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Charles L. EPSTEIN

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INTRODUCTION TO MAGNETIC RESONANCE IMAGING FOR MATHEMATICIANS

by Charles L. EPSTEIN (*)

1. Introduction.

Nuclear magnetic resonance (NMR) is a subtle quantum mechanical phenomenon that has played a major role in the revolution in medical imaging over the last 30 years. Before being used in imaging, NMR was employed by chemists to do spectroscopy, and remains a very important technique for determining the structure of complex chemical compounds like proteins. There are many points of contact between these technologies, and problems of interest to mathematicians. Spectroscopy is an applied form of spectral theory. NMR imaging is connected to Fourier analysis, and more general Fourier integral operators. The problem of *selective excitation* in NMR is easily translated into a classical inverse scattering problem, and in this formulation, is easily solved. On the other hand, practical problems in NMR suggest interesting mathematical questions in Fourier theory and inverse scattering theory.

In this note, which is adapted from my lecture, presented in Paris on June 27th, 2003 at the conference in honor of Professor Louis Boutet de Monvel, I give a rapid introduction to nuclear magnetic resonance imaging. Special emphasis is placed on the more mathematical aspects of the problem. After presenting an empirical semiclassical description of the basic NMR phenomenon, and the elementary techniques used in NMR

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imaging, I describe the application of inverse scattering to the problem of selective excitation.

Scant attention is paid to both the NMR spectroscopy, and the quantum description of NMR. Those seeking a more complete introduction to these subjects should consult the monographs of Abragam, [Ab], or Ernst, Bodenhausen and Wokaun, [EBW], for spectroscopy, and that of Callaghan, [Cal], for imaging. All three books consider the quantum mechanical description of the these phenomena.

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2. Nuclear magnetic resonance.

A proton is a spin- $\frac{1}{2}$ particle. In NMR, the spin state of a proton is described by a \mathbb{C}^2 -valued function, ψ . The *intrinsic* angular momentum, \mathbf{J}_p and magnetic moment, $\boldsymbol{\mu}_p$ are \mathbb{R}^3 -valued quantum mechanical observables, which transform, under the action of $\text{SO}(3)$, by the standard 3-dimensional representation. As there is a unique such representation, there is a constant, γ_p , such that

$$(1) \quad \boldsymbol{\mu}_p = \gamma_p \mathbf{J}_p.$$

This constant is called the *gyromagnetic ratio*, see [Me]. In the physics literature this relation is a special case of the Wigner-Eckart theorem.

As quantum mechanical observables, \mathbf{J}_p and $\boldsymbol{\mu}_p$ are operators which act on ψ . In this context they are represented in terms of the Pauli spin matrices,

$$(2) \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

with

$$\mathbf{J}_p = \frac{\hbar}{2} (\sigma_x, \sigma_y, \sigma_z).$$

Recall that Plank's constant $\hbar = 1.0545 \times 10^{-27}$ erg sec. If \mathbf{B} is a magnetic field, then the Schrödinger equation, describing the time evolution of the spin of a proton in this field, is given by

$$(3) \quad \hbar \partial_t \psi = i \mathbf{B} \cdot \boldsymbol{\mu}_p \psi, \text{ where } \mathbf{B} \cdot \boldsymbol{\mu}_p = \frac{\gamma \hbar}{2} [B_x \sigma_x + B_y \sigma_y + B_z \sigma_z].$$

The *expectation* of an observable is a quantum mechanical model for a measurement. The expectations of \mathbf{J}_p and $\boldsymbol{\mu}_p$ are defined by the inner products:

$$\langle \mathbf{J}_p \rangle = \langle \mathbf{J}_p \psi, \psi \rangle, \quad \langle \boldsymbol{\mu}_p \rangle = \langle \boldsymbol{\mu}_p \psi, \psi \rangle.$$

These expectations are \mathbb{R}^3 -valued functions.

The Schrödinger equation implies that $\langle \mathbf{J}_p \rangle$ satisfies the ordinary differential equation:

$$(4) \quad \frac{d\langle \mathbf{J}_p \rangle}{dt} = \langle \boldsymbol{\mu}_p \rangle \times \mathbf{B}.$$

In light of equation (1), this implies that the expectation of $\boldsymbol{\mu}_p$ satisfies

$$(5) \quad \frac{d\langle \boldsymbol{\mu}_p \rangle}{dt} = \gamma_p \langle \boldsymbol{\mu}_p \rangle \times \mathbf{B}.$$

If \mathbf{B} is a static field of the form $(0, 0, b_0)$, then equation (5) implies that $\langle \boldsymbol{\mu}_p \rangle$ precesses about the z -axis with a characteristic angular frequency, $\omega_0 = \gamma_p b_0$. This is the resonance phenomenon which characterizes NMR. The frequency ω_0 is called the *Larmor frequency*; it is proportional to the strength of the magnetic field. Note that there are no spatial variables in this model, i.e. the Schrödinger equation does not involve spatial derivatives. This is a low temperature approximation that is suitable for most medical applications of NMR.

In a classical NMR experiment, the proton would be placed in a static magnetic field of the form $\mathbf{B}_0 = (0, 0, b_0)$. The proton would then be irradiated by a time varying magnetic field of the form $\mathbf{B}_1 = (b_1 \cos \omega t, b_1 \sin \omega t, 0)$. The angular frequency ω would then be slowly varied through a range of values. By observing the power *absorbed* by this system at different frequencies, one could determine the resonant frequency, and thereby measure γ_p , see [Ab]. This is the “old” approach to NMR spectroscopy, called continuous wave, or CW spectroscopy.

