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Time Optimal Control of Nonlinear Bloch Equations

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Abstract

We deal with time optimal control of nonlinear Bloch equations describing the influence of Coulomb parameters on particle dynamics. The dynamic is analyzed using tools of geometric optimal control theory. We present different time optimal syntheses by varying the parameters of a two energy levels quantum dots system. We show the nontrivial role of Coulomb parameters on the time minimal trajectories.

Keywords: Geometric optimal control, Optimal control synthesis, Quantum dots

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1. Introduction

Rapid advances in semiconductor technologies have led to the fabrication of very small semiconductors, called quantum dots. Due to the effects of quantum confinement, quantum dots act as artificial atoms, showing discrete levels of controllable electronic energies. These energy levels are arranged in the conduction and valence band, forming an accessible energy continuum. Inside the quantum dots several interactions occur such as the phenomena of attractions and repulsions between charged particles called Coulomb interaction. The Coulomb interaction is considered as a perturbation in quantum dots and plays a significant role in determining of the characteristics laser fields that are able to excite quantum levels for population transfer in quantum dots. In these recent years, quantum systems have been the subject of several studies. Indeed, in [1] from electron-hole modeling and by considering the Heisenberg formalism, the authors give a modeling of the quantum dots. In [9] the time minimal control problem of two-level dissipative quantum systems based on the Lindblad equation was studied. Also, in [2] the minimum time population transfer problem for a spin particle driven by a magnetic field on Bloch sphere, where the population dynamics are influenced by a parameter which depends on the maximum amplitude of control field and the energy level, was solved. In [7] the time minimal of control problem taking into account the dissipative terms and the effects of damping which act on the population dynamics was studied, the system is modeled by the nonlinear Bloch equation which one finds in Nuclear Magnetic Resonance.

Here, we consider the time optimal control problem of two energy levels quantums dots systems in presence of Coulomb interaction. This problem is modeled by a nonlinear Bloch equation. We give the minimal time trajectories

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using Pontryagin Maximum Principle and we show the nontrivial role of Coulomb parameters on particle dynamics. Applying recent developments in geometric optimal control, we realize different minimal time syntheses by varying the system parameters. The aim of the paper is to study the changes made by Coulombian effects on population dynamics taking into account inter-band transition frequencies of quantum dots. Some analyses of modifications of electrons dynamics due to the presence of Coulomb parameters are given (see Figure 1). Also, the time optimal syntheses in the cases when the Coulomb parameter is great than, and weak than transition frequency are presented (see Figure 2 and Figure 3, respectively).

The paper is organized as follows. In Section 2, we first introduce the nonlinear Bloch model for quantum dots for two-level quantum systems and we bring out an affine control system on the two-dimensional manifold S^2. We also present some tools of geometric optimal control theory on two-dimensional manifolds which allow to carry out the time optimal synthesis. Section 3 is devoted to the study of time optimal problem for the considered nonlinear Bloch model. The analysis of numerical simulations of the electron optimal trajectories and of the optimal synthesis of the considered control system is given.

2. Problem Formulation and Preliminaries

We consider the following nonlinear Bloch model [1] whose nonlinear terms come from Coulomb interaction.

$$i\hbar\dot{\rho}(t) = [H,\rho] + [V(\rho),\rho] \qquad (1),$$

where $\hbar$ is the constant of Plancks (we will assume $\hbar = 1$, in this paper), $\rho(t)$ is the density matrix which is hermitian, positive and with trace equal to 1. It represents pure and mixed quantum states if and only if trace$(\rho(t)^2) \leq 1$. The matrix $V(\rho)$ is the *Coulomb interaction matrix*, which is hermitian. The total hamiltonian $H = H_0 + H_L$, with H_0 is the free hamiltonian of the system and H_L is the hamiltonian of interaction between quantum dot and laser field.

