CYBERNETICS AND PHYSICS, VOL. 1, NO. 4, 2012 , 243–251

EXCEPTIONAL TRAJECTORIES IN THE CONTRAST PROBLEM IN NUCLEAR MAGNETIC RESONANCE

Monique Chyba
Department of Mathematics
University of Hawai'i at Mānoa
USA
mchyba@math.hawaii.edu

John Marriott
Department of Mathematics
University of Hawai'i at Mānoa
USA
marriott@math.hawaii.edu

Abstract
In this paper we focus on the contrast problem in medical imaging. It consists of using a single magnetic field to control a pair of non-interacting spins, each representing a specific substance, with the goal of maximizing the difference of the moduli of the magnetization vectors of the two substances. Prior work analyzed the saturation contrast problem which brings one of the spins to magnetization zero while maximizing the modulus of the other. Here we relax the saturation constraint that one of the spins must reach magnetization zero, providing more flexibility to obtain a higher contrast. We focus on the study of exceptional arcs and construct bang-exceptional extremals based on a methodology that searches for the highest possible contrast. Numerical calculations are provided, and we graphically illustrate the results.

Key words
Geometric optimal control, nuclear magnetic resonance, contrast problem, exceptional singular arcs.

1 Introduction

Nuclear magnetic resonance (NMR) is a powerful tool in a variety of scientific fields, and is employed in applications such as quantum computing and medical imaging. In magnetic resonance imaging, nuclear spins are controlled via interaction with magnetic fields. We consider a physical system controlled in this way, and take a problem motivated by the application to medical imaging. In this imaging, the modulus of the magnetization vector of a substance determines its brightness in the resulting image. Thus, achieving a high visual contrast between two substances being imaged amounts to maximizing the difference of the moduli of the magnetization vectors of the two substances. This goal defines the *contrast problem*: given two substances initially at equilibrium, use a magnetic field to prepare two substances for imaging by maximizing the difference of the moduli of their magnetization vectors.

Using techniques from geometric control has proved to be a very efficient approach to analyze the contrast problem. First, numerical tools such as the creation of the gradient ascent pulse engineering algorithm [Khaneja *et al.*, 2005; Gershenzon *et al.*, 2008], a numerical tool for pulse sequence optimization, were developed. More recently geometric control has been used to complement those approaches. The main advantage of geometric control is that it provides an understanding of the qualitative structure of the optimal control and of the role of the physical parameters [Lapert *et al.*, 2010a]. The geometric approach has been complemented with experimental validation. See [Lapert *et al.*, 2012] for a survey and [Bonnard and Cots, 2012] for recent results. We embrace this point of view and contribute to the problem here. The maximum principle [Pontryagin *et al.*, 1962] shows that in the contrast problem, optimal controls are concatenations of *bang* and *singular* arcs (defined below). Among the singular arcs, there is a class called the *exceptional* singular arcs which are intrinsic to the system in the sense that they are independent of the cost. Our goal is to understand the role that the exceptional singular arcs can play in the resolution of the contrast problem. More precisely, we first develop an algorithm to construct bang-exceptional extremals and provide a solution to the saturation contrast problem using such a structure for the trajectory. Second we analyze bang-exceptional extremals in the non-saturation contrast problem, wherein the constraint that one spin reaches a magnetization of zero at the final time is removed. We develop a numerical scheme to search for solutions with a fixed contrast. The idea is to integrate our system backward along an exceptional arc from a terminal position representing the magnetization vectors for the pair of spin that produces a target contrast, requiring neither of the spins to be at zero magnetization. The difficulty lies in the fact that this exceptional arc integrated backward does not necessarily intersect a bang arc, and so would not produce a bang-exceptional extremal. A search determines the minimum distance of the exceptional arc from a bang arc, after which we apply the forward algorithm developed for the saturated case. The final result displays a slightly improved contrast and a control of shorter duration with respect to the saturation contrast problem. A very interesting observation is that the solution provided by our exhaustive algorithm in the non-saturated case is very similar to the solution of the saturated case. This similarity suggests that the saturation contrast problem is a good approximation of the general (i.e., not necessarily saturated) contrast problem and that by relaxing the saturated constraint the gain is not significant. A forthcoming work is to analyze other types of extremals in the non-saturated case to confirm this observation or prove that other strategies might be valuable.

The outline of this paper is as follows: in Section 2 we give the problem statement and outline recent work on the problem. We then apply the maximum principle to this problem in Section 3. In the final section, we describe a numerical algorithm for resolution of bang-exceptional contrast, and present the results of this algorithm.

2 Problem Statement

The contrast problem is introduced in detail in [Bonnard *et al.*, 2012], and the reader can find an introduction to the problem in a physical framework in [Lapert *et al.*, 2010b]. We here repeat only the main definitions in the control theory framework necessary to our work.

2.1 Bloch Equations

We consider a pair of non-interacting spins that are controlled by the same magnetic control field. The control is a bounded measurable function denoted by $u = (u_x, u_y)$ with $|u| \leq 2\pi$. Each spin particle is modeled by a magnetization vector, and the two spins have different relaxation parameters. After some normalization, the dynamics of the magnetization of the uncoupled spins can be written as a pair of Bloch equations. More precisely, if we denote by $q_i = (x_i, y_i, z_i)$ the magnetization vector of spin i, $i = 1, 2$, we have:

$$\begin{aligned} \dot{x}_i &= -\Gamma_i x_i + u_y z_i, \\ \dot{y}_i &= -\Gamma_i y_i - u_x z_i, \\ \dot{z}_i &= \gamma_i(1 - z_i) + (u_x y_i - u_y x_i), \end{aligned} \tag{1}$$

