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Structured matrix algorithms for inverse scattering on the line

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Abstract In this article the Marchenko integral equations leading to the solution of the inverse scattering problem for the 1-D Schrödinger equation on the line are solved numerically. The linear system obtained by discretization has a structured matrix which allows one to apply FFT based techniques to solve the inverse scattering problem with minimal computational complexity. The numerical results agree with exact solutions when available. A proof of the convergence of the discretization scheme is given.

Keywords Structured matrix systems, 1-D inverse scattering, Marchenko integral equation

1 Introduction

In this article we propose a numerical method for solving the inverse scattering problem for the Schrödinger equation

$$\psi''(k,x) + k^2\psi(k,x) = V(x)\psi(k,x), \quad x \in \mathbb{R}, \tag{1.1}$$

where V is a Faddeev class potential, i.e., a real function satisfying

$$\|V\|_{L^1_1(\mathbb{R})} \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} dx\,(1+|x|)|V(x)| < \infty.$$

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This method is based on the application of structured matrix algorithms for solving the linear systems obtained by discretizing the Marchenko integral equations whose solution allows one to identify the potential V, as explained in Sect. 2.

Traditionally inverse scattering problems on the line were solved numerically by methods not relying on the Marchenko integral equation method. Most effort went into the development of the layer stripping method [2,5,7, 21] which is based on either the trace formula or on causality and the Riesz transform. Basically these methods rely on the time domain description of direct and inverse scattering rather than on the frequency domain description. In [22] a time domain description of the direct and inverse problems and finite difference schemes are applied to solve the same inverse scattering problem. Only in [2,13] was the Marchenko integral equation method adopted, but without using structured matrix techniques. In [2] the Marchenko method served to construct the scattering matrices for the restrictions of the potential on the positive and negative half-lines and to employ the latter data in the layer stripping method, while in [13] an integral equation method was applied to solve the inverse spectral problem of the Schrödinger equation on a finite interval numerically. As a result, the method has a computational complexity of $O(n^3)$ for a number of x values that is proportional to n. Our method allows one to compute $V(x)$, for the same set of x values, by an algorithm of computational complexity $O(n^2 \log n)$. We also prove the convergence of the scheme adopted at the approximation of the Marchenko integral equation, by observing that the approximation amounts to quadratic spline interpolation. This approximation is similar but not identical to that given in [19] for convolution equations on the half-line. For the approximation inspired by that given in [19] and for the approximation obtained by applying the corresponding Nyström method we also give convergence proofs.

The outline of the paper is as follows. In Sect. 2 we introduce the Marchenko integral equation and explain how its solution allows one to identify the potential V if the scattering data satisfy the hypotheses which we specify. In Sect. 3 we discuss the boundedness and compactness of the Marchenko integral operator and the unique solvability of the Marchenko integral equation on various Sobolev spaces. These well-posedness results, as well as auxiliary results presented in Appendix A, are used in Sects. 4.1 and 4.2 to prove the convergence of two approximation schemes for the Marchenko equation in certain Sobolev spaces. In Sect. 3.2 we derive the explicit solution of this equation for rational scattering data by control theory methods. Some of them are used to assess the effectiveness of our numerical method. In Sect. 4.3 we describe the (preconditioned) Richardson iteration algorithm and present numerical results. We draw conclusions in Sect. 5.

2 The Marchenko integral equation method: statements and discussion

We first discuss conditions on the scattering data that assure the identificability of the potential V by the Marchenko integral equation method. To explain this issue, we introduce the Jost solutions $f_l(k,x)$ and $f_r(k,x)$ as those solutions of (1.1) that satisfy

$$\begin{cases} f_l(k,x) = e^{ikx}[1+o(1)], & x \to +\infty, \\ f_r(k,x) = e^{-ikx}[1+o(1)], & x \to -\infty, \end{cases}$$

and define the transmission coefficient $T(k)$ and the reflection coefficients $R(k)$ from the right and $L(k)$ from the left by means of the asymptotic relations

$$\begin{cases} f_l(k,x) = \dfrac{1}{T(k)}e^{ikx} + \dfrac{L(k)}{T(k)}e^{-ikx} + o(1), & x \to -\infty, \\ f_r(k,x) = \dfrac{1}{T(k)}e^{-ikx} + \dfrac{R(k)}{T(k)}e^{ikx} + o(1), & x \to +\infty, \end{cases}$$

such that the scattering matrix

$$S(k) = \begin{pmatrix} T(k) & R(k) \\ L(k) & T(k) \end{pmatrix}, \quad k \in \mathbb{R},$$

is unitary. Let $i\kappa_1, \ldots, i\kappa_{\mathcal{N}}$, with $0 < \kappa_1 < \ldots < \kappa_{\mathcal{N}}$, be the finitely many (necessarily simple) poles of $T(k)$ in the upper half-plane $\mathbb{C}^+$ and let $it_1, \ldots, it_{\mathcal{N}}$ be the residues of $T(k)$ at these poles. Then the inverse scattering problem consists of determining the unique Faddeev class potential $V(x)$ from the following scattering data [6,8,10,17]:

a. *to determine $V(x)$ for $x > 0$* from the reflection coefficient $R(k)$ from the right, the distinct positive numbers $\kappa_1, \ldots, \kappa_{\mathcal{N}}$ relating to the poles of $T(k)$ in $\mathbb{C}^+$, and the constant ratios $c_j = f_r(i\kappa_j, x)/f_l(i\kappa_j, x)$ (the so-called norming constants) such that $\Gamma_j = c_j t_j > 0$ $(j = 1, \ldots, \mathcal{N})$;
b. *to determine $V(x)$ for $x < 0$* from the reflection coefficient $L(k)$ from the left, the distinct positive numbers $\kappa_1, \ldots, \kappa_{\mathcal{N}}$ relating to the poles of $T(k)$ in $\mathbb{C}^+$, and the constant ratios $(1/c_j) = f_l(i\kappa_j, x)/f_r(i\kappa_j, x)$ (the so-called reciprocal norming constants) such that $(t_j/c_j) > 0$ $(j = 1, \ldots, \mathcal{N})$.

The potential $V(x)$ is to be found from the unique solutions $B_l(x,y)$ (for $x, y > 0$) and $B_r(x,y)$ (for $x < 0$ and $y > 0$) of the two Marchenko integral equations

$$B_l(x,y) + \Omega_l(2x+y) + \int_0^\infty dz\, \Omega_l(2x+y+z) B_l(x,z) = 0, \qquad (2.1)$$

$$B_r(x,y) + \Omega_r(-2x+y) + \int_0^\infty dz\, \Omega_r(-2x+y+z) B_r(x,z) = 0, \qquad (2.2)$$

by means of the identities

$$V(x) = \begin{cases} -2(\partial/\partial x)B_l(x, 0^+), & x > 0, \\ +2(\partial/\partial x)B_r(x, 0^+), & x < 0. \end{cases} \tag{2.3}$$

Here the kernels of the above integral equations are connected to the scattering data as follows:

$$\Omega_l(y) = \hat{R}(y) + \sum_{j=1}^{\mathcal{N}} t_j c_j e^{-\kappa_j y}, \quad \Omega_l(y) = \hat{L}(y) + \sum_{j=1}^{\mathcal{N}} (t_j/c_j) e^{-\kappa_j y}, \tag{2.4}$$

where

$$\hat{R}(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{iky} R(k), \quad \hat{L}(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{iky} L(k).$$

We note that the integral kernels of the Marchenko equations (2.1) and (2.2) are functions of the sums of their arguments. This property motivated us to solve them by applying structured matrix algorithms to the linear systems obtained by their discretization and thus to reduce the computational complexity of the algorithm substantially. The same property holds true for the integral kernels of the equations characterizing $V(x)$ for $x > 0$ and $x < 0$ as, given B_l and B_r, $\partial B_l/\partial x$ and $\partial B_r/\partial x$ are the solutions of the integral equations

$$\begin{aligned} \frac{\partial B_l}{\partial x}(x, y) + \int_0^{\infty} dz\, \Omega_l(2x + y + z) \frac{\partial B_l}{\partial x}(x, z) &= -2\Omega_l'(2x + y) \\ &\quad - 2 \int_0^{\infty} dz\, \Omega_l'(2x + y + z) B_l(x, z), \end{aligned} \tag{2.5}$$

$$\begin{aligned} \frac{\partial B_r}{\partial x}(x, y) + \int_0^{\infty} dz\, \Omega_r(-2x + y + z) \frac{\partial B_r}{\partial x}(x, z) &= 2\Omega_r'(-2x + y) \\ &\quad + 2 \int_0^{\infty} dz\, \Omega_r'(-2x + y + z) B_r(x, z). \end{aligned} \tag{2.6}$$

Consequently, we can apply the structured matrix algorithms for solving Eqs. (2.5)–(2.6), which allows us to obtain better results than by applying numerical differentiation to the solution of the Marchenko integral equations, but without increasing the order of computational complexity.

Calculations for $x > 0$ and $x < 0$ are done independently. Once the algorithm for computing $V(x)$ for $x > 0$ is in place, it is sufficient to recall that the scattering data $\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\}$ for $V(-x)$ for $x > 0$ are exactly $\{L(k), \{\kappa_j, (1/c_j)\}_{j=1}^{\mathcal{N}}\}$, where $L(k)$ is computed from $R(k)$ and $\kappa_1, \ldots, \kappa_{\mathcal{N}}$ in a straightforward way [6,8,17].

To test the method we make use of explicit expressions for the potential $V(x)$ with $x > 0$ based on a so-called realization of rational reflection coefficient $R(k)$ in the form [4]

$$R(k) = -i\mathcal{C}(k - i\mathcal{A})^{-1}\mathcal{B}, \tag{2.7}$$

where $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ are real $p \times p$, $p \times 1$ and $1 \times p$ matrices and p is minimal and is in fact equal to the McMillan degree of $R(k)$. Under the realization (2.7) the integral equation (2.1) can be solved explicitly by separation of variables if $x > 0$. Moreover, by using symbolic calculus the explicit solution thus obtained can be employed to determine the error in the numerical computation. When $R(k)$ is not rational, in general no explicit solution of (2.1) is known.

3 Analysis of the Marchenko equations

In this section we prove the compactness of the Marchenko integral operator between various function spaces.

