Inversion of the Bloch equations with T_2 relaxation: An application of the dressing method

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The Bloch equations, with time-varying driving field, and T_2 relaxation, are expressed as a scattering problem, with $\Gamma_2 = 1/T_2$ as the scattering parameter, or eigenvalue. When the rf pulse, describing the driving field, is real, this system is equivalent to the 2×2 Zakharov-Shabat eigenvalue problem. In general, for complex rf pulses, the system is a third-order scattering problem. These systems can be inverted, to provide the rf pulse needed to obtain a given magnetization response as a function of Γ_2. In particular, the class of ''soliton pulses'' are described, which have utility as T_2-selective pulses. For the third-order case, the dressing method is used to calculate these pulses. Constraints on the dressing data used in this method are derived, as a consequence of the structure of the Bloch equations. Nonlinear superposition formulas are obtained, which enable soliton pulses to be calculated efficiently. Examples of one-soliton and three-soliton pulses are given. A closed-form expression for the effect of T_1 relaxation for the one-soliton pulse is obtained. The pulses are tested numerically and experimentally, and found to work as predicted. [S1063-651X(98)03006-2]

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I. INTRODUCTION

This paper is concerned with the determination of T_2-selective pulses for systems obeying the Bloch equations

$$\frac{\partial \boldsymbol{m}}{\partial t} = A\boldsymbol{m} + \boldsymbol{b}, \tag{1.1a}$$

where

$$A = \begin{pmatrix} -\Gamma_2 & -\omega_3(t) & \omega_2(t) \\ \omega_3(t) & -\Gamma_2 & -\omega_1(t) \\ -\omega_2(t) & \omega_1(t) & -\Gamma_1 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 0 \\ 0 \\ \Gamma_1 \end{pmatrix}. \tag{1.1b}$$

These equations are found in studies of nuclear magnetic resonance (nmr) [1–3], electron paramagnetic resonance [4], quantum electronics [5], and optics [6]. In nmr, $\boldsymbol{m}(t)^T = (m_1, m_2, m_3)$ corresponds to the bulk magnetization of the sample, which is taken to have an equilibrium value of $\boldsymbol{m}^T = (0,0,1)$ (T denotes the transpose of a vector or matrix). $\boldsymbol{\Omega}(t)^T = (\omega_1(t), \omega_2(t), \omega_3(t))$ is the driving field of the system. It is usually decomposed into the complex radiofrequency (rf) pulse $\omega = \omega_1 + i\omega_2$ and the detuning (or resonance offset) ω_3. The constants Γ_1 and Γ_2 are the T_1 and T_2 relaxation rates, respectively. This terminology will be used, even though the results are not specific to nmr.

In more detail it is well known that any two-level system in the presence of a driving field has a Hamiltonian of the form $\mathcal{H} = \frac{1}{2}\hbar \boldsymbol{\Omega}^T \boldsymbol{\sigma}$, where $\hbar$ is Planck's constant, $\boldsymbol{\sigma}^T = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli spin matrices, and $\boldsymbol{\Omega}^T = (\omega_1, \omega_2, \omega_3)$ is a time-varying vector of scalars with units of angular velocity. Let the unitary matrix describing the evolution under this Hamiltonian be U. Then the time derivative of U is $\dot{U} = (1/i\hbar)\mathcal{H}U$, and the quantity $M = U\sigma U^{-1}$, where σ is any linear combination of the σ_j (with time-constant coefficients), has the form

$$M = \begin{pmatrix} m_3 & m_1 - im_2 \\ m_1 + im_2 & -m_3 \end{pmatrix}, \tag{1.2}$$

with m_1, m_2, and m_3 real. It is well known that the vector $\boldsymbol{m}^T = (m_1, m_2, m_3)$ evolves in time such that its instantaneous angular velocity about the origin is $\boldsymbol{\Omega}(t)$, and hence that it obeys the Bloch equations with $\Gamma_1 = \Gamma_2 = 0$. Furthermore, suppose the system is initially at thermal equilibrium, with (time-constant) Hamiltonian $\mathcal{H}_0 = \frac{1}{2}\hbar\sigma$. Then the density matrix is $\rho = (1/Z)\exp(-\mathcal{H}_0/kT)$ at temperature T, with k the Boltzmann constant, and Z the partition function. Hence, in the high-temperature regime, M is proportional to the excess over the scalar part of the density matrix, both at thermal equilibrium, and subsequently, after the application of a driving field, when the Hamiltonian becomes time varying. (The scalar part ρ_s of ρ is defined by $\rho = \rho_s + \rho_0$, where ρ_s is a multiple of the unit matrix, and ρ_0 has zero trace.) Thus the vector $\boldsymbol{m}$ represents this excess, or ''polarization.''

In nmr, for a nucleus with spin $\frac{1}{2}$ in a magnetic field $\boldsymbol{H}$, the quantity $\boldsymbol{\Omega}$ defining the Hamiltonian equals $-\gamma\boldsymbol{H}$, where γ is the gyromagnetic constant of the nucleus. In practice, the object whose nuclei are being studied is placed in a strong, time-constant, spatially uniform field $(0,0,H_0)$, and a magnetic field $2\cos\omega_{\rm rf}t\ (H_1(t), H_2(t), 0)$ is applied in the x-y plane. $\omega_{\rm rf}$ is chosen to be equal, or very close, to the transition frequency ω_0 of the system under just H_0, i.e., $\omega_0 = -\gamma H_0$ (the sign indicates the sense of rotation of $\boldsymbol{m}$ about the z axis), and in practice $\omega_{\rm rf}$ will be radio frequency.

H_1 and H_2 are slowly varying functions describing the envelope of the applied alternating field. Under the rotating-wave approximation [7,8], and in a frame rotating at $\omega_{\rm rf}$ about the z axis, it is well known that the Hamiltonian has

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the same form as before, but now ω_1, ω_2, and ω_3 in $\mathbf{\Omega}$ are given by $\omega_1 + i\omega_2 = \omega = -\gamma(H_1 + iH_2)$ and $\omega_3 = \omega_0 - \omega_{\mathrm{rf}}$.

It has been shown [2] that the Bloch equations in the rotating frame are appropriate in many cases to describe the evolution of a system of nuclei with spin greater than $\frac{1}{2}$ and in the presence of spin-lattice and spin-spin coupling. The latter two effects are described by relaxation rates Γ_1 and Γ_2, respectively. The quantity $\boldsymbol{m}$ then describes the bulk magnetization density, only the transverse component of which, i.e., $m_1 + im_2$, can be detected in a receiver coil, which is placed around the sample.

Hence, most nmr experiments attempt to align the magnetization of all the nuclei that are of interest along a common axis in the x-y plane, and to leave uninteresting spins along the z axis. For example, the signal due to ^{1}H spins from a dilute solute would be dominated by that from the ^{1}H nuclei in an aqueous solvent. Since, in many cases, the resonance offset ω_3 of solvent spins differs from the solute spins (because the nuclei are in different electronic environments), rf pulses have been designed to ''selectively excite'' spins according to their resonance offset.

When relaxation is neglected, the design of such ''frequency selective'' pulses is a solved problem. The most efficient approach is to reduce the Bloch equations to a 2×2 scattering problem—the Zakharov-Shabat (ZS) eigenvalue problem [9,10]—and then further reduce this problem to the calculation of soliton pulses, which in this context means pulses that return magnetization initially at $(0,0,1)$ back to $(0,0,1)$, irrespective of the resonance offset [11–13].

Sometimes, it is more convenient to select spins according to their relaxation behavior—usually because the spins to be distinguished are not well separated by their resonance offsets. A typical application is in magnetic resonance imaging, where the signal from ^{1}H in fat is often inconvenient, whereas the signal from water is desired. The general method is to null the magnetization, in some way, of the spins not of interest, i.e., make their final magnetization $\boldsymbol{m}^T = (0,0,0)$. If the method is to work, the other spins will have a non-null magnetization at this instant—often the method is designed so these spins all have magnetization along the z axis. These can then be detected with a short, intense, constant phase, rf pulse of total angle $\int|\omega|\,dt = \pi/2$ to flip these spins into the x-y plane. [Such a pulse is called a hard $\pi/2$ pulse. Assuming the rf field is applied along the x axis, it is ideally represented by $w_1(t) = (\pi/2)\delta(t)$, where $\delta(t)$ is the Dirac delta function.]

Existing schemes of spin selection via relaxation [14–19] (and also of spin contrast [20,21]) work by having short rf pulses, where relaxation is neglected, and separate periods of free-precession, i.e., where no rf is applied and the spins evolve only due to the field along the z axis, and due to relaxation.

An example of a T_1-selective method is the use of ''inversion nulling,'' i.e., the water eliminated Fourier transform (WEFT) and the driven equilibrium Fourier transform (DEFT) techniques [14–17]. In the simplest version [14], a hard π pulse is applied, causing all magnetization, assumed to be initially at $(0,0,1)$, to be rotated to $(0,0,-1)$. It then starts relaxing by T_1 relaxation towards the positive z axis. Suppose it is left to free precess for a time τ. For a spin with relaxation rate Γ_1, the Bloch equations can be easily solved with these conditions to find the evolution of m_3. In particular, at $\tau = (1/\Gamma_1)\ln 2$, the magnetization will be $(0,0,0)$, i.e., the magnetization will be nulled. Spins with different T_1 relaxation rates will not be nulled at that moment, and hence can be detected.

Note that this method also allows the measurement of T_1 for a spin species [22]. The period of free precession τ following the π hard pulse is varied. After each such period, a hard $\pi/2$ pulse is applied to flip any magnetization from the z axis to the x-y plane, and the magnitude of the signal is measured. Since the variation of the signal with τ is due to the value of T_1, its value can be calculated. This is called an inversion recovery sequence.

This decoupling of evolution to periods of just rf pulse and to just free precession is done because these regimes are more completely understood than the general case of both time-varying rf pulse and relaxation together causing the evolution. Since it may not always be valid to neglect relaxation during an rf pulse, and since the selectivity of existing relaxation based schemes is not very flexible, it is useful to consider the design of rf pulses that work simultaneously with relaxation to obtain selectivity.

In this paper, T_1 relaxation will be neglected, except qualitatively and for a special case, see Secs. IV B and IV C. Since $T_1 \gg T_2$ for many systems, this is often a valid assumption. Also, ω_3 is not a parameter used to select particular spins, but is considered part of the driving field. That is, all spins see the same ω_3 (which can be allowed to be time varying).

It is then easily shown that, by suitably choosing the reference frame, $\omega_3(t)$ can be made identically zero (see Appendix A). Its effect can be ''absorbed'' as a time-varying extra phase of the rf pulse. Henceforth, it should be assumed that this choice of reference frames has been made.

