

Time-optimal Control of independent Spin-1/2 Systems under Simultaneous Control

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Introduction

Time-optimal control (TOC) problems in quantum systems are ubiquitous and important in multiple applications. Because the inevitable noise from the environment degrades quantum states and operations over time, inducing quantum dynamics in minimal time utilizing TOC becomes a preferable choice.

Different mathematical approaches exist to obtain accurate TOC protocols, with the Pontryagin Maximum Principle (PMP) unifying some of them. However, independently of the method used, analytic solutions are rare in optimal control and theoretical calculations have to be complemented by difficult numerical experiments, with known problems of convergence to the actual solution. Previous works mainly consider time optimization with controls which address spin individually. However this is difficult in many experiments, and is a common scenario.

In this paper, we use the Pontryagin Maximum Principle (PMP) and a novel symmetry reduction technique, to obtain the optimal control laws for a system of two uncoupled spin-1/2 particles, under simultaneous control. Our symmetry reduction technique allows us to reduce the number of unknown parameters and to obtain analytic solutions. We implemented the TOC law using zero-field NMR, obtaining experimental fidelity as high as 99% and a gain of about 70% ~ 80% in the experiment time over previously known schemes.

Theory

The model is as follows: Two spin-1/2 particles with different gyromagnetic ratios are simultaneously subject to a global control field, as illustrated in Fig.1. The Hamiltonian is $H(\vec{u}) = \sum_{j=x,y,z} (\gamma_1 \sigma_j \otimes \mathbf{1}_2 + \gamma_2 \mathbf{1}_2 \otimes \sigma_j) u_j$.

The problem is to steer the identity evolution operator to any desired matrix under a constraint of the form $|\vec{u}| \leq D, D \neq 0$. We assume $\gamma_1 \neq \gamma_2$ (heteronuclear spins) which implies full controllability. The problem of optimal control can be stated as finding a function where H is the above Hamiltonian, so that the solution of the Schrodinger equation reaches $U_{f,1} \otimes U_{f,2}$ in minimum time.

The obtained TOC is illustrated in Fig.2. The main points of the protocol to find the optimal control field can be summarized as follows:

1. The PMP gives the form of optimal control $X = \sum_{j=x,y,z} -i(\sigma_j \otimes \mathbf{1} + \gamma_1 \mathbf{1} \otimes \sigma_j) u_j = X_1 \otimes \mathbf{1} + \gamma_1 \mathbf{1} \otimes X_1$, and trajectory, $U(t) = U_1(t) \otimes U_2(t)$. These are given by $X_1 = e^{At} P e^{-At}$, $U_1 = e^{At} e^{(P-A)t}$, $U_2 = e^{At} e^{(\gamma P - A)t}$, where A and P are constants in $su(2)$, parametrized therefore by 6 real parameters.

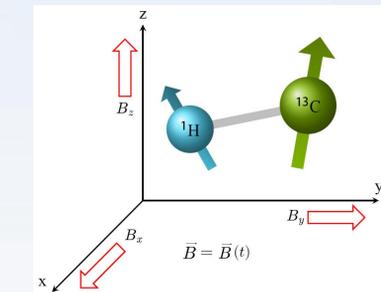


Fig.1

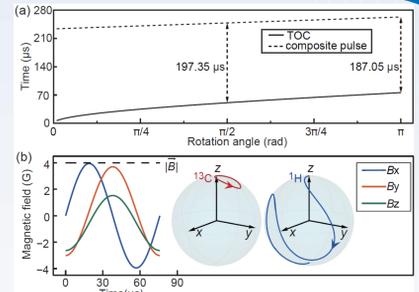


Fig.2

2. Symmetry reduction further reduces the number of unknown parameters to 3: If the control X and trajectory U are an optimal pair with optimal time t_{min} , then $\hat{Y}X\hat{Y}^\dagger$ and $\hat{Y}U\hat{Y}^\dagger$ is also an optimal pair with t_{min} (20). There are, $\omega, t_{min}, a(b)$, with $\sqrt{a^2 + b^2} = L$, 3 unknown parameters to be determined now (\hat{Y} is also unknown, but it can be determined if the above three parameters are known).

3. Find real values $\omega, t = t_{min}, a(b)$ (see point 1 above and (20)), such that

$$(e^{i\omega\sigma_z t} e^{(ia\sigma_z - ib\sigma_y - i\omega\sigma_z)t}, e^{i\omega\sigma_z t} e^{(i\gamma a\sigma_z - i\gamma b\sigma_y - i\omega\sigma_z)t})$$

is in the same class as $(U_{f,1}, U_{f,2})$ (Use Corollary 2.3), and t is minimum.

