The hard pulse approximation for the AKNS 2×2-system

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Abstract

In the hard pulse approximation, commonly used in nuclear magnetic resonance, one considers potentials for the AKNS system that are sums of δ-functions. The system of differential equations does not, strictly speaking make sense for such potentials. In [8] an analogous discrete forward and inverse problem are analyzed. We review these results and show that pulses obtained using the inverse scattering transform for this *hard pulse* approximation converge to the expected continuum potential pointwise and in the L^1-norm. We also show that the AKNS system makes sense with potentials that are nonatomic measures with finite total variation.

1 Introduction

To solve the problem of RF-pulse synthesis in nuclear magnetic resonance it is convenient to introduce the spin domain formulation of the Bloch equation. This describes the evolution of a $\mathbb{C}^2$-valued function $\boldsymbol{\psi}$, under the influence of a potential q :

$$\frac{d\boldsymbol{\psi}}{dt}(\xi;t) = \begin{bmatrix} -i\xi & q(t) \\ -q^*(t) & i\xi \end{bmatrix} \boldsymbol{\psi}(\xi;t). \tag{1}$$

Here ξ is a frequency variable and we follow the convention in MR of denoting complex conjugation with an asterisk, e.g. z^*. This is known in the mathematics literature as the Zakharov-Sabat system or the 2×2-AKNS system.

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Scattering theory for an equation like (1) relates the behavior of $\lim_{t\to-\infty}\boldsymbol{\psi}(\xi;t)$ to that of $\lim_{t\to\infty}\boldsymbol{\psi}(\xi;t)$, or vice versa. If q has bounded support, then the functions

$$\begin{bmatrix} e^{-i\xi t} \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ e^{i\xi t} \end{bmatrix}$$

are a basis of solutions for (1) outside the support of q. If the L^1-norm of q is finite, then it is shown in [1] that (1) has solutions which are asymptotic to these solutions as $t \to \pm\infty$. The basic result is:

Theorem 1. *If $\|q\|_{L^1}$ is finite, then, for every real ξ, there are* unique *solutions*

$$\boldsymbol{\psi}_{1+}(\xi), \boldsymbol{\psi}_{2+}(\xi) \text{ and } \boldsymbol{\psi}_{1-}(\xi), \boldsymbol{\psi}_{2-}(\xi)$$

to equation (1) *which satisfy*

$$\lim_{t\to-\infty} e^{i\xi t}\boldsymbol{\psi}_{1-}(\xi;t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \lim_{t\to-\infty} e^{-i\xi t}\boldsymbol{\psi}_{2-}(\xi;t) = \begin{bmatrix} 0 \\ -1 \end{bmatrix} \tag{2}$$

$$\lim_{t\to\infty} e^{i\xi t}\boldsymbol{\psi}_{1+}(\xi;t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \lim_{t\to\infty} e^{-i\xi t}\boldsymbol{\psi}_{2+}(\xi;t) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{3}$$

The solutions $\boldsymbol{\psi}_{1-}(\xi)$, $\boldsymbol{\psi}_{2+}(\xi)$ extend as analytic functions of ξ to the upper half plane, $\operatorname{Im}\xi > 0$ *and $\boldsymbol{\psi}_{2-}(\xi)$, $\boldsymbol{\psi}_{1+}(\xi)$ extend as analytic functions of ξ to the lower half plane,* $\operatorname{Im}\xi < 0$.

The proof of this theorem can be found in [1]. Among other things they show that if we set

$$Q_1(t) = \int_{-\infty}^{t} |q(s)|ds,$$

then

$$|\psi_{11-}(\xi;t)e^{i\xi t}| \le I_0(2Q_1(t)), \quad |\psi_{22-}(\xi;t)e^{-i\xi t}| \le I_0(2Q_1(t)). \tag{4}$$

Here I_0 is the classical I_0-Bessel function. The same argument applies *mutatis mutandis* to obtain $\boldsymbol{\psi}_{1+}$ and $\boldsymbol{\psi}_{2+}$. Indeed, essentially the same arguments show that these estimates hold for potentials that are nonatomic measures of finite total variation. In Theorem 2 we show that the eigenfunctions depend continuously on the potential in the total variation norm.

For real values of ξ, the solutions normalized at $-\infty$ can be expressed in terms of the solutions normalized at $+\infty$ by the linear relations

$$\begin{aligned} \boldsymbol{\psi}_{1-}(\xi;t) &= a(\xi)\boldsymbol{\psi}_{1+}(\xi;t) + b(\xi)\boldsymbol{\psi}_{2+}(\xi;t), \\ \boldsymbol{\psi}_{2-}(\xi;t) &= b^*(\xi)\boldsymbol{\psi}_{1+}(\xi;t) - a^*(\xi)\boldsymbol{\psi}_{2+}(\xi;t). \end{aligned} \tag{5}$$

The functions a, b are called the *scattering coefficients* for the potential q. The 2×2-matrices $[\boldsymbol{\psi}_{1-}\boldsymbol{\psi}_{2-}]$, $[\boldsymbol{\psi}_{1+}\boldsymbol{\psi}_{2+}]$ satisfy

$$[\boldsymbol{\psi}_{1-}\boldsymbol{\psi}_{2-}] = [\boldsymbol{\psi}_{1+}\boldsymbol{\psi}_{2+}] \begin{bmatrix} a(\xi) & b^*(\xi) \\ b(\xi) & -a^*(\xi) \end{bmatrix}. \tag{6}$$

It is well known that a extends to the upper half plane as an analytic function. If q has an integrable derivative, then, it can be shown that

$$a(\xi) = 1 + \frac{1}{2i\xi}\int_{-\infty}^{\infty} |q(s)|^2 ds + O(\frac{1}{\xi^2}), \tag{7}$$

as $|\xi|$ tends to infinity in $\operatorname{Im}\xi \geq 0$. As the Wronskian, $W(\boldsymbol{\psi}_{1-}, \boldsymbol{\psi}_{2-}) = -1$, it follows that

$$|a(\xi)|^2 + |b(\xi)|^2 = 1, \tag{8}$$

and therefore (7) implies that

$$|b(\xi)| = O(\frac{1}{|\xi|}) \quad \text{as } \xi \to \pm\infty. \tag{9}$$

Assuming that $t^j q(t)$ is integrable for all j, it is shown in [1] that a has finitely many zeros in $\operatorname{Im}\xi \geq 0$. Let $\{\xi_1, \ldots, \xi_N\}$ be a list of the zeros of a. For each j there is a *nonzero* complex number C_j' so that

$$\boldsymbol{\psi}_{1-}(\xi_j) = C_j' \boldsymbol{\psi}_{2+}(\xi_j), \quad j = 1, \ldots, N. \tag{10}$$

The constants $\{C_1', \ldots, C_N'\}$ appearing in (10) are called *norming constants*. Equation (1) can be rewritten in the form

$$\begin{bmatrix} i\partial_t & -iq \\ -iq^* & -i\partial_t \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \xi \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \tag{11}$$

From this formulation it is clear that ξ should be regarded as a spectral parameter. If ξ has positive imaginary part, then $\boldsymbol{\psi}_{1-}(\xi; t)$ decays exponentially as t tends to $-\infty$ and $\boldsymbol{\psi}_{2+}(\xi; t)$ decays exponentially as t tends to $+\infty$. If $a(\xi_j) = 0$, then (10) implies that $\boldsymbol{\psi}_{1-}(\xi_j; t)$ decays exponentially at both $\pm\infty$ and therefore the function $\boldsymbol{\psi}_{1-}(\xi_j; t)$ belongs to $L^2(\mathbb{R}; \mathbb{C}^2)$. Thus the operator on the left hand side of (11) has *bound states* for these values of ξ.

***Definition* 1.** The pair of functions $(a(\xi), b(\xi))$, for $\xi \in \mathbb{R}$, and the collection of pairs $\{(\xi_j, C_j) \ : \ j = 1, \ldots, N\}$ define the *scattering data* for equation (1).

