NUMERICAL APPROXIMATION IN OPTIMAL CONTROL OF TWO-LEVEL QUANTUM SYSTEMS

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Abstract
In this paper, we discuss the application of two quantum control algorithms, the Krotov's algorithm and the Rabitz's algorithm, to Nuclear Magnetic Resonance (NMR), based on a numerical method for iterative optimization. Specifically, we address the problem of the determination of external optimal pulses (controls) with minimal cost, over a two-level quantum system. We use the numerical approximation to find the optimal control in the case of one control, integrating the adjoint equations of the Pontryagin Maximum Principle (PMP), and propose a new algorithm, based on the algorithms of H. Rabitz et al. and V. F. Krotov et al., which unifies and generalizes them for the case of two controls. We compare the efficiency of these algorithms with the solutions found by analytical methods.

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

1 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 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

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

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 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).

We report, on the one hand, the application of two iterative algorithms, used on Quantum Molecular Dynamics, to Optimal Control of Two-Level Quantum Systems with one external electromagnetic field, the first one due to H. Rabitz and W. Zhu and the second one due to V. F. Krotov et al. On the other hand, we have devised an algorithm inspired in [Maday, 2003], which unifies and generalizes both algorithms for the case of two external electromagnetic fields. We use the approach adopted in [D'Alessandro, 2001]. Using numerical approximation to find the optimal control, we integrate the adjoint equations of the Pontryagin Maximum Principle (PMP). It's important to use an algorithm with an appropriate performance to solve the control quantum equations and so, reduce the cost.

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

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

where the state $\vec{\psi} : [0, T] \to \mathbb{C}^2$ is a vector representing the unitary ket $|\psi\rangle$, $T \in \mathbb{R}$, the control $u : [0, T] \to \mathbb{R}$ 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

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

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 moment and the angular momentum). Therefore

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

We study the simplest control system of a $-\frac{1}{2}$ spin particle interacting with the magnetic field, neglecting other interactions. 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, $S_x = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$, $S_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

2 Problem Statement

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

$$\left.\begin{array}{l} \dfrac{d}{dt}\vec{\psi}(t) = (S_z + u_x(t)S_x + u_y(t)S_y)\vec{\psi}(t) \\ \vec{\psi}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{array}\right\} \tag{5}$$

with $\vec{\psi} = (\psi_1, \psi_2) : [0, \frac{\pi}{\sqrt{2}}] \to \mathbb{C}^2$, $u : [0, \frac{\pi}{\sqrt{2}}] \to \mathbb{R}$ a Lebesgue integrable function, given the final state

$$\vec{\psi}(\frac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ i \end{pmatrix} \tag{6}$$

minimizing the cost functional

$$J(u) = \langle(\psi)^t(\frac{\pi}{\sqrt{2}})|O|\psi(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u_x^2(t) + u_y^2(t))\, dt \tag{7}$$

where O is the observable with target information:

$$O = \vec{\psi}(\frac{\pi}{\sqrt{2}})\vec{\psi}^t(\frac{\pi}{\sqrt{2}}) \tag{8}$$

which will allow an optimal evolution of the system.

Since $span\{S_z, S_x, S_y\} = su(2)$ and S_z, S_x, S_y are orthogonal and linearly independent, the optimal control for the system (5) with the final condition (6) exists [D'Alessandro, 2001].

We consider the *realification* of the system (5):

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

$$\vec{x}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \vec{x}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{9}$$

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

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

2.1 System with one control

In this section we consider the case where the system is subjeted to varing external electromagnetic field along the Y-axis, $u_y(t)$, denoted $u(t)$. Let us consider the system

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

$$\vec{x}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{10}$$

$$\min \to J(u) = \langle(\vec{x}^t(\frac{\pi}{\sqrt{2}})|O|\vec{x}(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} u^2(t)\, dt \tag{11}$$

2.1.1 Algorithm I: Rabitz et al.

In order to solve the system (10), we consider the following algorithm due to H. Rabitz et al. and presented in [Maday, 2003]