where Γ_i, γ_i are the substances parameters determined by the relaxation times. The system (1) can be written as an affine control system $\dot{q}_i = F^i(q, u) = F_0^i(q) + F_1^i(q)u$. In this paper we focus on the contrast between deoxygenated and oxygenated blood: $\gamma_1 = 1/(32.3 \cdot 1.35) = 0.023, \Gamma_1 = 1/(32.3 \cdot 0.05) = 0.619, \gamma_2 = \gamma_1, \Gamma_2 = 1/(32.3 \cdot 0.2) = 0.155$. This choice is motivated by its applicability to medical imaging. To summarize, we have an affine control system:

$$\dot{q}(t) = F(q(t), u(t)) = F_0(q(t)) + F_1(q(t))u$$

where $q = (q_1, q_2)$, and $F_j = (F_j^1, F_j^2)$. The initial value of the two spins is fixed the north pole: $q_i(0) = (0, 0, 1)$, $i = 1, 2$, the equilibrium of the uncontrolled system. We restrict ourselves in this paper to the case when the magnetic control field is real, this is equivalent to assume that $u_y \equiv 0$. As a consequence we can consider a 4-dimensional system with $q_i = (y_i, z_i)$, and write u_x simply as u. We then have

$$\begin{aligned} F_0^i &= (-\Gamma_i y_i, \gamma_i(1 - z_i))^T \\ F_1^i &= (-z_i, y_i)^T. \end{aligned}$$

2.2 Contrast Problem

The problem statement of the contrast problem is as follows: from the initial configuration $q(0) = (q_1(0), q_2(0)) = ((0, 1), (0, 1))$, find a control u defined on $[0, T]$ that maximizes $||q_1(T)| - |q_2(T)||$.

A sub-case of the contrast problem known as the *saturation contrast problem* is: from the initial configuration $q(0) = (q_1(0), q_2(0)) = ((0, 1), (0, 1))$, find a control u defined on $[0, T]$ with $q_1(T) = 0$ that maximizes $|q_2(T)|$ (which is the contrast since q_1 = 0) or, identically, minimizes $c(q(T)) = -|q_2(T)|^2$.

Results on the saturation contrast problem can be found in a series of articles, see [Bonnard *et al.*, 2012] and references therein. More precisely, a current approach is the use of differential geometric optimal control software. In [Bonnard and Cots, 2012], the authors use HAMPATH [Caillau, Cots and Gergaud, 2010] for this purpose. In this work, the authors consider controls of the form bang-singular, in the non-exceptional case. Such a control is determined by the switching time and the initial value of the adjoint vector $p(\cdot)$. The authors define a homotopy and a multiple shooting method to determine a locally optimal control. The homotopy is used on the augmented cost functional:

$$c(x(t_f)) + (1 - \lambda) \int_0^{t_f} |u|^{2-\lambda} dt, \quad \lambda \in [0, 1].$$

With $\lambda = 0$, the added convexity of the problem allows local minima to be easily found. As this parameter is taken from 0 to 1, the solution approaches a solution of the true problem. The final time is fixed to $t_f = 1.1 \times \min t_f$, where $\min t_f$ is the minimum time required for the first spin to reach the origin [Bonnard, Chyba and Sugny, 2009]. The result of this method is a control meeting the terminal condition $q_1(t_f) = 0$, with contrast $|q_2(t_f)| = 0.449$.

In the experimental setting, the apparatus consists of two vertical test tubes, a smaller tube placed inside of a larger one, containing the fluids to be imaged on a horizontal cross-section. The resulting image is of two concentric circles, each colored according to the modulus of the substance's magnetization. In the theoretical setting we assume that the magnetization is uniform throughout a substance. With this presentation, the contrast of the method described above is shown in Figure 1.

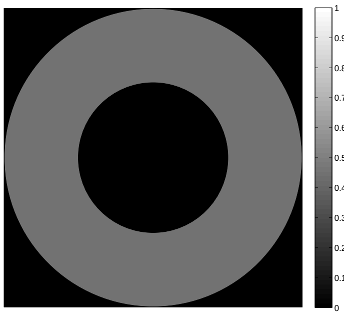

Figure 1. Contrast of 0.449 produced by current methods in the saturation contrast problem. The first spin (inner circle) is at the origin and the second spin (outer circle) is at a radius of 0.449.

In this paper we analyze extremals of the form bang-exceptional singular to complement this prior study. Moreover we expand our search to not only the saturation case but the general contrast problem.

3 First Order Necessary Conditions

The maximum principle [Pontryagin *et al.*, 1962] provides first order necessary conditions for a control to be optimal. See [Bonnard *et al.*, 2012] for more details on its application to the contrast problem, we here only recall the statement. Denote the final time as T and let us define the Hamiltonian function $H(q,p,u) = \langle p, F(q,u)\rangle$, a Mayer-type cost $c(q(T))$, and a terminal set as $\{q \mid \psi(q) = 0\}$. By the maximum principle, an optimal control has to satisfy the following necessary optimality conditions:

(i) $\dot{q} = \frac{\partial H}{\partial p}(q,p,u), \quad \dot{p} = -\frac{\partial H}{\partial q}(q,p,u)$
(ii) $H(q,p,u) = \max_{|v|\le M} H(q,p,v)$
(iii) $\psi(q(T)) = 0$
(iv) $p(T) = p_0 \frac{\partial c}{\partial q} + \delta^T \frac{\partial \psi}{\partial q}$, where $\delta^T \in \mathbb{R}^k$ and $p_0 \le 0$

A pair (q,p) which satisfies the maximum principle, in the sense just stated, is called an *extremal*. We refer the reader to [Bonnard and Chyba, 2003] for more details about bang arcs, singular arcs, and singular surfaces.

