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AN ITERATIVE ALGORITHM FOR OPTIMAL CONTROL OF TWO-LEVEL QUANTUM SYSTEMS

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Abstract
This paper addresses the numerical resolution of a state transfer problem in a single spin qubit using three different Optimal Control algorithms: Krotov algorithm, Rabitz algorithm, used on Quantum Molecular Dynamics, and a new algorithm that we propose. In the problem of finding the optimal control in the spin transference between two given states with a minimal cost in Nuclear Magnetic Resonance (NMR), we present the application of the two algorithms mentioned above to control a quantum system with one varying external electromagnetic field. Then, we propose a new algorithm, inspired in the Maday-Turinici algorithm, to compute the optimal controls for a system with two varying external electromagnetic fields, integrating the adjoint equations of the Pontryagin Maximum Principle (PMP). We compare the numerical results with the analytic solutions known for both problems and analyze the performance of these algorithms.

Key words
Optimal control, quantum control systems, nuclear magnetic resonance.

1 Organization of the Paper

In the next section we give an introduction to the basic concepts used in Quantum Optimal Control applied to Nuclear Magnetic Resonance. In the third section we establish the optimal control problem to be solved: controlling a single spin immersed in a static electromagnetic field and an external radio frequency magnetic field, with a minimal cost. In the first subsection we treat a system with a single external radio frequency magnetic field along the Y axis, we present the algorithm of H. Rabitz et al. and apply it to obtain the optimal control so that the system performs a unitary transformation and compute the corresponding cost. In the following subsection we apply the algorithm of V. F. Krotov et al. to the same system and obtain the optimal control and the corresponding cost for the realization of that unit transformation. In the fourth section we treat the problem with two varying external radio frequency magnetic fields along the X and Y axes. We have devised a general algorithm based on the two algorithms presented above and the Maday-Turinici algorithm. We get the optimal controls in this problem and the corresponding cost. We compar of the results with the analytic solutions for both problems.

2 Introduction

A sample is placed in a uniform and longitudinal static magnetic field B_z in the direction of the Z axis, aligning the magnetic moments of this sample. Then, it is exposed to variable radio frequency fields (r.f.) along the X-Y axes, $u_x(t)$, $u_y(t)$, absorbing the energy through a sequence of transverse magnetic pulses. The total magnetic field to which the sample is subjected is

$$\mathbf{B}(t) = u_x(t)\vec{\imath} + u_y(t)\vec{\jmath} + B_z\vec{k} \qquad (1)$$

When the magnetic moment vector of the system is transferred to the XY plane, the sequence of transverse magnetic pulses is stopped, causing the magnetic moment vector to precess. Repetitions of this process produce fluctuations in B_z and eventually, decoherence. The pulse sequence should be as short as possible to minimize the effects of relaxation, to optimize the sensitivity to the experiment and the contrast of the obtained image. This is achieved by controlling the sequence of pulses that create a unitary transformation in the shortest possible time. For Control Theory the minimization in time of a sequence of pulses equals the minimization of lengths of trajectories of vector states (in homogeneous spaces).

A quantum control system describes the dynamics of a system like an n-level quantum system, governed by the Schrödinger equation for a pure state (we set $\hbar = 1$)

$$\frac{d}{dt}\vec{\psi}(t) = -iH(u(t))\vec{\psi}(t) \quad (2)$$

where the state $\vec{\psi} : [0, T] \rightarrow \mathbb{C}^2$ is a vector representing the unitary ket $|\psi\rangle$, $T \in \mathbb{R}$ is the duration oh the process, the control $u : [0, T] \rightarrow \mathbb{R}$ is the external magnetic field and the energy of the system is represented by the Hamiltonian $H(t)$ that, in our case, is the interaction of the spin angular momentum with the external magnetic field. So, we can write

$$H(t) = -\gamma \mathbf{S} \cdot \mathbf{B}(t) \quad (3)$$

where $\mathbf{S} = s_x\vec{\imath} + s_y\vec{\jmath} + s_z\vec{k}$ is the spin angular momentum operator and γ is the gyromagnetic ratio of the system (i.e. the proportionality constant between the magnetic momentum and the angular moment). Therefore

$$H(u(t)) = -\gamma s_z B_z - \gamma s_x u_x(t) - \gamma s_y u_y(t) \quad (4)$$

We study the simplest control system of a $-\frac{1}{2}$ spin particle interacting with the magnetic field, neglecting other interactions with the system. We use the approach adopted on [D'Alessandro, 2001]. Rescaling the time and denoting $-\gamma s_z B_z = S_z$, $-\gamma s_x = S_x$ and $-\gamma s_y = S_y$, the state vector is written as $|\psi(t)\rangle = \alpha|+\rangle + \beta|-\rangle$, where $|+\rangle$ and $|-\rangle$ are the orthonormal eigenvectors corresponding to eigenvalues $+\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, respectively, of S_z. So, in the $\{|+\rangle, |-\rangle\}$ basis, the matrix representing S_z is $S_z = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$. In the same way, we have $S_x = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$, $S_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

