Half solitons as solutions to the Zakharov-Shabat eigenvalue problem for rational reflection coefficient with application in the design of selective pulses in nuclear magnetic resonance

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It is shown how the Zakharov-Shabat (ZS) eigenvalue problem for rational reflection coefficient may be reduced to the ZS problem with zero reflection coefficient. The soliton solutions to this reduced problem are obtained using the Bäcklund transform. Hence the solutions to the original problem are shown to be half solitons. It is demonstrated how selective pulses in nuclear magnetic resonance may be calculated using this technique. In particular, almost perfect 90° self-refocused and 180° refocusing selective pulses are demonstrated.

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I. INTRODUCTION

The Zakharov-Shabat (ZS) eigenvalue problem

$$\hat{L}v=\begin{bmatrix} i\dfrac{\partial}{\partial\tau} & -iq^{(-)} \\ iq^{(+)} & -i\dfrac{\partial}{\partial\tau}\end{bmatrix}v=\xi v \tag{1}$$

has been used to model two-level systems such as are found in, for example, optics [1] and nuclear magnetic resonance (NMR) [2]. It is also used to solve a class of nonlinear evolution equations [3].

The inverse problem is to determine the form of $q^{(+)}(\tau)$ and $q^{(-)}(\tau)$ given the asymptotic behavior of v as a function of ξ. For example, in NMR, we typically wish to determine the form of a radio-frequency pulse to be applied to a nuclear spin system in order to excite some spins and to leave others unaffected. It can be shown [2] that this problem of designing selective pulses is equivalent to inverting the ZS problem. In that case, the quantities in Eq. (1) have the following meanings. $v(\tau,\xi)$ is the spinor [4] describing the rotation of a spin at time $t=\tau T$, resonance offset $\nu=2\xi/T$ (T is an arbitrary scale factor with dimension time). The complex radio-frequency pulse is described in frequency units by $\omega(\tau T)=(2i/T)q^{(+)}(\tau)$. In this example, we require

$$q^{(-)}=-q^{(+)*}\ . \tag{2}$$

Using the notation of Ref. [3], we define ϕ, $\bar{\phi}$, ψ, and $\bar{\psi}$ to be fundamental solutions of Eq. (1) with asymptotic behavior

$$\phi(\tau,\xi)\to\begin{cases}\begin{bmatrix}1\\0\end{bmatrix}e^{-i\xi\tau} & \text{as } \tau\to-\infty\\ \begin{bmatrix}a(\xi)e^{-i\xi\tau}\\ b(\xi)e^{i\xi\tau}\end{bmatrix} & \text{as } \tau\to\infty\ ,\end{cases} \tag{3}$$

$$\bar{\phi}(\tau,\xi)\to\begin{cases}\begin{bmatrix}0\\-1\end{bmatrix}e^{i\xi\tau} & \text{as } \tau\to-\infty\\ \begin{bmatrix}\bar{b}(\xi)e^{-i\xi\tau}\\ -\bar{a}(\xi)e^{i\xi\tau}\end{bmatrix} & \text{as } \tau\to\infty\ ,\end{cases} \tag{4}$$

$$\psi(\tau,\xi)\to\begin{cases}\begin{bmatrix}0\\1\end{bmatrix}e^{i\xi\tau} & \text{as } \tau\to\infty\\ \begin{bmatrix}\bar{b}(\xi)e^{-i\xi\tau}\\ a(\xi)e^{i\xi\tau}\end{bmatrix} & \text{as } \tau\to-\infty\ ,\end{cases} \tag{5}$$

$$\bar{\psi}(\tau,\xi)\to\begin{cases}\begin{bmatrix}1\\0\end{bmatrix}e^{-i\xi\tau} & \text{as } \tau\to\infty\\ \begin{bmatrix}\bar{a}(\xi)e^{-i\xi\tau}\\ -b(\xi)e^{i\xi\tau}\end{bmatrix} & \text{as } \tau\to-\infty\ ,\end{cases} \tag{6}$$

where a, b, $\bar{a}$, and $\bar{b}$ are the scattering coefficients of the system. Under the symmetry of Eq. (2), they are related by $\bar{a}(\xi)=a^*(\xi^*)$ and $\bar{b}(\xi)=b^*(\xi^*)$.