In this paper, we consider the quantum dot as a quantum system with two energy levels. Write the density matrix $\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \overline{\rho_{12}} & 1-\rho_{11} \end{pmatrix}$, where $\overline{\rho_{12}}$ is the conjugate of ρ_{12}. For a two energy levels quantum system, we have [1] the Coulomb interaction matrix $V(\rho) = \begin{pmatrix} -R\rho_{11} & -R\rho_{12} \\ -R\overline{\rho_{12}} & R\rho_{11} \end{pmatrix}$, where R is *the Coulomb parameter* which is a real constant. To give the hamiltonian of the system we consider the case when the quantum dot is placed in a laser radiation modeled by an electromagnetic field. So we have $H=\begin{pmatrix} E_1^c & E(t)M \\ \overline{E(t)M} & E_2^v \end{pmatrix}$, where $E(t)$ is an electric field, M is a dipolar operator moment and $H_0 = \begin{pmatrix} E_1^c & 0 \\ 0 & E_2^v \end{pmatrix}$, where E_1^c and E_2^v are free energies for the conduction and valence band respectively. We write $E(t)M = \omega_1(t) + i\omega_2(t)$, where ω_1, ω_2 are the control functions which are real and bounded. Also, we assume that the *Rabi frequency* of laser field is equal to *transition frequency* $E_1^c - E_2^v$.

It is well known [5] that a good parametrization of the density matrix for two-level quantum system, which is hermitian, positive and of trace equal to 1, with only 3 real degrees of freedom, is given by using Pauli matrix and Bloch vector as follows :

$$\rho(x) = \frac{1}{2}(I_2 + \sum_{i=1}^{3} x_i\sigma_i),$$

where σ_i, $i \in \{1,2,3\}$ are Pauli matrix, I_2 is identity matrix of two order and $x =^t (x_1, x_2, x_3)$ is the column Bloch vector, that belongs to the unit ball $\left\{x \in \mathbf{R^3}, \| x \| \leq 1\right\}$. We get $x_1 = \rho_{12} + \overline{\rho_{12}}$, $x_2 = Im(\overline{\rho_{12}} - \rho_{12})$ and $x_3 = 2\rho_{11} - 1$. Clearly, $trace(\rho^2) = \frac{1}{2}(1 + \| x \|) = 1$ if $\| x \| = 1$ which means that all pure states are on the sphere S^2.

This parametrization $\rho(t) = \rho(x(t))$ in Equation (1) gives by simple calculations the following affine control system with two control functions $u_i(t) = 2\omega_i(t)$, $i \in \{1,2\}$:

$$\begin{cases} \dot{x}_1 = ((E_2^v - E_1^c) + R)x_2 - u_2x_3, \\ \dot{x}_2 = ((E_1^c - E_2^v) - R)x_1 - u_1x_3, \\ \dot{x}_3 = u_1x_2 + u_2x_1. \end{cases}$$

We clearly have that $x_1\dot{x}_1 + x_2\dot{x}_2 + x_3\dot{x}_3 = 0$, for any control functions $u_1(t)$ and $u_2(t)$. This implies $\|x(t)\| = \|x(0)\|$ and then if $\|x(0)\| = 1$ we get $\|x(t)\| = 1$ and then $x(t)$ belongs to the sphere S^2.

In this paper, we assume that $u_2 = 0$ and set $u_1 = u$, which means that the control field is real and the dynamics of electrons is only driven by the real control field u. Recall that the control is bounded and then there exist a real M such that $|u(t)| \leq M$. We obtain a single input affine control system of the form $\dot{x} = F(x) + uG(x)$, with $x \in S^2$ and $|u| \leq M$ as follows:

$$(\Sigma) : \quad \begin{cases} \dot{x_1} = ((E_2^v - E_1^c) + R)x_2, \\ \dot{x_2} = ((E_1^c - E_2^v) - R)x_1 - ux_3, \\ \dot{x_3} = ux_2. \end{cases}$$

We are interested in following time optimal problem:
we will find pair trajectory-control $(x(t), u(t))$ defined on $[0, T]$ joining an initial point $x(0) = x_0$ to a final point $x(T) = x_f$ in minimal time T.

