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Recovery of jumps and singularities of an unknown potential from limited data in dimension 1

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Abstract
We prove that in dimension 1 the jumps and singularities of an unknown potential appearing in the Schrödinger equation can be recovered using the Born approximation. The result is based on an accurate determination of the first nonlinear term of the Born series. We shall also work in wider function space than the previous publications on this topic. Numerical examples illustrate the feasibility of this technique.

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1. Introduction

Let us consider the one-dimensional Schrödinger operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) \tag{1}$$

with the real-valued potential $q(x)$ belonging to the weighted space $L^1_\sigma(\mathbb{R})$ defined by the norm

$$\|q\|_{L^1_\sigma(\mathbb{R})} = \int_{-\infty}^{\infty} (1+|x|)^\sigma |q(x)|\,\mathrm{d}x,$$

where $\sigma \geqslant 0$ will be specified later. For such potential the operator H is known to be self-adjoint in $L^2(\mathbb{R})$ (at least in terms of quadratic forms) with domain $D(H)$ in Sobolev space $W^1_2(\mathbb{R})$. If $q(x) \in L^1_\sigma(\mathbb{R})$ with $\sigma \geqslant 1$, then the spectrum of H can be described precisely (see for example [1]). Namely, it consists of an absolutely continuous spectrum, filling out the non-negative real axis $[0, \infty)$ and a possible finite negative discrete spectrum of finite multiplicity

$$-\lambda_n^2 < -\lambda_{n-1}^2 < \cdots < -\lambda_1^2 \tag{2}$$

with corresponding eigenfunctions from $L^2(\mathbb{R})$.

In scattering theory one considers the generalized eigenfunctions (which correspond to continuous spectrum) that are the solutions of

$$Hu = k^2 u, \qquad u = u_0 + u_{\mathrm{sc}}, \qquad u_0 = \mathrm{e}^{\mathrm{i}kx}.$$

They are the responses to an incoming wave u_0. Observe that the outgoing wave u_{sc} satisfies the equation

$$(-\Delta - k^2) u_{\mathrm{sc}} = -q u_0 - q u_{\mathrm{sc}}.$$

Applying the outgoing resolvent, i.e. the integral operator $\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - k^2 - \mathrm{i}0\right)^{-1}$, we obtain the so-called Lippmann–Schwinger integral equation

$$u(x,k) = \mathrm{e}^{\mathrm{i}kx} + \frac{1}{2\mathrm{i}|k|} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}|k||x-y|} q(y) u(y,k)\,\mathrm{d}y, \tag{3}$$

where $k \neq 0$. Note that for $k = 0$ we will have the equation

$$u(x) = 1 + \frac{1}{2} \int_{-\infty}^{\infty} |x-y| q(y) u(y)\,\mathrm{d}y.$$

It is not so difficult to check that for any fixed $k > 0$, the solutions $u(x,k)$ of (3) admit asymptotically the representations

$$u(x,k) = \mathrm{e}^{\mathrm{i}kx} a(k) + o(1), \qquad x \to +\infty,$$
$$u(x,k) = \mathrm{e}^{\mathrm{i}kx} + b(k)\,\mathrm{e}^{-\mathrm{i}kx} + o(1), \qquad x \to -\infty,$$

where

$$a(k) = 1 + \frac{1}{2\mathrm{i}k} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}ky} q(y) u(y,k)\,\mathrm{d}y,$$
$$b(k) = \frac{1}{2\mathrm{i}k} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}ky} q(y) u(y,k)\,\mathrm{d}y.$$

The inverse scattering problem for the Hamiltonian (1) is formulated as follows: to recover the potential $q(x)$ given scattering data, i.e. the coefficients $a(k)$ and $b(k)$ and the negative discrete spectrum (2), if it exists.