3.1 The Marchenko integral operator

For $1 \leq p \leq +\infty$ and $m = 0, 1, 2, \ldots$ we define the Sobolev spaces $W^{p,m}(\mathbb{R}^+)$ as the (real or complex) spaces of those measurable f for which f and its first m distributional derivatives $f', f'', \ldots, f^{(m)}$ belong to $L^p(\mathbb{R}^+)$, endowed with the norm

$$\|f\|_{p,m} = \begin{cases} \left[\displaystyle\sum_{j=0}^{m} \|f^{(j)}\|_p^p\right]^{1/p}, & 1 \leq p < +\infty, \\ \max(\|f\|_\infty, \|f'\|_\infty, \ldots, \|f^{(m)}\|_\infty), & p = +\infty. \end{cases}$$

We write $f^{(0)} = f$ and $W^{p,0}(\mathbb{R}^+) = L^p(\mathbb{R}^+)$. We write $BC(\mathbb{R}^+)$ for the Banach space of bounded continuous complex-valued functions on $[0, \infty)$ endowed with the supremum norm.

Proposition 3.1 *Let $1 \leq p \leq +\infty$ and $\mathcal{K} \in W^{1,m}(\mathbb{R}^+)$. Then the integral operator K defined by*

$$(Kf)(y) = \int_0^\infty dz\, \mathcal{K}(y + z) f(z) \tag{3.1}$$

acts as a compact linear operator from $L^p(\mathbb{R}^+)$ into $W^{p,m}(\mathbb{R}^+)$. As a result, K is a compact linear operator on $W^{p,m}(\mathbb{R}^+)$. The operator K is compact on $BC(\mathbb{R}^+)$ whenever $\mathcal{K} \in L^1(\mathbb{R}^+)$.

Proof It is easy to see that K is a bounded linear operator on $L^p(\mathbb{R}^+)$ with norm bounded above by $\|\mathcal{K}\|_1$. In fact, this is a straightforward estimate for $p = 1$ (using the convolution theorem), $p = 2$ (using the unitarity of the Fourier transform), and $p = +\infty$ (trivial). It follows for the remaining p-values by the Riesz interpolation theorem. Next, if $\mathcal{K} \in W^{1,m}(\mathbb{R}^+)$, then for $j = 0, 1, \ldots, m$ we have

$$(Kf)^{(j)}(y) = \int_0^\infty dz\, \mathcal{K}^{(j)}(y+z) f(z), \quad y \in \mathbb{R}^+,$$

in the distributional sense and therefore

$$\|(Kf)^{(j)}\|_p \leq \|\mathcal{K}^{(j)}\|_1 \|f\|_p, \quad f \in L^p(\mathbb{R}^+).$$

As a result, for $1 \leq p < +\infty$ we have

$$\begin{aligned}\|Kf\|_{p,m} &= \left[\sum_{j=0}^m \|(Kf)^{(j)}\|_p^p\right]^{1/p} \leq \left[\sum_{j=0}^m \|\mathcal{K}^{(j)}\|_1^p\right]^{1/p} \|f\|_p \\ &\leq (m+1)^{1/p} \|\mathcal{K}\|_{1,m} \|f\|_p \leq (m+1)^{1/p} \|\mathcal{K}\|_{1,m} \|f\|_{p,m}.\end{aligned}$$

For $p = +\infty$ we have $\|Kf\|_{\infty,m} \leq \|\mathcal{K}\|_{1,m} \|f\|_\infty \leq \|\mathcal{K}\|_{1,m} \|f\|_{\infty,m}$.

The compactness of K on $L^p(\mathbb{R}^+)$ and $BC(\mathbb{R}^+)$ under the condition $\mathcal{K} \in L^1(\mathbb{R}^+)$ is a well-known result ([11], Lemma XII 2.4, its proof generalized to $p \in [1, \infty]$). When $\mathcal{K} \in W^{1,m}(\mathbb{R}^+)$, we have $\mathcal{K}^{(j)} \in L^1(\mathbb{R}^+)$ and hence the integral operator K^j of the type (3.1) with kernel function $\mathcal{K}^{(j)}$ is compact on $L^p(\mathbb{R}^+)$ ($j = 0, 1, \ldots, m$). Thus choosing a bounded sequence $\{f_n\}_{n=1}^\infty$ in $L^p(\mathbb{R}^+)$ one can extract a subsequence $\{f_{n_k}\}_{k=1}^\infty$ and find $\{g_0, \ldots, g_m\}$ in $L^p(\mathbb{R}^+)$ such that, for $j = 0, 1, \ldots, m$, $\|K^{(j)} f_{n_k} - g_j\|_p \to 0$ as $k \to \infty$. From the fact that the (distributional) differentiation operator on $L^p(\mathbb{R}^+)$ is closed it follows that $g_j = (d/dx)^j g_0$ in the distributional sense. As a result, $\|Kf_{n_k} - g_0\|_{p,m} \to 0$ as $k \to \infty$, which proves the compactness of K as an operator from $L^p(\mathbb{R}^+)$ into $W^{p,m}(\mathbb{R}^+)$. □

To determine if $\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\}$ are scattering data for a (unique) Faddeev class potential, let $T_0(k)$ be the unique continuous function of $k \in \overline{\mathbb{C}^+}$ such that $k/T_0(k)$ is analytic in $k \in \mathbb{C}^+$, $T_0(k) \to 1$ as $k \to \infty$ in $\overline{\mathbb{C}^+}$, and $T_0(k)T_0(-k) = 1 - R(k)R(-k)$ for $k \in \mathbb{R}$ (cf. [8]). Put

$$T(k) = T_0(k) \prod_{j=1}^{\mathcal{N}} \frac{k + i\kappa_j}{k - i\kappa_j}, \quad L(k) = -\frac{T(k)}{T(-k)} R(-k).$$

Then $\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\}$ are scattering data for a (unique) Faddeev class potential [18, 17, 1] if and only if

a. $R(-k) = \overline{R(k)}$ for $k \in \mathbb{R}$,
b. $R(k)$ is continuous for $k \in \mathbb{R}$,
c. $-1 \le R(0) < 1$,
d. the function $k/T(k)$ is continuous in $\overline{\mathbb{C}^+}$,
e. $R(k) \le 1 - C(k^2/(1+k^2))$ on $\mathbb{R}$ for some positive constant C,
f. $R(k) = o(1/k)$ as $k \to \pm\infty$,
g. the functions $\hat{R}$ and $\hat{L}$ are absolutely continuous, while

$$\int_a^\infty dy\,(1+|y|)\big(|\hat{R}'(y)| + |\hat{L}'(y)|\big) < +\infty, \quad a \in \mathbb{R},$$

h. $\Gamma_j \stackrel{\text{def}}{=} t_j c_j > 0$ for $it_j = \mathrm{Res}_{i\kappa_j} T(k)$ $(j = 1, \dots, \mathcal{N})$.

When $\big\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\big\}$ are scattering data for a Faddeev class potential $V(x)$, then $\big\{L(k), \{\kappa_j, 1/c_j\}_{j=1}^{\mathcal{N}}\big\}$ are scattering data for a Faddeev class potential (namely, for $V(-x)$).

The following result is well-known, as far as unique solvability in $L^1(\mathbb{R}^+)$ and $L^2(\mathbb{R}^+)$ is concerned (see [6,8,9]). The other statements follow from it by the compactness of the integral operator and the symmetry of its kernel.

Theorem 3.2 *Let $\big\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\big\}$ be scattering data for a Faddeev class potential. Then, for $1 \le p < \infty$ and any $x \in \mathbb{R}^+$, the integral equation*

$$C_l(y) + \int_0^\infty dz\,\Omega_l(2x+y+z)C_l(z) = F_l(y), \quad y \in \mathbb{R}^+, \tag{3.2}$$

is uniquely solvable in $L^p(\mathbb{R}^+)$ for any $F_l \in L^p(\mathbb{R}^+)$. Moreover, if $\Omega_l \in W^{1,m}(\mathbb{R}^+)$ for some $m \in \mathbb{N}$, then (3.2) *is uniquely solvable in $W^{p,m}(\mathbb{R}^+)$ for any $F_l \in W^{p,m}(\mathbb{R}^+)$. Analogously, for $1 \le p < \infty$ and any $x \in \mathbb{R}^-$, the integral equation*

$$C_r(y) + \int_0^\infty dz\,\Omega_r(-2x+y+z)C_r(z) = F_r(y), \quad y \in \mathbb{R}^+, \tag{3.3}$$

is uniquely solvable in $L^p(\mathbb{R}^+)$ for any $F_r \in L^p(\mathbb{R}^+)$. Moreover, if $\Omega_r \in W^{1,m}(\mathbb{R}^+)$ for some $m \in \mathbb{N}$, then (3.3) *is uniquely solvable in $W^{p,m}(\mathbb{R}^+)$ for any $F_r \in W^{p,m}(\mathbb{R}^+)$.*

With $\mathcal{F}$ standing for the Fourier transform operator, it is well-known [15] that $\mathcal{F}$ maps the orthogonal decomposition $L^2(\mathbb{R}) = L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^+)$ into the orthogonal decomposition $L^2(\mathbb{R}) = H_-^2(\mathbb{R}) \oplus H_+^2(\mathbb{R})$, where the spaces $H_\pm^2(\mathbb{R})$ are the Hardy spaces of analytic functions f on $\mathbb{C}^\pm$ for which $\sup_{b>0} \|f(\cdot \pm ib)\|_2 < +\infty$. Letting Q_+ stand for the natural projection of $L^2(\mathbb{R})$ onto $H_+^2(\mathbb{R})$, j_+ for the natural imbedding of $L^2(\mathbb{R}^+)$ into $L^2(\mathbb{R})$, and J for the sign

inversion $(Jf)(k) = f(-k)$, we can write the Marchenko integral operator K in (3.1) on $L^2(\mathbb{R}^+)$ in the form

$$Kf = \mathcal{F}^{-1} Q_+ (\hat{\mathcal{K}} J \mathcal{F} j_+ f),$$

where $\mathcal{F}^{-1}$ maps $H^2_+(\mathbb{R})$ onto $L^2(\mathbb{R}^+)$ and $\hat{\mathcal{K}}$ is the Fourier transform of $\mathcal{K}$. As a result,

$$\|K\|_{L^2(\mathbb{R}^+)\to L^2(\mathbb{R}^+)} \leq \inf\{\|\hat{\mathcal{K}} - \phi\|_\infty : \phi \in H^\infty(\mathbb{C}^-)\},$$

where $H^\infty(\mathbb{C}^-)$ is the Banach space of bounded analytic functions on $\mathbb{C}^-$, which can be compared to functions of $k \in \mathbb{R}$ through their almost everywhere existing nontangential limits in $k \in \mathbb{R}$. In fact, equality holds according to the Hartman-Wintner theorem [14]. Therefore, if there are no bound states, then the Marchenko integral operator in (3.2) has the spectral radius

$$\min_{\phi \in H^\infty(\mathbb{C}^-)} \operatorname*{ess\,sup}_{k\in\mathbb{R}} |R(k)e^{ikx} - \phi(k)|.$$

As a result, if $R(k) \in [r_-, r_+]$ for $-1 \leq r_- < r_+ < 1$, then by choosing $\phi(k) = 1 - \frac{1}{2}[r_+ - r_-]$ we see that the Marchenko integral operator in (3.2) has a spectral radius $\leq \frac{1}{2}[r_+ - r_-]$.