These symbols will be used consistently to denote a solution to the ZS problem with that particular asymptotic behavior. For example, $\phi^{(2)}$ would denote the solution to the ZS problem with pulse $q^{(2)(+)}$ and with asymptotic behavior

$$\phi^{(2)}(\tau,\xi)\to\begin{cases}\begin{bmatrix}1\\0\end{bmatrix}e^{-i\xi\tau} & \text{as } \tau\to-\infty\\ \begin{bmatrix}a^{(2)}(\xi)e^{-i\xi\tau}\\ b^{(2)}(\xi)e^{i\xi\tau}\end{bmatrix} & \text{as } \tau\to\infty\ .\end{cases} \tag{7}$$

Note that if $v(\tau,\xi)=\binom{v_1(\tau,\xi)}{v_2(\tau,\xi)}$ is a solution to Eq. (1), then $v_T(\tau,\xi)=\binom{-v_2(-\tau,\xi)}{v_1(-\tau,\xi)}$ is a solution to

$$\hat{L}_T v_T = \begin{bmatrix} i\dfrac{\partial}{\partial\tau} & -iq_T^{(-)} \\ iq_T^{(+)} & -i\dfrac{\partial}{\partial\tau} \end{bmatrix} v_T = \xi v_T \ , \tag{8}$$

where $q_T^{(+)}(\tau)=q^{(-)}(-\tau)$ and $q_T^{(-)}(\tau)=q^{(+)}(-\tau)$.

Hence Eq. (8) has fundamental solution

$$\phi_T(\tau,\xi) = \begin{bmatrix} \psi_2(-\tau,\xi) \\ -\psi_1(-\tau,\xi) \end{bmatrix} \tag{9}$$

and therefore has scattering coefficients [obtained by letting $\tau\to\infty$ in Eq. (9)]

$$\begin{aligned} a_T(\xi) &= a(\xi) \ , \\ b_T(\xi) &= -\bar{b}(\xi) \ . \end{aligned} \tag{10}$$

With regard to designing selective pulses in NMR, we describe the desired effect of the pulse by giving initial and final magnetizations as functions of frequency offset. Assuming that the magnetization vector $m(t,\nu)=(m_1,m_2,m_3)$ equals (0,0,1) at $t=-\infty$ for all ν, Ref. [2] shows that the final magnetization vector is related to the scattering coefficients by

$$\begin{aligned} m(T\tau) &= m_1+im_2 \to 2a^* b e^{2i\xi\tau} \quad \text{as } \tau\to\infty \ , \\ m_3(T\tau) &\to |a|^2-|b|^2 \quad \text{as } \tau\to\infty \ . \end{aligned} \tag{11}$$

If we define $r(\xi)$, the reflection coefficient, by $r(\xi)=b(\xi)/a(\xi)$ then

$$r(\xi)=\lim_{\tau\to\infty} \frac{me^{-2i\xi\tau}}{1+m_3} \tag{12}$$

and, inversely

$$\begin{aligned} \lim_{\tau\to\infty} me^{-2i\xi\tau} &= \frac{2r}{1+|r|^2} \ , \\ \lim_{\tau\to\infty} m_3 &= \frac{1-|r|^2}{1+|r|^2} \ . \end{aligned} \tag{13}$$

Hence inverting the Bloch equation [the equation of motion for $m(t,\nu)$] for a given magnetization is equivalent to inverting the ZS eigenvalue problem for a given reflection coefficient. Several methods have been described for inverting the ZS problem for a given reflection coefficient [2,5–7]. The inversion is particularly simple if the reflection coefficient is zero for real ξ—the solutions being known as solitons. Calogero and Degasperis [5] described two methods of determining soliton solutions. One involved a matrix inversion, the other used the Bäcklund transform.

We have found a method of reducing the ZS problem for rational reflection coefficient to one for zero reflection coefficient. We have then used the Bäcklund transform to solve this reduced problem. This method is simple both conceptually and with regard to numerical implementation. We shall assume that $q^{(+)}=-q^{(-)*}$ throughout. However, the results are simply extended to the general case where $q^{(+)}$ and $q^{(-)}$ are independent.

We note that the pulses corresponding to the class of rational reflection coefficients are particularly suitable as NMR selective pulses, since the pulse is guaranteed to be zero for all $t>0$, and hence we can guarantee the correct phase of m at $t=0$ [2].

II. MAKING THE SYSTEM REFLECTIONLESS

The method is based on the observation that any (in general complex) pulse $q^{(+)}(\tau)$ which is zero for $\tau>0$ can always be made into a soliton pulse (i.e., a pulse corresponding to a zero reflection coefficient) by following it with a suitably chosen pulse $q'^{(+)}(\tau)$, which is zero for $\tau<0$.

