Optimal control of a three-level quantum system by laser fields plus von Neumann measurements

D. Sugny^{*} and C. Kontz

Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9 Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex,

France

(Received 28 March 2008; published 24 June 2008)

We investigate the control of a three-level quantum system by laser fields assisted by von Neumann measurements. We consider a system which is not completely controllable by unitary evolution but which becomes controllable if particular measurements are used. The optimal control is defined from a cost functional which takes into account the measurements. The cost corresponds either to the minimization of the duration of the control or to the minimization of the energy of the laser field. Using the Pontryagin maximum principle, we determine the optimal control which steers the system from a given initial state toward a desired target state. This allows one to determine which observable has to be chosen for the measurement and the time at which the measurement has to be performed.

DOI: 10.1103/PhysRevA.77.063420

PACS number(s): 32.80.Qk, 03.65.Yz, 78.20.Bh

I. INTRODUCTION

Geometric control theory has a long history dating back to the 17th century and the Euler-Lagrange equation, which leads to the classical calculus of variations. The interest for this theory has been renewed since the complete proof of the Pontryagin maximum principle (PMP) in the late 1950s [1-3]. This theorem is, for example, the main tool allowing us to determine an optimal laser field which achieves the objective of the control and which minimizes a given cost functional as the energy of the pulse or its duration [3-5]. The PMP has been applied for controlling both classical and quantum dynamics. For quantum systems with multiple degrees of freedom, the optimal equations are generally solved by purely numerical techniques such as the monotonically convergent algorithms [6-8]. These approaches have been largely explored for molecular systems [9–14]. More geometrical aspects of the control can be formulated only for simple quantum systems having, for instance, few levels. In recent years, a large amount of works dealing with the geometric control of closed quantum systems has been published [15–24]. Recently, these tools have also been applied to dissipative quantum systems, which present the difficulty to have a pure drift term due to dissipation [25,26]. Finally, we point out that all these geometrical tools allow us to answer some physical questions such as the fact that optimality implies resonance [27] or the benefit that can be gained from dissipation [25,26].

The aim of this paper is to study another aspect of geometric control of quantum systems, i.e., the control by laser fields assisted by von Neumann measurements (VNMs) [28]. The VNMs can be classified into two types: the instantaneous measurements and the continuous ones. Among instantaneous measurements, we also distinguish the selective ones where the state after the measurement is known (with a given probability) and the nonselective ones where this state is unknown [29]. In this paper, we will only consider selective instantaneous measurements. The question of measurement driven quantum evolution has already been discussed in a series of works mainly from a numerical point of view [29–34], either with or without a laser field assisting the control. In particular, it has been shown that the measurement process can modify the characteristics of the optimal laser field. We propose in this work to revisit this problem by using the PMP and a more geometrical point of view. For that purpose, we consider a very simple problem, the control of a three-level system. The interaction with the laser field consists of a dipolar interaction with constant dipolar terms coupling only neighboring states. It is known that this type of system is not completely controllable by unitary evolution, the dynamical Lie algebra being so(3) [35]. This point can be understood more geometrically as follows. We show in this paper that the dynamics evolves on the manifold $S^2 \times S^2$. A quantum state is described by one point on each sphere. The radius of each sphere depends on the state we consider. The simplest case corresponds to the case where one radius is equal to 1 and the other to 0. We can then assume that the quantum state only belongs to one sphere since the dynamics on the other sphere is trivial. In this case, if only unitary controls are used then the state will remain on this sphere and the system will not be controllable. The question of controllability of quantum systems subject to VNMs has been analyzed in Ref. [36]. It has been shown that systems which are not completely controllable with a so(N) dynamical Lie algebra become controllable by the action of particular VNMs. Note, however, that a judicious choice of the measured observable in relation with the target state has to be made. In the context of our problem, this remark can be expressed as follows. We consider an initial state and a target state belonging to two different spheres (in the sense detailed above), respectively S_i and S_f , and we choose an observable Q whose measure allows passage from S_i to S_f . This is possible if all the eigenvectors of Q belong to S_{f} . We thus see that the introduction of measurements allows us to create a path from the initial state to the target state but does not say nothing about the way to reach it. More precisely, we can ask several questions on this control: Which observable Q to use, at which time to perform the measurement, and which control fields to use. To answer these questions, we define a cost functional taking into account the VNMs and we introduce the PMP to determine the optimal laser field. We assume that according to the result of the measurement, the operator can modify the laser field applied to the system.