The soliton pulses mentioned above also occur in the context of designing T_2-selective pulses. In general, a soliton pulse means one whose associated scattering matrix is J diagonal (these terms are defined later). Here, however, it should be taken as meaning a pulse that, given an initial magnetization $\boldsymbol{m}^T = (0,0,1)$, results in a final magnetization $\boldsymbol{m}^T = (0,0,m_3(\Gamma_2))$, where

$$m_3 = \prod_{j=1}^{m} \frac{\Gamma_2 - iz_j^\star}{\Gamma_2 - iz_j}, \tag{1.3}$$

for a spin species with T_2 relaxation rate Γ_2. Here, the z_j are in the upper half complex plane, and $\star$ means the complex conjugate. Hence, for a suitable choice of z_j, $\boldsymbol{m}$ can be made zero for particular values of Γ_2, and thus a soliton pulse can be used to null the magnetization of spin species with these values (there will be a zero of m_3 for each z_j on the positive imaginary axis).

This paper is mostly concerned with the calculation of soliton pulses. For the special case when $\omega(t)$ is real, i.e., $\omega_2(t) = 0$, it shows that the Bloch equations can be reduced to the ZS problem, and hence existing, well-known methods may be used to calculate T_2-selective (not just soliton) pulses.

In general, though, the system must be treated as a third-order scattering problem, with Γ_2 as the scattering parameter, and $\omega(t)$ as the ''potential.''

A powerful technique, the dressing method [23,24], may be used to construct a ladder of soliton pulses. In order to apply this method, which is applicable to general $n\times n$ scattering problems, constraints have to be found on the parameters, or ''dressing data,'' used in soliton pulse construction. It is also necessary to connect the dressing data to the T_2 selectivity of the pulses (since it is the latter that will be specified). Finally, an efficient method of calculating these pulses, using ''nonlinear superposition formulas,'' will be given.

The jth step in the ladder of soliton pulses is made given dressing data $\{z_j,\overline{z_j},v_j,\tilde{w}_j\}$, where z_j and $\overline{z_j}$ are complex numbers, and v_j and $\tilde{w}_j$ are vectors. Appendix B proves that all the z_j, and $\overline{z_j}$, may be taken to be in the upper, and lower, half complex planes, respectively. Appendix C gives the connection between the calculation of pulses via the reduction to the ZS problem, to the calculation of the same (necessarily real) pulses via the dressing method.

II. REAL PULSE

If the rf pulse $\omega(t)$ is real, system (1.1) decouples, and can be reduced to a 2×2 system. For $\omega_2(t)=0$ and $\Gamma_1=0$, Eq. (1.1) can be rewritten:

$$\frac{\partial}{\partial t}\begin{pmatrix} m_1\\ m_2\\ m_3\end{pmatrix}=\begin{pmatrix} -\Gamma_2 & 0 & 0\\ 0 & -\Gamma_2 & -\omega_1\\ 0 & \omega_1 & 0\end{pmatrix}\begin{pmatrix} m_1\\ m_2\\ m_3\end{pmatrix}. \qquad (2.1)$$

Hence, assuming

$$\boldsymbol{m}\rightarrow\begin{pmatrix}0\\0\\1\end{pmatrix}, \qquad (2.2)$$

as $t\rightarrow-\infty$, then $m_1=0$ for all t. Further,

$$\frac{\partial}{\partial t}\left[e^{\Gamma_2 t/2}\begin{pmatrix} m_2\\ m_3\end{pmatrix}\right]=\begin{pmatrix} -\frac{\Gamma_2}{2} & -\omega_1\\ \omega_1 & \frac{\Gamma_2}{2}\end{pmatrix}\left[e^{\Gamma_2 t/2}\begin{pmatrix} m_2\\ m_3\end{pmatrix}\right]. \qquad (2.3)$$

But this is a special case of the Zakharov-Shabat eigenvalue problem [9],

$$\frac{\partial v}{\partial t}=\begin{pmatrix} -i\zeta & -q^{\star}(t)\\ q(t) & i\zeta\end{pmatrix}v, \qquad (2.4)$$

identifying $\zeta=-i\Gamma_2/2$ and $q(t)=\omega_1(t)=q^{\star}(t)$.

The ZS problem has been extensively studied both as a forward problem, where the behavior of v is determined, given the parameter ζ and function $q(t)$, and as an inverse problem. Here, the behavior of v is specified by giving the ''scattering data'' of the system. For each such set of scattering data, a ''potential'' $q(t)$ may be uniquely determined [9,10,25–27].

Suppose the ZS system (2.4) has scattering coefficients $a(\zeta),b(\zeta),\overline{a(\zeta)},\overline{b(\zeta)}$ for real ζ. It also has bound states, given in standard notation [10], by data $\{\zeta_j,b_j,\overline{\zeta_j},\overline{b_j}\}$. For example, the ζ_j are the zeroes of $a(\zeta)$ in the upper half complex plane. Since, for system (2.3), q is purely real, it can be shown that [10,28] $\overline{b(\zeta)}=b^{\star}(\zeta^{\star})=b(-\zeta)$, $\overline{a(\zeta)}=a^{\star}(\zeta^{\star})=a(-\zeta)$, $\overline{\zeta_j}=\zeta_j^{\star}$, and $\overline{b_j}=b_j^{\star}$. Also, the ζ_j occur in pairs $(\zeta_j,-\zeta_j^{\star})$, or lie on the imaginary axis. For a ζ_j on the imaginary axis, b_j is pure real, else it is in a $(b_j,b_j^{\star})$ pair.

Thus, for real ζ and assuming $q(t)$ is absolutely integrable, if the ZS system has a 2×2 fundamental solution with asymptotic behavior

$$V\rightarrow\begin{pmatrix} e^{-i\zeta t} & 0\\ 0 & e^{i\zeta t}\end{pmatrix} \quad \text{as } t\rightarrow-\infty, \qquad (2.5a)$$

it will have behavior

$$V\rightarrow\begin{pmatrix} a e^{-i\zeta t} & -\overline{b}e^{-i\zeta t}\\ b e^{i\zeta t} & \overline{a}e^{i\zeta t}\end{pmatrix} \quad \text{as } t\rightarrow\infty. \qquad (2.5b)$$

Then the corresponding solution to Eq. (2.3), with boundary conditions (2.2), can be shown to be

$$m_2\rightarrow-\overline{b}(-i\Gamma_2/2)e^{-\Gamma_2 t}, \qquad (2.6a)$$

$$m_3\rightarrow\overline{a}(-i\Gamma_2/2), \qquad (2.6b)$$

as $t\rightarrow\infty$. It is assumed here that $\overline{a(\zeta)}$ and $\overline{b(\zeta)}$ are defined at $\zeta=-i\Gamma_2/2$. For absolutely integrable $\omega_1(t)$, $\overline{a(\zeta)}$ can be analytically continued from the real axis to the whole lower half complex plane, including $\zeta=-i\Gamma_2/2$ [10]. In general, $\overline{b(\zeta)}$ exists for real ζ, and can be analytically continued to a strip surrounding the real axis, the width of the strip below the real axis depending on the rate at which $\omega_1(t)$ decays to zero as $t\rightarrow\infty$ [10]. $\overline{b}$ also exists at the ''bound states'' of the system in the lower half complex plane, i.e., at the zeroes of $\overline{a(\zeta)}$ in the lower half plane.

A useful class of pulses exists if $\overline{b(\zeta)}$ is zero throughout its strip of analyticity. Then $\overline{a(\zeta)}$ has the form

$$\overline{a(\zeta)}=\prod_{j=1}^{m}\frac{\zeta-\zeta_j^{\star}}{\zeta-\zeta_j}, \qquad (2.7)$$

for ζ real and in the lower half complex plane. This corresponds to a final magnetization response

$$m_1=m_2=0, \qquad (2.8a)$$

$$m_3=\prod_{j=1}^{m}\frac{\Gamma_2-2i\zeta_j^{\star}}{\Gamma_2-2i\zeta_j}, \qquad (2.8b)$$

and hence these pulses belong to the soliton class described in the Introduction. It is well known how to invert the ZS problem for $\overline{a(\zeta)}$ [and $a(\zeta)$] zero for real ζ. Methods such as the Bäcklund transform [11,29,30], or the dressing method of Neugebauer [31] are particularly efficient.

III. THE GENERAL CASE

For a complex rf pulse, it is not possible to reduce system (1.1) to a linear system of lower degree. It is necessary to treat the system as a third-order scattering system, and use more general techniques than for the ZS problem to find rf pulses. As described in the Introduction, pulses in the soliton class will be calculated using the dressing method.

It is convenient for this method to change variables in Eq. (1.1) so that the Hamiltonian becomes traceless. Then, since $\Gamma_1=0$ and $\omega_3(t)=0$,

$$\frac{\partial}{\partial t}\left[e^{2\Gamma_2 t/3}\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix}\right]=\begin{pmatrix} 2\Gamma_2/3 & -i\omega^\star/\sqrt{2} & i\omega/\sqrt{2} \\ -i\omega/\sqrt{2} & -\Gamma_2/3 & 0 \\ i\omega^\star/\sqrt{2} & 0 & -\Gamma_2/3 \end{pmatrix}\left[e^{2\Gamma_2 t/3}\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix}\right], \tag{3.1}$$

where $m=(1/\sqrt{2})[m_1+im_2]$, the factor $1/\sqrt{2}$ being chosen so that the matrix in Eq. (3.1) has a symmetry about the leading diagonal.

Let Φ be the fundamental 3×3 matrix solution to Eq. (3.1). Then Φ is the solution to the scattering system,

$$\frac{\partial \Phi}{\partial t}=[i\zeta J+V(t)]\Phi(t,\zeta), \tag{3.2a}$$

where $\zeta=-i\Gamma_2$ is the scattering parameter, or eigenvalue. Here, J is a time constant, traceless diagonal matrix with elements down the diagonal in nonincreasing order,

$$J=\begin{pmatrix} 2/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & -1/3 \end{pmatrix}, \tag{3.2b}$$

and V, the ''potential,'' is a time varying, absolutely integrable, ''J-off-diagonal'' matrix [32]. Being J-off-diagonal means that there exists a matrix W such that $V=[J,W]=JW-WJ$. Since

$$V=\begin{pmatrix} 0 & -i\omega^\star/\sqrt{2} & i\omega/\sqrt{2} \\ -i\omega/\sqrt{2} & 0 & 0 \\ i\omega^\star/\sqrt{2} & 0 & 0 \end{pmatrix}, \tag{3.2c}$$

a possible choice of W is

$$W=\begin{pmatrix} 0 & -i\omega^\star/\sqrt{2} & i\omega/\sqrt{2} \\ i\omega/\sqrt{2} & 0 & 0 \\ -i\omega^\star/\sqrt{2} & 0 & 0 \end{pmatrix}. \tag{3.3}$$

It is important that V is J-off-diagonal, since the dressing method naturally constructs such potentials from the ''vacuum,'' as described below [see especially Eq. (3.7)].

