Geometric Optimal Control Theory in spin systems

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Workshop quantum control IHP, Paris 2010

9/12/2010

Optimal control theory

A joint work between mathematicians, physicists and chemists.

- B. Bonnard, J.-B. Caillau, O. Cots, N. Scherbakova (IMB, Dijon)
- Group of S. J. Glaser, Y. Zhang, M. Braun (Chemistry department, Munich)
- M. Lapert (PhD, ICB, Dijon), E. Assémat (PhD, ICB, Dijon)

Rem.: Other results of our research project will be given in the conferences of B. Bonnard and S. J. Glaser

Quantum control

Application of tools of control theory to quantum dynamics.

- Photochemistry, femtosecond laser fields
- Condensed matter:
  - superconducting Josephson junction
  - cold atoms
- Nuclear Magnetic Resonance
  - liquid phase
  - solid phase

NMR in liquid phase

A promising field of applications.

- fundamental problems
- quantum computing
- NMR spectroscopy and imaging
(increase of the sensitivity and resolution of standard NMR techniques)

Advantages of the NMR domain

- Accuracy of the models, even in presence of dissipation
- low and finite-dimensional problems $\Longrightarrow$ geometry
- very good agreement between theory and experiment

Rem.: Such points are not true in Photochemistry

Optimal control in NMR

- Numerical approaches, e.g. the GRAPE and monotonic algorithms
- Geometric approach
  Ex.: Lie group methods for unbounded controls
  N. Khaneja, S. J. Glaser et al.

Our work: use of geometric optimal control theory to analyze NMR systems (Pontryagin Maximum Principle, indirect methods, analytic and numerical computations)

$\longrightarrow$ From mathematics (group of B. Bonnard) to experiments (group of S. J. Glaser)

The Bloch equations

$$\begin{pmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{pmatrix} = \begin{pmatrix} -\omega M_y + \omega_y M_z \\ \omega M_x - \omega_x M_z \\ \omega_x M_y - \omega_y M_x \end{pmatrix} + \begin{pmatrix} -M_x/T_2 \\ -M_y/T_2 \\ (M_0 - M_z)/T_1 \end{pmatrix} + RDE$$

with T_1, T_2 dissipation terms, ω: offset.

$$RDE = \frac{1}{M_0 T_r} \begin{pmatrix} -M_x M_z \\ -M_y M_z \\ M_x^2 + M_y^2 \end{pmatrix}$$

RDE: Radiation damping effect
T_r: Radiation damping constant.

Time-optimal control of a spin 1/2 particle

Saturation control problem in NMR:

North pole (equilibrium point) $\longrightarrow$ center of the Bloch ball.
Constraint: $|\omega| \leq \omega_{max}$, $\omega = 0$

Rem.: standard problem in NMR (remove the corresponding spin contribution).

Geometric analysis: symmetry of revolution $\Longrightarrow$ use of one control:

$$\dot{y} = -uz - y/T_2 - yz/T_r$$
$$\dot{z} = uy + (1-z)/T_1 + y^2/T_r$$

(y, z): reduced coordinates and $|u| \leq u_0$.

PMP and geometric analysis of the extremals: $u = \pm u_0$ or singular.
Rem.: structure depends on the dissipative parameters and on the bound of the control.

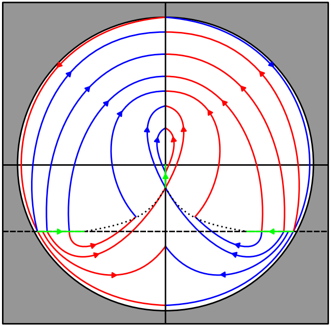


Figure: Schematic representation of the optimal synthesis

A concrete example

Ex.: The proton spins of H_2O in an organic solvent ($T_1 = 740$ ms, $T_2 = 60$ ms and $\omega_{max} = 32.3$ Hz)

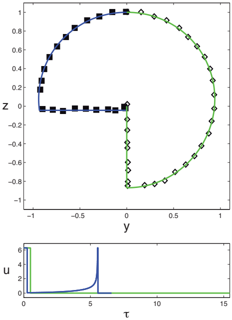
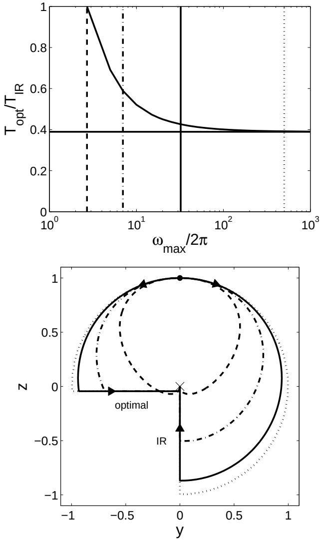


Figure: Time-optimal saturation of a spin 1/2 particle

Rem.: Comparison with the inversion recovery sequence: gain of 60% in the control duration.

Analysis in the unbounded case

Rem.: In the limit $\omega_{max} \to +\infty$, the structure is B-S-S.



Analytic computation in the unbounded case

Neglecting the duration of the first bang pulse, we get:

$$T_{opt} \rightarrow \frac{T_2}{2}\ln[1-\frac{2}{\alpha T_2}] + T_1 \ln[\frac{2T_1 - T_2}{2(T_1 - T_2)}]$$
$$T_{IR} \rightarrow T_1 \ln 2$$

Rem.: The physical limit of the control process is due to the dissipative parameters: Use of the dissipation to reach the target.

