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# Geometric and numerical methods in optimal control for the time minimal saturation in Magnetic Resonance Imaging

*DYNAMICS, CONTROL, and GEOMETRY*

In honor of Bronisław Jakubczyk's 70th birthday

12.09.2018 - 15.09.2018 | Banach Center, Warsaw

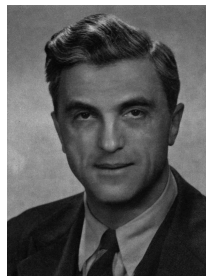
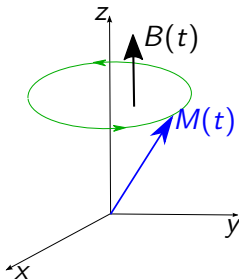
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# Magnetization vector

- **Bloch equation:**  $M$ : magnetization vector of the spin-1/2 particle in a magnetic field  $B(t)$ .

$$\dot{M}(t) = -\kappa M(t) \times B(t)$$



F. Bloch Nobel Prize (1952)

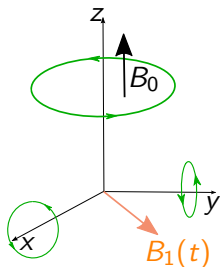
# Experimental model in Nuclear Magnetic Resonance

- **Two magnetic fields** : controlled field  $B_1(t)$  and a strong static field  $B_0$

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$$\begin{pmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{pmatrix} = \begin{pmatrix} -\Gamma M_x \\ -\Gamma M_y \\ -\gamma(M_0 - M_z) \end{pmatrix} + \begin{pmatrix} 0 & -\omega_0 & \omega_y \\ \omega_0 & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix}$$

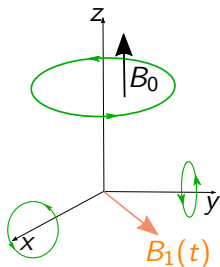


- $\Gamma, \gamma$  are parameters related to the observed species
- $\omega_0$  is fixed and associated to  $\mathbf{B}_0$
- $\omega_x, \omega_y$  are related to the controlled magnetic field  $B_1(t)$

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- $\Gamma, \gamma$  are parameters related to the observed species
  - $\omega_0$  is fixed and associated to  $\mathbf{B}_0$
  - $\omega_x, \omega_y$  are related to the controlled magnetic field  $B_1(t)$
- $M(t) \in S(O, |M(0)|)$ ,  
 $B_1 \equiv 0 \Rightarrow$  relaxation to the stable equilibrium  $M = (0, 0, |M(0)|)$ .

- Normalized Bloch equation in the *rotating frame*  $(\omega_0, (Oz))$

$$\dot{x}(t) = -\Gamma x(t) + u_y(t) z(t),$$

$$\dot{y}(t) = -\Gamma y(t) - u_x(t) z(t),$$

$$\dot{z}(t) = \gamma(1 - z(t)) - u_y(t) x(t) + u_x(t) y(t).$$

- $q = (x, y, z) = M/M(0)$  is the normalized magnetization vector,
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- $q = (x, y, z) = M/M(0)$  is the normalized magnetization vector,
  - $(u_x, u_y)$  is the control.
- Symmetry of revolution around  $(Oz)$ , we set:  $u_y = 0$  and we obtain the **planar control system**

$$\dot{y}(t) = -\Gamma y(t) - u(t) z(t),$$

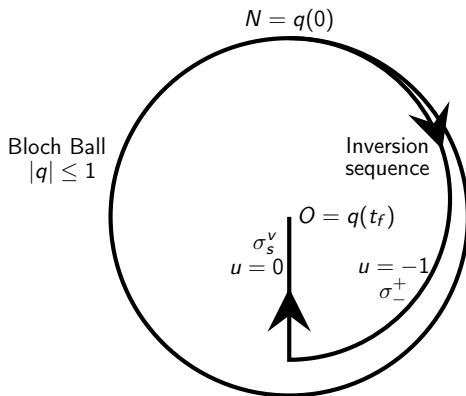
$$\dot{z}(t) = \gamma(1 - z(t)) + u(t) y(t),$$

and  $u = u_x$  is the control satisfying  $|u| \leq 1$ .



