrete and continuum problems have different asymptotes. Note, however, that this undesired behavior is due to the *ad hoc choice of the grids*.

In this paper, we show that, with a proper discretization, on so-called optimal grids finite difference methods can be used very successfully to solve inverse Sturm-Liouville problems (1.1). To our knowledge, this is the first established link between discrete inversion, such as inverse spectral problems for Jacobi matrices [18] or the impedance tomography problem for graphs [22, 20, 21, 40, 45, 48], and continuous inversion. Discrete studies consider k fixed and, in general, it is not known if the limit $k \to \infty$ gives convergence to the continuous solution. As we show in this paper, optimal grids play a key role in answering this convergence question.

Optimal grids have been introduced in [28, 29] for obtaining very accurate, yet inexpensive finite difference approximations of the Neumann-to-Dirichlet map. The idea in [28, 29] is to seek the locations of $2k$ grid points so that $2k$ prescribed measurements of $F^\sigma(\lambda)$ are satisfied *exactly*. As the number k of measurements increases, the grids are optimally refined to achieve convergence of the finite difference Neumann-to-Dirichlet map to the continuum one at a fast rate, usually exponential, in the spectral interval of interest. Since their introduction in [28, 29], optimal grids have been analyzed further in [6, 47], and their connection to spectral Galerkin methods has been investigated in [31, 30]. Extensions to higher-dimensional problems using tensor product grids and domain decomposition ideas are given in [6, 29, 31]. Anisotropic, three-dimensional, low-frequency Maxwell's equations are considered in [23]. Finally, optimal grids have also been used for the discretization of perfectly matched layer-absorbing boundary conditions for wave equations in [5]. All these studies apply to forward problems, but, as it was first proposed in [10], optimal grids play a very important role in inversion as well. In this paper, we give a rigorous foundation to the inversion approach proposed in [10].

In short, the inversion method proceeds as follows: We design the staggered, optimal grid with $2k$ points by asking that the finite difference approximation

$F_k^\sigma(\lambda)$ of the Neumann-to-Dirichlet map, corresponding to the discrete finite difference operator (a $k \times k$ tridiagonal Jacobi matrix), satisfy exactly the given $2k$ measurements of $F^\sigma(\lambda)$. In general, one can have various types of measurements, as explained later in the paper, and the corresponding grids depend *strongly* on the data that we have. In any case, for all types of data that we consider, we can recover uniquely the entries in the Jacobi matrix (discrete operator), which are grid cell averages of $\sigma(z)$. If $\sigma(z)$ is known, we can find the grid, and we call it optimal because it gives, by design, perfect prediction of the data. However, in inversion, neither $\sigma(z)$ nor the grid is known. Fortunately, as we show here, the grid dependence on the unknown coefficients is weak, so the inversion can be done on a precomputed grid for an a priori guess of the unknown coefficients.

We establish two fundamental properties of the optimal grids:

(1) Consider a compact set $\mathcal{S}$ of coefficients $\sigma(z)$ that are sufficiently similar. For example, $\mathcal{S}$ can be a set of sufficiently smooth functions $\sigma(z)$. As $k \to \infty$, the optimal grids corresponding to arbitrary $\sigma \in \mathcal{S}$ are asymptotically close. This means that any precomputed grid, for an a priori known coefficient $\sigma^0 \in \mathcal{S}$, gives a proper parametrization of the unknown $\sigma(z)$.

(2) The optimal grids provide an implicit total variation regularization of the reconstructed sequence of coefficients, so pointwise convergence of the solution is achieved as we let $k \to \infty$.

Our analysis is based on Kac and Krein's spectral theory of strings [51] and a novel, explicit perturbation analysis of Lanczos recursions [18, 78] and on a discrete Gel′fand-Levitan formulation [14, 35, 36, 42, 57, 62, 67].

This paper is organized as follows: In Section 2, we formulate the inverse problem and make the connection with Kac and Krein's spectral theory of strings [51]. We describe the finite difference approximation of the Neumann-to-Dirichlet map, and we show how to recover uniquely the discrete difference operator from $2k$ measurements of this map. In Section 3, we define the optimal grids and discuss some of their asymptotic properties. In Section 4, we describe our imaging algorithm and illustrate its performance with numerical simulations. In Section 5, we prove convergence of the inversion algorithm for a special class of coefficients $\sigma(z)$, which vary exponentially in z. The motivation for this section is twofold: First, the proof in this case is quite simple, since it follows just from algebraic calculations. Second, we need the results in Section 6 in order to prove convergence for more general $\sigma(z)$.

The main convergence result is proven in Section 6. Here we use the discrete Gel′fand-Levitan formulation due to Natterer [67] and develop a new perturbation theory for Lanczos recursions. The proof of bounded total variation of the reconstructed sequence of coefficients follows from this perturbation analysis, at least for sufficiently smooth $\sigma(z)$. While the analysis in this paper is for the so-called truncated measure data set for $F^\sigma(\lambda)$, where the first k eigenvalues and the values at $z = 0$ of the corresponding orthonormal eigenfunctions of the differential operator in (1.1) are given, we discuss in Section 7 extensions to other types of measurements. Finally, we end with concluding remarks in Section 8.

2 Formulation of the Inverse Problem

We consider the following inverse problem:

Problem 1. Find coefficient $\sigma(z)$, for $z \in [0, 1]$, given the Neumann-to-Dirichlet map (impedance function) (1.4).

It is known [11, 35, 43, 56, 57, 61, 63] that sufficiently smooth σ can be determined uniquely from the spectral measure of the differential operator in (1.1), with Neumann and Dirichlet boundary conditions at $z = 0$ and $z = 1$, respectively,

$$\mu^\sigma(s) = -\sum_{p=1}^{\infty} \xi_p H(-s - \theta_p^2), \tag{2.1}$$

where H is the Heaviside (step) function. This operator has distinct eigenvalues $-\theta_p^2$ that tend to $-\infty$ as $p \to \infty$, the eigenfunctions $y(z, \theta_p)$ are orthonormal with respect to the inner product

$$(f, g) = \int_0^1 \sigma(z) f(z) g(z)\, dz \quad \text{for arbitrary } f, g \in L^2([0, 1]), \tag{2.2}$$

and the weights in (2.1) are given by $\xi_p = y(0, \theta_p)^2$.

The connection between data F^σ in Problem 1 and the spectral measure μ^σ follows from the classic study of Kac and Krein [51] of impedance functions of oscillating strings. In our case, the string oscillates at frequency $\sqrt{\lambda}$, and its equations of motion are obtained from (1.1) by defining the coordinate transformation

$$x(z) = \int_0^z \frac{ds}{\sigma(s)} \tag{2.3}$$

and the mass distribution

$$M : [0, x(1)] \to [0, \widehat{x}(1)], \quad M(x(z)) = \widehat{x}(z) = \int_0^z \sigma(s)\, ds. \tag{2.4}$$

Because $\sigma(z)$ is positive and bounded, we have a regular string with finite length

$$L = x(1) = \int_0^1 \frac{ds}{\sigma(s)} \tag{2.5}$$

and mass

$$M(L) = \widehat{x}(1) = \int_0^1 \sigma(s)\, ds. \tag{2.6}$$

Under a change of coordinates (2.3), the solution u of (1.1) becomes a function of x, which can be interpreted as the displacement of the string. In an abuse of notation, we denote the displacement by $u(x)$ and write the equations of motion of the string as

$$\begin{aligned} \frac{d}{dM(x)}\left[\frac{du(x)}{dx}\right] - \lambda u(x) = 0 \quad \text{for } 0 < x < L, \\ -\frac{du(0)}{dx} = 1, \\ u(L) = 0. \end{aligned} \tag{2.7}$$

The asymptotic behavior of eigenvalues $-\theta_p^2 = O(p^2)$ and weights $\xi_p = O(1)$ for $p \to \infty$ [15, 19, 70] guarantees Kac and Krein's criterion for μ^σ to be a so-called spectral function of the string [51],

$$\int_{-\infty}^{0} \frac{d\mu^\sigma(s)}{\lambda - s} = \sum_{p=1}^{\infty} \frac{\xi_p}{\lambda + \theta_p^2} < \infty \quad \text{for } \lambda \geq 0. \tag{2.8}$$

We have from [51] the following:

LEMMA 2.1 ([32], Kac and Krein [51]) *The impedance function of the string is given by*

$$F^\sigma(\lambda) = \sum_{p=1}^{\infty} \frac{\xi_p}{\lambda + \theta_p^2}, \tag{2.9}$$

and it is bounded on $[0, \infty)$. *There is a bijection between* $F^\sigma(\lambda)$ *and finite measure* [71] M *on* $[0, L)$ (*the mass distribution of the string*). *Moreover, the map* $M(x) \in L^\infty[0, L] \to F^\sigma(\lambda) \in L^\infty[0, \infty)$ *is continuous.*[1]

Lemma 2.1 and (2.9) allow us to reformulate the inverse problem, Problem 1, in terms of the spectral function (measure) of the string and thus to obtain its unique solvability. Alternatively, we can draw the same conclusion from the uniqueness studies [12, 26, 55, 65, 77, 79] of the inverse problem of electrical impedance tomography [9].

2.1 Finite Difference Discretization

In practice, we do not have full knowledge of the map $F^\sigma(\lambda)$ or, equivalently, of the measure μ^σ. Instead, we have a finite number of data points or measurements that can be linear or nonlinear functionals of F^σ (or its Stieltjes measure μ^σ). Examples of such measurement sets include:

(a) The values of $F^\sigma(\lambda_p)$ are given for some $2k$ noncoinciding values λ_p, or, alternatively, we know $F^\sigma(\lambda_0)$ and its first $2k-1$ derivatives at λ_0. These pieces of information determine the corresponding multipoint or simple Padé approximants of F^σ [7].

[1] The topology in the space of M can be significantly relaxed in this statement. The impedance is also continuous as a function of L.

(b) The first k poles and zeros of $F^\sigma(\lambda)$ are given.
(c) The first k poles and residues of $F^\sigma(\lambda)$ are given. Equivalently, we know the truncated measure (TM)

$$\mu_k^\sigma(s) = -\sum_{p=1}^{k} \xi_p H(-s-\theta_p^2). \tag{2.10}$$

Here we concentrate on the last example, because it is simpler to analyze in the context of inversion. The other measurement sets will be discussed briefly in Section 7.

Let us consider the following problem:

Problem 2. Find an approximation of $\sigma(z)$ for $z \in [0,1]$ that predicts measurements $\{\theta_p, \xi_p\}$ for $1 \le p \le k$.

In this paper, we propose a finite difference solution of this inverse problem, where equation (1.1) is discretized as follows: Consider a staggered grid, with primary nodes z_j and dual nodes $\widehat{z}_j$, satisfying

$$z_{j+1} = z_j + h_j, \quad \widehat{z}_j = \widehat{z}_{j-1} + \widehat{h}_j, \quad \text{where } z_1 = \widehat{z}_0 = 0 \text{ and } j = 1, \ldots, k. \tag{2.11}$$

Let U_j be the numerical approximation of u at z_j and discretize (1.1) as

$$\begin{aligned} &\frac{1}{\widehat{h}_j}\left[\widehat{\sigma}_j\left(\frac{U_{j+1}-U_j}{h_j}\right) - \widehat{\sigma}_{j-1}\left(\frac{U_j - U_{j-1}}{h_{j-1}}\right)\right] \\ &\qquad\qquad - \lambda\sigma_j U_j = 0, \quad j = 2,3,\ldots,k, \\ &\frac{1}{\widehat{h}_1}\left[\widehat{\sigma}_1\left(\frac{U_2-U_1}{h_1}\right)+1\right] - \lambda\sigma_1 U_1 = 0, \\ &U_{k+1} = 0, \end{aligned} \tag{2.12}$$

where σ_j and $\widehat{\sigma}_j$ are algebraic and harmonic averages of σ on the grid defined by the equalities

$$\gamma_j = \frac{h_j}{\widehat{\sigma}_j} = \int_{z_j}^{z_{j+1}} \frac{dz}{\sigma(z)} \quad \text{and} \quad \widehat{\gamma}_j = \widehat{h}_j \sigma_j = \int_{\widehat{z}_{j-1}}^{\widehat{z}_j} \sigma(z)\, dz \tag{2.13}$$

(the quantities γ_j and $\widehat{\gamma}_j$ are introduced for further use).

Similarly to the derivation of (2.7) in the continuum setting, we introduce next the discrete version of coordinate transformation (2.3),

$$x_{j+1} = \sum_{i=1}^{j} \gamma_i \quad \text{for } 1 \le j \le k, \; x_1 = 0, \tag{2.14}$$

for a discrete string with point masses $\widehat{\gamma}_j$ and piecewise constant, monotone increasing mass distribution

$$M_k(x) = \widehat{x}_j = \sum_{i=1}^{j} \widehat{\gamma}_i, \quad \text{if } x \in [x_j, x_{j+1}) \text{ for } 1 \le j \le k, \tag{2.15}$$
$$M_k(x_{k+1}) = M_k(x_{k+1} - 0) = M_k(x_k).$$

The equations of motion of the string are derived from (2.12) and (2.13) as

$$(\Gamma - \lambda I)\,\mathbf{U} = -\frac{1}{\widehat{\gamma}_1}\mathbf{e}_1, \tag{2.16}$$

where $\mathbf{U} = (U_1, \ldots, U_k)^{\mathsf{T}}$ is the vector of displacements, I is the $k \times k$ identity matrix, $\mathbf{e}_1$ is the first vector in the canonical basis of $\mathbb{R}^k$, Γ is the tridiagonal difference operator (matrix)

$$\Gamma_{ij} = \begin{cases} -\dfrac{1}{\widehat{\gamma}_i}\left(\dfrac{1}{\gamma_i} + \dfrac{1}{\gamma_{i-1}}\right)\delta_{ij} & \\ \quad + \dfrac{1}{\widehat{\gamma}_i \gamma_i}\delta_{i+1j} + \dfrac{1}{\widehat{\gamma}_i \gamma_{i-1}}\delta_{i-1j}, & 1 < i \le k,\ 1 \le j \le k, \\ -\dfrac{1}{\widehat{\gamma}_1 \gamma_1}\delta_{j1} + \dfrac{1}{\widehat{\gamma}_1 \gamma_1}\delta_{j2}, & i = 1,\ 1 \le j \le k, \end{cases} \tag{2.17}$$

and δ_{ij} is the Kronecker delta symbol.

It is easy to check that

$$\operatorname{diag}\left(\widehat{\gamma}_1^{1/2}, \ldots, \widehat{\gamma}_k^{1/2}\right)\Gamma \operatorname{diag}\left(\widehat{\gamma}_1^{-1/2}, \ldots, \widehat{\gamma}_k^{-1/2}\right) \tag{2.18}$$

is a Jacobi matrix [18], so Γ has simple, negative eigenvalues $-\theta_{j,k}^2$, ordered as

$$\theta_{1,k} < \cdots < \theta_{k,k}, \tag{2.19}$$

and eigenvectors

$$\mathbf{Y}(\theta_{j,k}) = \left(Y_1(\theta_{j,k}), \ldots, Y_k(\theta_{j,k})\right)^{\mathsf{T}}, \quad 1 \le j \le k, \tag{2.20}$$

which are orthonormal with respect to the inner product

$$\langle \mathbf{a}, \mathbf{b} \rangle_{\widehat{\gamma}} = \sum_{p=1}^{k} \widehat{\gamma}_p a_p b_p \tag{2.21}$$
$$\text{for arbitrary } \mathbf{a} = (a_1, \ldots a_k)^{\mathsf{T}} \text{ and } \mathbf{b} = (b_1, \ldots b_k)^{\mathsf{T}} \text{ in } \mathbb{R}^k.$$

Then, the spectral function (measure) of the discrete string is of the form

$$\mu_k^{\sigma}(s) = -\sum_{p=1}^{k} \xi_{p,k} H\left(-s - \theta_{p,k}^2\right) \tag{2.22}$$

where $\xi_{p,k} = Y_1^2(\theta_{p,k})$.