Recursion formulas, $k \geq 1$

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

$$\vec{x}^{(k)}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{12}$$

$$u^{(k)}(t) = -\lambda^{(k-1)}(t)\bar{S}_y\vec{x}^{(k)}(t) \tag{13}$$

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

$$\vec{\lambda}^{(k)}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ x_4^k(\frac{\pi}{\sqrt{2}}) \end{pmatrix} \tag{14}$$

$$v^{(k)}(t) = -\lambda^{(k)}(t)\bar{S}_y\vec{x}^{(k)}(t) \tag{15}$$

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

We start with the selection

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{16}$$

The process converged for the previous selection and the cost was $J = 0.59545$ for $k = 100$.
In a second selection

$$\lambda^{(0)}(t) = \begin{pmatrix} 10 \\ 10 \\ 10 \\ 10 \end{pmatrix} \tag{17}$$

the process converged. We obtained the optimal control and the cost was $J = 0.56956$ for $k = 100$.
In a third selection

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ t^2 \\ 10 \\ 10 \end{pmatrix} \tag{18}$$

the process converged. We obtained the optimal control and the cost was $J = 0.569545$ for $k = 100$.

In a fourth selection

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ 20 \\ 20 \\ 20 \end{pmatrix} \tag{19}$$

the process converged. We obtained the optimal control in figure (1) and the cost was $J = 0.59545$ for $k = 100$.

2.1.2 Algorithm II: Krotov et al.

In order to solve the system (10), we consider the following algorithm due to V. F. Krotov et al. and presented in [Maday, 2003]

Recursion formulas, $k \geq 1$

$$\frac{d}{dt}\vec{x}^{(k)} = (\bar{S}_z + u^{(k)}(t)\bar{S}_y)\vec{x}^{(k)}$$
$$\vec{x}^{(k)}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{20}$$

$$u^{(k)}(t) = -\lambda^{(k-1)}(t)\bar{S}_y\vec{x}^{(k)}(t) \tag{21}$$

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

$$\vec{\lambda}^{(k)}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ x_4^k(\frac{\pi}{\sqrt{2}}) \end{pmatrix} \tag{22}$$

the procedure 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 (21).
3. Replace $u^{(1)}(t)$ in the equation (20).
4. Integrate forward (20) 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 (22).
7. Integrate backwards (22) from the final state $x(T)$ to get $\lambda^{(1)}(t)$.
8. $\lambda^{(k+1)}(t) \to \lambda^{(k)}(t)$
9. $x^{(k+1)}(t) \to x^{(k)}(t)$
10. $u^{(k+1)}(t) \to u^{(k)}(t)$
11. Continue until convergence

We started with the selection

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{23}$$

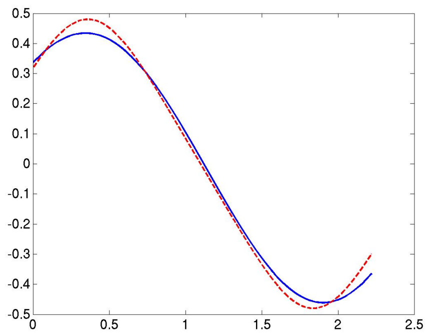

Figure 1. Optimal control $u(t)$ for one external electromagnetic field. Rabitz's algorithm. Numerical solution (blue continuous line) for k=100. Analytical solution (red dotted line).

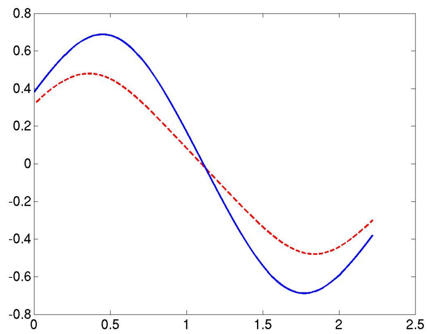

Figure 2. Optimal control $u(t)$ for one external electromagnetic field. Krotov's algorithm. Numerical solution (blue continuous line) for k=100. Analytical solution (red dotted line).