A direct application to the saturation contrast imaging problem gives $\psi(q_1(T)) = q_1(T) = (0,0)$ and splitting $p = (p_1,p_2)$, $p_2(T) = -2p_0 q_2(T)$, $p_0 \le 0$, since $c(q) = -|q_2|^2$ in the contrast problem. In the normal case $p_0 \ne 0$, we normalize by setting $p_0 = -\frac{1}{2}$.

In the general (non-saturation) contrast problem, the terminal constraint $\psi(q)$ is removed and by assuming that $|q_2(T)| > |q_1(T)|$, (swapping indices as necessary) we have $\phi(q) = -(|q_2| - |q_1|)$. Thus $p(T) = -2p_0 q(T)$, and again we normalize $p_0 = -\frac{1}{2}$.

In both cases, the optimal control problem can be mainly reduced to the analysis of the so-called singular trajectories since the optimal solution is a concatenation of a sequence of bang-singular arcs. More precisely, in both contrast problems the Hamiltonian function is given by:

$$
\begin{aligned}
H(q,p,u) &= p_{y_1}(-\Gamma_1 y_1 - u z_1) \\
&+ p_{z_1}(\gamma_1(1-z_1) + u y_1) + p_{y_2}(-\Gamma_2 y_2 - u z_2) \\
&\qquad + p_{z_2}(\gamma_2(1-z_2) + u y_2).
\end{aligned}
$$

The Hamiltonian function can also be written $H = \langle p, F_0\rangle + u\langle p, F_1\rangle$ where $F_0 = (F_0^1, F_0^2)$ and $F_1 = (F_1^1, F_1^2)$. The maximization condition (ii) implies that if $\langle p, F_1\rangle$ does not vanish on a given interval, u takes either its maximum or minimum value. In such a case the control is called *bang*, and the resulting trajectory is a *bang arc*. If however $\langle p, F_1\rangle = 0$ on an non-empty time interval, the control is called *singular* and its value is computed by other means.

The vector fields F_0 and F_1, and their respective Lie brackets up to length three play a major role in the calculation of the singular control. They are given by

$$
F_0 = \begin{pmatrix} -\Gamma_1 y_1 \\ \gamma_1(1-z_1) \\ -\Gamma_2 y_2 \\ \gamma_2(1-z_2))^T \end{pmatrix} \quad F_1 = \begin{pmatrix} -z_1 \\ y_1 \\ -z_2 \\ y_2 \end{pmatrix}
$$

$$
[F_0, F_1] = \begin{pmatrix} \gamma_1 - \delta_1 z_1 \\ -\delta_1 y_1 \\ \gamma_2 - \delta_2 z_2 \\ -\delta_2 y_2 \end{pmatrix}
$$

$$
[F_1, [F_0, F_1]] = \begin{pmatrix} 2y_1\delta_1 \\ \gamma_1 - 2\delta_1 z_1 \\ 2y_2\delta_2 \\ \gamma_2 - 2\delta_2 z_2 \end{pmatrix}
$$

$$
[F_0, [F_0, F_1]] = \begin{pmatrix} \gamma_1(\delta_1 - \Gamma_1) - \delta_1^2 z_1 \\ \delta_1^2 y_1 \\ \gamma_2(\delta_2 - \Gamma_2) - \delta_2^2 z_2 \\ \delta_2^2 y_2 \end{pmatrix}
$$

where $\delta_i = \gamma_i - \Gamma_i$.

Given the fact that the optimal solution is a concatenation of bang-singular arcs, we study a specific problem here: what is the highest contrast attainable by a control of the form bang-exceptional? First we analyze each component of such a control in detail.

3.1 Bang Arcs in the Contrast Problem

Due to the symmetry of the system about the z-axis we restrict our discussion to arcs with $u = +2\pi$ (indeed, if the initial point of an arc lies on the z-axis, the bang arcs produced by $\pm 2\pi$ are symmetric about the z-axis), and starting at the north pole $q(0) = ((0,1),(0,1))$. From the maximum principle the spin's dynamics for a bang arc associated to $u = +2\pi$ is given by

$$\begin{pmatrix}\dot{y}_1\\ \dot{z}_1\\ \dot{y}_2\\ \dot{z}_2\end{pmatrix} = \begin{pmatrix}-\Gamma_1 y_1 - 2\pi z_1\\ \gamma_1(1-z_1) + 2\pi y_1\\ -\Gamma_2 y_2 - 2\pi z_2\\ \gamma_2(1-z_2) + 2\pi y_2\end{pmatrix}$$

with corresponding adjoint dynamic

$$\begin{pmatrix}\dot{p}_{y_1}\\ \dot{p}_{z_1}\\ \dot{p}_{y_2}\\ \dot{p}_{z_2}\end{pmatrix} = \begin{pmatrix}\Gamma_1 p_{y_1} - 2\pi p_{z_1}\\ \gamma_1 p_{z_1} + 2\pi p_{y_1}\\ \Gamma_2 p_{y_2} - 2\pi p_{z_2}\\ \gamma_2 p_{z_2} + 2\pi p_{y_2}\end{pmatrix}$$

Notice that for our set of parameters the projection of a solution onto a plane (y_i, z_i) is dominated by a rotation (the $\dot{y}_i = -2\pi z_i, \dot{z}_i = 2\pi y_i$ component) since the 2π coefficient of these terms dominates the Γ_i, γ_i coefficients of the other terms, and the same can be said for the (p_{y_i}, p_{z_i}) pairs as well.