We generally assume that the zeros of a are simple and that their imaginary parts are positive. This is mostly to simplify the exposition, there is no difficulty, in principle, if a has real zeros or higher order zeros. There is a very useful "Plancherel relation" or energy formula relating the L^2-norm of q to the scattering data:

$$\int_{-\infty}^{\infty} |q(t)|^2 dt = \frac{1}{\pi}\int_{-\infty}^{\infty} \log(1 + |r(\xi)|^2) d\xi + 4\sum_{j=1}^{N} \operatorname{Im}\xi_j. \tag{12}$$

The scattering data are not quite independent. The *reflection* coefficient is defined by

$$r(\xi) = \frac{b(\xi)}{a(\xi)}. \tag{13}$$

A priori the reflection coefficient is only defined on the real axis. We can express a in terms of r and the locations of its zeros:

$$a(\xi) = \prod_{j=1}^{n}\left(\frac{\xi-\xi_j}{\xi-\xi_j^*}\right)\exp\left[\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{\log(1+|r(\zeta)|^2)d\zeta}{\zeta-\xi}\right]. \tag{14}$$

Equation (14) has a well defined limit as ξ approaches the real axis. Assuming that a has simple zeros, we let

$$C_j = \frac{C_j'}{a'(\xi_j)} \text{ for } j = 1, \dots, N. \tag{15}$$

***Definition* 2.** The function $r(\xi)$, for $\xi \in \mathbb{R}$ and the collection of pairs $\{(\xi_j, C_j) : j = 1, \dots, N\}$ define the *reduced scattering data* for equation (1).

Implicitly the reduced scattering data is a function of the potential q. In inverse scattering theory, the data $\{r; (\xi_1, C_1), \dots, (\xi_N, C_N)\}$ are specified, and we seek a potential q which has this reduced scattering data. The map from this data to q is often called the *Inverse Scattering Transform* or *IST*.

In applications to NMR, the refelction coefficient is specified and one seeks a potential that produces it. This is explained in detail in [5]. A standard technique for solving this problem is to find a potential that is a sum of equally spaced δ-functions or *hard pulses*:

$$q_h(t) = \sum_{j=-\infty}^{\infty}\mu_j\delta_0(t - j\Delta). \tag{16}$$

It is easy to see that any solution, $\boldsymbol{\psi}$, to (1), with a potential of this form, would have to be discontinuous at each $j\Delta$ for which $\mu_j \neq 0$. As the wave front sets at $t = j\Delta$ of $\boldsymbol{\psi}(\xi; t)$ and $\mu_j\delta_0(t - j\Delta)$ are nonempty and equal, one cannot make sense, even as distributions, of the product $\boldsymbol{\psi}(\xi; t)q_h(t)$. For this reason, neither the differential equation nor the equivalent integral equation make any obvious sense for a potential of this form. Nonetheless, if one considers q_h as a limit of the "softened" potentials:

$$q_\epsilon = \sum_{j=-\infty}^{\infty}\frac{\mu_j}{\epsilon}\chi_{[0,\epsilon)}(t - j\Delta), \tag{17}$$

then the corresponding normalized solutions, $\boldsymbol{\psi}_\epsilon$ have limits as $\epsilon \to 0^+$, which are piecwise smooth functions of t having jump discontinuities at $\operatorname{supp} q_h$. This is the approach taken in the physics and NMR literature. In second author's thesis, a discrete analogue of the ZS-system is introduced, see [8]. It is shown that there is a scattering and inverse scattering theory entirely analogous to that for (1) with a smooth potential. Moreover, explicit, non-iterative algorithms are given for the solution of the inverse problem. These algorithms are much more stable than the standard approaches to solving the Marchenko equations, especially when there are bound states.

In this paper we show that, under relatively weak assumptions, the potentials found using the discrete approximation converge, as $\Delta \to 0$, to the solution of the continuum inverse scattering problem with limiting scattering data. We also show that the scattering data of the softened potential q_1 approximates that of hard potential q_h, for frequencies in the natural range $[-\frac{\pi}{2\Delta}, \frac{\pi}{2\Delta}]$.

We close this section with a result showing that the forward scattering data depends continuously on the potential in the total variation norm.

Theorem 2. *Suppose that $h_1(s)ds$ and $h_2(s)ds$ are non-atomic measures with finite total variation, and that $F_i^{\pm}(\xi), i = 1, 2$ solves the ZS-system with potential $h_i, i = 1, 2$. Let*

$$\begin{aligned} H^-(t) &= \|h_1(s)ds - h_2(s)ds\|_{\mathrm{TV}(-\infty,t)} \quad Q^-(t) = \|h_1(s)ds\|_{\mathrm{TV}(-\infty,t)} \\ H^+(t) &= \|h_1(s)ds - h_2(s)ds\|_{\mathrm{TV}(t,\infty)} \quad Q^+(t) = \|h_1(s)ds\|_{\mathrm{TV}(t,\infty)}, \end{aligned} \tag{18}$$

If

$$\lim_{t\to\pm\infty} \|F_1^{\pm}(\xi; t) - F_2^{\pm}(\xi; t)\| = 0.$$

Then, for $\xi \in \mathbb{R}$ the differences satisfy the estimates

$$\|F_1^{\pm}(\xi; t) - F_2^{\pm}(\xi; t)\| \le 2I_0(2\|h_2\|_{\mathrm{TV}})H^{\pm}(t)\exp(Q^{\pm}(t)). \tag{19}$$

Proof. The proof of this result is a small modification of the proof of the estimate (4) given in [1]. Let σ denote the 2×2-matrix

$$\sigma = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

and let

$$D^{\pm}(\xi; t) = e^{-it\xi\sigma}(F_1^{\pm} - F_2^{\pm}).$$

For real ξ and t, the matrices $e^{\pm it\xi\sigma}$ are unitary and therefore

$$\|F_1^{\pm} - F_2^{\pm}\| = \|D^{\pm}\|.$$

The vector valued functions $D^{\pm}$ satisfy the equations

$$\begin{aligned} &\partial_t D^{\pm} = e^{-it\xi\sigma}\begin{bmatrix} 0 & h_1 \\ -h_1^* & 0 \end{bmatrix} e^{it\xi\sigma} D^{\pm} + e^{-it\xi\sigma}\begin{bmatrix} 0 & (h_1 - h_2) \\ -(h_1^* - h_2^*) & 0 \end{bmatrix} F_2^{\pm}. \\ &\lim_{t\to\pm\infty} D^{\pm}(\xi; t) = 0. \end{aligned} \tag{20}$$

We now restrict our attention to the $-$ case, the $+$ case is handled by an essentially identical argument.

The differential equation in (20) is equivalent to the integral equation

$$\begin{aligned} D^-(\xi; t) = &\int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & h_1(s) \\ -h_1^*(s) & 0 \end{bmatrix} e^{is\xi\sigma} D^-(\xi; s)ds + \\ &\int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & (h_1 - h_2)(s) \\ -(h_1^* - h_2^*)(s) & 0 \end{bmatrix} F_2^-(s)ds. \end{aligned} \tag{21}$$

This is a Volterra equation that can be solved by the following iteration:

$$\begin{aligned} D_0^-(\xi;t) &= \int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & (h_1-h_2)(s) \\ -(h_1^*-h_2^*)(s) & 0 \end{bmatrix} F_2^-(s)ds \\ D_j^-(\xi;t) &= D_0^-(\xi;t) + \int_{-\infty}^{t} e^{-is\xi\sigma}\begin{bmatrix} 0 & h_1(s) \\ -h_1^*(s) & 0 \end{bmatrix} e^{is\xi\sigma} D_{j-1}^-(\xi;s)ds, \end{aligned} \tag{22}$$

for $j \geq 1$.

First observe that the operator norm defined by the Euclidean norm satisfies

$$\left\| \begin{bmatrix} 0 & \alpha \\ -\alpha^* & 0 \end{bmatrix} \right\| = |\alpha|,$$

and therefore (4) implies that

$$\|D_0^-(\xi;t)\| \leq 2I_0(\|h_2\|_{\mathrm{TV}})H^-(t).$$

We make the inductive assumption that

$$\|D_j^-(\xi;t)\| \leq 2I_0(\|h_2\|_{\mathrm{TV}})H^-(t)\left[\sum_{k=0}^{j} \frac{(Q^-(t))^k}{k!}\right]. \tag{23}$$

From these assumptions and (22) it follows that

$$\|D_{j+1}^-(\xi;t)\| \leq 2I_0(\|h_2\|_{\mathrm{TV}})\left(H^-(t) + \int_{-\infty}^{t} |h_1(s)|H^-(s)\left[\sum_{k=0}^{j} \frac{(Q^-(s))^k}{k!}\right]\right). \tag{24}$$

If $h_1(s)$ is an L^1-function, then the definition of Q^- implies that

$$|h_1(s)| = \partial_s Q^-(s).$$

In general, using a simple approximation argument we can show that

$$\int_{-\infty}^{t} |h_-(s)ds|(Q^-(s))^k \leq \frac{(Q^-(t))^{k+1}}{k+1}, \tag{25}$$

and therefore (24) implies that

$$\|D_{j+1}^-(\xi;t)\| \leq 2I_0(\|h_2\|_{\mathrm{TV}})H^-(t)\left(\sum_{k=0}^{j+1} \frac{(Q^-(s))^k}{k!}\right). \tag{26}$$

This completes the proof of the induction step. As

$$\lim_{j\to\infty} D_j^- = D^-,$$

letting j tend to infinity, completes the proof of the theorem.