## Saturation of a single spin in minimum time

- **Aim.** Steer the North pole  $N = (0, 1)$  of the Bloch ball  $\{|q| \leq 1\}$  to the center  $O$  in minimum time.



The inversion sequence  $\sigma_-^+ \sigma_s^v$  is not optimal in many physical cases

- **Pontryagin Maximum Principle.**

- Pseudo-Hamiltonian:  $H(q, p, u) = p \cdot (F(q) + u G(q)) = H_F + u H_G$
- $u(\cdot)$  optimal  $\Rightarrow \exists p(\cdot) \in \mathbb{R}^2 \setminus \{0\}$ :

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$$

$$H(q(t), p(t), u(t)) = \max_{|v| \leq 1} H(q(t), p(t), v) = cst \geq 0$$

- Regular and bang-bang controls:  
 $u(t) = \text{sign}(H_G(q(t), p(t))), H_G(q(t), p(t)) \neq 0$
- Singular trajectories are contained in  $\{q, \det(G, [F, G])(q) = 0\}$ :

$$z = \gamma / (2\delta) = z_s(\gamma, \Gamma), \quad \delta = \gamma - \Gamma \quad \text{and} \quad y = 0.$$

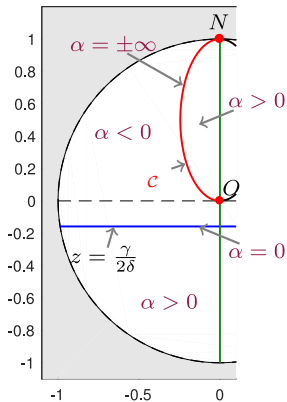
## Computations:

$$D'(q) + u D(q) = 0$$

with  $D = \det(G, [G, [F, G]])$  and  $D' = \det(G, [F, [F, G]])$ .

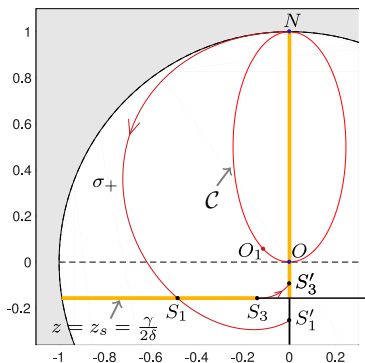
We obtain:

- $u_s = \gamma(2\Gamma - \gamma)/(2\delta\gamma)$  on the horizontal singular line.
- $u_s = 0$  on the vertical singular line



- Symmetry:  $u \leftarrow -u$  corresponds to  $y \leftarrow -y$
- Collinearity set:  
 $\mathcal{C} = \{q \mid \det(F, G)(q) = 0\}$
- Switching function:  
 $\Phi(t) = p(t) \cdot G(q(t))$  and outside the set  $\mathcal{C}$ ,  
 $\text{sign}(\dot{\Phi}(t)) = \text{sign}(\alpha(q)), \alpha(q) \neq 0$   
 where  $\alpha(q(t)) = \frac{\det(G, [F, G])(q)}{\det(G, F)(q)}$ .

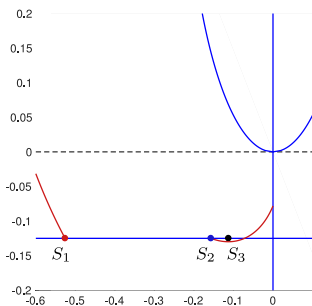
## Definition of the points $S_1, S_3$



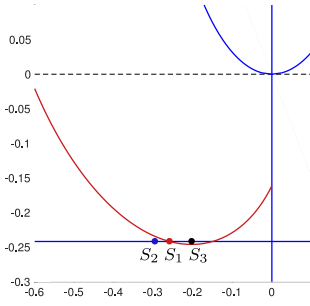
The singular trajectory  $q(\cdot)$  is called

- *Hyperbolic* if  $p(t) \cdot [G, [F, G]](q(t)) = \frac{\partial}{\partial u} \frac{d^2}{dt^2} \frac{\partial H}{\partial u}(q(t), p(t)) > 0$ .
- *Elliptic* if  $p(t) \cdot [G, [F, G]](q(t)) = \frac{\partial}{\partial u} \frac{d^2}{dt^2} \frac{\partial H}{\partial u}(q(t), p(t)) < 0$ .