For our parameter values the solution for a bang arc starting at the north pole is given by

$$\begin{aligned} y_i(t) &= -\alpha_i^1 + e^{-\mu_i t}(\alpha_i^1 \cos(\omega_i t) - \alpha_i^2 \sin(\omega_i t))\\ z_i(t) &= \beta_i + e^{-\mu_i t}(\zeta_i^1 \cos(\omega_i t) + \zeta_i^2 \sin(\omega_i t)) \end{aligned} \tag{2}$$

for the state, and

$$p_i(t) = P_i(t) p_i(0)$$

for the adjoint, where $P_i(t) = \rho_i e^{\mu_i t} P_i'(t)$ and $P_i'(t)$ is

$$\begin{pmatrix}\sigma_i^1 \cos(\omega_i t) + \sigma_i^2 \sin(\omega_i t) & -\sigma_i^3 \sin(\omega_i t)\\ \sigma_i^3 \sin(\omega_i t) & \sigma_i^1 \cos(\omega_i t) - \sigma_i^2 \sin(\omega_i t)\end{pmatrix}$$

where $p_i(0)$ is the initial value of the adjoint vector at the north pole. The above coefficients are $\alpha_1^1 = 3.65 \times 10^{-3}$, $\alpha_1^2 = 1.001$, $\beta_1 = 3.60 \times 10^{-4}$, $\zeta_1^1 = 0.999$, $\zeta_1^2 = 0.0511$, $\mu_1 = 0.321$, $\rho_1 = 6.34 \times 10^{-3}$, $\sigma_1^1 = 157.74$, $\sigma_1^2 = 7.49$, and $\sigma_1^3 = 157.91$, $\omega_1 = 6.276$; and $\alpha_2^1 = 3.65 \times 10^{-3}$, $\alpha_2^2 = 1$, $\beta_2 = 8.99 \times 10^{-5}$, $\zeta_2^1 = 0.999$, $\zeta_2^2 = 0.0141$, $\mu_2 = 0.0888$, $\rho_2 = 6.33 \times 10^{-3}$, $\sigma_2^1 = 157.90$, $\sigma_2^2 = 1.65707$, $\sigma_2^3 = 157.91$, and $\omega_2 = 6.283$.

This analytic expression will be useful in our numerical algorithm to find concatenations of bang and exceptional arcs. The evolution of the adjoint vector will allow us to verify that the sign of $\langle p, F_1\rangle$ does not change during a bang arc.

3.2 Exceptional Singular Arcs in the Contrast Problem

Definition 1. *For system* (2.1)*, an extremal pair* (q, p) *is called* singular *if* $\langle p, F_1\rangle = 0$ *is satisfied almost everywhere along the extremal. If additionally* $\langle p, F_0\rangle = 0$ *is satisfied, it is called* exceptional. *An* exceptional arc *is a system trajectory under an exceptional singular control.*

The following lemma provides the expression for an exceptional control as a feedback in terms of the state variable [Bonnard and Chyba, 2003].

Lemma 1. *For a Mayer-type optimal control problem such as the contrast problem with* $\dot{q} = F_0 + uF_1$, $q \in \mathbb{R}^4$*, an exceptional singular control is calculated by*

$$u_s = -\frac{D'(q)}{D(q)}$$

where

$$\begin{aligned} D' &= \det(F_0, F_1, [F_1,F_0], [[F_1,F_0],F_0])\\ D &= \det(F_0, F_1, [F_1,F_0], [[F_1,F_0],F_1]), \end{aligned}$$

outside of $D(q) = 0$.

In an equivalent way, outside $D(q) = 0$ the exceptional control is given by

$$u_s = \delta_3(q)$$

where $\delta_3(q)$ is the component of $[[F_1,F_0],F_0]$ in the basis $ad^2_{F_0}F_1 = F_0, F_1, [F_1,F_0], [[F_1,F_0],F_1]$,

$$ad^2_{F_0}F_1 = \delta_1 F_0 + \delta_2 F_1 + \delta_3 [F_1,F_0] + \delta_4 [[F_1,F_0],F_1]$$

The components D and D' are degree four polynomials in the y_i, z_i, and for our parameter values they are

$$\begin{aligned} D(q) = &-1.12 \times 10^{-5} y_1 + 1.12 \times 10^{-5} y_2\\ &+ 1.79 \times 10^{-4} y_1 z_1 + 5.69 \times 10^{-5} y_2 z_1\\ &- 6.32 \times 10^{-4} y_1 z_2 + 1.69 \times 10^{-4} y_2 z_2\\ &- 6.69 \times 10^{-3} y_1^2 y_2 + 3.20 \times 10^{-3} y_1 y_2^2\\ &- 6.81 \times 10^{-5} y_2 z_1^2 - 9.43 \times 10^{-3} y_1 z_1 z_2\\ &+ 1.88 \times 10^{-3} y_2 z_1 z_2 + 6.43 \times 10^{-4} y_1 z_2^2\\ &+ 6.24 \times 10^{-2} y_1 y_2^2 z_1 - 5.52 \times 10^{-3} y_1^2 y_2 z_2\\ &- 2.05 \times 10^{-3} y_2 z_1^2 z_2 + 9.25 \times 10^{-3} y_1 z_1 z_2^2 \end{aligned}$$

and

$$\begin{aligned}D'(q) = &-3.02\times 10^{-4}y_1^2 + 3.58\times 10^{-4}y_1y_2\\ &-5.72\times 10^{-5}y_2^2 - 7.90\times 10^{-4}z_1z_2\\ &+6.39\times 10^{-4}z_1^2 + 1.51\times 10^{-4}z_2^2\\ &-1.46\times 10^{-3}y_1y_2z_1 + 2.39\times 10^{-3}y_1y_2z_2\\ &-5.20\times 10^{-3}y_1^2z_2 + 2.55\times 10^{-3}y_2^2z_1\\ &-0.013z_1^2z_2 + 3.54\times 10^{-3}z_1z_2^2\\ &-0.258y_1y_2z_1z_2 + 9.90\times 10^{-3}y_1^2y_2^2\\ &+0.139y_1^2z_2^2 + 0.139y_2^2z_1^2\\ &+9.89\times 10^{-3}z_1^2z_2^2\end{aligned}$$

Notice that associated to the exceptional flow defined by the integral curves of the vector field $F_0(q) + u_s(q)F_1(q)$ is a one dimensional foliation of the Bloch balls. Additionally it can be verified that the north pole is a singularity for the exceptional flow since at $q = ((0,1),(0,1))$ both D and D' are 0.