The impedance

$$F_k^\sigma(\lambda) = U_1 \tag{2.23}$$

satisfies the following:

LEMMA 2.2 *The impedance function F_k^σ is given by*

$$F_k^\sigma(\lambda) = \int_{-\infty}^{0} \frac{d\mu_k^\sigma(s)}{\lambda - s} = \sum_{p=1}^{k} \frac{\xi_{p,k}}{\lambda + \theta_{p,k}^2}, \tag{2.24}$$

and it can be written explicitly, in terms of parameters γ_j and $\widehat{\gamma}_j$, as

$$F_k^\sigma(\lambda) = \cfrac{1}{\widehat{\gamma}_1\lambda + \cfrac{1}{\gamma_1 + \cfrac{1}{\widehat{\gamma}_2\lambda + \cdots \cfrac{1}{\gamma_{k-1} + \cfrac{1}{\widehat{\gamma}_k\lambda + \cfrac{1}{\gamma_k}}}}}}. \tag{2.25}$$

PROOF: Expand the solution $\mathbf{U}$ of (2.16) in the basis of the eigenvectors of Γ:

$$\mathbf{U} = \sum_{j=1}^{k} C_j \mathbf{Y}(\theta_{j,k}) \quad \text{where } C_j = \frac{Y_1(\theta_{j,k})}{\lambda + \theta_{j,k}^2} \tag{2.26}$$

and take the first component in (2.26) to obtain (2.24). The continued fraction representation (2.25) is known in the theory of rational function approximations, and it can be found, for example, in [7, 51, 68]. □

2.2 The Discrete Inverse Problem for the String

Note that the impedance $F_k^\sigma(\lambda)$ and the spectral measure μ_k^σ of a discrete string are independent of σ per se, but depend on its primitives γ_j and $\widehat{\gamma}_j$ on the grid, so we change notation as $F_k^\sigma(\lambda) \rightsquigarrow F_k^\gamma(\lambda)$ and $\mu_k^\sigma \rightsquigarrow \mu_k^\gamma$. Note also that, so far, the grid and parameters γ_j and $\widehat{\gamma}_j$ have been arbitrary, and there are many choices that one can make. Our approach is to choose $\{\gamma_j, \widehat{\gamma}_j\}_{1\le j\le k}$ so that the measurements are satisfied exactly. Explicitly, we ask that

$$\theta_{p,k} = \theta_p \quad \text{and} \quad \xi_{p,k} = \xi_p \quad \text{for } p = 1, \ldots, k, \tag{2.27}$$

so μ_k^γ is the same as the truncated measure (2.10).

By our choice (2.13) of coefficients σ_j and $\widehat{\sigma}_j$, we have

$$x_j = x(z_j) \quad \text{and} \quad \widehat{x}_j = \widehat{x}(\widehat{z}_j) \quad \text{for } j = 1, \ldots, k, \tag{2.28}$$

so the mass distribution $M_k(x)$ of the discrete string is a piecewise constant approximation of the continuous $M(x)$. In fact, since (2.15) is just a particular case of mass distributions of the regular strings considered by Kac and Krein [51], M_k satisfies the following counterpart of Lemma 2.1:

LEMMA 2.3 (Kac and Krein [51]; Stieljes [76]) *There is a bijection between piecewise constant, monotone increasing mass distributions taking on k values, as $M_k(x)$, and impedance functions*

$$F_k^\gamma(\lambda) = \int_{-\infty}^0 \frac{d\mu_k^\gamma(s)}{\lambda - s} = \sum_{p=1}^{k} \frac{\xi_p}{\lambda + \theta_p^2} \tag{2.29}$$

with positive residues ξ_p and distinct, negative poles $-\theta_p^2$ for $p = 1, \dots, k$.

The inverse problem of calculating M_k from μ_k^γ is as follows:

Problem 3. Find parameters γ_j and $\widehat{\gamma}_j$, for $j = 1, \dots, k$, given the discrete spectral measure (2.10).

Remark 2.4. Problem 3 is equivalent to the inverse eigenvalue problem for tridiagonal matrix Γ or the Jacobi inverse eigenvalue problem [8, 18, 44]. It can be solved numerically, for example, with Lanczos's method [18, 78] or Stieljes's method [68, 76].

3 The Optimal Finite Difference Grid

In the forward problem, $\sigma(z)$ is known and, after solving Problem 3 to obtain parameters $\{\gamma_j, \widehat{\gamma}_j\}_{j\geq 1}$ and, consequently, discrete coordinate transformations x_j and $\widehat{x}_j$, given by (2.14) and (2.15), we can determine the grid points as follows:

Algorithm 1. Find $\widehat{z}_j$ and z_{j+1} from equations (recall (2.13))

$$\int_0^{\widehat{z}_j} \sigma(s)\, ds = \sum_{p=1}^{j} \widehat{\gamma}_p \quad \text{and} \quad \int_0^{z_{j+1}} \frac{ds}{\sigma(s)} = \sum_{p=1}^{j} \gamma_p,$$

where $j = 1, \dots, k,\ \widehat{z}_0 = z_1 = 0$.

Remark 3.1. It follows easily from (2.9), (2.25), and (2.29) that

$$x_{k+1} = F_k^\gamma(0) < F^\sigma(0) = L.$$

Together with the strict positivity of $\sigma(z)$, this gives solvability of the algorithm with respect to z_j. The solvability with respect to $\widehat{z}_j$ would similarly follow from the strict positivity of $\sigma(z)$ and the bound $\widehat{x}_k \leq L$. The latter is given by Lemma 3.2 in the case of constant coefficient $\sigma(z) = 1$. For $\sigma(z)$ variable, the bound is verified numerically, but it remains a conjecture at this point. However, even if $\widehat{x}_k$ were greater than L, we could make Algorithm 1 solvable with respect to $\widehat{z}_j$ by extending $\sigma(z) = \sigma(1)$ for $z > 1$.

FIGURE 3.1. The grid $\mathcal{G}_{10}^0$. The stars are the primary points z_i^0 and the dots are the dual points $\widehat{z}_i^0$.

We denote the grid by

$$\mathcal{G}_k^\sigma = \{z_i,\ 1 \le i \le k+1,\ \text{and}\ \widehat{z}_i,\ 0 \le i \le k,\ z_1 = \widehat{z}_0 = 0\}, \tag{3.1}$$

where the index σ reminds us that it is obtained for a given $\sigma(z)$ in Algorithm 1. We call $\mathcal{G}_k^\sigma$ an optimal grid, because the finite difference solution on $\mathcal{G}_k^\sigma$ produces exactly the measurements in (2.10). Note that, since γ_p, $\widehat{\gamma}_p$, and $\sigma(z)$ are positive, Algorithm 1 generates grid points satisfying

$$0 = z_1 < z_2 < \cdots < z_{k+1} \le 1,$$
$$0 = \widehat{z}_0 < \widehat{z}_1 < \cdots < \widehat{z}_k.$$

Before ending this section, let us consider the optimal TM grid $\mathcal{G}_k^0$, corresponding to the problem with homogeneous coefficient $\sigma = \sigma^0 = 1$. This grid is of importance because we use it in inversion. We calculate $\mathcal{G}_k^0$ *explicitly* in Appendix A. In Figure 3.1, we show $\mathcal{G}_k^0$ for $k = 10$. Here, we give a number of qualitative and asymptotic results for $\mathcal{G}_k^0$:

LEMMA 3.2 *The steps of the TM grid $\mathcal{G}_k^0$ satisfy the monotonic refinement property*

$$\widehat{h}_1^0 < h_1^0 < \widehat{h}_2^0 < h_2^0 < \cdots < \widehat{h}_k^0 < h_k^0, \tag{3.2}$$

and their asymptotic behavior, for large k, is given by

$$h_j^0 = \frac{2 + O[(k-j)^{-1} + j^{-2}]}{\pi\sqrt{k^2 - j^2}}$$
$$\text{for } 1 \le j \le k-1 \text{ and } h_k^0 = \frac{\sqrt{2} + O(k^{-1})}{\sqrt{\pi k}}, \tag{3.3}$$
$$\widehat{h}_j^0 = \frac{2 + O[(k+1-j)^{-1} + j^{-2}]}{\pi\sqrt{k^2 - (j-1/2)^2}} \quad \text{for } 1 \le j \le k.$$

Remark 3.3. The main convergence result of this work allows us to extend (in a weak sense) asymptotic formulae (3.3) to grids $\mathcal{G}_k^\sigma$ corresponding to general smooth coefficients $\sigma(z)$.

Remark 3.4. Condition (3.2) implies the alternating property for the nodes of $\mathcal{G}_k^0$

$$0 = \widehat{z}_0^0 = z_1^0 < \widehat{z}_1^0 < z_2^0 < \widehat{z}_2^0 < \cdots < z_k^0 < \widehat{z}_k^0 < z_{k+1}^0. \tag{3.4}$$

We experimentally found that this property also holds for $\mathcal{G}_k^\sigma$ with at least smooth enough variable $\sigma(z)$ as well as other measurement sets but have not had a proof at this point.

4 Imaging on Optimal Grids

Although the string with mass distribution $M_k(x)$ is defined uniquely by the discrete measure (2.10), in inversion, there is ambiguity in the determination of $\sigma(z)$. This is because, as it is defined in (2.13), γ_j and $\widehat{\gamma}_j$ are the primitives of $\sigma(z)^{-1}$ and $\sigma(z)$ on the grid, respectively, and thus, to find $\sigma(z)$, we must choose the grid. Typically, sequences $\{\sigma_j, \widehat{\sigma}_j\}_{j\geq 1}$ reconstructed on arbitrary grids are oscillatory (see, e.g., [10]) and additional smoothness constraints (i.e., regularization) on σ are needed to achieve convergence. Our objective in this paper is to use grids that give unconstrained convergence of the solution of the discrete inverse problem, Problem 2.

Remark 4.1. It was conjectured in [46] that one of the consequences of Krein's theory of oscillating strings is the pointwise convergence of $M_k(x)$ to $M(x)$ on $[0, L)$. For the case of sufficiently smooth σ, this hypothesis follows from the main convergence result of this work, so it may appear that we can obtain $\sigma = \sqrt{dM/dx}$ and thus the coordinate transformation $x(z)$. However, this approach requires artificial smoothing (regularization) of the sequence M_k of piecewise constant functions. Instead, we show next that the optimal grids give the desired coordinate transformation directly, without differentiation.

Let us consider a set $\mathcal{S}$ of functions satisfying the following:

Assumption 1. $\mathcal{S}$ is a compact set of bounded, positive, and sufficiently smooth functions $\sigma(z)$ that contains the constant function $\sigma^0 = 1$.[2]

We seek grids

$$\mathcal{G}_k = \{z_i,\ 1 \leq i \leq k+1,\ \text{and}\ \widehat{z}_i,\ 0 \leq i \leq k,\ z_1 = \widehat{z}_0 = 0\},$$

which are essentially independent of $\sigma(z) \in \mathcal{S}$, as $k \to \infty$, so that

$$\max_{1\leq i\leq k}\max_{\sigma\in\mathcal{S}}\left|\int_0^{\widehat{z}_i}\sigma(z)dz - \sum_{j=1}^{i}\widehat{\gamma}_j\right| < \epsilon_k,\ \max_{1\leq i\leq k}\max_{\sigma\in\mathcal{S}}\left|\int_0^{z_{i+1}}\frac{dz}{\sigma(z)} - \sum_{j=1}^{i}\gamma_j\right| < \epsilon_k, \tag{4.1}$$

where γ_j and $\widehat{\gamma}_j$ are obtained from the truncated spectral measurements (2.10) and $\lim_{k\to\infty}\epsilon_k = 0$. If such grids exist, we have by (2.13) that the reconstructed conductivities $\widehat{\sigma}_i$ and σ_i converge to the true σ (in weak norms).

In [10], we relied on a high-frequency asymptotics argument and the smoothness of the conductivities in the set $\mathcal{S}$ to introduce an imaging algorithm on grid $\mathcal{G}_k^0$ that is optimal for $\sigma(z) = \sigma^0 = 1$. Moreover, we proved that the necessary

[2] The compactness of $\mathcal{S}$ may be with respect to any norm placing it within the class of strings satisfying Lemma 2.1, but to fix ideas, we can consider the total variation norm that arises naturally in the convergence results of Section 6.

We say that $\sigma(z)$ is a sufficiently smooth function if the differential operator in (1.1) has spectral data θ_n, ξ_n that converges to θ_n^0, ξ_n^0, the spectral data for the reference $\sigma^0 = 1$, in the limit $n \to \infty$, as (5.1).

condition for convergence of the inversion process, on any grid, is that this be asymptotically close to $\mathcal{G}_k^0$:

PROPOSITION 4.2 *Let γ_j and $\widehat{\gamma}_j$, for $1 \le j \le k$, be obtained from the measurements in* (2.10) *by solving Problem* 3. *Let z_j^0 and $\widehat{z}_j^0$ be the nodes of $\mathcal{G}_k^0$. We have, for any grid* (*not necessarily optimal*) *with primary nodes z_j and dual nodes $\widehat{z}_i$* (*not necessarily interlaced*), *where $1 \le j \le k+1$ and $0 \le i \le k$, that*

$$\begin{aligned} &\max_{\sigma \in \mathcal{S}} \left| \int_0^{\widehat{z}_i} \sigma(z) dz - \sum_{j=1}^{i} \widehat{\gamma}_j \right| \ge \left| \widehat{z}_i^0 - \widehat{z}_i \right|, \\ &\max_{\sigma \in \mathcal{S}} \left| \int_0^{z_{i+1}} \frac{dz}{\sigma(z)} - \sum_{j=1}^{i} \gamma_j \right| \ge \left| z_{i+1}^0 - z_{i+1} \right|, \quad i = 1, \dots, k. \end{aligned} \tag{4.2}$$

Therefore, conditions (4.1) *can be satisfied only by grids that are asymptotically close to $\mathcal{G}_k^0$ as $k \to \infty$.*

This proposition is proven in [10] by simply noting that, for the test function $\sigma(z) = \sigma^0(z) = 1$, formulae (4.2) become equalities. In this paper, we prove that imaging on a grid that is asymptotically close to $\mathcal{G}_k^0$ is not only necessary for convergence but sufficient as well. The inversion algorithm is as follows:

Algorithm 2. To solve the discrete inverse problem, Problem 2, proceed as follows:

(1) Calculate the grid $\mathcal{G}_k^0$ for $\sigma^0 = 1$ by solving Problem 3 with data $-(\theta_p^0)^2$ and ξ_p^0 for $p = 1, \dots, k$. Here, $-(\theta_p^0)^2$ and ξ_p^0 are the eigenvalues and weights, respectively, of the differential operator in (1.1) for $\sigma = \sigma^0 = 1$.
(2) Find γ_j and $\widehat{\gamma}_j$, for $1 \le j \le k$, by solving Problem 3 with truncated spectral data $-\theta_p^2$ and ξ_p, $p = 1, \dots, k$, of the differential operator in (1.1), with the unknown σ that we wish to find.
(3) Obtain the solution by substituting $\mathcal{G}_k^0$, γ, and $\widehat{\gamma}$ into (2.13), i.e., put

$$\sigma_j = \frac{\widehat{\gamma}_j}{\widehat{h}_j^0} \quad \text{and} \quad \widehat{\sigma}_j = \frac{h_j^0}{\gamma_j}, \quad 1 \le j \le k. \tag{4.3}$$

The convergence of Algorithm 2 is stated in Theorem 6.1 and proven in Section 6. Explicitly, we show that, for sets $\mathcal{S}$ of smooth enough $\sigma(z)$ (see (6.1)), the reconstructed sequence of conductivities, defined as the piecewise constant interpolation of point values σ_j and $\widehat{\sigma}_j$, $j = 1, \dots, k$, given by (4.3), has uniformly bounded total variation. Then, standard compactness results [71, 72] imply the pointwise convergence of the reconstructed sequence and, by the uniqueness of solution of the inverse problem, the limit is $\sigma(z)$, the true conductivity in the set $\mathcal{S}$. Finally, the asymptotic closeness of the optimal grids to the homogeneous medium one, i.e.,

$$\max_{1 \le j \le k} |z_j - z_j^0| \to 0, \quad \max_{1 \le j \le k} |\widehat{z}_j - \widehat{z}_j^0| \to 0, \quad \text{as } k \to \infty,$$

follows as a corollary to Theorem 6.1.

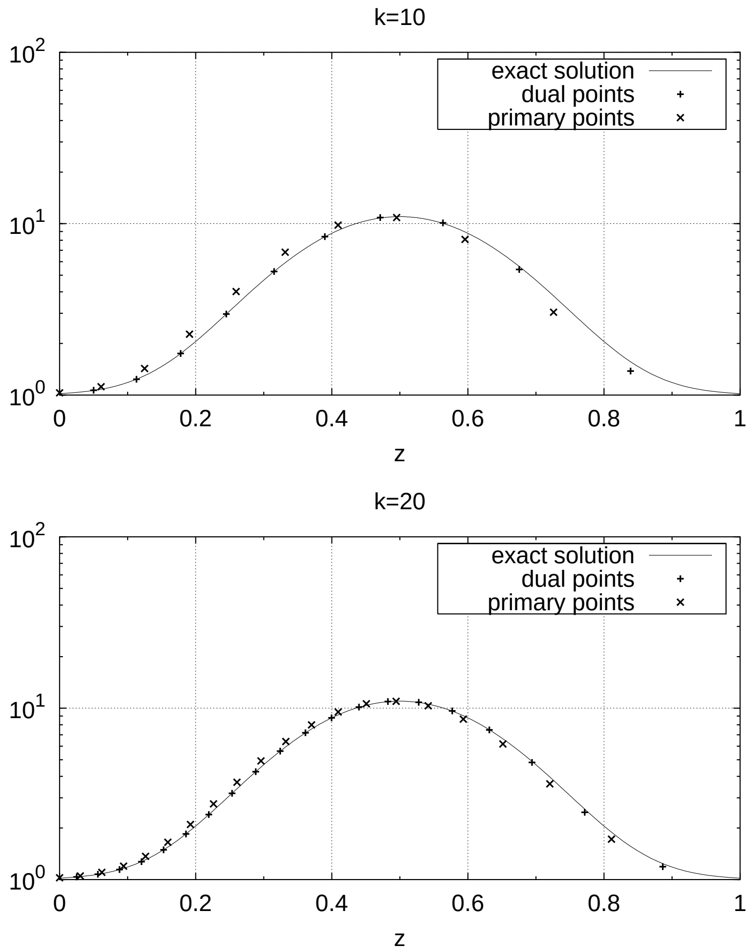

FIGURE 4.1. Inversion for the Gaussian bell

$$\sigma(z) = 1 + 10 \exp[-25(x - 0.5)^2],$$

with TM data on optimal grids $\mathcal{G}^0_{10}$ and $\mathcal{G}^0_{20}$.