Of course one cannot obtain an isolated proton, so the constant γ_p has never been measured directly. What can actually be measured are resonances for protons contained in nuclei of molecules. The electron cloud in a molecule affects the magnetic field at the nuclei, leading to small shifts in the observed resonances. This phenomenon is one of the basic ingredients needed to use NMR spectroscopy to determine molecular structure. For hydrogen protons in water molecules

$$(6) \quad \gamma \approx 2\pi \times 42.5764 \times 10^6 \frac{\text{rad}}{\text{Tesla}}.$$

For hydrogen protons in other molecules, the gyromagnetic ratio is expressed in the form $(1 - \sigma)\gamma$. The coefficient σ is called the *chemical shift*. It is typically between 10^{-6} and 10^{-4} . In the sequel we use γ to denote a gyromagnetic ratio, which can safely be thought of as that of a hydrogen proton in a water molecule.

For purposes of comparison, the strength of the earth's magnetic field is about 5×10^{-5} Tesla. The strength of a standard magnet used in a hospital MR imaging device is in the 1–3 Tesla range, and spectrometers typically use magnets in the 5–15 Tesla range. For imaging magnets, the resonance frequencies are in the 40–120 MHz range. That this is the standard radio frequency (RF) band turns out to be a great piece of luck for medical applications. The quantum mechanical energy ($E = \hbar\omega_0$) at these frequencies is too small to break chemical bonds, and so the radiation used in MR is fundamentally “safe” in ways that X-rays are not. Technologically, it is also a relatively simple frequency band to work in.

In most NMR imaging applications one is attempting to determine the distribution of water molecules in an extended object. Let (x, y, z) denote orthogonal coordinates in the region occupied by the sample, and $\rho(x, y, z)$ denote the density of water molecules at (x, y, z) . The nuclear spins in a complex, extended object interact with one another. If the object is placed within a static magnetic field \mathbf{B}_0 (no longer assumed to be homogeneous) then the spins become *polarized* leading to a net bulk *equilibrium magnetization* \mathbf{M}_0 . The strength of \mathbf{M}_0 is determined by thermodynamic considerations: there is a universal constant C so that

$$(7) \quad \mathbf{M}_0(x, y, z) = \frac{C}{T} \rho(x, y, z) \mathbf{B}_0(x, y, z).$$

Here T is the absolute temperature. At room temperature, in a 1 Tesla field, roughly 1 in 10^6 moments are aligned with \mathbf{B}_0 . Thus \mathbf{M}_0 is a tiny perturbation of \mathbf{B}_0 , which would be very difficult to directly detect.

Felix Bloch introduced a phenomenological equation, which describes the interactions of the bulk magnetization, resulting from the nuclear spins, with one another, and with an applied field. If \mathbf{B} is a magnetic field of the form $\mathbf{B}_0(x, y, z) + \tilde{\mathbf{B}}(x, y, z; t)$, with the time dependent parts much smaller than \mathbf{B}_0 , then the bulk magnetization, \mathbf{M} , satisfies the equation

$$(8) \quad \frac{d\mathbf{M}(x, y, z; t)}{dt} = \gamma \mathbf{M}(x, y, z; t) \times \mathbf{B}(x, y, z; t) - \frac{1}{T_2} \mathbf{M}^\perp(x, y, z; t) + \frac{1}{T_1} (\mathbf{M}_0(x, y, z) - \mathbf{M}^\parallel(x, y, z; t)).$$

Here M^\perp is the component of M , perpendicular to B_0 , (called the *transverse component*), and M^\parallel is the component of M , parallel to B_0 , (called the *longitudinal component*). Much of the analysis in NMR amounts to understanding the behavior of solutions to equation (8) with different choices of B . We now consider some important special cases.

If B has no time dependent component, then this equation predicts that the sample becomes polarized with the transverse part of M decaying as e^{-t/T_2} , and the longitudinal component approaching the equilibrium field, M_0 as $1 - e^{-t/T_1}$. In Bloch’s model, the spins at different points do not directly interact. Instead, the relaxation terms describe averaged interactions with “spin baths.” This simple model is adequate for most imaging applications. Indeed, for many purposes, it is sufficient to use the Bloch equation without the relaxation terms. See [Bl] and [To].

Typically, B_0 , the *background field*, is assumed to be a strong uniform field, $B_0 = (0, 0, b_0)$, and B takes the form

$$(9) \quad B = B_0 + G + B_1,$$

where G is a *gradient field*. Usually the gradient fields are “piecewise time independent” fields, small relative to B_0 . By piecewise time independent field we mean a collection of static fields that, in the course of the experiment, are turned on and off. The B_1 component is a time dependent radio frequency field, nominally at right angles to B_0 . It is usually taken to be spatially homogeneous, with time dependence of the form:

$$(10) \quad B_1(t) = \begin{pmatrix} \operatorname{Re}[(\alpha(t) + i\beta(t))e^{i\omega_0 t}] \\ \operatorname{Im}[(\alpha(t) + i\beta(t))e^{i\omega_0 t}] \\ 0 \end{pmatrix},$$

as before $\omega_0 = \gamma b_0$.