To prove this, let $a^{(1)}$ and $b^{(1)}$ be the scattering coefficients corresponding to the pulse $q^{(1)(+)}(\tau)$ (which is zero for $\tau>0$). Further, let $a^{(2)}$ and $b^{(2)}$ be the scattering coefficients for the pulse $q^{(2)(+)}(\tau)$ (also zero for $\tau>0$).

Hence, from Eq. (10), the scattering coefficients associated with the pulse $q_T^{(2)(+)}$ will be $a^{(2)}(\xi)$ and $-\bar{b}^{(2)}(\xi)$.

Consider the composite pulse,

$$q^{(+)}(\tau) = \begin{cases} q^{(1)(+)}(\tau) & \text{for } \tau\le 0 \\ q_T^{(2)(+)}(\tau) & \text{for } \tau\ge 0 \ . \end{cases} \tag{14}$$

This will have fundamental solutions ϕ, $\bar{\phi}$, ψ, and $\bar{\psi}$. We must have that

$$\phi(\tau,\xi)=\phi^{(1)}(\tau,\xi) \quad \text{for } \tau\le 0 \ , \tag{15}$$

$$\bar{\phi}(\tau,\xi)=\bar{\phi}^{(1)}(\tau,\xi) \quad \text{for } \tau\le 0 \ , \tag{16}$$

$$\psi(\tau,\xi)=\psi_T^{(2)}(\tau,\xi) \quad \text{for } \tau\ge 0 \ , \tag{17}$$

$$\bar{\psi}(\tau,\xi)=\bar{\psi}_T^{(2)}(\tau,\xi) \quad \text{for } \tau\ge 0 \ . \tag{18}$$

Hence from Eqs. (3) and (15) and since $q^{(1)(+)}=0$ for $\tau>0$,

$$\phi(\tau=0,\xi) = \begin{bmatrix} a^{(1)}(\xi) \\ b^{(1)}(\xi) \end{bmatrix} \tag{19}$$

and therefore

$$\phi(\tau\ge 0,\xi)=a^{(1)}\phi_T^{(2)}-b^{(1)}\bar{\phi}_T^{(2)} \ . \tag{20}$$

From the asymptotic behavior of ϕ and $\bar{\phi}$ as $\tau\to\infty$ [Eqs. (3) and (4)], and assuming symmetry (2), we can conclude that

$$\phi(\tau,\xi)\to \begin{bmatrix} [a^{(1)}(\xi)a^{(2)}(\xi)+b^{(1)}(\xi)b^{(2)}(\xi)]e^{-i\xi\tau} \\ [-a^{(1)}(\xi)b^{(2)*}(\xi^*)+b^{(1)}(\xi)a^{(2)*}(\xi^*)]e^{i\xi\tau} \end{bmatrix} \quad \text{as } \tau\to\infty \tag{21}$$

and so the scattering coefficients of the composite pulse are

$$\begin{aligned} a(\xi) &= a^{(1)}(\xi)a^{(2)}(\xi)+b^{(1)}(\xi)b^{(2)}(\xi) \\ &= a^{(1)}(\xi)a^{(2)}(\xi)[1+r^{(1)}(\xi)r^{(2)}(\xi)] \ , \end{aligned} \tag{22}$$

$$\begin{aligned} b(\xi) &= -a^{(1)}(\xi)b^{(2)*}(\xi^*)+b^{(1)}(\xi)a^{(2)*}(\xi^*) \\ &= a^{(1)}(\xi)a^{(2)*}(\xi^*)[r^{(1)}(\xi)-r^{(2)*}(\xi^*)] \ , \end{aligned} \tag{23}$$

where $r^{(1)}=b^{(1)}/a^{(1)}$ and $r^{(2)}=b^{(2)}/a^{(2)}$.

Therefore, if we choose $q^{(2)(+)}$ such that $r^{(2)}(\xi)=r^{(1)*}(\xi^*)$ (which we can always do) then $b(\xi)=0$

and we have a soliton pulse.

$a(\xi)$ is then given by

$$a(\xi)=a^{(1)}(\xi)a^{(2)}(\xi)[1+r^{(1)}(\xi)r^{(1)*}(\xi^*)] \qquad (24)$$

and the bound states of the soliton pulse are located at the roots q_j of $1+r^{(1)}(\xi)r^{(1)*}(\xi^*)=0$ in the upper half complex plane. It is assumed that $r^{(1)}(\xi)$ has no factors of the form $(\xi-\alpha_j^*)/(\xi-\alpha_j)$. If any such factors are introduced, the algorithm in Sec. III should include additional "bound states" $q_{j'}=\alpha_j$ (which may be in the lower-half complex plane), but no additional poles p_k.

