Geometric Optimal Control Theory in spin systems

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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
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 $\rightarrow$ 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)

→ 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, \( \omega \): 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.
Saturation control problem in NMR:

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

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

Geometric analysis: symmetry of revolution \(\implies\) use of one control:

\[
\begin{align*}
\dot{y} &= -uz - y/T_2 - yz/T_r \\
\dot{z} &= uy + (1 - z)/T_1 + y^2/T_r
\end{align*}
\]

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

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](image)

**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.
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 \( \frac{d\dot{r}}{d\theta} \).
The GRAPE algorithm

Iterative algorithm to solve the optimal equations:

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

Fixed control duration $T$ and bound $\omega_{\text{max}}$ on the control field.

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

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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
  - Two spins with different offsets
  - The contrast problem
The radiation damping effect

**Experimental constraint:** Inhomogeneous ensemble with different offsets.

![Figure: Optimal trajectory computed with the GRAPE algorithm.](image)

**Rem.** Example of coupling between geometric methods and the GRAPE algorithm.
Two spins with different offsets: the symmetric case

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

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


**Optimal solution**: bang-bang controls
Inversion of two spins

two spins with two controls $\iff$ two spins with one control
Two proton spins of methyl acetate $\text{CH}_3\text{OOCCH}_3$. 

Figure: Dominique Sugny
Geometric Optimal Control Theory in spin systems
The contrast problem: the blood

Two uncoupled spins describing the oxygenated/desoxyngeated blood

**Structure of the optimal control**: Bang-Singular

![Optimization of the distance between the two spins](image-url)
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.
References

- B. Bonnard et al., IEEE Trans. AC 54, 2598 (2009)

page web:
http://icb.u-bourgogne.fr/OMR/DQNL/Sugny/professionel.html