Because of the compactness of K on all of the function spaces mentioned above, the result remains true on these spaces. Indeed, let E and $\tilde{E}$ be two of these function spaces, let K be compact on either, and let $I - K$ be invertible on E. Then $E \cap \tilde{E}$, which is dense in both E and $\tilde{E}$, is a Banach space when endowed with the sum of the norms on E and $\tilde{E}$ and K is a compact operator on $E \cap \tilde{E}$. Since $\operatorname{Ker}(I - K) = \{0\}$ on $E \cap \tilde{E}$, the Fredholm alternative implies the invertibility of $I - K$ on $E \cap \tilde{E}$. Then the density of $E \cap \tilde{E}$ in $\tilde{E}$ implies that $I - K$ has a dense range on $\tilde{E}$. By the Fredholm alternative, $I - K$ is invertible on $\tilde{E}$, as claimed.

3.2 Explicit solutions in the rational case

If the reflection coefficient $R(k)$ is a rational function satisfying the characterization conditions (a)-(h) for corresponding to a Faddeev class potential, then there exist real matrices $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$, of sizes $p \times p$, $p \times 1$ and $1 \times p$, respectively, such that $\mathcal{A}$ does not have zero or purely imaginary eigenvalues and the realization (2.7) is valid. Letting $P^{(+)}_{\mathcal{A}}$ and $P^{(-)}_{\mathcal{A}}$ stand for the projections onto the maximal $\mathcal{A}$-invariant subspaces of $\mathbb{C}^p$ on which the restriction of $\mathcal{A}$ only has eigenvalues in the right and left half-planes, we have

$$\hat{R}(y) = \mathcal{C}E(y; -\mathcal{A})\mathcal{B}, \tag{3.4}$$

where

$$E(y;-\mathcal{A}) = \begin{cases} +\mathcal{C}e^{-y\mathcal{A}}P_{\mathcal{A}}^{(+)}\mathcal{B}, & y > 0, \\ -\mathcal{C}e^{-y\mathcal{A}}P_{\mathcal{A}}^{(-)}\mathcal{B}, & y < 0. \end{cases}$$

We now easily arrive at the following result (cf. [3]).

Theorem 3.3 *Let* $\left\{R(k), \{\kappa_j, c_j\}_{j=1}^{\mathcal{N}}\right\}$ *be valid scattering data satisfying the conditions (a)-(h), and let* $R(k)$ *have the realization* (2.7)*. Put*

$$\tilde{\mathcal{B}} = \begin{pmatrix} \mathcal{B} \\ 1 \\ \vdots \\ 1 \end{pmatrix}, \quad \begin{cases} \tilde{\mathcal{A}} = \mathcal{A} \oplus \operatorname{diag}(\kappa_1, \ldots, \kappa_{\mathcal{N}}), \\ \tilde{\mathcal{C}} = \begin{pmatrix} \mathcal{C} & t_1 c_1 & \ldots & t_{\mathcal{N}} c_{\mathcal{N}} \end{pmatrix}. \end{cases}$$

Then for $x \in \mathbb{R}^+$ *the unique solution of the Marchenko equation* (2.1) *is given by*

$$B_l(x, y) = -\tilde{\mathcal{C}}E(2x + y; -\tilde{\mathcal{A}})\left[I + \tilde{\mathcal{X}}E(2x; -\tilde{\mathcal{A}})\right]^{-1}\tilde{\mathcal{B}},$$

where

$$\tilde{\mathcal{X}} = \int_0^\infty dy\, E(y; -\tilde{\mathcal{A}})\tilde{\mathcal{B}}\tilde{\mathcal{C}}E(y; -\tilde{\mathcal{A}}). \tag{3.5}$$

For $x \in \mathbb{R}^+$ *the corresponding potential is given by*

$$V(x) = -4\tilde{\mathcal{C}}E(2x; -\tilde{\mathcal{A}})\left[I + \tilde{\mathcal{X}}E(2x; -\tilde{\mathcal{A}})\right]^{-1} \tilde{\mathcal{A}}\left[I + \tilde{\mathcal{X}}E(2x; -\tilde{\mathcal{A}})\right]^{-1}\tilde{\mathcal{B}}. \tag{3.6}$$

Proof From (3.4) and (2.4) we easily derive that

$$\hat{\Omega}_l(y) = \tilde{\mathcal{C}}E(y; -\tilde{\mathcal{A}})\tilde{\mathcal{B}}, \tag{3.7}$$

where $E(y; -\tilde{\mathcal{A}}) = E(y; -\mathcal{A}) \oplus \operatorname{diag}(e^{-\kappa_1 y}, \ldots, e^{-\kappa_{\mathcal{N}} y})$ for $y > 0$. Further, for $x \in \mathbb{R}^+$ the integral equation (2.1) has a separated kernel and hence

$$B_l(x, y) = -\tilde{\mathcal{C}}E(2x + y; -\tilde{\mathcal{A}})\left[\tilde{\mathcal{B}} + \int_0^\infty dz\, E(z; -\tilde{\mathcal{A}})\tilde{\mathcal{B}}B_l(x, z)\right],$$

which implies that

$$\left[I + \tilde{\mathcal{X}}E(2x; -\tilde{\mathcal{A}})\right]\int_0^\infty dy\, E(y; -\tilde{\mathcal{A}})\tilde{\mathcal{B}}B_l(x, y) = -\tilde{\mathcal{X}}E(2x; -\tilde{\mathcal{A}})\tilde{\mathcal{B}},$$

which immediately gives (3.5). Equation (3.6) then follows using (2.3). □

4 Discretization schemes and algorithms

In this section we introduce an approximation scheme which makes use of an exact calculation of integrals of the type $\int_0^\infty dz\, \mathcal{K}(y+z)s(z)$, where s is a quadratic spline, and prove its convergence in several Sobolev spaces. When these integrals can be evaluated exactly, as in all of the examples given in Sect. 5 except for Example 5.3, the resulting linear system is of diagonal-plus-Hankel type. Moreover, we describe an algorithm for solving Eqs. (2.1)–(2.2) and (2.5)–(2.6) which relies on the evaluation of these integrals by composite Simpson quadrature, thus leading to Nyström's method [16]. In all cases the resulting linear system is of diagonal-plus-Hankel type. The former method, to be described in Sect. 4.1, leads to an approximation error of the type

$$\int_0^\infty dz\, \mathcal{K}(y+z)\big[(I-\Pi_\Gamma)f\big](z),$$

with Π_Γ defined below in (4.2), whereas the second method, to be described in Sect. 4.2, leads to the additional quadrature error

$$\int_0^\infty dz\, \big[(I-\Pi_\Gamma)(\mathcal{K}(y+\cdot)f)\big](z).$$

which is of the order of the square of the step size.

4.1 Convergence of the approximation scheme

By a *mesh* we mean a set of the form

$$\Gamma = \{0 = x_0 < x_1 < x_2 < \ldots < x_n < \ldots < +\infty\}, \tag{4.1}$$

where $x_n \to +\infty$ as $n \to \infty$. The points x_n are called *division points*. We write $h_j = x_j - x_{j-1}$ $(j = 1, 2, \ldots)$. For each mesh we write $\|\Gamma\| \stackrel{\text{def}}{=} \sup_{j\in\mathbb{N}} h_j$.

Given the mesh Γ of type (4.1) and a continuous function $f : \mathbb{R}^+ \to \mathbb{C}$ we define its corresponding quadratic spline interpolant as:

$$\begin{aligned}(\Pi_\Gamma f)(y) = {} & f(x_{j-1})\frac{\big(y-\frac{1}{2}[x_{j-1}+x_j]\big)(y-x_j)}{h_j^2/2} \\ & - f\left(\frac{1}{2}[x_{j-1}+x_j]\right)\frac{(y-x_{j-1})(y-x_j)}{h_j^2/4} \\ & + f(x_j)\frac{(y-x_{j-1})\big(y-\frac{1}{2}[x_{j-1}+x_j]\big)}{h_j^2/2},\end{aligned} \tag{4.2}$$

where $x_{j-1} \le y \le x_j$ for $j = 1, 2, 3, \ldots,$. Using a C^∞-function g of compact support to compute $\langle (\Pi_\Gamma f)' f, g\rangle = -\langle \Pi_\Gamma f, g'\rangle$ and $g(x_0) = g(0) = 0$, we obtain (in the sense of a function defined a.e.)

$$\begin{aligned}(\Pi_\Gamma f)'(y) = f(x_{j-1})\frac{y - \left(\frac{1}{4}x_{j-1} + \frac{3}{4}x_j\right)}{h_j^2/4}\\ -f\left(\frac{1}{2}[x_{j-1} + x_j]\right)\frac{y - \frac{1}{2}[x_{j-1} + x_j]}{h_j^2/8}\\ +f(x_j)\frac{y - \left(\frac{3}{4}x_{j-1} + \frac{1}{4}x_j\right)}{h_j^2/4},\end{aligned} \tag{4.3}$$

where $x_{j-1} < y < x_j$ and $j = 1, 2, 3, \ldots$. For details see Appendix B.