$\square$

2 Inverse Scattering for the ZS-System

There are several different approaches to solving the inverse scattering problem, see [1], [2], [3] or [6]. In this section we summarize the solution of this problem via the Marchenko equations. We generally suppose that the $\{\xi_j\}$ are distinct complex numbers with positive imaginary parts. We assume that the reflection coefficient is smooth and rapidly vanishing at $\pm\infty$. Using limiting arguments, the latter restriction is easily relaxed.

The Marchenko equations are systems of integral equations of Fredholm type. We follow the slightly non-standard presentation given in [8], as both the continuous and discrete theories are presented with a consistent notation. Suppose we are given the scattering data $\{r(\xi),\ \xi \in \mathbb{R};\ (\xi_1, C_1), \ldots, (\xi_N, C_N)\}$. Applying the Fourier transform to equation (2.3.13) in [8] we obtain the following integral equation:

$$\begin{aligned} k_t(s) + \int_0^\infty R_t(s,\sigma) k_t(\sigma) \frac{d\sigma}{2\pi} = \\ - \left[\hat{r}^*(-s-2t) + 2\pi i \sum_{j=1}^N C_k^* e^{-i\xi_k^*(s+2t)} \right], \text{ for } s \in [0,\infty). \end{aligned} \tag{27}$$

Here the kernel function R_t is defined by

$$\begin{aligned} R_t(s,\sigma) = \int_{-\infty}^0 & \left[\hat{r}^*(\tau - s - 2t) + 2\pi i \sum_{j=1}^N C_k^* e^{-i\xi_k^*(s-\tau+2t)} \right] \times \\ & \left[\hat{r}(\tau - \sigma - 2t) - 2\pi i \sum_{j=1}^N C_k e^{-i\xi_k(\tau-\sigma-2t)} \right] \frac{d\tau}{2\pi}, \end{aligned} \tag{28}$$

for later use we set:

$$g_t(s) = \hat{r}^*(-s-2t) + 2\pi i \sum_{j=1}^N C_k^* e^{-i\xi_k^*(s+2t)}. \tag{29}$$

Equation (27), the right Marchenko equation, is of the form

$$(\mathrm{Id} + F_t^* F_t) k_t(s) = -g_t(s).$$

Under very mild regularity hypotheses on r the operator F_t^* is easily shown to be bounded and in fact compact, so the $L^2[t,\infty)$-solvability of these equations is trivial. In [4], conditions are given to assure the solvability in higher Sobolev spaces as well.

The connection between the inverse scattering problem and the Marchenko equation is summarized in the following theorem:

Theorem 3. *Given a smooth, rapidly decaying reflection coefficient* r, *and a finite set of pairs* $\{(\xi_j, C_j) \; : \; j = 1, \ldots, N\}$, *with the* $\{\xi_j\}$ *distinct,* $\operatorname{Im}\xi_j > 0$ *and* $C_j \neq 0$ *for* $j = 1, \ldots, N$, *the equation* (27) *has a unique solution for every* $t \in \mathbb{R}$. *If*

$$q(t) = \frac{1}{\pi} k_t(0), \tag{30}$$

then the ZS-system, with this potential, has reflection coefficient r. *It has exactly* N *bound states for frequencies* $\{\xi_1, \ldots, \xi_N\}$ *and the relations* (10) *hold at these points.*

This theorem is proved in [8],[6] and, in a slightly different formulation in [2].

Equation (27) involves integration over positive half rays. If there are bound states, or the reflection coefficient is large, then this system of equations become exponentially ill-conditioned as t decreases towards $-\infty$. It is therefore useful to work both ends against the middle. For that purpose one can derive the *left* Marchenko equation, which involves integration over negative half rays. As we do not consider this equation in detail, we only explain how the left reduced scattering data is related to the right scattering data. Recall that $r = b/a$; given r, we can use (14) to determine a and therefore b. The left reflection coefficient is

$$\tilde{r}(\xi) = -\frac{b^*(\xi)}{a(\xi)}.$$

The left norming constants are related to the right norming constants by the relations:

$$\widetilde{C}_k = -\frac{\xi_k^{-1}}{C_k [a'(\xi_k)]^2}. \tag{31}$$

For the left equation, the exponential correction terms are exponentially decaying as t tends to $-\infty$. In most circumstances one is given the right reduced scattering data. In order to use the left equation one needs to numerically determine both a and b as well as the left norming constants $\{\widetilde{C}_j\}$. This is very difficult to do stably and with sufficient accuracy and is a primary motivation for introducting the hard pulse approximation. The details of this problem and its solution are described in [9]

In the remainder of our analysis we concentrate on the right Marchenko equation, (27), with the understanding that everything said applies, *mutatis mutandis,* to the left formulation as well.

The following Paley-Wiener type theorem is useful in applications:

Theorem 4. *Suppose that* q *is a potential for the ZS-system with support in the half line* $(-\infty, t_+]$. *Then the kernel function*

$$g(s) = \hat{r}(s) - 2\pi i \sum_{j=1}^{N} C_k e^{-i\xi_k s}, \tag{32}$$

for the right Marchenko equation is supported in the ray $[-2t_+, \infty)$. *A similar statement holds for the kernel function of the left Marchenko equation.*

***Remark* 1.** The kernel of the operator $F_t^* F_t$ in the right Marchenko equation is expressible as

$$R_t(s,\sigma) = \int_{-\infty}^{0} g^*(\tau - s - 2t) g(\tau - \sigma - 2t) \frac{d\tau}{2\pi}. \tag{33}$$

Proof of Theorem (4). If q has support in $(-\infty, t_+]$, then the scattering coefficient b has an analytic extension to the upper half plane. This is because $\boldsymbol{\psi}_{1+} = [e^{-i\xi t}, 0]^\dagger$ for $t \geq t_+$, and therefore equation (5) shows that

$$b(\xi) = \boldsymbol{\psi}_{21-}(\xi; t_+) e^{-i\xi t_+}.$$

When r has a meromorphic extension to the upper half plane, then the integrand, g, has a different representation. If the zeros of a in the upper half plane have imaginary parts less than η_0, then

$$g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{b(\xi + i\eta_0)}{a(\xi + i\eta_0)} e^{i(\xi + i\eta_0)t} d\xi, \tag{34}$$

see [1]. Using the well known asymptotics for $\boldsymbol{\psi}_{21-}$, we conclude that $e^{2i\xi t_+} r$ satisfies the hypotheses of the Paley-Wiener Theorem in the half plane $\operatorname{Im}\xi \geq \eta_0$. This function is therefore the Fourier transform of a function with support in $(-\infty, 0]$. Hence g is supported in $[-2t_+, \infty)]$. This argument applies *mutatis mutandis* to the kernel of the left Marchenko equation. □

***Remark* 2.** If a has only simple zeros then (34) implies that the norming constants are given by

$$C_i = \frac{b(\xi_i)}{a'(\xi_i)}.$$

Given that the potential has support in an appropriate half line, the formula (34) defines the kernel functions for the right Marchenko equation, whether or not the zeros of a are simple.

3 The Hard Pulse Approximation

Consider a potential of the form

$$q_h(t) = \sum_{j=-\infty}^{\infty} \mu_j \delta(t - j\Delta),$$

such that

$$\sum_{j=-\infty}^{\infty} |\mu_j| < \infty.$$

We call such a function a *discrete potential*. For potentials this singular, the differential equation (1) does not make sense and is replaced by the recursion:

$$\mathbf{\Psi}_{j+1}(\xi) = \begin{bmatrix} e^{-i\xi\Delta} & 0 \\ 0 & e^{i\xi\Delta} \end{bmatrix} \begin{bmatrix} \cos|\mu_j| & \frac{\mu_j}{|\mu_j|}\sin|\mu_j| \\ -\frac{\mu_j^*}{|\mu_j|}\sin|\mu_j| & \cos|\mu_j| \end{bmatrix} \mathbf{\Psi}_j(\xi). \tag{35}$$

This describes the jump at $t = j\Delta$, in a "solution" to the differential equation with the singular potential. The solutions, $\mathbf{\Psi}_j(\xi)$, of the recursion (35), with standard asymptotic boundary conditions as $j \to \pm\infty$, (see (37)), are periodic in ξ of period $\frac{\pi}{\Delta}$. We therefore use $w = e^{2i\xi\Delta}$ as the spectral parameter for the discrete problem. We suppose that $\Psi_{\pm,j}(w)$ are solutions to (35) with

$$\Psi_{\pm,j}(w) = \begin{bmatrix} A_{\pm,j}(w)w^{-\frac{j}{2}} \\ B_{\pm,j}(w)w^{\frac{j}{2}} \end{bmatrix}, \tag{36}$$

where

$$\lim_{j\to\pm\infty} \begin{bmatrix} A_{\pm,j}(w) \\ B_{\pm,j}(w) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{for all } w \in S^1. \tag{37}$$