$b(\xi)=0$ for all $\xi\neq q_j$. At $\xi=q_j$, $a(\xi)=0$ and hence a solution $\phi(\tau,q_j)$ of the composite system will have asymptotic behavior

$$\phi(\tau,q_j)\rightarrow \begin{bmatrix} 0 \\ b \end{bmatrix} e^{iq_j\tau} \quad \text{as } \tau\rightarrow\infty \ . \qquad (25)$$

We also know $\phi(\tau=0,q_j)$ [Eq. (19)]. Hence under pulse $q_T^{(2)(+)}$, ϕ has boundary conditions at $\tau=0$ and $\tau\rightarrow\infty$. Consider instead the system under $q^{(2)(+)}$. It will have boundary conditions

$$v(\tau\rightarrow-\infty,q_j)=\begin{bmatrix} b \\ 0 \end{bmatrix} e^{-iq_j\tau}=b\phi^{(2)} \ , \qquad (26)$$

$$v(\tau=0,q_j)=\begin{bmatrix} b^{(1)} \\ -a^{(1)} \end{bmatrix} . \qquad (27)$$

Therefore

$$b(q_j)\phi^{(2)}(\tau=0,q_j)=\begin{bmatrix} b^{(1)}(q_j) \\ -a^{(1)}(q_j) \end{bmatrix} . \qquad (28)$$

But

$$\phi^{(2)}(\tau=0,q_j)=\begin{bmatrix} a^{(2)}(q_j) \\ b^{(2)}(q_j) \end{bmatrix} . \qquad (29)$$

Comparing Eqs. (28) and (29), we conclude

$$b(q_j)=\frac{b^{(1)}(q_j)}{a^{(2)}(q_j)}=-\frac{a^{(1)}(q_j)}{b^{(2)}(q_j)}=r^{(1)}(q_j)\frac{a^{(1)}(q_j)}{a^{(2)}(q_j)} . \qquad (30)$$

Now if $a^{(1)}(\xi)$ has zeros at $\xi=p_j$, it must have the form

$$a^{(1)}(\xi)=\frac{\prod_k \xi-p_k}{\prod_k \xi-q_k^*} \qquad (31)$$

since we require $a^{(1)}(\xi)$ to be analytic in the upper half plane, $a^{(1)}\rightarrow 1$ as $|\xi|\rightarrow\infty$, and $a^{(1)}(\xi)a^{(1)*}(\xi^*)+b^{(1)}(\xi)b^{(1)*}(\xi^*)=1$. Similarly,

$$a^{(2)}(\xi)=\frac{\prod_k \xi-p_k^*}{\prod_k \xi-q_k^*} . \qquad (32)$$

We conclude, Eqs. (30)–(32),

$$b(q_j)=r^{(1)}(q_j)\frac{\prod_k q_j-p_k}{\prod_k q_j-p_k^*} . \qquad (33)$$

Furthermore, if $a(\xi)$ is the scattering coefficient for a soliton pulse, it must have the form

$$a(\xi)=\frac{\prod_k \xi-q_k}{\prod_k \xi-q_k^*} . \qquad (34)$$

So

$$\left.\frac{da}{d\xi}\right|_{\xi=q_j}=a'(q_j)=\frac{\prod_{k\neq j} q_j-q_k}{\prod_k q_j-q_k^*} . \qquad (35)$$

Therefore, assuming that the q_j are all distinct, the soliton pulse has residues

$$c_j=\frac{b(q_j)}{a'(q_j)}=r^{(1)}(q_j)\frac{\prod_k q_j-p_k}{\prod_k q_j-p_k^*}\frac{\prod_k q_j-q_k^*}{\prod_{k\neq j} q_j-q_k} . \qquad (36)$$

III. CREATING THE SOLITON PULSE WITH THE BÄCKLUND TRANSFORM

Let this pulse correspond to an N-soliton (i.e., there are N q_j). Using the Bäcklund transform described by Calogero and Degasperis [5], we see that this soliton can be considered built up from plane waves

$$\chi_j^{(0)}(\tau)=\rho_j e^{2iq_j\tau} \ , \qquad (37)$$

where

$$\rho_j=-ir^{(1)}(q_j)\frac{\prod_k q_j-p_k}{\prod_k q_j-p_k^*} \qquad (38)$$

are the plane-wave residues. Note that if the p_k occur in complex conjugate pairs, then Eq. (38) reduces to

$$\rho_j=-ir^{(1)}(q_j) \ . \qquad (39)$$

The N-soliton is built up by constructing the lower triangular half of an $(N+1)\times(N+1)$ "soliton lattice." The base of the lattice is known explicitly in terms of the plane waves $\chi_j^{(0)}$. Each successively higher row of the lattice is then constructed in an algebraic way from previously calculated points. Figure 1 shows how the first two rows of the lattice are constructed.