4. Repeat step 3 with the substitution: $(U_{f,1}, U_{f,2}) \rightarrow (-U_{f,1}, -U_{f,2})$. Choose the minimum time between these two cases, and the corresponding $\omega, t = t_{min}, a(b)$

5. Find $Y \in SU(2)$ such that

$$\pm U_{f,1} = Y^\dagger e^{i\omega\sigma_z t} e^{(ia\sigma_z - ib\sigma_y - i\omega\sigma_z)t} Y,$$

$$\pm U_{f,2} = Y^\dagger e^{i\omega\sigma_z t} e^{(i\gamma a\sigma_z - i\gamma b\sigma_y - i\omega\sigma_z)t} Y,$$

with $t = t_{min}$. The \pm sign is chosen according to step 4.

6. The optimal control is $X = X_1 \otimes \mathbf{1}_2 + \gamma_1 \mathbf{1}_2 \otimes X_1$ with $X_1 = Y^\dagger e^{i\omega\sigma_z t} (ia\sigma_z - ib\sigma_y) e^{-i\omega\sigma_z t} Y$.

Experiment

The experimental control magnetic field $\vec{B} = (B_x, B_y, B_z) := -2(u_x, u_y, u_z)$ ($|\vec{B}| = 2D$) are given by

$$B_x \approx 1.98D \sin(1.54D\gamma_1 t);$$

$$B_y \approx 0.18D - 1.68D \cos(1.54D\gamma_1 t);$$

$$B_z \approx -0.28D - 1.04D \cos(1.54D\gamma_1 t).$$

Its experimental implementation is illustrated in Fig.3

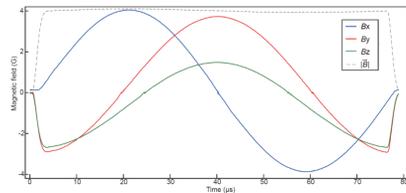


Fig.3

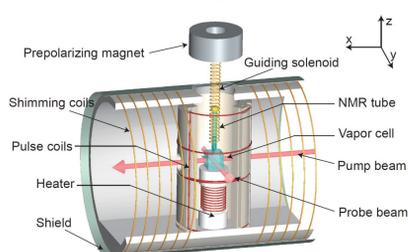


Fig.4

TOC experiments were performed using a home-built zero-field NMR spectrometer, as illustrated in FIG. 4. Nuclear spins in the ¹³C-formic acid sample ($\approx 230\mu\text{L}$) were polarized in a 1.3-T prepolarizing magnet, after which the sample was shuttled into a magnetically shielded region, such that the bottom of the sample tube is $\sim 1\text{mm}$ above a ⁸⁷Rb vapor cell of an atomic magnetometer. The ⁸⁷Rb atoms in the vapor cell were pumped with a circularly polarized laser beam propagating in the x direction. The magnetic field were measured via optical rotation of linearly polarized probe laser light at the D_2 transition propagating in the y direction. The magnetometer was primarily sensitive to z component of the nuclear magnetization, i.e., $M_z \propto \text{Tr}[\rho(t)(\gamma_H \sigma_z \otimes \mathbf{1}_2 + \gamma_C \mathbf{1}_2 \otimes \sigma_z)]$, with a noise floor of about $15 \text{ fT}/\sqrt{Hz}$ above 100 Hz, here $\rho(t)$ is the density matrix of the ¹H-¹³C system. A guiding magnetic field ($\approx 1\text{G}$) was applied during the transfer, and was adiabatically switched to zero after the sample reached the zero-field region. In our experiment, to ensure adiabaticity, the decay time to turn off the guiding field is 1 s. Thus the spin system is initially prepared in the adiabatic state [32]: $\rho(0) = \mathbf{1}_4/4 + \frac{\epsilon_H + \epsilon_C}{2} (\sigma_z \otimes \mathbf{1}_2 + \mathbf{1}_2 \otimes \sigma_z) - \frac{\epsilon_H - \epsilon_C}{4} (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)$ with the polarizations $\epsilon_H, \epsilon_C \sim 10^{-6}$. The TOC pulses were generated by three sets of mutually orthogonal low-inductance pulse coils, which were individually controlled by arbitrary waveform generators (Keysight 33512B with two channels, Keysight 33511B with single channel), and amplified individually with linear power amplifiers (AE TECHRON 7224) with 300 KHz bandwidth.

The average fidelity for ¹H single-spin TOC control is estimated to be around 0.99 via randomized benchmarking.

Discussion and Outlook

Typical optimal control techniques and applications to quantum systems use numerical methods which involve the repeated numerical integration of a system of differential equations with variable initial conditions (parameters). In our case, there is no need of numerical integration since the solution is given in explicit form. Moreover the number of parameters is reduced to a minimum with the technique of symmetry reduction.

Ideas presented here can be applied more in general for quantum systems displaying symmetries such as the KP systems. The analytic knowledge of the TOC is useful even in cases where such a control is not the one physically implemented. It gives information about the inherent time limitations of the system, therefore indicating a benchmark to which to compare the time for any control law. The knowledge of the TOC law for any final condition is also equivalent to a description of the reachable sets which, in the presence of symmetries, can be carried out in the (reduced) orbit space.