If $G = 0$ and $\beta \equiv 0$, then the solution operator for Bloch’s equation, without relaxation terms, is

$$(11) \quad U(t) = \begin{pmatrix} \cos \omega_0 t & -\sin \omega_0 t & 0 \\ \sin \omega_0 t & \cos \omega_0 t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta(t) & -\sin \theta(t) \\ 0 & \sin \theta(t) & \cos \theta(t) \end{pmatrix},$$

where

$$(12) \quad \theta(t) = \int_0^t \alpha(s) ds.$$

Up to the “resonance rotation” about the z -axis, at time t (the first factor on the r.h.s. of (11)) this is simply a rotation about the x -axis through the angle $\theta(t)$. If, on the other hand, $\mathbf{B}_1 = 0$ and $\mathbf{G}_\ell = (0, 0, \ell(x, y, z))$, where $\ell(\cdot)$ is a linear function, then U depends on (x, y, z) , and is given by

$$(13) \quad U(x, y, z; t) = \begin{pmatrix} \cos(\omega_0 + \gamma\ell(x, y, z))t & -\sin(\omega_0 + \gamma\ell(x, y, z))t & 0 \\ \sin(\omega_0 + \gamma\ell(x, y, z))t & \cos(\omega_0 + \gamma\ell(x, y, z))t & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The field \mathbf{G}_ℓ , defined above, is not divergence free, and therefore cannot be a solution to Maxwell’s equations. For any linear function ℓ there is a solution to Maxwell’s equations of the form $\tilde{\mathbf{G}}_\ell = (\ell_1, \ell_2, \ell)$, where ℓ_1 and ℓ_2 are also linear functions, with coefficients bounded by those of ℓ . So long as ℓ , and therefore also ℓ_1 and ℓ_2 are small, relative to $\|\mathbf{B}_0\|$, it is safe to simply ignore the components of $\tilde{\mathbf{G}}_\ell$ orthogonal to \mathbf{B}_0 . Over the duration of a realistic MR experiment, they have a negligible effect. In most of the MR-literature, when one speaks of “field gradients” one is referring only to the component in the direction of \mathbf{B}_0 of a relatively small, piecewise time independent magnetic field.

3. A basic imaging experiment.

With these preliminaries we can describe the basic measurements in magnetic resonance imaging. The sample is polarized, and then an RF-field, of the form given in (10), (with $\beta \equiv 0$) is turned on for a finite time T . This is called an *RF-excitation*. For the purposes of this discussion we suppose that the time is chosen so that $\theta(T) = 90^\circ$, see equation (12). As \mathbf{B}_0 and \mathbf{B}_1 are spatially homogeneous, the magnetization vectors within the sample remain parallel throughout the RF-excitation. At the conclusion of the RF-excitation, \mathbf{M} is orthogonal to \mathbf{B}_0 .

After time T , the RF is turned off, and the vector field $\mathbf{M}(x, y, z; t)$ precesses about \mathbf{B}_0 , *in phase*, with angular velocity ω_0 . The transverse component of \mathbf{M} decays exponentially. If we normalize the time so that $t = 0$ corresponds to the conclusion of the RF-pulse, then

$$(14) \quad \mathbf{M}(x, y, z; t) = \frac{C\omega_0\rho(x, y, z)}{\gamma T} [e^{-t/T_2} e^{i(\omega_0 t + \phi)}, (1 - e^{-t/T_1})].$$

Here ϕ is a fixed real phase. In this formula and in the sequel we follow the standard practice in MR, expressing the magnetization in the form $[M_x + iM_y, M_z]$.

Recall Faraday’s Law: A changing magnetic field induces an electromotive force (EMF) in a loop of wire according to the relation

$$(15) \quad \text{EMF}_{\text{loop}} \propto \frac{d\Phi_{\text{loop}}}{dt}.$$

Here Φ_{loop} denotes the flux of the field through the loop of wire. A loop is an oriented, simple closed curve, c ; if Σ is an oriented surface with boundary equal to c , then Φ_c , the flux of \mathbf{M} through c , is given by

$$(16) \quad \Phi_c = \int_{\Sigma} \mathbf{M} \cdot \boldsymbol{\nu} dS,$$

here $\boldsymbol{\nu}$ is the outward pointing unit normal to Σ .

The transverse components of \mathbf{M} are a rapidly varying magnetic field, which, according to Faraday’s law, induce a current in a loop of wire. In fact, by placing several such loops near to the sample we can measure a signal of the form:

$$(17) \quad S_0(t) = \frac{C' \omega_0^2 e^{-t/T_2} e^{i\omega_0 t}}{\gamma T} \int_{\text{sample}} \rho(x, y, z) b_{1\text{rec}}(x, y, z) dx dy dz.$$

Here $b_{1\text{rec}}(x, y, z)$ quantifies the sensitivity of the detector to the precessing magnetization located at (x, y, z) . From $S(t)$ we easily obtain a measurement of the integral of the function $\rho b_{1\text{rec}}$. By using a carefully designed detector, $b_{1\text{rec}}$ can be taken to be a constant, and therefore we can determine the total spin density within the object of interest. For the rest of this section we assume that $b_{1\text{rec}}$ is a constant. Note that the size of the measured signal is proportional to ω_0^2 , which is, in turn, proportional to $\|\mathbf{B}_0\|^2$. This explains, in part, why it is so useful to have a very strong background field. Though even with a 1.5 T magnet, the measured signal is only in the micro-watt range, see [Ho1], [Ho2].

Let $\ell(x, y, z) = \langle (x, y, z), (k_x, k_y, k_z) \rangle$, for a constant vector $k = (k_x, k_y, k_z)$. Suppose that at the end of the RF-excitation, we turn on \mathbf{G}_ℓ . As the magnetic field $\mathbf{B} = \mathbf{B}_0 + \mathbf{G}_\ell$ now has a nontrivial spatial dependence, the precessional frequency of the spins, which equals $\gamma\|\mathbf{B}\|$, also has a spatial dependence. In fact, it follows from (13) that the measured signal would now be given by

$$(18) \quad S_\ell(t) \approx \frac{C' b_{1\text{rec}} \omega_0^2 e^{-t/T_2} e^{i\omega_0 t}}{\gamma T} \times \int_{\text{sample}} \rho(x, y, z) e^{it\gamma \langle (x, y, z), (k_x, k_y, k_z) \rangle} dx dy dz.$$

Up to a constant, $e^{t/T_2} e^{-i\omega_0 t} S_\ell(t)$ is simply the Fourier transform of ρ at $-t\gamma k$. By sampling in time and using a variety of different linear functions ℓ , we can sample the Fourier transform of ρ in neighborhood of 0. This suffices to reconstruct an approximation to ρ .