We associate each point (j^+,j^-) of the lattice with a pair of values $q^{(+)}(j^+,j^-)$ and $q^{(-)}(j^+,j^-)$. We define the base of the lattice by, for $j^+=1,\ldots,N$,

$$q^{(-)}(0,0)=0 \ , \qquad (40)$$

$$q^{(+)}(0,0)=0 \ , \qquad (41)$$

$$q^{(-)}(j^+,0)=0 \ , \qquad (42)$$

$$q^{(+)}(j^+,0)=2\sum_{k=1}^{j^+}\chi_k^{(j^+)} \ , \qquad (43)$$

where $\chi_k^{(j^+)}$ are inductively defined by Eq. (37) and, for $j^+\geq 1$, $k=1,\ldots,N$,

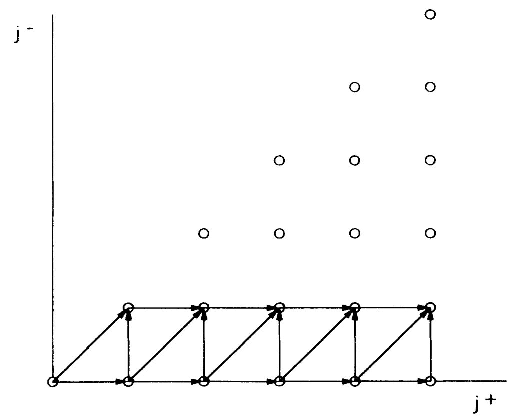

FIG. 1. Diagram to show how the points of the first two rows of the soliton lattice are built up. An arrow pointing from one point to a second point shows that the value of the second point depends on the value of the first.

$$\chi_k^{(j^+)}=\begin{cases}\dfrac{\chi_k^{(j^+-1)}}{q_k-q_{j^+}} & \text{if } k\neq j^+\\ \chi_k^{(j^+-1)} & \text{if } k=j^+ .\end{cases} \tag{44}$$

To build up the rest of the lattice, we distinguish between points on and off the diagonal. Points on the diagonal are inductively defined, for $k=1,\ldots,N$,

$$q^{(+)}(k,k)=q^{(+)}(k-1,k-1)+\frac{2(q_k-q_k^*)}{2/q^{(+)}(k,k-1)+q^{(+)*}(k,k-1)/2}, \tag{45}$$

$$q^{(-)}(k,k)=-q^{(+)*}(k,k) . \tag{46}$$

Points off the diagonal are defined by, for $j=1,\ldots,N$ and $k=1,\ldots,j-1$,

$$q^{(+)}(j,k)=q^{(+)}(j-1,k-1)+\frac{2(q_j-q_k^*)}{2/q^{(+)}(j,k-1)-q^{(-)}(j-1,k)/2}, \tag{47}$$

$$q^{(-)}(j,k)=q^{(-)}(j-1,k-1)+\frac{2(q_k^*-q_j)}{2/q^{(-)}(j-1,k)-q^{(+)}(j,k-1)/2} . \tag{48}$$

Finally, the N-soliton pulse is given by $q^{(+)}(N,N)$. Hence the pulse corresponding to reflection coefficient $r^{(1)}(\xi)$ is given by $q^{(1)(+)}(\tau)=q^{(+)}(N,N)(\tau)\Theta(-\tau)$ where

$$\Theta(\tau)=\begin{cases}0 & \text{for } \tau<0\\ 1 & \text{for } \tau\geq 0 .\end{cases} \tag{49}$$

Recalling the definition $q^{(+)}=-\frac{1}{2}i\omega T$, we can determine the pulse $\omega(t)$ in frequency units. Note that we only need to store one row of the lattice at a time, and hence this algorithm requires storage of size N and $O(N^2)$ arithmetic operations.