We end this section with the following notes:

Remark 4.3. The reference coefficient does not have to be constant. For example, one may take any $\sigma^0(z)$ that is given as a priori information in inversion and construct the corresponding reference grid $\mathcal{G}^0_k$ using Algorithm 1.

4.1 Illustration of the Inversion Approach

In Figure 4.1 we show the inversion result for a Gaussian conductivity profile, using Algorithm 2 with TM data. The recovered coefficients give a good approximation of $\sigma(z)$. In Figure 4.2 we show the inversion of the same data but on the equidistant grid. The results are not even remotely close to the true model. If we substituted the asymptotic expression of $\mathcal{G}_k^0$ from Lemma 3.2 into Proposition 4.2, we would see that the error does not vanish as $k \to \infty$. The equidistant grid does not give the correct limit for the TM data set. In fact, our numerical experiments show that equidistant grids don't give the correct limit for any of the measurement sets mentioned in Section 2.1.

As we can observe from Figure 4.2, coefficients σ_i and $\widehat{\sigma}_i$ live on different manifolds; i.e., equidistant grids lead to false anisotropy and, consequently, to unbounded variation (as $k \to \infty$) of the reconstructed function $\sigma^k(z)$, defined as some interpolation, say piecewise constant, of the point values σ_p and $\widehat{\sigma}_p$ for $p = 1, \dots, k$. In contrast, grid $\mathcal{G}_k^0$ guarantees the uniformly bounded total variation of the reconstructed $\sigma^k(z)$, as proven in Section 6, and subsequently, convergence to the true solution of the inverse problem. In this context, optimal grids can be considered as an implicit method of total variation regularization.

Finally, we point out that, as is well-known [54], an anisotropic problem can be transformed by a coordinate stretching to an isotropic one, with the same impedance data. As a by-product of our analysis, we obtain that optimal grids perform implicitly such transformations.

5 Convergence of the Inversion Algorithm for a Special Class of Exponential Coefficients

The convergence analysis of Algorithm 2, given in Section 6, is based on the assumption that, in the asymptotic limit $n \to \infty$, perturbations $\Delta\theta_n = \theta_n - \theta_n^0$ and $\Delta\xi_n = \xi_n - \xi_n^0$ decay as $O(1/(n^\alpha \log n))$ and $O(1/n^\alpha)$, respectively, for some $\alpha > 1$. Asymptotic expansions of θ_n and ξ_n, using various smoothness requirements on $\sigma(z)$, are well-known [15, 19, 70]. For example, if $\sigma(z) \in H^3([0,1])$, we have [15, 70]

$$(5.1)\quad \Delta\theta_n = \theta_n - \theta_n^0 = \frac{\int_0^1 Q(z)dz}{(2n-1)\pi} + O(n^{-2}) \quad \text{and} \quad \Delta\xi_n = \xi_n - \xi_n^0 = O(n^{-2}),$$

where

$$(5.2)\qquad Q(z) = \sigma(z)^{-\frac{1}{2}} \frac{d^2\sigma(z)^{\frac{1}{2}}}{dz^2}$$

is the Schrödinger potential and

$$(5.3)\qquad \theta_n^0 = \left(n - \frac{1}{2}\right)\pi, \quad y(z,\theta_n^0) = \sqrt{2}\cos\left[\left(n - \frac{1}{2}\right)z\right], \quad \text{and} \quad \xi_n^0 = y(0,\theta_n^0)^2 = 2$$

are the eigenvalues, eigenfunctions, and weights of the homogeneous problem, respectively. Because only zero mean potentials $Q(z)$ give the desired asymptotic

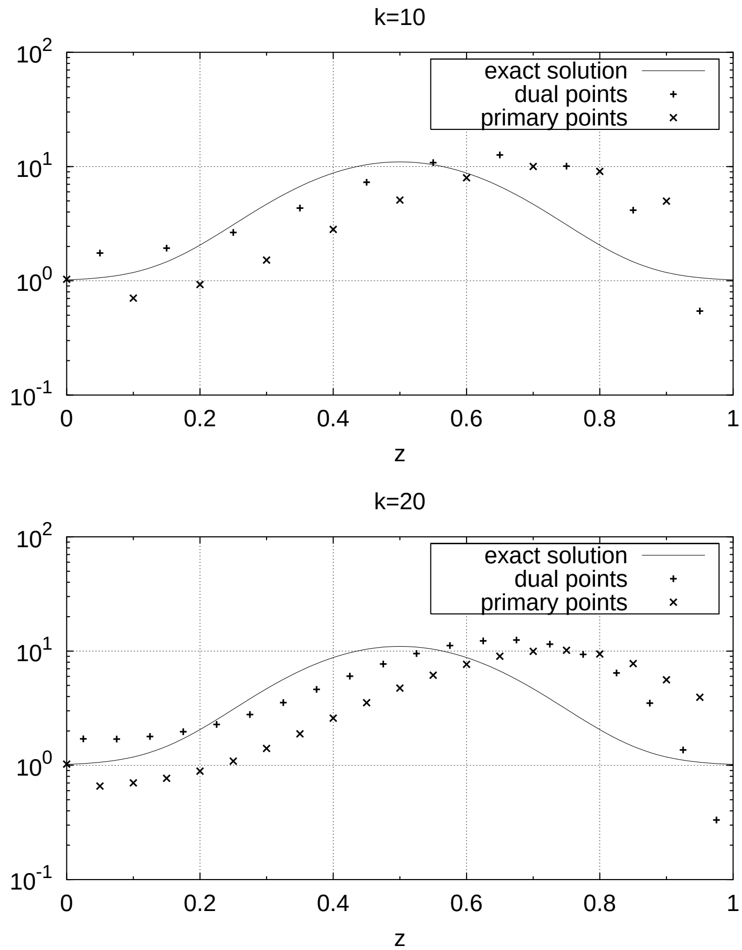

FIGURE 4.2. Inversion for the Gaussian bell

$$\sigma(z) = 1 + 10\exp[-25(x-0.5)^2],$$

with TM data on equidistant grids with 10 and 20 nodes.

behavior of $\Delta\theta_n$, it appears that the analysis in Section 6 applies to a much restricted class of functions $\sigma(z)$. However, in case of general, nonzero mean potentials, we can modify Algorithm 2 by replacing the uniform reference coefficient σ^0 with function

$$\sigma^{\overline{Q}}(z) = \frac{1}{4}\left(e^{\sqrt{\overline{Q}}z} + e^{-\sqrt{\overline{Q}}z}\right)^2 \tag{5.4}$$

satisfying the initial value problem

$$
\begin{aligned}
\frac{d^2\sqrt{\sigma^{\overline{Q}}(z)}}{dz^2} &= \overline{Q}\sqrt{\sigma^{\overline{Q}}(z)} \quad \text{for } 0 < z \le 1, \\
\frac{d\sigma^{\overline{Q}}(0)}{dz} &= 0, \quad \sigma^{\overline{Q}}(0) = 1,
\end{aligned} \tag{5.5}
$$

where $\overline{Q}$ is a constant obeying the condition

$$
\overline{Q} > -\frac{\pi^2}{4}, \tag{5.6}
$$

so that (5.4) remains strictly positive in the unit interval $z \in [0, 1]$. Of course, here $\overline{Q}$ plays the role of the mean value of Schrödinger's potential (5.2).

Using (5.4) as the reference coefficient, we obtain the desired decay of $\Delta\theta_n$ and the analysis in Section 6 applies. The remaining question is, What does the optimal grid for coefficient (5.4) look like? We prove in this section that the grid is the same as $\mathcal{G}_k^0$ in the asymptotic limit $k \to \infty$, so Algorithm 2 converges after all, without modifying the reference coefficient from σ^0 to $\sigma^{\overline{Q}}$.

THEOREM 5.1 *Let $\{\sigma_j^{\overline{Q}}, \widehat{\sigma}_j^{\overline{Q}}\}_{j\ge 1}$ be the sequence of parameters generated by Algorithm* 2, *with the TM data set corresponding to the function $\sigma^{\overline{Q}}(z)$. Then, $\sigma_j^{\overline{Q}}$ satisfy the finite difference discretization of initial value problem* (5.5),

$$
\begin{aligned}
\frac{1}{\widehat{h}_j^0}\left[\left(\frac{\sqrt{\sigma_{j+1}^{\overline{Q}}} - \sqrt{\sigma_j^{\overline{Q}}}}{h_j^0}\right) - \left(\frac{\sqrt{\sigma_j^{\overline{Q}}} - \sqrt{\sigma_{j-1}^{\overline{Q}}}}{h_{j-1}^0}\right)\right]& \\
- \overline{Q}\sqrt{\sigma_j^{\overline{Q}}} = 0, &\quad j = 2, 3, \dots, k, \\
\frac{1}{\widehat{h}_1^0}\left(\frac{\sqrt{\sigma_2^{\overline{Q}}} - \sqrt{\sigma_1^{\overline{Q}}}}{h_1^0}\right) - \overline{Q}\sqrt{\sigma_1^{\overline{Q}}} = 0, &\quad \sigma_1 = 1,
\end{aligned} \tag{5.7}
$$

and $\widehat{\sigma}_j^{\overline{Q}}$ are given by

$$
\widehat{\sigma}_j^{\overline{Q}} = \sqrt{\sigma_j^{\overline{Q}}\sigma_{j+1}^{\overline{Q}}} \quad \textit{for } j = 1, \dots, k. \tag{5.8}
$$

In the limit $k \to \infty$, we have

$$
\max_{1\le j\le k}\left|\sigma_j^{\overline{Q}} - \sigma^{\overline{Q}}\big(z_j^0\big)\right| \to 0 \quad \textit{and} \quad \max_{1\le j\le k}\left|\widehat{\sigma}_j^{\overline{Q}} - \sigma^{\overline{Q}}\big(\widehat{z}_j^0\big)\right| \to 0. \tag{5.9}
$$

Finally, letting $\sigma^{k,\overline{Q}}(z)$ *be the piecewise constant interpolation of point values* $\{\sigma_j^{\overline{Q}}, \widehat{\sigma}_j^{\overline{Q}}\}_{1\le j\le k}$,

$$\sigma^{k,\overline{Q}}(z) = \begin{cases} \sigma_j^{\overline{Q}} & \text{for } z \in \left[z_j^0, \widehat{z}_j^0\right), \; j = 1, \dots, k, \\ \widehat{\sigma}_j^{\overline{Q}} & \text{for } z \in \left[\widehat{z}_j^0, z_{j+1}^0\right), \; j = 1, \dots, k, \\ \widehat{\sigma}_k^{\overline{Q}} & \text{for } z \in \left[z_{k+1}^0, 1\right], \end{cases} \tag{5.10}$$

we have

$$\sigma^{k,\overline{Q}}(z) \to \sigma^{\overline{Q}}(z) \quad \text{as } k \to \infty \text{ in } L^\infty[0,1]. \tag{5.11}$$

PROOF: Take coefficient (5.4) in (1.1) and rewrite the equation in Schrödinger form

$$\begin{gathered} \frac{d^2 w(z)}{dz^2} - \lambda w(z) - \overline{Q} w(z) = 0 \qquad \text{for } 0 < z < 1, \\ \frac{dw(0)}{dz} = -1, \\ w(1) = 0, \end{gathered} \tag{5.12}$$

where

$$w(z) = \sqrt{\sigma^{\overline{Q}}(z)}\, u(z). \tag{5.13}$$

The Schrödinger operator in (5.13) has the same eigenfunctions as the homogeneous ($\overline{Q} = 0$) one, and, because $\sigma^{\overline{Q}}(0) = 1$, transformation (5.13) gives the same weights

$$\xi_n^{\overline{Q}} = \xi_n^0. \tag{5.14}$$

The eigenvalues are shifted as

$$-(\theta_n^{\overline{Q}})^2 = -\left(n - \frac{1}{2}\right)^2 \pi^2 - \overline{Q} = -(\theta_n^0)^2 - \overline{Q} \quad \text{for } n \ge 1, \tag{5.15}$$

and they remain strictly negative due to assumption (5.6).

Now, let us solve Problem 3 with spectral data $\{\theta_n^0, \xi_n^0\}_{1\le n\le k}$ to find the tridiagonal matrix Γ^0 with entries in terms of h_j^0 and $\widehat{h}_j^0$ for $j = 1, \dots, k$ (recall (2.17)). Similarly, use shifted data $\{\theta_n^{\overline{Q}}, \xi_n^{\overline{Q}}\}_{1\le n\le k}$ to find the tridiagonal matrix $\Gamma^{\overline{Q}}$, with entries in terms of $\gamma_j^{\overline{Q}}$ and $\widehat{\gamma}_j^{\overline{Q}}$ for $j = 1, \dots, k$. We denote by

$$\mathcal{Y}^0 = \left(\mathbf{Y}(\theta_1^0), \dots, \mathbf{Y}(\theta_k^0)\right) \quad \text{and} \quad \mathcal{Y}^{\overline{Q}} = \left(\mathbf{Y}(\theta_1^{\overline{Q}}), \dots, \mathbf{Y}(\theta_k^{\overline{Q}})\right) \tag{5.16}$$

the matrices of eigenvectors of Γ^0 and $\Gamma^{\overline{Q}}$, respectively, and we recall from Section 2.1 that

$$\mathcal{Z}^0 = \operatorname{diag}\left(\sqrt{\widehat{h}_1^0}, \dots, \sqrt{\widehat{h}_k^0}\right)\mathcal{Y}^0, \qquad \mathcal{Z}^{\overline{Q}} = \operatorname{diag}\left(\sqrt{\widehat{\gamma}_1^{\overline{Q}}}, \dots, \sqrt{\widehat{\gamma}_k^{\overline{Q}}}\right)\mathcal{Y}^{\overline{Q}}, \tag{5.17}$$

are orthogonal. Thus, in view of (5.14),

$$\left(\mathcal{Z}^{\overline{Q}}\mathcal{Z}^{\overline{Q}^\star}\right)_{11} = \widehat{\gamma}_1^{\overline{Q}}\sum_{n=1}^{k}\xi_n^{\overline{Q}} = \widehat{\gamma}_1^{\overline{Q}}\sum_{n=1}^{k}\xi_n^0 = 1 = \left(\mathcal{Z}^0\mathcal{Z}^{0^\star}\right)_{11} = \widehat{h}_1^0\sum_{n=1}^{k}\xi_n^0 \tag{5.18}$$

and

$$\sigma_1^{\overline{Q}} = \frac{\widehat{\gamma}_1^{\overline{Q}}}{\widehat{h}_1^0} = 1 = \sigma^{\overline{Q}}(0), \tag{5.19}$$

as stated in (5.7).

To obtain the remaining equations in Theorem 5.1, we note that, up to a diagonal scaling, $\Gamma^{\overline{Q}}$ and Γ^0 are Jacobi matrices [18], so the unique solution of the inverse spectral problem is

$$\operatorname{diag}\left(\sqrt{\widehat{\gamma}_1^{\overline{Q}}/\widehat{h}_1^0}, \dots, \sqrt{\widehat{\gamma}_k^{\overline{Q}}/\widehat{h}_k^0}\right)\Gamma^{\overline{Q}}\operatorname{diag}\left(\sqrt{\widehat{h}_1^0/\widehat{\gamma}_1^{\overline{Q}}}, \dots, \sqrt{\widehat{h}_k^0/\widehat{\gamma}_k^{\overline{Q}}}\right) = \Gamma^0 - \overline{Q}I. \tag{5.20}$$

Then, using (2.13), (5.20), and definitions (2.17) of the entries of Γ, we derive, with straightforward algebra, equations (5.7) and (5.8) (first, comparing the off-diagonal components, we establish (5.8); then, comparing the diagonal ones and utilizing (5.8), we derive (5.7)).