By an *allowable sequence of meshes* we mean a sequence $\{\Gamma_m\}_{m=1}^\infty$ of meshes

$$\begin{cases}\Gamma_m = \{0 = x_0^m < x_1^m < x_2^m < \ldots < x_n^m < \ldots < +\infty\},\\ h_j^m = x_j^m - x_{j-1}^m, \quad j = 1, 2, \ldots,\end{cases} \tag{4.4}$$

where

$$\lim_{m\to\infty} \|\Gamma_m\| = 0.$$

Given the integral operator K defined by (3.1), we now define the approximant K_Γ of K as:

$$\begin{cases}(K_\Gamma f)(y) = (\Pi_\Gamma g)(y),\\ g(y) = \displaystyle\int_0^\infty dz\, \mathcal{K}(y+z)(\Pi_\Gamma f)(z).\end{cases} \tag{4.5}$$

Proposition 4.1 *Let $1 \le p < \infty$. Then for any allowable sequence of meshes $\{\Gamma_m\}_{m=1}^\infty$ we have as $m \to \infty$*

$$\|K - K_{\Gamma_m}\| = O(\|\Gamma_m\|) \tag{4.6}$$

if $\mathcal{K} \in W^{1,2}(\mathbb{R}^+)$, in the operator norm of any of the Banach spaces $W^{p,1}(\mathbb{R}^+)$.

Proof Writing $K_{\Gamma_m} = \Pi_{\Gamma_m} K \Pi_{\Gamma_m}$ we have

$$K - K_{\Gamma_m} = K(I - \Pi_{\Gamma_m}) + (I - \Pi_{\Gamma_m})K - (I - \Pi_{\Gamma_m})K(I - \Pi_{\Gamma_m}). \tag{4.7}$$

We estimate each term separately as depicted in the following diagrams:

$$\begin{aligned}&W^{p,1}(\mathbb{R}^+) \xrightarrow{I-\Pi_{\Gamma_m}} L^p(\mathbb{R}^+) \xrightarrow{K} W^{p,1}(\mathbb{R}^+),\\ &W^{p,1}(\mathbb{R}^+) \xrightarrow{K} W^{p,2}(\mathbb{R}^+) \xrightarrow{I-\Pi_{\Gamma_m}} W^{p,1}(\mathbb{R}^+),\\ &W^{p,1}(\mathbb{R}^+) \xrightarrow{I-\Pi_{\Gamma_m}} L^p(\mathbb{R}^+) \xrightarrow{K} W^{p,2}(\mathbb{R}^+) \xrightarrow{I-\Pi_{\Gamma_m}} W^{p,1}(\mathbb{R}^+).\end{aligned}$$

The first estimate requires $\mathcal{K} \in W^{1,1}(\mathbb{R}^+)$, the second and third require $\mathcal{K} \in W^{1,2}(\mathbb{R}^+)$, and Lemma A.2 and the p-additivity of the L^p-norm are applied to get the norm estimates on $I - \Pi_{\Gamma_m}$. In all of these cases we only need $\Pi_{\Gamma_m} f$ and $(\Pi_{\Gamma_m} f)'$ for continuous f, but no higher order derivatives of $\Pi_{\Gamma_m} f$.

Indeed, applying Lemma A.2 to each interval (x_{j-1}^m, x_j^m) for $j = 1, 2, \ldots$ and Proposition 3.1 for $m = 1$, we obtain, for $1 \leq p < \infty$,

$$\begin{aligned}
\|K(I - \Pi_{\Gamma_m})f\|_{p,1}^p &\leq (\|K\|_{L^p \to W^{p,1}})^p \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy \, |\big[(I - \Pi_{\Gamma_m})f\big](y)|^p \\
&\leq (\|K\|_{L^p \to W^{p,1}})^p \sum_{j=1}^{\infty} \left(\frac{3}{4} h_j\right)^p \int_{x_{j-1}}^{x_j} dy \, |f'(y)|^p \\
&\leq 2 \left(\frac{3}{4} \|\mathcal{K}\|_{1,1} \|\Gamma_m\|\right)^p \|f\|_{p,1}^p,
\end{aligned}$$

so that, for $f \in W^{p,1}(\mathbb{R}^+)$,

$$\|K(I - \Pi_{\Gamma_m})f\|_{p,1} \leq 2^{1/p} \|\Gamma_m\| \|\mathcal{K}\|_{1,1} \|f\|_{p,1}. \tag{4.8}$$

Next, using the facts that K acts as a bounded linear operator from $W^{p,1}(\mathbb{R}^+)$ into $W^{p,2}(\mathbb{R}^+)$ whenever $\mathcal{K} \in W^{1,2}(\mathbb{R}^+)$ with norm bounded above by $\|\mathcal{K}\|_{1,2}$ and that $I - \Pi_{\Gamma_m}$ acts as a bounded linear operator from $W^{p,2}(\mathbb{R}^+)$ into $W^{p,1}(\mathbb{R}^+)$ [see (A.13a)] with norm of the order of $O(\|\Gamma_m\|)$, we see that, for $f \in W^{p,1}(\mathbb{R}^+)$,

$$\|(I - \Pi_{\Gamma_m})Kf\|_{p,1} \leq 3^{1/p} \|\Gamma_m\| \|\mathcal{K}\|_{1,2} \|f\|_{p,1}. \tag{4.9}$$

Also, using the facts that $I - \Pi_{\Gamma_m}$ acts as a bounded operator from $W^{p,1}(\mathbb{R}^+)$ into $L^p(\mathbb{R}^+)$ with norm of the order of $O(\|\Gamma_m\|)$, that K acts as a bounded operator from $L^p(\mathbb{R}^+)$ into $W^{p,2}(\mathbb{R}^+)$ whenever $\mathcal{K} \in W^{1,2}(\mathbb{R}^+)$ with norm bounded above by $3^{1/p}\|\mathcal{K}\|_{1,2}$, and that $I - \Pi_{\Gamma_m}$ acts as a bounded operator from $W^{p,2}(\mathbb{R}^+)$ into $W^{p,1}(\mathbb{R}^+)$ with norm of the order of $O(\|\Gamma_m\|)$, we have, for $f \in W^{p,1}(\mathbb{R}^+)$,

$$\|(I - \Pi_{\Gamma_m})K(I - \Pi_{\Gamma_m})f\|_{p,1} \leq 3^{1/p} \|\Gamma_m\| \|\mathcal{K}\|_{1,2} \|f\|_{p,1}. \tag{4.10}$$

From (4.8)–(4.10) we immediately obtain (4.6). □

The unique solvability of the Marchenko integral equations implies that, under the conditions of Proposition 4.1, the solution of the discretized equation

$$(I + K_{\Gamma_m})B_m = -\Pi_{\Gamma_m} W \tag{4.11}$$

converges to the unique solution of the Marchenko integral equation

$$(I + K)B = -W$$

in the norm of the function space $W^{p,1}(\mathbb{R}^+)$, irrespective of the choice of $W \in W^{p,2}(\mathbb{R}^+)$.

Theorem 4.2 *Let $1 \le p < \infty$ and let $I + K$ be invertible on $L^p(\mathbb{R}^+)$. If $\mathcal{K} \in W^{1,2}(\mathbb{R}^+)$, then for any allowable sequence of meshes $\{\Gamma_m\}_{m=1}^{\infty}$ there exists $m_0 \in \mathbb{N}$ such that, for $m \ge m_0$,* (4.11) *has a unique solution $B_m \in W^{p,1}(\mathbb{R}^+)$ for any $W \in W^{p,2}(\mathbb{R}^+)$. Moreover, for $m \ge m_0$ we have*

$$\|B - B_m\|_{p,1} = O(\|\mathcal{K}\|_{1,2}\|\Gamma_m\|\,\|W\|_{p,2}), \tag{4.12}$$

where the order constant does not depend on $m \ge m_0$ and $B \in W^{p,2}(\mathbb{R}^+)$.

Proof The invertibility of $I + K$ on $W^{p,1}(\mathbb{R}^+)$ and the relation

$$\lim_{m\to\infty} \left\| K - K_{\Gamma_m} \right\|_{W^{p,1}\to W^{p,1}} = 0$$

imply that, for sufficiently large m, the inverses $(I + K_{\Gamma_m})^{-1}$ exist and are uniformly bounded on $W^{p,1}(\mathbb{R}^+)$:

$$\left\|(I + K_{\Gamma_m})^{-1}\right\|_{W^{p,1}\to W^{p,1}} \le c_0, \quad m \ge m_0.$$

Now let $B_m \in W^{p,1}(\mathbb{R}^+)$ be the solution of (4.11). Then for $m \ge m_0$ it follows that

$$\begin{aligned}
\|B - B_m\|_{p,1} &\le c_0\|(I + K_{\Gamma_m})(B - B_m)\|_{p,1} \\
&\le c_0\big(\|(I + K)B - (I + K_{\Gamma_m})B_m\|_{p,1} + \|(K_{\Gamma_m} - K)B\|_{p,1}\big) \\
&\le c_0\big(\|W - \Pi_{\Gamma_m}W\|_{p,1} + 3^{1+\frac{1}{p}}\|\Gamma_m\|\,\|\mathcal{K}\|_{1,2}\|B\|_{p,1}\big) \\
&\le O(\|\Gamma_m\|\,\|\mathcal{K}\|_{1,2})\big(\|W\|_{p,2} + \|B\|_{p,1}\big) \\
&\le O(\|\Gamma_m\|\,\|\mathcal{K}\|_{1,2})\|W\|_{p,2},
\end{aligned}$$

which establishes (4.12). □

4.2 Applying Nyström's method

Apart from (4.5), we now consider the Nyström approximation scheme [16]

$$\begin{cases}
(K_{[\Gamma]}f)(y) = \displaystyle\int_0^\infty dz\,(K^\Gamma f)(y, z), \\
(K^\Gamma f)(z) = [\Pi_\Gamma \mathcal{K}(y + \cdot)f(\cdot)](z).
\end{cases}$$

Given the mesh (4.1) and putting $h_{-1} = h_{n+1} = 0$, it is easily verified that

$$\int_0^\infty dy\,(\Pi_\Gamma f)(y) = \sum_{j=0}^{n+1} \frac{h_{j-1}+h_j}{6} f(x_j) + \frac{h_n}{6} f(x_n) + \sum_{j=1}^{n} \frac{2}{3} h_{j-1} f\left(\frac{1}{2}[x_{j-1}+x_j]\right)$$

is the result of truncating f for $y > x_n$ and integrating f over $[0, x_n]$ by Simpson's rule. Here we note that the sum of the weights equals x_n. Thus, the integral in the integral equation $(I-K)B = -W$ is confined to the interval $[0, x_n]$ and evaluated by Simpson's quadrature rule.