4 Second Order Necessary Conditions

The concept of a conjugate point is related to second-order optimality conditions—a trajectory is locally optimal prior to a conjugate point, and therefore it plays an important role in the study of optimal synthesis. We will apply the theory derived in [Bonnard, Caillau and Trélat, 2007] to compute the conjugate points along the exceptional arcs since in this situation the exceptional control is derived as a smooth function and therefore exceptional extremals are smooth.

Definition 2. *Let $\hat{H}(q,p) = \langle p, F(q,u)\rangle$ where u is the exceptional singular control. Let $z = (q,p)$ be the reference extremal defined on $[0,T]$. The variational equation*

$$\delta\dot{z} = d\vec{\hat{H}}(z(t))\delta z$$

is called the Jacobi equation. A Jacobi field $J(t)$, a nontrivial solution $\delta z = (\delta q, \delta p)$, is said to be vertical at time t if $\delta q(t) = d\Pi_{z(t)}\delta z(t) = 0$, where Π is the canonical projection $(q,p)\mapsto q$.

Definition 3. *Define the exponential mapping for fixed $q(0) = q_0$ as the mapping $\exp_{q_0} : (t, p_0) \mapsto \Pi(z(t, z_0))$ where $z(\cdot)$ is the solution of $\hat{H}$ with initial condition $z_0 = (q_0, p_0)$, p_0 being normalized by $|p_0| = 1$. A time $t_c > 0$ is said to be geometrically conjugate to zero if the exponential mapping is not of maximal rank $(n-1)$ at $t = t_c$ and the associated point $q(t_c)$ is said to be geometrically conjugate to q_0.*

With these definitions, the conjugate point test is as follows. Taking a reference extremal of the exceptional dynamics, $\frac{dq}{dt} = F^s(q(t)) := F(q(t), u_s(t))$ where u_s is the exceptional singular control, the variational equation is $\frac{d\delta q}{dt} = \frac{\partial F^s}{\partial q}(q(t))\delta q$. We compute a single Jacobi field $J_0(t)$, denoting by δq_0 its projection on the q-space, which is a solution of the variational equation with initial condition $\delta q(0) = F_1(q(0))$. Then a conjugate point is characterized by $\delta q_0(t) \in \mathrm{span}\{F_0(q(t)), F_1(q(t))\}$, or equivalently,

$$\det[\delta q_0(t), F_0(q(t)), F_1(q(t)), \mathrm{ad}^2 F_1.F_0(q(t))] = 0. \tag{3}$$

This last description allows straightforward numerical calculation of conjugate points by singular value decomposition of the matrix in (3).

5 Bang-Exceptional Extremals

A *bang-exceptional extremal* is a concatenation of a bang and exceptional singular arc that is an extremal of the system. Due to the symmetry of the system, it is sufficient to consider only bang arcs with $u = +2\pi$.

The goal of this section is to determine the conditions to construct a bang-exceptional extremal starting from the north pole with no constraint on the final configuration for a given switching time t_1. This will be used in following sections for the saturation and the non-saturation contrast problem.

Denote $H_{F_i} = \langle p, F_i\rangle$, $i = 0,1$. By definition along an exceptional arc the Hamiltonian vanishes. Therefore to construct a bang-exceptional extremal on the time interval $[0,T]$ with switching time t_1, we must verify $H = H_{F_0} + uH_{F_1} = 0$ along the exceptional arc. On the interval $[0,t_1]$, we must have $\mathrm{sgn}\, H_{F_1} = 1$ almost everywhere so that $u \equiv +2\pi$ on this interval. Satisfying these conditions amounts to the proper choice of the adjoint vector $p(\cdot)$, or equivalently its value at a particular time. The switching time t_1 is fixed, then from equations (2) the state $q(t_1)$ of the two spins at t_1 is completely determined. Along an exceptional arc, the adjoint vector is uniquely determined (up to a scalar) by satisfying the conditions $H_{F_0} = H_{F_1} = \dot{H}_{F_1} = 0$ where $\dot{H}_{F_1} = \{H_{F_0}, H_{F_1}\} = \langle p, [F_i, F_j]\rangle$. This imposes that at the switching point we have

$$p(t_1) \in \ker\{F_0, F_1, [F_0, F_1]\}.$$

It determines $p(t_1)$ up to a nonzero scalar. We choose the normalization such that $p(t_1)$ is a unit vector with orientation so that the initial bang arc is $u = +2\pi$. The initial value of the adjoint vector is calculated from (3.1): $p_i(0) = P_i^{-1}(t_1)p_i(t_1)$. The bang-exceptional concatenation is now completely determined on $[0,T]$, indeed we have the first arc defined on $[0,t_1]$ and the junction conditions at t_1 to switch to an exceptional arc are met by our construction. Finally, to guarantee that the first arc is indeed a bang arc, it is necessary that $\mathrm{sgn}\, H_{F_1} = 1$ almost everywhere on $[0,t_1]$. Notably, this can fail for some choices of t_1. We illustrate this fact in Figure 2: for $t_1 = 0.45$, $H_{F_1} > 0$ on $(0,t_1)$, but this fails for $t_1 = 0.55$. Since the mapping $t \mapsto H_{F_1}$ is smooth, there are intervals of admissible and non-admissible switching times. This provides the single restriction in the construction of a bang-exceptional extremal: that the switching time must be admissible with respect to the value of H_{F_1} on $[0, t_1]$.