The discrete scattering matrix is defined to be

$$\begin{bmatrix} a & -b^* \\ b & a^* \end{bmatrix} = \begin{bmatrix} \Psi_{1+,j}^* & \Psi_{2+,j}^* \\ -\Psi_{2+,j} & \Psi_{1+,j} \end{bmatrix} \begin{bmatrix} \Psi_{1-,j} & -\Psi_{2-,j}^* \\ \Psi_{2-,j} & \Psi_{1-,j}^* \end{bmatrix}, \tag{38}$$

which is easily shown to be independent of j. The reflection coefficient is defined to be

$$r(w) = \frac{b(w)}{a(w)}.$$

The following basic results are established in [8]:

Proposition 1. *Let $\mu : \mathbb{Z} \to \mathbb{C}$ be a sequence of complex numbers such that*

$$\sum_{j=-\infty}^{\infty} |\mu_j| < \infty.$$

Then there are unique solutions $\mathbf{\Psi}_{\pm,j}$ to equations (35), satisfying (36) and (37). Furthermore, for each integer j, the functions $A_{-,j}$, $w^{-1}B_{-,j}$, $A_{+,j}^*$ and $B_{+,j}^*$ extend analytically to the unit disk in w.

1. The functions a and b are in $L^2(S^1)$ and satisfy
$$|a(w)|^2 + |b(w)|^2 = 1 \quad \text{for } w \in S^1 \text{ and } \hat{a}(0) > 0. \tag{39}$$
2. The function $a = A_{+,j}^* A_{-,j} + B_{+,j}^* B_{-,j}$ has an analytic extension to the unit disk. We assume that a has finitely many zeros $\{w_1, \ldots, w_m\}$ in the unit disk, which are all simple. For each zero w_k of a, there is a constant c_k' such that
$$\begin{bmatrix} A_{-,j}(w_k) \\ B_{-,j}(w_k) \end{bmatrix} = c_k' \begin{bmatrix} -B_{+,j}^*(w_k)w_k^j \\ A_{+,j}^*(w_k)w_k^j \end{bmatrix} \text{ for all } j \in \mathbb{Z}. \tag{40}$$

Set

$$c_k = \frac{c'_k}{a'(w_k)} \tag{41}$$

3. The functions $A_\pm$ and $B_\pm$ are in $L^2(S^1)$ and satisfy

$$|A_{\pm,j}(w)|^2 + |B_{\pm,j}(w)|^2 = 1 \text{ for } w \in S^1 \text{ and } \hat{A}_{\pm,j}(0) > 0. \tag{42}$$

4. The data $(a, b; w_1, \ldots, w_m; c'_1, \ldots, c'_m)$ is called the *discrete scattering data* for the potential q, and the data $(r; w_1, \ldots, w_m; c_1, \ldots, c_m)$ is called the *reduced discrete scattering data* for the potential q.

5. The functions a and b can be determined from the reduced scattering data by the formulas

$$\begin{aligned} a &= \prod_{k=1}^{m} \left(\frac{w_k^*}{|w_k|} \frac{w_k - w}{1 - w_k^* w} \right) \cdot \exp(-\tilde{\Pi}_+(1 + |r|^2)) \\ b &= ra. \end{aligned} \tag{43}$$

Here Π_+ is the projection onto the positive Fourier components and:

$$\tilde{\Pi}_+ \left(\sum_{j=-\infty}^{\infty} a_j w^j \right) = \sum_{j=1}^{\infty} a_j w^j + \frac{1}{2} a_0, \tag{44}$$

and Π_- is the analogous projection onto the negative Fourier components.

6. The function $\frac{w B^*_{+,j}}{\hat{A}_{+,j}(0)}$ can be determined from the reduced scattering data. It is the unique solution to the discrete right Marchenko equation:

$$(1 + \Pi_+ r_j^* \Pi_- r_j \Pi_+) \left(\frac{w B^*_{+,j}}{\hat{A}_{+,j}(0)} \right) = -\Pi_+ r_j^*, \tag{45}$$

where

$$r_j = \Pi_- r w^{j-1} - \sum_{k=1}^{m} \frac{c_k w_k^j}{w - w_k}. \tag{46}$$

7. The potential $q(t) = \sum_{j=-\infty}^{\infty} \mu_j \delta(t - j\Delta)$ can be recovered using

$$\mu_j = \frac{\gamma_j}{|\gamma_j|} \arctan |\gamma_j| \text{ with } \gamma_j = \mathscr{F}(\frac{w B^*_{+,j}}{\hat{A}_{+,j}(0)})(1). \tag{47}$$

Here $\mathscr{F}$ denotes the Fourier transforms as the map from $L^2(S^1) \to \ell^2(\mathbb{Z})$ defined by

$$\mathscr{F}(f)(n) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-in\theta} d\theta. \tag{48}$$

Theorem 5. *Let $S = (r; w_1, \ldots, w_m; c_1, \ldots, c_m)$ be arbitrary discrete reduced scattering data, as above, such that r is in $H^1(S^1)$. Then there is a well defined discrete potential $q(t) = \sum_{j=-\infty}^{\infty} \mu_j \delta(t - j\Delta)$ for the ZS-system such that S is the corresponding discrete scattering data. This potential can be found by solving equation* (45) *and using* (47)*.*

There is entirely analogous left scattering data and a left Marchenko equation. The left reflection coefficient $s = -\frac{b^*}{a}$ and the left norming constants are related to the right by:

$$\tilde{c}_k = \frac{-w_k^{-1}}{c_k\,[a'(w_k)]^2}. \tag{49}$$

In their frequency domain formulation, equations (45) and (46), the Marchenko equations, admit of a recursive solution. It is both extremely efficient and very stable; for the details see [8].

4 Convergence of Hard Pulses

Let $S = (r; \xi_1, \ldots, \xi_N; C_1, \ldots, C_N)$ be reduced continuum scattering data with $r \in H^1(\mathbb{R})$. There is a unique potential $q : \mathbb{R} \to \mathbb{C}$ corresponding to S. However, to practically compute $q(t)$ for some $t \in \mathbb{R}$, one needs to use a finite, discrete approximation to the Marchenko equation. We describe a method of doing this, using the hard pulse approximation, and then show the pointwise convergence of the softened pulses $\{q_1^\Delta\}$ to q as $\Delta \to 0$.

Choose a time step Δ. As the reflection coefficient for the discrete inverse problem we use the periodic function

$$r^\Delta(\xi) = e^{2i\xi\Delta} \sum_{n=-\infty}^{\infty} r(\xi + \frac{n\pi}{\Delta}). \tag{50}$$

As in ordinary signal processing, there is obviously a notion of Nyquist sampling rate for discrete approximation in inverse scattering. We assume that r is smooth enough and decays rapidly enough so that this sum and its term by term derivative converge absolutely and uniformly. The bound states are defined by the pairs $\{(w_k, 2\Delta i w_k C_k)\}$ where $w_k = e^{2\Delta i \xi_k}$.

If we conjugate the discrete Marchenko equation,

$$(1 + \Pi_+ r_j^{\Delta *} \Pi_- r_j^\Delta \Pi_+) h_{j\Delta} = -\Pi_+ r_j^{\Delta *},$$

by the Fourier transform then, for each j, we obtain the equation:

$$\begin{aligned} \tilde{K}_{j\Delta}^\Delta(m) + \sum_{n=1}^{\infty} \tilde{R}_{j\Delta}^\Delta(m,n) \tilde{K}_{j\Delta}^\Delta \frac{\Delta}{\pi} &= \\ -\left[\frac{\Delta}{\pi} \hat{r}^*(-2\Delta(m+j)) + 2\Delta i \sum_{l=1}^{m} C_l^* e^{-2i\Delta(m+j)\xi_l^*}\right] &\text{ for } m > 0. \end{aligned} \tag{51}$$

The discrete kernel function is given by

$$\tilde{R}^{\Delta}_{j\Delta}(m,n) = \sum_{l=-\infty}^{-1} \hat{r}^*(2\Delta(l-m-j))\hat{r}(2\Delta(l-n-j))\frac{\Delta}{\pi}. \tag{52}$$

This is simply the Riemann sum approximation to equation (27), with $t = j\Delta$ and sample spacing 2Δ. The jth coefficient of the hard pulse is

$$\mu_j = \frac{\gamma_j}{|\gamma_j|} \arctan|\gamma_j|$$

where $\gamma_j = \tilde{K}^{\Delta}_{j\Delta}(1)$.