Fix $M > 0$. Let $\{\Gamma_m\}_{m=1}^\infty$ be a sequence of meshes such that

$$\Gamma_m = \{0 = x_0^m < x_1^m < \ldots < x_{n_m}^m = M\}, \quad \lim_{m\to\infty} \max_{j=1,\ldots,n_m} (x_j^m - x_{j-1}^m) = 0. \tag{4.13}$$

Then it follows from [16, Theorems 12.2 and 12.4] that the sequence of quadrature rules corresponding to such a sequence of meshes is convergent in the sense that

$$\lim_{n\to\infty} \int_0^M dy\,[f(y) - (\Pi_{\Gamma_m} f)(y)] = 0$$

for every $f \in C[0, M]$. According to [16, Theorem 12.8], the sequence of integral operators $\{K^{\Gamma_m}\}_{m=1}^\infty$ is collectively compact and converges pointwise to the integral operator $K^{(M)}$ defined on $C[0, M]$ by

$$(K^{(M)} f)(y) = \int_0^M dz\,\mathcal{K}(y+z) f(z), \quad 0 \le y \le M. \tag{4.14}$$

In the sequel we write χ_A for the characteristic function of the set A.

Theorem 4.3 *Suppose $\mathcal{K} \in W^{1,1}(\mathbb{R}^+)$, $W \in BC(\mathbb{R}^+)$, and that the homogeneous equation $(I+K)f = 0$ has only the trivial solution in $L^\infty(\mathbb{R}^+)$. Then, for sufficiently large $M > 0$ and for any sequence of meshes $\{\Gamma_m\}_{m=1}^\infty$ satisfying* (4.13)*, there exists $m_0 = m_0(M) \in \mathbb{N}$ such that the equations*

$$B_M(y) + \chi_{[0,M]}(y) \int_0^M dz\,\mathcal{K}(y+z) B_M(z) = -W(y), \quad y \ge 0,$$

and, for $m \ge m_0$,

$$(I + K_{[\Gamma_m]}) B_{[m]} = -\Pi_{\Gamma_m}\left(W|_{[0,M]}\right)$$

have unique solutions $B_M \in L^\infty(\mathbb{R}^+)$ and $B_{[m]} \in C[0, M]$, respectively. Moreover,

$$\lim_{m\to\infty} \|B_{[m]} - B_M\|_{\infty,[0,M]} = 0 \text{ for sufficiently large } M, \tag{4.15}$$

where $\|f\|_{\infty,[0,M]} = \sup_{x\in[0,M]} |f(x)|$, *and*

$$\lim_{M\to\infty} \|B_M - B\|_\infty = 0. \tag{4.16}$$

Proof For $M > 0$ define $\tilde{K}^{(M)} = P_M K P_M : L^\infty(\mathbb{R}^+) \to L^\infty(\mathbb{R}^+)$, where

$$(P_M f)(x) = \begin{cases} f(x), & x \in [0, M], \\ 0, & x > M. \end{cases}$$

Since P_M has unit norm on $L^\infty(\mathbb{R}^+)$, for $f \in L^\infty(\mathbb{R}^+)$ we can estimate

$$\begin{aligned} \left\| Kf - \tilde{K}^{(M)} f \right\|_\infty &\le \|Kf - K P_M f\|_\infty + \|P_M(Kf - K P_M f)\|_\infty \\ &\le 2\|Kf - K P_M f\|_\infty \\ &= 2 \sup_{y\ge 0} \left| \int_M^\infty dz\, \mathcal{K}(y+z) f(z) \right| \\ &\le 2\|f\|_\infty \int_M^\infty dz\, |\mathcal{K}(z)|, \end{aligned}$$

which vanishes as $M \to +\infty$. This means that

$$\lim_{M\to\infty} \left\| K - \tilde{K}^{(M)} \right\|_{L^\infty(\mathbb{R}^+)\to L^\infty(\mathbb{R}^+)} = 0. \tag{4.17}$$

Consequently, since $I + K$ is invertible on $L^\infty(\mathbb{R}^+)$, the operators $I + \tilde{K}^{(M)}$ are invertible for sufficiently large M.

To prove that the operator $I + K^{(M)} : C[0, M] \to C[0, M]$ defined by (4.14) is invertible for sufficiently large M, it is sufficient to show that, for sufficiently large M, the homogeneous equation

$$\tilde{f} + K^{(M)} \tilde{f} = 0 \tag{4.18}$$

has only the trivial solution in $C[0, M]$. Indeed, if $\tilde{f} \in C[0, M]$ is a solution of (4.18), define

$$f(x) = \begin{cases} \tilde{f}(x), & x \in [0, M], \\ 0, & x > M. \end{cases}$$

Then, since P_M is a projection operator, we have

$$0 = \tilde{f} + \tilde{K}^{(M)} \tilde{f} = P_M f + P_M K P_M P_M f = \left(I + \tilde{K}^{(M)}\right) P_M f.$$

Due to the invertibility of $I + \tilde{K}^{(M)}$ on $L^\infty(\mathbb{R}^+)$ for sufficiently large M, we obtain $P_M f = 0$ and hence $\tilde{f} = 0$, thus proving the uniqueness statement.

Let B and B_M denote the solutions of the equations $(I + K)B = -W$ and $\left(I + \tilde{K}^{(M)}\right) B_M = -W$, respectively. Then, due to (4.17), $\|B_M - B\|_\infty \to 0$ as $M \to +\infty$. With the help of [16, Theorem 10.9] one obtains the convergence (in the norm of $C[0, M]$) of $B_{[m]}$ to the restriction of B_M to the interval $[0, M]$. Thus we have proved (4.15) as well as (4.16). □

The choice of M is not an easy task. However, in our numerical experiments we found it effective to choose M such that $\|\mathcal{K}\chi_{[M,\infty)}\|_1 \simeq \|\Gamma\|$, where $\chi_{[M,\infty)}$ is the characteristic function of $[M,\infty)$. This choice of M is motivated by the fact that, on the one hand, $\|K - K^{(M)}\| = O(\|\mathcal{K}\chi_{[M,\infty)}\|_1)$ and, on the other hand, $\|K - K_{[\Gamma]}\| = O(\|\Gamma\|)$.

4.3 Algorithms

Our numerical method is based on Nyström's method, i.e., on the evaluation of the integrals in (2.1)–(2.2) and (2.5)–(2.6) by Simpson's method for $y \in (0,\alpha)$ for sufficiently large α. When applied to (2.1) by selecting an odd integer n and a step size h such that $(n-1)h = \alpha$, by taking $x_l = (l-1)h$ for $l = 1,\ldots,n$, and by selecting $y_i = (i-i)h$ for $i = 1,\ldots,n$ with $(n-1)h = \alpha$ for each given l value, we obtain the linear system

$$B_i + \sum_{j=1}^{n} H_{i+j} d_j B_j = -H_i, \quad i = 1,\ldots,n, \tag{4.19}$$

where

$$H_i = \hat{R}\big(2x_l + (i-1)h\big) + \sum_{s=1}^{\mathcal{N}} t_s c_s e^{-\kappa_s[2x_l+(i-1)h]},$$

$d_1 = d_n = (h/3)$, $d_i = (4h/3)$ for $i = 2,4,6,\ldots,n-1$, and $d_i = (2h/3)$ for $i = 3,5,7,\ldots,n-2$. Thus the linear system (4.19) has the form

$$(I + HD)b = -w, \tag{4.20}$$

where I is the identity matrix, $H = (H_{i+j})_{i,j=1}^{n}$ is a Hankel matrix, $D = \mathrm{diag}(d_1,\ldots,d_n)$ is a diagonal matrix, and w is a known column vector. After the computation of B_l, the application of the same technique to (2.5) leads to a linear system whose matrix is exactly the same but whose right-hand side is different. For this reason the analysis of the algorithm is focused on the solution of (2.1). We note that solving Eq. (2.1) and then Eq. (2.5) leads to more accurate results than computing $V(x)$ by numerical differentiation of B_l without increasing the computational complexity of the algorithm.

When there are no bound states, the Marchenko equations (2.1) and (2.2) can be solved uniquely by iteration in a variety of function spaces [6,8,9,17]. In this case the linear system (4.20) is solved by Richardson iteration [12], since the Marchenko integral operator is a strict contraction. When there are bound states, the Marchenko integral operator is a strict contraction plus a positive selfadjoint operator of rank $\mathcal{N}$, which makes (2.1) and (2.2) uniquely solvable in many function spaces ([9], also the discussion at the end of Sect. 2). In this case the Hankel matrix H can be written as the sum $H = H^{(R)} + H^{(K)}$ of a

Hankel matrix for which $H^{(R)}D$ is contractive, and a positive Hankel matrix of rank $\mathcal{N}$. We then solve the preconditioned system

$$\big(I + [I + H^{(K)}D]^{-1}H^{(R)}D\big)b = -[I + H^{(K)}D]^{-1}w,$$

by Richardson iteration. The Hankel matrix-vector products arising during execution are computed by applying the FFT, leading to a reduction of the computational complexity from $O(n^2)$ [for each x] to $O(n\log(n))$ [for each x].

If there are no bound states, the linear system

$$\big[I + H^{(R)}D\big]b = -\omega$$

can be solved by the Richardson iteration scheme:

$$\begin{cases} \tilde{b}^{(r)} = Db_r, \\ b^{(r+1)} = -\omega - H^{(R)}\tilde{b}^{(r)}. \end{cases} \tag{4.21}$$

Then the absolute error $b - b^{(r)}$ of the r-th iterate behaves as follows:

$$b - b^{(r+1)} = \big[-\omega - H^{(R)}Db\big] + \omega + H^{(R)}Db^{(r)} = -H^{(R)}D\big(b - b^{(r)}\big).$$

Therefore,

$$b - b^{(r)} = (-1)^r D^{-1/2}[D^{1/2}H^{(R)}D^{1/2}]^r D^{1/2}\big(b - b^{(0)}\big).$$

Consequently, the relative error decreases exponentially in r, i,.e.,

$$\frac{\|b - b^{(r)}\|}{\|b - b^{(0)}\|} \le \|D^{-1/2}\|\,\|D^{1/2}\|\,\|D^{1/2}H^{(R)}D^{1/2}\|^r,$$

where $\|D^{1/2}H^{(R)}D^{1/2}\|$ coincides with the spectral radius of $H^{(R)}D$, because of the selfadjointness of $D^{1/2}H^{(R)}D^{1/2}$. It should be observed that in (4.21) the first line can be implemented in $O(n)$ operations and (by FFT) the second line in $O(n\log(n))$ operations for each iteration step. To get the relative error $\|b - b^{(r)}\|/\|b - b^{(0)}\|$ below $\varepsilon > 0$ we need about

$$\frac{\log\big(\|D^{1/2}\|\,\|D^{-1/2}\|/\varepsilon\big)}{\log(1/\|D^{1/2}H^{(R)}D^{1/2}\|)}$$

iterations.