This is an idealized model for the measurement process. The fact that the objects being studied are often electrically conductive, leads to noise in the measurements. The amplitude of the noise is proportional to the bandwidth of the measured data and the volume of the sample. The measurement apparatus itself also produces noise. From the Riemann Lebesgue lemma, it follows that $|e^{t/T_2} S_\ell(t)| \propto |\widehat{\rho}(-t\gamma k)|$, is decaying as t increases. As the noise has a constant mean amplitude, there is a practical limit on how long the signal can be sampled. This translates into a maximum absolute frequency in Fourier space that can reasonably be measured. This maximum absolute frequency in turn limits the resolution attainable in the reconstructed image.

The foregoing remarks indicate that the measurements made in an MR experiment should be regarded as samples of a random variable. Real MR experiments are often repeated many times. As these constitute essentially independent measurements, the noise is uncorrelated from trial to trial. By repeating the same measurement N times, and averaging the results, the variance is reduced by a factor of \sqrt{N} .

The approach to imaging described above captures the spirit of the methods used in real applications. It is however, not representative in several particulars. It is unusual to sample the 3-dimensional Fourier transform of ρ . Rather, a specially shaped RF-pulse is used in the presence of nontrivial field gradients, to excite the spins in a thin, essentially 2-dimensional, slice of the sample. The spins slightly outside this slice remain in the equilibrium state. This means that any measured signal comes predominately from the excited slice. This process is called *selective excitation*. In the next section we explain a technique used to design RF-pulses to produce such a selective excitation. It is also much more common to sample the Fourier domain in a rectilinear fashion, rather than in the radial fashion described above. This makes it possible to use the “fast Fourier transform” algorithm to reconstruct the image, vastly reducing the computational requirements of the reconstruction step. We do not consider this aspect of the problem in any detail, the interested reader is referred to [Cal] or [Ha].

4. Selective excitation.

As noted above, it is unusual to excite the entire sample at once. By using carefully designed RF-pulses, applied in the presence of gradient fields, we can excite the spins in a thin slice of the sample while leaving those outside a slightly larger slice in the equilibrium state. In this section we show how the design of such a pulse is actually an inverse scattering problem for the classical Zakharov-Shabat 2×2 -system. This fact was first recognized in the early 1980s and appears in papers of, *inter alia*, Alberto Grünbaum, M. Shinnar, and John Leigh, see [GH], [SL1], [SL2]. The approach we describe can be found in the work of Carlson, and Morris and Rourke, see [Ca1], [Ca2], [MR], and [Ep]

The Bloch equation is usually analyzed in a *rotating reference frame*, related to the *laboratory frame* by a time dependent orthogonal transformation of the form

$$(19) \quad \mathbf{F}(t) = \begin{pmatrix} \cos \vartheta(t) & -\sin \vartheta(t) & 0 \\ \sin \vartheta(t) & \cos \vartheta(t) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We set

$$(20) \quad \mathbf{M}(t) = \mathbf{F}(t)\mathbf{m}(t),$$

so that \mathbf{m} denotes the bulk magnetization in the rotating reference frame. Larmor's theorem implies that if \mathbf{M} satisfies $\partial_t \mathbf{M} = \gamma \mathbf{M} \times \mathbf{B}$, then \mathbf{m} satisfies

$$(21) \quad \frac{d\mathbf{m}}{dt} = \gamma \mathbf{m} \times \mathbf{B}_{\text{eff}},$$

where

$$(22) \quad \mathbf{B}_{\text{eff}}(t) = \mathbf{F}^{-1}(t)\mathbf{B}(t) + \frac{1}{\gamma} \boldsymbol{\Omega}(t), \quad \text{and} \quad \boldsymbol{\Omega}(t) = [0, 0, \vartheta'(t)]^t.$$

In this section we assume that $\mathbf{B}_0 = (0, 0, b_0)$ and $\mathbf{G} = (0, 0, gz)$. In this case, setting $\vartheta(t) = -\omega_0 t$, gives

$$(23) \quad \mathbf{B}_{\text{eff}}(\nu; t) = (\omega_1(t), \omega_2(t), \gamma^{-1}\nu).$$

The constant value $\nu = gz$ is called the *offset frequency* or *resonance offset*. In the laboratory frame, the radio frequency magnetic field takes the form

$$(24) \quad \mathbf{B}_1(t) = [\text{Re } e^{i\omega_0 t}(\omega_1(t) + i\omega_2(t)), \text{Im } e^{i\omega_0 t}(\omega_1(t) + i\omega_2(t)), 0]^t.$$

A *magnetization profile* is a unit vector valued function defined for $\nu \in \mathbb{R}$,

$$(25) \quad \mathbf{m}^\infty(\nu) = \begin{pmatrix} m_1^\infty(\nu) \\ m_2^\infty(\nu) \\ m_3^\infty(\nu) \end{pmatrix}.$$

In essentially all MR applications, $\mathbf{m}^\infty(\nu) = (0, 0, 1)^t$, for ν outside of a bounded interval. The problem of RF-pulse synthesis is to find a time dependent complex pulse envelope, $\omega_1(t) + i\omega_2(t)$, so that, if $\mathbf{B}_{\text{eff}}(\nu)$ is given by (23), then the solution of

$$(26) \quad \frac{d\mathbf{m}}{dt}(\nu; t) = \gamma \mathbf{m}(\nu; t) \times \mathbf{B}_{\text{eff}}(\nu; t),$$

with

$$(27) \quad \lim_{t \rightarrow -\infty} \mathbf{m}(\nu; t) = (0, 0, 1)^t,$$

satisfies

$$(28) \quad \lim_{t \rightarrow \infty} (e^{-i\nu t} (m_1 + im_2)(\nu; t), m_3(\nu; t)) = ((m_1^\infty + im_2^\infty)(\nu), m_3^\infty(\nu)).$$