2.1. Pontryagin Maximum Principle

We use some notions developed in the literature to solve time-optimal control problem for an affine system on two-dimensional manifolds, for more details see [3, 4, 8, 10]. The main tool is the Pontryagin Maximum Principle (PMP), here we give a version adapted to the affine control system

$$\dot{x} = F(x) + uG(x),\ x \in S^2 \text{ and } |u| \leq M$$

. It states [3] that the optimal trajectories are solutions of the following equations, for almost any $t \in [0, T]$:

1. $\dot{x}(t) = \frac{\partial H}{\partial p}(x(t), p(t), u(t))$ and $\dot{p}(t) = -\frac{\partial H}{\partial x(t)}(x(t), p(t), u(t))$,
2. $H(x(t), p(t), u(t)) = max_{v(t)\in[-M,M]} \{H(x(t), p(t), v(t))\}$, and
3. $H(x(t), p(t), u(t)) = 0$.

where,

$$H(x(t), p(t), v(t)) = p(t)(F(x(t)) + v(t)G(x(t)) + p_0,$$

with $p_0 \leq 0$ a constant and $p(t)$ is the nonzero line adjoint vector. If $p_0 \neq 0$ (resp. $p_0 = 0$), the trajectory is called a *normal extremal.* (resp. an *abnormal extremal*).

The maximization condition of the PMP gives that

$$max_{|v(t)|\leq M} \{H(x(t), p(t), v(t))\} = max_{|v(t)|\leq M} \{v(t)\Phi(t)\},$$

where $\Phi(t) = p(t)G(x(t))$ called the *switching function.* The analyze of $\Phi(t)$ gives a strategy of switching [3].

1. If $\Phi(t) > 0$ (resp. $\Phi(t) < 0$) for $t \in]t_1, t_2[\subset [0, T]$, then the optimal control is given by $u(t) = M$, (resp. $u(t) = -M$) and the solution of $\dot{x}(t) = (F + uG)(x(t))$ on the interval $]t_1, t_2[$ is a *bang* optimal trajectory.
2. If Φ vanishes in an isolated point with a nonzero derivative we get a *bang – bang* optimal trajectory as follows: Assume that for some $t \in]0, T[$, we have $\Phi(t) = 0$, $\dot{\Phi}(t)$ exists and $\dot{\Phi}(t) > 0$ (resp. $\dot{\Phi}(t) < 0$), then there exists $\varepsilon > 0$ such that $x(t)$ corresponds to the control $u = -M$ on $]t - \varepsilon, t[$ and $u = M$ on $]t, t + \varepsilon[$ (resp. $u = M$ on $]t - \varepsilon, t[$ and $u = -M$ on $]t + \varepsilon, t[$); so the trajectory is *bang-bang*, it is a concatenation of two *bang* trajectories.
3. On the other hand, if Φ vanishes on an interval $I = [t_1, t_2]$, we say that $x(t)$ is a singular extremal and the corresponding singular control u_s can be obtained by using the fact that the first and the second derivatives of with respect to time are zero. One can verify (see [3] for more details) that for $t \in I \subset [0, T]$,

$$\dot{\Phi}(t) = p(t)[F, G](x(t)) = 0.$$

Without loss of generality we can assume that $M = 1$ and $|u(t)| \leq 1$, (we normalize $u(t)$).

2.2. **Minimum time on the sphere S^2**

We consider the following functions and sets:

$$\Delta_1(x) = F(x) \wedge G(x) \text{ and } \Delta_2(x) = G(x) \wedge [F,G](x),$$

where $\wedge$ is vector product. The set $\Delta_1^{-1}(0) = \left\{x \in S^2 : \Delta_1(x) = 0\right\}$, called collinear locus (that is the set of points x, where $F(x)$ and $G(x)$ are parallel), it is useful for the study of abnormal trajectories, and the switching of abnormal extremal happens on the set $\Delta_1^{-1}(0)$. While the set $\Delta_2^{-1}(0) = \left\{x \in S^2 : \Delta_2(x) = 0\right\}$, called singular locus (that is the set of points x, where $G(x)$ and $[F,G](x)$ are parallel), it is used to locate singular trajectories and it is characterized by two types of subsets *turnpike* (resp. *antiturnpike*). The optimal singular locus is *turnpike* and can contain singular trajectory when the singular control, denoted by u_s is admissible ($|u_s| < 1$) [3]. Whereas, the non optimal singular locus is *antiturnpike*.