For the potentials from the weighted space $L^1_\sigma(\mathbb{R})$ with $\sigma \geqslant 1$, this problem was solved in the frame of the Gelfand–Levitan–Marchenko approach, see [2–7] and [1]. These studies provide the uniqueness theorems for direct and inverse problems as well as transformation formulae and exact formula for recovering the potential $q(x)$ in one form or another. However, the entire spectrum must be known. The reflection coefficient (in our case $b(k)$) must be known for all $k \neq 0$ and also in the case of discrete spectrum normalizing constants, and this discrete spectrum is required. There is a large literature for potentials that are not in the standard class $L^1_1(\mathbb{R})$. We refer to the book of Chadan and Sabatier [7], see chapter XVII, sections 4 and 5, and see also the references therein.

If the potential $q(x)$ belongs to $L^1_\sigma(\mathbb{R})$, with $0 \leqslant \sigma < 1$, then we cannot describe the spectrum of the Hamiltonian as above. We may only say (see [8]) that the essential spectrum of H is $[0, \infty)$. But if in addition we assume that the potential has the special behaviour

$$|q(x)| \leqslant C|x|^{-\mu}, \qquad |x| > R,$$

where R is large enough and $\mu > 1$, then the spectrum consists of a continuous spectrum filling out the positive real axis and a possible negative discrete spectrum of finite multiplicity with zero as the only possible accumulation point, see [9]. Here and in the following, $C > 0$ shall designate a generic constant that may change from one step to another. For potentials from $L^1_\sigma(\mathbb{R})$ with $0 \leqslant \sigma < 1$, the uniqueness theorem in the one-dimensional inverse scattering problem does no longer hold, see [10]. Let us note here that there are some interesting examples of potentials with Dirac delta function for which the uniqueness theorem also does not hold, see [11–13]. For our considerations we do not need the uniqueness theorem for the inverse scattering problem.

In the present paper we will consider the potential $q(x)$ from $L^1(\mathbb{R})$ and investigate an approximate method to recover partial information about the potential, namely the jumps and discontinuities of it. This method works if we know only one of the data coefficients, $b(k)$. Furthermore, it is not required to be known for all $k \in \mathbb{R}$, but for all k which are as large as we want in absolute value. Actually, in the frame of this method the unknown potential, up to a C^∞ function, is simply the inverse Fourier transform of the data $b(k)$. It is well known that if the potential is small (in the sense of having small norm), then this approximation is very good. But even if the potential is not small, we can obtain very essential information about it from this approximation. In the present paper we improve some of the results obtained in the paper [14–16].

This paper is organized as follows. In section 2 we give the incident direction $u_0 = \mathrm{e}^{\mathrm{i}kx}$ full treatment in terms of defining the Born approximation and then studying the first nonlinear term of the Born series. We give estimates for the remaining terms in this series so concluding the recovery of jumps and singularities of the unknown potential. Section 3 lists the corresponding results without proofs for the second incident direction $u_0 = \mathrm{e}^{-\mathrm{i}kx}$. We finish the paper by giving a selection of numerical examples illustrating the usefulness of the method.

2. The first incident direction

Let $u_0(x,k) = \mathrm{e}^{\mathrm{i}kx}$. Defining

$$u(x,k) = \overline{u(x,-k)} \tag{4}$$

for $k < 0$, we can consider equation (3) for all $k \neq 0$ in the form

$$u(x,k) = \mathrm{e}^{\,\mathrm{i}kx} + \frac{1}{2\mathrm{i}k}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k|x-y|} q(y) u(y,k)\,\mathrm{d}y. \tag{5}$$

Lemma 1. *Suppose that the potential $q(x)$ belongs to $L^1(\mathbb{R})$. Then for any $|k| > \|q\|_1/2$, there exist solutions of the integral equation (5) satisfying the estimate*

$$|u(x,k)| \leqslant \frac{2|k|}{2|k| - \|q\|_1}$$

uniformly in $x \in \mathbb{R}$.