A. The dressing method

The dressing method states that if Φ_0 is the solution to the, in general, $n\times n$ scattering system

$$\frac{\partial \Phi_0}{\partial t}=[i\zeta J+V_0(t)]\Phi_0(t,\zeta), \tag{3.4}$$

with given boundary conditions, then there exists a Φ_1, related to Φ_0 by

$$\Phi_1=[1+R/(\zeta-z)]\Phi_0, \tag{3.5}$$

and that has a similar evolution to Φ_0, namely,

$$\frac{\partial \Phi_1}{\partial t}=[i\zeta J+V_1(t)]\Phi_1(t,\zeta), \tag{3.6}$$

with boundary conditions determined below, and with

$$V_1-V_0=i[R,J]. \tag{3.7}$$

Here, $R(t)$ is an $n\times n$ matrix, to be determined. It is obtained in terms of Φ_0, z (which is where Φ_1 becomes singular), and some other parameters. The set of parameters needed to determine Φ_1 given Φ_0 will be called ''dressing data.''

Thus, given a known solution to an equation of the form Eq. (3.4), a ladder of new solutions can be built up. Since the matrix dressing operator R is known in terms of the known solution Φ_0, both Φ_1 and V_1 may be explicitly determined. This process may then be repeated, with a new matrix R determined in terms of Φ_1. Typically, the initial system is the ''vacuum,'' where $V_0(t)=0$, and hence $\Phi_0(t,\zeta)$ may be taken as $\exp[i\zeta Jt]$. This ladder is then called a ''soliton-ladder.'' That these are solitons as defined in the Introduction is shown in Sec. III C.

It can be shown [24,33] that R satisfies

$$\frac{dR}{dt}=L_0(\bar{z})R-RL_0(z)+iRJR, \tag{3.8a}$$

and

$$R^2=(z-\bar{z})R. \tag{3.8b}$$

Here, $L_0(\zeta)=i\zeta J+V_0$, and the time dependence in quantities above is not shown explicitly unless needed. $\bar{z}$ is another parameter in the dressing method, and is most naturally taken as $\bar{z}=z^\star$ for the system (3.2), as shown later. Further, z is assumed to be off the real axis. Given this assumption, it is shown in Appendix B that z may be taken, without loss of generality, to be in the upper half complex plane. Hence, solutions in the soliton ladder may always be chosen to be analytic in the lower half complex plane.

This result is not surprising. J in Eq. (3.2b) has only two distinct elements on the diagonal. It is therefore reasonable to expect that the fundamental solution Φ would share some analytic properties with the solution to the 2×2 ZS problem. One property of the latter is that the fundamental solution may be chosen to be analytic in the lower half complex plane.

Under the assumption that z is off the real axis, $z-\overline{z}\neq 0$, and then Eq. (3.8b) implies that

$$R(t)=(z-\overline{z})\hat{T}(t), \tag{3.9}$$

where $\hat{T}(t)$ is a projection matrix, i.e., $\hat{T}^2=\hat{T}$. Thus, Eq. (3.5) can be rewritten

$$\Phi_1(t,\zeta)=\left[1+\frac{z-\overline{z}}{\zeta-z}\hat{T}(t)\right]\Phi_0(t,\zeta) \tag{3.10a}$$

or, inversely,

$$\Phi_0(t,\zeta)=\left[1-\frac{z-\overline{z}}{\zeta-\overline{z}}\hat{T}(t)\right]\Phi_1(t,\zeta). \tag{3.10b}$$

The change in V, i.e., V_1-V_0 can be rewritten [Eq. (3.7)]:

$$V_1-V_0=i(z-\overline{z})[\hat{T},J]. \tag{3.11}$$

Further, the image and kernel of $\hat{T}$ can be shown to have the general form [23,24]

$$\text{im }\hat{T}=\Phi_0(\overline{z})v, \tag{3.12a}$$

$$\ker\hat{T}=\Phi_0(z)w, \tag{3.12b}$$

with v and w constant vector spaces. Hence, they are given as $n\times d$ and $n\times(n-d)$ matrices, where d is the dimension of the image of $\hat{T}$, with each column of the matrix a linearly independent vector in the respective space. Then, the general form of $\hat{T}$ is

$$\hat{T}=\Phi_0(\overline{z})v[\tilde{w}^T\Phi_0^{-1}(z)\Phi_0(\overline{z})v]^{-1}\tilde{w}^T\Phi_0^{-1}(z). \tag{3.13}$$

Here, $\tilde{w}$ refers to the space orthogonal to w, i.e., it is an $n\times d$ matrix such that $\tilde{w}^Tw=0$. Note that $\tilde{w}$ is not a uniquely defined matrix. However, the value of $\hat{T}$ is independent of the choice of the forms of both $\tilde{w}$ and of v.

However, for the 3×3 system considered here, d must equal 1 or 2, if $\hat{T}$ is to be nontrivial. If $d=1$, then $\hat{T}$ can be written more simply. Since, for $d=1$, $\tilde{w}^T\Phi_0^{-1}(z)\Phi_0(\overline{z})v$ is a number, it is convenient to define

$$T(t)=\Phi_0(t,\overline{z})P\Phi_0^{-1}(t,z), \tag{3.14}$$

where

$$P=v\tilde{w}^T \tag{3.15}$$

is (up to an arbitrary scale factor) an ''undressed'' constant projection matrix with a one-dimensional image.

Then,

$$\hat{T}=\frac{\Phi_0(\overline{z})v\tilde{w}^T\Phi_0^{-1}(z)}{\tilde{w}^T\Phi_0^{-1}(z)\Phi_0(\overline{z})v} \tag{3.16a}$$

$$=T/\text{tr}(T), \tag{3.16b}$$

where tr(T) denotes the trace of T. Note that, here, $\tilde{w}$ is an n-component vector that is uniquely defined, up to an overall scale factor.

If $\hat{T}$ is a two-dimensional projection, then $1-\hat{T}$ is a one-dimensional projection, with image and kernel equal to the kernel and image, respectively, of $\hat{T}$. Then,

$$1-\hat{T}=\frac{\Phi_0(z)w\tilde{v}^T\Phi_0^{-1}(\overline{z})}{\tilde{v}^T\Phi_0^{-1}(\overline{z})\Phi_0(z)w}, \tag{3.17}$$

where $\tilde{v}$ is defined in the same way as $\tilde{w}$ was above, that is $\tilde{v}$ is the space orthogonal to v, in this case it is a uniquely defined vector (up to an overall constant multiplier). Defining $\hat{T}'=1-\hat{T}$, and from Eq. (3.10a),

$$\Phi_1=\left[1+\frac{z-\overline{z}}{\zeta-z}\hat{T}\right]\Phi_0=\left[1+\frac{z-\overline{z}}{\zeta-z}(1-\hat{T}')\right]\Phi_0$$
$$=\frac{\zeta-\overline{z}}{\zeta-z}\left[1+\frac{\overline{z}-z}{\zeta-\overline{z}}\hat{T}'\right]\Phi_0. \tag{3.18}$$

Hence, using a two-dimensional $\hat{T}$ with $(z,\overline{z})$, in the dressing data is equivalent to using a one-dimensional $\hat{T}'$ with $(\overline{z},z)$ in its dressing data. Therefore, for system (3.2), $\hat{T}$ may always be taken to have the form of Eq. (3.16), i.e., it may always be taken to have a one-dimensional image.

Returning to the general $n\times n$ system, it follows from Eqs. (3.10) and (3.12) that

$$\Phi_1(\overline{z})v=0, \tag{3.19a}$$

$$\Phi_1^{-1^T}(z)\tilde{w}=0. \tag{3.19b}$$

That is, Φ_1 and $\Phi_1^{-1^T}$ become degenerate at $\zeta=\overline{z}$ and $\zeta=z$, respectively, with v and $\tilde{w}$ giving the linear dependence of the columns. Typically, the dressing method is used to create an ''m soliton'' Φ_m, as the final rung in the ladder $\Phi_0,\Phi_1,\ldots,\Phi_m$. Each Φ_j is determined from Φ_{j-1} by specifying dressing data $s_j=\{z_j,\overline{z}_j,v_j,\tilde{w}_j\}$, i.e., by specifying the extra degeneracy of Φ_j over Φ_{j-1}. Assuming each z_j is distinct from all other z_j and $\overline{z}_j$, this degeneracy cannot be taken away. Hence,

$$\Phi_m(\overline{z}_j)v_j=0, \tag{3.20a}$$

$$\Phi_m^{-1^T}(z_j)\tilde{w}_j=0 \tag{3.20b}$$

for $j=1,\ldots,m$. Therefore, the order in which the s_j are specified is not important. Actually, the s_j can be split up into $s_{j+}=\{z_j,\tilde{w}_j\}$ and $s_{j-}=\{\overline{z_j},v_j\}$ and these can be paired up in any order. The same Φ_m will result. This ability to build up an m-soliton using dressing data in any order is the basis of the nonlinear superposition formulas [33].

B. Symmetries

For the system (3.2), there are constraints on the form of the Hamiltonian. Define

$$L_m(t,\zeta)=i\zeta J+V_m(t). \tag{3.21}$$

which corresponds to the evolution of Φ_m, the final soliton constructed by the dressing method. V_m is the corresponding potential. L_m has the following symmetries:

$$L_m(t,\zeta)=-L_m^{\dagger}(t,\zeta^{\star}), \tag{3.22a}$$

$$L_m(t,\zeta)=-BL_m^{T}(t,-\zeta)B^{-1}, \tag{3.22b}$$

where † denotes the Hermitian transpose, and

$$B=\begin{pmatrix} 1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}. \tag{3.22c}$$

Of course, $B=B^{-1}$, here, but the constraints Eqs. (3.24) and (3.25) below hold for general (time-constant, invertible) B.

Studying how such constraints affect the allowed dressing data is known as a reduction problem [24,34]. Note that only the constraints upon L_m will be considered, and not the Hamiltonians of solitons lower down the ladder, since ultimately only Φ_m and V_m are of interest.

