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Spectral Resolution and Inversion of the Bloch Equations with Relaxation

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Abstract. It is demonstrated that the linear Bloch equations, describing near-resonant excitation of two-level media with relaxation, can be resolved into a $3n$-dimensional nonlinear system associated with a special spectral problem, generalizing the classical Zakharov–Shabat spectral problem. Remarkably, for $n=1$ it is the well-known Lorenz system, and for $n>1$ several such systems coupled with each other in a manner dependant on the excitation pulse. The unstable manifold of a saddle equilibrium point in this ensemble characterizes possible excitations of the spins from the initial equilibrium state. This enables us to get a straightforward geometric extension of the inverse scattering method to the damped Bloch equations and hence invert them, i.e., design frequency selective pulses automatically compensated for the effect of relaxation. The latter are essential, for example, in nuclear magnetic resonance and extreme nonlinear optics.

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1. Introduction

The near-resonant interaction of two-level media with classical radiation is well modelled by the Bloch equations, which in dimensionless form (and the rotating frame) are

$$\dot{m}=(-r_2+i\lambda)m-i\omega(t)m_z,\quad \dot{m}_z=-r_1(m_z-1)+\frac{i}{2}(\omega(t)\bar{m}-\bar{\omega}(t)m). \tag{1}$$

Here m_z is the population difference between the levels, m is the complex transverse component of the "spin vector", ω is the complex time-varying excitation pulse, λ is the detuning from resonance, and r_1, $r_2>0$ are the longitudinal and the transverse relaxation rates, respectively (throughout, $\bar{\chi}$ means the complex conjugate of χ, and $\dot{}=\mathrm{d}/\mathrm{d}t$).

Equations (1) occurred first in the theory of nuclear magnetic resonance [4], where they describe the excitation of two-level (and, in some cases, spin $>1/2$)

nuclei by radio-frequency pulses. Later they also occurred in coherent optics [3, 5], where they are used, for example, in the theory of ultrafast optoelectronic devices.

Since the excitation is localized in time, relaxation makes the system return rapidly to the equilibrium state

$$m = 0, \quad m_z = 1 \tag{2}$$

as $t \to +\infty$, so the semi-infinite boundary conditions are of a key interest

$$m \to 0, \quad m_z \to 1, \quad t \to -\infty, \tag{3}$$

$$m = f(\lambda), \quad m_z = g(\lambda), \quad t = 0. \tag{4}$$

Two problems are the most important for applications. The first (or the direct) one is to find corresponding profiles $f(\lambda)$, $g(\lambda)$ for a given pulse $\omega(t)$. The second (or the inverse) one is to find a pulse $\omega(t)$ providing specified profiles $f(\lambda)$, $g(\lambda)$. While the direct problem can be solved numerically using standard methods, analytical and numerical aspects of the inverse problem are both of great interest, as in the absence of regular algorithms, frequency selective pulses are still designed fully ignoring the effect of relaxation.

However, this effect becomes appreciable when the relaxation times are comparable to, or shorter than, the total duration of the excitation. For example, in magnetic resonance imaging, a driving field is typically used to selectively excite spins into a coherent superposition, with spins with only a particular range of Larmor frequencies being excited. This enables images to be obtained of an object one slice a time. Relaxation (caused by spin–lattice and spin–spin interactions) makes this selection less sharp, with less uniform excitation within the slice. In magnetic resonance spectroscopy, relaxational distortions of frequency-domain excitation patterns (especially for narrow chemical shift bands) cause an undesirable broadening of the spectrum. Relaxation is also of critical importance in the control of qubits, imposing a limit on the number of gates that can be implemented in a quantum computer, and in optical coherence techniques, where relaxation (caused by atomic interactions) makes the induced polarization decay rapidly to the unexcited state.

Some attempts have been made to include relaxation into mathematically simple inversion schemes, concerning though very special cases, such as $r_1 = 0$ and $r_1 = r_2$ (see, for example, [12–14]). Complete analysis of the damped Bloch equations is still an open question, and no inverse results have been known for general r_1, r_2.

Many methods have been suggested to solve the inverse problem for $r_1 = r_2 = 0$ (see, for example, [6, 8, 15]). The most advantageous are the inverse scattering techniques based on the spinor equations of motion, or the Zakharov-Shabat spectral problem (see [9–11])

$$B\psi = \lambda\psi, \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \tag{5}$$

where B is the linear operator

$$B = \begin{pmatrix} 2i\partial_t & -\bar{\omega} \\ \omega & -2i\partial_t \end{pmatrix}.$$

Problem (5) (with the symbol t being regarded as the spatial coordinate) was suggested first in [16] for the exact solution of the so-called nonlinear Schrödinger equation and then generalized [2] to other important evolution equations. For $r_1 = r_2 = 0$, solutions to (1), (5) are related as

$$m = 2\bar{\psi}_1\psi_2, \quad m_z = \psi_1\bar{\psi}_1 - \psi_2\bar{\psi}_2,$$

which allows the inverse scattering method to be applied to Equations (1).