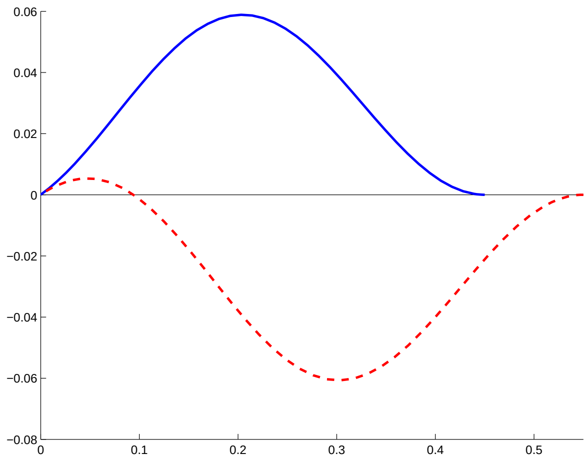

Figure 2. The component H_{F_1} of the Hamiltonian for switching times $t_1 = 0.45$ in solid blue, and $t_1 = 0.55$ in dashed red, showing that some switching times are not permissible for the construction of bang-exceptional arcs.

This construction will be used in the methods described below for the saturation and non-saturation contrast problems, which are mainly motivated by the lack of flexibility in the choice of a particular bang-exceptional arc (only the switching time is chosen) and the difficulty of predicting the behavior of the exceptional portion.

6 Results in the Saturation Problem

The constraint in the saturation contrast problem is to bring one of the spins to zero magnetization. The difficulty is to find switching times such that we have an admissible bang-exceptional trajectory and such that the saturation constraint is met. It is done numerically as described below.

From the one-parameter family of trajectories characterized by the switching time t_1, regions where the first spin passes through a neighborhood of the origin are identified. In such a region, a pair of times such that the trajectory crosses the y_1-axis on opposite sides of the origin is identified, and bisection is used to find t_1 such that $q_1(T) = 0$.

Among such solutions identified in this procedure, the extremal producing the highest contrast is given by the switching time $t_1 = 0.3858$, with final time $T = 8.9081$ and contrast $\|q_2(T)\| = 0.4272$. Along the exceptional arc, the first conjugate point is found at $t_c = 4.8776$, and therefore this extremal is not locally optimal in its entirety. The highest (non-saturation) contrast produced along this trajectory is 0.4738, occurring at time $t = 4.0376$. This result is illustrated in Figures 3 and 4, which show the state trajectory and associated control. We also note that this is an admissible switching time with respect to the sign of H_{F_1} on the bang arc. The components of the Hamiltonian along the extremal are shown in Figure 5. The contrast produced by this method is shown in Figure 11.

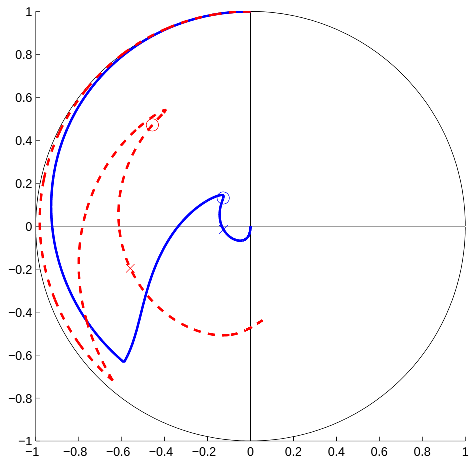

Figure 3. The state trajectory of the bang-exceptional arc of the saturation problem with $t_1 = 0.3858$. The spin q_1 is shown as a solid blue line, with q_2 as a dashed red line. The circle marks the point of highest contrast at $t = 4.0376$, which notably is not at the final time $T = 8.9081$. The conjugate point is marked with an $\times$.

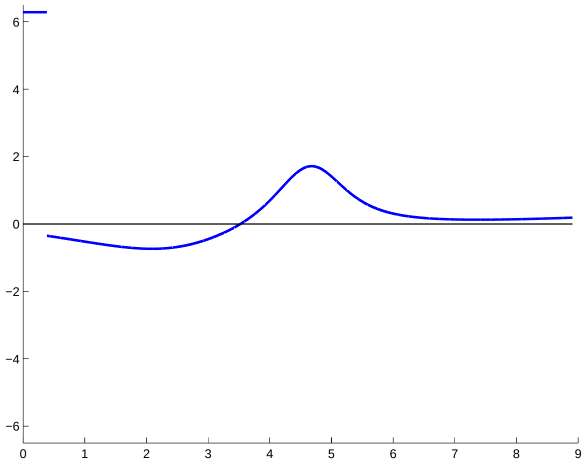

Figure 4. The control associated with the bang-exceptional arc of the saturation problem with $t_1 = 0.3858$.

7 Results in the Non-saturation Problem

In the non-saturation case there is no constraint on the final configuration for q. As a consequence a shooting method is impractical to use. Instead, we integrate backward from a set of final states for the spins with a target contrast, and attempt to find an intersection with

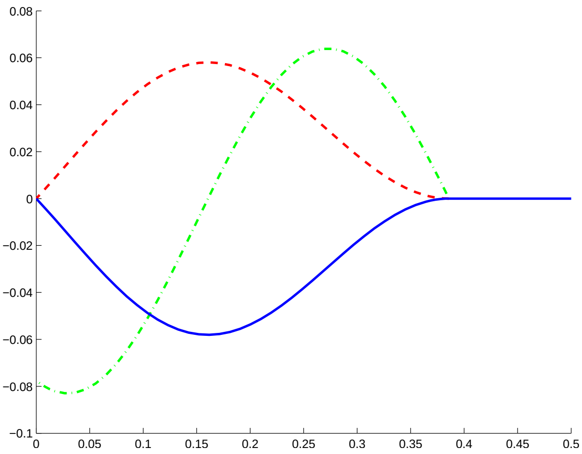

Figure 5. Components of the Hamiltonian for the bang-exceptional arc of the saturation problem with $t_1 = 0.3858$. The components are H_{F_0} in a dashed red line, uH_{F_1} in a solid blue line, and $\{H_{F_0}, H_{F_1}\}$ in a dot-dashed green line. All three of these are identically zero on the exceptional arc, after the switching time t_1.