It is well known [34] that the symmetries (3.22) give rise to automorphisms on the solution sets to system (3.2). This means that if Φ_m has asymptotic behavior,

$$\Phi_m(t,\zeta)\to e^{i\zeta Jt}A_m(\zeta) \tag{3.23}$$

as $t\to-\infty$, then Eqs. (3.22a) and (3.22b) imply, respectively,

$$\Phi_m(t,\zeta)=\Phi_m^{-1^{\dagger}}(t,\zeta^{\star})A_m^{\dagger}(\zeta^{\star})A_m(\zeta), \tag{3.24a}$$

$$\Phi_m(t,\zeta)=B\Phi_m^{-1^{T}}(t,-\zeta)A_m^{T}(-\zeta)B^{-1}A_m(\zeta). \tag{3.24b}$$

Assume that Φ_m is normalized so that $A_m^{\dagger}(\zeta^{\star})A_m(\zeta)=1$ and $A_m^{T}(-\zeta)B^{-1}A_m(\zeta)=B^{-1}$. This can always be done. Then, by considering Eqs. (3.20), it follows that the above constraints on Φ_m imply (modulo reordering, and scaling of the vectors by arbitrary constants), for $j=1,\ldots,m$,

$$z_j=\overline{z_j^{\star}}, \tag{3.25a}$$

$$\tilde{w}_j=v_j^{\star}, \tag{3.25b}$$

and either

$$z_j \text{ is purely imaginary and } \tilde{w}_j=B^{-1}v_j, \tag{3.25c}$$

or

$$z_j \ \text{ occurs in a } (z_j,z_k=-z_j^{\star}) \text{ pair,}$$

$$\text{with } v_k=B\tilde{w}_j \text{ and } \tilde{w}_k=B^{-1}v_j. \tag{3.25d}$$

Further, by considering how imposing the above conditions (3.25) gives rise to symmetries on the dressed projection operators $\hat{T}_j$ used to determine Φ_j from Φ_{j-1}, it can be shown that these conditions are sufficient to give the desired symmetries on L_m. Notice, though, that constraint (3.25d) allows intermediate Φ_j to exist that do not have the same symmetries as Φ_m [Eqs. (3.24)].

Finally, the form of Eqs. (3.2) implies that each v_j (and hence $\tilde{w}_j$) may be normalized so that its first component is one, i.e., v_j has the form $v_j^T=(1,a_{j2},a_{j3})$. Such a normalization would only be impossible if the first component of v_j, and hence $\tilde{w}_j$, were zero. Then the undressed projection matrix P_j defined by Eq. (3.15) would be nonzero only in its lower 2×2 block. Thus the dressed projection matrix $\hat{T}_j$ would also have this structure, and hence would be J diagonal, i.e., by definition, $[\hat{T}_j,J]=0$. Thus, the subsequent application of the dressing method would not change the potential. Therefore, v_j must have a nonzero first component if the dressing method is to have a nontrivial effect, and so the above normalization is valid.

C. The asymptotic behavior of the system

In order to determine the effect of the m-soliton potential $V_m(t)$ calculated by the dressing method, the behavior of $\Phi_m(t,\zeta)$ as $t\to\pm\infty$ must be determined.

Consider an intermediate soliton solution of system (3.2), $\Phi_{j-1}(t,\zeta)$. It will, in general, have asymptotic forms

$$\Phi_{j-1}(t,\zeta)\to\begin{cases} e^{i\zeta Jt}A_{j-1}(\zeta) & \text{as } t\to-\infty\\ e^{i\zeta Jt}S_{j-1}(\zeta)A_{j-1}(\zeta) & \text{as } t\to\infty\end{cases} \tag{3.26}$$

for real ζ, where $S_{j-1}(\zeta)$ is the ‘‘scattering matrix’’ of the system.

The dressed projection matrix $\hat{T}_j(t)$ used to determine $\Phi_j(t,\zeta)$ will then have asymptotic forms (which are independent of t),

$$\hat{T}_j(t)\to\begin{cases}[\mathbb{1}_-A_{j-1}(\overline{z_j})P_jA_{j-1}^{-1}(z_j)\mathbb{1}_-]/\mathrm{tr}[\cdots] & \text{as } t\to-\infty\\ [\mathbb{1}_+S_{j-1}(\overline{z_j})A_{j-1}(\overline{z_j})P_jA_{j-1}^{-1}(z_j)S_{j-1}^{-1}(z_j)\mathbb{1}_+]/\mathrm{tr}[\cdots] & \text{as } t\to\infty,\end{cases} \tag{3.27}$$

where $P_j = v_j \tilde{w}_j^T$, and $\{z_j, \overline{z_j}, v_j, \tilde{w}_j\}$ are the dressing data used to construct Φ_j. The notation $X/\mathrm{tr}[\cdots]$ stands for X divided by its trace. The matrices $\mathbb{1}_+$ and $\mathbb{1}_-$ are

$$\mathbb{1}_+ = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.28a}$$

$$\mathbb{1}_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.28b}$$

The above results rely on the fact that J in Eq. (3.2) has its elements in nonincreasing order, and that z_j is in the upper half complex plane, with $\overline{z_j} = z_j^\star$. The particular structure of $\mathbb{1}_+$ and $\mathbb{1}_-$ follows from J having a unique highest element, and two equal lowest elements.

The asymptotic forms (3.27) can be written as

$$\hat{T}_j(t) \to \begin{cases} \begin{bmatrix} 0 & \\ & \hat{T}_j^- \end{bmatrix} & \text{as } t \to -\infty \\ \begin{bmatrix} \hat{T}_j^+ & \\ & 0 \end{bmatrix} & \text{as } t \to \infty, \end{cases} \tag{3.29}$$

where 0 signifies a zero matrix of appropriate size, $\hat{T}_j^-$ is a 2×2 matrix, and $\hat{T}_j^+$ is a number. Clearly, $\hat{T}_j^+ = 1$, as it must have a trace of one. Here, and later, a matrix in square brackets signifies that it is built up from smaller matrices or vectors, as well as numbers, in an obvious way.

The asymptotic forms of $\Phi_j(t,\zeta)$ can then be shown to be

$$\Phi_j(t,\zeta) \to \begin{cases} e^{i\zeta Jt} A_j(\zeta) & \text{as } t \to -\infty \\ e^{i\zeta Jt} S_j(\zeta) A_j(\zeta) & \text{as } t \to \infty, \end{cases} \tag{3.30}$$

where

$$A_j(\zeta) = \begin{bmatrix} 1 & \\ & 1 + \dfrac{z_j - \overline{z_j}}{\zeta - z_j} \hat{T}_j^- \end{bmatrix} A_{j-1}(\zeta), \tag{3.31a}$$

$$S_j(\zeta) = \begin{bmatrix} 1 + \dfrac{z_j - \overline{z_j}}{\zeta - z_j} \hat{T}_j^+ & \\ & 1 \end{bmatrix} S_{j-1}(\zeta) \begin{bmatrix} 1 & \\ & 1 - \dfrac{z_j - \overline{z_j}}{\zeta - \overline{z_j}} \hat{T}_j^- \end{bmatrix}, \tag{3.31b}$$

where the 1's are unit matrices of appropriate size.

Given a "vacuum" solution $\Phi_0 = \exp[i\zeta Jt]$, then $A_0(\zeta) = S_0(\zeta) = 1$. The final $A_m(\zeta)$ and $S_m(\zeta)$ can then be obtained via Eqs. (3.31). Note that all the S_j will be J diagonal.

Equation (3.31b) gives the connection between the calculation of the soliton potential, V_m, and the calculation of T_2-selective pulses. The m-soliton solution Φ_m is a fundamental solution to the traceless equation of motion of the magnetization, Eq. (3.1). Now assume that the initial magnetization is $m_3 = 1$, $m = 0$ for all Γ_2, i.e.,

$$e^{2\Gamma_2 t/3} \begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix} \to \begin{pmatrix} e^{2\Gamma_2 t/3} \\ 0 \\ 0 \end{pmatrix} \tag{3.32}$$

as $t \to -\infty$.

However, $\Phi_m(t,\zeta) \to \exp[i\zeta Jt] A_m(\zeta)$ as $t \to -\infty$, and so

$$\Phi_m(t, -i\Gamma_2) A_m^{-1}(-i\Gamma_2) \hat{e}_1 \to \begin{pmatrix} e^{2\Gamma_2 t/3} \\ 0 \\ 0 \end{pmatrix} \tag{3.33}$$

as $t \to -\infty$, where $\hat{e}_1^T = (1,0,0)$.

Hence, the magnetization response is related to Φ_m,

$$\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix} = e^{-2\Gamma_2 t/3} \Phi_m(t, -i\Gamma_2) A_m^{-1}(-i\Gamma_2) \hat{e}_1. \tag{3.34}$$

Therefore, after the rf pulse $\omega(t)$ corresponding to the soliton potential $V_m(t)$ via Eq. (3.2c), is applied,

$$\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix} \to e^{-2\Gamma_2 t/3} e^{\Gamma_2 Jt} S_m(-i\Gamma_2) \hat{e}_1$$
$$\to \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-\Gamma_2 t} & 0 \\ 0 & 0 & e^{-\Gamma_2 t} \end{pmatrix} S_m(-i\Gamma_2) \hat{e}_1, \tag{3.35}$$

as $t \to \infty$. Just as in Sec. II, the elements of $S_m(\zeta)$ are, in general, not defined over the whole complex ζ plane. Let S_m have $S_m^{(i,j)}$ as the element in row i and column j. Then the element $S_m^{(1,1)}$ is defined for real ζ, and may be analytically continued to the entire lower half complex plane. $S_m^{(2,1)}$ and $S_m^{(3,1)}$ are defined for real ζ and may be analytically continued to a strip surrounding the real axis.

For real ζ, Eq. (3.31b) allows the calculation of $S_m(\zeta)$. From Eq. (3.35), only its first column is of interest. Since $\hat{T}_j^+ = 1$, it gives

$$S_m(\zeta) \hat{e}_1 = \begin{pmatrix} \prod_{j=1}^{m} \dfrac{\zeta - \overline{z_j}}{\zeta - z_j} \\ 0 \\ 0 \end{pmatrix}, \tag{3.36}$$

and hence

$$\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix} \to \begin{pmatrix} \prod_{j=1}^{m} \dfrac{\Gamma_2 - i\overline{z_j}}{\Gamma_2 - iz_j} \\ 0 \\ 0 \end{pmatrix} \tag{3.37}$$

as $t \to \infty$. This expression is correct even if $-i\Gamma_2$ is outside the strip of analyticity referred to above, as then the transverse magnetization will still decay to zero as $t\rightarrow\infty$, and the expression for m_3 is correct for all Γ_2.