In connection with the semi-infinite problem (3), (4), the "half-soliton" method is efficient. It is based on the observation (details are in [10, 11]) that the unique solution to the inverse scattering problem (5) with rational reflection coefficient $\rho(\lambda)$ and $\omega(t) = 0$ for $t > 0$ is exactly the n-soliton (truncated at $t > 0$) with the bound states defined by the equation

$$1 + \rho(\lambda)\bar{\rho}(\bar{\lambda}) = 0$$

and the residues also easily reconstructed from the reflection coefficient. The corresponding solutions to (1) at $t = 0$ can be written as

$$f = \frac{2\rho}{1 + \rho\bar{\rho}}, \quad g = \frac{1 - \rho\bar{\rho}}{1 + \rho\bar{\rho}}.$$

These are then simple rational polynomials in λ with poles coinciding with the bound states.

We show that a direct extension of the inverse scattering method to the case $r_{1,2} > 0$ leads to a new spectral problem, generalizing the Zakharov–Shabat problem. The solutions $m(\lambda, t)$, $m_z(\lambda, t)$ are still rational polynomials in λ, while the corresponding pulses $\omega(t)$ satisfy a special nonlinear integro-differential equation. This equation can be recast as a $3n$-dimensional ODE system, generalizing the well-known Lorenz system. Thus, the problem receives a straightforward geometric interpretation: each achievable profile (4) is associated with a point on the n-dimensional unstable manifold of a saddle equilibrium point of this system. This enables us to invert the damped Bloch equations in full analogy with the classical inverse scattering method.

The latter has been applied before to problems close to that considered here. For example, the propagation of a pulse through a resonant two-level medium is described by the following Maxwell–Bloch equations (preserving our notations)

$$\begin{aligned} &\omega_x = i\langle m\rangle = i\int_{-\infty}^{+\infty} \kappa(\lambda) m(\lambda, x, t)\,\mathrm{d}\lambda, \\ &\dot{m} = i\lambda m - i\omega m_z, \quad \dot{m}_z = \frac{i}{2}(\omega\bar{m} - \bar{\omega}m), \end{aligned} \tag{6}$$

where ω is the electric field envelope (propagating along the spatial x axis), m, m_z are the induced polarization and the population inversion, respectively, and the density $\kappa(\lambda)$ characterizes the inhomogeneous broadening of the medium.

Problem (6) can be treated as lossy, as, in general, an incident pulse decomposes not only into "soliton" pulses to which the medium is transparent but also yields radiation which is absorbed. In [1], it has been shown that in this case the inverse scattering technique still can be applied.

However, we deal with a spatially localized situation (typical, for example, for nuclear magnetic resonance), where ω can be treated as an external field simply acting on the polarization, and so the problem of polarization (or magnetization) dynamics (1) becomes more important than the pulse propagation problem (6).

Moreover, the presence of spin–lattice (r_1) and spin–spin (r_2) relaxations, completely neglected in (6), makes including the general Bloch equations into mathematically elegant schemes a really difficult problem. The analysis developed below can be regarded as a step in this direction.

2. Spectral Resolution of the Bloch Equations

Noting that

$$m_z = 1 + \frac{i}{2}\,\mathrm{e}^{-r_1 t}\int_{-\infty}^{t} \mathrm{e}^{r_1 t'}(\omega\bar{m} - \bar{\omega}m)\,\mathrm{d}t', \tag{7}$$

rewrite Equations (1) in the 2-dimensional form

$$Av = \lambda v - u, \tag{8}$$

where

$$v = \begin{pmatrix} \bar{m} \\ m \end{pmatrix}, \quad u = \begin{pmatrix} \bar{\omega} \\ \omega \end{pmatrix},$$

and A is the linear integro-differential operator

$$A = i\begin{pmatrix} \partial_t + r_2 + \frac{1}{2}\bar{\omega}\mathrm{e}^{-r_1 t}\int_{-\infty}^{t}\mathrm{d}t'\,\omega\mathrm{e}^{r_1 t'} & -\frac{1}{2}\bar{\omega}\mathrm{e}^{-r_1 t}\int_{-\infty}^{t}\mathrm{d}t'\,\bar{\omega}\mathrm{e}^{r_1 t'} \\ \frac{1}{2}\omega\mathrm{e}^{-r_1 t}\int_{-\infty}^{t}\mathrm{d}t'\,\omega\mathrm{e}^{r_1 t'} & -\partial_t - r_2 - \frac{1}{2}\omega\mathrm{e}^{-r_1 t}\int_{-\infty}^{t}\mathrm{d}t'\,\bar{\omega}\mathrm{e}^{r_1 t'} \end{pmatrix}.$$