Proof. The Lippmann–Schwinger equation (5) is a Fredholm integral equation of the second kind whose solution is found via Neumann series

$$u(x,k) = \sum_{j=0}^{\infty} u_j(x,k), \tag{6}$$

where

$$u_j(x,k) = \frac{1}{2\mathrm{i}k}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k|x-y|} q(y) u_{j-1}(y,k)\,\mathrm{d}y, \qquad j = 1, 2, \ldots$$

$$u_0(x,k) = \mathrm{e}^{\mathrm{i}kx}.$$

It follows by induction that

$$|u_j(x,k)| \leqslant \left(\frac{\|q\|_1}{2|k|}\right)^j, \qquad j = 1, 2, \ldots.$$

Hence, series (6) converges if

$$|k| > \frac{\|q\|_1}{2}.$$

For such k, there holds

$$|u(x,k)| \leqslant \sum_{j=0}^{\infty} \left(\frac{\|q\|_1}{2|k|}\right)^j = \frac{1}{1-\frac{\|q\|_1}{2|k|}} = \frac{2|k|}{2|k|-\|q\|_1}$$

proving the lemma. □

Corollary 2. *The remaining terms of series (6) satisfy the estimate*

$$\sum_{j=m}^{\infty} |u_j(x,k)| \leqslant \frac{c_m}{|k|^m}, \qquad m = 0, 1, \ldots$$

for $|k| \geqslant \|q\|_1$ *with* $c_m = 2\left(\frac{\|q\|_1}{2}\right)^m$.

Proof. For $|k| \geqslant \|q\|_1$, we have the estimates

$$\sum_{j=m}^{\infty} |u_j(x,k)| \leqslant \sum_{j=m}^{\infty} \left(\frac{\|q\|_1}{2|k|}\right)^j = \left(\frac{\|q\|_1}{2|k|}\right)^m \frac{1}{1-\frac{\|q\|_1}{2|k|}} \leqslant \frac{2\|q\|_1^m}{(2|k|)^m} = \frac{c_m}{|k|^m},$$

for $m = 0, 1, \ldots$. □

Since

$$u(x,k) \approx \mathrm{e}^{\mathrm{i}kx}, \qquad k \to \infty,$$

we have the asymptotics

$$a(k) \approx 1 + \frac{1}{2\mathrm{i}k}\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y \approx 1, \qquad k \to \infty,$$

$$b(k) \approx \frac{1}{2\mathrm{i}k}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}2ky} q(y)\,\mathrm{d}y, \qquad k \to \infty.$$

That is why we choose $b(k)$ as our data in the inverse problem which is to recover jumps and singularities of q. For $|k| < \|q\|_1$ we set $b(k) = 0$. An easy computation using (4) shows that $b(k) = \overline{b(-k)}$.

We observe that for large k,

$$b(k) \approx \frac{\sqrt{2\pi}}{2\mathrm{i}k}(Fq)(2k),$$

where F designates the Fourier transform defined by

$$(Ff)(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}ky} f(y)\,\mathrm{d}y.$$

Correspondingly, the inverse Fourier transform F^{-1} is defined by

$$(F^{-1}f)(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}kx} f(k)\,\mathrm{d}k.$$

This motivates the following.

Definition 3. *The inverse scattering Born approximation* $q_{\mathrm{B}}(x)$ *of the potential* $q(x)$ *is defined by*

$$q_{\mathrm{B}}(x) = F^{-1}\left(\frac{\mathrm{i}kb(k/2)}{\sqrt{2\pi}}\right) = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty} kb(k/2)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}k. \tag{7}$$

Remark 4. Since

$$q_B(x) = \frac{i}{2\pi}(f(x) - \overline{f(x)}),$$

where

$$f(x) = \int_0^\infty kb(k/2)\,e^{-ikx}\,dk,$$

we note that $q_B(x)$ is real valued.