We have used the standard complex notation, $m_1 + im_2$, for the transverse components of the magnetization. If $\omega_1(t) + i\omega_2(t)$ is supported in the interval $[t_0, t_1]$, then these asymptotic conditions are replaced by

$$(29) \quad \begin{cases} \mathbf{m}(\nu; t_0) = (0, 0, 1)^t, \\ (e^{-i\nu t_1} (m_1 + im_2)(\nu; t_1), m_3(\nu; t_1)) = ((m_1^\infty + im_2^\infty)(\nu), m_3^\infty(\nu)). \end{cases}$$

With the offset frequency, ν , interpreted as a spectral parameter, it is clear that this is an inverse scattering problem.

In the rotating reference frame, the Bloch equation without relaxation can be rewritten in the form

$$(30) \quad \frac{d\mathbf{M}}{dt} = X_{\mathbf{B}} \mathbf{M}.$$

where $X_{\mathbf{B}}$ is the skew symmetric matrix

$$(31) \quad X_{\mathbf{B}} = \begin{pmatrix} 0 & \nu & -\gamma\omega_2 \\ \nu & 0 & \gamma\omega_1 \\ \gamma\omega_2 & -\gamma\omega_1 & 0 \end{pmatrix}.$$

By appending two additional orthogonal columns to \mathbf{M} this equation can be extended to the canonical equation on $\text{SO}(3)$: $\partial_t \mathbf{O}\mathbf{O}^{-1} = X_B$. This equation can in turn be lifted to the double cover, $\text{SU}(2)$. The lifted equation is known, in MR, as the *spin domain* Bloch equation. It is given by

$$(32) \quad \frac{d\boldsymbol{\psi}}{dt}(\xi;t) = \begin{pmatrix} -i\xi & q(t) \\ -\bar{q}(t) & i\xi \end{pmatrix} \boldsymbol{\psi}(\xi;t),$$

with $\boldsymbol{\psi}$ a \mathbb{C}^2 -valued function, $\xi = \frac{1}{2}\nu$, and $q(t) = -\frac{1}{2}i\gamma(\omega_1(t) - i\omega_2(t))$.

A simple recipe takes a solution of (32) and produces a solution of (26). If $\boldsymbol{\psi}(\xi;t) = [\psi_1(\xi;t), \psi_2(\xi;t)]^t$ satisfies (32), then the 3-vector valued function

$$(33) \quad \mathbf{m}(\nu;t) = (2 \operatorname{Re}(\psi_1^* \psi_2), 2 \operatorname{Im}(\psi_1^* \psi_2), |\psi_1|^2 - |\psi_2|^2)^t \left(\frac{\nu}{2}; t\right)$$

satisfies (26). If in addition

$$(34) \quad \lim_{t \rightarrow -\infty} e^{i\xi t} \boldsymbol{\psi}(\xi;t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

then \mathbf{m} satisfies (27). Thus the RF-pulse synthesis problem is easily translated into an inverse scattering problem for equation (32).

Scattering theory, for an equation like (32), relates the behavior of $\boldsymbol{\psi}(\xi;t)$, as $t \rightarrow -\infty$ to that of $\boldsymbol{\psi}(\xi;t)$, as $t \rightarrow +\infty$. If q has bounded support, then, outside the support of q , the functions

$$(35) \quad \begin{pmatrix} e^{-i\xi t} \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ e^{i\xi t} \end{pmatrix}$$

are a basis of solutions for (32). If the L^1 -norm of q is finite, then, it is shown in [AKNS], that (32) has solutions that are asymptotic to these solutions as $t \rightarrow \pm\infty$.

THEOREM 1. — *If $\|q\|_{L^1}$ is finite, then, for every $\xi \in \mathbb{R}$, there are unique solutions*

$$(36) \quad \boldsymbol{\psi}_{1+}(\xi), \boldsymbol{\psi}_{2+}(\xi) \quad \text{and} \quad \boldsymbol{\psi}_{1-}(\xi), \boldsymbol{\psi}_{2-}(\xi)$$

to equation (32), which satisfy

$$(37) \quad \lim_{t \rightarrow -\infty} e^{i\xi t} \boldsymbol{\psi}_{1-}(\xi;t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \lim_{t \rightarrow -\infty} e^{-i\xi t} \boldsymbol{\psi}_{2-}(\xi;t) = \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$

$$(38) \quad \lim_{t \rightarrow \infty} e^{i\xi t} \boldsymbol{\psi}_{1+}(\xi;t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \lim_{t \rightarrow \infty} e^{-i\xi t} \boldsymbol{\psi}_{2+}(\xi;t) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

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

The proof of this theorem can be found in [AKNS].

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

$$(39) \quad \begin{cases} \psi_{1-}(\xi;t) = a(\xi)\psi_{1+}(\xi;t) + b(\xi)\psi_{2+}(\xi;t), \\ \psi_{2-}(\xi;t) = b^*(\xi)\psi_{1+}(\xi;t) - a^*(\xi)\psi_{2+}(\xi;t). \end{cases}$$

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

$$(40) \quad [\psi_{1-} \ \psi_{2-}] = [\psi_{1+} \ \psi_{2+}] \begin{pmatrix} a(\xi) & b^*(\xi) \\ b(\xi) & -a^*(\xi) \end{pmatrix}.$$

The *scattering matrix* for the potential q is defined to be

$$(41) \quad s(\xi) = \begin{pmatrix} a(\xi) & b^*(\xi) \\ b(\xi) & -a^*(\xi) \end{pmatrix}.$$

It is well known that a extends to the upper half plane as an analytic function. On the real axis we have

$$(42) \quad |a(\xi)|^2 + |b(\xi)|^2 = 1.$$

These results are proved in [AKNS].