A geometric representation for a $-\frac{1}{2}$ spin quantum system is the Bloch sphere $S_{\mathbf{B}} \subset \mathbb{R}^3$. We can observe the evolution of the state of a single qubit as a trajectory on the Bloch sphere. We use the Hopf projection $\Pi : S^3 \subset \mathbb{C}^2 \rightarrow S_{\mathbf{B}}$,

$$\Pi : \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \mapsto \begin{pmatrix} -2Re(\psi_1^* \psi_2) \\ 2Im(\psi_1^* \psi_2) \\ \|\psi_1\|^2 - \|\psi_2\|^2 \end{pmatrix} \quad (5)$$

with ψ_1^* the conjugate of ψ_1 in $\mathbb{C}$.

3 The Model

Let us consider a single particle with spin $-\frac{1}{2}$. The optimal control problem for the pure state is:

$$\left.\begin{array}{l} \frac{d}{dt}\vec{\psi}(t) = (S_z + u_x(t)S_x + u_y(t)S_y)\vec{\psi}(t) \\ \vec{\psi}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{array}\right\} \quad (6)$$

where $\vec{\psi}(t) = (\psi_1(t), \psi_2(t)) : [0, \frac{\pi}{\sqrt{2}}] \rightarrow \mathbb{C}^2$, the Lebesgue integrable function $u : [0, \frac{\pi}{\sqrt{2}}] \rightarrow \mathbb{R}$ represents the intensity of the laser pulsed control field and the final state

$$\vec{\psi}(\frac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ i \end{pmatrix} \quad (7)$$

minimizing the following cost functional

$$J(u) = \langle (\psi)^t (\frac{\pi}{\sqrt{2}}) | O | \psi(\frac{\pi}{\sqrt{2}}) \rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u_x^2(t) + u_y^2(t))\, dt \quad (8)$$

where O is the observable with target information:

$$O = \vec{\psi}(\frac{\pi}{\sqrt{2}}) \vec{\psi}^t (\frac{\pi}{\sqrt{2}}) \quad (9)$$

which will allow an optimal evolution of the system. The first term in the cost functional (8) represents the fidelity component of the signal and the second one is the pulse energy component.

We have $Lie\{S_z, S_x, S_y\} = su(2)$, so the optimal control for the system (6) with the final condition (7) exists [D'Alessandro, 2001].

We transform the system (6) into a real one:

$$\frac{d}{dt}\vec{x} = (\bar{S}_z + u_x(t)\bar{S}_x + u_y(t)\bar{S}_y)\vec{x}$$

$$\vec{x}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \vec{x}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (10)$$

where $\bar{S}_z = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$, $\bar{S}_y = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$,

$$\bar{S}_x = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} Re(\psi_1) \\ Re(\psi_2) \\ Im(\psi_1) \\ Im(\psi_2) \end{pmatrix}$$

3.1 System Subjected to a One r.f. Magnetic Field

In this section we discuss the case where the system is subjected to a varying radio frequency magnetic field along the Y-axes, $u_y(t)$, denoted $u(t)$. Let us consider the control problem

$$\frac{d}{dt}\vec{x} = (\bar{S}_z + u(t)\bar{S}_y)\vec{x}$$
$$\vec{x}(0) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$$
$$\min \rightarrow J(u) = \langle(\vec{x}^{\,t}(\tfrac{\pi}{\sqrt{2}})|O|\vec{x}(\tfrac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} u^2(t)\,dt \quad (11)$$

also we use an adjoint state or costate (Lagrange multiplier) $\lambda(t)$, which satisfies

$$\frac{d}{dt}\vec{\lambda} = (\bar{S}_z + u(t)\bar{S}_y)\vec{\lambda} \quad (12)$$

3.1.1 Numerical Approximation The development of monotonic algorithms applied to Quantum Control Theory generates approximative procedures to get pulse sequences in a state transfer problem with a single spin. Several algorithms exist to compute the approximate solution of (11) and (12), as those developed by V. F. Krotov, W. Zhu and H. Rabitz, or Y. Maday and G. Turinici, [Krotov, 1988], [Rabitz, 1998], [Maday and Turinici, 2003]. Those procedures compute teratively sequences of states, controls and adjoint functions, $\{\vec{\psi}^{(k)}(t), u^{(k)}(t), x^{(k)}(t), \vec{\lambda}^{(k)}(t)\}_{k\in\mathbb{N}}$ solving repeatedly the Schrödinger equation to approximate the solution $\{\vec{\psi}(t), u(t), x(t), \vec{\lambda}(t)\}$.