Now note that $\|D^{1/2}\|\,\|D^{-1/2}\|$ equals the square root of the ratio between the largest and the smallest weight, namely $q = 2$ for Simpson's rule. Writing $\Delta = \Delta(h)$ for the value of $\|D^{1/2}H^{(R)}D^{1/2}\|$ we need about

$$\frac{\log(q/\varepsilon)}{\log(1/\Delta)}$$

iterations, where $q = 2$. Richardson iteration works properly only if

$$\|D^{1/2}H^{(R)}D^{1/2}\| = \Delta(h) < 1. \tag{4.22}$$

This condition is satisfied, since $\Delta(h)$ tends to the spectral radius of K (which is less than 1) monotonically as $h \to 0^+$. Hence the iteration scheme works in the approximately

$$\frac{\log(1/\|D^{1/2}H^{(R)}D^{1/2}\|)}{\log(1/\varepsilon)}$$

iterations needed to attain a relative error of less than ε.

If there are $\mathcal{N}$ bound states, we should solve the full linear system

$$\big[I + \{H^{(K)} + H^{(R)}\}D\big]b = -\omega, \tag{4.23}$$

where $H^{(K)}$ is a Hankel matrix of rank $\mathcal{N}$ such that the nonzero eigenvalues if $H^{(K)}D$ are all positive. This means that linear systems which are of the form $[I + H^{(K)}D]b = -\hat{b}$ can easily be solved uniquely in $O(\mathcal{N}^2)$ operations, without using any of its structure apart from its rank. We then write (4.23) in the form

$$\begin{aligned} \hat{b} &= -\omega - H^{(R)}Db, \\ \big[I + H^{(K)}D\big]b &= \hat{b}, \end{aligned}$$

which can be solved by the Richardson iteration scheme:

$$\begin{cases} \tilde{b}^{(r)} = Db^{(r)}, \\ \hat{b}^{(r+1)} = -\omega - H^{(R)}\tilde{b}^{(r)}, \\ b^{(r+1)} = \big[I + H^{(K)}D\big]^{-1}\hat{b}^{(r+1)}. \end{cases}$$

The rate of exponential convergence is determined by the spectral radius of the matrix

$$\big[I + H^{(K)}D\big]^{-1}H^{(R)}D,$$

which equals the spectral radius (and hence the norm) of

$$\big[I + D^{1/2}H^{(K)}D^{1/2}\big]^{-1/2}D^{1/2}H^{(R)}D^{1/2}\big[I + D^{1/2}H^{(K)}D^{1/2}\big]^{-1/2},$$

which is strictly less than the spectral radius of $H^{(R)}D$, due to the nonnegative selfadjointness of $D^{1/2}H^{(K)}D^{1/2}$. Thus taking into account bound state information tends to accelerate the Richardson iteration scheme. Once (4.22) is satisfied, the iteration scheme works in the approximately

$$\frac{\log\big(1/\|[I + D^{1/2}H^{(K)}D^{1/2}]^{-1/2}D^{1/2}H^{(R)}D^{1/2}[I + D^{1/2}H^{(K)}D^{1/2}]^{-1/2}\|\big)}{\log(1/\varepsilon)}$$

iterations needed to attain a relative error of less than ε.

To compute the inverse of the matrix $I + H^{(K)}D$, we first observe that

$$H^{(K)}D = UV^T,$$

where U and V are the real $n \times \mathcal{N}$ matrices given by

$$U_{is} = t_s c_s e^{-\kappa_s(i-1)h},$$
$$V_{js} = w_j e^{-\kappa_s(j-1)h},$$

$i, j = 1, \ldots, n$ and $s = 1, \ldots, \mathcal{N}$. According to the Sherman-Morrison-Woodbury formula ([12], Sect. 2.1.3), we have

$$\left(I + H^{(K)}D\right)^{-1} = I_{n\times n} - U(I + V^T U)^{-1}V^T,$$

where $(I + V^T U)^{-1}$ is an $\mathcal{N} \times \mathcal{N}$-matrix which is to be computed before performing the iterations. As a result, we have $O\big(n \log(n)\big)$ operations per iteration, as if there were no bound states.

5 Numerical results and conclusions

5.1 Numerical results

In order to assess the effectiveness of the method proposed, we carried out extensive experimentation on various models, some of which are quoted in the literature. More precisely, we considered three models without bound states, a model with one bound state, and a model with two bound states. The results are presented in Figs. 5.1–5.5 in logarithmic scale (except for Fig. 5.3). Furthermore, the results presented were obtained by taking $\alpha = 10.24$, which corresponds to $n = 2^{10} + 1$ and $h = \frac{1}{100}$. These values of α and n correspond to a choice for which $\|\Gamma_m\|$ and $\|\mathcal{K}\chi_{[\alpha,\infty)}\|_1$ are essentially equivalent.

Example 5.1 Following [2] we consider the Schrödinger potential without bound states, where

$$R(k) = \frac{(k+i)(k+2i)(101k^2 - 3ik - 400)}{(k-i)(k-2i)(50k^4 + 280ik^3 - 609k^2 - 653ik + 400)}.$$

Then for $y > 0$ we have

$$\hat{R}(y) = -\frac{3}{2}e^{-y} + \frac{4}{3}e^{-2y}, \quad \hat{L}(y) = (8 - 6\sqrt{2})e^{-y\sqrt{2}}.$$

Moreover, for $x > 0$ the potentials $V(x)$ and $V(-x)$ are given by (3.6), where $\tilde{\mathcal{A}} = \mathcal{A} = \mathrm{diag}(1, 2)$, $\tilde{\mathcal{B}} = \mathcal{B} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and $\tilde{\mathcal{C}} = \mathcal{C} = \left(-\frac{3}{2}\ \frac{4}{3}\right)$ [for $V(x)$], and

$\tilde{\mathcal{A}} = \mathcal{A} = \big(\sqrt{2}\big)$, $\tilde{\mathcal{B}} = \mathcal{B} = \big(1\big)$, and $\tilde{\mathcal{C}} = \mathcal{C} = \big(8 - 6\sqrt{2}\big)$ [for $V(-x)$], which corresponds with the expressions given in [2].

Figure 5.1 highlights the effectiveness of the algorithm illustrated in Sect. 3.1. Indeed, it shows the behavior of both the analytical expression for the potential for $x > 0$ and the potential computed by solving (2.1) and (2.5) as explained above.

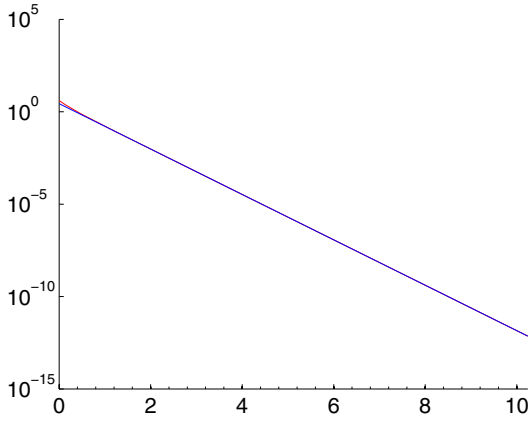

Fig. 5.1 Potential without bound states and with exponentially decaying Marchenko kernel: numerical (blue) and exact (red) results

Example 5.2 We next consider the potential without bound states whose Marchenko integral kernel for $x > 0$ is given by (3.4), where

$$\tilde{\mathcal{A}} = \mathcal{A} = \begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}, \quad \tilde{\mathcal{B}} = \mathcal{B} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \tilde{\mathcal{C}} = \mathcal{C} = \big(\tfrac{1}{2}\ \tfrac{1}{5}\big).$$

Then

$$\hat{R}(y) = e^{-4y} \left(\frac{7}{10} \cos(y) - \frac{3}{10} \sin(y) \right).$$

Figure 5.2 gives a geometrical idea of the accuracy of the results for this model.

Example 5.3 We now study the Schrödinger potential without bound states, where $R(k) = \gamma\, \pi\, e^{-|k|}$ for $\gamma\, \pi\, \in [-1, 1)$. Then, for $y > 0$, we have

$$\hat{R}(y) = \frac{\gamma}{1 + y^2},$$

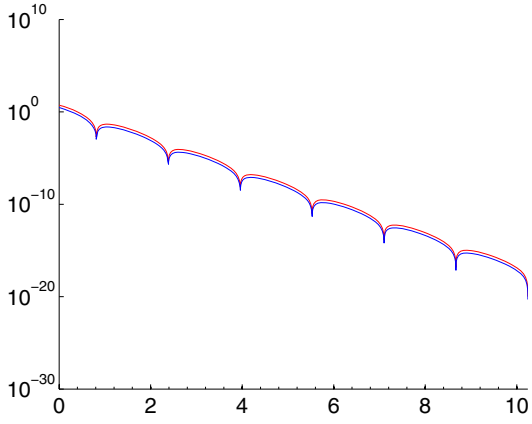

Fig. 5.2 Potential without bound states and with oscillatory Marchenko kernel: numerical (blue) and exact (red) results

where the spectral radius of the Marchenko integral operator is bounded above by $|\gamma|\pi/2$. In this case no explicit solution of the inverse scattering problem is known. Further, as $\alpha \to +\infty$, we have

$$\int_\alpha^\infty dy\,(|\hat{R}(y)| + |\hat{R}'(y)|) = \arctan(1/\alpha) + \frac{1}{1+\alpha^2} = (1/\alpha)[1 + O(1/\alpha)].$$

Example 5.4 Here we consider the Schrödinger equation with one bound state pole at $k = i\kappa$, norming constant $\Gamma_1 = t_1 c_1 = \Gamma > 0$, and reflection coefficient