We define a piecewise constant function on $[0,\infty)$ by setting

$$K^{\Delta}_{j\Delta}(s) = \frac{\pi}{\Delta}\tilde{K}^{\Delta}_{j\Delta}(m) \text{ for } \quad 2(m-1)\Delta \leq s < 2m\Delta. \tag{53}$$

We denote the piecewise constant extension, in both variables, of $\tilde{R}^{\Delta}_{j\Delta}$ to $[0,\infty) \times [0,\infty)$ by $R^{\Delta}_{j\Delta}(s,\sigma)$, and set

$$\begin{aligned} G^{\Delta}_{j\Delta}(s) =& \hat{r}^*(-2\Delta(m+j)) + 2\pi i \sum_{l=1}^{N} C_l^* e^{-2i\Delta(m+j)\xi_l^*} \quad \text{for } 2(m-1)\Delta \leq s < 2m\Delta \\ =& g_{j\Delta}(-2\Delta(m+j)) \quad \text{for } 2(m-1)\Delta \leq s < 2m\Delta, \end{aligned} \tag{54}$$

where g_t is defined in (29). With these definitions we see that, except possibly for a discrete set of points,

$$K^{\Delta}_{j\Delta}(s) + \int_0^{\infty} R^{\Delta}_{j\Delta}(s,\sigma)K^{\Delta}_{j\Delta}(\sigma)\frac{d\sigma}{2\pi} = -G^{\Delta}_{j\Delta}(s), \text{ for } s \geq 0. \tag{55}$$

For the remainder of this section we assume that $\hat{r}$, $\partial_s\hat{r}$ and $\partial_s^2\hat{r}$ are in $L^1(\mathbb{R})$ and tend to zero as $|s| \to \infty$, which is the case if r is sufficiently smooth and decays sufficiently rapidly. We let $A_t : L^2[0,\infty) \to L^2[0,\infty)$ denote the operator defined by R_t and $A^{\Delta}_{j\Delta} : L^2[0,\infty) \to L^2[0,\infty)$ denote the operator defined by $R^{\Delta}_{j\Delta}$.

Lemma 1. *If $j\Delta \leq t < (j+1)\Delta$, then the L^2-operator norm of the difference $A_t - A^{\Delta}_{j\Delta}$ satisfies the estimate*

$$\|A_t - A^{\Delta}_{j\Delta}\| \leq 12(\Delta + |j\Delta - t|)N(t) \tag{56}$$

where

$$\begin{aligned} M_0(y) = \sup_{x\leq 0}|g(x-y)| \textit{ and } M_1(y) = \int_{-\infty}^{0} |\partial_s g(x-y)|dx \\ N(t)^2 = \left[\int_0^{\infty} M_0^2(s+2t)ds\right]\left[\int_0^{\infty} M_1^2(s+2t)ds\right]. \end{aligned} \tag{57}$$

***Remark* 3.** The function g is defined in (32). Our assumptions on $\hat{r}$ imply that M_0 and M_1 are uniformly bounded and $N(t)$ is finite for each t.

Proof. These estimates follow from the elementary fact that the L^2-operator norm satisfies the estimate

$$\|A_t - A^{\Delta}_{j\Delta}\| \leq \|R_t - R^{\Delta}_{j\Delta}\|_{L^2([0,\infty)^2)}, \tag{58}$$

and pointwise estimates for $|R_t - R^{\Delta}_{j\Delta}|$. To derive the pointwise estimate we see that

$$\begin{aligned} &|R_t(s,\sigma) - R^{\Delta}_{j\Delta}(s,\sigma)| \leq \\ &\sum_{n=-\infty}^{-1}\Bigg[\int\limits_{2\Delta n}^{2\Delta(n+1)} |g(\tau - s - 2t) - g(2\Delta(n-k-j))||g(\tau-\sigma-2t)|d\tau + \\ &\int\limits_{2\Delta n}^{2\Delta(n+1)} |g(\tau - s - 2t) - g(2\Delta(n-m-j))||g(2\Delta(n-k-j))|d\tau\Bigg]. \end{aligned} \tag{59}$$

Here k and m satisfy $2\Delta k \leq s < 2\Delta(k+1)$ and $2\Delta m \leq \sigma < 2\Delta(m+1)$. Assuming that $j\Delta \leq t < (j+1)\Delta$, then these estimates imply that the sum on the right is bounded by

$$6(\Delta + |j\Delta - t|)[M_0(\sigma + 2t)M_1(s+2t) + M_0(s+2t)M_1(\sigma+2t)].$$

The estimate in (56), follows from (58), by using this estimate to bound the L^2-norm of the difference $R_t - R^{\Delta}_{j\Delta}$. □

Using the lemma we can obtain uniform bounds on the difference $|k_t(s) - K^{\Delta}_{j\Delta}(s)|$, for t in any positive ray $[t_0,\infty)$, however the constant in these estimates diverges as $t \to -\infty$. In most applications this is not an issue because, using the left Marchenko equation, we can show that both $k_t(0)$ and $K^{\Delta}_{j\Delta}(0)$ tend uniformly and rapidly to zero as t or $j\Delta$ go to $-\infty$. To prove the bounds on $|k_t(s) - K^{\Delta}_{j\Delta}(s)|$ we need to estimate $\|g_t - G^{\Delta}_{j\Delta}\|_{L^2}$.

Lemma 2. *If* $j\Delta \leq t < (j+1)\Delta$, *then*

$$\|g_t - G^{\Delta}_{j\Delta}\|_{L^2([0,\infty))} \leq (\Delta + |t - j\Delta|)\|\mathcal{M}^{\Delta}\partial_s g\|_{L^2((-\infty,-2t))}, \tag{60}$$

here

$$\mathcal{M}^{\Delta}h(s) = \sup_{|\sigma - s|\leq 4\Delta}|h(\sigma)|.$$

If $2n\Delta \leq s \leq 2(n+1)\Delta$, *then*

$$|g_t(s) - G^{\Delta}_{j\Delta}(s)| \leq (\Delta + |t - j\Delta|)\mathcal{M}^{\Delta}\partial_s g_t(s) \tag{61}$$

Proof. The second estimate is an immediate consequence of the definition of $G^{\Delta}_{j\Delta}$ and the mean value theorem. The first estimate follows from the second by integration. Our assumptions on $\hat{r}$ imply that the right hand side of (60) is finite and tends to zero as $t \to \infty$. □

Using the lemmas we can prove our convergence results.

Theorem 6. *If $\hat{r}$, $\partial_s\hat{r}$, and $\partial_s^2\hat{r}$ are in $L^1(\mathbb{R})$ and tend to zero as $|s| \to \infty$, and $j\Delta \leq t < (j+1)\Delta$, then*

$$\|k_t - K^{\Delta}_{j\Delta}\|_{L^2([0,\infty))} \leq (\Delta + |t - j\Delta|)[\|\mathcal{M}^{\Delta}\partial_s g_t\|_{L^2([0,\infty))} + 12\|G^{\Delta}_{j\Delta}\|_{L^2([0,\infty))}]. \quad (62)$$

Proof. Throughout this argument, L^2 means $L^2([0,\infty))$. Because A_t is a positive self adjoint operator, it follows that

$$\|k_t - K^{\Delta}_{j\Delta}\|_{L^2} \leq \|(\mathrm{Id} + A_t)(k_t - K^{\Delta}_{j\Delta})\|_{L^2}. \quad (63)$$

This estimate implies that

$$\|k_t - K^{\Delta}_{j\Delta}\|_{L^2} \leq \|g_t - G^{\Delta}_{j\Delta}\|_{L^2} + \|(A_t - A^{\Delta}_{j\Delta})K^{\Delta}_{j\Delta}\|_{L^2}. \quad (64)$$

Because the operator in the discrete Marchenko equation is also positive, it follows that $\|K^{\Delta}_{j\Delta}\|_{L^2} \leq \|G^{\Delta}_{j\Delta}\|_{L^2}$. Combining these estimates with (56), and (60) gives (62). □

The uniform pointwise convergence is an immediate consequence. We express the pointwise difference $k_t(s) - K^{\Delta}_{j\Delta}(s)$ as

$$k_t(s) - K^{\Delta}_{j\Delta}(s) = -g_t(s) + G^{\Delta}_{j\Delta}(s) - A_t(k_t - K^{\Delta}_{j\Delta})(s) + (A^{\Delta}_{j\Delta} - A_t)K^{\Delta}_{j\Delta}(s). \quad (65)$$

From this identity we obtain the estimate

$$|k_t(s) - K^{\Delta}_{j\Delta}(s)| \leq |g_t(s) - G^{\Delta}_{j\Delta}(s)| + \sqrt{\int_0^\infty |R_t(s,\sigma)|^2 d\sigma}\,\|k_t - K^{\Delta}_{j\Delta}\|_{L^2} + 12N(t)(\Delta + |t - j\Delta|)\|G^{\Delta}_{j\Delta}\|_{L^2}. \quad (66)$$

Putting this together with the estimates above gives the uniform convergence of $K^{\Delta}_{j\Delta}$ to k_t, as $\Delta \to 0$.