3.1.2 Optimization Algorithm I In order to solve the system (11), we consider the following algorithm due to H. Rabitz et al. [Maday and Turinici, 2003]. The recursion formulas, $k \geq 1$, are:

$$\frac{d}{dt}\vec{x}^{(k)} = (\bar{S}_z + u^{(k)}(t)\bar{S}_y)\vec{x}^{(k)}$$
$$\vec{x}^{(k)}(0) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \quad (13)$$

$$u^{(k)}(t) = -\lambda^{(k-1)}(t)\bar{S}_y\vec{x}^{(k)}(t) \quad (14)$$

$$\tfrac{d}{dt}\vec{\lambda}^{(k)} = v^{(k)}(t)\bar{S}_y\vec{\lambda}^{(k)}$$
$$\vec{\lambda}^{(k)}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix}0\\0\\0\\x_4^k(\frac{\pi}{\sqrt{2}})\end{pmatrix} \quad (15)$$

$$v^{(k)}(t) = -\lambda^{(k)}(t)\bar{S}_y\vec{x}^{(k)}(t) \quad (16)$$

So, the procedure (Algorithm I) for finding the optimal control $u(t)$ and minimizing the cost $J(u)$ is the following:

1. Choose the initial $\lambda^{(0)}(t)$.
2. Replace $\lambda^{(0)}(t)$ in the equation (14).
3. Replace $u^{(1)}(t)$ in the equation (13).
4. Integrate forward (13) to obtain $x^{(1)}(t)$ from the initial state $x^{(1)}(0)$.
5. Obtain $u^{(1)}(t)$ from (14).
6. Replace $x^{(1)}(t)$ in the equation (16) to obtain $v^{(1)}$ in terms of $\lambda^{(1)}(t)$.
7. Replace $\lambda^{(1)}(t)$ in the equation (15).
8. Integrate backwards (15) from the final state $x(T) = \lambda^1(\frac{\pi}{\sqrt{2}})$ to get $\lambda^{(1)}(t)$.
9. Obtain $v^{(1)}(t)$, replacing $\lambda^{(1)}(t)$ on (16).
10. $\{v^{(k+1)}(t),\ \lambda^{(k+1)}(t)\} \rightarrow \{v^{(k)}(t),\ \lambda^{(k)}(t)\}$
11. $\{x^{(k+1)}(t),\ u^{(k+1)}(t)\} \rightarrow \{x^{(k)}(t),\ u^{(k)}(t)\}$
12. Continue until convergence

We chose as the initial costate $\lambda^{(0)}(t)$ each of the following vectors:

$$\left\{\begin{pmatrix}t\\0\\0\\0\end{pmatrix}, \begin{pmatrix}10\\10\\10\\10\end{pmatrix}, \begin{pmatrix}t\\t^2\\10\\10\end{pmatrix}, \begin{pmatrix}t\\20\\20\\20\end{pmatrix}\right\} \quad (17)$$

In the first selection the process converged and the cost functional was $J = 0.59545$ for $k = 100$. In the second one, the process converged and the cost functional was $J = 0.56956$ for $k = 100$. In the third selection the process was convergent also. We obtained the optimal control and the cost was again $J = 0.59545$ for $k = 100$. In the fourth selection the process was convergent. We obtained the optimal control shown in figure (2) and the cost was again $J = 0.59545$ for $k = 100$.

3.1.3 Optimization Algorithm II We consider the following algorithm due to V. F. Krotov et al. mentioned in [Maday and Turinici, 2003]. The recursion formulas, $k \geq 1$, are:

$$\frac{d}{dt}\vec{x}^{(k)} = (\bar{S}_z + u^{(k)}(t)\bar{S}_y)\vec{x}^{(k)}$$
$$\vec{x}^{(k)}(0) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \quad (18)$$

$$u^{(k)}(t) = -\lambda^{(k-1)}(t)\bar{S}_y\vec{x}^{(k)}(t) \quad (19)$$

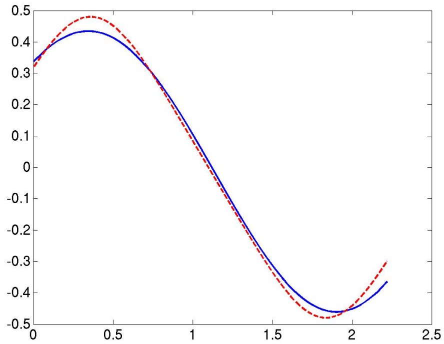

Figure 1. Optimal control $u(t)$ for one external electromagnetic field. Rabitz's algorithm. Numerical solution (blue continuous line) for k=100. Analytical solution (red dotted line).