The process converged for that selection and the cost was $J = 1.2999$ for $k = 100$.
In a second selection

$$\lambda^{(0)}(t) = \begin{pmatrix} 10 \\ 10 \\ 10 \\ 10 \end{pmatrix} \tag{24}$$

the process converged. We obtained the optimal control and the cost was $J = 1.2992$ for $k = 100$.
In a third selection

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ t^2 \\ 10 \\ 10 \end{pmatrix} \tag{25}$$

the process converged. We obtained the optimal control and the cost was again $J = 1.2992$ for $k = 100$.
In a fourth choose

$$\lambda^{(0)}(t) = \begin{pmatrix} t \\ 20 \\ 20 \\ 20 \end{pmatrix} \tag{26}$$

the process converged. We obtained the optimal control in figure (2) and the cost was again $J = 1.2992$ for $k = 100$. We mention the following theorem:

Theorem [Maday-Turinici]
The algorithms I and II converge monotonically:

$$J(u^{(k+1)}) \leq J(u^{(k)}) \quad \forall k \geq 1,\, k \in \mathbb{N} \tag{27}$$

where

$$J(u^{(k)}) = \langle (\vec{x}^{(k)})^t(\frac{\pi}{\sqrt{2}})|O|\vec{x}^{(k)}(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u^{(k)})^2(t)\, dt \tag{28}$$

For a demonstration, see [Maday, 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, 2003].

3 Case of two-controls

In this section we consider the case where two varying external electromagnetic fields, $u_x(t), u_y(t)$, act along the X and Y-axes. Again, let us consider the system

$$\begin{gathered} \frac{d}{dt}\vec{x} = (\bar{S}_z + u_x(t)\bar{S}_x + u_y(t)\bar{S}_y)\vec{x} \\ \vec{x}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \vec{x}(\tfrac{\pi}{\sqrt{2}}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \end{gathered} \tag{29}$$

minimizing the cost functional:

$$J(u_x, u_y) = \langle (\psi)^t(\frac{\pi}{\sqrt{2}})|O|\psi(\frac{\pi}{\sqrt{2}})\rangle + \int_0^{\frac{\pi}{\sqrt{2}}} (u_x^2 + u_y^2)\, dt \tag{30}$$

3.1 Algorithm III

We devised and tested an algorithm based on those Rabitz and Krotov which unifies and generalizes them for the case of two controls. Given δ_1, δ_2, η_1, $\eta_2, \in$

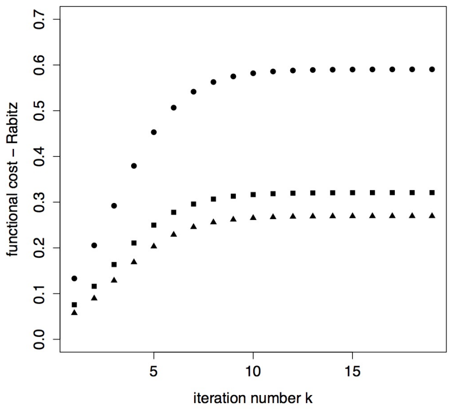

Figure 3. Evolution of the cost functional for Rabitz's algorithm (dotted line with circles). The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

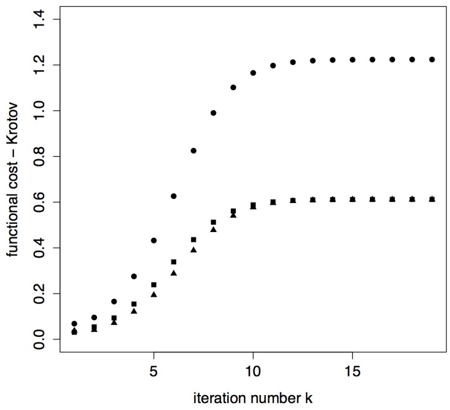

Figure 4. Evolution of the cost functional for Krotov's algorithm (dotted line with circles). The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