Consider special solutions to (8), which are simple rational polynomials in λ

$$v = \frac{V_1(t)}{\lambda - \zeta_1} + \cdots + \frac{V_N(t)}{\lambda - \zeta_N}. \tag{9}$$

This is possible only when ζ_j are eigenvalues of the operator A, and V_j are the corresponding eigenfunctions,

$$AV_j = \zeta_j V_j, \quad j \in \overline{1, N}. \tag{10}$$

Indeed, substitution of (9) into (8) gives (10) and the additional relation

$$u = V_1 + \cdots + V_N. \tag{11}$$

The latter follows also from the asymptotics for solutions to (1) as (real) $\lambda \to \infty$

$$m = \frac{\omega(t)}{\lambda} + O\left(\frac{1}{\lambda^2}\right), \quad m_z = 1 + O\left(\frac{1}{\lambda^2}\right). \tag{12}$$

Look at the spectral problem generated by the operator A

$$Av = \lambda v. \tag{13}$$

Since $\omega(t)$ vanishes as $t \to -\infty$, the fundamental solutions to (13) have the asymptotics

$$v \to \begin{pmatrix} 1 \\ 0 \end{pmatrix} \mathrm{e}^{-(i\lambda + r_2)t}, \quad v' \to \begin{pmatrix} 0 \\ 1 \end{pmatrix} \mathrm{e}^{(i\lambda - r_2)t}, \ \ t \to -\infty.$$

Using the symmetry

$$\sigma_1 \bar{A} = A\sigma_1, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and requirement (3), i.e.,

$$V_j \to 0, \quad t \to -\infty, \quad j \in \overline{1, N},$$

we conclude that actually $N = 2n$ is even, and the eigenvalues ζ_j and the eigenfunctions V_j form the pairs

$$\{\zeta_j\}_{j=1}^N = \{\lambda_k, \bar{\lambda}_k\}_{k=1}^n, \quad \{V_j\}_{j=1}^N = \{v_k, v_k'\}_{k=1}^n$$

with

$$Av_k = \lambda_k v_k, \quad Av_k' = \bar{\lambda}_k v_k', \quad v_k' = \sigma_1 \bar{v}_k, \quad \operatorname{Im} \lambda_k > r_2. \tag{14}$$

Then relations (9), (11) take the form

$$v = \sum_{k=1}^n \frac{v_k}{\lambda - \lambda_k} + \frac{v_k'}{\lambda - \bar{\lambda}_k}, \quad u = \sum_{k=1}^n v_k + v_k'. \tag{15}$$

It is natural to call relations (15) the spectral resolution of Equations (1).

Since real values of λ do not belong to the spectrum, we are not interested in formal scattering theory for the operator A. We do not even care whether $\omega(t)$ vanishes as $t \to +\infty$. What we need is to invert inhomogeneous problem (8) on the semi-axis $-\infty < t \leq 0$. This can be done in the following way.

3. Inversion of the Bloch Equations

As a consequence of (14), (15), u satisfies the nonlinear integro-differential equation

$$\left[\prod_{k=1}^{n}(A-\lambda_k)(A-\bar{\lambda}_k)\right]u=0. \tag{16}$$

Equation (16) allows the reconstraction of $\omega(t)$, given the poles of solution (15), up to n arbitrary complex constants c_k. These constants are to be determined by the specification of the corresponding residues at $t=0$.

We see a direct analogy with the classical inverse scattering method, where $\omega(t)$, $\lambda_1, \ldots, \lambda_n$ and $c_1, \ldots, c_n$ play the parts of the potential, the bound states and the residues, respectively.