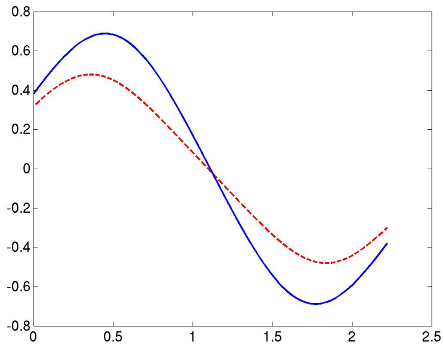

Figure 2. Optimal control $u(t)$ for one external electromagnetic field. Krotov's algorithm. Numerical solution (blue continuous line) for k=100. Analytical solution (red dotted line).

$$\frac{d}{dt}\vec{\lambda}^{(k)} = u^{(k)}(t)\bar{S}_y\vec{\lambda}^{(k)}$$

$$\vec{\lambda}^{(k)}\left(\tfrac{\pi}{\sqrt{2}}\right) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ x_4^k\left(\tfrac{\pi}{\sqrt{2}}\right) \end{pmatrix} \tag{20}$$

The procedure (Algorithm II) to compute the optimal control $u(t)$ minimizing the cost $J(u)$ is the following:

1. Choose the initial $\lambda^{(0)}(t)$.
2. Replace $\lambda^{(0)}(t)$ in the equation (19).
3. Replace $u^{(1)}(t)$ in the equation (18).
4. Integrate forward (18) to obtain $x^{(1)}(t)$ from the initial state $x^{(1)}(0)$.
5. Obtain $u^{(1)}(t)$.
6. Replace $x^{(1)}(t)$ and $u^{(1)}(t)$ in the equation (20).
7. Integrate backwards (20) from the final state $x(T) = \lambda^1(\frac{\pi}{\sqrt{2}})$ to get $\lambda^{(1)}(t)$.
8. $\{\lambda^{(k+1)}, x^{(k+1)}, u^{(k+1)}\} \to \{\lambda^{(k)}, x^{(k)}, u^{(k)}\}$

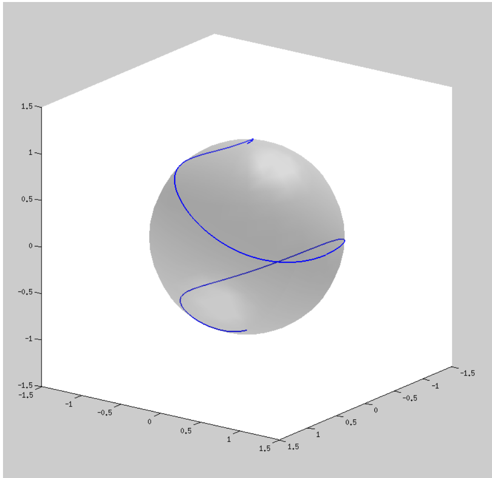

Figure 3. State transfer trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere, using the optimal control in figure 1 for Rabitz algorithm.

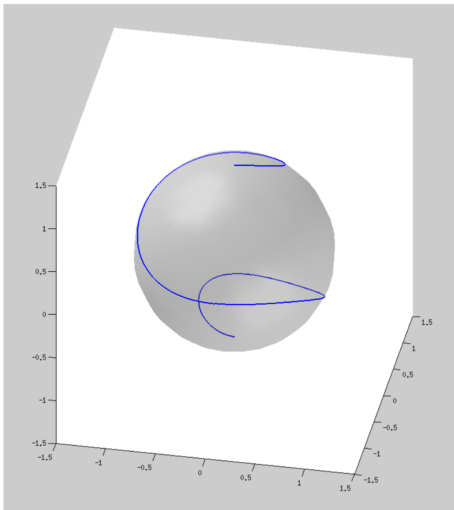

Figure 4. State transfer trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere, using the optimal control in figure 2 for Krotov algorithm.

9. Continue until convergence

As in the previous algorithm, we chose as the costate $\lambda^{(0)}(t)$ the vectors shown in (17). In the first choice of the costate the process was convergent and the cost functional was $J = 1.2999$ for $k = 100$. In the second one, the process was convergent and the cost functional was $J = 1.2992$ for $k = 100$. In the third selection the process was convergent also. We have obtained the optimal control and the cost was again $J = 1.2992$ for $k = 100$. In the fourth selection the process was convergent. We obtain the optimal control in the figure (2) and the cost was again $J = 1.2992$ for $k = 100$.

We represent the trajectories of the states transfer on the Bloch sphere $S_{\mathbf{B}}$, corresponding to the optimal controls obtained, figures (3), (4).

Finally, we mention a theorem about the monotonic convergence of the algorithms I and II.

