Time-optimal control of a spin 1/2 particle with radiation damping and relaxation effects

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We apply recent developments in geometric optimal control to analyze the time minimum control problem of a spin 1/2 particle with radiation damping and relaxation effects. The dynamics of the system is governed by the Bloch equations in which nonlinear terms due to the radiation damping are included [5, 9]. This work can also be applied to the control of a dissipative two-level quantum system by two laser pulses [1]. The dynamics of the system is governed by the Lindblad equation. The nonlinear terms can be interpreted as the influence of a third unstable quantum level on the two-level system [7].

For a spin 1/2 particle, the dynamics of the system is described in terms of coordinates of the magnetization (M_x, M_y, M_z) . Introducing normalized coordinates q = (x, y, z), the system can be written as the following system of inhomogeneous differential equations :

$$\dot{x} = -\Gamma x + u_2 z - kxz
\dot{y} = -\Gamma y - u_1 z - kyz
\dot{z} = \gamma_- - \gamma_+ z + u_1 y - u_2 x + k(x^2 + y^2).$$
(1)

In (1), $\Lambda = (\Gamma, \gamma_{-}, \gamma_{+})$ is the set of dissipative parameters such that $\Gamma \geq \gamma_{+}/2 > 0$ and $\gamma_{+} \geq |\gamma_{-}|$ which describes the interaction of the spin system with the environment. Radiation damping effects are incorporated through the nonlinear terms depending on the parameter k. The control is composed of two normalized magnetic fields u_{1} and u_{2} which are assumed to be in resonance with the transition frequency of the spin system. The physical state belongs to the *Bloch ball*, $|q| \leq 1$, which is invariant for the dynamics considered.

The system can be written shortly as

$$\dot{q} = F_0(q) + u_1 F_1(q) + u_2 F_2(q) \tag{2}$$

and in order to minimize the effect of dissipation, we consider the time minimum control problem for which, up to a rescaling on the set of parameters Λ and k, the control bound is $|u| \leq 1$.

A first step in the analysis of such systems is contained in [8]. Assuming $u_2 = 0$, the problem can be reduced to the time-optimal control of a two-dimensional system with the constraint $|u_1| \leq 1$. Using cylindrical coordinates, one can also show that this case corresponds to the general case when the initial state is on the z-axis. For such a problem, the geometric optimal control techniques for single-input two-dimensional systems presented in [4] succeed to make the time-optimal synthesis for every values of parameters (Γ , γ_- , γ_+ , k). We present the different optimal syntheses that can be encountered [3] and some examples with experimentally realistic parameters in Nuclear Magnetic Resonance [6]. The role of the nonlinear parameter with respect to dissipative ones will be also analyzed.

In the bi-input case, we use geometrical and numerical techniques to conclude [2]. The maximum principle first selects extremal trajectories, candidates as minimizers and solutions of an Hamiltonian equation. A consequence of this analysis is the fact that, in the cases $(\gamma_{-} = 0, k = 0)$ and $(\Gamma = \gamma_{+} = \gamma_{-} = 0, k \neq 0)$, the extremal system is integrable. In the first case, if $\Gamma = \gamma_+$, the problem can be in addition reduced to a 2D-almost Riemannian problem on a two-sphere of revolution (Grushin model). We take advantage of this property to analyze the general integrable case ($\gamma_{-} = 0, k = 0$) using continuation methods on the set of parameters, while the analysis fits in the geometrical framework of Zermelo navigation problems. The same work can be done in the second case to study the effect of nonlinear terms. Secondly, having selected extremal trajectories, second-order conditions using the variational equation allow to determine first *conjugate points* forming the conjugate locus which are points where locally extremals cease to be optimal. We numerically determine the deformation of the conjugate locus with respect to the one of the Grushin model when the different parameters are varied.

The behavior of the controlled system in the general case will be also discussed from a numerical point of view. We determine the different asymptotic behaviors of the extremals according to the values of the dissipative and nonlinear parameters. We show that the extremals having a non periodic behavior have no conjugate point and remain locally optimal. In contract, periodic extremals have conjugate points which appear after the first oscillation of the extremal trajectory.

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References

- [1] B. BONNARD AND D. SUGNY, Optimal control theory with applications in space and quantum dynamics, submitted (2008).
- [2] B. BONNARD AND D. SUGNY, Time-Minimal control of dissipative twolevel quantum systems: The integrable case, to be publised in SIAM, J. Control and Opt. (2009).
- [3] B. BONNARD, M. CHYBA AND D. SUGNY, Time-Minimal control of dissipative two-level quantum systems: The generic case, submitted to IEEE Trans. Automatic Control (2009).
- [4] U. BOSCAIN AND B. PICCOLI, Optimal syntheses for control systems on 2-D manifolds, Springer-Verlag, Berlin, 2003.
- [5] J.-H. CHEN, B. CUTTING AND G. BODENHAUSEN, Measurement of radiation damping rate constants in nuclear magnetic resonance by inversion recovery and automated compensation of selective pulses, J. Chem. Phys., **112**, 6511 (2000).
- [6] N. I. GERSHENZON, K. KOBZAR, B. LUY, S. J. GLASER AND T. E. SKINNER, Optimal control design of excitation pulses that accomodate relaxation, J. Magn. Reson., 188, 330 (2007).
- [7] M. MIRRAHIMI AND P. ROUCHON, Singular perturbations and Lindblad-Kossakowski differential equations, to be publised in IEEE Trans. Automatic Control (2009).
- [8] D. SUGNY, C. KONTZ AND H. R. JAUSLIN, Time-optimal control of a two-level dissipative quantum system, Phys. Rev. A, 76, 023419 (2007).
- [9] W. S. WARREN, S. L. HAMMES AND J. L. BATES, Dynamics of radiation damping in nuclear magnetic resonance, J. Chem. Phys, 91, 5896 (1989).