This analogy is not accidental. Indeed, let $r_1=r_2=\gamma$. Then from (5), (13) we find that

$$B\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=\lambda\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{17}$$

implies

$$A\left[\begin{pmatrix}\psi_1^2\\ -\psi_2^2\end{pmatrix}\mathrm{e}^{-\gamma t}\right]=\lambda\left[\begin{pmatrix}\psi_1^2\\ -\psi_2^2\end{pmatrix}\mathrm{e}^{-\gamma t}\right], \tag{18}$$

which easily follows from the relation

$$\int_{-\infty}^{t}(\omega\psi_1^2+\bar{\omega}\psi_2^2)\,\mathrm{d}t'=2i\psi_1\psi_2.$$

Thus, in the case $r_1=r_2$, eigenfunctions of the operator A are algebraically expressed in terms of those of the operator B, so problem (13) can be regarded as a generalization of problem (5).

In general, Equation (16) cannot be solved in closed form, but yet admits a straightforward geometric interpretation. Denoting

$$v_k=\begin{pmatrix}\bar{\eta}_k\\ \mu_k\end{pmatrix},\quad \nu_k=\frac{i}{2}\mathrm{e}^{-r_1t}\int_{-\infty}^{t}\mathrm{e}^{r_1t'}(\omega\bar{\eta}_k-\bar{\omega}\mu_k)\,\mathrm{d}t',$$

we obtain from Equations (14) and (15)

$$\begin{gathered}\dot{\mu}_k=(-r_2+i\lambda_k)\mu_k-i\omega\nu_k,\quad \dot{\eta}_k=(-r_2+i\bar{\lambda}_k)\eta_k-i\omega\bar{\nu}_k,\\ \dot{\nu}_k=-r_1\nu_k+\frac{i}{2}(\omega\bar{\eta}_k-\bar{\omega}\mu_k),\end{gathered} \tag{19}$$

where

$$\omega=\sum_{k=1}^{n}\mu_k+\eta_k. \tag{20}$$

In terms of system (19), solutions to (1) take the form

$$m = \sum_{k=1}^{n} \frac{\mu_k}{\lambda - \lambda_k} + \frac{\eta_k}{\lambda - \bar{\lambda}_k}, \quad m_z = 1 + \sum_{k=1}^{n} \frac{\nu_k}{\lambda - \lambda_k} + \frac{\bar{\nu}_k}{\lambda - \bar{\lambda}_k}, \tag{21}$$

and boundary conditions (3) become

$$\mu_k, \eta_k, \nu_k \to 0, \quad t \to -\infty. \tag{22}$$

System (19) is a $3n$-dimensisonal autonomous nonlinear system. It has the equilibrium

$$\mu_k = \eta_k = \nu_k = 0, \quad k \in \overline{1, n}, \tag{23}$$

corresponding to equilibrium (2). Linearization near (23) shows that equilibrium (23) is of the saddle type: exactly n of its eigenvalues are in the right complex half-plane, and the remaining $2n$ are in the left one. All solutions satisfying (22) fill an n-dimensional complex manifold, namely, the unstable manifold U of the saddle (23).

Thus, boundary problem (3) and (4) receives a straightforward geometric interpretation: each achievable profile f, g is associated with a point on the manifold U. The profile

$$f(\lambda) = \sum_{k=1}^{n} \frac{\mu_k(0)}{\lambda - \lambda_k} + \frac{\eta_k(0)}{\lambda - \bar{\lambda}_k}, \quad g(\lambda) = 1 + \sum_{k=1}^{n} \frac{\nu_k(0)}{\lambda - \lambda_k} + \frac{\bar{\nu}_k(0)}{\lambda - \bar{\lambda}_k} \tag{24}$$

is achievable if and only if the point, having the coordinates

$$(\mu_1(0), \eta_1(0), \nu_1(0), \ldots, \mu_n(0), \eta_n(0), \nu_n(0)), \tag{25}$$

belongs to U. Inversely, taking a point (25) on U, and solving Equations (19) and (20) with this initial data, we get a pulse $\omega(t)$ that provides the corresponding profile (24).

Due to the symmetry of the Bloch equations

$$\omega \to \omega e^{i(st+\theta)}, \quad m \to m e^{i(st+\theta)}, \quad \lambda \to \lambda + s \tag{26}$$

with the arbitrary real parameters s, θ, system (19) possesses the 1-parametric symmetry

$$\mu_k \to \mu_k e^{i\theta}, \quad \eta_k \to \eta_k e^{i\theta}. \tag{27}$$

It follows from asymptotics (12) that the system always has the integral

$$\sum_{k=1}^{n} \nu_k + \bar{\nu}_k = 0. \tag{28}$$

In the case $r_1 = 2r_2$, it has the integral

$$|\omega|^2 + 2\sum_{k=1}^{n}(\lambda_k \nu_k + \bar{\lambda}_k \bar{\nu}_k) = 0,$$