$[0,2]$, $\lambda^0(t)$, $v^0(t)$, $w^0(t)$ and $k \geq 1$ let be

$$\left.\begin{aligned} \frac{d}{dt}\vec{x}^{(k)} &= \begin{pmatrix} 0 & -u_y^{(k)}(t) & -1 & -u_x^{(k)}(t) \\ u_y^{(k)}(t) & 0 & -u_x^{(k)}(t) & 1 \\ 1 & u_x^{(k)}(t) & 0 & -u_y^{(k)}(t) \\ u_x^{(k)}(t) & -1 & u_y^{(k)}(t) & 0 \end{pmatrix} \vec{x}^{(k)} \\ \vec{x}^{(k)}(0) &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned}\right\} \tag{31}$$

$$u_y^{(k)} = (1-\delta_1)v^{(k-1)}(t)+\delta_1\lambda^{t(k-1)} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \vec{x}^{(k)} \tag{32}$$

$$u_x^{(k)} = (1-\delta_2)w^{(k-1)}(t)+\delta_2\lambda^{t(k-1)} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \vec{x}^{(k)} \tag{33}$$

$$\left.\begin{aligned} \frac{d}{dt}\lambda^{(k)} &= \begin{pmatrix} 0 & -v^{(k)}(t) & -1 & -w^{(k)}(t) \\ v^{(k)}(t) & 0 & -w^{(k)}(t) & 1 \\ 1 & w^{(k)}(t) & 0 & -v^{(k)}(t) \\ w^{(k)}(t) & -1 & v^{(k)}(t) & 0 \end{pmatrix} \lambda^{(k)} \\ \lambda^{(\mathbf{k})}\left(\frac{\pi}{\sqrt{\mathbf{2}}}\right) &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ x_4^{(k)}\left(\frac{\pi}{\sqrt{2}}\right) \end{pmatrix} \end{aligned}\right\} \tag{34}$$

$$v^{(k)}(t) = (1-\eta_1)u_y^{(k)} + \eta_1\,\lambda^{t(k)} \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \vec{x}^{(k)} \tag{35}$$

$$w^{(k)}(t) = (1-\eta_2)u_x^{(k)} + \eta_2\,\lambda^{t(k)} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \vec{x}^{(k)} \tag{36}$$

the recursion equations. The following algorithm allows to find the optimal controls $u_x(t)$, $u_y(t)$ of the problem (9), 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 (32) to get $u_y^{(1)}(t)$.
4. Replace δ_2, $\lambda^0(t)$, $w^0(t)$ in (33) to get $u_x^{(1)}(t)$.
5. In (35) replace $u_y^{(1)}(t)$ and η_1.
6. In (36) replace $u_x^{(1)}(t)$ and η_2.
7. Integrate (31) forward to get $x^{(1)}(t)$, using $u_y^{(1)}(t)$ and $u_x^{(1)}(t)$.
8. Integrate (34) 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. $\{u_y^{(k+1)}(t), u_x^{(k+1)}(t)\} \to \{u_y^{(k)}(t), u_x^{(k)}(t)\}$
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 obtained the optimal control in figure (5) and the cost was again $J = 1.112498$ for $k = 100$.

4 Discussion

In the case of one external electromagnetic field, the analytic solution [D'Alessandro, 2001] is

$$u(t) = 1.21cn(2.49\,t - 1.0, 0.487) \qquad (37)$$

which was found defining two auxiliary controls, using the Pontryagin's Maximum Principle [Pontryagin, 1962] and carrying up the system (10) to one of the Duffing types. Solving that system we express the solution in terms of Jacobi elliptic functions and eventually it has the form (37). We can observe in figure (1) that the Rabitz's algorithm I has a better performance for finding the optimal control in this case, in contrast with Krotov's algorithm II that has a poor performance, figure (2). In figures (3), (4) 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 (4), that the cost functional converges to the expected value (J=1.312828). It's not the case for the Rabitz's algorithm I, figure (3).