Assuming that $t^j q(t)$ is integrable for all j , it is shown in [AKNS] that a has finitely many zeros in $\text{Im } \xi \geq 0$. The function a vanishes at ξ if and only if the functions $\psi_{1-}(\xi)$ and $\psi_{2+}(\xi)$ are linearly dependent. Let $\{\xi_1, \dots, \xi_N\}$ be a list of the zeros of a . For each j there is a *nonzero* complex number C'_j so that

$$(43) \quad \psi_{1-}(\xi_j) = C'_j \psi_{2+}(\xi_j), \quad j = 1, \dots, N.$$

If $\text{Im } \xi_j > 0$, then is not hard to show that, in this case, the functions $\{\psi_{1-}(\xi_j)\}$ belong to $L^2(\mathbb{R})$, and therefore define *bound states*. We generally assume that the zeros of a are simple and that their imaginary parts are positive. This is mostly to simplify the exposition, there is no difficulty, in principle, if a has real zeros or higher order zeros.

DEFINITION 1. — The pair of functions $(a(\xi), b(\xi))$, for $\xi \in \mathbb{R}$, and the collection of pairs $\{(\xi_j, C'_j) : j = 1, \dots, N\}$ define the *scattering data* for equation (32).

The scattering data are not independent. If $\{\xi_j : j = 1, \dots, N\}$ are the zeros of $a(\xi)$ in the upper half plane, then

$$(44) \quad \tilde{a}(\xi) = \prod_{j=1}^N \left(\frac{\xi - \xi_j^*}{\xi - \xi_j} \right) a(\xi)$$

is an analytic function without zeros in the upper half plane. Moreover $|a(\xi)| = |\tilde{a}(\xi)|$ on the real axis. The function $\log \tilde{a}$ is also analytic in the upper half plane, and $|\log \tilde{a}(\xi)|$ is $O(|\xi|^{-1})$ as $|\xi|$ tends to infinity. The Cauchy integral formula therefore applies to give a representation of $\log \tilde{a}$ in $\text{Im } \xi > 0$:

$$(45) \quad \log \tilde{a}(\xi) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log(|a(\zeta)|^2) d\zeta}{\zeta - \xi}.$$

Exponentiating, and putting the zeros of a back in gives

$$(46) \quad a(\xi) = \prod_{j=1}^N \left(\frac{\xi - \xi_j}{\xi - \xi_j^*} \right) \exp \left(\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log(|a(\zeta)|^2) d\zeta}{\zeta - \xi} \right),$$

see [FT]. The *reflection* coefficient is defined by

$$(47) \quad r(\xi) = \frac{b(\xi)}{a(\xi)}.$$

A priori the reflection coefficient is only defined on the real axis. Using (42) we rewrite (46) in terms of r :

$$(48) \quad a(\xi) = \prod_{j=1}^n \left(\frac{\xi - \xi_j}{\xi - \xi_j^*} \right) \exp \left(\frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{\log(1 + |r(\zeta)|^2) d\zeta}{\zeta - \xi} \right).$$

Both (46) and (48) have well defined limits as ξ approaches the real axis.

If a has simple zeros at the points $\{\xi_1, \dots, \xi_N\}$ (so that $a'(\xi_j) \neq 0$), then we define the *norming constants* by setting

$$(49) \quad C_j = \frac{C'_j}{a'(\xi_j)},$$

where the $\{C'_j\}$ are defined in (43). The definition needs to be modified if a has nonsimple zeros. The pairs $\{(\xi_j, C_j)\}$ are often referred to as the *discrete data*. A complete discussion of inverse scattering for the ZS-system can be found in [Ma].

DEFINITION 2. — The function $r(\xi)$, for $\xi \in \mathbb{R}$, and the collection of pairs $\{(\xi_j, C_j) : j = 1, \dots, N\}$ define the *reduced scattering data* for equation (32).

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

We now rephrase the RF-pulse synthesis problem as an inverse scattering problem. Recall that the data for the pulse synthesis problem is the magnetization profile \mathbf{m}^∞ , which we now think of as a function of $\xi = \frac{1}{2}\nu$. Using (33), the solution ψ_{1-} to the ZS-system defines a solution \mathbf{m}_{1-} to (26), satisfying (27). It follows from (38) and (39) that

$$(50) \quad \psi_{1-}(\xi; t) \sim \begin{pmatrix} a(\xi)e^{-i\xi t} \\ b(\xi)e^{i\xi t} \end{pmatrix}, \quad \text{as } t \rightarrow +\infty.$$

Therefore

$$(51) \quad \mathbf{m}_{1-}(\xi; t) \sim \begin{pmatrix} 2b(\xi)a^*(\xi)e^{2i\xi t} \\ |a(\xi)|^2 - |b(\xi)|^2 \end{pmatrix}, \quad \text{as } t \rightarrow +\infty.$$

As before, we use the complex notation for the transverse components of \mathbf{m}_{1-} . If \mathbf{m}_{1-} also satisfies (28), then it follows from (51) and (42) that

$$(52) \quad r(\xi) = \frac{b(\xi)}{a(\xi)} = \lim_{t \rightarrow \infty} \frac{(m_{11-} + im_{21-})(\xi; t)e^{-2i\xi t}}{1 + m_{31-}(\xi; t)} = \frac{(m_1^\infty + im_2^\infty)(\xi)}{1 + m_3^\infty(\xi)}.$$

As $\mathbf{m}^\infty(\xi)$ is a unit vector valued function, we see that the reflection coefficient $r(\xi)$ uniquely determines $\mathbf{m}^\infty(\xi)$ and vice-versa. Thus the RF-pulse synthesis problem can be rephrased as the following inverse scattering problem: *Find a potential $q(t)$ for the ZS-system so that the reflection coefficient $r(\xi)$ satisfies (52) for all real ξ .* Note that the pulse synthesis problem makes no reference to the data connected to the bound states, i.e. $\{(\xi_j, C_j)\}$. Indeed these are *free* parameters in the RF-pulse synthesis problem, making the problem highly underdetermined.