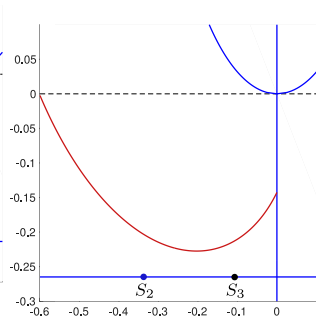
Optimal synthesis depends on the ratio  $\frac{\gamma}{\Gamma}$ .



**Case 1:**  $S_1$  exists and  $S_2 \in S_1 S_3$

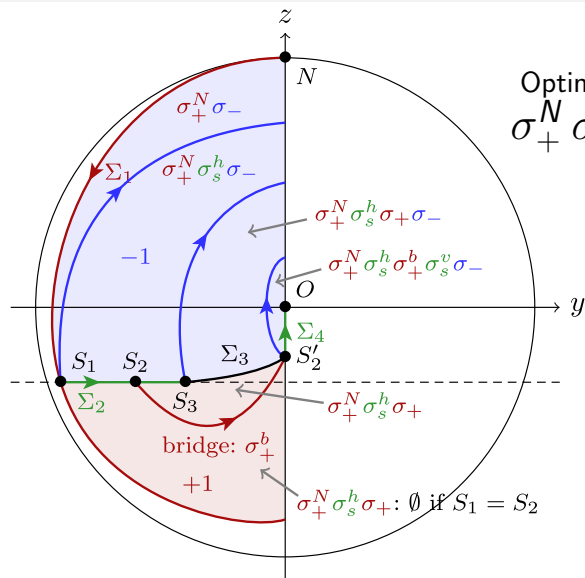


**Case 2:**  $S_1$  exists and  $S_2 \notin S_1 S_3$



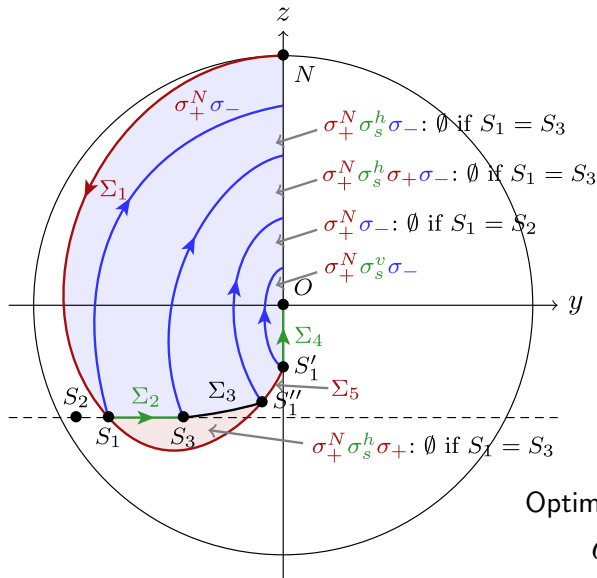
**Case 3:**  $S_1$  doesn't exist

# Case 1: $S_1$ exists and $S_2 \in S_1 S_3$

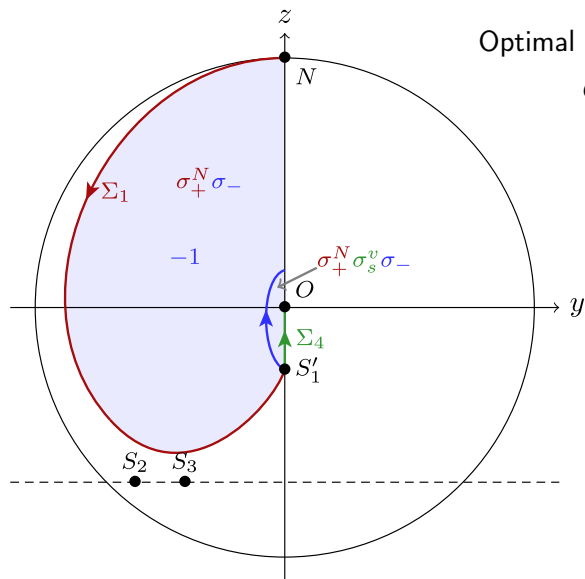


Optimal trajectory from  $N$  to  $O$ :  
 $\sigma_+^N \sigma_s^h \sigma_+^b \sigma_s^v$