For two external electromagnetic fields, the analytic solution [D'Alessandro, 2001],

$$\begin{aligned} u_x(t) &= -\frac{1}{2}\cos(\frac{2\pi}{3}t - (\sqrt{2}-1)\frac{\pi}{\sqrt{2}}) \\ u_y(t) &= -\frac{1}{2}\sin(\frac{2\pi}{3}t - (\sqrt{2}-1)\frac{\pi}{\sqrt{2}}) \end{aligned} \qquad (38)$$

was found using again the equations of PMP. We can observe in figure (5) that the algorithm III has a good performance for finding the optimal controls in this case. In figure (6) we show the evolution of the cost functional and their split in fidelity and pulse energy, for two external electromagnetic fields case with our unified algorithm. We note that the cost functional does not converge to the expected value (J=1.543119).

5 Conclusions

In this paper we have addressed the problem of the optimal time to perform a unitary spin transition from the state spin $\frac{1}{2}$ to the state spin $-\frac{1}{2}$ in a two-level quantum system, in the cases of we have one or two controls.

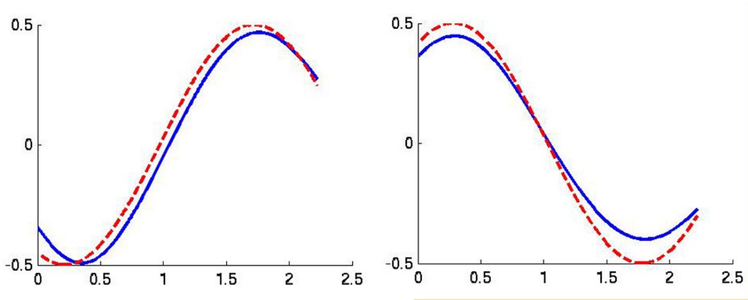

Figure 5. Optimal controls $u_x(t), u_y(t)$, for two external electromagnetic fields. Unified algorithm. Numerical solutions (blue continuous lines) for k=100. Analytical solutions (red dotted lines).

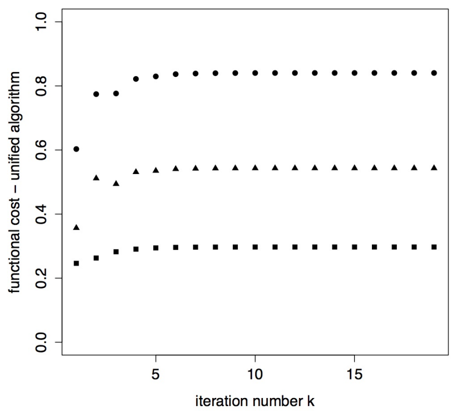

Figure 6. Evolution of the cost functional for two external electromagnetic fields case (dotted line with circles), unified algorithm. The fidelity component of the cost functional (dotted line with triangles). The pulse energy component of the cost functional (dotted line with squares).

In the first instance, one control 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 mentioned. The corresponding optimal control and the minimal cost were calculated. The results were compared with the analytical solution in each case. This is an elliptic function of Jacobi which is obtained by introducing two auxiliary controls and carrying up the system to one of the Duffing oscillator types and whose parameters depend on the initial conditions of the original problem. The limit of the recursive process is a function that takes the form of the elliptic function of Jacobi cosine type. The minimum value of the cost is close to that obtained in reports like [D'Alessandro, 2001]. Secondly, in the case of two controls, we have devised an algorithm that is a combination of the algorithms of H. Rabitz and V. F. Krotov and implement it to the mentioned problem of two controls. Again, the algorithm converges rapidly to known analytical solutions, which are sine and cosine functions. The minimum cost was calculated. This strategy yields a good performances in the case-study we have analyzed: we have compared with the analytic solution. Of course, a structured validation of the new algorithm is required. Finally, we consider very important the implementation and development of iterative numerical algorithms to solve quantum control problems in the case of a quantum multilevel.

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