Now, note that the reconstructed coefficients $\sigma_j^{\overline{Q}} = \widehat{\gamma}_j^{\overline{Q}}/\widehat{h}_j^0$ solve the finite difference approximation of initial value problem (5.5) on the grid $\mathcal{G}_k^0$. Lemma 3.2 together with the standard finite difference error analysis [37] show that $\mathcal{G}_k^0$ is regular enough for the convergence of the finite difference solution, i.e., $\sigma_j^{\overline{Q}}$. Then (5.8) and the alternating property (3.4) give convergence of $\widehat{\sigma}_j^{\overline{Q}}$. □

6 Convergence Analysis for the Discrete Inverse Problem

In this section, we study the convergence of Algorithm 2 for reconstructing coefficients $\sigma(z) \in \mathcal{S}$ that are smooth enough, so that perturbations $\Delta\theta_n = \theta_n - \theta_n^0$ and $\Delta\xi_n = \xi_n - \xi_n^0$ have the asymptotic behavior

$$\Delta\theta_n = O\left(\frac{1}{n^\alpha \log n}\right) \quad \text{and} \quad \Delta\xi_n = O\left(\frac{1}{n^\alpha}\right) \quad \text{for some } \alpha > 1 \text{ as } n \to \infty. \tag{6.1}$$

It follows from (5.1) that asymptotic behavior (6.1) holds for sufficiently smooth $\sigma(z)$ satisfying

$$\overline{Q} = \int_0^1 Q(z)dz = 0, \tag{6.2}$$

where $Q(z)$ is the Schrödinger potential (5.2). For simplicity of explanation, we present the convergence analysis for such coefficients $\sigma(z)$. Then, we extend the result to the general case $\overline{Q} \neq 0$ in Section 6.5.

We have the following convergence result:

THEOREM 6.1 *Suppose that coefficient $\sigma(z) \in \mathcal{S}$ that we wish to find gives spectral data with perturbations*

$$\Delta\theta_n = \theta_n - \theta_n^0 \quad \textit{and} \quad \Delta\xi_n = \xi_n - \xi_n^0, \tag{6.3}$$

having asymptotic behavior (6.1). *Let $\{\sigma_j, \widehat{\sigma}_j\}_{1\le j\le k}$ be the coefficients generated by Algorithm* 2 *and define $\sigma^k(z)$, the piecewise constant interpolation of point values σ_j and $\widehat{\sigma}_j$ for $j = 1, \dots, k$,*

$$\sigma^k(z) = \begin{cases} \sigma_j & \textit{for } z \in \left[z_j^0, \widehat{z}_j^0\right), \ j = 1, \dots, k, \\ \widehat{\sigma}_j & \textit{for } z \in \left[\widehat{z}_j^0, z_{j+1}^0\right), \ j = 1, \dots, k, \\ \widehat{\sigma}_k & \textit{for } z \in \left[z_{k+1}^0, 1\right]. \end{cases} \tag{6.4}$$

As $k \to \infty$, $\sigma^k(z)$ converges to $\sigma(z)$ pointwise and in $L^1[0, 1]$.

The main steps in the convergence proof are: We begin in Section 6.1 by rewriting the finite difference forward problem in first-order system form. This reformulation introduces $2k - 1$ new parameters

$$\begin{aligned} \beta_{2p-1} &= \frac{1}{\sqrt{\gamma_p \widehat{\gamma}_p}} = \frac{1}{\sqrt{h_p^0 \widehat{h}_p^0}} \sqrt{\frac{\widehat{\sigma}_p}{\sigma_p}}, \\ \beta_{2p} &= \frac{1}{\sqrt{\gamma_p \widehat{\gamma}_{p+1}}} = \frac{1}{\sqrt{h_p^0 \widehat{h}_{p+1}^0}} \sqrt{\frac{\widehat{\sigma}_p}{\sigma_{p+1}}}. \end{aligned} \tag{6.5}$$

As we prove in Section 6.3, these parameters satisfy the bounded variation criterion

$$\sum_{p=1}^{2k-1} \left| \log \frac{\beta_p}{\beta_p^0} \right| = \frac{1}{2} \sum_{p=1}^{k} \left| \log \widehat{\sigma}_p - \log \sigma_p \right| + \frac{1}{2} \sum_{p=1}^{k-1} \left| \log \widehat{\sigma}_p - \log \sigma_{p+1} \right| \le C \tag{6.6}$$

uniformly with respect to k. The left-hand side in (6.6) is the variation of $\sigma^k(z)$, and convergence follows from standard compactness arguments and the uniqueness of the solution of the inverse problem, Problem 1.

The proof of the bounded variation criterion (6.6) is the most technical part of the paper, and it is based on the method of small perturbations as follows: Write for an arbitrary continuation parameter $r \in [0,1]$,

$$\Delta\theta_n^r = r\,\Delta\theta_n \quad \text{and} \quad \Delta\xi_n^r = r\,\Delta\xi_n, \quad n = 1,\dots,k, \tag{6.7}$$

and let β_p^r be the entries in the tridiagonal skew-symmetric matrix B^r with spectral data $\theta_n^r = \theta_n^0 + \Delta\theta_n^r$ and $\xi_n^r = \xi_n^0 + \Delta\xi_n^r$. Obviously, for $r = 1$, $\beta_p^1 = \beta_p$, and for $r = 0$ we have the unperturbed problem entries β_p^0. Using a novel perturbation analysis, we derive in Section 6.3 explicit formulae for perturbations $d\log\beta_p^r$ in terms of the eigenvalues and eigenvectors of matrix B^r and perturbations $d\theta_n^r = \Delta\theta_n\,dr$ and $d\xi_n^r = \Delta\xi_n\,dr$, respectively. Further, we obtain the uniform bound

$$\sum_{p=1}^{2k-1} \left| d\log\beta_p^r \right| \le C\,|dr| \tag{6.8}$$

with a constant C independent of k and r. Then, the magnitudes

$$\log\frac{\beta_p}{\beta_p^0} = \int_0^1 d(\log\beta_p^r) \tag{6.9}$$

satisfy (6.6) uniformly with k.

The novel perturbation analysis introduced in Section 6.3 is based on a discrete Gel′fand-Levitan formulation, due to Natterer [67], and reviewed, for completeness, in Section 6.2. We gather all our results and finalize the proof of Theorem 6.1 in Section 6.4.

We end this section with a corollary to Theorem 6.1 that establishes the asymptotic behavior of optimal grids mentioned in Section 4:

COROLLARY 6.2 *The optimal grids corresponding to coefficients $\sigma(z) \in \mathcal{S}$ that give spectral data with asymptotic behavior* (6.1) *satisfy*

$$\max_{1\le j\le k} \left| z_j - z_j^0 \right| \to 0, \quad \max_{1\le j\le k} \left| \widehat{z}_j - \widehat{z}_j^0 \right| \to 0 \quad \text{as } k \to \infty. \tag{6.10}$$

PROOF: It follows from the L^1 convergence result of Theorem 6.1, the smoothness of σ, and the regularity of steps h_j^0 and $\widehat{h}_j^0$ (Lemma 3.2) that

$$\sum_{i=1}^{j} \widehat{h}_i^0 \sigma^k\left(z_i^0\right) - \sum_{i=1}^{j} \widehat{h}_i^0 \sigma\left(z_i^0\right) = o(1)$$

uniformly in j. Now, Algorithm 2 and (2.13), for any $1 \le j \le k$, give

$$\sum_{i=1}^{j} \widehat{\gamma}_i = \int_0^{\widehat{z}_j} \sigma(z)\,dz = \sum_{i=1}^{j} \widehat{h}_i^0 \sigma^k\left(z_i^0\right) = \sum_{i=1}^{j} \widehat{h}_i^0 \sigma\left(z_i^0\right) + o(1).$$

From the above equation we obtain

$$\int_{\widehat{z}_j^0}^{\widehat{z}_j} \sigma(z)\,dz = \sum_{i=1}^{j} \widehat{h}_i^0 \sigma^k\big(z_i^0\big) - \int_0^{\widehat{z}_j^0} \sigma(z)\,dz$$

$$= \sum_{i=1}^{j} \widehat{h}_i^0 \sigma\big(z_i^0\big) - \int_0^{\widehat{z}_j^0} \sigma(z)\,dz + o(1),$$

and with the help of the triangle inequality we arrive at

$$|\widehat{z}_j^0 - \widehat{z}_j| \min_z \sigma(z) \le \left| \int_{\widehat{z}_j^0}^{\widehat{z}_j} \sigma(z)\,dz \right| \le \left| \int_0^{\widehat{z}_j^0} \sigma(z)\,dz - \sum_{i=1}^{j} \widehat{h}_i^0 \sigma\big(z_i^0\big) \right| + o(1). \tag{6.11}$$

One of the consequences of Lemma 3.2 is that grids $\mathcal{G}_k^0$ generate a sequence of convergent quadratures with nodes z_i^0 and weights $\widehat{h}_i^0$. These quadratures and the smoothness and boundedness of $\sigma(z)$ allow us to estimate the first term in the right-hand side of (6.11) as $o(1)$, uniformly in j. Finally, since $\sigma(z)$ is strictly positive, we have

$$\max_{1\le j\le k} \left|\widehat{z}_j - \widehat{z}_j^0\right| \to 0 \quad \text{as } k \to \infty.$$

The result

$$\max_{1\le j\le k} |z_j - z_j^0| \to 0 \quad \text{as } k \to \infty$$

follows similarly from equality

$$\sum_{i=1}^{j} \gamma_i = \int_0^{z_{j+1}} \frac{dz}{\sigma(z)} = \sum_{i=1}^{j} \frac{h_i^0}{\sigma^k(\widehat{z}_i^0)}, \qquad j = 1, \dots, k.$$

□

6.1 The First-Order System Formulation

The reduction of second-order differential equation (1.1) to a first-order system is a standard and useful transformation that can be found, for example, in [12]. In the discrete, finite difference setting, the transformation of system (2.16) is[3]

$$B\mathcal{H}^{\frac{1}{2}}\mathbf{W} - \sqrt{\lambda}\,\mathcal{H}^{\frac{1}{2}}\mathbf{W} = -\frac{\mathbf{e}_1}{\sqrt{\lambda\widehat{\gamma}_1}}, \tag{6.12}$$

where the unknown vector is

$$\mathbf{W} = \big(W_1, \widehat{W}_1, W_2, \widehat{W}_2, \dots, W_k, \widehat{W}_k\big)^{\mathsf{T}}, \tag{6.13}$$

$$W_j = \sqrt{\sigma_j}\, U_j, \quad \widehat{W}_j = \frac{\widehat{\sigma}_j}{\sqrt{\lambda\widehat{\sigma}_j}} \frac{U_{j+1} - U_j}{h_j^0}, \quad \text{for } j = 1, \dots, k, \tag{6.14}$$

$\mathcal{H}$ is the scaling diagonal matrix

$$\mathcal{H} = \operatorname{diag}\big(\widehat{h}_1^0, h_1^0, \dots, \widehat{h}_k^0, h_k^0\big), \tag{6.15}$$

[3] Equations (6.12) can be verified directly by using (2.12).

and

$$B = \begin{pmatrix} 0 & \beta_1 & 0 & \cdots & 0 \\ -\beta_1 & 0 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \beta_{2k-2} & 0 \\ \vdots & \ddots & -\beta_{2k-2} & 0 & \beta_{2k-1} \\ 0 & \dots & 0 & -\beta_{2k-1} & 0 \end{pmatrix} \tag{6.16}$$

is the tridiagonal, skew-symmetric matrix with entries (6.5).

The skew-symmetric matrix B has purely imaginary eigenvalues and orthonormal eigenvectors

$$\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \dots, \zeta_{2k})^{\mathsf{T}}, \tag{6.17}$$

given in terms of the eigenvectors of Γ as follows:

LEMMA 6.3 *The eigenvalues of B are given by $\pm i\theta_j$, where $-\theta_j^2$ are the eigenvalues of Γ for $1 \le j \le k$. Consider then the orthonormal vectors*

$$\boldsymbol{\eta}(\theta_j) = \operatorname{diag}\left(\widehat{\gamma}_1^{1/2}, \dots, \widehat{\gamma}_k^{1/2}\right) \mathbf{Y}(\theta_j) \tag{6.18}$$

and

$$\widehat{\boldsymbol{\eta}}(\theta_j) = \operatorname{diag}\left(\gamma_1^{1/2}, \dots, \gamma_k^{1/2}\right) \widehat{\mathbf{Y}}(\theta_j), \tag{6.19}$$

where $\mathbf{Y}(\theta_j)$ are eigenvectors of Γ and where $\widehat{\mathbf{Y}}(\theta_j) = \left(\widehat{Y}_1(\theta_j), \dots, \widehat{Y}_k(\theta_j)\right)^{\mathsf{T}}$ satisfies

$$\widehat{Y}_p(\theta_j) = \frac{Y_{p+1}(\theta_j) - Y_p(\theta_j)}{\theta_j \gamma_p}, \quad 1 \le p \le k. \tag{6.20}$$

The eigenvectors of B are given by

$$\boldsymbol{\zeta}(\pm\theta_j) = \frac{1}{\sqrt{2}}\left(\eta_1(\theta_j), \pm i\, \widehat{\eta}_1(\theta_j), \dots, \eta_k(\theta_k), \pm i\, \widehat{\eta}_k(\theta_k)\right)^{\mathsf{T}}. \tag{6.21}$$

Lemma 6.3 is proven in Appendix B.

Finally, let us note that, since spectral data $\{\theta_j, \xi_j\}_{1\le j\le k}$ determines uniquely the tridiagonal matrix Γ, it also determines uniquely matrix B, with entries β_j given by (6.5).

6.2 The Discrete Gel′fand-Levitan Formulation for the Skew-Symmetric, First-Order System of Equations

We base our perturbation analysis for estimating (6.8) on a discrete Gel′fand-Levitan formulation, shown here as derived by Natterer in [67]. Let us consider the "reference" matrix B^r for an arbitrary but fixed $r \in [0, 1]$, and define the lower triangular, transmutation matrix G satisfying

$$EGB = EB^rG, \quad \mathbf{e}_1^{\mathsf{T}} G = \mathbf{e}_1^{\mathsf{T}}, \tag{6.22}$$

where $E = I - \mathbf{e}_{2k}\mathbf{e}_{2k}^{\mathsf{T}}$. The fact that such a matrix G is uniquely determined by (6.22) follows easily from the Lanczos process, which considers equation (6.22) row by row. Indeed, letting $\mathbf{g}_j^{\mathsf{T}}$ be the j^{th} row of G, we have

$$\mathbf{g}_1 = \mathbf{e}_1,$$

$$\beta_1^r \mathbf{g}_2 = B\mathbf{g}_1 = \beta_1 \mathbf{e}_2,$$

$$\beta_1^r \mathbf{g}_1 - \beta_2^r \mathbf{g}_3 = B\mathbf{g}_2 = \frac{\beta_1^2}{\beta_1^r}\mathbf{e}_1 - \frac{\beta_1\beta_2}{\beta_1^r}\mathbf{e}_3, \quad \text{and so on.}$$

Clearly, if $B = B^r$, then $G = I$.

Next, consider the initial value problem

$$EB\boldsymbol{\phi}(\lambda) = i\lambda E\boldsymbol{\phi}(\lambda), \quad \mathbf{e}_1^{\mathsf{T}}\boldsymbol{\phi}(\lambda) = 1. \tag{6.23}$$

One easily shows, with the same method as above, that (6.23) has a unique solution $\boldsymbol{\phi}(\lambda)$. Note in particular that, for $\lambda = \pm\theta_j$,

$$\boldsymbol{\phi}(\pm\theta_j) = \frac{\boldsymbol{\zeta}(\pm\theta_j)}{\zeta_1(\pm\theta_j)} = \sqrt{\frac{2}{\widehat{\gamma}_1\xi_j}}\,\boldsymbol{\zeta}(\pm\theta_j), \tag{6.24}$$

and (6.23) holds even for E replaced by the identity matrix. For the reference matrix, we have

$$EB^r\boldsymbol{\phi}^r(\lambda) = i\lambda E\boldsymbol{\phi}^r(\lambda), \quad \mathbf{e}_1^{\mathsf{T}}\boldsymbol{\phi}^r(\lambda) = 1, \tag{6.25}$$

and, using (6.22), we obtain

$$\boldsymbol{\phi}^r(\pm\theta_j) = G\boldsymbol{\phi}(\pm\theta_j), \quad 1 \le j \le k. \tag{6.26}$$

We write (6.26) in matrix form as

$$\Phi^r = G\Phi = GZ\mathcal{P}, \quad \mathcal{P} = \sqrt{\frac{2}{\widehat{\gamma}_1}}\,\text{diag}\left(\xi_1^{-1/2}, \xi_1^{-1/2}, \ldots, \xi_k^{-1/2}, \xi_k^{-1/2}\right), \tag{6.27}$$

where Z is the orthonormal matrix of eigenvectors of B,

$$\Phi = \left(\boldsymbol{\phi}(\theta_1), \boldsymbol{\phi}(-\theta_1), \ldots, \boldsymbol{\phi}(-\theta_k)\right) = Z\mathcal{P},$$
$$\Phi^r = \left(\boldsymbol{\phi}^r(\theta_1), \boldsymbol{\phi}^r(-\theta_1), \ldots, \boldsymbol{\phi}^r(-\theta_k)\right).$$

Then, letting

$$F = \Phi^r\mathcal{P}^{-1} = GZ, \tag{6.28}$$

we have

$$FF^\star = GG^\star. \tag{6.29}$$

Finally, equations (6.28) and (6.22) give

$$EB^rF = EB^rGZ = EGBZ = iEGZ\Theta = iEF\Theta, \tag{6.30}$$

where

$$\Theta = \operatorname{diag}(\theta_1, -\theta_1, \dots, \theta_k, -\theta_k). \tag{6.31}$$

Remark 6.4. The discrete Gel′fand-Levitan inversion method proceeds as follows: Start with a known reference matrix B^r for some $r \in [0, 1]$. (The usual choice is B^0, the matrix corresponding to the constant coefficient $\sigma^0 = 1$.) Determine Φ^r and $F = \Phi^r \mathcal{P}^{-1}$ from spectral data θ_j^r and ξ_j^r for $1 \le j \le k$. Then calculate G from (6.29) by a Cholesky factorization and obtain B from (6.22).