Remark 1. — Our discussion of inverse scattering and its applications to RF-pulse design is largely adapted from [AKNS], [MR], [PRNM] and [Ep].

Remark 2. — In the mid 1980s Patrick Le Roux, and Jack Leigh and Meir Shinnar introduced a method for RF-pulse synthesis now known as the *SLR method*. In this approach, one looks for a potential of the special form

$$q_0(t) = \sum_{j=1}^N a_j \delta(t - j\Delta t).$$

The scattering data for such a potential are periodic functions. For scattering data of this type, the inverse problem can be solved using a simple, and efficient recursive algorithm. The potential q_0 is not physically realizable, instead one uses a smoothed version, for example,

$$q_1 = \sum_{j=1}^N \frac{a_j}{\Delta t} \chi_{[0, \Delta t)}(t - j\Delta t).$$

If Δt is sufficiently small then q_0 and q_1 have very similar reflection coefficients for frequencies in the interval $(-\Delta t^{-1} \frac{1}{2} \pi, \Delta t^{-1} \frac{1}{2} \pi)$. See [SL1], [SL2], [PRNM], [Ep], [Ma].

We conclude our discussion with a formula for the energy of the pulse envelope in terms of the reduced scattering data. The underlying results from inverse scattering theory are due to Zakharov, Faddeev, and Manakov.

THEOREM 2. — *Suppose that $q(t)$ is a sufficiently rapidly decaying potential for the ZS-system, with reflection coefficient $r(\xi)$, and discrete data $\{(\xi_j, C_j), j = 1, \dots, N\}$, then*

$$(53) \quad \int_{-\infty}^{\infty} |q(t)|^2 dt = \frac{1}{\pi} \int_{-\infty}^{\infty} \log(1 + |r(\xi)|^2) d\xi + 4 \sum_{j=1}^N \text{Im } \xi_j.$$

The proof of this result can be found in [AKNS] or [FT]. Note that the norming constants play no role in this formula.

Combining (52) with (53) we obtain the following simple corollary.

COROLLARY 1. — *If m^∞ is a sufficiently smooth magnetization profile, such that $m_1^\infty + im_2^\infty$ decays to zero as $|\xi| \rightarrow \infty$, and is absolutely*

integrable, then the total energy of any RF-envelope, $\omega_1(t) + i\omega_2(t)$, which produces this magnetization profile, satisfies the estimate

$$(54) \quad \int_{-\infty}^{\infty} |\omega_1(t) + i\omega_2(t)|^2 dt \geq \frac{2}{\pi\gamma^2} \int_{-\infty}^{\infty} \log \left(1 + \left| \frac{m_1^\infty(\xi) + im_2^\infty(\xi)}{1 + m_3^\infty(\xi)} \right|^2 \right) d\xi.$$

Equality holds in this estimate if and only if the ZS-system with the corresponding potential has no bound states.

From the corollary it is evident that the lowest energy RF-envelope is obtained by solving the inverse scattering problem with *no* bound states.

5. Some examples and questions.

The inverse scattering problem stated in the previous section can be solved numerically in a variety of different ways. In [Ep] we present an algorithm using the left and right Marchenko equations. This improves an earlier approach given in [MR] in that it allows for an essentially arbitrary specification of bound states. Without bound states the problem is numerically well behaved; if there are bound states one is faced with solving highly ill conditioned linear systems. A very effective approach to this has been found, in collaboration with Jeremy Magland, and is described in his PhD thesis, see [Ma]. In this section we present solutions to some typical selective excitation problems, and then consider some open questions.

As described in Section 3, a fundamental problem is to flip the magnetization 90° for offset frequencies in a certain interval, $[\xi_0, \xi_1]$, while leaving those outside a slightly larger interval fixed. The “ideal” reflection coefficient is given by $r_i(\xi) = \chi_{[\xi_0, \xi_1]}(\xi)$. The mapping properties of the IST are quite similar to those of the Fourier transform. In particular, the quantitative smoothness of the reflection coefficient determines the rate of decay of the potential and vice versa, see [BC]. In real applications it is important to have a potential with small effective support; this translates into a requirement to smooth r_i .

Example 1. — For our first example we use piecewise polynomial functions, with three continuous derivatives, to design pulses. Figure 1 (a) shows several such approximations to r_i and Figure 1 (b)–(d) shows