Theorem 1 [Maday-Turinici]

The algorithms I and II converge monotonically:

$$J(u^{(k+1)}) \geq J(u^{(k)}) \quad \forall k \geq 1,\, k \in \mathbb{N} \tag{21}$$

where

$$J(u^{(k)}) = \langle (\vec{x}^{(k)})^t(\frac{\pi}{\sqrt{2}})|O|\vec{x}^{(k)}(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u^{(k)})^2(t)\, dt \tag{22}$$

For a demonstration, see [Maday and Turinici, 2003]

Remark.
The rigorous proof of the convergence $\{u^{(k)}(t), \vec{x}^{(k)}(t)\} \rightarrow \{u(t), \vec{x}(t)\}$ is still an open problem [Maday and Turinici, 2003].

4 System Subjected to Two r.f. Magnetic Fields

In this section we consider the case where two time varying external electromagnetic fields, $u_x(t), u_y(t)$, act along the X and Y-axes. We have the control problem

$$\frac{d}{dt}\vec{x} = (\bar{S}_z + u_x(t)\bar{S}_x + u_y(t)\bar{S}_y)\vec{x}$$
$$\vec{x}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{23}$$

minimizing the cost functional:

$$J(u_x, u_y) = \langle (\psi)^t(\frac{\pi}{\sqrt{2}})|O|\psi(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u_x^2 + u_y^2)\, dt \tag{24}$$

4.1 Optimization Algorithm III

We devised and tested an algorithm, inspired on [Maday and Turinici, 2003] and based on those of algorithms of H. Rabitz and V. F. Krotov which unifies and generalizes them for the case of two controls. Given four constants $\delta_1,\, \delta_2,\, \eta_1,\, \eta_2, \in (0, 2), \lambda^0(t),\, v^0(t),\, w^0(t)$ and $k \geq 1$ let be

$$\left.\begin{aligned} \frac{d}{dt}\vec{x}^{(k)} &= \begin{pmatrix} 0 & -u_y^{(k)}(t) & -1 & -u_x^{(k)}(t) \\ u_y^{(k)}(t) & 0 & -u_x^{(k)}(t) & 1 \\ 1 & u_x^{(k)}(t) & 0 & -u_y^{(k)}(t) \\ u_x^{(k)}(t) & -1 & u_y^{(k)}(t) & 0 \end{pmatrix} \vec{x}^{(k)} \\ \vec{x}^{(k)}(0) &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned}\right\} \tag{25}$$

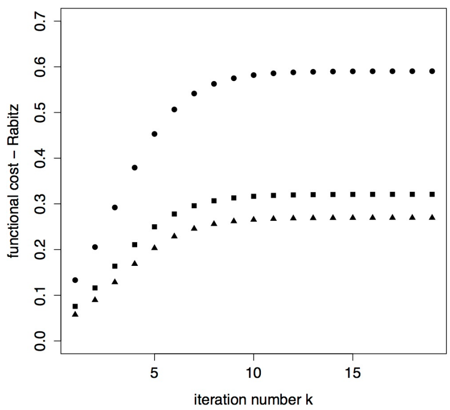

Figure 5. Evolution of the cost functional for Rabitz's algorithm (dotted line with circles). The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

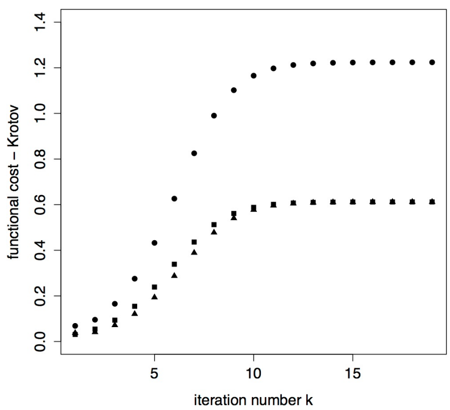

Figure 6. Evolution of the cost functional for Krotov's algorithm (dotted line with circles). The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

$$u_y^{(k)} = (1-\delta_1)v^{(k-1)}(t)+\delta_1\lambda^{t(k-1)}\begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\end{pmatrix}\vec{x}^{(k)} \tag{26}$$

$$u_x^{(k)} = (1-\delta_2)w^{(k-1)}(t)+\delta_2\lambda^{t(k-1)}\begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}\vec{x}^{(k)} \tag{27}$$