6.3 The Perturbation Analysis

Consider small perturbations $d\theta_n = \Delta\theta_n\, dr$ and $d\xi_n = \Delta\xi_n\, dr$ of the spectral data of reference matrix B^r and take the linearization of the Gel′fand-Levitan equations in Section 6.2 around B^r. Throughout this section, we denote the perturbed quantities by a tilde ($\tilde{}$). We write in short

$$\widetilde{\Theta} = \Theta^r + d\Theta, \quad \widetilde{\mathcal{P}} = \mathcal{P}^r + d\mathcal{P}, \quad \widetilde{Z} = Z^r + dZ, \tag{6.32}$$

and, using (6.32) in (6.30), we have

$$E B^r\, dF = i E Z^r\, d\Theta + i E\, dF\, \Theta^r, \tag{6.33}$$

because $G^r = I$ and $F^r = Z^r$. Now multiply (6.33) by $Z^{r\star}$ on the right and note that, since $\Theta^r Z^{r\star} = -i Z^{r\star} B^r$, the differential form

$$dV = dF\, Z^{r\star} \tag{6.34}$$

satisfies

$$E B^r\, dV - E\, dV\, B^r = i E Z^r\, d\Theta Z^{r\star}, \tag{6.35}$$

$$\mathbf{e}_1^{\mathsf{T}}\, dV = \mathbf{e}_1^{\mathsf{T}}\, dF\, Z^{r\star} = (d\chi_1, d\chi_1, \dots, d\chi_k, d\chi_k)\, Z^{r\star}, \tag{6.36}$$

where $d\chi_j$ is the differential of

$$\chi_j = \zeta_1(\pm\theta_j^r) = \sqrt{\frac{\widehat{\gamma}_1^r \xi_j^r}{2}} = \sqrt{\frac{\xi_j^r}{2\sum_{p=1}^k \xi_p^r}} \quad \text{for } 1 \le j \le k. \tag{6.37}$$

Similarly, differentiating (6.22), we have

$$E\, dB + E\, dG\, B^r = E B^r\, dG, \quad \mathbf{e}_1^{\mathsf{T}}\, dG = \mathbf{0}^{\mathsf{T}}. \tag{6.38}$$

Finally, differentiating (6.29) and recalling that $F^r = Z^r$, we obtain

$$dF\, Z^{r\star} + Z^r\, dF^\star = dV + dV^\star = dG + dG^\star. \tag{6.39}$$

Equations (6.38) and (6.39) allow us to obtain the relative perturbations of the entries β_j^r of the matrix B^r. Indeed, taking the $j, j+1$ component in (6.38), we get

$$\frac{d\beta_j^r}{\beta_j^r} = dG_{j+1j+1} - dG_{jj} = dV_{j+1j+1} - dV_{jj}, \tag{6.40}$$

and we prove next the following result:

LEMMA 6.5 *Assume that $\Delta\theta_n$ and $\Delta\xi_n$, and therefore $d\theta_n$ and $d\xi_n$, have asymptotic behavior* (6.1). *Then, the linearized perturbations of* $\log\beta_j^r$ *satisfy*

$$\sum_{j=1}^{2k-1}\left|\frac{d\beta_j^r}{\beta_j^r}\right| \le C|dr|, \tag{6.41}$$

where C is independent of k and r is a positive constant.

Because of linearity, we prove (6.41) by examining separately the effect of the small perturbations of the eigenvalues and of the weights, respectively, on the linearized relative perturbation of β_j^r for $1 \le j \le 2k-1$.

Perturbation of the Eigenvalues

Assume that only the eigenvalues are perturbed. We get from (6.35) and (6.36) that

$$EB^r\,dV - E\,dV\,B^r = iEZ^r\,d\Theta\,Z^{r\star}, \quad \mathbf{e}_1^{\mathsf{T}}\,dV = \mathbf{0}^{\mathsf{T}}, \tag{6.42}$$

and the solution, which we derive in Appendix C, is

$$\begin{cases} \widehat{\gamma}_p^r \displaystyle\sum_{q=1}^{k}\sum_{\substack{l=1\\ l\neq q}}^{k} \frac{2\theta_q^r\,d\theta_q^r}{(\theta_q^r)^2-(\theta_l^r)^2}\left[Y_p(\theta_l^r)^2 - \sqrt{\frac{\xi_l^r}{\xi_q^r}}\,Y_p(\theta_l^r)Y_p(\theta_q^r)\right] \\ \quad \text{if } j = 2p-1, \\ \gamma_p^r \displaystyle\sum_{q=1}^{k}\sum_{\substack{l=1\\ l\neq q}}^{k}\left[\frac{2\theta_q^r\,d\theta_q^r}{(\theta_q^r)^2-(\theta_l^r)^2}\,\widehat{Y}_p(\theta_l^r)^2 - \frac{2\theta_l^r\,d\theta_q^r}{(\theta_q^r)^2-(\theta_l^r)^2}\sqrt{\frac{\xi_l^r}{\xi_q^r}}\,\widehat{Y}_p(\theta_l^r)\widehat{Y}_p(\theta_q^r)\right] \\ \qquad\qquad + \displaystyle\sum_{q=1}^{k}\frac{d\theta_q^r}{\theta_q^r}\,\gamma_p^r\widehat{Y}_p(\theta_q^r)^2 \quad \text{if } j = 2p, \end{cases} \tag{6.43}$$

where γ_p^r and $\widehat{\gamma}_p^r$ are the components in matrix Γ^r with eigenvalues $-(\theta_n^r)^2$ and eigenvectors $\mathbf{Y}(\theta_n^r)$, $1 \le n \le k$. We obtain the following estimate:

LEMMA 6.6 *There exists a positive constant C that is independent of k and r such that*

$$\sum_{j=1}^{2k-1}\left|dV_{j+1\,j+1} - dV_{jj}\right| \le C|dr|. \tag{6.44}$$

PROOF: Recall that

$$\begin{aligned} \boldsymbol{\eta}(\theta_p^r) &= \operatorname{diag}\left(\sqrt{\widehat{\gamma}_1^r},\dots,\sqrt{\widehat{\gamma}_k^r}\right)\mathbf{Y}(\theta_p^r), \\ \widehat{\boldsymbol{\eta}}(\theta_p^r) &= \operatorname{diag}\left(\sqrt{\gamma_1^r},\dots,\sqrt{\gamma_k^r}\right)\widehat{\mathbf{Y}}(\theta_p^r), \end{aligned} \tag{6.45}$$

are orthonormal eigenvectors satisfying

$$\boldsymbol{\eta}(\theta_p^r)^{\mathsf{T}}\boldsymbol{\eta}(\theta_j^r) = \widehat{\boldsymbol{\eta}}(\theta_p^r)^{\mathsf{T}}\widehat{\boldsymbol{\eta}}(\theta_j^r) = \delta_{pj}. \tag{6.46}$$

Then, (6.43) gives

$$\sum_{p=1}^{k} \left|dV_{2p-1,2p-1}\right| \leq \sum_{q=1}^{k}\sum_{\substack{l=1\\l\neq q}}^{k} \frac{2\theta_q^r\,|d\theta_q^r|}{|(\theta_q^r)^2-(\theta_l^r)^2|}\sum_{p=1}^{k}\left[\eta_p(\theta_l^r)^2+\sqrt{\frac{\xi_l^r}{\xi_q^r}}\,\left|\eta_p(\theta_l^r)\eta_p(\theta_q^r)\right|\right], \tag{6.47}$$

and, from (6.46) and the Cauchy-Schwartz inequality, we have

$$\sum_{p=1}^{k} \left|dV_{2p-1,2p-1}\right| \leq \sum_{q=1}^{k}\left|d\theta_q^r\right|\mathcal{F}(q), \tag{6.48}$$

where

$$\mathcal{F}(q)=\sum_{\substack{l=1\\l\neq q}}^{k}\left(1+\sqrt{\frac{\xi_l^r}{\xi_q^r}}\right)\frac{2\theta_q^r}{\left|\left(\theta_q^r\right)^2-\left(\theta_l^r\right)^2\right|}.$$

Now note that, for $r=1$, $\xi_l^1=\xi_l$ satisfies $\xi_l/\xi_q=O(1)$ for all $l,q=1,\dots,k$ [15] and that, as $l\to\infty$, $\xi_l=\xi_l^0+\Delta\xi_l=2+O(l^{-2})$. Then, surely, uniformly for $r\in[0,1]$, $\xi_l^r=\xi_l^0+r\,\Delta\xi_l$ satisfies $\xi_l^r/\xi_q^r=O(1)$, so we can write

$$\mathcal{F}(q)\leq C_1\sum_{\substack{l=1\\l\neq q}}^{k}\frac{2\theta_q^r}{\left|\left(\theta_q^r\right)^2-\left(\theta_l^r\right)^2\right|} \tag{6.49}$$

for a positive constant C_1 that is independent of k and r.

Next, we show that

$$\mathcal{F}(q)=O(\log q) \tag{6.50}$$

and, since by assumption $d\theta_q^r=\Delta\theta_q\,dr$ decays as $O(1/(q^\alpha\log q))$ for large q and some $\alpha>1$, we obtain

$$\sum_{p=1}^{k}|dV_{2p-1,2p-1}|\leq C_2|dr| \tag{6.51}$$

for yet another positive constant C_2 that is independent of k and r.

Let us then prove (6.50). Since all we care about is the order of magnitude of $\mathcal{F}(q)$, we recall the asymptotic behavior of the eigenvalues and write

$$\mathcal{F}(q)=O[\mathcal{F}^0(q)],$$

where

$$\mathcal{F}^0(q) = 2\sum_{\substack{l=1\\l\neq q}}^{k} \frac{2\theta_q^0}{\left|\left(\theta_q^0\right)^2 - \left(\theta_l^0\right)^2\right|} = O\left[\sum_{\substack{l=1\\l\neq q}}^{k} \frac{2q-1}{|(l-q)(l+q-1)|}\right].$$

Now, expand this upper bound for $\mathcal{F}^0(q)$ as

$$\mathcal{F}^0(q) = O\left[\sum_{l=1}^{q-1}\left(\frac{1}{q-l} + \frac{1}{l+q-1}\right) + \sum_{l=q+1}^{k}\left(\frac{1}{l-q} - \frac{1}{l+q-1}\right)\right]$$

and use that [13]

$$\sum_{m=1}^{j} \frac{1}{m} = O(\log j),$$

to obtain (6.50).

To complete the proof of Lemma 6.6, we show next that

$$\begin{aligned}\sum_{p=1}^{k}\left|dV_{2p,2p}\right| \leq &\sum_{q=1}^{k}\sum_{\substack{l=1\\l\neq q}}^{k}\left|d\theta_q^r\right| \frac{2\theta_q^r}{\left|\left(\theta_q^r\right)^2 - \left(\theta_l^r\right)^2\right|}\sum_{p=1}^{k}\widehat{\eta}_p(\theta_l^r)^2 \\ &+ \sum_{q=1}^{k}\left|d\theta_q^r\right|\sum_{p=1}^{k}\left|\widehat{\eta}_p\left(\theta_q^r\right)\right|\left|\widehat{a}_p\left(\theta_q^r\right)\right| \\ &+ \sum_{q=1}^{k}\frac{\left|d\theta_q^r\right|}{\theta_q^r}\sum_{p=1}^{k}\widehat{\eta}_p\left(\theta_q^r\right)^2 \leq C_3|dr|,\end{aligned} \tag{6.52}$$

where C_3 is a positive constant, independent of k and r, and where

$$\widehat{a}_p(\theta_q^r) = \sum_{\substack{l=1\\l\neq q}}^{k}\sqrt{\frac{\xi_l^r}{\xi_q^r}}\,\frac{2\theta_l^r}{\left(\theta_q^r\right)^2 - \left(\theta_l^r\right)^2}\,\widehat{\eta}_p\left(\theta_l^r\right). \tag{6.53}$$

The first term in the right-hand side of (6.52) is basically the same as (6.48), and it is bounded by $O(|dr|)$ uniformly in k and r. The third term in the right-hand side of (6.52) is

$$\sum_{q=1}^{k}\frac{\left|d\theta_q^r\right|}{\theta_q^r}\sum_{p=1}^{k}\widehat{\eta}_p\left(\theta_q^r\right)^2 = \sum_{q=1}^{k}\frac{\left|d\theta_q^r\right|}{\theta_q^r} = O(|dr|) \tag{6.54}$$

because of the assumed decay of $d\theta_q^r$. For the second term we use the Cauchy-Schwartz inequality and the identity

$$\begin{aligned}
&\sum_{p=1}^{k} a_p\big(\theta_q^r\big)^2 \\
&= \sum_{\substack{l=1\\ l\neq q}}^{k}\sum_{\substack{l'=1\\ l'\neq q}}^{k} \frac{\sqrt{\xi_l^r\xi_{l'}^r}}{\xi_q} \frac{4\theta_l^r\theta_{l'}^r}{\big[\big(\theta_q^r\big)^2-\big(\theta_l^r\big)^2\big]\big[\big(\theta_q^r\big)^2-(\theta_{l'}^r)^2\big]} \sum_{p=1}^{k}\widehat{\eta}_p\big(\theta_l^r\big)\eta_p\big(\theta_{l'}^r\big) \qquad (6.55)\\
&= \sum_{\substack{l=1\\ l\neq q}}^{k} \frac{\xi_l^r}{\xi_q^r}\frac{4\big(\theta_l^r\big)^2}{\big[\big(\theta_q^r\big)^2-\big(\theta_l^r\big)^2\big]^2} = \widetilde{\mathcal{F}}(q),
\end{aligned}$$

to obtain

$$\sum_{q=1}^{k}\big|d\theta_q^r\big|\sum_{p=1}^{k}\big|\widehat{\eta}_p\big(\theta_q^r\big)\big|\,\big|\widehat{a}_p\big(\theta_q^r\big)\big| \leq \sum_{q=1}^{k}\big|d\theta_q^r\big|\sqrt{\widetilde{\mathcal{F}}(q)}. \qquad (6.56)$$

Now we show that $\widetilde{\mathcal{F}}(q) = O(1)$ and, given our assumption of the asymptotic behavior of $d\theta_q^r$ for large q, we obtain the summability of the right-hand side in (6.55) and thus the desired bound (6.52). Proceeding as before, we have that

$$\widetilde{\mathcal{F}}(q) = O\left[\widetilde{\mathcal{F}}^0(q)\right],$$

where

$$\widetilde{\mathcal{F}}^0(q) = \sum_{\substack{l=1\\ l\neq q}}^{k}\frac{4(\theta_l^0)^2}{\big[\big(\theta_q^0\big)^2-\big(\theta_l^0\big)^2\big]^2} = O\left\{\sum_{\substack{l=1\\ l\neq q}}^{k}\left[\frac{1}{(q-l)^2}+\frac{1}{(q+l-1)^2}\right]\right\},$$

and since

$$\sum_{m=1}^{j}\frac{1}{m^2} = O(1) \quad \text{uniformly in } j,$$

$\widetilde{\mathcal{F}}(q) = O(1)$ [13]. Inequality (6.52) follows from (6.56). Finally, (6.51) and (6.52) give (6.44). ☐

Perturbation of the Weights

Assuming that only the weights are perturbed, we have from (6.35) that

$$E B^r\, dV - E\, dV\, B^r = \mathbf{0}, \quad \mathbf{e}_1^\top\, dV = (d\chi_1, d\chi_1, \ldots, d\chi_k)Z^{r\star}, \qquad (6.57)$$

where

$$\frac{d\chi_n^r}{\chi_n^r} = \frac{1}{2}\left(\frac{d\widehat{\gamma}_1^r}{\widehat{\gamma}_1^r}+\frac{d\xi_n^r}{\xi_n^r}\right) \quad \text{and} \quad \frac{d\widehat{\gamma}_1^r}{\widehat{\gamma}_1^r} = -\widehat{\gamma}_1^r\sum_{q=1}^{k} d\xi_q^r. \qquad (6.58)$$