and, in the case $r_1 = r_2$, the n integrals

$$\mu_k \bar{\eta}_k + \nu_k^2 = 0, \quad k \in \overline{1, n}. \tag{29}$$

In this case, in accordance with (17) and (18) after the change

$$\mu_k = -\varphi_{k2}^2, \quad \eta_k = \bar{\varphi}_{k1}^2$$

system (19) is reduced to the $2n$-dimensional system

$$\begin{pmatrix} \varphi_{k1} \\ \varphi_{k2} \end{pmatrix}^{\cdot} = -\frac{i}{2}\begin{pmatrix} \lambda_k - i\gamma & \bar{\omega} \\ \omega & -\lambda_k - i\gamma \end{pmatrix}\begin{pmatrix} \varphi_{k1} \\ \varphi_{k2} \end{pmatrix}, \quad \omega = \sum_{k=1}^{n}\left(\bar{\varphi}_{k1}^2 - \varphi_{k2}^2\right).$$

We have shown recently [14] that, in this case, a simple general connection exists between solutions to the Bloch equations (1) and the spinor Equations (5). This allows, in particular, a straightforward inversion in terms of the relaxation rate γ to be made.

A. THE CASE $n = 1$

Look at the case $n = 1$, for general r_1 and r_2. As a result of symmetry (26), we may assume λ_1 to be purely imaginary

$$\lambda_1 = i\beta_1, \quad \beta_1 > r_2.$$

Equation (16) takes the form

$$\begin{gathered} \ddot{\omega} + 2r_2\dot{\omega} + \left(\frac{1}{2}|\omega|^2 - \Delta^2\right)\omega - p\,\mathrm{e}^{-r_1 t}\omega\int_{-\infty}^{t}\mathrm{e}^{r_1 t'}|\omega|^2\,\mathrm{d}t' = 0, \\ \Delta^2 = \beta_1^2 - r_2^2, \quad p = r_2 - \frac{r_1}{2}, \end{gathered} \tag{30}$$

which is a complicated integro-differential equation. In the case $p = 0$, the equation becomes purely differential, representing a dissipative nonlinear oscillatory system. When $r_1 = r_2 = 0$, it is completely integrable and gives the solution

$$\omega = 2\mathrm{e}^{i\theta}\Delta\,\mathrm{sech}\,\Delta(t - t_0)$$

with arbitrary real constants θ, t_0, which is the 1-soliton pulse in full accordance with the inverse scattering method.

Let now in (19)

$$\begin{gathered} \eta_1 + \mu_1 = r_2 X, \quad \beta_1(\eta_1 - \mu_1) = r_2^2 Y, \\ i\beta_1(\bar{\nu}_1 - \nu_1) = r_2^2 Z, \quad r_2 t = \tau. \end{gathered} \tag{31}$$

Then, to within symmetry (27), X, Y, Z are real and satisfy the equations

$$\frac{\mathrm{d}X}{\mathrm{d}\tau}=\sigma(Y-X),\quad \frac{dY}{d\tau}=-Y+(r-Z)X,\\ \frac{dZ}{d\tau}=-bZ+XY \tag{32}$$

with the parameters

$$\sigma=1,\quad r=\frac{\beta_1^2}{r_2^2}>1,\quad b=\frac{r_1}{r_2}>0. \tag{33}$$

System (32) is the well-known Lorenz system [7], which is non-integrable except for certain values of the parameters, and exhibits extremely irregular behaviour (the strange attractor) on an open set of them.

In our case, though, the behaviour of system (32) is regular. The unstable manifold U is 1-dimensional and consists of two symmetric (with respect to the symmetry $X\to -X$, $Y\to -Y$ of the Lorenz system) "moustaches" $U_\pm$. For almost all values of the parameters r_1, r_2 and β_1, the moustaches $U_\pm$ go from the saddle equilibrium

$$X=Y=Z=0 \tag{34}$$

to the two symmetric stable equilibria, or the foci

$$O_\pm:\quad Z=r-1,\quad X=Y=\pm\sqrt{b(r-1)}. \tag{35}$$

These equilibria are the only attractors in the case (33).

The only bifurcation here is a constraint on the parameters in the form

$$r=C(b), \tag{36}$$

for which $U_\pm$ go from equilibrium (34) to two symmetric limit cycles, representing unstable saddle periodic solutions to system (32). On one side of curve (36), U_+ [respectively, U_-] goes to O_+ [O_-], and on the other side, inversely, U_+ [U_-] goes to O_- [O_+]. Numerical analysis shows that the function $C(b)$ is defined for $b<1$ only, it is a smooth increasing function of b with the vertical asymptote $b=1$. The existence of this constraint allows an interesting conclusion that there are real pulses $\omega(t)$ periodic in t, for which solutions to the Bloch equations are rational in λ and periodic in t.