Therefore, after the application of the rf pulse, the magnetization will once again lie on the z axis. The m_3 response must take the form

$$m_3(\Gamma_2)=\prod_{j=1}^{m}\frac{\Gamma_2-iz_j^{\star}}{\Gamma_2-iz_j}, \tag{3.38}$$

with z_j in the upper half complex plane. Hence, the dressing method indeed creates soliton pulses as defined in the Introduction. It also demonstrates that the general definition of soliton pulse [one whose scattering matrix is J diagonal] corresponds to the specific definition used for this system [one whose final magnetization response has the form of Eq. (3.37)].

D. Computing the soliton potential

Given the set of dressing data $s_j=\{z_j,\overline{z_j},v_j,\widetilde{w}_j\}$ for $j=1,\ldots,m$, the most straightforward way to numerically calculate the soliton potential $V_m(t)$ is with nonlinear superposition formulas. This method obviates the need to determine any Φ_j, for $j>0$. Only the $\hat{T}_j$ are needed, and they can be easily determined from previously calculated $\hat{T}_j$.

Nonlinear superposition formulas are well known for the ZS problem [29] and for higher-order systems [33]. The formulas given below are specific to systems where all the $\hat{T}_j$ have one-dimensional images. However, they are computationally advantageous, as no matrix inverses need be calculated, unlike those in Ref. [33].

Consider a fundamental solution Φ to system (3.2). Let Φ_{12} be the solution after the addition of dressing data s_1 and s_2. Φ_{12} can be obtained in two ways, represented as

$$\begin{array}{ccccc} & & \Phi_1 & & \\ s_1,\hat{T}_1 & \nearrow & & \searrow & s_2,\hat{T}_{12} \\ \Phi & & & & \Phi_{12}. \\ s_2,\hat{T}_2 & \searrow & & \nearrow & s_1,\hat{T}_{21} \\ & & \Phi_2 & & \end{array} \tag{3.39}$$

Hence, Φ_{12} is created via intermediate solutions Φ_1 or Φ_2, corresponding to adding dressing data in the order s_1,s_2 or s_2,s_1, respectively.

Given the general form of the $\hat{T}$ projections [Eq. (3.16)], it is straightforward to show that $\hat{T}_{12}$, the projection needed to go from Φ_1 to Φ_{12} is

$$\hat{T}_{12}=\left\{\left[1+\frac{z_1-\overline{z_1}}{\overline{z_2}-z_1}\hat{T}_1\right]\hat{T}_2\left[1-\frac{z_1-\overline{z_1}}{z_2-\overline{z_1}}\hat{T}_1\right]\right\}\Big/\ \mathrm{tr}[\cdots]. \tag{3.40a}$$

Similarly,

$$\hat{T}_{21}=\left\{\left[1+\frac{z_2-\overline{z_2}}{\overline{z_1}-z_2}\hat{T}_2\right]\hat{T}_1\left[1-\frac{z_2-\overline{z_2}}{z_1-\overline{z_2}}\hat{T}_2\right]\right\}\Big/\ \mathrm{tr}[\cdots]. \tag{3.40b}$$

As previously, $X/\mathrm{tr}[\cdots]$ denotes X divided by its trace.

Consider now the problem of building up the m-soliton potential V_m from the vacuum. This can be done by constructing a lattice whose base is the vacuum. For example, for $m=3$, the lattice would look like

$$\begin{array}{ccccccc} \Phi_0 & & & & & & \\ & \searrow s_1 & & & & & \\ & & \Phi_1 & & & & \\ & \nearrow s_1 & & \searrow s_2 & & & \\ \Phi_0 & & & & \Phi_{12} & & \\ & \searrow s_2 & & \nearrow s_1 & & \searrow s_3 & \\ & & \Phi_2 & & & & \Phi_{123}. \\ & \nearrow s_2 & & \searrow s_3 & & \nearrow s_1 & \\ \Phi_0 & & & & \Phi_{23} & & \\ & \searrow s_3 & & \nearrow s_2 & & & \\ & & \Phi_3 & & & & \\ & \nearrow s_3 & & & & & \\ \Phi_0 & & & & & & \end{array} \tag{3.41}$$

Here, each element in the first column represents the vacuum solution, $\Phi_0=\exp[i\zeta Jt]$ at a given time t. The second column represents solutions where a single soliton has been added via s_1, s_2, or s_3.

The $\hat{T}$ projection matrices needed to go from the Φ_0's to the second column can be easily obtained, given the dressing data s_j, $j=1,\ldots,m$, and Eq. (3.16). Then the projection matrices to get to the 2-soliton solutions in the third column may be determined from the nonlinear superposition formulas, Eqs. (3.40). This is repeated until the end of the lattice has been reached. Finally, the m-soliton potential $V_m(t)$ may be obtained from

$$V_m(t)=i\sum_{j=1}^{m}(z_j-\overline{z_j})[\hat{T}_{12\cdots j},J], \tag{3.42}$$

where $\hat{T}_{12\cdots j}$ is the projection matrix needed to go from $\Phi_{12\cdots(j-1)}$ to $\Phi_{12\cdots j}$ along the top edge of the lattice. Note that V_m is expressed in terms only of the $\hat{T}$ matrices, and thus the soliton solutions Φ in the lattice never need to be determined.

IV. EXAMPLES

A. One-soliton potential

The simplest nontrivial real soliton pulse, as calculated in Sec. II, would have, with scattering data $\{\zeta_1, \overline{\zeta_1}, b_1, \overline{b_1}\}$, the magnetization response [Eqs. (2.8)]

$$m=0, \tag{4.1a}$$

$$m_3=\frac{\Gamma_2-\eta}{\Gamma_2+\eta}, \tag{4.1b}$$

where $\zeta_1=i\eta/2$ and $\eta\in\mathbb{R}^+$. This pulse could therefore be used to null the magnetization of spins with $\Gamma_2=\eta$. The general form of the one-soliton potential is well known [10,27], and hence the real rf pulse giving rise to the above response is

$$\omega_1(t)=\frac{b_1}{|b_1|}\eta\ \mathrm{sech}[\eta t-\ln|b_1|], \tag{4.2}$$

where b_1 is real. The requirements that ζ_1 is imaginary and b_1 is real follow from the symmetry constraints on the scattering data given in Sec. II.

The general form of a one-soliton potential calculated with the dressing method with dressing data $\{z,\overline{z},v,w\}$ is

$$V=\begin{pmatrix} 0 & v_{12} & v_{13} \\ v_{21} & 0 & 0 \\ v_{31} & 0 & 0 \end{pmatrix}, \tag{4.3a}$$

where, for example,

$$v_{21}(t)=-\frac{\eta a_2 e^{-i\lambda t}}{\sqrt{|a_2|^2+|a_3|^2}}\ \mathrm{sech}\ [\eta t-\ln\sqrt{|a_2|^2+|a_3|^2}]. \tag{4.3b}$$

Here, $z=\lambda+i\eta$, with $\lambda\in\mathbb{R}$ and $\eta\in\mathbb{R}^+$, and $v^T=(1,a_2,a_3)$.

The above expression assumed the constraints (3.25a) and (3.25b), but not (3.25c) or (3.25d). To get a physically realizable one-soliton rf pulse, constraint (3.25c) must be satisfied, and hence $z=i\eta$ and $a_3=a_2^{\star}$. The associated magnetization response [Eq. (3.38)] would be

$$m_3=\frac{\Gamma_2-\eta}{\Gamma_2+\eta}. \tag{4.4}$$

The general form of the rf pulse, $\omega(t)$, is then

$$\omega(t)=-i\eta e^{i\phi_2}\mathrm{sech}[\eta t-\ln(\sqrt{2}|a_2|)], \tag{4.5}$$

where ϕ_2 is defined by $a2=|a2|e^{i\phi_2}$.

From Appendix C, $\omega(t)$ in Eq. (4.5) should correspond with that in Eq. (4.2) when $a_2=i\overline{b_1}/\sqrt{2}$. Since $\overline{b_1}=b_1^{\star}$ in general, and here b_1 is real, this prediction is easily verified.

The rf pulse calculated by the dressing method, Eq. (4.5), is just a trivial generalization of the rf pulse calculated by the reduction to the ZS problem, Eq. (4.2), since it just has an extra constant phase. It is necessary to calculate higher-order soliton pulses to get a nontrivial difference.

B. One-soliton potential with both T_1 and T_2 relaxation

Although this paper describes the calculation of pulses whose response is a function of Γ_2, and Γ_1 is assumed to be zero, in many cases this assumption is not valid. It is therefore useful to see the effect of T_1 relaxation on the one-soliton pulse of Sec. IV A. This pulse can be taken, without loss of generality, to be

$$\omega(t)=\mathrm{sech}(t). \tag{4.6}$$

System (1.1), with $\omega_3=0$, can be solved for this pulse. For example, the method in Ref. [35], where $\Gamma_1=\gamma$ and $\Gamma_2=\frac{1}{2}\gamma$, can be generalized. Given the initial condition

$$\boldsymbol{m}(t)\to\begin{pmatrix}0\\0\\1\end{pmatrix}, \tag{4.7}$$

as $t\to-\infty$, the magnetization at time t will have the form

$$\boldsymbol{m}(t)=\frac{1}{(2\Gamma-1)(2\Gamma+1)}\begin{pmatrix} 0 \\ \frac{2\Gamma_1}{\Gamma_2+1}[\tanh(t)+2\Gamma]f(t)-\mathrm{sech}(t)[1+2\Gamma-2g(t)] \\ -\frac{2\Gamma_1}{\Gamma_2+1}\mathrm{sech}(t)f(t)-[\tanh(t)-2\Gamma][1+2\Gamma-2g(t)] \end{pmatrix}, \tag{4.8}$$

where $\Gamma=\frac{1}{2}(\Gamma_2-\Gamma_1)$, and

$$f(t)={}_2F_1(1,[\Gamma_2+1]/2;[\Gamma_2+3]/2;-e^{2t})e^t,$$

$$g(t)={}_2F_1(1,\Gamma_1/2;1+\Gamma_1/2;-e^{2t}), \tag{4.9}$$

with ${}_2F_1$ the hypergeometric function [36].

Hence, the asymptotic form of $m(t)$ can be shown to be, for $\Gamma_2<1$ and $\Gamma_1<\Gamma_2+1$,

$$\boldsymbol{m}(t)\to\begin{pmatrix} 0 \\ \dfrac{\pi\Gamma_1 e^{-\Gamma_2 t}}{(2\Gamma_1-1)\sin\left[\dfrac{\pi}{2}(\Gamma_2+1)\right]} \\ 1-\dfrac{\pi\Gamma_1 e^{-\Gamma_1 t}}{(\Gamma_2-\Gamma_1+1)\sin\left(\dfrac{\pi}{2}\Gamma_1\right)} \end{pmatrix} \tag{4.10}$$

as $t\to\infty$. Note that in the limit $\Gamma_1\to 0$, this becomes $\boldsymbol{m}(t)^T \to(0,0,(\Gamma_2-1)/(\Gamma_2+1))$, as expected from the previous example.