Recall that using the fact that on $\Delta_2^{-1}(0)$, we have

$$\Delta_2(x(t)) = 0, \text{ and then } \tfrac{\partial \Delta_2}{\partial x(t)} F(x(t)) + u(t) \tfrac{\partial \Delta_2}{\partial x(t)} G(x(t)) = 0.$$

This equality gives the singular control $u = u_s$.
Also, on the set $\{x \in S^2, x \notin \Delta_1^{-1}(0) \cup \Delta_2^{-1}(0)\}$, we have $(F(x), G(x))$ is a basis on the two-dimensional manifold and then we can write

$$[F,G](x) = f(x)F(x) + g(x)G(x),$$

with real scalar functions $f(x), g(x) \in \mathbf{R}$. So as $\Delta_2(x) = G(x) \wedge [F,G](x)$, we get

$$f(x) = -\frac{\Delta_2(x)}{\Delta_1(x)}.$$

The sign of f gives different domains that allow to specify when we can change the optimal control and characterize the switching time. Indeed, we have that if an optimal normal trajectory $(x(t), p(t))$ switches at a time $\bar{t} \in [0,T]$, then

$$\dot{\Phi}(\bar{t}) = f(x(\bar{t})).$$

Because we have $\Phi(\bar{t}) = p(t)G(x(\bar{t}))) = 0$ and $\dot{\Phi}(\bar{t}) = p(\bar{t})[F,G](x(\bar{t}))$. Then

$$\dot{\Phi}(\bar{t}) = p(\bar{t})(f(x(\bar{t})))F(x(\bar{t})) + g(x(\bar{t}))G(x(\bar{t}))) = f(x(\bar{t}))p(\bar{t})F(x(\bar{t})).$$

Using the condition (3) of the PMP,

$$H(x(t), p(t), u(t)) = p(t)(F(x(t) + u(t)G(x(t)) + p_0 = 0,$$

for almost any $t \in [0,T]$, we get $p(\bar{t})F(x(\bar{t})) = -p_0 = 1$ (for $p_0 \neq 0$ we can take $p_0 = -1$). Therefore, $\dot{\Phi}(\bar{t}) = f(x(\bar{t}))$.

Also if $f(x(\bar{t})) > 0$ (resp. $f(x(\bar{t})) < 0$), then the control can switch to the time $\bar{t}$ from $u = -1$ to $u = +1$ (resp. from $u = +1$ to $u = -1$).
Finally, the method to build the optimal synthesis is based on the properties of bang and singular trajectories. Also, under certain generic conditions, we know that there exists a finite number of bang and singular arcs contained in an optimally constructed trajectory [3, 8]. The synthesis is built recursively, by the number of extremal trajectory commutations.

3. Time optimal synthesis of the Bloch model

We apply the above notions to solve the time optimal control for our system (Σ). Denote by $-E_{21} = E_1^c - E_2^v$ the *inter-band transition frequencies*, and set $a = -E_{21} - R$. We will assume that $a \neq 0$.

$$(\Sigma) \quad \dot{x_1} = -ax_2\ ,\ \dot{x_2} = ax_1 - ux_3 \ \ \textit{and} \ \ \dot{x_3} = ux_2.$$

(Σ) is a single input affine control system (bilinear system) of the form $\dot{x} = F(x) + uG(x)$, with $x \in S^2$, $|u| \leq 1$, $F(x) = Ax$ and $G(x) = Bx$,

where $A = \begin{pmatrix} 0 & -a & 0 \\ a & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$.