The solution of (6.57) is

$$d\mathbf{V} = \sum_{p=1}^{k} \frac{d\chi_p^r}{\chi_p^r}\left[\boldsymbol{\zeta}\left(\theta_p^r\right)\boldsymbol{\zeta}\left(\theta_p^r\right)^\star + \boldsymbol{\zeta}\left(-\theta_p^r\right)\boldsymbol{\zeta}\left(-\theta_p^r\right)^\star\right], \tag{6.59}$$

and, using Lemma 6.3, definitions (6.45), and the orthogonality of the eigenvectors, we have

$$\begin{aligned} dV_{2p-1\,2p-1} &= \sum_{q=1}^{k}\left[-\frac{d\xi_q^r\,\widehat{\gamma}_1^r}{2}\sum_{l=1}^{k}\eta_p\left(\theta_l^r\right)^2 + \frac{d\xi_q^r}{2\xi_q^r}\,\eta_p\left(\theta_q^r\right)^2\right] \\ &= \sum_{q=1}^{k}\frac{d\xi_q^r}{2\xi_q^r}\left[-\xi_q^r\widehat{\gamma}_1^r + \eta_p\left(\theta_q^r\right)^2\right] \end{aligned} \tag{6.60}$$

and

$$\begin{aligned} dV_{2p\,2p} &= \sum_{q=1}^{k}\left[-\frac{d\xi_q^r\,\widehat{\gamma}_1^r}{2}\sum_{l=1}^{k}\widehat{\eta}_p\left(\theta_l^r\right)^2 + \frac{d\xi_q^r}{2\xi_q^r}\,\widehat{\eta}_p\left(\theta_q^r\right)^2\right] \\ &= \sum_{q=1}^{k}\frac{d\xi_q^r}{2\xi_q^r}\left[-\xi_q^r\widehat{\gamma}_1^r + \widehat{\eta}_p\left(\theta_q^r\right)^2\right], \end{aligned} \tag{6.61}$$

so that

$$dV_{2p2p} - dV_{2p-12p-1} = \sum_{q=1}^{k}\frac{d\xi_q^r}{2\xi_q^r}\left[\widehat{\eta}_p\left(\theta_q^r\right)^2 - \eta_p\left(\theta_q^r\right)^2\right] \tag{6.62}$$

and

$$dV_{2p+1\,2p+1} - dV_{2p\,2p} = \sum_{q=1}^{k}\frac{d\xi_q^r}{2\xi_q^r}\left[\eta_{p+1}\left(\theta_q^r\right)^2 - \widehat{\eta}_p\left(\theta_q^r\right)^2\right]. \tag{6.63}$$

Finally, recalling (6.46) and the asymptotic behavior (6.1) of the differentials $d\xi_q^r$ and summing the evident bounds for (6.62) and (6.63) over p, we obtain the following:

LEMMA 6.7 *There exists a positive constant C such that*

$$\sum_{j=1}^{2k-1}\left|dV_{j+1\,j+1} - dV_{jj}\right| \le C|dr| \tag{6.64}$$

uniformly with k and r.

PROOF: Lemma 6.5 follows from (6.40) and Lemmas 6.6 and 6.7. □

See also [27] for a similar perturbation analysis applied to tridiagonal symmetric matrices.

6.4 The Convergence Result: Proof of Theorem 6.1

Lemma 6.5 and (6.9) give (6.6), i.e., a uniform bound on the variation of function $\sigma^k(z)$, defined by (6.4). We also have from the identities[4]

$$\widehat{\gamma}_1 \sum_{p=1}^{k} \xi_p = 1, \qquad \widehat{h}_1^0 \sum_{p=1}^{k} \xi_p^0 = 1, \tag{6.65}$$

and the summability of $\Delta \xi_p$ that

$$\sigma_1 = \frac{\widehat{\gamma}_1}{\widehat{h}_1^0} = \frac{1}{1 + \widehat{h}_1^0 \sum_{p=1}^{k} \Delta \xi_p} = 1 + O(\widehat{h}_1^0) = 1 + O\left(\frac{1}{k}\right), \tag{6.66}$$

so $\sigma_1 \to \sigma(0) = 1$ as $k \to \infty$. But $\sigma^k(0) = \sigma_1$ and, since $\sigma^k(z)$ has uniformly bounded variation, $\sigma^k(z)$ remains uniformly bounded in $[0, 1]$.

PROOF: Assume for a proof by contradiction that $\sigma^k \not\to \sigma$ in $L^1[0, 1]$. Then there exist $\epsilon_1 > 0$ and a subsequence σ^{k_l} such that $\|\sigma^{k_l} - \sigma\|_{L^1[0,1]} \geq \epsilon_1$. By Helly's selection principle and by compactness of embedding of the space of functions of bounded total variation in $L^1([0, 1])$ [66, chap. 8, sec. 4; chap. 5, sec. 3], there exists a subsequence of σ^{k_l}, converging pointwise as well as in $L^1[0, 1]$, to limit $\widetilde{\sigma}(z)$. We again denote this subsequence by σ^{k_l} and note that its convergence in $L^1[0, 1]$ implies $M_{k_l} \to M^{\widetilde{\sigma}}$ by virtue of (2.3)–(2.4). Further, by Lemma 2.1, we have $F^{\sigma^{k_l}}(\lambda) \to F^{\widetilde{\sigma}}(\lambda)$. However, by construction, $F^{\sigma^k}(\lambda) \to F^{\sigma}(\lambda)$, and, by the uniqueness of solution of Problem 1, $\widetilde{\sigma} = \sigma$. We have now reached a contradiction. Since the pointwise convergence can be proved analogously, the proof of Theorem 6.1 is complete. □

6.5 Extension to General, Smooth Coefficients σ

For simplicity, we have considered above the case of coefficients $\sigma(z)$ with corresponding Schrödinger potential with mean $\overline{Q} = 0$. Here we extend the results to the general case $\overline{Q} \neq 0$. (We require $\overline{Q}$ to satisfy condition (5.6).)

As we discussed in Section 5, the spectral data corresponding to reference coefficient $\sigma^{\overline{Q}}(z)$, defined by (5.4), for constant potential $\overline{Q} \neq 0$, is given by (5.14) and (5.15), and, assuming that $\sigma(z)$ is sufficiently smooth, we have

$$\theta_n - \theta_n^{\overline{Q}} = O\left(\frac{1}{n^\alpha \log n}\right) \quad \text{and} \quad \xi_n - \xi_n^{\overline{Q}} = O\left(\frac{1}{n^\alpha}\right) \quad \text{for some } \alpha > 1 \text{ as } n \to \infty. \tag{6.67}$$

[4] The proof of (6.65) is identical to the proof of (5.18).

Using the same analysis that leads to (6.6), we get

$$\sum_{p=1}^{2k-1} \left| \log \frac{\beta_p}{\beta_p^{\overline{Q}}} \right| = \frac{1}{2} \sum_{p=1}^{k} \left| \log \frac{\widehat{\sigma}_p}{\widehat{\sigma}_p^{\overline{Q}}} - \log \frac{\sigma_p}{\sigma_p^{\overline{Q}}} \right| + \frac{1}{2} \sum_{p=1}^{k-1} \left| \log \frac{\widehat{\sigma}_p}{\widehat{\sigma}_p^{\overline{Q}}} - \log \frac{\sigma_{p+1}}{\sigma_{p+1}^{\overline{Q}}} \right| \leq C \tag{6.68}$$

uniformly in k. Then let us define function $\rho^k(z)$, the piecewise constant interpolation[5] of point values

$$\rho_j = \frac{\sigma_j}{\sigma_j^{\overline{Q}}} \quad \text{and} \quad \widehat{\rho}_j = \frac{\widehat{\sigma}_j}{\widehat{\sigma}_j^{\overline{Q}}}, \quad j = 1, \ldots, k. \tag{6.69}$$

By (6.66), $\sigma_1 \to \sigma(0) = 1$, and, by Theorem 5.1, $\sigma_1^{\overline{Q}} = 1$, so $\rho^k(0) \to 1$ as $k \to \infty$. But ρ^k is a function of bounded variation, so it remains uniformly bounded in [0, 1]. Then the L^1 and pointwise convergence of $\rho^k(z)$ to $\sigma(z)/\sigma^{\overline{Q}}(z)$ follows by the same arguments that we used in Section 6.4.

7 More General Measurement Sets and Optimal Grids

Here we show how imaging on optimal grids can be extended to more general measurement sets, e.g., sets (a) and (b) given in Section 2.1. Given a finite measurement set

$$\mathcal{D}_p(F^\sigma), \quad 1 \leq p \leq 2k, \tag{7.1}$$

where $\mathcal{D}_p$ are linear or nonlinear functionals of the impedance function, we reformulate the inverse problem as:

Problem 4. Find an approximation of $\sigma(z)$ that predicts measurements $\mathcal{D}_p(F^\sigma)$ for $1 \leq p \leq 2k$.

This can be done in a robust way, as explained below, if the data satisfy the following assumption:

Assumption 2. We suppose that:

(1) $\mathcal{D}_p(F^\sigma)$ is continuous with respect to the spectral data so that small perturbations of θ_p and ξ_p for $p = 1, \ldots, k$ result in small perturbations in the measurements.

(2) Conditions

$$\mathcal{D}_p(F^\sigma) = \mathcal{D}_p(F_k^\gamma), \quad p = 1, \ldots, 2k, \tag{7.2}$$

determine uniquely F_k^γ of the form (2.29) with positive residues ξ_p and distinct negative poles $-\theta_p^2$ for $1 \leq p \leq k$. Equivalently, they determine a discrete Stieltjes measure μ_k^γ given by (2.10).

[5] The definition is similar to (6.4).

(3) For all $\lambda \in \mathbb{C} \setminus (-\infty, 0)$,

$$\lim_{k \to \infty} F_k^\gamma(\lambda) = F^\sigma(\lambda). \tag{7.3}$$

All the measurement sets presented in Section 2.1 satisfy Assumption 2. The convergence rate in (7.3) depends on the data set. For example, the truncated measure (TM) measurement set gives a convergence rate of $O(1/k)$, as follows from Lemma 2.2 and the asymptotic formulae for θ_k and ξ_k [15]. Faster (exponential in k) convergence rates can be achieved with the (Padé) measurement set (a). This measurement set is most efficient for the numerical solution of the forward problem [10, 28, 29, 30, 47]. However, in this paper, we consider the TM measurement set, which, although it gives a slower rate of convergence of $F_k^\gamma(\lambda)$ to $F^\sigma(\lambda)$, is simpler to analyze in the context of inversion.

It follows from the uniqueness of the solution of Problem 3 that all measurement sets (7.1) satisfying Assumption 2 determine uniquely $M_k(x)$. The discrete inverse problem, in terms of M_k, for measurements other than the TM set is solved with a modified version of Algorithm 2 containing one extra step:

Algorithm 3. A two-stage algorithm of inversion for general measurement sets:

(1) From conditions (7.2), find $F_k^\gamma(\lambda)$ and therefore μ_k^γ. This step is trivial for the TM set.
(2) Solve Problem 3 using μ_k^γ as the entry data.

Numerous examples of different optimal grids are given in [10, 28, 29, 30, 47]. They all exhibit the refinement property (3.2), but the asymptotic refinement rates vary significantly from one measurement set to another. In other words, the distribution of the grid points in the interior of the domain depends strongly on the measurement set $\mathcal{D}_p(F^\sigma)$, as illustrated in Figure 7.1. However, the dependence of the grid on σ is much weaker, as we have seen in this paper, and this plays a key role in inversion. The imaging algorithm for general measurements is:

Algorithm 4. To solve the discrete inverse problem with data (7.1) satisfying Assumption 2, proceed as follows:

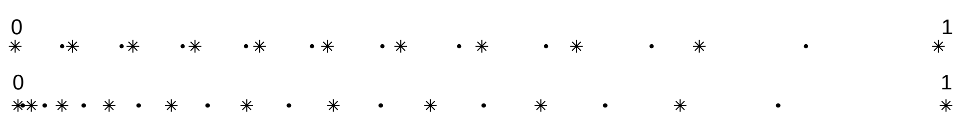

FIGURE 7.1. Examples of optimal grids in the unit interval, calculated with the TM measurement set (top figure) and with a simple Padé approximant at $\lambda = 0$ (bottom figure), respectively, for $k = 10$. The stars are the primary points z_i and the dots are the dual points $\widehat{z}_i$. The coefficient is $\sigma^0(z) = 1$.

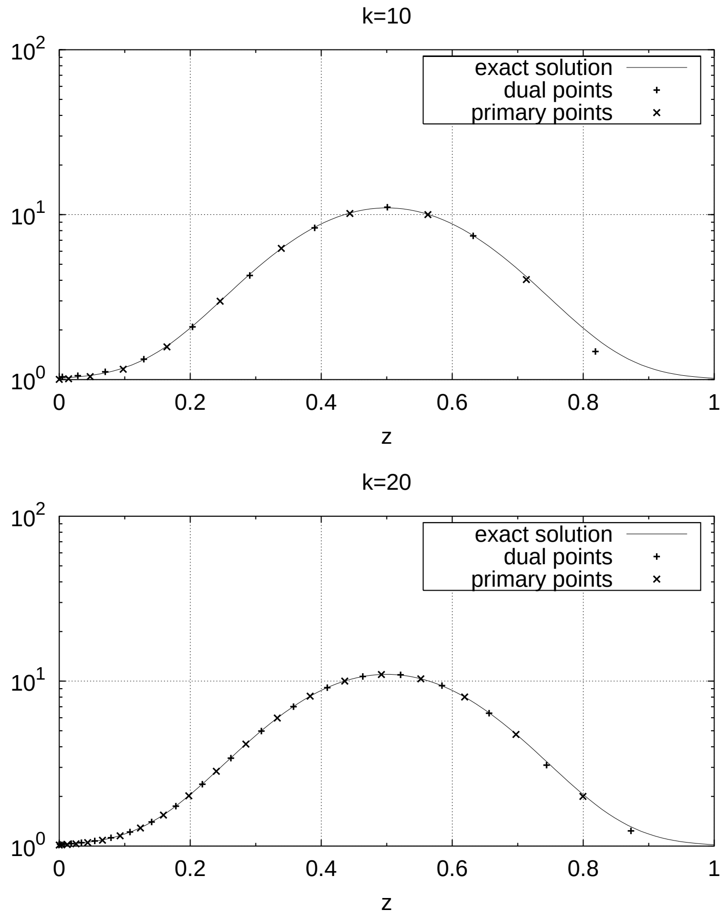

FIGURE 7.2. Inversion for the Gaussian bell

$$\sigma(z) = 1 + 10\exp[-25(x - 0.5)^2]$$

on the optimal grids with 10 and 20 nodes, corresponding to the simple Padé approximant at 0.

(1) Calculate a grid $\mathcal{G}_k^0$ with mesh sizes $h_j^0 = z_{j+1}^0 - z_j^0$ and $\widehat{h}_j^0 = \widehat{z}_j^0 - \widehat{z}_{j-1}^0$ for $1 \le j \le k$ by solving Problem 3 with data $\mathcal{D}_p(F^{\sigma^0}) = \mathcal{D}_p(F_k^{\gamma^0})$, $p = 1, \ldots, k$, where $\sigma^0 = 1$, $h_j^0 = \gamma_j^0$, and $\widehat{h}_j^0 = \widehat{\gamma}_j^0$ for $j = 1, \ldots, k$.

(2) Find γ_j and $\widehat{\gamma}_j$ for $1 \le j \le k$, using data (7.1) and matching conditions (7.2) (recall Problem 3).

(3) Obtain the solution as $\sigma_j = \widehat{\gamma}_j / \widehat{h}_j^0$ and $\widehat{\sigma}_j = h_j^0 / \gamma_j$, $1 \le j \le k$.

Proposition 4.2 remains valid for Algorithm 4, and as we illustrate in Figure 7.2, the numerical experiments using Algorithm 4 with Padé data show very good convergence. We hope that the convergence proof presented in this paper can be modified, with some effort, for the measurement sets (a) and (b) in Section 2.1.

8 Conclusions

In this paper, we have proven that finite difference solutions of inverse spectral problems on optimal grids have uniformly bounded total variation and, as such, that they converge pointwise and in L^1 to the true continuum limit. Thus, we have established the link between discrete inversion, such as inverse spectral problems for Jacobi matrices [18] or resistor network tomography [22, 45, 48] and continuous inversion.

The multidimensional problem remains open, but since all the resolution studies [16, 24, 25, 49, 73] show that the solution is most sensitive to the discretization in depth and since our results indicate a weak dependence of the grids on σ, we expect that our results will be useful in higher dimensions as well. The extension to two-dimensional problems seems especially promising due to recent results for planar graphs [22, 46, 48] and the ∂-bar approach [53, 65, 74] that can be considered as two-dimensional counterparts of the Stieltjes and Gel′fand-Levitan methods, respectively.

As a by-product of our analysis, we have obtained novel, explicit perturbation formulae for Lanczos recursions arising in inverse spectral problems for Jacobi matrices [18].