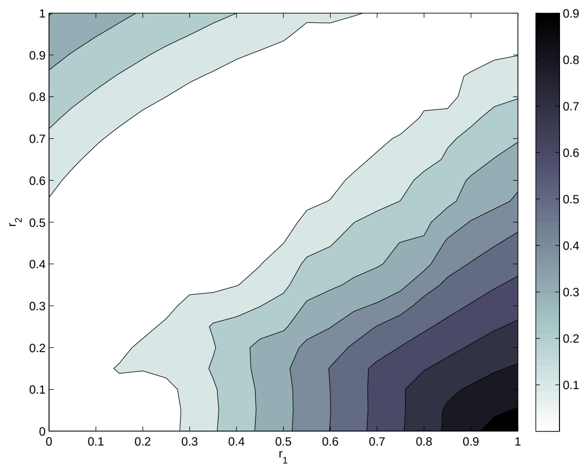

Figure 6. The minimum distance (value given by the color bar to the right) between a bang arc and an exceptional arc terminating at various radii r_1 and r_2.

a bang arc in order to construct a bang-exceptional arc with this contrast.

The set of final configurations $q(T) = (q_1(T), q_2(T))$ is parametrized using polar coordinates by $((r_1, \theta_1), (r_2, \theta_2))$, $r_i \in [0, 1]$, $\theta_i \in [0, 2\pi[$. We fix the contrast, $|r_1 - r_2|$ to a target value, and integrate the exceptional flow backward for a sufficiently long time duration. The bang arc departing from the north pole and associated to $u = +2\pi$ is computed on $[0, 20]$ which amounts to about 20 rotations around the origin. Given this exceptional arc and the bang arc we define the distance between them, $d((r_1, \theta_1), (r_2, \theta_2))$, as the smallest Euclidean distance between those two curves. The next step is to construct, using the algorithm described in Section 5, a bang-exceptional trajectory with the switching time such that we are on the bang arc at the point that is distance d from the backward integrated exceptional. Intuitively, the smaller the distance d is, the closer the achieved contrast will be to the target one.

On Figure 6, we display the distance function d between the bang arc $u = +2\pi$ starting at $((0, 1), (0, 1))$ and the exceptional arc integrated backward for various values of final states $q_1(T), q_2(T)$. The interval $[0, 2\pi[$ for the angles θ_i is discretized into 50 sub-intervals for our calculations. From this figure we identify the pairs of r_1 and r_2 that produce a small distance with a high contrast.

It can be observed that the choice of radii $r_1 = 0.1$, $r_2 = 0.6$ provides a good candidate for a high contrast and a small distance d (this is one chosen for illustration among many candidates that lead to the same solution). We fix these radii and then identify the θ_i that minimize the distance between the bang and the backward integrated exceptional arc, i.e., $\mathrm{argmin}_{\theta_1, \theta_2} d(r_1, \theta_1, r_2, \theta_2)$. First, all pairs in a discretization of pairs of θ_i are checked, as shown in Figure 7. There are two clear candidates that result from this search: $(0.859, 1.07)$ and $(2.30, 2.08)$; each belong to the interior of the two little islands that can be seen in the figure. The first corresponds to a switching time $t_1 = 0.596$, and the bang-exceptional arc with this switching time yields maximum contrast of 0.4840. A search in a neighborhood of t_1 for a switching time which produces a bang-exceptional arc with locally maximum contrast gives a refined $t_1' = 0.5939$ with contrast 0.4843 (this local maximum is identified clearly among nearby switching times). However this concatenation is not an extremal because the bang arc is not admissible in the sense that H_1 changes sign on $[0, t_1']$. The second candidate, after the same refinement, results in a switching time $t_1 = 0.4142$ and contrast 0.4845. The second choice is superior in terms of contrast and furthermore it is an extremal since the sign of H_{F_1} is constant along the bang trajectory. Thus, with an initial search among target contrasts of 0.5, we have achieved a realizable contrast of 0.4845.

The switching time $t_1 = 0.4142$ with contrast 0.4845 at $T = 5.5734$ is the highest contrast found by the method used here. By following the exceptional control past the final time, the first conjugate point at $t_c = 7.3565$ is located, showing the local optimality of this extremal. The state trajectory and associated control are shown in Figures 8 and 9, and the components of the Hamiltonian along the extremal are shown in Figure 10. Finally, we display the contrast produced by this method in Figure 11.

8 Conclusion

Future work will address the contrast attainable in the non-saturation case using different scenarios than bang-exceptional extremals. Aside from the possibility of increased contrast, another benefit of the non-saturation case is seen when repeated experiments are considered. In applications, successive images are

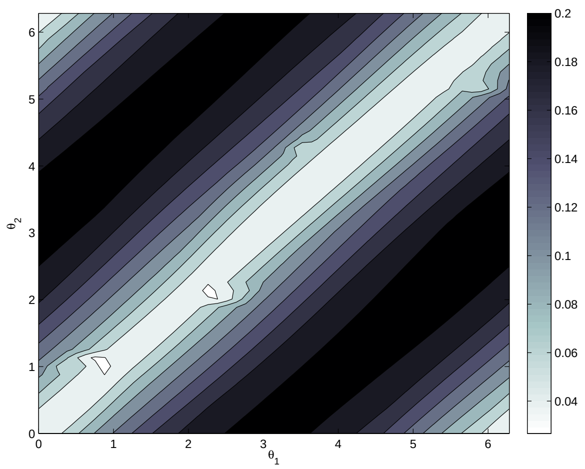

Figure 7. Minimum distance (value given on the color bar to the right) between a bang arc and an exceptional arc of the non-saturation problem terminating at radii $r_1 = 0.1$, $r_2 = 0.6$ for various θ_1 and θ_2.