$$\left.\begin{array}{l}\frac{d}{dt}\lambda^{(k)} = \begin{pmatrix}0 & -v^{(k)}(t) & -1 & -w^{(k)}(t)\\ v^{(k)}(t) & 0 & -w^{(k)}(t) & 1\\ 1 & w^{(k)}(t) & 0 & -v^{(k)}(t)\\ w^{(k)}(t) & -1 & v^{(k)}(t) & 0\end{pmatrix}\lambda^{(k)}\\ \lambda^{(\mathbf{k})}(\frac{\pi}{\sqrt{2}}) = \begin{pmatrix}0\\ 0\\ 0\\ x_4^{(k)}(\frac{\pi}{\sqrt{2}})\end{pmatrix}\end{array}\right\} \tag{28}$$

$$v^{(k)}(t) = (1-\eta_1)u_y^{(k)} + \eta_1\,\lambda^{t(k)}\begin{pmatrix}0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\end{pmatrix}\vec{x}^{(k)} \tag{29}$$

$$w^{(k)}(t) = (1-\eta_2)u_x^{(k)} + \eta_2\,\lambda^{t(k)}\begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}\vec{x}^{(k)} \tag{30}$$

the recursion equations. The following algorithm finds the optimal controls $u_x(t)$, $u_y(t)$ of the problem (10), minimizing the cost $J(u_x, u_y)$:

1. Select the initial $\lambda^0(t)$, $v^0(t)$, $w^0(t)$.
2. Select the values δ_1, δ_2, η_1, $\eta_2, \in [0, 2]$.
3. Replace δ_1, $\lambda^0(t)$, $v^0(t)$ in (26) to get $u_y^{(1)}(t)$.
4. Replace δ_2, $\lambda^0(t)$, $w^0(t)$ in (27) to get $u_x^{(1)}(t)$.
5. In (29) replace $u_y^{(1)}(t)$ and η_1.
6. In (30) replace $u_x^{(1)}(t)$ and η_2.
7. Integrate (25) forward to get $x^{(1)}(t)$, using $u_y^{(1)}(t)$ and $u_x^{(1)}(t)$.
8. Integrate (28) backwards to get $\lambda^{(1)}(t)$, using $u_y^{(1)}(t)$ and $u_x^{(1)}(t)$.
9. Replace $x^{(1)}(t)$ in the equation for $u^{(1)}(t)$.
10. $\{v^{(k+1)}, w^{(k+1)}, \lambda^{(k+1)}\} \to \{v^{(k)}, w^{(k)}, \lambda^{(k)}\}$
11. $\{u_y^{(k+1)}(t), u_x^{(k+1)}(t)\} \to \{u_y^{(k)}(t), u_x^{(k)}(t)\}$

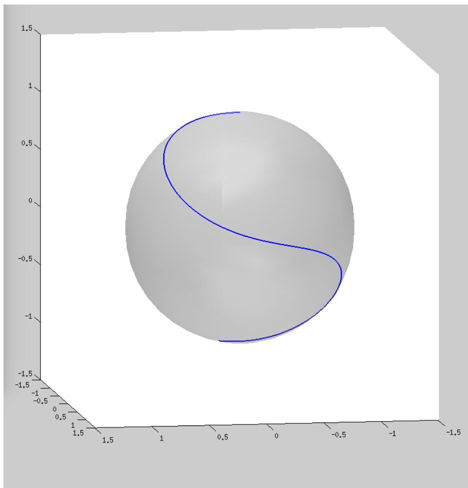

Figure 7. State transfer trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere, using the optimal controls in figure 8 for algorithm III.

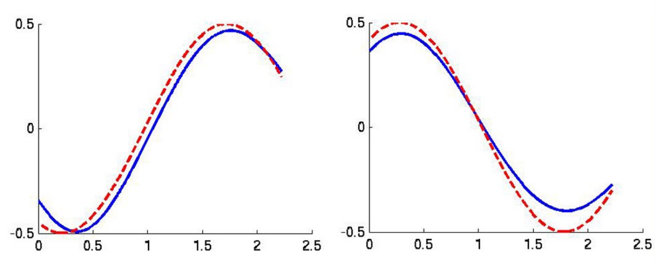

Figure 8. Optimal controls $u_x(t), u_y(t)$, for two external electromagnetic fields. Unified algorithm. Numerical solutions (blue continuous lines) for k=100. Analytical solutions (red dotted lines).

12. Continue until convergence

We start with the selection $\delta_1 = \frac{1}{2}, \delta_2 = \frac{1}{2}, \eta_1 = \frac{3}{2}, \eta_2 = \frac{3}{2}, v^{(0)} = \cos t, w^{(0)} = 1$. The process was convergent at $k = 15$ for the previous selection and the cost was $J = 1.112498$ for $k = 100$. In a second selection $\delta_1 = \frac{1}{2}, \delta_2 = \frac{3}{2}, \eta_1 = \frac{3}{2}, \eta_2 = \frac{1}{2}$, $v^{(0)} = \cos t$, $w^{(0)} = \cos t$, the process was convergent at $k = 15$. We obtain the optimal control in figure (8) and the cost was again $J = 1.112498$ for $k = 100$.