We can deduce an upper limit on $|q^{(+)}(N,N)|$. Since

$$\frac{1}{|z+1/z^*|}\leq\tfrac{1}{2} \quad \text{for all complex } z$$

the inductive definition of $q^{(+)}(k,k)$ [Eqs. (41) and (45)] gives

$$|q^{(+)}(N,N)|\leq\sum_{k=1}^{N}|q_k-q_k^*| . \tag{50}$$

IV. EXAMPLES

(1) Consider the reflection coefficient

$$r^{(1)}(\xi)=\frac{\alpha}{\xi-i\beta} \quad \text{where } \beta \text{ is real} . \tag{51}$$

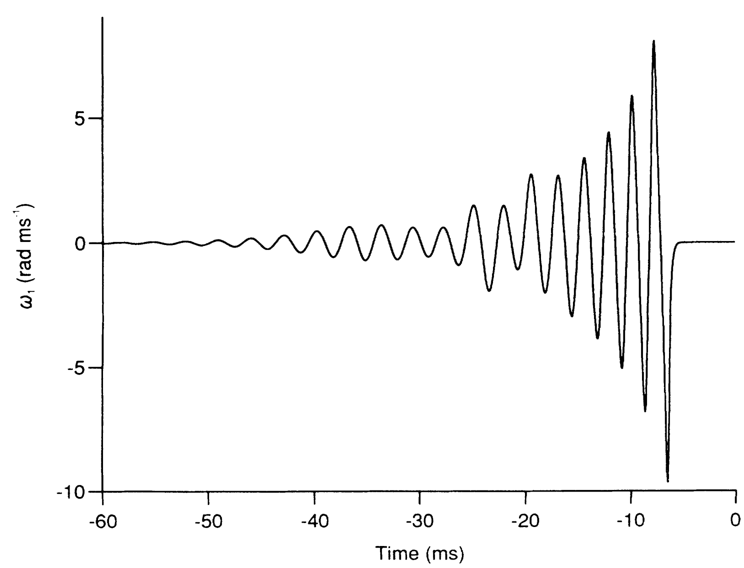

FIG. 2. The purely real pulse $\omega(t)$ which gives rise to the reflection coefficient of Eq. (60) with $n=16$ (and hence this is a self-refocused 90° pulse). In all the figures, $T=1$ ms.

The corresponding magnetization profiles will be given by Eq. (13). There is one root of $1+r^{(1)}(\xi)r^{(1)*}(\xi^*)=0$ in the upper half plane:

$$q_1=i\gamma=i(\alpha\alpha^*+\beta^2)^{1/2} . \tag{52}$$

The one plane-wave residue is [Eq. (38)]

$$\rho_1=-ir^{(1)}(i\gamma)\frac{q_1-i\beta}{q_1+i\beta}=\frac{-\alpha}{\gamma+\beta} . \tag{53}$$

We calculate $q^{(+)}(1,1)$ from Eqs. (40)–(45),

$$q^{(+)}(1,1)(\tau)=-2i\gamma\frac{\alpha}{|\alpha|}\text{sech}\left[2\gamma\tau+\text{arctanh}\left[\frac{\beta}{\gamma}\right]\right] . \tag{54}$$

This is the 1-soliton pulse. The pulse with the reflection coefficient $r^{(1)}(\xi)$ is given by $q^{(1)(+)}(\tau)=q^{(+)}(1,1)(\tau)\Theta(-\tau)$. Therefore the pulse in frequency units is given by

$$\omega(t)=\frac{4\gamma}{T}\frac{\alpha}{|\alpha|}\text{sech}\left[2\gamma t/T+\text{arctanh}\left[\frac{\beta}{\gamma}\right]\right]\Theta(-t) . \tag{55}$$

Note that we inverted the reflection coefficient (51) in Ref. [2] (and obtained the same result). However, the solution was obtained considerably more easily using the method described here.

(2) Consider the reflection coefficient

$$r^{(1)}(\xi)=\frac{i}{\xi^2+1} . \tag{56}$$

This has poles at $p_1=i$ and $p_2=-i$. The soliton has bound states at $q_1=2^{1/4}e^{i3\pi/8}$ and $q_2=2^{1/4}e^{i5\pi/8}=-q_1^*$. The plane-wave residues can be obtained from Eq. (39),

$$\rho_1=-i , \quad \rho_2=i . \tag{57}$$

It can be shown that the resultant 2-soliton has the form

$$q^{(+)}(2,2)(\tau)=4i\beta\,\text{sech}(2\beta\tau)\times\frac{[\sin(2\alpha\tau)+(\beta/\alpha)\cos(2\alpha\tau)\tanh(2\beta\tau)]}{1+[(\beta/\alpha)\cos(2\alpha\tau)\text{sech}(2\beta\tau)]^2} , \tag{58}$$