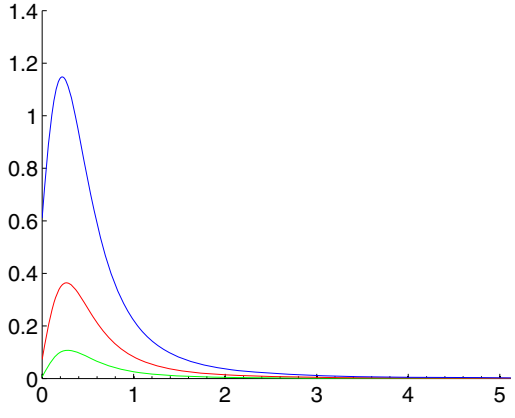

Fig. 5.3 Potential without bound states and with algebraically decaying Marchenko kernel: numerical results for $\gamma = -\frac{1}{\pi}$ (blue), $\gamma = -\frac{1}{8}$ (red), $\gamma = -\frac{1}{25}$ (green)

from the right and transmission coefficient

$$R(k) = \frac{2\gamma\beta}{k^2+\beta^2},$$
$$T(k) = \frac{(k+i\beta\sqrt{1+2(\gamma/\beta)})(k+i\beta\sqrt{1-2(\gamma/\beta)})}{(k+i\beta)^2}\,\frac{k+i\kappa}{k-i\kappa},$$

where $-1 \le 2(\gamma/\beta) < 1$. Then $\hat{R}(y)$ is given by (3.4), where $\mathcal{A} = (\beta)$, $\mathcal{B} = (1)$, and $\mathcal{C} = (\gamma)$, while

$$\tilde{\mathcal{A}} = \begin{pmatrix} \beta & 0 \\ 0 & \kappa \end{pmatrix}, \quad \tilde{\mathcal{B}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \tilde{\mathcal{C}} = (\gamma \ \ \Gamma).$$

The Marchenko integral kernel is given by

$$\Omega_l(y) = \gamma e^{-\beta y} + \Gamma e^{-\kappa y}, \quad y > 0.$$

The numerical and analytical results (for $\beta = 1$, $\gamma = -\frac{3}{2}$, $\kappa = 2$, and $\Gamma = \frac{4}{3}$) are presented in Fig. 5.4.

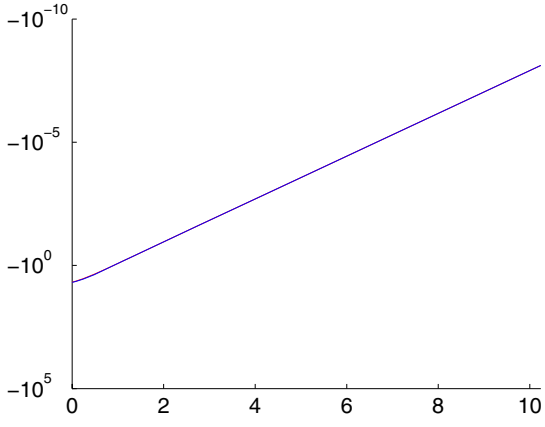

Fig. 5.4 Potential with one bound state and exponentially decaying Marchenko kernel: numerical (blue) and exact (red) results

Example 5.5 Lastly we consider the Schrödinger equation with two bound state poles at $i\kappa_1$ and $i\kappa_2$, norming constants $\Gamma_1 = t_1 c_1 > 0$ and $\Gamma_2 = t_2 c_2 > 0$, reflection coefficient from the right $R(k) = 2\gamma\beta/(k^2+\beta^2)$ with $-1 \le 2(\gamma/\beta) < 1$, and transmission coefficient

$$T(k) = \frac{(k+i\beta\sqrt{1+2(\gamma/\beta)})(k+i\beta\sqrt{1-2(\gamma/\beta)})}{(k+i\beta)^2}\,\frac{(k+i\kappa_1)(k+i\kappa_2)}{(k-i\kappa_1)(k-i\kappa_2)}.$$

Then the Marchenko integral kernel is given by

$$\Omega_l(y) = \gamma\, e^{-\beta y} + \Gamma_1 e^{-\kappa_1 y} + \Gamma_2 e^{-\kappa_2 y}, \quad y > 0,$$

which can be written in the form (3.7), where

$$\tilde{\mathcal{A}} = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \kappa_1 & 0 \\ 0 & 0 & \kappa_2 \end{pmatrix}, \quad \tilde{\mathcal{B}} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \tilde{\mathcal{C}} = \begin{pmatrix} \gamma & \Gamma_1 & \Gamma_2 \end{pmatrix}.$$

The numerical and analytical results (for $\beta = 1$, $\gamma = \frac{1}{5}$, $\kappa_1 = \frac{1}{2}$, $\kappa_2 = 2$, $\Gamma_1 = 3$, and $\Gamma_2 = 6$) are presented in Fig. 5.5.

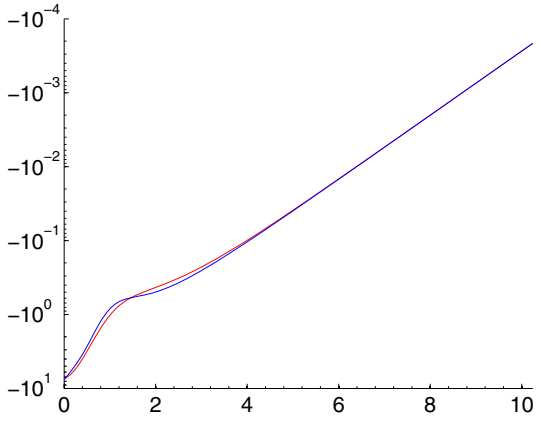

Fig. 5.5 Potential with two bound states and exponentially decaying Marchenko kernel: numerical (blue) and exact (red) results

5.2 Conclusions

Our numerical experiments highlight the effectiveness of the numerical algorithm, as might be expected from the convergence properties of the spline approximation to the exact solution of the Marchenko integral equation. Furthermore, in the absence of bound states the Marchenko integral operator has spectral radius less than one in suitable Sobolev spaces and therefore this is also the case for the iteration matrix in the Richardson iteration. When there are bound states, the bound state part of the Marchenko integral operator makes its spectrum shift to the right and hence the corresponding matrices have the same property, which leads to a preconditioned Richardson iteration matrix of spectral radius less than one. As a result, starting from $b^{(0)} = (0, \ldots, 0)^T$,

we always obtained good results with few iterations: at most 15 for the algebraically decaying case (Example 5.3) and at most 10 in the exponentially decaying cases (Examples 5.1–5.2 and 5.4–5.5). We emphasize that the computational complexity of our method is $O(n\log(n))$ for one x value, whereas it is $O(n^2)$ in all the methods for solving the Marchenko integral equation of which we are aware [2].

We remark that in the cases considered we have essentially the same results obtained with the same computational complexity if we adopt the approximation scheme based on the approximation of Kf by $K_\Gamma f$.

Acknowledgments. The authors are greatly indebted to Prof. Peter Junghanns for several useful remarks which have led to a substantial improvement of the contents of the paper, in particular for the formulation and proof of Theorem 4.3 on the Nyström method.

A Appendix: auxiliary approximation results

In this section we obtain results concerning the approximation by quadratic splines needed to study the convergence of our discretization schemes.

Consider $\alpha, \beta, \gamma \in \mathbb{R}$ such that $\alpha < \beta$ and $\gamma = \frac{1}{2}(\alpha+\beta)$, and put $h = \beta - \alpha$. For a continuous function $f : [\alpha, \beta] \to \mathbb{C}$, the unique quadratic polynomial $\mathcal{S}_2 f$ passing through the points $(\alpha, f(\alpha))$, $(\beta, f(\beta))$ and $(\gamma, f(\gamma))$ is given by each of the three identities

$$(\mathcal{S}_2 f)(x) = f(x) - E_n(f;\gamma,x) + \frac{E_n(f;\gamma,\beta)(x-\alpha)(x-\gamma) + E_n(f;\gamma,\alpha)(x-\beta)(x-\gamma)}{h^2/2}, \tag{A.1}$$

where $n = 0, 1, 2$. Here $E_n(f;\gamma,x)$ is the n-th order remainder term in the Taylor expansion of f in γ, i.e.,

$$f(x) = \sum_{j=0}^{n} \frac{f^{(j)}(\gamma)}{n!}(x-\gamma)^j + E_n(f;\gamma,x), \tag{A.2}$$

where

$$E_n(f;\gamma,x) = \frac{1}{n!}\int_\gamma^x dt\,(x-t)^n f^{(n+1)}(t), \tag{A.3}$$

provided that $f \in C^{(n+1)}[\alpha,\beta]$. Throughout the appendix norms are taken in function spaces over the interval $[\alpha,\beta]$.

The estimate (A.4) in the following lemma can be proved in a straightforward way for $p = 1$ and $p = \infty$ and by interpolation for $1 < p < \infty$. The estimate (A.5) follows by applying Hölder's inequality.

Lemma A.1 *For general $n = 0, 1, 2, \ldots$ and $1 \le p \le +\infty$ we have*

$$\|E_n(f;\gamma,\cdot)\|_p \le \frac{1}{2^{n+1}(n+1)!}h^{n+1}\|f^{(n+1)}\|_p \tag{A.4}$$

and

$$\|E_n(f;\gamma,\cdot)\|_\infty \le \begin{cases} (h/2)^{1/q}\|f'\|_p, & n=0,\\ \dfrac{h^{1+\frac{1}{q}}}{(q+1)^{1/q}2^{1+\frac{1}{q}}}\|f''\|_p, & n=1,\\ \dfrac{h^{n+\frac{1}{q}}}{n!(nq+1)^{1/q}2^{n+\frac{1}{q}}}\|f^{(n+1)}\|_p, & n=0,1,2,\ldots, \end{cases} \tag{A.5}$$

where $q = p/(p-1)$.

We now easily obtain the following result.