Corollary 1. *If $\hat{r}$, $\partial_s\hat{r}$, and $\partial_s^2\hat{r}$ are in $L^1(\mathbb{R})$ and tend to zero as $|s| \to \infty$, and $j\Delta \leq t < (j+1)\Delta$, then for $s \geq 0$ we have*

$$|k_t(s) - K^{\Delta}_{j\Delta}(s)| \leq (\Delta + |t - j\Delta|)\times \left[\|\mathcal{M}^{\Delta}\partial_s g_t\|_{L^2} + \|\mathcal{M}^{\Delta}\partial_s g_t\|_{L^2}\sqrt{\int_0^\infty |R_t(s,\sigma)|^2 d\sigma} + 12N(t)\|G^{\Delta}_{j\Delta}\|_{L^2}\right]. \quad (67)$$

Let μ_j denote the jth coefficient in the hard pulse $q_h(t)$ with scattering data

$$S_\Delta = \{r_\Delta(w); w_1, \ldots, w_N; 2iw_1C_1\Delta, \ldots, 2iw_NC_N\Delta\}, \tag{68}$$

and $q(t)$ the smooth potential with scattering data $S = \{r(\xi); \xi_1, \ldots, \xi_N, C_1; \ldots, C_N\}$. In light of the formulæ $q(t) = \frac{1}{\pi}k_t(0)$ and

$$\mu_j = \frac{K_{j\Delta}^{\Delta}(0)}{\Delta|K_{j\Delta}^{\Delta}(0)|}\arctan\left[\frac{\Delta}{\pi}|K_{j\Delta}^{\Delta}(0)|\right] = \frac{K_{j\Delta}^{\Delta}(0)}{\pi}[1 + O(\Delta^2|K_{j\Delta}^{\Delta}(0)|)] \tag{69}$$

with

$$q_1^{\Delta}(t) = \sum_{j=-\infty}^{\infty}\frac{\mu_j}{\Delta}\chi_{[0,\Delta)}(t - j\Delta),$$

we have that

$$|q(t) - q_1^{\Delta}(t)| \le C_t\Delta. \tag{70}$$

Here C_t is finite and tends to zero as $t \to \infty$. To summarize we have:

Theorem 7. *If $\hat{r}$, $\partial_s\hat{r}$, and $\partial_s^2\hat{r}$ are in $L^1(\mathbb{R})$ and tend to zero as $|s| \to \infty$, and q is the continuum potential with scattering data S and q_1^{Δ} is the softening of the hard pulse with scattering data S_Δ, then $|q(t) - q_1^{\Delta}(t)| \le C_t\Delta$, where $C_t \to 0$ as $t \to \infty$. Both $q(t)$ and $q_1^{\Delta}(t)$ tend to zero as $t \to -\infty$, at a rate that is uniform in Δ. Indeed $\|q - q_1^{\Delta}\|_{L^1}$ tends to zero as $\Delta \to 0$.*

Proof. From (67) and (69) it follows that

$$\int_t^{\infty} C_s ds < \infty \tag{71}$$

for any $t > -\infty$. All the statements have been proved but the last two. These follow from estimates given in Theorem 4 of [5], which we recall: if g^r (g^l) is the kernel function for the right (left) Marchenko equation, then we set

$$\begin{gathered} M_{g^r}(s) = \sup_{\sigma \ge s}|g^r(\sigma)| \text{ and } I_{g^r}(s) = \int_s^{\infty}|g^r(\sigma)|d\sigma \\ \left(M_{g^l}(s) = \sup_{\sigma \le s}|g^l(\sigma)| \text{ and } I_{g^l}(s) = \int_{-\infty}^{s}|g^l(\sigma)|d\sigma\right). \end{gathered} \tag{72}$$

If $I_{g^r}(2t) < 1$ ($I_{g^l}(2t) < 1$), then

$$|q(t)| \le \frac{M_{g^r}(2t)}{1 - I_{g^r}^2(2t)} \quad \left(|q(t)| \le \frac{M_{g^l}(2t)}{1 - I_{g^l}^2(2t)}\right) \tag{73}$$

These estimates are easily extended to the discrete approximation to the Marchenko equations. The estimates for the left Marchenko equation serve to establish the last two claims in the theorem. □

Beginning with the continuum left scattering data and using the left Marchenko equations, a similar result can be obtained as $t \to -\infty$. However, the left discrete potential is not exactly the same as the discrete potential obtained above: Discretizing the left and right continuum Marchenko equations, separately, in the above sense, does not produce consistent *discrete* scattering data. Such a discretization has been discussed in the literature, for example see [7]. In general, the $\frac{\pi}{\Delta}$-periodization of the left continuum scattering coefficient does not give the discrete left scattering coefficient that corresponds to $r^{\Delta}(w)$. In order to get consistent left and right discrete Marchenko equations, one must first replace the scattering data by discrete scattering data, in the above manner, and then derive the data for the discrete left equation from the data for the discrete right equation. The theorem implies that the left and right discrete potentials differ from the continuum potential, and hence one another, by $O(\Delta)$.

Empirically one finds that small errors in the approximate computation of the left scattering data can lead to large errors in the reconstructed potential. Moreover, as it entails locating the zeros $\{\xi_j\}$, of a and evaluating $a'(\xi_j)$, it is very difficult to compute the left continuum scattering data with sufficient accuracy. On the other hand, the determination of the left discrete scattering data from the right discrete scattering data can often be done with sufficient accuracy and guarantees that the resulting hard pulse has the correct scattering data. In particular, once Δ is small enough for the aliasing error:

$$\sum_{n\neq 0} r(\xi + \frac{\pi n}{\Delta}) \tag{74}$$

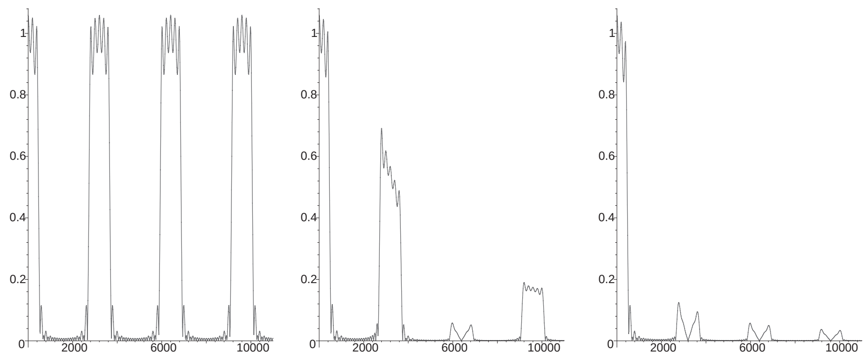
to be small, then the reflection coefficient corresponding to the discrete potential is a very good approximation to the original reflection coefficient in a neighborhood of zero.

The theorem states that $\|q_1^{\Delta} - q\|_{L^1}$ tends to zero as $\Delta \to 0$; one can easily show that the L^2-norms of the functions q_1^{Δ} are uniformly bounded as $\Delta \to 0$. Hence, if Z^{Δ} are the locations of the bound states of the potential q_1^{Δ}, then the energy formula implies that the sum

$$\sum_{\xi \in Z^{\Delta}} \operatorname{Im} \xi$$

is uniformly bounded. We can therefore use Theorem 2 to conclude that the bound state data for the potential q_1^{Δ}, at least for $\operatorname{Re}\xi$ in a fixed interval converges, as $\Delta \to 0$, to the bound state data of $q(t)$.

The behavior of $r_1^{\Delta}(\xi)$ for large $|\xi|$ is governed by the asymptotics for a piecewise constant potential. These are spelled out in Appendix A. We see the decaying side lobes, with periodicity $\frac{\pi}{\Delta}$ in Figure 1(c), which shows the magnitude of r_1^{Δ}, for an approximation to a 90°-sinc-pulse with a bandwidth of 1000 Hz. Note that $r_{\frac{1}{2}}^{\Delta}$ in Figure 1(b) has considerable support outside the fundamental period $[-500, 500]$. These side lobes appear whenever the soft pulse approximation is used.