## Case 2: $S_1$ exists and $S_2 \notin S_1 S_3$



### Case 3: $S_1$ doesn't exist



Optimal trajectory from  $N$  to  $O$ :

$$\sigma_+^N \sigma_s^v$$



## Theorem

*The time optimal trajectory for the saturation problem of 1-spin is of the form:*

$$\sigma_+^N \quad \underbrace{\sigma_s^h \quad \sigma_+^b}_{\text{empty if } S_2 \leq S_1} \quad \sigma_s^V$$

# Numerical validations using Moments/LMI techniques

*Aim:* Provide lower bounds on the global optimal time.

- Numerical times obtain with the `HamPath` software to validate :

Case	$\Gamma$	$\gamma$	$t_f$
$C_1$	$9.855 \times 10^{-2}$	$3.65 \times 10^{-3}$	42.685
$C_2$	$2.464 \times 10^{-2}$	$3.65 \times 10^{-3}$	110.44
$C_3$	$1.642 \times 10^{-2}$	$2.464 \times 10^{-3}$	164.46
$C_4$	$9.855 \times 10^{-2}$	$9.855 \times 10^{-2}$	8.7445

## Context

$$t_f = \inf_{u(\cdot)} T$$

$$\dot{x}(t) = f(x(t), u(t)),$$

$$x(t) \in X, \quad u(t) \in U, \quad x(0) \in X_0, \quad x(T) \in X_T$$

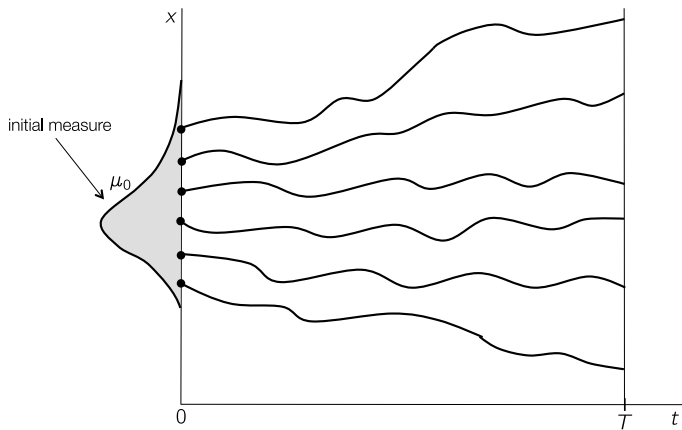
$X, U, X_0, X_T$  are subsets of  $\mathbb{R}^n$  which can be written as

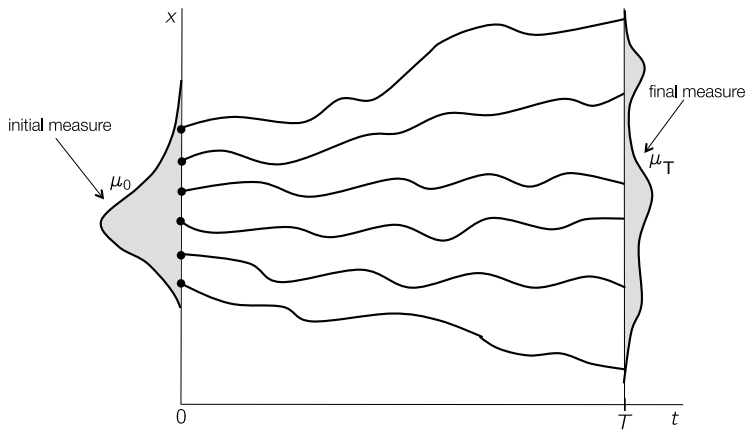
$$X = \{(t, x) : p_k(t, x) \geq 0, k = 0, \dots, n_X\}, \quad U = \{u : q_k(u) \geq 0, k = 0, \dots, n_U\}$$