The associated hamiltonian to (Σ) is given by:

$$H(x, p, u) = p(t)(A + uB)x(t) + p_0 = -ax_2p_1 + ax_1p_2 + u(t)(p_3x_2 - x_3p_2) + p_0.$$

The adjoint equation is $\dot{p}(t) = -p(t)(A + uB)$ with

$$\dot{p}_1(t) = -ap_2, \quad \dot{p}_2(t) = ap_1 - up_3 \quad and \quad \dot{p}_3(t) = up_2.$$

The switching function is $\Phi(t) = p(t)G(x(t)) = p(t)Bx(t) = p_3x_2 - p_2x_3$. If $\Phi(t) \geq 0$ (resp. $\Phi(t) \leq 0$) then the optimal control is $u = 1$ (resp. $u = -1$).

Proposition 3.1. *The bang optimal trajectories corresponding to the optimal controls $u = 1$ or $u = -1$ are*

$$x(t) = e^{t(A+uB)}x(0) \text{ and } p(t) = p(0)e^{-t(A+uB)}.$$

The switching function is

$$\Phi(t) = p(t)Bx(t) = p(0)e^{-t(A+uB)}Be^{t(A+uB)}x(0).$$

Proof We have $\dot{x}(t) = (A + uB)x(t)$ and $\dot{p}(t) = -p(t)(A + uB)$. Then

$$x(t) = e^{t(A+uB)}x(0) \quad and \quad p(t) = p(0)e^{-t(A+uB)}.$$

By simple calculations we get the matrix $e^{t(A+uB)}$ for any real constant u (in particular for the optimal control $u = 1$ or $u = -1$). Set $w = \sqrt{a^2 + u^2}$

$$e^{t(A+uB)} = \begin{pmatrix} \frac{u^2+a^2cos(wt)}{w^2} & \frac{asin(wt)}{w} & \frac{-au(1-cos(wt))}{w^2} \\ \frac{asin(wt)}{w} & cos(wt) & \frac{usin(wt)}{w} \\ \frac{-au(1-cos(wt)}{w^2} & \frac{usin(wt)}{w} & \frac{a^2+u^2cos(wt)}{w^2} \end{pmatrix}.$$

Notice that using the switching function one can find times of commutation and present the extremal trajectories for a given parameter a. Here, the aim of the paper is to represent the dynamics of electrons by varying the Coulomb parameter R ($a = -E_{21} - R$) and to give a numerical synthesis.

3.1. Analysis of dynamics

We consider two quantum dots D_1 and D_2 corresponding to two different inter-band transition frequency values given respectively in [11] and [6] by $-E_{21} = 0.287$ for D_1 and $-E_{21} = 0.154$ for D_2. We choose R great and weak than the transition frequency $-E_{21}$, namely $R = -10E_{21}$ and $R = -\frac{1}{10}E_{21}$.

To achieve our simulation we consider an optimal control field $u = -1$ and for each quantum dot, we represent the dynamics of an electron by varying the Coulomb parameter R. We can analyze the influence of the parameter $a = -E_{21} - R$ of (Σ) on the electrons dynamics for the two quantum dots. The two yellow points represent north pole and south pole of Bloch sphere. We specify these two points because in the process of population transfert from the first state to second state in two-level quantum system modeled by Bloch sphere, the north pole represent the first state of the system and denoted by the point $(0, 0, 1)$ and the second state is represented by south pole and denoted by the point $(0, 0, -1)$.

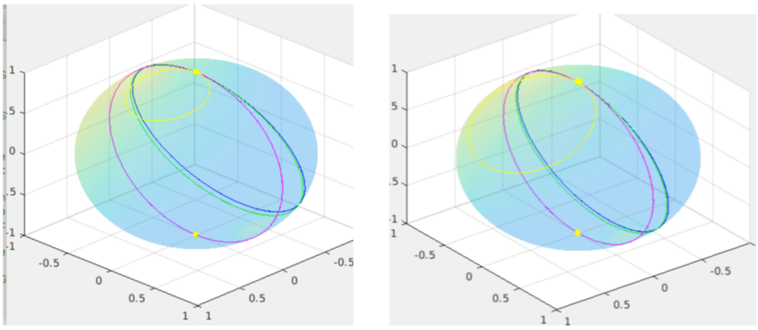

Figure 1. (Color online) D_1 left side; D_2 right side. $R = -10E_{21}$ corresponds to the yellow curve, $R = -\frac{1}{10}E_{21}$ the green curve, $R = -E_{21}$ the magenta curve and $R = 0$ the blue curve.