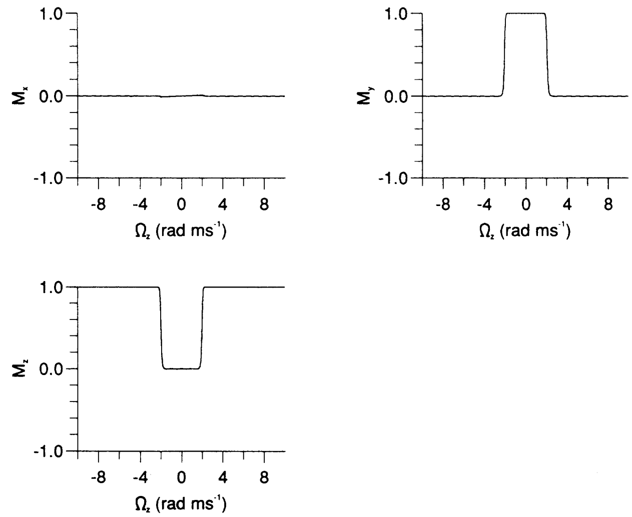

FIG. 3. The response to the pulse of Fig. 2 described as magnetization profiles. M_x, M_y, and M_z are the three components of the magnetization vector as a function of resonance offset Ω_z. We can recover the corresponding reflection coefficient from Eq. (12).

where $q_1=\alpha+i\beta$. We then obtain $\omega(t)$ from

$$\omega(t)=\frac{2i}{T}q^{(+)}(2,2)(t/T)\Theta(-t) . \tag{59}$$

(3) The reflection coefficient

$$r^{(1)}(\xi)=\frac{i}{\xi^{2n}+1} \tag{60}$$

tends to a "top hat" form as $n\rightarrow\infty$, where the top hat function $\mathcal{T}(\xi)$ is defined by

$$\mathcal{T}(\xi)=\begin{cases}1 & \text{for } |\xi|<1\\ 0 & \text{for } |\xi|>1 .\end{cases}$$

It is equivalent [Eq. (13)] to $m_1=0$, m_2 being a top hat and m_3 being an inverted top hat. For $n>1$, it is not easy to obtain the corresponding $2n$-soliton pulse in closed form. However, we can determine it numerically.

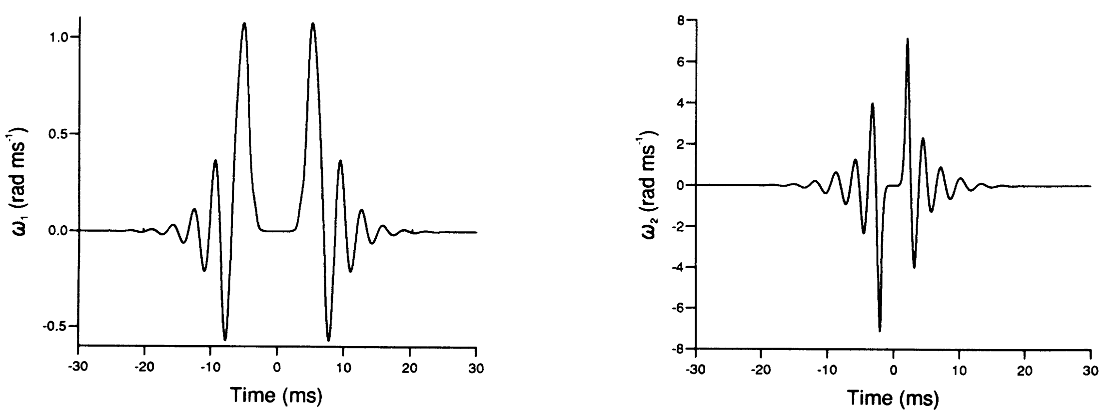

FIG. 4. The components ω_1 and ω_2 of the pulse which give rise to the scattering coefficient $b(\xi)$ of Eq. (61) with $n=8$. Hence this is a 180° refocusing pulse.