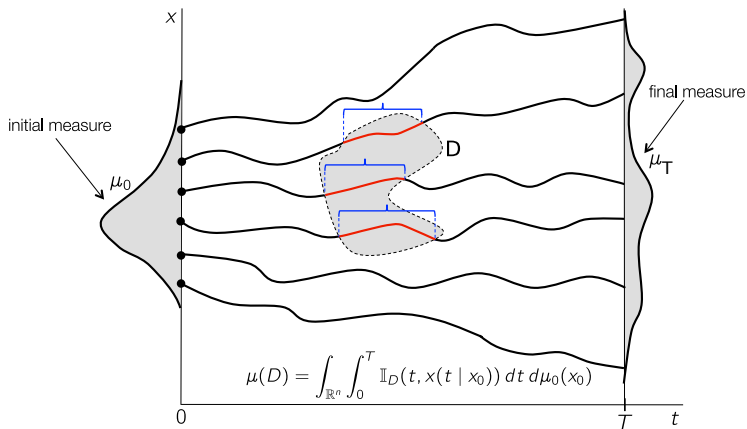
$$X_0 = \{x : r_k^0(x) \geq 0, k = 0, \dots, n_0\}, \quad X_T = \{(t, x) : r_k^T(t, x) \geq 0, k = 0, \dots, n_T\}$$

**Objective:** Compute  $\min_{u(\cdot)} T$  when  $f, p_k, q_k, r_k^0, r_k^T$  are polynomials and the above sets are compacts.

**Result:** [J. B. Lasserre, D. Henrion, C. Prieur, E. Trélat, 2008]  
Converging monotone nondecreasing sequence of lower bounds of  $t_f$ .







$$\int_0^T v(t, x(t)) dt = \int_0^T \int_X \int_U v(t, x) d\mu(t, x, u), \quad v \in C^0([0, T] \times X)$$

# Liouville's equation

Linear equation linking the measures  $\mu_0, \mu$  and  $\mu_T$ .

$$\int_{X_T} v(T, x) d\mu_T(x) - \int_{X_0} v(0, x) d\mu_0(x) = \int_{[0, T] \times Q \times U} \frac{\partial v}{\partial t} + \nabla_x \cdot f(x, u) d\mu(t, x, u)$$

for all test functions  $v \in \mathcal{C}^1([0, T] \times X)$ .

**Optimization over system trajectories**

$\Leftrightarrow$

**Optimization over measures satisfying Liouville equation.**

- **Relaxed controls:**  $u(t)$  is replaced for each  $t$  by a probability measure  $\omega_t(u)$  supported on  $U$ .
- **Relaxed problem:**

$$T_R = \min_{\omega} T$$

$$\text{s.t. } \dot{x}(t) = \int_U f(x(t), u) d\omega_t(u)$$

$$x(0) \in X_0, \quad x(t) \in X, \quad x(T) \in X_T$$



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- **Linear Problem on measures:**

$$d\mu(t, x, u) = dt d\delta_{x(t)}(x) d\omega_t(u) \in \mathcal{M}_+([0, T] \times X \times U)$$

$$T_{LP} = \min_{\mu, \mu_T, \mu_0} \int d\mu_T$$

$$\text{s.t. } \int \left( \frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} f(x, u) \right) d\mu$$

$$= \int v(\cdot, x_T) d\mu_T - \int v(0, x_0) d\mu_0, \quad \forall v \in \mathbb{R}[t, x],$$

$$\mu \in \mathcal{M}_+([0, T] \times X \times U), \quad \mu_T \in \mathcal{M}_+(X_T), \quad \mu_0 \in \mathcal{M}_+(X_0)$$

**Notation:**  $\alpha = (\alpha_1, \dots, \alpha_p) \in \mathbb{N}^p$ ,  $z = (z_1, \dots, z_p) \in \mathbb{R}^p$ . We denote by  $z^\alpha$  the monomial  $z_1^{\alpha_1} \dots z_p^{\alpha_p}$  and by  $\mathbb{N}_d^p$  the set  $\{\alpha \in \mathbb{N}^p, |\alpha|_1 = \sum_{i=1}^p \alpha_i \leq d\}$ .