A useful situation to consider is a range of spin species, with different T_2 values, and with each spin species having $\Gamma_1=\Gamma_2/\alpha$, where $\alpha>1$ is a constant. Imagine applying the sech pulse, and examining the magnetization response at a fixed time T, assumed large enough so that $\boldsymbol{m}(t)$ is in the regime of Eq. (4.10).

Then, as $\Gamma_2\to 0$,

$$\boldsymbol{m}(T)\to\begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}. \tag{4.11}$$

Equation (4.10) is not valid for $\Gamma_2\geqslant 1$. However, it is easily seen that

$$\boldsymbol{m}(T)\to\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{4.12}$$

as $\Gamma_2\to\infty$.

There will therefore always be a value of Γ_2, say g_2, for which $m_3(T)=0$, obtained by solving $m_3=0$ in Eq. (4.10). This always has a unique solution for $\alpha>1$ and $\Gamma_2<1$. As α decreases, so does g_2.

In general, T_2-selective pulses with odd m in Eq. (3.38) can still be used in the presence of T_1 relaxation, provided the corresponding shift in the value of g_2 is taken into account. It should also be noted that m_2 (and m_1, for complex rf pulses) will now be nonzero after the application of the pulse.

C. A higher-order soliton pulse

A higher-order soliton pulse was calculated numerically using the dressing data

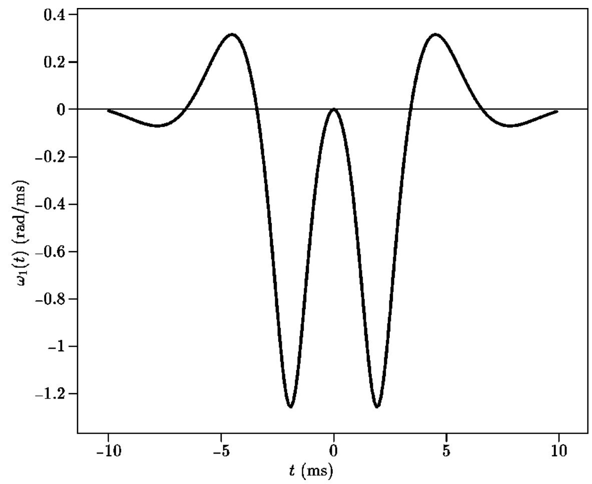

FIG. 1. Three-soliton real rf pulse, $\omega_1(t)$, with dressing data from Eq. (4.13).

$$z_1=i,\quad \overline{z_1}=z_1^\star,\quad v_1=\begin{pmatrix} 1 \\ -\dfrac{i}{\sqrt{2}} \\ \dfrac{i}{\sqrt{2}} \end{pmatrix},\quad \tilde{w}_1=v_1^\star,$$

$$z_2=(\sqrt{3}+i)/2,\quad \overline{z_2}=z_2^\star,\quad v_2=\begin{pmatrix} 1 \\ \dfrac{i}{\sqrt{2}} \\ -\dfrac{i}{\sqrt{2}} \end{pmatrix},\quad \tilde{w}_2=v_2^\star,$$

$$z_3=(-\sqrt{3}+i)/2,\quad \overline{z_3}=z_3^\star,\quad v_3=\begin{pmatrix} 1 \\ \dfrac{i}{\sqrt{2}} \\ -\dfrac{i}{\sqrt{2}} \end{pmatrix},\quad \tilde{w}_3=v_3^\star. \tag{4.13}$$

Note that the above data satisfy the constraints of Eqs. (3.25). These data were chosen somewhat arbitrarily, to demonstrate dressing data with one z_j on the imaginary axis, and two z_j as a $(z_j,-z_j^\star)$ pair.

Such dressing data would lead to a magnetization response

$$m_3(\Gamma_2)=\frac{(\Gamma_2-1)[(\Gamma_2)^2-\Gamma_2+1]}{(\Gamma_2+1)[(\Gamma_2)^2+\Gamma_2+1]}. \tag{4.14}$$

Choosing the unit of time as 1 ms, this would select out spins with $T_2=1$ ms. The corresponding rf pulse is shown in Fig. 1. Note that this pulse is real, and could have also been calculated by the method of Sec. II.

For soliton rf pulses, the final m_3 response is a function only of the z_j in the dressing data, and not of the v_j making up the undressed projection matrices. Further, the total ''energy'' of the pulse,

$$E=\int_{-\infty}^{\infty}|w(t)|^2\,dt, \tag{4.15}$$

is dependent only on the z_j. The effect of the v_j becomes apparent from the expression for the one-soliton potential [Eqs. (4.3)]. An m-soliton can be considered as m one-solitons superposed in a nonlinear fashion. However, if each soliton is widely separated from every other one, i.e., the values of $v_j^{\dagger}v_j$ are all well separated, the individual solitons will be independent, and hence temporally well resolved in the combined m-soliton.

If the values of $v_j^{\dagger}v_j$ are not well separated, it is sometimes useful to still think of the m-soliton as composed of individual one-solitons. For example, consider two solitons superposed, with v_j and v_{j+1} in their dressing data. If $v_j = v_{j+1}$, the maximum amplitude of the resultant rf pulse will often be larger than it would be if the components of v_{j+1} have different phases than those in v_j.

Consider a set of dressing data similar to that above, but with the phases of v_2 and v_3 changed,

$$z_1=i,\quad \overline{z_1}=z_1^{\star},\quad v_1=\begin{pmatrix}1\\ -\frac{i}{\sqrt{2}}\\ \frac{i}{\sqrt{2}}\end{pmatrix},\quad \tilde{w}_1=v_1^{\star},$$

$$z_2=(\sqrt{3}+i)/2,\quad \overline{z_2}=z_2^{\star},\quad v_2=\begin{pmatrix}1\\ \frac{-1}{\sqrt{2}}\\ -\frac{i}{\sqrt{2}}\end{pmatrix},\quad \tilde{w}_2=v_2^{\star},$$

$$z_3=(-\sqrt{3}+i)/2,\quad \overline{z_3}=z_3^{\star},\quad v_3=\begin{pmatrix}1\\ \frac{i}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix},\quad \tilde{w}_3=v_3^{\star}. \tag{4.16}$$

The corresponding, complex, rf pulse is shown in Fig. 2. This figure also shows $|\omega(t)|$. It can be seen that simply changing the phase of the middle components of v_2 and v_3 resulted in an approximately 20% decrease in maximum amplitude, without changing the pulse duration.

The pulse of Fig. 1 was tested experimentally on a series of copper sulphate solutions with varying concentrations, and hence varying T_2 times. In fact, the pulse was compressed to 14.5 ms, instead of 20 ms, and its amplitude was multiplied by a factor 20/14.5. The predicted response is then

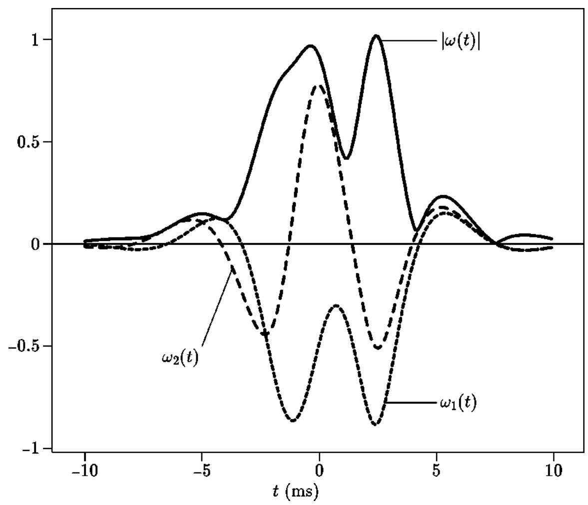

FIG. 2. Three-soliton complex rf pulse, with dressing data from Eq. (4.16). The real and imaginary parts of the rf pulse, $\omega_1(t)$ and $\omega_2(t)$, are shown together with the absolute value of the pulse, $|\omega(t)|$. The functions describing the pulse are in units of rad/ms.

$$m_3(\Gamma_2)=\frac{(\Gamma_2/\Gamma_0-1)[(\Gamma_2/\Gamma_0)^2-\Gamma_2/\Gamma_0+1]}{(\Gamma_2/\Gamma_0+1)[(\Gamma_2/\Gamma_0)^2+\Gamma_2/\Gamma_0+1]}, \tag{4.17}$$

where $\Gamma_0 = 20/14.5\ \ \mathrm{ms}^{-1}$. This response is plotted against $\log_{10}\Gamma_2$ as the dashed line in Fig. 3.

For each concentration, the T_2 was determined by a spin-echo sequence [37], and the T_1 was determined by an inversion-recovery method [22], as described in the Introduction.

Given a sample, the rf amplifier was calibrated by applying hard pulses of varying strengths and measuring the signal intensities. Thus, a π hard pulse would correspond to the first zero of the signal as a function of pulse strength. This then enabled the T_2-selective pulse to be played out at the correct amplitude. Following the pulse, a hard $\pi/2$ pulse was used to flip any z magnetization into the x-y plane, giving a measure of the m_3 component of magnetization following the selective pulse.

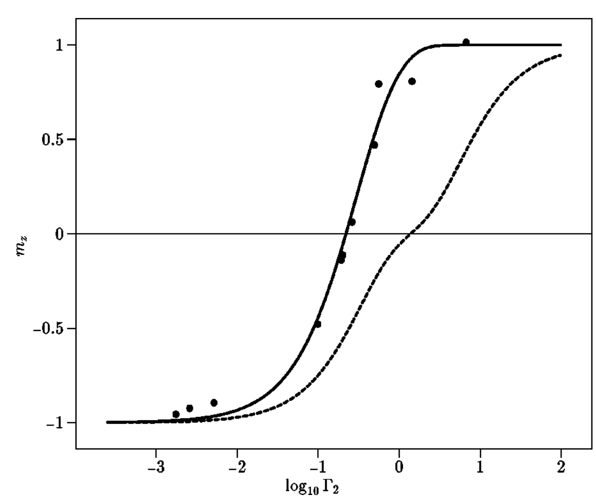

FIG. 3. Dashed line: predicted m_z response to the pulse of Fig. 1, with $\Gamma_1 = 1/T_1 = 0$, as a function of $\log_{10}\Gamma_2$. Solid line: predicted response with $\Gamma_1 = \frac{1}{3}\Gamma_2$. Dots: experimental results. Γ_2 has units ms^{-1}.