Finally, we have obtained a partial answer to a crucial question that arises in any practical inversion scheme: *How to parametrize properly the unknown $\sigma(z)$ that we wish to reconstruct*? Take for a moment the problem of electrical impedance tomography [3, 4, 9, 17, 26, 50, 79], where σ is the unknown electrical conductivity that we wish to find in the interior of some domain, given simultaneous measurements of electric currents and voltages at the boundary. Although, in theory, an isotropic σ can be recovered uniquely from the Neumann-to-Dirichlet map [12, 26, 55, 65, 77, 79], the problem is severely ill-posed [3, 4, 50, 60], and reconstruction methods require some form of regularization in order to converge to a solution [33, 52, 64, 69].

However, regularization often relies on prior assumptions on $\sigma(z)$, and it can create undesired artifacts in the resulting images. It is therefore desirable to avoid artificial penalties that we impose on the solution for the sake of achieving convergence by means of proper parametrizations (discretizations) of the unknown σ. This natural idea has been considered in the distinguishability studies [16, 24, 25, 49, 73], which rely on the presumably known noise level in the data in order to characterize the distinguishable perturbations in σ from an a priori guess profile σ^0. A complete characterization of the distinguishable perturbations is not known, in general, but there exist distinguishability bounds [24, 25, 41, 49, 73] which show that the resolution limits decrease dramatically deep down in the interior of the domain.

The critical issue is therefore how to parametrize the unknown profile, in depth, as we move away from the boundary. Adaptive discretizations of σ on distinguishability grids have been used in [17, 75] (and the references within), and they have helped to improve the quality of the reconstructed images. However, distinguishability grids are constructed with a linearization, heuristic approach, and rigorous answers to the question of optimal parametrization of σ have yet to be found in general, although there are some new, promising results in this direction [59, 58] that are reminiscent of stability studies of the electrical impedance tomography problem [2, 60].

In this paper, we have shown that optimal parametrizations of σ can be found and justified rigorously in the finite difference setting, at least in the case of layered media, as is commonly assumed in geophysical exploration. The practically important conclusion is that the parametrization depends strongly on the measurement method (the data) but is rather insensitive to regular perturbations of σ.

Appendix A: The TM Optimal Grid for the Constant Coefficient $\sigma^0 = 1$

For simplicity of notation, let us denote by H_j, $j = 1, \ldots, 2k$, all the grid spacings where $H_{2p} = h_p^0$ and $H_{2p-1} = \widehat{h}_p^0$. The eigenvalues of B^0 are $\pm i\theta_j^0$, where $\theta_j^0 = \pi(j - \frac{1}{2})$ and the weights are 2 for $j = 1, \ldots, k$. We extract from [34, 4.1] the expression

$$(\beta_j^0)^2 = \frac{1 - \left(\frac{j}{N}\right)^2}{4\left(4 - \frac{1}{j^2}\right)} \cdot (\pi N)^2, \quad 1 \le j \le N - 1. \tag{A.1}$$

Owing to the equality

$$\beta_j^0 = \frac{1}{\sqrt{H_j H_{j+1}}}, \quad 1 \le j \le N - 1,$$

we have the recurrence

$$H_1 = \frac{1}{\sum_{p=1}^k \xi_p^0} = \frac{1}{N}, \quad H_{j+1} = \frac{1}{H_j (\beta_j^0)^2}, \quad 1 \le j \le N - 1,$$

which gives

$$H_j = \begin{cases} \left(\frac{\beta_{j-2}^0 \beta_{j-4}^0 \cdots \beta_1^0}{\beta_{j-1}^0 \beta_{j-3}^0 \cdots \beta_2^0}\right)^2 \cdot H_1 & \text{if } j \equiv 1 \pmod 2, \\ \left(\frac{\beta_{j-2}^0 \beta_{j-4}^0 \cdots \beta_2^0}{\beta_{j-1}^0 \beta_{j-3}^0 \cdots \beta_3^0}\right)^2 \cdot \frac{1}{(\beta_1^0)^2 H_1} & \text{if } j \equiv 0 \pmod 2. \end{cases}$$

Noting that, in view of (A.1),

$$\left(\frac{\beta_{j-1}^0}{\beta_j^0}\right)^2 = a_j b_{j,N}, \quad 2 \le j \le N - 1,$$

with

$$a_j = \frac{4 - \frac{1}{j^2}}{4 - \frac{1}{(j-1)^2}}, \quad j \geq 2, \qquad b_{j,N} = \frac{1 - (\frac{j-1}{N})^2}{1 - (\frac{j}{N})^2}, \quad 2 \leq j \leq N-1,$$

and that

$$\frac{1}{(\beta_1^0)^2 H_1} = \frac{12N}{\pi^2(N^2-1)},$$

we have

$$H_j = A_j B_j, \quad 1 \leq j \leq N, \tag{A.2}$$

with

$$A_j = \begin{cases} \displaystyle\prod_{\substack{2 \leq l \leq j-1 \\ l \equiv 0 \pmod 2}} a_l, & j \equiv 1 \pmod 2, \\ \displaystyle\frac{12}{\pi^2} \prod_{\substack{3 \leq l \leq j-1 \\ l \equiv 1 \pmod 2}} a_l, & j \equiv 0 \pmod 2, \end{cases} \tag{A.3}$$

and

$$B_j = \begin{cases} \displaystyle\frac{1}{N} \prod_{\substack{2 \leq l \leq j-1 \\ l \equiv 0 \pmod 2}} b_{l,N}, & j \equiv 1 \pmod 2, \\ \displaystyle\frac{N}{N^2-1} \prod_{\substack{3 \leq l \leq j-1 \\ l \equiv 1 \pmod 2}} b_{l,N}, & j \equiv 0 \pmod 2 \end{cases} \tag{A.4}$$

(empty products are assumed to be 1 according to the definition).

In what follows, Γ denotes the Γ-function (see [1, chap. 6]; $\Gamma(z) = (z-1)!$) and !! denotes the double factorial

$$j!! = \prod_{\substack{1 \leq i \leq j \\ i \equiv j \pmod 2}} i.$$

LEMMA A.1 *We have the representation*

$$B_j = \frac{1}{2} \cdot \frac{\Gamma\left(\frac{N+j}{2}\right)\Gamma\left(\frac{N-j+1}{2}\right)}{\Gamma\left(\frac{N-j+2}{2}\right)\Gamma\left(\frac{N+j+1}{2}\right)}, \quad 1 \leq j \leq N. \tag{A.5}$$

PROOF: For an even $j \geq 4$, using (A.4) and

$$(2j)!! = 2^j j! \quad \text{and} \quad (2j-1)!! = \frac{2^j \Gamma\left(j + \frac{1}{2}\right)}{\sqrt{\pi}} \tag{A.6}$$

(see [38, 8.339.2]), we obtain

$$B_j = \frac{N}{N^2-1} \prod_{3 \leq j \leq j-1,\ j \equiv 1(2)} \frac{(N-j+1)(N+j-1)}{(N-j)(N+j)}$$

$$
\begin{aligned}
&= \frac{N}{N^2-1} \\
&\quad \times \frac{(N-j+2)(N-j+4)\cdots(N-2)\times(N+2)(N+4)\cdots(N+j-2)}{(N-j+1)(N-j+3)\cdots(N-3)\times(N+3)(N+5)\cdots(N+j-1)} \\
&= \frac{(N+j-2)!!(N-j-1)!!}{(N-j)!!(N+j-1)!!} \\
&= \frac{2^{\frac{N+j-2}{2}}\cdot\frac{N+j-2}{2}!}{2^{\frac{N-j}{2}}\cdot\frac{N-j}{2}!}\cdot\frac{2^{\frac{N-j}{2}}\Gamma\left(\frac{N-j+1}{2}\right)\pi^{-\frac{1}{2}}}{2^{\frac{N+j}{2}}\Gamma\left(\frac{N+j+1}{2}\right)\pi^{-\frac{1}{2}}},
\end{aligned}
$$

which coincides with the right-hand side of (A.5). For an odd $j \geq 3$, using (A.4) and (A.6), we deduce

$$
\begin{aligned}
B_j &= \frac{1}{N}\prod_{2\leq j\leq j-1,\ j\equiv 0(2)}\frac{(N-j+1)(N+j-1)}{(N-j)(N+j)} \\
&= \frac{1}{N} \\
&\quad\times\frac{(N-j+2)(N-j+4)\cdots(N-1)\times(N+1)(N+3)\cdots(N+j-2)}{(N-j+1)(N-j+3)\cdots(N-2)\times(N+2)(N+4)\cdots(N+j-1)} \\
&= \frac{(N+j-2)!!(N-j-1)!!}{(N-j)!!(N+j-1)!!} \\
&= \frac{2^{\frac{N+j-1}{2}}\Gamma\left(\frac{N+j}{2}\right)\pi^{-\frac{1}{2}}}{2^{\frac{N-j+1}{2}}\Gamma\left(\frac{N-j+2}{2}\right)\pi^{-\frac{1}{2}}}\cdot\frac{2^{\frac{N-j-1}{2}}\cdot\frac{N-j-1}{2}!}{2^{\frac{N+j-1}{2}}\cdot\frac{N+j-1}{2}!},
\end{aligned}
$$

which again equals the right-hand side of (A.5). The partial cases of (A.5), with $j = 1, 2$, are verified directly with the use of identity

$$\Gamma(z+1) = z\Gamma(z). \tag{A.7}$$

□

LEMMA A.2 *The representation*

$$A_j = \frac{(2j-1)2^{2j-2}}{\pi^2}\cdot\frac{\Gamma\left(\frac{j}{2}\right)^4}{\Gamma(j)^2}, \quad j \geq 1, \tag{A.8}$$

holds.

PROOF: We shall exploit (A.6) and the equality

$$a_j = \frac{(j-1)^2(2j+1)}{j^2(2j-3)}.$$

For an even $j \geq 4$, we have

$$A_j = \frac{12}{\pi^2} \prod_{\substack{3\le j\le j-1\\ j\equiv 1(2)}} a_j = \frac{12}{\pi^2} \prod_{\substack{3\le j\le j-1\\ j\equiv 1(2)}} \frac{(j-1)^2(2j+1)}{j^2(2j-3)} =$$

$$\frac{12}{\pi^2}\left[\frac{(j-2)!!}{(j-1)!!}\right]^2 \frac{2j-1}{3} = \frac{4(2j-1)}{\pi^2}\left(\frac{2^{\frac{j-2}{2}}\cdot\frac{j-2}{2}!}{\frac{(j-1)!}{2^{\frac{j-2}{2}}\cdot\frac{j-2}{2}!}}\right)^2 =$$

$$\frac{4(2j-1)2^{2j-4}}{\pi^2}\frac{\left(\frac{j-2}{2}!\right)^4}{[(j-1)!]^2},$$

which gives the right-hand side of (A.8). For an odd $j \geq 3$, using

$$\Gamma(z)\Gamma\left(z+\frac{1}{2}\right) = \frac{2\sqrt{\pi}\,\Gamma(2z)}{2^{2z}},$$

(see [1, (6.1.18)]), we derive

$$A_j = \prod_{\substack{2\le j\le j-1\\ j\equiv 0(2)}} a_j = \prod_{\substack{2\le j\le j-1\\ j\equiv 0(2)}} \frac{(j-1)^2(2j+1)}{j^2(2j-3)} =$$

$$\left[\frac{(j-2)!!}{(j-1)!!}\right]^2(2j-1) = \frac{(2j-1)\left[\frac{(j-2)!}{2^{\frac{j-3}{2}}\cdot\frac{j-3}{2}!}\right]^2}{\left(2^{\frac{j-1}{2}}\cdot\frac{j-1}{2}!\right)^2} = \frac{2j-1}{2^{2j-4}}\cdot\left[\frac{(j-2)!}{\frac{j-3}{2}!\,\frac{j-1}{2}!}\right]^2 =$$

$$\frac{2j-1}{2^{2j-4}}\cdot\left[\frac{\Gamma(j-1)}{\Gamma\left(\frac{j-1}{2}\right)\Gamma\left(\frac{j+1}{2}\right)}\right]^2 = \frac{2j-1}{2^{2j-4}}\cdot\left[\frac{\Gamma(j-1)}{\frac{2\sqrt{\pi}\,\Gamma(j-1)}{2^{j-1}\Gamma\left(\frac{j}{2}\right)}\cdot\frac{2\sqrt{\pi}\,\Gamma(j)}{2^{j}\Gamma\left(\frac{j}{2}\right)}}\right]^2.$$

This is also identical to the right-hand side of (A.8).

Cases $j = 1, 2$ are checked separately. For $j = 1$, we use that ([1, (6.1.8)])

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}. \tag{A.9}$$

□

In what follows, we use Stirling's formula

$$\Gamma(z) \sim e^{-z}z^{z-\frac{1}{2}}\sqrt{2\pi}\left(1+\frac{1}{12z}+\frac{1}{288z^2}-\frac{139}{51840z^3}-\frac{571}{2488320z^4}+\cdots\right) \tag{A.10}$$

(see [1, (6.1.37)]) and the formula

$$\frac{\Gamma\left(z+\frac{1}{2}\right)}{\Gamma(z)} \sim \sqrt{z}\left(1-\frac{1}{8z}+\frac{1}{128z^2}+\frac{5}{1024z^3}-\frac{21}{32768z^4}+\cdots\right) \tag{A.11}$$

[39, answer to problem 9.60]. It is shown in [38, (8.327)] that for a real and positive z, the remainder in the series in (A.10) is less than twice the first term thrown away. Since (A.11) may be deduced from (A.10), an analogous estimate is valid for (A.11).

PROPOSITION A.3 *Steps H_j satisfy the asymptotic relation*

$$\begin{aligned} H_j &= \frac{\frac{4}{\pi} + O\left[(N-j)^{-1} + j^{-2}\right]}{\sqrt{N^2 - j^2}}, \quad 1 \le j \le N-1, \\ H_N &= \frac{\frac{2}{\sqrt{\pi}} + O\left(N^{-1}\right)}{\sqrt{N}}. \end{aligned} \tag{A.12}$$

PROOF: Because of (A.2), we can obtain (A.12) by considering separately the asymptotic behavior of A_j and B_j.

As $j \to \infty$, Stirling's formula (A.10) applied to (A.8) implies

$$A_j \sim \frac{j 2^{2j-1}}{\pi^2} \cdot \frac{\left[\sqrt{2\pi}\sqrt{\frac{2}{j}}\left(\frac{j}{2}\right)^{\frac{j}{2}} e^{-\frac{j}{2}}\right]^4}{\left(\sqrt{2\pi}\,\frac{1}{\sqrt{j}}\, j^j e^{-j}\right)^2} = \frac{4}{\pi}.$$

Since

$$a_j = 1 + \frac{2j-1}{4j^2(j-1)^2 - j^2} = 1 + O(j^{-3}),$$

we have

$$A_j = \frac{4}{\pi} + O(j^{-2}) \quad \text{as } j \to \infty. \tag{A.13}$$

It follows from (A.5) and (A.11), for $j = 1, \ldots, N-1$, that

$$\begin{aligned} B_j &= \frac{1}{N-j} \cdot \frac{\Gamma\left(\frac{N+j}{2}\right)\Gamma\left(\frac{N-j+1}{2}\right)}{\Gamma\left(\frac{N+j+1}{2}\right)\Gamma\left(\frac{N-j}{2}\right)} \\ &= \frac{1}{N-j}\left(\frac{N+j}{2}\right)^{-\frac{1}{2}}\left[1 + O\left(\frac{1}{N+j}\right)\right]\left(\frac{N-j}{2}\right)^{\frac{1}{2}}\left[1 + O\left(\frac{1}{N-j}\right)\right] \\ &= \frac{1 + O\left(\frac{1}{N-j}\right)}{\sqrt{N^2 - j^2}}. \end{aligned} \tag{A.14}$$

Finally, for $j = N$, using (A.5), (A.9), and (A.11), we have

$$B_N = \frac{1}{2} \cdot \frac{\Gamma(N)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(N+\frac{1}{2}\right)\Gamma(1)} = \frac{\sqrt{\pi}}{2\sqrt{N}}\left[1 + O\left(N^{-1}\right)\right]. \tag{A.15}$$

Now, (A.12) is clear in view of (A.13), (A.14), and (A.15). □

COROLLARY A.4 *Given* $0 < u < v < 1$, *in the interval family* $u\sqrt{N} \le j \le vN$, *we have*

$$H_j = \frac{\frac{4}{\pi} + O\left(N^{-1}\right)}{\sqrt{N^2 - j^2}}$$

uniformly in j *as* $N \to +\infty$.

PROPOSITION A.5 *Steps* H_j *form a monotonically increasing sequence,*

$$H_1 < H_2 < \cdots < H_{N-1} < H_N.$$

PROOF: Because of (A.2), it is sufficient to demonstrate that sequences A_j and B_j are monotonically increasing.