Lemma 5. *Under the same assumptions for $q(x)$ as in lemma 1, the Born approximation (7) is of the form*

$$q_B = q + q_1 + \tilde{q} + q_{\mathrm{rest}},$$

where

$$q_1 = F^{-1}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)u_1\left(y, \frac{k}{2}\right) dy\right),$$

$$\tilde{q} = F^{-1}\left([\chi(k/2) - 1]\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)\left(u_0\left(y, \frac{k}{2}\right) + u_1\left(y, \frac{k}{2}\right)\right) dy\right),$$

$$q_{\mathrm{rest}} = F^{-1}\left(\chi(k/2)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)\sum_{j=2}^{\infty} u_j\left(y, \frac{k}{2}\right) dy\right),$$

with

$$\chi(k) = \begin{cases} 0, & |k| < \|q\|_1 \\ 1, & |k| \geqslant \|q\|_1. \end{cases}$$

Proof. Set

$$b(k) = \chi(k)\frac{1}{2ik}\int_{-\infty}^{\infty} e^{iky} q(y)u(y,k)\,dy$$

for all $k \in \mathbb{R}$. Then

$$\begin{aligned} q_B &= F^{-1}\left([1 + (\chi(k/2) - 1)]\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)u\left(y, \frac{k}{2}\right) dy\right) \\ &= F^{-1}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)u_0\left(y, \frac{k}{2}\right) dy\right) + F^{-1}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)u_1\left(y, \frac{k}{2}\right) dy\right) \\ &\quad + F^{-1}\left([\chi(k/2) - 1]\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)\left(u_0\left(y, \frac{k}{2}\right) + u_1\left(y, \frac{k}{2}\right)\right) dy\right) \\ &\quad + F^{-1}\left(\chi(k/2)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{i\frac{k}{2}y} q(y)\sum_{j=2}^{\infty} u_j\left(y, \frac{k}{2}\right) dy\right) \\ &= q + q_1 + \tilde{q} + q_{\mathrm{rest}}. \end{aligned}$$

□

Since F and F^{-1} map compactly supported distributions to C^∞ functions, we have $\tilde{q} \in C^\infty(\mathbb{R})$ and so

$$q_B - q - q_1 - q_{\mathrm{rest}} \in C^\infty(\mathbb{R}). \tag{8}$$

Our aim is to conclude that the difference $q_B - q$ is (at least) continuous. To that end it remains to estimate q_1 and q_{rest}. We start with q_1 for which we can even find an explicit formula.

Lemma 6. *Under the same assumptions for $q(x)$ as in lemma 1, the first nonlinear term of the Born expansion admits the representation*

$$q_1(x) = \frac{1}{2}\left(\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y\right)^2 - \left(\int_{-\infty}^{x} q(y)\,\mathrm{d}y\right)^2.$$

Proof. The proof is a straightforward computation starting from the definition

$$\begin{aligned} q_1(x) &= F^{-1}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{k}{2}y} q(y) u_1\left(y, \frac{k}{2}\right)\mathrm{d}y\right) \\ &= F^{-1}\left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{k}{2}y} q(y)\frac{1}{\mathrm{i}k}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k|y-z|/2} q(z) u_0\left(z, \frac{k}{2}\right)\mathrm{d}z\,\mathrm{d}y\right) \\ &= \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y\int_{-\infty}^{\infty} q(z)\,\mathrm{d}z\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{k}{2}(|y-z|+z+y-2x)}\frac{\mathrm{d}k}{k} \\ &= \frac{1}{\pi}\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y\int_{-\infty}^{\infty} q(z)\,\mathrm{d}z\int_{0}^{\infty} \frac{\sin\left(\frac{k}{2}(|y-z|+z+y-2x)\right)}{k}\,\mathrm{d}k. \end{aligned}$$