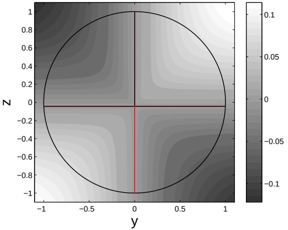


Figure: Contour plot of $d\dot{r}/d\theta$.

The GRAPE algorithm

Iterative algorithm to solve the optimal equations:

Cost: $\Phi_t = \sqrt{y^2 + z^2}$.

Fixed control duration T and bound ω_{max} on the control field.

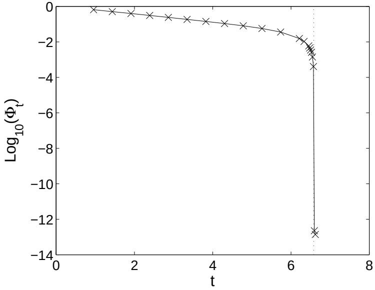


Figure: $\Phi_t \rightarrow 0$ when $T \rightarrow T_{geom}$.

Comparison of the different optimal solutions

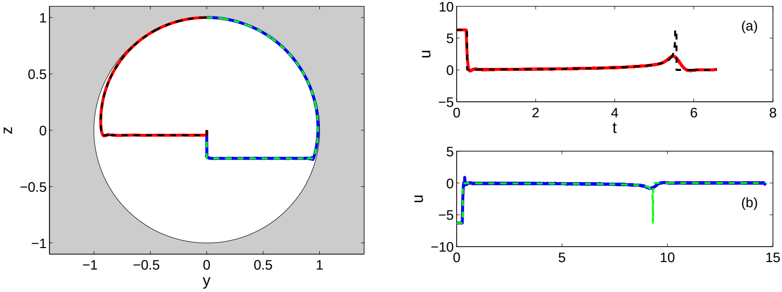


Figure: Smooth regularization of the geometric solution.

Results:

Geom.: $T_{geom.} = 6.58$, $\Phi_t = 5.34 \times 10^{-16}$

Grape: $T_{grape} = 6.60$, $\Phi_t = 2.25 \times 10^{-13}$.

Grape: $T_{grape} = 6.58$, $\Phi_t = 4.78 \times 10^{-6}$

Generalization to other systems

- Energy minimization problem (no singular extremal, a smooth solution)
- Radiation damping effect (smooth effect if $T_r > 0$).
- Optimal control of uncoupled spin systems
  $\longrightarrow$ Two spins with different offsets
  $\longrightarrow$ The contrast problem

The radiation damping effect

Experimental constraint: Inhomogeneous ensemble with different offsets.

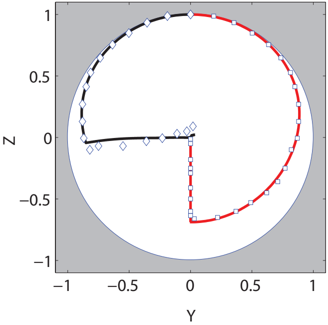


Figure: Optimal trajectory computed with the GRAPE algorithm.

Rem. Example of coupling between geometric methods and the GRAPE algorithm.

Two spins with different offsets: the symmetric case

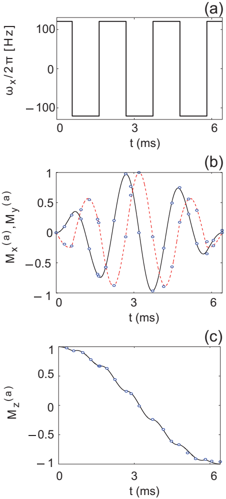
$$\begin{pmatrix} \dot{M}_{ax} \\ \dot{M}_{ay} \\ \dot{M}_{az} \end{pmatrix} = \begin{pmatrix} -\omega M_{ay} + \omega_y M_{az} \\ \omega M_{ax} - \omega_x M_{az} \\ \omega_x M_{ay} - \omega_y M_{ax} \end{pmatrix}$$

$$\begin{pmatrix} \dot{M}_{bx} \\ \dot{M}_{by} \\ \dot{M}_{bz} \end{pmatrix} = \begin{pmatrix} \omega M_{by} + \omega_y M_{bz} \\ -\omega M_{bx} - \omega_x M_{bz} \\ \omega_x M_{by} - \omega_y M_{bx} \end{pmatrix}$$

- One spin, one control: P. Mason, U. Boscain, JMP (2006)
  Optimal solution: bang-bang controls

Inversion of two spins

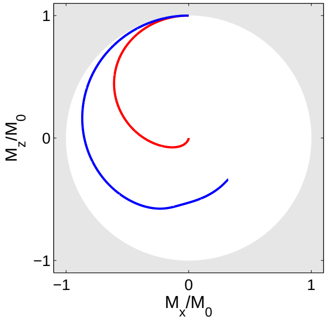
two spins with two controls $\Longleftrightarrow$ two spins with one control
Two proton spins of methyl acetate CH_3OOCCH_3.

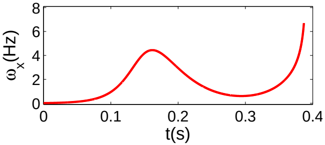


The contrast problem: the blood

Two uncoupled spins describing the oxygeneated/desoxygeneated blood

Structure of the optimal control: Bang-Singular





Conclusion

- Mathematical developments
  - Global understanding of the contrast problem
  - Classification of the different structure in the case of RDE
- Numerical applications
  - limit of indirect methods, continuation approach
  - coupling between GRAPE and geometric methods
- Experimental implementation of geometric solutions
  - Applications in NMR spectroscopy and NMR imaging.

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