This analysis makes the exact inversion in this case fairly simple. To within symmetry (27), in terms of change (31), we get

$$m(0)=f=r_2\frac{X(0)\lambda-ir_2Y(0)}{\lambda^2+\beta_1^2},\quad m_z(0)=g=1-\frac{r_2^2Z(0)}{\lambda^2+\beta_1^2},$$

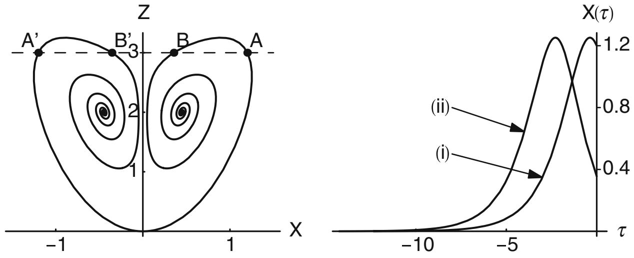

Figure 1. (*Left*) The XZ-projection of the manifolds $U_\pm$ for $r_1 = 1/(10\sqrt{3})$, $r_2 = 1/\sqrt{3}$, $\beta_1 = 1$ and their intersections A, B, A', B' with the plane $Z = 3$. (*Right*) The X-components of the solutions ending at (i) A, (ii) B. The corresponding pulses $\omega(t)$ calculated via (38) give the m_z-response of (37).

where the point $(X(0), Y(0), Z(0))$ belongs to U_+ (or U_-). For example, to provide the desired response

$$g = \frac{\lambda^2}{1+\lambda^2} = 1 - \frac{1}{\lambda^2+1}, \tag{37}$$

it is sufficient to take $\beta_1 = 1$ and find an intersection of the manifolds $U_\pm$ with the plane $Z = 1/r_2^2$, which can easily be done numerically for reasonable values of $r_{1,2}$. Here

$$\omega(t) = r_2 X(r_2 t), \tag{38}$$

where $X(\tau)$ is the X-component of the solution to (32) with the corresponding initial data. Since the solutions oscillate near equilibria (35), the suitable pulse is not unique (each pulse differs from others by a time shift), which gives an additional degree of freedom.

Figure 1 illustrates this example for

$$\beta_1 = 1, \quad r_1 = \frac{1}{10\sqrt{3}}, \quad r_2 = \frac{1}{\sqrt{3}} \quad \left(b = \frac{1}{10}, \quad r = 3\right).$$

On the left, the XZ-projection of the manifolds $U_\pm$ is shown. They intersect the plane $Z = 3$ at the points A, B, A', B'. On the right are shown $X(\tau)$ trajectories from the origin to (i) A and (ii) B, respectively (recall that $\tau = 0$ is defined as the point at the end of the trajectory). Numerical calculation confirms that both pulses given by (38) provide the same responses $g(\lambda)$ coinciding with (37).

B. THE CASE $n > 1$

In general, system (19) can be regarded as n Lorenz systems coupled with each other via the common nonlinear factor ω given by (20). This makes the full analysis much more complicated. However, since we are interested in the dynamics for

$-\infty < t < 0$ only, there is no need for us to analyze the limit behaviour of the manifold U as $t \to +\infty$, and the computation is not crucially difficult. Various approximate techniques are useful. The following heuristic algorithm turned out to be efficient for the important class of "frequency selective" responses

$$g = \frac{\lambda^{2n}}{\lambda^{2n}+1} = 1 + \frac{1}{2n}\sum_{k=1}^{n} \frac{\lambda_k}{\lambda - \lambda_k} + \frac{\bar{\lambda}_k}{\lambda - \bar{\lambda}_k} \tag{39}$$

with

$$\lambda_k = \exp\left(i\frac{(2k-1)\pi}{2n}\right).$$

When n is sufficiently large, (39) is close to the hat-like profile: $g \sim 0$ at $-1 < \lambda < 1$, and $g \sim 1$ for $|\lambda| > 1$.