In each figure, we notice that there is a great separation between blue and yellow curves. Also, yellow curve passes very far from south pole so that means that electron trajectory is greatly modified when Coulomb parameter is greatly added to the transition frequencies, it greatly affects the transfert of population. Secondly, the magenta curve deviate from blue curve and passes at south pole that means that when Coulomb parameter is equal to inter-band frequencies it greatly contribute to the transfert of population. Finally, we see that the green curve is very close to blue curve that means that when Coulomb parameter is weakly add to inter-band frequencies it doesn't bring enough modifications to the system able to affect a transfert of population.

3.2. Construction of time-optimal synthesis

The following propositions present a time optimal synthesis which involves Coulomb parameter R for quantum dot D_1. The case D_2 is similar.
Denote by x^+ and x^- the *bang* trajectories of (Σ) corresponding to $u = 1$ and $u = -1$ respectively. Singular trajectory is denoted by S.

Proposition 3.2. *Consider System* (Σ) *when* $-E_{21} = 0.287$ *and* $R = -10E_{21} = 2,87$. *Then:*

1. *a normal optimal trajectory starting from north pole and reaches a point over the plan* $x_3 = 0$ *is a finite concatenation of bang trajectories of the form* x^-; x^-x^+; $x^-x^+x^-$; $x^-x^+x^-x^+$ *and* $x^-x^+x^-x^+x^-$.

2. *every optimal abnormal trajectory switches at most five times before loses its optimality and the final bang-bang arc has the form* $x^-x^+x^-x^+x^-x^+$.

Proof : One can verify that $\Delta_1(x) = ax_2x$ and $\Delta_2(x) = -ax_3x$ with $x \in S^2$. Clearly, $\Delta_1^{-1}(0) = \{x_2 = 0\} \cap S^2$ and $\Delta_2^{-1}(0) = \{x_3 = 0\} \cap S^2$. Also, $f(x) = \frac{x_3}{x_2}$, where $x_2 \neq 0$ and $x_3 \neq 0$. It is easy to give the sign of f. We know that a normal trajectory solution of control system (Σ) can bifurcate at a possible switching time $\bar{t}$ if $\dot{\Phi}(\bar{t}) = \frac{x_3(\bar{t})}{x_2(\bar{t})}$, where $x_2(\bar{t})x_3(\bar{t}) \neq 0$.
We analyze the behavior of optimal trajectories in four areas depending on the sign of $f(x) = \frac{x_3}{x_2}$, $x_2 \neq 0$ and $x_3 \neq 0$. Set $d_1 = \left\{x \in S^2 : x_3 > 0; x_2 > 0\right\}$ and $d_2 = \left\{x \in S^2 : x_3 > 0; x_2 < 0\right\}$. From d_1 (resp. d_2) we get d_3 (resp. d_4) by taking $x_3 < 0$.
Along a normal optimal extremal with control $u = -1$ denoted by x^-, starting from north pole, switching can happen when it enters in the area d_1 at a certain time $\bar{t}$ from $u = -1$ to $u = +1$ because $\dot{\Phi}(\bar{t}) > 0$. A normal optimal extremal x^+ corresponding to the control $u = +1$ can not bifurcate from x^- in d_2, because in this part we have $\dot{\Phi}(\bar{t}) < 0$. When the trajectory x^- it self-intersects it loses its optimality.
• The trajectory x^+ bifurcating from the point $x^-(\bar{t})$ in d_1 can switch from $u = +1$ to $u = -1$ in the area d_2 at time $\overline{t_1} > \bar{t}$ due to $\dot{\Phi}(\overline{t_1}) < 0$. When the trajectory x^- is intersected in the area d_2 by trajectory x^+ coming from the point $x^-(\bar{t})$, it loses its optimality at the intersection point called a locus point.