**Moment of order  $\alpha$  for a measure  $\nu \in \mathcal{M}_+(Z)$ :**  $y_\alpha^\nu = \int z^\alpha d\nu(z)$ .

**Riesz linear functional:**  $l_{y^\nu} : \mathbb{R}[z] \rightarrow \mathbb{R}$  s.t.  $l_{y^\nu}(z^\alpha) = y_\alpha^\nu$ .

**Moment Matrix:**  $M_d(y^\nu)[i, j] = y_{i+j}^\nu, \forall i, j \in \mathbb{N}_d^p$ .

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Proposition (Putinar, 1993)

Let  $Z = \{z \in \mathbb{R}^p \mid g_k(z) \geq 0, k = 1, \dots, n_Z\}$ . The sequence  $(y_\alpha)_\alpha$  has a representing measure  $\nu \in \mathcal{M}_+(Z)$  if and only if

$$M_d(y) \succeq 0, \quad M_d(g_k y) \succeq 0, \quad \forall d \in \mathbb{N}, \forall k = 1, \text{Moment } \dots, n_Z.$$

## Moment Semidefinite Programming Problem:

$$T_{SDP} = \min_{y^\mu, y^{\mu T}} l_{y^{\mu T}}(1)$$

$$l_{y^\mu} \left( \frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} f(x, u) \right) = l_{y^{\mu T}}(v(\cdot, x_T)) - l_{y^{\mu_0}}(v(0, x_0)), \forall v \in \mathbb{R}[t, x],$$

$$M_d(y^\mu) \succeq 0, M_d(g_i y^\mu) \succeq 0, \forall i, \forall d \in \mathbb{N},$$

$$M_d(y^{\mu_0}) \succeq 0, M_d(g_i^0 y^{\mu T}) \succeq 0, \forall i \forall d \in \mathbb{N}$$

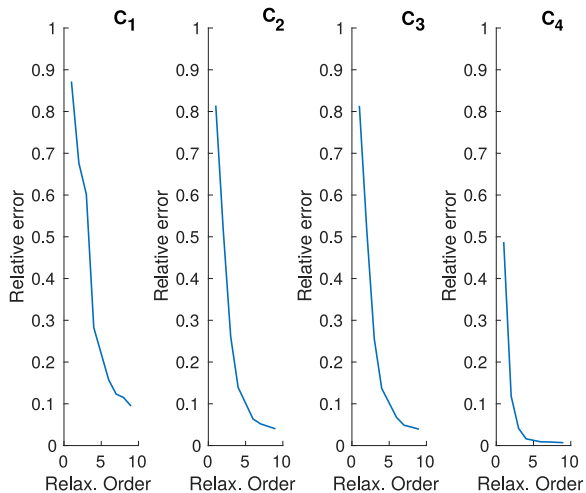
$$M_d(y^{\mu T}) \succeq 0, M_d(g_i^T y^{\mu T}) \succeq 0, \forall i \forall d \in \mathbb{N}$$

where  $g_i, g_i^0$  and  $g_i^T$  are polynomials defining the sets  $[0, T] \times X \times U, X_0$  and  $X_T$  respectively.

By truncating the sequences  $(y^\mu)$ ,  $(y^{\mu T})$  up to moments of length  $r$  (relaxation order), we have a **hierarchy of Semidefinite Programming Problems** and the lower bounds  $T_{sdp}^1, \dots, T_{sdp}^r, \dots$  of these problems satisfy:

$$t_f = T_{LP} = T_{SDP} \geq \dots \geq T_{sdp}^{r+1} \geq T_{sdp}^r \geq \dots \geq T_{sdp}^1.$$

# Numerical results on the saturation problem



- Generalization to an ensemble of pair of spins where Bloch equations are coupled and Inhomogeneities on the control field are taken into account.
- Contrast problem where we have two species to discriminate. Saturation of the first spin while the norm of the second spin is maximized.