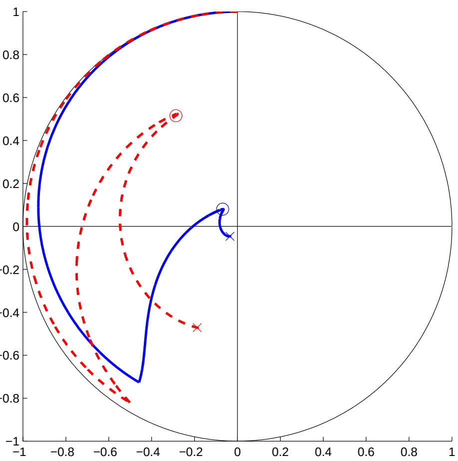

Figure 8. The state trajectory of the bang-exceptional arc of the non-saturation problem with $t_1 = 0.4142$. The spin q_1 is shown as a solid blue line, with q_2 as a dashed red line. The circle marks the point of highest contrast at $T = 5.5734$. For reference, the trajectory is continued past T until $t_c = 7.3565$ when the first conjugate point, marked with an $\times$ occurs.

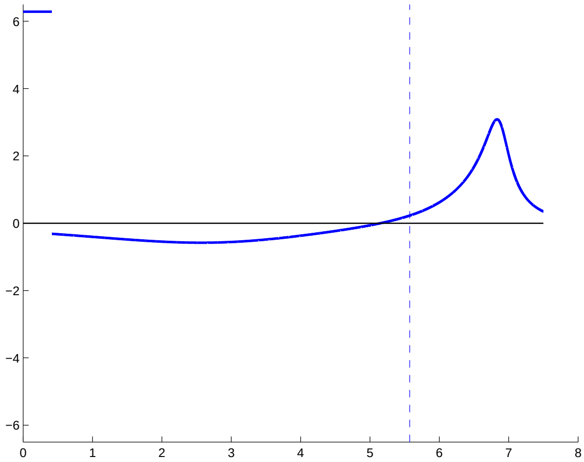

Figure 9. The control associated with the bang-exceptional arc of the non-saturation problem with $t_1 = 0.4142$. The dashed line marks the final time, $T = 5.5734$, when the highest contrast is reached along the trajectory. The control is shown up to the time of the first conjugate point for reference.

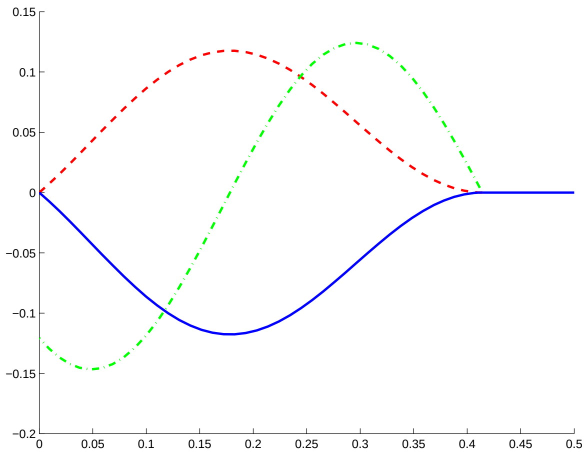

Figure 10. Components of the Hamiltonian for the bang-exceptional arc with $t_1 = 0.4142$. The components are H_{F_0} in a dashed red line, uH_{F_1} in a solid blue line, and $\{H_{F_0}, H_{F_1}\}$ in a dot-dashed green line. All three of these are identically zero on the exceptional arc, after the switching time t_1.

taken to separate the signal and noise, and so the system must return to equilibrium after the spins are controlled to a point ideal for imaging. This return trip has a relatively long duration compared to the time used to produce the contrast, and the length of this return trip is mostly influenced by the distance from the north pole in the z-direction, and thus in the saturation case the spin sent to the origin is the slowest to return to equilibrium. In the non-saturation case, both spins (possibly after rotation) are closer to the north pole than the origin, reducing the time of the return trip.

Acknowledgements

This work was supported by the National Science Foundation Division of Graduate Education, award #0841223 and the National Science Foundation Division of Mathematical Sciences, award #1109937.

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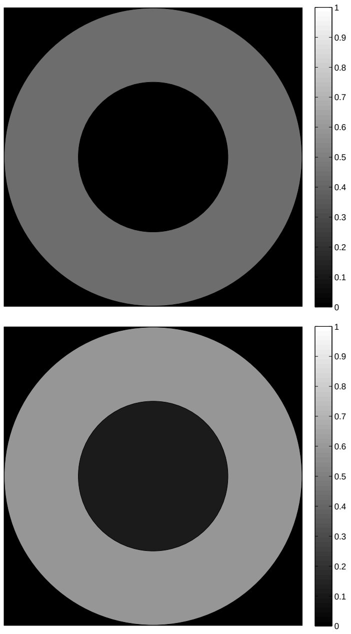

Figure 11. Top: contrast of 0.4272 produced by the bang-exceptional arc with $t_1 = 0.3858$ in the saturation contrast problem. The first spin (inner circle) is at a the origin and the second spin (outer circle) is at a radius of 0.4272. Bottom: contrast of 0.4548 produced by the bang-exceptional arc with $t_1 = 0.4142$ in the non-saturation contrast problem. The first spin (inner circle) is at a radius of 0.1058 and the second spin (outer circle) is at a radius of 0.5903.

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