• Trajectory x^- coming from point $x^+(\overline{t_1})$ in the area d_2 can switch from $u = -1$ to $u = +1$ in d_1 at a time $\overline{t_2} > \overline{t_1}$ due to $\dot{\Phi}(\overline{t_2}) > 0$ in this area.
• The trajectory x^+ bifurcating from the point $x^-(\overline{t_2})$ in d_1, is no longer optimal when it intersects a trajectory x^- located at the top of the Bloch sphere, as it is shown in left figure in Figure 2. This intersection point corresponds to a cut locus point.
• Therefore, when trajectory x^+ doesn't intersect a trajectory x^- located at the top of the Bloch sphere, it can switch at certain time $\overline{t_3} > \overline{t_2}$ when it enters in the area d_2 due to the fact that $\Phi(\overline{t_3}) < 0$, and the trajectory x^- bifurcating from the point $x^+(\overline{t_3})$ in d_2 is no longer optimal when it intersects a trajectory x^+ at a cut locus point in the same area.
• There is no optimal trajectory that reaches the south pole. There is not optimal singular trajectory. The left figure in Figure 2 represented optimal synthesis for normal trajectories described above. All the locus points are represented by magenta color.
• If a optimal extremal x^- starting from north pole with control $u = -1$ is abnormal then switching can happen on $\{x_2 = 0\} \cap S^2$. Therefore we see that trajectory makes half turn when it reaches the set $\{x_2 = 0\} \cap S^2$, so switching happen at the time $t = \pi$. After five switching, trajectory loses its optimality at a cut locus point represented with magenta color in Figure 1 at right side.

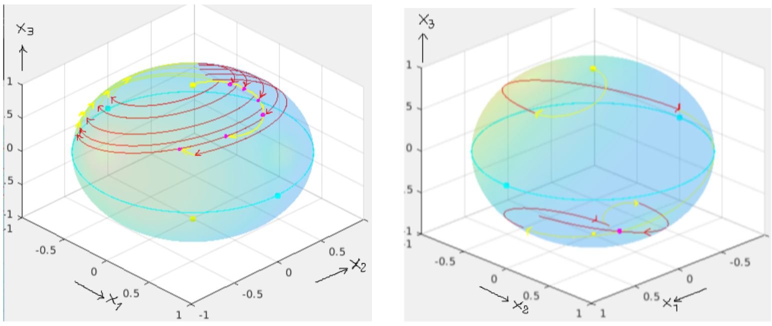

Figure 2. (Color online) Red and yellow color curves are for $u = +1$ and $u = -1$ respectively, the cyan curve is singular locus. In left figure: Normal *bang and bang-bang* optimal trajectories. In the right figure: Abnormal *bang-bang* optimal trajectory.

The previous proposition describes the possible optimal trajectories when Coulomb parameter greatly acts on transition frequency. In the following proposition, let us consider the case where Coulomb effect is relatively small than transition frequency.

Proposition 3.3. *Consider System* (Σ) *when* $-E_{21} = 0.287$ *and* $R = -\frac{1}{10}E_{21} = 0,0287$. *Then:*

1. *a normal optimal trajectory starting from north pole is finite concatenation of bang and singular trajectories of the form* x^-; x^-S; x^-Sx^+; x^-Sx^- *and* $x^-x^+x^-$.

2. *every optimal abnormal trajectory switches at most thirteen times before it loses its optimality and the final bang-bang arc has the form* $x^-x^+ ... x^-x^+$.