Lemma A.2 *For* $1 \le p < +\infty$ *we have*

$$\|f-\mathcal{S}_2 f\|_p \le h\left[\frac{1}{2}+\frac{1}{4}(p+1)^{-1/p}\right]\|f'\|_p \le \frac{3}{4}h\|f'\|_p, \tag{A.6a}$$

$$\|f-\mathcal{S}_2 f\|_p \le h^2\left[\frac{1}{8}+\frac{1}{8}(p+1)^{-1/p}\right]\|f''\|_p \le \frac{1}{4}h^2\|f''\|_p, \tag{A.6b}$$

$$\|f-\mathcal{S}_2 f\|_p \le h^3\left[\tfrac{1}{48}+\frac{1}{32}(p+1)^{-1/p}\right]\|f^{(3)}\|_p \le \frac{5}{96}h^3\|f^{(3)}\|_p, \tag{A.6c}$$

while, for $p=+\infty$, *we have*

$$\|f-\mathcal{S}_2 f\|_\infty \le \frac{3}{2}h\|f'\|_\infty, \tag{A.7a}$$

$$\|f-\mathcal{S}_2 f\|_\infty \le \frac{3}{8}h^2\|f''\|_\infty, \tag{A.7b}$$

$$\|f-\mathcal{S}_2 f\|_\infty \le \frac{1}{16}h^3\|f^{(3)}\|_\infty. \tag{A.7c}$$

Proof We begin by deriving the estimates

$$\|(\cdot-\beta)(\cdot-\gamma)\|_p = \|(\cdot-\alpha)(\cdot-\gamma)\|_p = \begin{cases} \left(\dfrac{h}{2}\right)^{2+\frac{1}{p}} K_p, & 1 \le p < +\infty,\\ \dfrac{h^2}{2}, & p=+\infty, \end{cases}$$

where

$$K_p = \left[\int_0^1 t^p(1-t)^p\,dt + \int_0^1 t^p(1+t)^p\,dt\right]^{1/p}.$$

For $1 \le p < +\infty$ and $n = 0, 1, 2$ we have [cf. (A.4) and (A.5)]

$$\frac{\|f - \mathcal{S}_2 f\|_p}{\|f^{(n+1)}\|_p} \le \frac{\|E_n(f;\gamma,\cdot)\|_p}{\|f^{(n+1)}\|_p} + \frac{4}{h^2}\frac{\|E_n(f;\gamma,\cdot)\|_\infty}{\|f^{(n+1)}\|_p} K_p \left(\frac{h}{2}\right)^{2+\frac{1}{p}}$$

$$\le \frac{h^{n+1}}{2^{n+1}(n+1)!} + \frac{K_p h^{n+1}}{n!(nq+1)^{1/q}2^{n+1}}$$

$$\le h^{n+1}\left[\frac{1}{2^{n+1}(n+1)!} + \frac{K_p}{n!\,2^{n+1}}\right],$$

where K_p is as above. On the other hand, for $p = \infty$ and $n = 0, 1, 2$ we have [cf. (A.5)]

$$\frac{\|f - \mathcal{S}_2 f\|_\infty}{\|f^{(n+1)}\|_\infty} \le \frac{\|E_n(f;\gamma,\cdot)\|_\infty}{\|f^{(n+1)}\|_\infty} + 2\frac{2}{h^2}\frac{\|E_n(f;\gamma,\cdot)\|_\infty}{\|f^{(n+1)}\|_\infty}\frac{h^2}{2} \le 3c_n h^{n+1},$$

where $c_0 = \frac{1}{2}$, $c_1 = \frac{1}{8}$ and $c_2 = \frac{1}{48}$, as claimed. □

We now compute the derivatives of the spline interpolants. First we have

$$\frac{d}{dx}E_n(f;\gamma,x) = \begin{cases} f'(x), & n = 0, \\ E_{n-1}(f';\gamma,x), & n = 1, 2, 3, \ldots. \end{cases} \tag{A.8}$$

From (A.1) we find that

$$\begin{aligned} f'(x) - (\mathcal{S}_2 f)'(x) &= f'(x) - \frac{E_0(f;\gamma,\beta)(x - \frac{\alpha+\gamma}{2}) + E_0(f;\gamma,\alpha)(x - \frac{\beta+\gamma}{2})}{h^2/4} \\ &= E_0(f';\gamma,x) - \frac{E_1(f;\gamma,\beta)(x - \frac{\alpha+\gamma}{2}) + E_1(f;\gamma,\alpha)(x - \frac{\beta+\gamma}{2})}{h^2/4} \\ &= E_1(f';\gamma,x) - \frac{E_2(f;\gamma,\beta)(x - \frac{\alpha+\gamma}{2}) + E_2(f;\gamma,\alpha)(x - \frac{\beta+\gamma}{2})}{h^2/4}, \end{aligned} \tag{A.9}$$

as well as that

$$\begin{aligned} f''(x) - (\mathcal{S}_2 f)''(x) &= f''(x) - \frac{E_0(f;\gamma,\beta) + E_0(f;\gamma,\alpha)}{h^2/4} \\ &= f''(x) - \frac{E_1(f;\gamma,\beta) + E_1(f;\gamma,\alpha)}{h^2/4} \\ &= E_0(f'';\gamma,x) - \frac{E_2(f;\gamma,\beta) + E_2(f;\gamma,\alpha)}{h^2/4}. \end{aligned} \tag{A.10}$$

Using the fact that

$$\left\|\cdot - \frac{\beta+\gamma}{2}\right\|_p = \left\|\cdot - \frac{\alpha+\gamma}{2}\right\|_p$$

$$= \begin{cases} \dfrac{h^{1+\frac{1}{p}}[3^{p+1}+1]^{1/p}}{4^{1+\frac{1}{p}}(p+1)^{1/p}}, & 1 \le p < +\infty, \\ \frac{3}{4}h, & p = +\infty, \end{cases}$$

we obtain

$$\left\| f' - (\mathcal{S}_2 f)' \right\|_p \le \left\| f' \right\|_p \left[1 + \frac{[3^{p+1}+1]^{1/p}}{2^{1/p}(p+1)^{1/p}} \right] \le 4 \left\| f' \right\|_p, \tag{A.11a}$$

$$\left\| f' - (\mathcal{S}_2 f)' \right\|_p \le \frac{1}{2} h \left\| f'' \right\|_p \left[1 + \frac{[3^{p+1}+1]^{1/p}}{2^{1/p}(p+1)^{1/p}(q+1)^{1/q}} \right] \le 2h \left\| f'' \right\|_p, \tag{A.11b}$$

$$\begin{aligned} \left\| f' - (\mathcal{S}_2 f)' \right\|_p &\le \frac{1}{8} h^2 \left\| f^{(3)} \right\|_p \left[1 + \frac{[3^{p+1}+1]^{1/p}}{2^{3+\frac{1}{p}}(p+1)^{1/p}(2q+1)^{1/q}} \right] \\ &\le \frac{11}{64} h^2 \left\| f^{(3)} \right\|_p, \end{aligned} \tag{A.11c}$$

$$\left\| f'' - (\mathcal{S}_2 f)'' \right\|_p \le \left\| f'' \right\|_p \left[1 + \frac{2^{1+\frac{1}{p}}}{(q+1)^{1/q}} \right] \le 5 \left\| f'' \right\|_p, \tag{A.12a}$$

$$\left\| f'' - (\mathcal{S}_2 f)'' \right\|_p \le \frac{1}{2} h \left\| f^{(3)} \right\|_p \left[1 + \frac{2^{1/p}}{(2q+1)^{1/q}} \right] \le \frac{3}{2} h \left\| f^{(3)} \right\|_p. \tag{A.12b}$$

We now arrive at the result to be applied when proving the convergence of the discretization method for the Marchenko integral equations. The constants can be chosen to be independent of $p \in [1, +\infty]$.

Theorem A.3 *For* $1 \le p \le +\infty$ *we have*

$$\| f - \mathcal{S}_2 f \|_{p,1} \le \text{const.} h \| f \|_{p,2}, \tag{A.13a}$$

$$\| f - \mathcal{S}_2 f \|_{p,1} \le \text{const.} h^2 \| f \|_{p,3}, \tag{A.13b}$$

$$\| f - \mathcal{S}_2 f \|_{p,2} \le \text{const.} h \| f \|_{p,3}. \tag{A.13c}$$

Proof Equations (A.6) and (A.11)-(A.12) imply that

$$\begin{aligned} \| f - \mathcal{S}_2 f \|_{p,1} &\le \text{const.} h \| f' \|_{p,1} \le \text{const.} h \| f \|_{p,2}, \\ \| f - \mathcal{S}_2 f \|_{p,1} &\le \text{const.} h^2 \| f'' \|_{p,1} \le \text{const.} h^2 \| f \|_{p,3}, \\ \| f - \mathcal{S}_2 f \|_{p,2} &\le \text{const.} h \| f' \|_{p,2} \le \text{const.} h \| f \|_{p,3}, \end{aligned}$$

as claimed. □

B Appendix: distributional derivatives $(\Pi_\Gamma f)'$ and $(\Pi_\Gamma f)''$

Put $\xi_j = \frac{1}{2}[x_{j-1} + x_j]$, where $j = 1, 2, 3, \ldots$. Given a C^∞-function g of compact support in $(0, \infty)$ and denoting the right-hand side of (4.3) by $H(y)$, we obtain, for a continuous function f on $[0, \infty)$,

$$
\begin{aligned}
\langle (\Pi_\Gamma f)', g\rangle &= -\langle \Pi_\Gamma f, g'\rangle \\
&= -\sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, (\Pi_\Gamma f)(y) g'(y) \\
&= -\sum_{j=1}^{\infty} [(\Pi_\Gamma f)(y) g(y)]_{y=x_{j-1}}^{x_j} + \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, H(y) g(y) \\
&= -\sum_{j=1}^{\infty} \big\{ f(x_j) g(x_j) - f(x_{j-1}) g(x_{j-1}) \big\} \\
&\quad + \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, H(y) g(y) \\
&= f(x_0) g(x_0) - \lim_{n\to\infty} f(x_n) g(x_n) + \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, H(y) g(y) \\
&= \int_0^{\infty} dy\, H(y) g(y).
\end{aligned}
$$

Here we have employed the fact that $g(x_0)$ and all but finitely many $g(x_j)$ vanish, which yields the absolute convergence of the first series in the fourth expression above. Thus $(\Pi_\Gamma f)'(y) = H(y)$ for a.e. $y \in \mathbb{R}^+$.

Computing $(\Pi_\Gamma f)''$ we obtain, for any C^∞-function g of compact support in $(0, \infty)$,

$$
\begin{aligned}
\langle (\Pi_\Gamma f)'', g\rangle &= -\langle (\Pi_\Gamma f)', g'\rangle = -\int_0^{\infty} dy\, H(y) g'(y) \\
&= -\sum_{j=1}^{\infty} [H(y) g(y)]_{y=x_{j-1}}^{x_j} + \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, H'(y) g(y) \\
&= \sum_{j=1}^{\infty} \{H(x_j^+) - H(x_j^-)\} g(x_j) + \sum_{j=1}^{\infty} \int_{x_{j-1}}^{x_j} dy\, H'(y) g(y).
\end{aligned}
$$

Consequently, $(\Pi_\Gamma f)''$ is the sum of the piecewise constant function H' and an infinite linear combination of delta functions centered at each of the points x_j $(j = 1, 2, 3, \ldots)$.

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