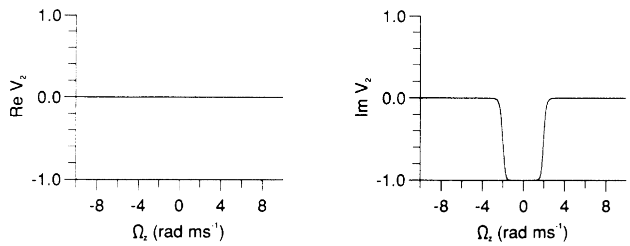

FIG. 5. The real and imaginary parts of the second spinor component, obtained by integrating the ZS problem (1) for the pulse of Fig. 4, starting with $v=\binom{1}{0}$ at the start of the pulse. They are plotted as a function of resonance offset Ω_z.

Figure 2 shows the (purely real) pulse $\omega(t)$ obtained from this reflection coefficient with $n=16$. It was determined at 8192 time points in about 2 CPU minutes on our RISC workstation. The magnetization responses at $t=0$ were then obtained from this pulse via numerical integration of the Bloch equation. They are shown in Fig. 3. We can see that we have an essentially perfect self-refocused 90° selective pulse.

(4) Suppose we wish to find a pulse $q^{(+)}(\tau)$ that leads to the scattering coefficient

$$b(\xi)=\frac{-i}{1+\xi^{2n}} . \tag{61}$$

(In NMR, such a pulse would be a 180° selective refocusing pulse as $n\rightarrow\infty$ [8].)

We can find such a pulse by first assuming that it has the symmetry $q^{(+)}(-\tau)=-q^{(+)*}(\tau)$. Let

$$q^{(+)}(\tau)=\begin{cases} q^{(1)(+)}(\tau) & \text{for } \tau\le 0 \\ -q^{(1)(+)*}(-\tau)=q_T^{(1)(+)}(\tau) & \text{for } \tau\ge 0 . \end{cases} \tag{62}$$

Then from Eq. (23), we see that

$$\begin{aligned} b(\xi)&=a^{(1)}(\xi)a^{(1)*}(\xi^*)[r^{(1)}(\xi)-r^{(1)*}(\xi^*)] \\ &=\frac{r^{(1)}(\xi)-r^{(1)*}(\xi^*)}{1+r^{(1)}(\xi)r^{(1)*}(\xi^*)} \end{aligned} \tag{63}$$

and so if we can find $r^{(1)}(\xi)$ such that $b(\xi)$ has the form (61), then we can find $q^{(1)(+)}$ and hence $q^{(+)}$.

There are many possible factorizations. The simplest is

$$r^{(1)}(\xi)=\frac{\alpha}{\prod_{j=0}^{n-1}\xi-p_j} , \tag{64}$$

where

$$\alpha=-\frac{1}{\sqrt{2}} , \tag{65}$$

$$p_j=\frac{1}{2^{1/(2n)}}e^{i\pi/2n}e^{i2\pi j/n} . \tag{66}$$

The bound states of the corresponding n-soliton pulse are given by, for $j=0,\ldots,n-1$,

$$q_j=e^{i\pi/2n}e^{i\pi j/n} \tag{67}$$

and from Eq. (38) the plane-wave residues are given by, for $j=0,\ldots,n-1$,

$$\rho_j=\begin{cases} \sqrt{2}-1 & \text{for even } j \\ -(\sqrt{2}+1) & \text{for odd } j . \end{cases} \tag{68}$$

We have numerically determined the pulse $\omega(t)=\omega_1(t)+i\omega_2(t)$ (in frequency units) corresponding to (61) with $n=8$. Note that the pulse is complex. It is shown in Fig. 4. We numerically integrated Eq. (1) with this pulse. Setting the spinor $\binom{v_1}{v_2}=\binom{1}{0}$ at the start of the pulse for all resonance offsets, we determined the spinor at the end of the pulse. Figure 5 shows the real and imaginary parts of v_2 at the end, confirming that we have a refocusing pulse.

We note that this pulse differs from that obtained by Carlson in Ref. [8]—who obtained purely real refocusing pulses. These would be obtained if we factorized $b(\xi)$ with the constraint that $r^{(1)}(\xi)=-r^{(1)*}(-\xi^*)$.

V. CONCLUSION

We have found a simple and fast method for inverting the Zakharov-Shabat eigenvalue problem for rational reflection coefficient. Since it shows how the problem may be reduced to one where the reflection coefficient is zero, and hence solutions must be half solitons, it is more satisfactory than existing methods, where the form of the solution is assumed.

It also enables us to use the Bäcklund transform as the main tool in the inversion—which is both quicker and simpler to use than techniques using matrix inversion.

We have concentrated on its application with regard to designing selective pulses in NMR. However, the results are applicable in any problem involving the ZS problem.

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