The paper is organized as follows. In Sec. II, we introduce the model system and the different approximations used. Section III details the geometrical aspect of the control and the way the VNM acts. We formulate in Sec. IV the PMP with a cost functional suited to the control. The cost corresponds either to the minimization of the duration of the control or to the minimization of the energy of the laser field (the duration of the control being fixed). In Sec. V, we solve the PMP and we determine the optimal controls. Conclusion and prospective views are given in Sec. VI. Some technical calculations on the Grusin model [3,26,37] are reported in the Appendix.

II. THE MODEL SYSTEM

We consider a three-level quantum system whose dynamics is governed by the Schrödinger equation. The system is described by a pure state $|\psi(t)\rangle$ belonging to a threedimensional Hilbert space \mathcal{H} . The time evolution of $|\psi(t)\rangle$ is given by

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = [H_0 + E_1(t)H_1 + E_2(t)H_2]|\psi(t)\rangle, \qquad (1)$$

where H_0 is the field-free Hamiltonian defined in matrix form as

$$\begin{pmatrix} -E_0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & E_0 \end{pmatrix}.$$
 (2)

 H_1 and H_2 read in the eigenbasis of H_0 as

$$H_1 = d \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad H_2 = d \begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix}, \tag{3}$$

where *d* is a real constant. Equation (1) is written in units such that $\hbar = 1$. A basis of \mathcal{H} is given by the eigenvectors $|1\rangle$, $|2\rangle$, and $|3\rangle$ of H_0 . $E_1(t)$ and $E_2(t)$ are two real components of the electric field along two orthogonal directions of polarization. $E_1(t)$ and $E_2(t)$ are assumed to be in resonance with the frequency E_0 . It has been shown that optimality implies resonance for three-level systems [27]. In the RWA approximation, the equation for the time evolution of $|\psi(t)\rangle$ can be written as

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \begin{pmatrix} 0 & ue^{iE_{0}t} & 0\\ u^{*}e^{-iE_{0}t} & E_{0} & ue^{iE_{0}t}\\ 0 & u^{*}e^{-iE_{0}t} & 2E_{0} \end{pmatrix} |\psi(t)\rangle, \quad (4)$$

where u is the complex Rabi frequency. In the interaction representation, Eq. (4) becomes

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \begin{pmatrix} 0 & u_1 + iu_2 & 0\\ u_1 - iu_2 & 0 & u_1 + iu_2\\ 0 & u_1 - iu_2 & 0 \end{pmatrix} |\psi(t)\rangle, \quad (5)$$

where u_1 and u_2 are, respectively, the real and imaginary parts of the complex Rabi frequency. We keep the same notation for the state $|\psi(t)\rangle$ after this transformation. The interaction representation means here that we have performed the unitary transformation U to the state $|\psi(t)\rangle$:

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-iE_0 t} & 0 \\ 0 & 0 & e^{-2iE_0 t} \end{pmatrix}.$$
 (6)

Note that this transformation allows us to eliminate the drift term due to the field-free Hamiltonian H_0 [15].

We denote by c_1 , c_2 , and c_3 the complex coefficients of the state $|\psi(t)\rangle$ in the basis $\{|1\rangle, |2\rangle, |3\rangle\}$. We introduce the real coefficients x_i ($i \in \{1, 2, ...6\}$) defined by

$$c_1 = x_1 + ix_2, \quad c_2 = x_3 + ix_4, \quad c_3 = x_5 + ix_6.$$
 (7)

Let **x** be the six-dimensional vector of coordinates x_i . Equation (6) reads in a more compact form as

$$\dot{\mathbf{x}} = u_1 F_1 + u_2 F_2, \tag{8}$$

where F_1 and F_2 are the vector fields

$$F_{1} = \begin{pmatrix} x_{4} \\ -x_{3} \\ x_{2} + x_{6} \\ -x_{1} - x_{5} \\ x_{4} \\ -x_{3} \end{pmatrix}, \quad F_{2} = \begin{pmatrix} x_{3} \\ x_{4} \\ x_{5} - x_{1} \\ x_{6} - x_{2} \\ -x_{3} \\ -x_{4} \end{pmatrix}.$$
(9)

The dynamics takes place on a five dimensional sphere S^5 since $\sum_{i=1}^{6} x_i^2 = 1$.