First, we have

$$\begin{aligned}
\frac{B_{j+1}}{B_j} &= \frac{\Gamma\left(\frac{N+j+1}{2}\right)\Gamma\left(\frac{N-j}{2}\right)}{\Gamma\left(\frac{N+j+2}{2}\right)\Gamma\left(\frac{N-j+1}{2}\right)} \Bigg/ \frac{\Gamma\left(\frac{N+j}{2}\right)\Gamma\left(\frac{N-j+1}{2}\right)}{\Gamma\left(\frac{N+j+1}{2}\right)\Gamma\left(\frac{N-j+2}{2}\right)} \\
&= \frac{\Gamma\left(\frac{N+j+1}{2}\right)^2}{\Gamma\left(\frac{N+j+2}{2}\right)\Gamma\left(\frac{N+j}{2}\right)} \cdot \frac{\Gamma\left(\frac{N-j}{2}\right)\Gamma\left(\frac{N-j+2}{2}\right)}{\Gamma\left(\frac{N-j+1}{2}\right)^2} \\
&= \prod_{j=0}^{\infty} \frac{1 - \frac{1}{(N+j+1+2j)^2}}{1 - \frac{1}{(N-j+1+2j)^2}} > 1,
\end{aligned}$$

where we used the infinite product decomposition [38, 8.325.1]

$$\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\gamma)\Gamma(\beta-\gamma)} = \prod_{j=0}^{+\infty}\left[\left(1 + \frac{\gamma}{\alpha+j}\right)\left(1 - \frac{\gamma}{\beta+j}\right)\right],$$

with $\alpha = \beta$ and $\gamma = \frac{1}{2}$.

Second, (A.8) and (A.7) give

$$\begin{aligned}
\frac{A_{j+1}}{A_j} = \frac{(2j+1)4^{j+1}\frac{\Gamma\left(\frac{j+1}{2}\right)^4}{\Gamma(j+1)^2}}{(2j-1)4^j\frac{\Gamma\left(\frac{j}{2}\right)^4}{\Gamma(j)^2}} &= 4\frac{2j+1}{2j-1} \cdot \frac{\Gamma\left(\frac{j+1}{2}\right)^4}{\Gamma\left(\frac{j}{2}\right)^4} \cdot \frac{\Gamma(j)^2}{\Gamma(j+1)^2} \\
&= \frac{4(2j+1)}{j^2(2j-1)} \cdot \left[\frac{\Gamma\left(\frac{j+1}{2}\right)}{\Gamma\left(\frac{j}{2}\right)}\right]^4.
\end{aligned}$$

Then, using (A.11) and manipulating power series in $1/j$ gives

$$\frac{A_{j+1}}{A_j} = \frac{2j+1}{2j-1}\left[1 - \frac{1}{4j} + \frac{1}{32j^2} + \frac{5}{128j^3} + O\left(j^{-4}\right)\right]^4$$
$$= 1 + \frac{1}{4j^3} + O(j^{-4}),$$

which is greater than 1 for j exceeding some constant. For smaller values of j, that $A_{j+1}/A_j > 1$ follows by direct computation. □

Appendix B: Proof of Lemma 6.3

First, we prove that the two first and the two last components of eigenvectors $\boldsymbol{\zeta}$ do not vanish. Writing explicitly the equation $B\boldsymbol{\zeta} = i\theta\boldsymbol{\zeta}$, we have

$$\begin{aligned} \beta_1\zeta_2 &= i\theta\zeta_1, \\ -\beta_1\zeta_1 + \beta_2\zeta_3 &= i\theta\zeta_2, \\ &\vdots \\ -\beta_{2k-1}\zeta_{2k-1} &= i\theta\zeta_{2k}. \end{aligned} \tag{B.1}$$

Note that $\theta \neq 0$; otherwise $\boldsymbol{\zeta} = \mathbf{0}$. Now, suppose that $\zeta_p = 0$ for at least one of the indices $p = 1, 2, 2k-1$, or $2k$. Since $\beta_j \neq 0$ for all $1 \leq j \leq 2k-1$, we obtain from (B.1) that $\boldsymbol{\zeta} = \mathbf{0}$, which is a contradiction.

Next, let us denote by

$$\boldsymbol{\eta} = (\zeta_1, \zeta_3, \ldots, \zeta_{2k-1})^\mathsf{T} \quad \text{and} \quad \widehat{\boldsymbol{\eta}} = (\zeta_2, \zeta_4, \ldots, \zeta_{2k})^\mathsf{T} \tag{B.2}$$

the vectors of odd and even components in eigenvector (6.17), respectively. By direct calculation, we have

$$B^2\boldsymbol{\zeta} = -\theta^2\boldsymbol{\zeta} = \left((\mathcal{T}\boldsymbol{\eta})_1, (\widehat{\mathcal{T}}\widehat{\boldsymbol{\eta}})_1, \ldots, (\mathcal{T}\boldsymbol{\eta})_k, (\widehat{\mathcal{T}}\widehat{\boldsymbol{\eta}})_k\right)^\mathsf{T}, \tag{B.3}$$

where

$$\mathcal{T} = \operatorname{diag}\left(\widehat{\gamma}_1^{1/2}, \ldots, \widehat{\gamma}_k^{1/2}\right)\Gamma \operatorname{diag}\left(\widehat{\gamma}_1^{-1/2}, \ldots, \widehat{\gamma}_k^{-1/2}\right) \tag{B.4}$$

is a symmetric, negative definite, tridiagonal matrix, as explained in Section 2.1, and similarly,

$$\widehat{\mathcal{T}} = \operatorname{diag}\left(\gamma_1^{1/2}, \ldots, \gamma_k^{1/2}\right)\widehat{\Gamma} \operatorname{diag}\left(\gamma_1^{-1/2}, \ldots, \gamma_k^{-1/2}\right) \tag{B.5}$$

with

$$\widehat{\Gamma}_{ij} = \begin{cases} -\frac{1}{\gamma_i}\left(\frac{1}{\widehat{\gamma}_i} + \frac{1}{\widehat{\gamma}_{i+1}}\right)\delta_{ij} + \frac{1}{\gamma_i\widehat{\gamma}_i}\delta_{i-1j} + \frac{1}{\gamma_i\widehat{\gamma}_{i+1}}\delta_{i+1j}, & 1 \leq i < k,\ 1 \leq j \leq k, \\ -\frac{1}{\gamma_k\widehat{\gamma}_k}\delta_{jk} + \frac{1}{\gamma_k\widehat{\gamma}_k}\delta_{jk-1}, & i = k,\ 1 \leq j \leq k, \end{cases} \tag{B.6}$$

is the matrix corresponding to the discretization of the problem dual to (1.1), with the Dirichlet boundary condition at $z = 0$ and the Neumann boundary condition at $z = 1$, respectively. Then, using equation (B.3), we conclude that $\boldsymbol{\eta}$ and $\widehat{\boldsymbol{\eta}}$ are eigenvectors of $\mathcal{T}$ and $\widehat{\mathcal{T}}$, respectively, for an eigenvalue $-\theta^2$. Since $\boldsymbol{\eta}$ and $\widehat{\boldsymbol{\eta}}$ are orthonormal, we easily obtain that (6.19) and (6.21) hold. Finally, equation (6.20) is verified by substitution in the dual eigenvalue problem for the matrix $\widehat{\Gamma}$.

Appendix C: Derivation of Solutions (6.43)

The unique solvability of (6.42) is easily established as follows: Let $\mathbf{v}_j^{\mathsf{T}}$ for $j = 1, \ldots, 2k$ be the rows of matrix dV that we wish to find. Clearly, $\mathbf{v}_1 = \mathbf{0}$. Then, writing equations (6.42) row by row and using that $\beta_j^r > 0$ for all $j = 1, \ldots, 2k-1$ allows us to determine uniquely all the rows of dV.

Next, we decompose the solution of (6.42) as

$$dV = dV_0 + dV_1 + dV_2, \tag{C.1}$$

where the matrices dV_0, dV_1, and dV_2 satisfy

$$B^r dV_0 - dV_0\, B^r = i\, Z^r d\Theta\, Z^{r\star} + i\,\mathbf{e}_j \mathbf{b}^\star, \tag{C.2}$$

$$\boldsymbol{\zeta}\left(\theta_p^r\right)^\star dV_0\, \boldsymbol{\zeta}\left(\theta_p^r\right) = \boldsymbol{\zeta}\left(-\theta_p^r\right)^\star dV_0\, \boldsymbol{\zeta}\left(-\theta_p^r\right) = 0 \quad \text{for } p = 1, \ldots, k, \tag{C.3}$$

$$E B^r dV_1 - E\, dV_1 B^r = 0, \quad \mathbf{e}_1^{\mathsf{T}} dV_1 = -\mathbf{e}_1^{\mathsf{T}} dV_0, \tag{C.4}$$

and

$$E B^r dV_2 - E\, dV_2\, B^r = -i\,\mathbf{e}_j \mathbf{b}^\star, \quad \mathbf{e}_1^{\mathsf{T}}\, dV_2 = \mathbf{0}^{\mathsf{T}}, \tag{C.5}$$

respectively, for a fixed index j satisfying $1 \le j \le 2k$ and a vector

$$\mathbf{b} = \sum_{p=1}^{k} \left[C_p^+ \boldsymbol{\zeta}\left(\theta_p^r\right) + C_p^- \boldsymbol{\zeta}\left(-\theta_p^r\right) \right] \tag{C.6}$$

to be determined. It follows easily from (C.5) that the first j rows of dV_2 are identically zero, so we calculate explicitly just $(dV_0)_{jj} + (dV_1)_{jj}$.

To find dV_0, we multiply (C.2) to the left and right by $Z^{r\star}$ and Z^r, respectively, and, since $B^r = i\, Z^r\, \Theta^r\, Z^{r\star}$, we have

$$\Theta^r Z^{r\star} dV_0\, Z^r - Z^{r\star} dV_0\, Z^r\, \Theta^r = d\Theta + Z^{r\star} \mathbf{e}_j \mathbf{b}^\star Z^r. \tag{C.7}$$

Clearly, the diagonal entries in the left-hand side of (C.7) vanish so that

$$(d\Theta)_{nn} + (Z^{r\star} \mathbf{e}_j \mathbf{b}^\star Z^r)_{nn} = 0 \quad \text{for } n = 1, \ldots, 2k, \tag{C.8}$$

and, using (C.6), we find that

$$C_p^+ = -\frac{d\theta_p^r}{\zeta_j\left(\theta_p^r\right)}, \quad C_p^- = \frac{d\theta_p^r}{\zeta_j(-\theta_p^r)}. \tag{C.9}$$

Next, we substitute (C.9) in (C.6) and rewrite (C.7) as

$$\Theta^r Z^{r\star} dV_0\, Z^r - Z^{r\star} dV_0\, Z^r \Theta^r = d\Theta - Z^{r\star}\mathbf{e}_j \sum_{p=1}^{k} d\theta_p^r \left[\frac{\boldsymbol{\zeta}\left(\theta_p^r\right)^\star}{\overline{\zeta_j\left(\theta_p^r\right)}} - \frac{\boldsymbol{\zeta}\left(-\theta_p^r\right)^\star}{\overline{\zeta_j\left(-\theta_p^r\right)}} \right] Z^r. \tag{C.10}$$

In light of condition (C.3), one has that

$$\begin{aligned} dV_0 = &\sum_{q=1}^{k} \sum_{\substack{l=1\\ l\neq q}}^{k} \left[c_{lq}^{++} \boldsymbol{\zeta}\left(\theta_l^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star + c_{lq}^{--} \boldsymbol{\zeta}\left(-\theta_l^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \right] \\ &+ \sum_{q=1}^{k} \sum_{l=1}^{k} \left[c_{lq}^{+-} \boldsymbol{\zeta}\left(\theta_l^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star + c_{lq}^{-+} \boldsymbol{\zeta}\left(-\theta_l^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \right], \end{aligned} \tag{C.11}$$

where the coefficients

$$c_{lq}^{\pm\pm} = \boldsymbol{\zeta}\left(\pm\theta_l^r\right)^\star dV_0\, \boldsymbol{\zeta}\left(\pm\theta_q^r\right) \tag{C.12}$$

are obtained from (C.10) as follows: To get c_{lq}^{++}, multiply (C.10) to the left and right by $\mathbf{e}_{2l-1}^{\mathsf{T}}$ and $\mathbf{e}_{2q-1}$, respectively, and obtain

$$c_{lq}^{++} = \boldsymbol{\zeta}\left(\theta_l^r\right)^\star dV_0\, \boldsymbol{\zeta}\left(\theta_q^r\right) = \frac{d\theta_q^r}{\theta_q^r - \theta_l^r} \overline{\left(\frac{\zeta_j\left(\theta_l^r\right)}{\zeta_j\left(\theta_q^r\right)} \right)}. \tag{C.13}$$

Similarly, we find all the other coefficients in (C.12) and (C.11), which gives

$$\begin{aligned} dV_0 = &\sum_{q=1}^{k} \sum_{\substack{l=1\\ l\neq q}}^{k} \frac{d\theta_q^r}{\theta_q^r - \theta_l^r} \left[\overline{\left(\frac{\zeta_j\left(\theta_l^r\right)}{\zeta_j\left(\theta_q^r\right)} \right)} \boldsymbol{\zeta}\left(\theta_l^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \right. \\ &\qquad \left. + \overline{\left(\frac{\zeta_j\left(-\theta_l^r\right)}{\zeta_j\left(-\theta_q^r\right)} \right)} \boldsymbol{\zeta}\left(-\theta_l^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \right] \\ &+ \sum_{q=1}^{k} \sum_{l=1}^{k} \frac{d\theta_q^r}{\theta_q^r + \theta_l^r} \left[\overline{\left(\frac{\zeta_j\left(\theta_l^r\right)}{\zeta_j\left(-\theta_q^r\right)} \right)} \boldsymbol{\zeta}\left(\theta_l^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \right. \\ &\qquad \left. + \overline{\left(\frac{\zeta_j\left(-\theta_l^r\right)}{\zeta_j\left(\theta_q^r\right)} \right)} \boldsymbol{\zeta}\left(-\theta_l^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \right]. \end{aligned} \tag{C.14}$$

Next, we observe that the solution of (C.4) is of the form

$$dV_1 = \sum_{q=1}^{k} \left[c_q^+ \boldsymbol{\zeta}\left(\theta_q^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star + c_q^- \boldsymbol{\zeta}\left(-\theta_q^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \right], \tag{C.15}$$

where the coefficients c_q^+ and c_q^- are found from the initial conditions

$$\mathbf{e}_1^\mathsf{T} dV_1 = \sum_{q=1}^{k} \left[c_q^+ \zeta_1\left(\theta_q^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star + c_q^- \zeta_1\left(-\theta_q^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \right] = -\mathbf{e}_1^\mathsf{T}\, dV_0. \tag{C.16}$$

Using (C.14) and (C.16), we find

$$\begin{aligned} dV_1 = \sum_{q=1}^{k} \sum_{\substack{l=1 \\ l \neq q}}^{k} \sqrt{\frac{\xi_l^r}{\xi_q^r}}\, \frac{d\theta_q^r}{\theta_l^r - \theta_q^r} \Bigg[& \overline{\left(\frac{\zeta_j(\theta_l^r)}{\zeta_j\left(\theta_q^r\right)}\right)} \boldsymbol{\zeta}\left(\theta_q^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \\ & + \overline{\left(\frac{\zeta_j(-\theta_l^r)}{\zeta_j(-\theta_q^r)}\right)} \boldsymbol{\zeta}\left(-\theta_q^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \Bigg] \\ - \sum_{q=1}^{k} \sum_{l=1}^{k} \sqrt{\frac{\xi_l^r}{\xi_q^r}}\, \frac{d\theta_q^r}{\theta_q^r + \theta_l^r} \Bigg[& \overline{\left(\frac{\zeta_j(-\theta_l^r)}{\zeta_j\left(\theta_q^r\right)}\right)} \boldsymbol{\zeta}\left(\theta_q^r\right) \boldsymbol{\zeta}\left(\theta_q^r\right)^\star \\ & + \overline{\left(\frac{\zeta_j(\theta_l^r)}{\zeta_j\left(-\theta_q^r\right)}\right)} \boldsymbol{\zeta}\left(-\theta_q^r\right) \boldsymbol{\zeta}\left(-\theta_q^r\right)^\star \Bigg]. \end{aligned} \tag{C.17}$$

Finally, we sum the jj components in (C.14) and (C.17) and, using Lemma 6.3, we obtain formula (6.43). □

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LILIANA BORCEA
Computational
and Applied Mathematics
MS 134
Rice University
6100 Main St.
Houston, TX
77005-1892
E-mail: borcea@caam.rice.ed

VLADIMIR DRUSKIN
Schlumberger–Doll Research Center
Old Quarry Rd.
Ridgefield, CT
06877-4108
E-mail: vdruskin@ridgefield.oilfield.slb.com

LEONID KNIZHNERMAN
Central Geophysical Expedition, Russia
Moscow
Narodnogo Opolcheniya St.
House 38, Bldg. 3
E-mail: mmd@cge.ru

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