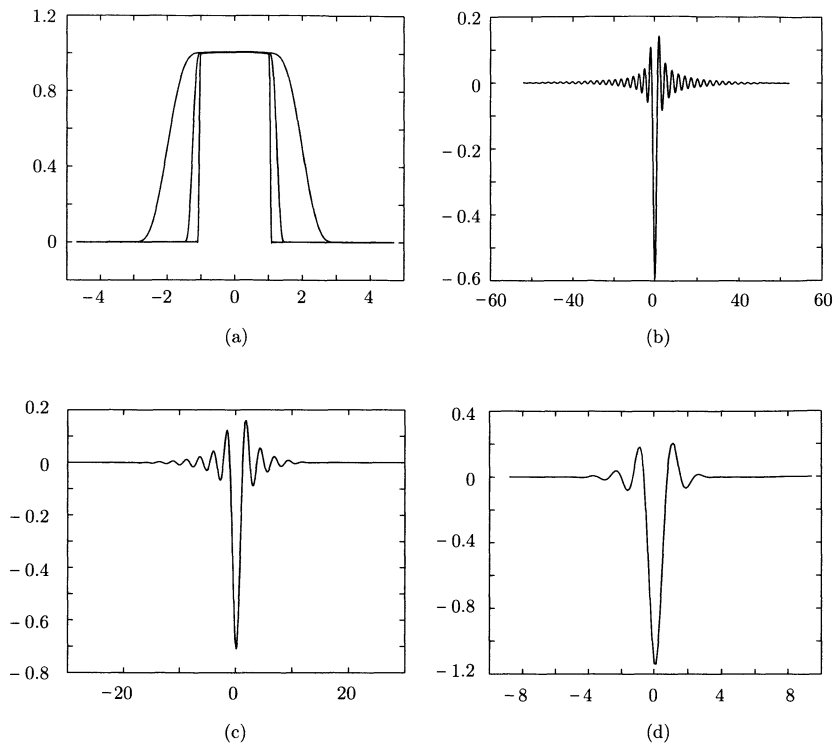
the corresponding minimum energy (no bound states) potentials. The relationship between the quantitative smoothness of r and the effective support of q is quite apparent in these examples.

Example 2. — For our next example we consider the effects of adding bound states. We use the rational function $r_{18}(\xi) = (1 + \xi^{18})^{-1}$ as an approximation to r_i . We use 9 bound states with $\{\xi_1, \dots, \xi_9\}$ given by the poles of r_{18} in the upper half. For the norming constants, we use the residues of r_{18} at the corresponding points. As is well known, this produces a potential supported in $(0, \infty]$. In the MR-literature this is called a *self refocused* pulse. The pulse and its corresponding reflection coefficient are shown in Figure 2.

The physical problem of selective excitation fixes only the reflection coefficient. The discrete data for the inverse scattering problem are free parameters. In medical applications it is usually important to keep the total energy and maximum amplitude of the pulse small; this makes the minimum energy pulse an attractive choice. There are however other considerations which might make a pulse with higher energy more useful. The main desideratum is to reduce the “effective” support of the potential. In real applications one might truncate the potential produced by the IST to obtain a function of the form $w(t)q(t)$, with support in a finite interval. This leads one to ask the following questions:

- 1) For a given reflection coefficient r , is it possible to choose discrete data, $\{(\xi_j, C_j)\}$, so that the potential with this reduced scattering data has arbitrarily small *effective* support?
- 2) For a given reflection coefficient r , is it possible to choose discrete data, $\{(\xi_j, C_j)\}$, so that the effective support of the potential with this reduced scattering data is reduced by a definite factor over that of the minimum energy potential, e.g., cut in half?
- 3) Is there a nonlinear Heisenberg uncertainty principle for the IST?

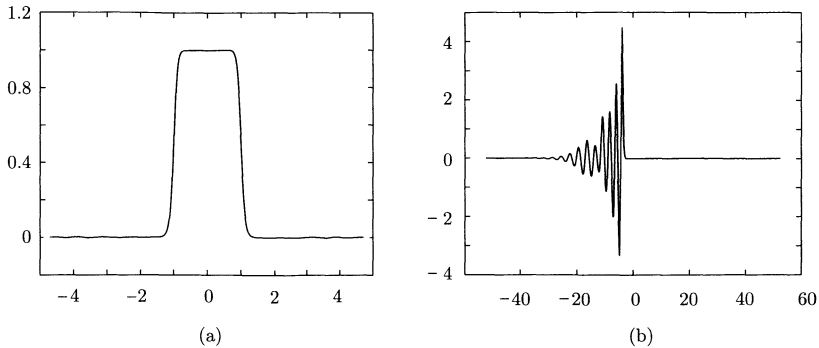
These problems beg the question of what is meant by effective support. The main goal is to attain a good approximation to the given reflection coefficient, r . Hence, we say that an interval I contains the effective support of q if there is a window function w supported in I so that r_w is a good approximation to r . From experiments we have done, it is fairly clear that, for minimum energy pulses, the effective support can be described as an interval where the potential assumes at least some fraction of its maximum value. On the other hand, for pulses with bound states, parts of the pulse



- (a) A plot showing the different approximations to r_i used to design the potentials in (b)–(d).
 (b) Potential with reflection coefficient supported in $(-1.1, 1.1)$.
 (c) Potential with reflection coefficient supported in $(-1.5, 1.5)$.
 (d) Potential with reflection coefficient supported in $(-3, 3)$.

Figure 1. Several minimum energy potentials which approximate a 90° flip. Note the different time scales used in the plots (b)–(d). A smoother reflection coefficient produces a potential with smaller effective support.

with very small relative amplitude seem to be important for attaining a good approximation to r . It is therefore an interesting question to give sufficient conditions for I to contain the effective support of q . Questions of this sort appear in papers of Grünbaum, see [Gr2], [Gr1]. Another problem in the application of RF-pulses is the lack of spatial homogeneity across the extent of the sample. One therefore would like to find discrete data $\{(\xi_j, C_j)\}$ which “stabilizes” the effect of the pulse under small errors in either the amplitude or phase.



(a) A plot the reflection coefficient produced by the potential shown in (b).
 (b) Potential with reflection coefficient r_{18} and bound states corresponding to poles of r_{18} .

Figure 2. A self refocused pulse. Note the much large amplitude, by comparison to the minimum energy pulses.

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Charles L. EPSTEIN,
University of Pennsylvania
Department of Mathematics
and
LSNI, Hospital of the University of Pennsylvania
Philadelphia, PA (USA).
cle@math.upenn.edu