It was found that the T_1 for these samples was not negligible, and was approximately $\Gamma_1=\frac{1}{3}\Gamma_2$ for all the samples. The solid line in Fig. 3 shows the response for the pulse of Fig. 1, but with $\Gamma_1=\frac{1}{3}\Gamma_2$, as calculated by numerically integrating Eqs. (1.1), with $\omega_3=0$. This curve compares very well with the experimental results, shown as dots.

This pulse gives $m_3=0$ at $\Gamma_2\approx 0.22\ \text{ms}^{-1}$ when there is T_1 relaxation as described above. The maximum value of m_2 over all values of Γ_2 was found numerically to be approximately 0.038, when determined at the end of the pulse. Hence, similarly to the one-soliton pulse in Sec. IV B, this pulse would be suitable as a T_2-selective pulse for this system.

V. CONCLUSION

The Bloch equations are usually inverted in order to design driving fields to produce a given final response as a function of resonance offset, neglecting relaxation. This paper describes a method of exploiting T_2 relaxation in order to null the magnetization of spins with particular relaxation rates.

The inclusion of relaxation with the rf pulse in the analytic study of the Bloch equations is not new [35,38–41]. For the purpose of inversion of the equations, it seems of little practical value to obtain closed-form expressions of the response, e.g., as quadratures or series expansions. Rather, it is useful to express the problem as a scattering problem, and use inverse scattering techniques, such as the dressing method, to perform the inversion.

It is interesting to note that Manakov [42] showed that the pair of coupled nonlinear Schrödinger equations describing the evolution of a sum of left and right handed polarized electromagnetic waves through a nonlinear medium can be studied using the inverse scattering method, with associated eigenvalue problem a generalization of Eq. (3.1). The potentials q_1 and q_2 used in Manakov reduce to the system here, when

$$q_1=q_2^\star=-i\omega^\star/\sqrt{2}. \tag{5.1}$$

Hence, the properties of the scattering system described there, namely the analyticity and unitarity of the scattering matrix form a subset of the properties derived here in Secs. III B and III C. The expression for the one-soliton pulse in Manakov is equivalent to that here, Eq. (4.3b). The ability to reduce the third order system Eq. (3.1) to the ZS problem, for a real pulse, is paralleled by a similar ability in Manakov for the case of a single polarization.

However, the purposes of Manakov's and this paper are very different. The former was mainly interested in the asymptotic behavior, as $t\rightarrow\infty$, of a group of colliding one-solitons (our ''time'' corresponds to ''space'' in that paper). We are more concerned with the practical application to nmr (and other systems obeying the Bloch equations). Hence, we have constructed an explicit and efficient solution to the eigenvalue problem, including a determination of the necessary and sufficient set of dressing data needed for its solution, and the relationship of the dressing data to the magnetization response as a function of relaxation rate Γ_2.

The pulses calculated here by the dressing method belong to the ''soliton'' class of pulses. Such pulses can be used to return all spins that were initially aligned along the main magnetic field (the z axis) back to the z axis, but with the magnitude of the magnetization dependent on the spin's T_2. This magnitude can be made zero for particular T_2 values, and hence this is a way of obtaining T_2-selective pulses.

It has been demonstrated experimentally that these pulses work as predicted. One application of such pulses is the selection of a spectral line that is hidden by another at the same resonance offset. An application in imaging would be the nulling of magnetization of spins that are not of interest, e.g., fat or water. These are normally well distinguished from other spins by their T_2.

The T_2-selective pulses designed here rely on T_1 being much longer than T_2. If T_1 is not negligible, these pulses will still work, provided T_1 is taken into account. Currently, this would need to be done numerically for all such pulses, other than the one-soliton pulse of Examples IV A and IV B.

Future work will include the extension of the 3×3 inverse scattering method described here to a broader class of pulses than soliton pulses. This should enable the design of pulses with more flexible responses than that of Eq. (3.38), such as sharper ''notch-filter'' responses.

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APPENDIX A: ABSORBING THE DETUNING, $\omega_3(t)$, INTO THE RF PULSE

The Bloch equations, Eqs. (1.1), can be written as

$$\frac{\partial}{\partial t}\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix}=\begin{pmatrix} -\Gamma_1 & -i\omega^\star/\sqrt{2} & i\omega/\sqrt{2} \\ -i\omega/\sqrt{2} & i\omega_3-\Gamma_2 & 0 \\ i\omega^\star/\sqrt{2} & 0 & -i\omega_3-\Gamma_2 \end{pmatrix}\begin{pmatrix} m_3 \\ m \\ m^\star \end{pmatrix} + \begin{pmatrix} \Gamma_1 \\ 0 \\ 0 \end{pmatrix}, \tag{A1}$$

where the transverse magnetization m is defined by $m=1/\sqrt{2}[m_1+im_2]$, the factor $1/\sqrt{2}$ being chosen to be consistent with Eq. (3.1) in Sec. III. As defined in the Introduction, $\omega=\omega_1+i\omega_2$.

Then define $m'(t)$ and $\phi(t)$ by

$$m'(t)=m(t)\exp\left[i\int_t^{t_1}\omega_3(t')\ dt'\right]=m(t)e^{i\phi(t)}, \tag{A2}$$

where t_1 is the time at which the driving field ends.

Equation (A1) becomes

$$\frac{\partial}{\partial t}\begin{pmatrix} m_3 \\ m' \\ m'^{\star} \end{pmatrix} = \begin{pmatrix} -\Gamma_1 & -i\omega'^{\star}/\sqrt{2} & i\omega'/\sqrt{2} \\ -i\omega'/\sqrt{2} & -\Gamma_2 & 0 \\ i\omega'^{\star}/\sqrt{2} & 0 & -\Gamma_2 \end{pmatrix}\begin{pmatrix} m_3 \\ m' \\ m'^{\star} \end{pmatrix} + \begin{pmatrix} \Gamma_1 \\ 0 \\ 0 \end{pmatrix}, \tag{A3}$$

where $\omega'(t)=\omega(t)e^{i\phi(t)}$.

Hence, the evolution of $\boldsymbol{m}$ under arbitrary $\omega_3(t)$ is equivalent to evolution in the frame defined by Eq. (A2) with $\omega_3 = 0$.

Consider the converse case. Let evolution under the rf pulse $\omega(t)$, with detuning $\omega_3(t)$, be denoted by $\{\omega(t),\omega_3(t)\}$. Given initial transverse and longitudinal magnetization $\{m(t_0),m_3(t_0)\}$, let this evolution lead to final transverse and longitudinal magnetization $\{m(t_1),m_3(t_1)\}$. Then by going into the m' frame, an initial magnetization given by $\{m(t_0)e^{i\phi(t_0)},m_3(t_0)\}$, with $\phi(t)$ defined in Eq. (A2), will also evolve under $\{\omega(t)e^{i\phi(t)},0\}$ to $\{m(t_1),m_3(t_1)\}$.

Hence, all final magnetizations reachable by an rf pulse-detuning pair, $\{\omega(t),\omega_3(t)\}$, are also reachable with no detuning if either $e^{i\phi(t_0)}=1$ or if $m(t_0)=0$. In almost all cases of interest, the initial magnetization is $\boldsymbol{m}^T=(0,0,1)$, so the latter condition is satisfied. In general, it would be necessary to apply a detuning ''blip,'' $\omega_3(t)=\phi(t_0)\delta(t-t_0)$, where $\delta(t)$ is the Dirac delta function, before the evolution under $\{\omega(t)e^{i\phi(t)},0\}$, for this to be equivalent to evolution under $\{\omega(t),\omega_3(t)\}$. Since this blip acts to rotate the initial magnetization about the z axis by $\phi(t_0)$, this could be replaced by three rf pulse blips, i.e., hard pulses, of (in order) $R_y(\pi/2)$, $R_x(\phi(t_0))$, and $R_y(-\pi/2)$. [Here, for example, $R_y(\pi/2)$ means an rf pulse blip producing a rotation of angle $\pi/2$ about the y axis, and could be obtained from an rf pulse of the form $\omega(t)=i(\pi/2)\delta(t)$.] This follows from the identity

$$R_{\boldsymbol{n}'}(\theta)=R_{\boldsymbol{m}}(\alpha)R_{\boldsymbol{n}}(\theta)R_{\boldsymbol{m}}(-\alpha), \tag{A4}$$

where, for example, $R_{\boldsymbol{m}}(\alpha)$ represents a rotation of α about a unit axis $\boldsymbol{m}$, and $\boldsymbol{n}'$ is obtained from $\boldsymbol{n}$ by the rotation $R_{\boldsymbol{m}}(\alpha)$, i.e.,

$$\boldsymbol{n}'=R_{\boldsymbol{m}}(\alpha)\boldsymbol{n}. \tag{A5}$$

Hence, any evolution under a nonzero detuning can be replaced by evolution under zero detuning, possibly with initial preparation of the spin system with rf pulse blips (but these are not necessary when the initial magnetization lies along the z axis).

APPENDIX B: SWAPPING $z\leftrightarrow\bar{z}$ AND ''UNDOING'' THE SWAP

The soliton ladder of solutions to Eq. (3.2) is composed of solutions $\Phi_j(t,\zeta)$, $j=0,1,\ldots$, and potentials $V_j(t)$, $j=0,1,\ldots$, with $\Phi_0=\exp[i\zeta Jt]$ and $V_0(t)=0$. Each Φ_j, and hence V_j, is constructed from Φ_{j-1} with the dressing data $s_j=\{z_j,\bar{z}_j,v_j,\tilde{w}_j\}$.

For this system, it will be shown that any pair $(z_j,\bar{z}_j)$ can be swapped to the pair $(\bar{z}_j,z_j)$ without changing the V_j, and right-multiplying all the Φ_j for $j>0$ by a time-constant matrix, $G(\zeta)$. To achieve this, all the v_j and $\tilde{w}_j$ must be modified.

Since $\bar{z}_j=z_j^{\star}$ for this system, the above result means that, without loss of generality, all the z_j may be taken to be in the upper half complex plane. (It is assumed in this paper that the z_j are all off the real axis.)

Suppose a pair $(z,\bar{z})$ are to be swapped. Since the dressing method can use the dressing data in any order, it can be assumed without loss of generality that this pair corresponds to $(z_1,\bar{z}_1)$.