(a) A plot of $|r_0^\Delta|$, the hard pulse approximation.

(b) A plot of $|r_{\frac{1}{2}}^\Delta|$, an intermediate case.

(c) A plot of $|r_1^\Delta|$, the soft pulse approximation.

Figure 1. Plots of the absolute reflection coefficients for various approximations to a 90°-sinc pulse showing several fundamental periods.

5 Softening Hard Pulses

A hard pulse is a sum of δ-function which is nonphysical. The RF-envelope which is actually used, e.g. in an NMR experiment, is a *finite* sum of "softened" pulses. For example one could replace each $\mu_j \delta(t - j\Delta)$ by a characteristic function of width Δ with the same integral, leading to the softened pulse:

$$q_1^\Delta = \sum_{j=-P_-}^{P_+} \frac{\mu_j}{\Delta} \chi_{[0,\Delta)}(t - j\Delta);$$

see [10]. The reflection coefficient r_1^Δ corresponding to q_1^Δ tends to zero at infinity. The difference $q_h^\Delta - q_1^\Delta$ is only "small" in the weak distributional sense. Nonetheless, under certain conditions, the difference $|r_0^\Delta(\xi) - r_1^\Delta(\xi)|$ can be made small for ξ in any fixed disk in the complex plane. The relationship between r_0^Δ and r_1^Δ is studied below.

For our analysis of this approximation, we consider pulses defined by the scattering data S_Δ, given in (68). We assume that the corresponding continuum scattering data satsifies the hypotheses of the previous section. For each Δ, we consider the one parameter family of pulses

$$q_\epsilon^\Delta = \sum_{j=-P_-}^{P_+} \frac{\mu_j}{\epsilon\Delta} \chi_{[0,\epsilon\Delta)}(t - j\Delta), \quad \epsilon \in [0, 1], \tag{75}$$

with the understanding that q_0^Δ is the sum of δ-pulses given above. While we do not make the dependence explicit, the limits of summation P_-, P_+ depend on Δ. In general they would be chosen to ensure that the scattering data of the truncated softened pulse differs very little from that of the hard pulse for $|\xi| < \frac{\pi}{2\Delta}$. If we fix an error then this would imply that $\Delta(P_+ + P_-) \approx L$, for some fixed L.

Let r_ϵ^Δ denote the reflection coefficient defined by q_ϵ^Δ. The potential q_ϵ^Δ is supported in the interval $[-P_-\Delta, P_+\Delta]$. In order to study r_ϵ^Δ we need to find a formula for $\boldsymbol{\psi}_{\epsilon 1-}(\xi; P_+\Delta)$. To simplify the exposition, we translate in time to replace P_- with 1 and P_+ by

$$P = P_- + P_+.$$

This just has the effect of multiplying the reflection coefficient by a linear phase $e^{2\Delta i P_- \xi}$.

As is well known, $\boldsymbol{\psi}_{\epsilon 1-}(\xi; P\Delta)$ can be conveniently expressed in terms of a product of 2×2-matrices. The solution operator at time $t_0+\Delta$ to the ZS-system with potential given by

$$\epsilon^{-1}\mu\chi_{[0,\epsilon\Delta)}(t-t_0)$$

is

$$U_{\mu,\epsilon,\Delta}(\xi) = \begin{bmatrix} e^{-i(1-\epsilon)\xi\Delta}\left(\frac{\alpha\cos(\alpha)-i\epsilon\xi\Delta\sin(\alpha)}{\alpha}\right) & e^{-i(1-\epsilon)\xi\Delta}\left(\frac{\mu\sin(\alpha)}{\alpha}\right) \\ -e^{i(1-\epsilon)\xi\Delta}\left(\frac{\mu^*\sin(\alpha)}{\alpha}\right) & e^{i(1-\epsilon)\xi\Delta}\left(\frac{\alpha\cos(\alpha)+i\epsilon\xi\Delta\sin(\alpha)}{\alpha}\right)\end{bmatrix}, \tag{76}$$

where

$$\alpha = \sqrt{(\epsilon\xi\Delta)^2+|\mu|^2}. \tag{77}$$

The solution operator for the ZS-system, at time $P\Delta$ with the potential given by (75) is therefore the product of the 2×2-matrices:

$$\begin{aligned} U_{\epsilon,\Delta}(\xi) &= U_{\mu_P,\epsilon,\Delta}(\xi)\cdots U_{\mu_1,\epsilon,\Delta}(\xi) \\ &= \begin{bmatrix} A_\epsilon^\Delta(\xi) & -B_\epsilon^{\Delta *}(\xi) \\ B_\epsilon^\Delta(\xi) & A_\epsilon^{\Delta *}(\xi)\end{bmatrix}. \end{aligned} \tag{78}$$

From the definition we see that

$$r_\epsilon^\Delta(\xi) = \frac{B_\epsilon^\Delta(\xi)e^{-2iP\xi\Delta}}{A_\epsilon^\Delta(\xi)}. \tag{79}$$

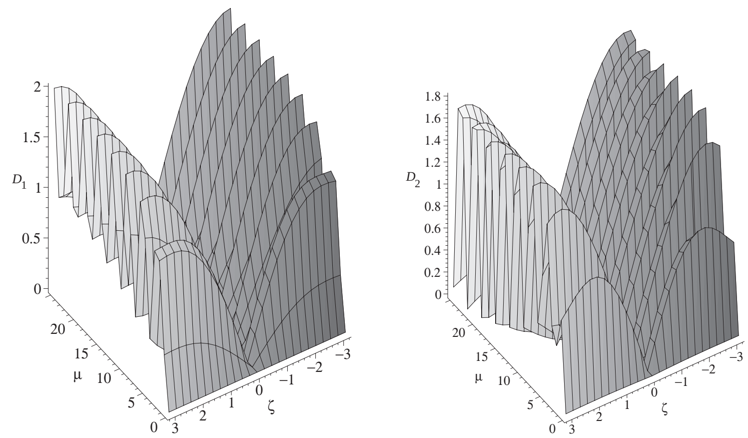
The entries of (76), and (78) are continuous at $\epsilon=0$. The functions $(A_\epsilon^\Delta, B_\epsilon^\Delta)$ are none other than the scattering coefficients for the ZS-system with potential q_ϵ^Δ. If $\epsilon=0$ then A_0^Δ and B_0^Δ can be expressed as

$$A_0^\Delta(\xi) = e^{2iM\xi\Delta}P(e^{2i\xi\Delta}), \quad B_0^\Delta(\xi) = e^{2iM'\xi\Delta}Q(e^{2i\xi\Delta}),$$

Where P and Q are polynomials of degree $P-1$. As expected A_0^Δ and B_0^Δ are $\Delta^{-1}\pi$-periodic functions.

The questions of principal interest are:

1. How well does $r_1^\Delta(\xi)$ approximate $r_0^\Delta(\xi)$ over the interval $[-\frac{\pi}{2\Delta}, \frac{\pi}{2\Delta}]$?
2. How rapidly does r_1^Δ decay outside of $[-\frac{\pi}{2\Delta}, \frac{\pi}{2\Delta}]$?
3. How are the zeros of A_1^Δ in the upper half plane related to those of A_0^Δ?



(a) A plot of D_1.

(b) A plot of D_2.

Figure 2. Plots of the error functions D_1 and D_2 for $\mu \in [0, 25]$.

The first question admits of a fairly simple analysis. We first consider a single term in the product expansion (78), examining the dependence of the difference $\|U_{\mu,1,\Delta}(\xi) - U_{\mu,0,\Delta}(\xi)\|$ on (μ, Δ), for small $\Delta|\xi|$. By setting $\zeta = \xi\Delta$ this reduces to consideration of the differences

$$\begin{aligned} D_1(\mu,\zeta) &= \left| e^{i\zeta}\left(\cos\sqrt{|\mu|^2+\zeta^2} - \frac{i\zeta\sin\sqrt{|\mu|^2+\zeta^2}}{\sqrt{|\mu|^2+\zeta^2}}\right) - \cos|\mu|\right| \\ D_2(\mu,\zeta) &= \left| e^{i\zeta}\frac{\mu\sin\sqrt{|\mu|^2+\zeta^2}}{\sqrt{|\mu|^2+\zeta^2}} - \frac{\mu\sin|\mu|}{|\mu|}\right|, \end{aligned} \tag{80}$$

for $\zeta \in [-\pi, \pi]$. As the plots in Figures 2 and 3 show, the only way to make both differences small is to take $|\mu|$ small.