Since

$$\int_0^{\infty} \frac{\sin(k\beta)}{k}\,\mathrm{d}k = \frac{\pi}{2}\,\mathrm{sgn}\,\beta$$

and

$$|y-z| + z + y = 2\max(y, z),$$

we get

$$\begin{aligned} q_1(x) &= \frac{1}{2}\int_{-\infty}^{\infty} q(y)\int_{-\infty}^{\infty} q(z)\,\mathrm{sgn}(|y-z|+z+y-2x)\,\mathrm{d}y\,\mathrm{d}z \\ &= \frac{1}{2}\int_{-\infty}^{\infty} q(y)\int_{-\infty}^{\infty} q(z)\,\mathrm{sgn}(\max(y,z)-x)\,\mathrm{d}y\,\mathrm{d}z. \end{aligned}$$

Elementary considerations of the signum function above yield

$$q_1(x) = \frac{1}{2}\left(\int_{x}^{\infty} q(y)\,\mathrm{d}y\right)^2 + \int_{-\infty}^{x} q(y)\int_{x}^{\infty} q(z)\,\mathrm{d}y\,\mathrm{d}z - \frac{1}{2}\left(\int_{-\infty}^{x} q(y)\,\mathrm{d}y\right)^2$$

or

$$q_1(x) = \frac{1}{2}\left(\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y\right)^2 - \left(\int_{-\infty}^{x} q(y)\,\mathrm{d}y\right)^2$$

after completing the square. □

We conclude from lemma 6 that $q_1(x)$ is bounded and continuous. The same turns out to be true for $q_{\mathrm{rest}}(x)$.

Lemma 7. *Under the same assumptions for $q(x)$ as in lemma 1, the term $q_{\mathrm{rest}}(x)$ in the Born expansion is bounded and continuous.*

Proof. We start with the elementary estimate

$$\left|\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\frac{k}{2}y} q(y)\sum_{j=2}^{\infty} u_j\left(y, \frac{k}{2}\right)\mathrm{d}y\right| \leqslant \int_{-\infty}^{\infty} |q(y)|\sum_{j=2}^{\infty}\left|u_j\left(y, \frac{k}{2}\right)\right|\mathrm{d}y \leqslant \frac{C\|q\|_1}{k^2},$$

for $|k| \geqslant 2\|q\|_1$. It follows that

$$|\hat{q}_{\mathrm{rest}}(k)| \leqslant \frac{C}{k^2}, \qquad |k| \geqslant 2\|q\|_1,$$

where the hat denotes the Fourier transform. Hence,

$$\|q_{\mathrm{rest}}\|^2_{H^s(\mathbb{R})} = \int_{-\infty}^{\infty} (1+|k|^2)^s |\hat{q}_{\mathrm{rest}}(k)|^2 \, \mathrm{d}k \leqslant \int_{|k| \geqslant 2\|q\|_1} \frac{C(1+|k|^2)^s}{|k|^4} \, \mathrm{d}k$$
$$\leqslant C \int_{2\|q\|_1}^{\infty} \frac{1}{|k|^{4-2s}} \, \mathrm{d}k < \infty$$

if and only if $s < 3/2$. Here, we have used the fact that

$$\frac{(1+k^2)^s}{(k^2)^s} = \left(1 + \frac{1}{k^2}\right)^s \leqslant \left(1 + \frac{1}{k_0^2}\right)^s, \qquad k \geqslant k_0 > 0, \quad s > 0,$$

i.e. $(1+k^2)^s \leqslant Ck^{2s}$, for $k \geqslant k_0 > 0$, $s > 0$. So

$$q_{\mathrm{rest}} \in H^s(\mathbb{R}),$$

for any $s < 3/2$. Since $H^s(\mathbb{R}) \subset C(\mathbb{R}) \cap L^\infty(\mathbb{R})$, $s > 1/2$, we can conclude that q_{rest} is bounded and continuous. □

Remark 8. The function $q_{\mathrm{rest}}(x)$ is even in $C^\alpha(\mathbb{R})$, $0 < \alpha < 1$, but we do not need this additional smoothness.

We thus have the following result.