III. GEOMETRICAL DESCRIPTION OF THE CONTROL

We begin this section by analyzing the controllability of the process. In matrix form, this can be done by computing the dynamical Lie algebra \mathcal{L} generated by iH_0 , iH_1 , and iH_2 . A standard calculation shows that $\mathcal{L}=so(3)$ and that the system is not completely controllable [35]. We recall that a possible characterization of a matrix A with complex entries belonging to so(3) [38] is

$$A \in \operatorname{so}(3) \Leftrightarrow \begin{cases} A = -A \dagger \\ AJ + JA = 0, \end{cases}$$
(10)

where J is the matrix

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$
 (11)

The noncomplete controllability of the system can be understood more geometrically as follows. We define new coordinates X_i by

$$X_{1} = \frac{1}{\sqrt{2}}(x_{1} - x_{5}), \quad X_{2} = \frac{1}{\sqrt{2}}(x_{1} + x_{5}),$$
$$X_{3} = x_{3}, \quad X_{4} = x_{4}, \quad X_{5} = \frac{1}{\sqrt{2}}(x_{2} + x_{6}), \quad X_{6} = \frac{1}{\sqrt{2}}(x_{2} - x_{6}).$$
(12)

For any choice of the controls u_1 and u_2 in Eq. (8), only the coordinates $\{X_1, X_3, X_5\}$ and $\{X_2, X_4, X_6\}$ are coupled between each other. In addition, they fulfill the following relations:

$$X_1^2 + X_3^2 + X_5^2 = R_i^2, \quad X_2^2 + X_4^2 + X_6^2 = R_f^2,$$
(13)

where R_i and R_f are two real constants such that $R_i^2 + R_f^2 = 1$. The system thus evolves on two spheres that we denote S_i and S_f . The radii R_i and R_f of the two spheres are determined from the initial state of the system and are constant for unitary evolution. To simplify the geometrical description of the control, we consider in this paper that one radius is equal to 1 and the other to 0. In this case, we can assume that the state belongs only to one sphere since the dynamics on the other sphere is trivial. Using this description, one deduces that if the system is initially on one of the two spheres then it will remain on this sphere by unitary evolution and it will not reach a state belonging, for instance, to the other sphere. The description of the control is more difficult if the two radii are different from zero. In particular, due to the symmetry of Eq. (8), the optimal trajectories on the two spheres are the same and cannot be controlled independently.

We now describe the control assisted by measurements. As explained above, we assume that the initial and the target states belong, respectively, to S_i and S_f . We can choose, for instance, $|\psi_i\rangle = |2\rangle$ and $|\psi_f\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |3\rangle)$. For the measurement process, the idea is to determine an observable Q for which the system passes from S_i to S_f after a measurement. This is possible if all the eigenvectors of Q belong to S_f and form a basis of \mathcal{H} . A possible choice is given by the vectors

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |3\rangle), \quad |\phi_2\rangle = i|2\rangle, \quad |\phi_3\rangle = \frac{i}{\sqrt{2}}(|1\rangle - |3\rangle).$$
(14)

The corresponding observable Q is equal to $Q = \sum_{i=1}^{3} q_i |\phi_i\rangle \langle \phi_i|$ where the q_i 's are real numbers. Let $|\psi\rangle = \sum_{i=1}^{3} a_i |\phi_i\rangle$ be the state of the system at time t. Then after the measurement, this state becomes $|\phi_i\rangle$ ($i \in \{1, 2, 3\}$) with the probability $|a_i|^2$. Since all the eigenvectors of Q belong to S_f , the sphere of the target state, one sees that, whatever the result of the measurement, the target state can now be reached by unitary evolution. Note also that the control by laser field on the sphere S_f will depend on the result of the measurement. As mentioned in the Introduction, we assume that the operator knows this result and can modify the control field according to the result of the measurement.

IV. PONTRYAGIN MAXIMUM PRINCIPLE AND COST FUNCTIONAL

We analyze the optimal control of this three-level system either with the constraint of minimizing the duration of the control or the energy of the laser field. The solutions of these two problems are intrinsically related [15]. We recall that this is not the case when the system has a purely drift term which can be due to dissipation [25,26].