Proof : Recall that, the functions f and $\dot{\Phi}$ are defined by, $f(x) = \frac{x_3}{x_2}$, $\dot{\Phi}(\bar{t}) = \frac{x_3(\bar{t})}{x_2(\bar{t})}$. Also, one can easily verify that the singular admissible control is $u_s = 0$. We use the same techniques as in the previous proposition to describe the optimal trajectories in the different areas by using the sign of f. But the difference here is that the trajectory x^- coming from north pole cross the *turnpike* singular locus and along this trajectory switching can happen from $u = -1$ to $u = 1$ in area d_4 due to $\dot{\Phi} > 0$. Furthermore, let $\bar{t}$ the first time at which it reaches this singular locus at point $x^-(\bar{t}) = \bar{x}$, switching can happen from $u = -1$ to $u = +1$ at the point $\bar{x}$ in a small neighborhood of $\bar{x}$ in d_1 or the control becomes singular. Trajectory x^+ coming from the point $\bar{x}$ passes by the south pole, so the south pole is reached by optimal *bang-bang* trajectory. On the other hand, singular locus can contain optimal singular trajectory and this one is guiding by control $u_s = 0$. If an optimal extremal x^- starting from north pole with control $u = -1$ is abnormal switching happen at time $t = \pi$ on $\{x_2 = 0\} \cap S^2$. By simulation on Figure 2 at right side, this trajectory loses its optimality after thirteen switching.

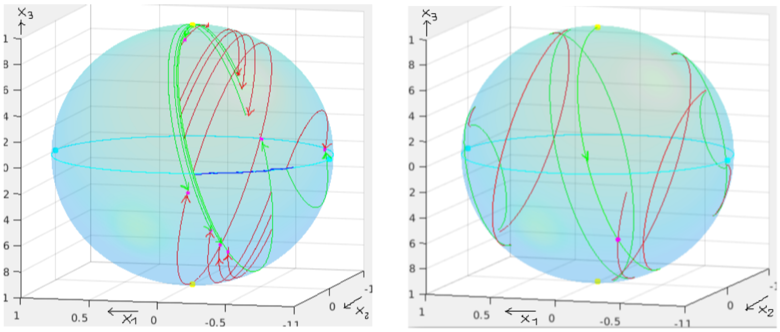

Figure 3. (Color online) Red and green color curves are for $u = +1$ and $u = -1$ respectively, blue curve is singular optimal trajectory. The cyan curve is singular locus and magenta color points are cut locus points. Left figure: Normal *bang-bang; bang and singular* optimal trajectories. Right figure: Abnormal *bang-bang* optimal trajectory, magenta color point is cut locus point.

Consider the remaining case when $-E_{21} = R$. Clearly, if $a = -E_{21} - R = 0$, then the optimal trajectory x^- coming from north pole is contained in the circle $\{x_1 = 0\} \cap S^2$ because in System (Σ) we get $\dot{x}_1 = 0$ and $x_1(0) = 0$. So the technique used previously for the description of optimal trajectories on two-dimensional manifold is no longer applicable here. The south pole is optimally reach at time $t = \pi$ by the trajectory x^- because this trajectory makes a half turn until reaching the south pole. The optimal control field steering the electron to north pole to the south one is only *bang*.

4. Conclusion

In this paper, using the nonlinear Bloch model, we have provided an optimal synthesis, taking into account the disturbance of Coulomb parameter on *transition frequency*. For the value of Coulomb parameter greater than *transition frequency*, we show that there is no optimal trajectories that reach south pole and all the optimal trajectories are only *bang-bang*. When Coulomb parameter value is weaker than *transition frequency* optimal synthesis exhibits optimal trajectories containing singular trajectory, moreover, we have found in this case that there are optimal trajectories steering the system state from north pole to reach south pole.

From practical point of view, the results given in *proposition 3.2 and proposition 3.3* could allow to understand two essential points in the physical frame. First of all, in the design of resonant laser fields for population inversion in two-level quantum system when the transition frequency is strongly disturbed by the Coulomb energy, *i.e.* $-E_{21} < R$, this may not allow a population inversion. Then when Coulomb's energy is weakly added to the transition frequency such that $-E_{21} > R$, a population transfer can be carried out. Therefore, Coulomb energy can have a bad effect on population inversion or a factor that contributes to population inversion when its influence on the *transition frequency* is minimal.

In a futur work we are interesting in the study of the above system with two controls. We also study the model (1) with three energy levels.

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