Theorem 9. *Suppose that the potential $q(x)$ belongs to $L^1(\mathbb{R})$. Then the difference $q_{\mathrm{B}} - q$ is a continuous function, i.e. the jumps and singularities of q can be recovered from q_{B}.*

Proof. It follows from lemmas 6 and 7 that we can remove q_1 and q_{rest} from the smoothness result (8). This establishes the theorem. □

Remark 10. In particular, we can recover from q_{B} any unknown bounded interval on the line.

3. The second incident direction

In dimension 1 we can study all (both) possible incident directions. The second choice is $u_0(x,k) = \mathrm{e}^{-\mathrm{i}kx}$. Now, we are led to the Lippmann–Schwinger equation

$$u(x,k) = \mathrm{e}^{-\mathrm{i}kx} + \frac{1}{2\mathrm{i}k} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}k|x-y|} q(y) u(y,k) \, \mathrm{d}y.$$

In this case the asymptotics become

$$u(x,k) = \mathrm{e}^{-\mathrm{i}kx} a_1(k) + o(1), \qquad x \to -\infty,$$
$$u(x,k) = \mathrm{e}^{-\mathrm{i}kx} + b_1(k)\,\mathrm{e}^{\mathrm{i}kx} + o(1), \qquad x \to +\infty,$$

where

$$a_1(k) = 1 + \frac{1}{2\mathrm{i}k} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}ky} q(y) u(y,k) \, \mathrm{d}y,$$
$$b_1(k) = \frac{1}{2\mathrm{i}k} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}ky} q(y) u(y,k) \, \mathrm{d}y.$$

Hence, we define

$$q_{\mathrm{B}}^{-}(x) = F\left(\frac{\mathrm{i}k}{\sqrt{2\pi}} b_1(k/2)\right) = \frac{\mathrm{i}}{2\pi}\int_{-\infty}^{\infty} k b_1(k/2)\,\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k.$$

The Born series of $q_{\mathrm{B}}^{-}(x)$ can be analysed as above to arrive at the conclusion of theorem 9. Furthermore, the first nonlinear term becomes

$$q_1^{-}(x) = \frac{1}{2}\left(\int_{-\infty}^{\infty} q(y)\,\mathrm{d}y\right)^2 - \left(\int_{x}^{\infty} q(y)\,\mathrm{d}y\right)^2.$$

It follows that the average of q_1 terms assumes the beautiful symmetrical form

$$\frac{q_1^{-}(x) + q_1(x)}{2} = \int_{-\infty}^{x} q(y)\,\mathrm{d}y \int_{x}^{\infty} q(y)\,\mathrm{d}y$$

so that, e.g.

$$\lim_{x\to\pm\infty} \frac{q_1^{-}(x) + q_1(x)}{2} = 0.$$

4. Numerical examples

In this section we give some examples of discontinuities of q and how they can be recovered from q_{B}. We assume that $\operatorname{supp} q \subset [0, 1]$.

As is already noted, for q_{B} it remains to compute

$$f(x) = \int_0^{\infty} k b(k/2)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}k.$$

We do this using the Gauss–Laguerre quadrature rule of order $l \in \mathbb{N}$,

$$\int_0^{\infty} \mathrm{e}^{-k} g(k)\,\mathrm{d}k \approx \sum_{j=1}^{l} \omega_j g(k_j),$$

where the abscissas k_j are the roots of the Laguerre polynomial $L_l(x)$ and the weights ω_j are given by

$$\omega_j = \frac{1}{k_j L_l'(k_j)^2}, \qquad j = 1, 2, \ldots, l.$$

The Laguerre polynomials are defined by

$$L_j(x) = \frac{\mathrm{e}^x}{j!}\frac{\mathrm{d}^j}{\mathrm{d}x^j}(x^j\,\mathrm{e}^{-x}), \qquad j = 0, 1, \ldots,$$

but we compute them from the recurrence relation

$$L_0(x) = 1, \qquad L_1(x) = 1 - x,$$
$$(j+1)L_{j+1}(x) = (2j + 1 - x)L_j(x) - jL_{j-1}(x), \qquad j = 1, 2, \ldots.$$