In terms of pulse design, this means that Δ should be taken to be small, which in turn generally forces P to be large. A computation with Taylor series shows that, near $(0, 0)$,

$$\begin{aligned} D_1(\mu,\zeta) &= |\mu|^2 F(|\mu|,\zeta), \\ D_2(\mu,\zeta) &= |\mu\zeta| G(|\mu|,\zeta), \end{aligned} \tag{81}$$

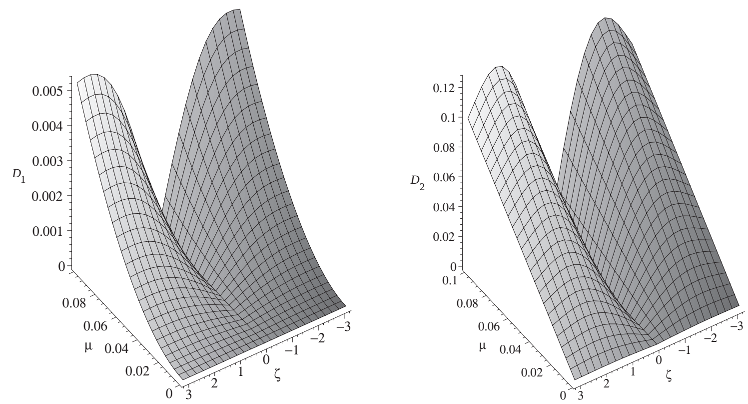
where F and G are entire functions. For a fixed r, Theorem 7 shows that the $\{\mu_j\}$ appearing in (78) satisfy

$$|\mu_j| = O(\Delta).$$

For ξ restricted to a *fixed* disk in the complex plane, ζ also behaves like $O(\Delta)$. Provided $\Delta \operatorname{Im}\xi$ is bounded, both error functions are $O((1+|\xi|)\Delta^2)$ as Δ tends to zero.

We express $U_{1,\Delta}$ as

$$U_{1,\Delta} = U_{\mu_P,0,\Delta}(\mathrm{Id}_2 + E_P)U_{\mu_{P-1},0,\Delta}(\mathrm{Id}_2 + E_{P-1})\cdots U_{\mu_1,0,\Delta}(\mathrm{Id}_2 + E_1),$$



(a) A plot of D_1. (b) A plot of D_2.

Figure 3. Plots of the error functions D_1 and D_2 for $\mu \in [0, 0.1]$.

where

$$\mathrm{Id}_2 + E_j = U^{-1}_{\mu_j,0,\Delta} U_{\mu_j,1,\Delta}.$$

The estimates shows that $\|E_j\| \leq C(1 + |\xi|)\Delta^2$. Using this expression, the estimates above and Theorem 7, one can show that, the difference satisfies

$$\begin{aligned} \|U_{1,\Delta}(\xi) - U_{0,\Delta}(\xi)\| \leq & \sum_{(\epsilon_1,\dots,\epsilon_P)\in 2'_P} \|E_1\|^{\epsilon_1} \dots \|E_P\|^{\epsilon_P} \\ \leq & (1 + C(1 + |\xi|)\Delta^2)^P - 1 \end{aligned} \tag{82}$$

Here $2'_P$ are the binary sequences of length P, excluding $(0, \dots, 0)$. Provided that $(1 + |\xi|)P$, is $o(\Delta^{-2})$ this estimate implies that implies that the differences

$$|A^{\Delta}_1(\xi) - A^{\Delta}_0(\xi)|, \quad |B^{\Delta}_1(\xi) - B^{\Delta}_0(\xi)|$$

can be made uniformly $O(P(1 + |\xi|)\Delta^2)$. In particular, the zeros of A^{Δ}_1 in the upper half plane converge to those of A^{Δ}_0.

A Asymptotics with simple jumps

Suppose that φ is a function with two continuous derivatives and $-\infty < \alpha < \beta < \infty$. We establish asymptotic formulæ and estimates for the scattering data (a_c, b_c) for the ZS-system with a potential $\chi_{[\alpha,\beta]}\varphi$ having simple jumps:

$$\begin{aligned} a_c(\xi) =& 1 + \frac{\|\varphi\|^2_{L^2[\alpha,\beta]}}{2i\xi} + O\left(\frac{1}{(1 + |\xi|)^2}\right), \\ e^{2i\xi\beta} b_c(\xi) =& e^{2i\xi\beta} \hat{T}_{[\alpha,\beta;\varphi^*(\alpha),\varphi^*(\beta)]}(2\xi) + O\left(\frac{1}{(1 + |\xi|)^2}\right). \end{aligned} \tag{83}$$

Here $T_{[\mu,\nu;A,B]}$ is the piecewise, linear function

$$T_{[\mu,\nu;A,B]}(t) = \chi_{[\mu,\nu]}(t)\frac{B(t-\mu)+A(\nu-t)}{\nu-\mu}. \tag{84}$$

For large real ξ this implies that

$$r_c(\xi) = \frac{b_c(\xi)}{a_c(\xi)} = \hat{T}_{[\alpha,\beta;\varphi^*(\alpha),\varphi^*(\beta)]}(2\xi)(1-\frac{\|\varphi\|^2_{L^2[\alpha,\beta]}}{2i\xi}) + O(|\xi|^{-3}). \tag{85}$$

Using the composition rules for the scattering data of potentials with dijoint support, it is easy to use this formula to work out asymptotics for the reflection coefficient of a potential on the form in (17). Figures 1(b,c) show the predicted sidelobes quite clearly.

We use the standard integral equations, defining the components of $\boldsymbol{\psi}_{1-}$, see [5]. Let

$$f_1(\xi;t) = \psi_{11-}(\xi;t)e^{i\xi t}.$$

It follows from (3), and (5) that

$$\begin{aligned} a_c(\xi) &= 1 + \int_\alpha^\beta M_1(\xi;\infty,s)\, f_1(\xi;s)ds,\\ b_c(\xi) &= -\int_\alpha^\beta e^{-2i\xi s}\varphi^*(s)\, f_1(\xi;s)ds. \end{aligned} \tag{86}$$

Where, in light of the simple form assumed by the potential we have that

$$\begin{aligned} M_1(\xi;\infty,s) &= -\varphi^*(s)\chi_{[\alpha,\beta]}(s)\int_s^\beta e^{2i\xi(x-s)}\varphi(x)dx\\ &= -\varphi^*(s)\chi_{[\alpha,\beta]}(s)\left[\frac{e^{2i\xi(\beta-s)}\varphi(\beta)-\varphi(s)}{2i\xi} - \int_s^\beta \frac{e^{2i\xi(x-s)}\varphi'(x)}{2i\xi}dx\right] \end{aligned} \tag{87}$$

Since $(x-s)\geq 0$ in the integral, this expression remains uniformly bounded for ξ in the upper half plane, and implies that

$$M_1(\xi;\infty,s) = -\varphi^*(s)\chi_{[\alpha,\beta]}(s)\left[\frac{e^{2i\xi(\beta-s)}\varphi(\beta)-\varphi(s)}{2i\xi} + O\left(\frac{1}{1+|\xi|^2}\right)\right]. \tag{88}$$

This formula holds for ξ with nonnegative real part, with the implied constant in the O-term only depending on the $\mathscr{C}^2[\alpha,\beta]$-norm of φ.

Using this formula for $M_1(\xi;\infty,s)$ in (86) gives

$$\begin{aligned} a_c(\xi) &= 1+\frac{\|\varphi\chi_{[\alpha,\beta]}\|^2_{L^2}}{2i\xi}+O\left(\frac{1}{1+|\xi|^2}\right)\\ b_c(\xi) &= -\int\limits_{\alpha}^{\beta} e^{-2i\xi s}\varphi^*(s)ds+O\left(\frac{1}{1+|\xi|^2}\right). \end{aligned} \tag{89}$$

This completes the analysis of a_c; for b_c we integrate by parts again to get:

$$b_c(\xi)=\frac{e^{-2i\xi\beta}\varphi^*(\beta)-e^{-2i\xi\alpha}\varphi^*(\alpha)}{2i\xi}+O\left(\frac{1}{1+|\xi|^2}\right). \tag{90}$$

The proof is completed by observing that

$$\hat{T}_{[\mu,\nu;A,B]}=-\frac{Be^{-i\nu\xi}-Ae^{-i\mu\xi}}{i\xi}+\frac{B-A}{\beta-\alpha}\frac{e^{-i\nu\xi}-e^{-i\mu\xi}}{\xi^2}.$$

If φ has $k+1$ derivatives, then we can integrate by parts in (87) k-times to get an asymptotic expansion for M_1 with an error term of order $O(|\xi|^{-(k+1)})$. This can, in turn, be used in (86) to obtain higher order asymptotic expansions for a_c and b_c. For smooth potentials, vanishing at infinity, expansions of this type are well known in the inverse scattering literature.

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