Finally, we obtain the optimal trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere $S_{\mathbf{B}}$, figure 7, corresponding to algorithm III. We have the following result:

Theorem 2

The algorithm III converges monotonically for δ_1, δ_2, η_1, $\eta_2 \in (0, 2)$, i.e., if

$$J_\Delta := J(u_x^{(k+1)}, u_y^{(k+1)}) - J(u_x^{(k)}, u_y^{(k)})$$

then $J_\Delta \geq 0$.

Proof: The proof is a generalization of that of Theorem 1.

$$
\begin{aligned}
J_\Delta &= \langle(\vec{x}^{(k+1)})^t(T)|O|\vec{x}^{(k+1)}(T)\rangle \\
&+ \int_0^T \left((u_x^{(k+1)})^2 + (u_y^{(k+1)})^2\right) dt \\
&- \langle(\vec{x}^{(k)})^t(T)|O|\vec{x}^{(k)}(T)\rangle \\
&- \int_0^T ((u_x^{(k)})^2(t) + (u_y^{(k)})^2(t))\, dt \\
&= \langle((\vec{x}^{(k+1)})^t - (\vec{x}^{(k)})^t)(T)|O|(\vec{x}^{(k+1)} - \vec{x}^{(k)})(T)\rangle \\
&+ 2Re\langle(\vec{x}^{(k+1)})^t(T) - (\vec{x}^{(k)})^t(T)|O|\vec{x}^{(k)}(T)\rangle \\
&+ \int_0^T \left((u_x^{(k+1)})^2 - (u_x^{(k)})^2 + (u_y^{(k+1)})^2 - (u_y^{(k)})^2\right) dt
\end{aligned}
$$

Now, we have

$$
\begin{aligned}
&2Re\langle(\vec{x}^{(k+1)} - \vec{x}^{(k)})(T)|O|\vec{x}^{(k)}(T)\rangle = \\
&2Re\langle(\vec{x}^{(k+1)} - \vec{x}^{(k)})(T), \vec{\lambda}^{(k)}(T)\rangle = \\
&2Re \int_0^T \Big(\langle(S_z + u_x^{k+1}S_x + u_y^{k+1}S_y)\vec{x}^{(k+1)}(t) - \\
&(S_z + u_x^k S_x + u_y^k S_y)\vec{x}^{(k)}(t), \vec{\lambda}^{(k)}(t)\rangle + \\
&\langle(\vec{x}^{(k+1)} - \vec{x}^{(k)})(t), (S_z + v^k S_y + w^k S_x)\vec{\lambda}^{(k)}(t)\rangle\Big) dt = \\
&2Re \int_0^T \Big(\langle S_z x^{k+1}, \vec{\lambda}^{(k)}(t)\rangle + u_x^{k+1}\langle S_x x^{k+1}, \vec{\lambda}^{(k)}(t)\rangle + \\
&u_y^{k+1}\langle S_y x^{k+1}, \vec{\lambda}^{(k)}(t)\rangle - \langle S_z x^k, \vec{\lambda}^{(k)}(t)\rangle - \\
&u_x^k\langle S_x x^k, \vec{\lambda}^{(k)}(t)\rangle - u_y^{k+1}\langle S_y x^k, \vec{\lambda}^{(k)}(t)\rangle + \\
&\langle x^{k+1}, S_z\vec{\lambda}^{(k)}(t)\rangle + v^k\langle x^{k+1}, S_y\vec{\lambda}^{(k)}(t)\rangle + \\
&w^k\langle x^{k+1}, S_x\vec{\lambda}^{(k)}(t)\rangle - \langle x^k, S_z\vec{\lambda}^{(k)}(t)\rangle - \\
&v^k\langle x^k, S_y\vec{\lambda}^{(k)}(t)\rangle - w^k\langle x^k, S_x\vec{\lambda}^{(k)}(t)\rangle\Big) dt = \\
&2Re \int_0^T \Big(u_x^{k+1}\big(\tfrac{u_x^{k+1} - (1-\delta_2)w^k}{\delta_2}\big) - u_x^k\big(\tfrac{w^k - (1-\eta_2)u_x^k}{\eta_2}\big) + \\
&u_y^{k+1}\big(\tfrac{u_y^{k+1} - (1-\delta_1)v^k}{\delta_1}\big) - u_y^k\big(\tfrac{v^k - (1-\eta_1)u_y^k}{\eta_1}\big) + \\
&v^k\big(\tfrac{u_y^{k+1} - (1-\delta_1)v^k}{\delta_1}\big) - v^k\big(\tfrac{v^k - (1-\eta_1)u_y^k}{\eta_1}\big) + \\
&w^k\big(\tfrac{u_x^{k+1} - (1-\delta_2)w^k}{\delta_2}\big) - w^k\big(\tfrac{w^k - (1-\eta_2)u_x^k}{\eta_2}\big)\Big) dt
\end{aligned}
$$