In the linear approximation near equilibrium (23), in accordance with (19), the manifold U is given by

$$\mu_k = \nu_k = 0, \quad \eta_k = c_k e^{\gamma_k t}, \quad \gamma_k = i\bar{\lambda}_k - r_2, \quad k \in \overline{1,n},$$

where c_k are arbitrary complex constants. When values of the c_k are small, the manifold U admits a series expansion with respect to $c_1, \ldots, c_n$ and their complex conjugates, where the expansion for ν_k starts from terms of second order, and that for μ_k starts from terms of third order. More precisely, we have

$$\eta_k = \eta_k^{(1)} + \eta_k^{(3)} + \cdots, \quad \mu_k = \mu_k^{(3)} + \mu_k^{(5)} + \cdots, \quad \nu_k = \nu_k^{(2)} + \nu_k^{(4)} + \cdots,$$

where $\chi^{(j)}$ denotes a form of the jth order with respect to c_k, $\bar{c}_k$, $k \in \overline{1,n}$. Due to (20), also

$$\omega = \omega^{(1)} + \omega^{(3)} + \cdots$$

Noting that

$$\eta_k^{(1)} = c_k e^{\gamma_k t}, \quad \omega^{(1)} = \sum_{k=1}^{n} \eta_k^{(1)}, \quad \dot{\nu}_k^{(2)} = -r_2 \nu_k^{(2)} + \frac{i}{2}\omega^{(1)}\bar{\eta}_k^{(1)},$$

we find

$$\nu_k^{(2)} = \frac{i}{2}\bar{c}_k e^{\bar{\gamma}_k t}\sum_{j=1}^{n} a_{kj} c_j e^{\gamma_j t}, \quad a_{kj} = \frac{1}{r_1 + \gamma_j + \bar{\gamma}_k}.$$

Restricting ourselves to the second order term in ν_k only, we get from (39), (24)

$$\nu_k(0) = \frac{\lambda_k}{2n} \sim \frac{i}{2}\bar{c}_k \sum_{j=1}^{n} a_{kj} c_j,$$

which leads to the approximate equations for c_k

$$i\bar{c}_k \sum_{j=1}^{n} a_{kj} c_j = \frac{\lambda_k}{n}, \quad k \in \overline{1, n}. \tag{40}$$

Symmetry (27) implies the symmetry $c_k \to e^{i\theta} c_k$, so one of the constants (say, c_1) can be chosen to be real.

Instead of solving Equations (40) (which is a nontrivial problem of algebraic geometry), rewrite them as

$$\bar{c}_k = \frac{\lambda_k}{in \sum_{j=1}^{n} a_{kj} c_j}$$

and apply the iteration method

$$\bar{c}_k^{(q+1)} = \frac{\lambda_k}{in \sum_{j=1}^{n} a_{kj} c_j^{(q)}}, \quad k \in \overline{1, n}, \quad q = 0, 1, \ldots, \tag{41}$$

starting from some initial $c_1^{(0)}, \ldots, c_n^{(0)}$. We have found by numerical experiment that iterations (41) possess the remarkable property that the mathematical expectations, or the averages

$$m_k = \lim_{N \to \infty} \frac{1}{N} \sum_{q=1}^{N} |c_k^{(q)}|,$$

exist independent of the initial data. Since c_1 is assumed to be real, we take $c_1 = m_1$ and then find the remaining constants by the rule

$$c_k = \lim_{N \to \infty} \frac{1}{N} \sum_{q=1}^{N} c_k^{(q)}, \quad k \in \overline{2, n},$$

where the iterations in the right-hand side are calculated now for that fixed c_1.

This gives an approximate complex pulse in the form

$$\omega' = \sum_{k=1}^{n} c_k e^{\gamma_k (t + T_+)}, \tag{42}$$

where the shift T_+ is defined by the earliest instant of time when $m_z(T_+) = 0$ at $\lambda = 0$. Numerical analysis shows that the response to this approximate pulse is non-symmetric with respect to the change $\lambda \to -\lambda$, although qualitatively close to the desired (39). Note that if the pulse $\omega(t)$ gives a response $g(\lambda)$ then the pulse $\bar{\omega}$ gives the response $g(-\lambda)$. We then take the "geometric average", the smooth real function $\omega(t)$, where $\omega^2 = \omega' \bar{\omega}'$, as the pulse. Numerical results show that

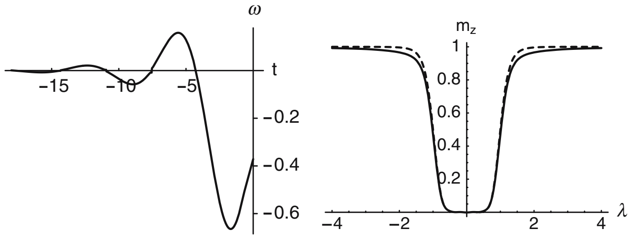

Figure 2. The pulse $\omega(t)$ (*left*) providing the approximate "frequency selective" response (*right*) close to that given by (39) for $n=4$, $r_1=1/25$ and $r_2=1/12$.

the response is very close to the desired response (39). The algorithm is the most efficient when $n=4$.