So

$$f(x) \approx \sum_{j=1}^{l} \omega_j\,\mathrm{e}^{k_j(1-\mathrm{i}x)} k_j b(k_j/2). \tag{9}$$

For (9) we need to compute an approximation to our data $b(k)$. For $|k| \geqslant \|q\|_1$, we use the Simpson quadrature rule to get

$$b(k) = \frac{1}{2\mathrm{i}k}\int_0^1 \mathrm{e}^{\mathrm{i}ky} q(y)u(y,k)\,\mathrm{d}y \approx \frac{1}{2\mathrm{i}k}\sum_{j=0}^{2n} w_j\,\mathrm{e}^{\mathrm{i}ky_j} q(y_j)u(y_j,k), \tag{10}$$

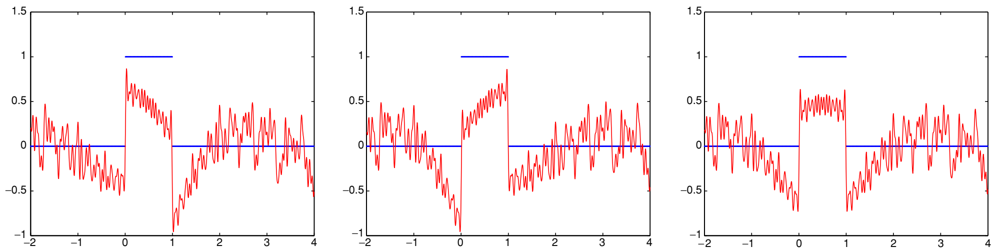

Figure 1. Recovery of jump discontinuity of height 1.

where $y_j = \frac{j}{2n}$, $j = 0, 1, 2, \ldots, 2n$, and

$$w_j = \frac{1}{6n} \times \begin{cases} 1, & j = 0, 2n \\ 4, & j = 1, 3, 5, \ldots, 2n-1 \\ 2, & j = 2, 4, 6, \ldots, 2n-2. \end{cases}$$

Finally, given $k \in \mathbb{R}$, for (10) we need the (approximate) solution $u(y_j, k)$ of

$$u(x,k) = \mathrm{e}^{\mathrm{i}kx} + \frac{1}{2\mathrm{i}k} \int_0^1 \mathrm{e}^{\mathrm{i}k|x-y|} q(y) u(y,k)\,\mathrm{d}y \tag{11}$$

at isolated points y_j. An application of the Simpson rule gives

$$u(x,k) \approx \mathrm{e}^{\mathrm{i}kx} + \frac{1}{2\mathrm{i}k} \sum_{j=0}^{2n} w_j\, \mathrm{e}^{\mathrm{i}k|x-y_j|} q(y_j) u(y_j,k).$$

Evaluating this at $x = y_s$, $s = 0, 1, 2, \ldots, 2n$, results in the (approximate) linear system

$$u(y_s,k) \approx \mathrm{e}^{\mathrm{i}ky_s} + \frac{1}{2\mathrm{i}k} \sum_{j=0}^{2n} w_j\, \mathrm{e}^{\mathrm{i}k|y_s-y_j|} q(y_j) u(y_j,k), \qquad s = 0, 1, 2, \ldots, 2n.$$

From this system we find $u(y_j, k)$, $j = 0, 1, 2, \ldots, 2n$, for $|k| \geqslant \|q\|_1$. The other incident direction is treated in an analogous manner.

We remark that while the Gaussian quadrature is often more suitable for singular integration, it loses its appeal when we need to have excessively many abscissas in the Nyström method above. Furthermore, we ignore the possible singularities in (10) and (11), as is justified in [17], by setting $q(x) = 0$ at the points of singularity. Fortunately, this simplification will not deteriorate the resolution of the singularities of q. Recall also that the Born approximation is better if q is small in norm.