Therefore, the value of J_Δ is

$$
\begin{aligned}
&\langle(\vec{x}^{(k+1)})^t - \vec{x}^{(k)})^t|O|\vec{x}^{(k+1)} - \vec{x}^{(k)}\rangle(T) \\
&+ \int_0^T ((\tfrac{2}{\delta_1} - 1)(u_y^{(k+1)} - v^{(k)})^2 + (\tfrac{2}{\eta_1} - 1)(v^{(k)} - u_y^{(k)})^2 \\
&+ (\tfrac{2}{\delta_2} - 1)(u_x^{(k+1)} - w^{(k)})^2 + (\tfrac{2}{\eta_2} - 1)(w^{(k)} - u_x^{(k)})^2) dt \\
&\geq 0
\end{aligned}
$$

5 Concluding Remarks

In the case of the control with one external electromagnetic field, the analytic solution [D'Alessandro, 2001] is $u(t) = 1.21cn(2.49\,t - 1.0, 0.487)$, which was found using the Pontryagin's Maximum Principle [Pontryagin et al., 1962], defining two auxiliary controls and carrying up the system (11) to one of the Duffing oscillator types. Solving that system, the form of the solution is a Jacobi elliptic function. We can observe in figure (1) that the Rabitz's algorithm I has a better performance for finding the optimal control

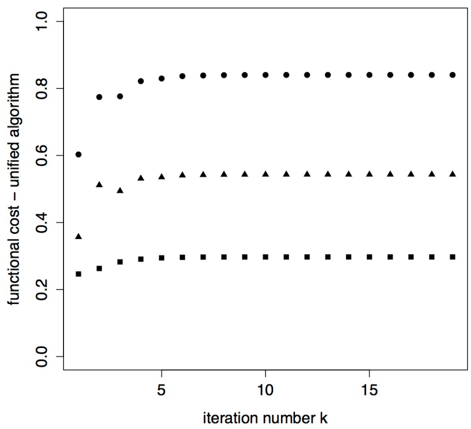

Figure 9. Evolution of the cost functional for two external electromagnetic fields (dotted line with circles), unified algorithm. The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

in this case, in contrast, with Krotov's algorithm II that has a poor performance, figure (2). In figures (5), (6) we show the evolution of the cost functional and their split in fidelity and pulse energy, for one external electromagnetic field with Rabitz's algorithm I and Krotov's algorithm II, respectively. In the case of Krotov's algorithm II we note, figure (6), that the cost functional converges to the expected value (J=1.312828). This is not the case for the Rabitz algorithm I, figure (5). For two external electromagnetic fields, the analytic solution, [D'Alessandro, 2001], $u_x(t) = -\dfrac{1}{2}\cos(\dfrac{2\pi}{3}t - (\sqrt{2}-1)\dfrac{\pi}{\sqrt{2}})$, $u_y(t) = -\dfrac{1}{2}\sin(\dfrac{2\pi}{3}t - (\sqrt{2}-1)\dfrac{\pi}{\sqrt{2}})$ was found using again the equations of PMP. We can observe in figure (8) that the algorithm III has a good performance for finding the optimal controls in this case. In figure (9) we show the evolution of the cost functional and their split in fidelity and pulse energy, for two external electromagnetic fields with our unified algorithm. Note that the cost functional does not converge to the expected value (J=1.543119).

6 Conclusions

In this paper we have addressed the problem of finding the optimal control corresponding to the minimal time to perform a unitary spin transition from the state $\frac{1}{2}$ to the state $-\frac{1}{2}$, subjected to a minimal cost, in a two-level quantum system. We have considered one or two time varying external electromagnetic fields along the Y axes, and the X and Y-axes, respectively. In the first case we have implemented two monotonic convergent algorithms, devised by H. Rabitz et al. and V. F. Krotov et al. , respectively, for their application in the problem highlighted. The corresponding optimal control and the minimum cost were calculated. The results were compared with the analytical solution in each case: the minimum value of the cost is close to that obtained in reports like [D'Alessandro, 2001]. We have obtained the state trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere, using the optimal control for algorithm I and algorithm II. In the second case we have devised and implemented a new algorithm, which converges rapidly to the known analytical solutions. This strategy yields good performances in our case-study. The minimum cost was calculated, but this numerical result was far of the analytic result, nevertheless, the state trajectory from $|0\rangle$ to $|1\rangle$ on the Bloch sphere, using the optimal controls for algorithm III, is the best.

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