On Figure 2, left, the pulse $\omega(t)$ obtained by the above algorithm is shown with the corresponding response, right (solid line), which is in good agreement with the desired response (39) (dashed line) for $n=4$. Here $r_1=1/25$ and $r_2=1/12$.

4. Conclusion

We have shown that the Bloch equations containing relaxation terms can be inverted in full analogy with the classical inverse scattering method valid when relaxation is neglected. This is possible by considering a special spectral problem, which generalizes the classical Zakharov–Shabat spectral problem. To obtain it, the assumption that the solutions are rational polynomials in the resonance offset was used. Hence, we gave a geometric extension of the classical inverse scattering method to the damped Bloch equations. This extension is based on the observation that each achievable response can be associated with a point on the n-dimensional unstable invariant manifold of a saddle equilibrium point of a special $3n$-dimensional ODE system. This system is obtained as a result of the resolution of the Bloch equations into a linear combination of eigenfunctions of the generalized spectral problem. For $n=1$, it turned out to be the well-known Lorenz system, which allowed a simple exact inversion to be made in this case. For $n>1$, we described a fast approximate algorithm to calculate frequency selective pulses compensated for relaxation. The suggested results can be used in nuclear magnetic resonance imaging and spectroscopy, as well as extreme nonlinear optics.

References

1. Ablowitz, M.J., Kaup, D.J., Newell, A.C.: Coherent pulse propagation, a dispersive, irreversible phenomenon. J. Math. Phys. **15**, 1852–1858 (1974)
2. Ablowitz, M.J., Kaup, D.J., Newell, A.C., Segur, H.: The inverse scattering transform–Fourier analysis for nonlinear problems. Stud. Appl. Math. **53**, 249–315 (1974)

3. Allen, L., Eberly, J.H.: Optical Resonance and Two-Level Atoms. Dover Publications, New York (1987)
4. Bloch, F.: Nuclear induction. Phys. Rev. **70**, 460–474 (1946)
5. Feynman, R.P., Vernon, F.L. (Jr)., Hellwarth, R.W.: Geometrical representation of the Schrödinger equation for solving maser problems. J. Appl. Phys. **28**, 49–52 (1957)
6. Le Roux, P.: Exact Synthesis of Radiofrequency waveforms. Society of Magnetic Resonance in Medicine, San Francisco, p. 1049 (1988)
7. Lorenz, E.N.: Deterministic nonperiodic flow. J. Atmos. Sci. **20**, 130–141 (1963)
8. Pauly, J., Le Roux, P., Nishimura, D., Macovski, A.: Parameter relations for the Shinnar-Le Roux selective excitation pulse design algorithm. IEEE Trans. Med. Imag. **10**, 53–65 (1991)
9. Rourke, D.E., Morris, P.G.: The inverse scattering transform and its use in the exact inversion of the Bloch equation for noninteracting spins. J. Magn. Reson. **99**, 118–138 (1992)
10. Rourke, D.E., Morris, P.G.: 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. Phys. Rev. A **46**, 3631–3636 (1992)
11. Rourke, D.E., Saunders, J.K.: Half-solitons as solutions to the Zakharov-Shabat eigenvalue problem for rational reflection coefficient. II. Potentials on infinite support. J. Math. Phys. **35**, 848–872 (1994)
12. Rourke, D.E., Bush, S.D.: Inversion of the Bloch equations with T_2 relaxation: An application of the dressing method. Phys. Rev. E **57**, 7216–7230 (1998)
13. Rourke, D.E., Khodarinova, L., Karabanov, A.A.: Two-level systems with relaxation. Phys. Rev. Lett. **92**, 163003 (2004)
14. Rourke, D.E., Karabanov, A.A., Booth, G.H., Frantsuzov, I.: The Bloch equations when $T_1 = T_2$. Inverse Probl. **23**, 609–623 (2007)
15. Shinnar, M., Leigh, J.S.: The application of spinors to pulse synthesis and analysis. Magn. Reson. Med. **12**, 93–98 (1989)
16. Zakharov, V.E., Shabat, A.B.: Exact theory of two-dimensional self-focusing and one-dimensional self-modulation of waves in nonlinear media, Zh. Eksp. Teor. Fiz. **61**, 118–134 (1971) [Sov. Phys. JETP **34**, 62–69 (1972)]