Our basic example is the jump discontinuity in the form of the characteristic function of an interval. The potential $q(x) = \chi_{(0,1)}(x)$ is presented in figure 1 together with $q_{\mathrm{B}}(x)$ (left), $q_{\mathrm{B}}^-(x)$ (middle) and $\frac{q_{\mathrm{B}}(x)+q_{\mathrm{B}}^-(x)}{2}$ (right). Figure 2 presents what in our minds is an excellent recovery of the smaller jump $q(x) = 0.1\chi_{(0,1)}(x)$. In figure 3 we consider the algebraic and logarithmic singularities,

$$q(x) = \chi_{(0,1)}(x)\left(\frac{1}{\sqrt{x}} - 1\right) \qquad \text{and} \qquad q(x) = \chi_{(0,1)}(x)\log x,$$

respectively. For the latter three examples, it suffices to look at $q_{\mathrm{B}}(x)$ only. We report without details that $q_{\mathrm{B}}^-(x)$ and $\frac{q_{\mathrm{B}}(x)+q_{\mathrm{B}}^-(x)}{2}$ give a comparable resolution of the jump and singularities in these cases.

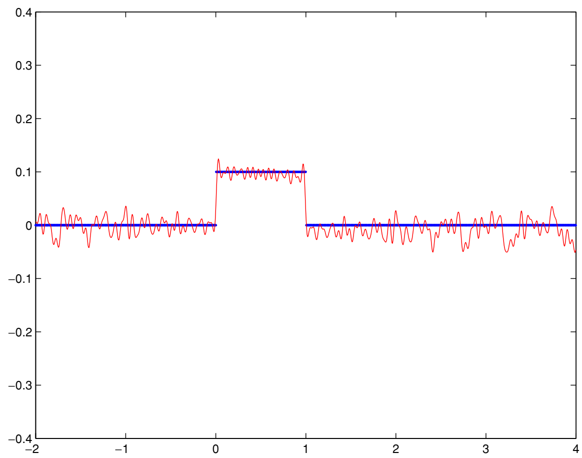

Figure 2. Recovery of jump discontinuity of height 0.1.

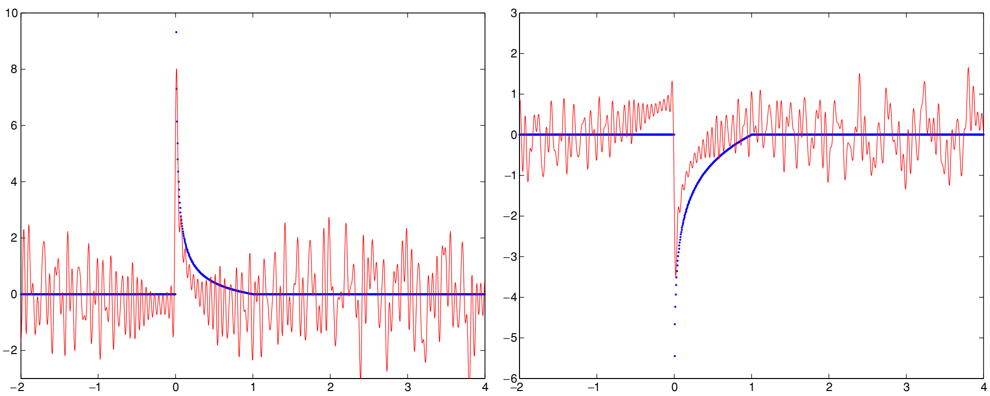

Figure 3. Recovery of algebraic and logarithmic singularities.

In all of the experiments we have used the values $n = 128$ and $l = 32$. We see that in all the cases, the location and type of the singularity are recovered reasonably well, but the higher jump remains rather inaccurate. Moreover, these experiments suggest that especially in the search for 'higher' jumps, one should look at the average of q_B terms in order to identify the unknown interval. Luckily enough this does not become a problem as the computation of q_B is relatively simple (and fast) once the data are available.

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