Let Φ_1 be the solution according to dressing data z_1, $\bar{z}_1$, v_1, and $\tilde{w}_1$. Then [Eqs. (3.10a) and (3.16)]

$$\Phi_1=\left[1+\frac{z_1-\bar{z}_1}{\zeta-z_1}\hat{T}_1\right]\Phi_0, \tag{B1}$$

where

$$\hat{T}_1=\frac{\Phi_0(\bar{z}_1)v_1\tilde{w}_1^T\Phi_0^{-1}(z_1)}{\tilde{w}_1^T\Phi_0^{-1}(z_1)\Phi_0(\bar{z}_1)v_1}. \tag{B2}$$

Similarly, let Φ_1' be the solution obtained from Φ_0 with dressing data $\bar{z}_1$, z_1, v_1', and $\tilde{w}_1'$. Its construction will require the formation of a projection matrix $\hat{T}_1'$, defined as in Eq. (B2), but using different dressing data.

Hence, defining

$$G(t,\zeta)=\Phi_1^{-1}(t,\zeta)\Phi_1'(t,\zeta), \tag{B3}$$

then

$$G(t,\zeta)=\Phi_0^{-1}\left[1-\frac{z_1-\bar{z}_1}{\zeta-\bar{z}_0}(\hat{T}_1+\hat{T}_1')+\left(\frac{z_1-\bar{z}_1}{\zeta-\bar{z}_1}\right)^2\hat{T}_1\hat{T}_1'\right]\Phi_0. \tag{B4}$$

Hence, choosing $\hat{T}_1'$ such that

$$\hat{T}_1\hat{T}_1'=0 \tag{B5a}$$

and

$$\hat{T}_1+\hat{T}_1' \text{ is constant and } J \text{ diagonal} \tag{B5b}$$

will result in G being a function of ζ only, that is

$$G(\zeta)=1-\frac{z_1-\bar{z}_1}{\zeta-\bar{z}_1}(\hat{T}_1+\hat{T}_1'). \tag{B6}$$

By definition, choosing $\hat{T}_1+\hat{T}_1'$ as J diagonal means that $[\hat{T}_1+\hat{T}_1',J]=0$. Then, since $\Phi_0=\exp[i\zeta Jt]$,

$$\Phi_0^{-1}[\hat{T}_1+\hat{T}_1']\Phi_0=\hat{T}_1+\hat{T}_1', \tag{B7}$$

from which Eq. (B6) follows. It also means, from Eq. (3.11), that the potentials $V_1(t)$ and $V_1'(t)$, corresponding to Φ_1 and Φ_1', will be equal.

For the system (3.2), constraints (B5) can be solved to give

$$v_1' = \lambda[\hat{e}_1 \tilde{w}_1^T - \tilde{w}_1^T \hat{e}_1] v_1, \tag{B8a}$$

$$\tilde{w}_1' = \mu[\hat{e}_1 v_1^T - v_1^T \hat{e}_1] \tilde{w}_1, \tag{B8b}$$

where $\hat{e}_1^T = (1,0,0)$ and λ and μ are arbitrary scale factors.

Explicitly,

$$v_1' = \lambda \begin{pmatrix} a_2 b_2 + a_3 b_3 \\ -a_2 b_1 \\ -a_3 b_1 \end{pmatrix} \quad \text{and} \quad \tilde{w}_1' = \mu \begin{pmatrix} a_2 b_2 + a_3 b_3 \\ -a_1 b_2 \\ -a_1 b_3 \end{pmatrix}, \tag{B9}$$

where $v_1^T = (a_1, a_2, a_3)$ and $\tilde{w}_1^T = (b_1, b_2, b_3)$. Then, it can be shown that

$$\hat{T}_1 + \hat{T}_1' = \begin{bmatrix} 1 & \\ & \hat{P}_- \end{bmatrix}, \tag{B10}$$

where $\hat{P}_-$ is the projection matrix

$$\hat{P}_- = \frac{1}{a_2 b_2 + a_3 b_3} \begin{pmatrix} a_2 b_2 & a_2 b_3 \\ a_3 b_2 & a_3 b_3 \end{pmatrix}. \tag{B11}$$

Hence [Eq. (B6)],

$$G(\zeta) = 1 - \frac{z_1 - \bar{z}_1}{\zeta - \bar{z}_1} \begin{bmatrix} 1 & \\ & \hat{P}_- \end{bmatrix}. \tag{B12}$$

Now consider the addition of another soliton, to get Φ_2 when starting at Φ_1, and Φ_2' when starting at Φ_1'. The projection matrix $\hat{T}_2$ needed to get from Φ_1 to Φ_2 is, given the dressing data z_2, $\bar{z}_2$, v_2, and $\tilde{w}_2$,

$$\hat{T}_2 = \frac{\Phi_1(\bar{z}_2) v_2 \tilde{w}_2^T \Phi_1^{-1}(z_2)}{\tilde{w}_2^T \Phi_1^{-1}(z_2) \Phi_1(\bar{z}_2) v_2}. \tag{B13}$$

The projection matrix $\hat{T}_2'$ to get from Φ_1' to Φ_2' is defined similarly in terms of z_2, $\bar{z}_2$, v_2', and $\tilde{w}_2'$.

The parameters v_2' and $\tilde{w}_2'$ are to be chosen such that $\hat{T}_2' = \hat{T}_2$. This will ensure that $\Phi_2' = \Phi_2 G(\zeta)$, and hence the corresponding potentials calculated by the two routes V_2 and V_2' are the same. Since $\Phi_1' = \Phi_1 G(\zeta)$, this implies that, for $j = 2$,

$$v_j' = G^{-1}(z_j) v_j, \tag{B14a}$$

$$\tilde{w}_j' = G^T(\bar{z}_j) \tilde{w}_j. \tag{B14b}$$

The same argument can be made for all the subsequent parameters v_j' and $\tilde{w}_j'$, and hence Eqs. (B14) must be true for all $j \geqslant 2$.

Finally, this procedure works if more than one $(z, \bar{z})$ pair are to be swapped. For each pair, it can be imagined that the dressing data are reordered, so the pair to be swapped is in the data for the first soliton calculated from the vacuum. The above procedure is undertaken. The dressing data are again reordered so that the next pair is in the first lot of dressing data, and so on.

APPENDIX C: CONNECTION BETWEEN REAL PULSE AND GENERAL CASE

This Appendix gives the connection between the methods of calculating real soliton pulses in Secs. II and III. That is, given that such a pulse, $\omega_1(t)$, was determined in Sec. II with scattering data $\{\zeta_j, b_j, \bar{\zeta}_j, \bar{b}_j\}$, it shows what dressing data $\{z_j, \bar{z}_j, v_j, \tilde{w}_j\}$ are needed in Sec. III to calculate the same pulse.

Since all the z_j used in the dressing method were chosen in the upper half complex plane, the soliton solution Φ calculated by that method will be analytic in the lower half complex plane. It is then natural to consider a fundamental solution to the ZS problem (2.4) of Sec. II that is also analytic in the lower half complex plane.

It is well known [10] that the solutions $\bar{\psi}(t,\zeta)$ and $\bar{\phi}(t,\zeta)$ to the ZS problem with asymptotic behavior

$$\bar{\psi}(t,\zeta) \to \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\zeta t} \quad \text{as} \quad t \to \infty, \tag{C1a}$$

$$\bar{\phi}(t,\zeta) \to \begin{pmatrix} 0 \\ -1 \end{pmatrix} e^{i\zeta t} \quad \text{as} \quad t \to -\infty, \tag{C1b}$$

are analytic in the lower half complex plane. Hence define the 3×3 matrix-valued function Ψ as

$$\Psi = \begin{bmatrix} 1 & \\ & [\bar{\psi} \quad -\bar{\phi}] \end{bmatrix}. \tag{C2}$$

This function satisfies

$$\frac{\partial \Psi}{\partial t} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -i\zeta & -\omega_1(t) \\ 0 & \omega_1(t) & i\zeta \end{pmatrix} \Psi(t,\zeta), \tag{C3}$$

where $q(t)$ in the ZS problem has been set equal to the real function $\omega_1(t)$ describing the rf pulse.

Let $\Phi(t,\zeta)$ be a fundamental solution to Eq. (3.1) in Sec. III, built up by the dressing method. Consider

$$\tilde{\Phi}(t,\zeta) = EC\Phi(t,\zeta)C^{-1}, \tag{C4a}$$

where

$$E = \begin{pmatrix} e^{i\zeta t/3} & 0 & 0 \\ 0 & e^{-i\zeta t/6} & 0 \\ 0 & 0 & e^{-i\zeta t/6} \end{pmatrix} \tag{C4b}$$

and

$$C = \begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & -i/\sqrt{2} & i/\sqrt{2} \\ 1 & 0 & 0 \end{pmatrix}. \tag{C4c}$$

Then, since the rf pulse is real, $\tilde{\Phi}$ satisfies

$$\frac{\partial\tilde{\Phi}(t,2\zeta)}{\partial t}=\begin{pmatrix} 0 & 0 & 0 \\ 0 & -i\zeta & -\omega_1(t) \\ 0 & \omega_1(t) & i\zeta \end{pmatrix}\tilde{\Phi}(t,2\zeta), \quad \text{(C5)}$$

noting that this is the same evolution equation as satisfied by $\Psi(t,\zeta)$.

Finally, it can be checked that both $\Psi(t,\zeta)$ and $\tilde{\Phi}(t,2\zeta)$ have the same asymptotic behavior as $|\zeta|\to\infty$ in the lower half complex plane. Thus, it can be concluded that

$$\Psi(t,\zeta)=EC\Phi(t,2\zeta)C^{-1}. \quad \text{(C6)}$$

Now, the scattering data $\overline{\zeta_j}$ and $\overline{b_j}$ are defined by [10]

$$\overline{\phi}(t,\overline{\zeta_j})=\overline{b_j}\overline{\psi}(t,\overline{\zeta_j}). \quad \text{(C7)}$$

Hence,

$$\Psi(t,\overline{\zeta_j})\begin{pmatrix} 0 \\ \overline{b_j} \\ 1 \end{pmatrix}=0. \quad \text{(C8)}$$

But the corresponding dressing data are defined by [Eq. (3.19a)]

$$\Phi(t,\overline{z_j})v_j=0. \quad \text{(C9)}$$

Equation (C6) then implies that

$$\overline{z_j}=2\overline{\zeta_j} \quad \text{(C10a)}$$

and

$$v_j=C^{-1}\begin{pmatrix} 0 \\ \overline{b_j} \\ 1 \end{pmatrix}=\begin{pmatrix} 1 \\ i\overline{b_j}/\sqrt{2} \\ -i\overline{b_j}/\sqrt{2} \end{pmatrix}. \quad \text{(C10b)}$$

The other dressing data, z_j and $\tilde{w}_j$, can be obtained from the symmetries (3.25).

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