We denote by $U \subset \mathbb{R}^2$ the manifold of admissible control fields. For the time minimum cost, we have the condition $u_1^2 + u_2^2 \leq 1$ on the control field, whereas there is no restriction on laser fields if the cost minimizes the energy. The total duration *T* of the control is fixed for the energy cost problem.

We begin by the standard formulation of the Pontryagin maximum principle, i.e., without measurement. The Pontryagin maximum principle [1,2,4] is formulated from the pseudo-Hamiltonian H_P which can be written as follows:

$$H_p = \mathbf{p} \cdot (u_1 F_1 + u_2 F_2) + p_0 f_0(u_1, u_2), \tag{15}$$

where $\mathbf{p} \in \mathbb{R}^6$ is the adjoint state and p_0 is a negative constant such that \mathbf{p} and p_0 are not simultaneously zero. f_0 is a function of u_1 and u_2 whose integral over time gives the associated cost *C*. We have

$$C_E = \int_0^T f_0(u_1(t), u_2(t)) dt = \int_0^T \left[u_1^2(t) + u_2^2(t) \right] dt \quad (16)$$

for the energy minimization problem and

$$C_T = \int_0^T dt = T \tag{17}$$

for the time-minimum optimal control. The Pontryagin maximum principle states that the coordinates of the extremal vector state \mathbf{x} and of the corresponding adjoint state \mathbf{p} fulfill the Hamiltonian's equations associated to a Hamiltonian H,

$$\dot{\mathbf{x}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{x}},$$
 (18)

defined as

$$H(\mathbf{x},\mathbf{p}) = \operatorname{Max}_{\{u_1,u_2\} \in U} H_P(\mathbf{x},\mathbf{p},u_1,u_2).$$
(19)

The optimal controls are given explicitly by

$$u_1^E = P_1, \quad u_2^E = P_2$$
 (20)

and

$$u_1^T = P_1 / \sqrt{P_1^2 + P_2^2}, \quad u_2^T = P_2 / \sqrt{P_1^2 + P_2^2},$$
 (21)

where $P_1 = \mathbf{p} \cdot F_1$ and $P_2 = \mathbf{p} \cdot F_2$ [3]. The *E* and *T* labels correspond, respectively, to the energy and the time cost cases.

We assume now that a measurement is performed at a time $t \in [0, T]$. The definition of the cost given below can be extended straightforwardly to the case of several measurements. Let $Q = \sum_{i=1}^{3} q_i |\phi_i\rangle\langle\phi_i|$ be the observable associated to the measurement. We denote by $|\psi(t)\rangle$ the state of the system at time t at which the measurement is performed. Since $\{\phi_i\}_{i=1,...,3}$ is a basis of \mathcal{H} , $|\psi(t)\rangle$ can be written as

$$|\psi(t)\rangle = \sum_{i} a_{i}(t) |\phi_{i}\rangle.$$
(22)

Let $C_0(t)$ be the cost corresponding to the optimal path from $|\psi_i\rangle$ to $|\psi(t)\rangle$. Note that C_0 is equal to zero if t=0. We also

introduce the costs C_i , (i=1,...,3) which are respectively associated to the optimal passage from $|\phi_i\rangle$ to $|\psi_j\rangle$. The total cost of the control C(t) is then defined by

$$C(t) = C_0(t) + \sum_{i=1}^{3} |a_i(t)|^2 C_i.$$
 (23)

The choice of C(t) is related to the fact that the operator knows the result of the measurement and can modify the electric field accordingly. $\sum_{i=1}^{3} |a_i(t)|^2 C_i$ can be viewed as an average of the three costs C_i . From the cost C(t), the goal is then to determine the control fields, the observable Q and the time t at which the measurement is performed to minimize C(t). We will solve this problem by using twice the Pontryagin maximum principle: once on S_i and once on S_f . Indeed, for a fixed observable Q, it is clear that the trajectories which minimize C correspond to the concatenation of extremal trajectories on S_i and S_f . We solve this optimal control problem in Sec. V for particular examples. The general solution is very complex and can only be determined numerically.

V. OPTIMAL CONTROL

A. Preliminary

To describe the dynamics of the system on the two spheres, we introduce two sets of spherical coordinates (θ_i, ϕ_i) and (θ_f, ϕ_f) such that

$$X_1 = \sin \theta_i \cos \phi_i, \quad X_3 = \cos \theta_i, \quad X_5 = \sin \theta_i \sin \phi_i$$
(24)

and

$$X_2 = \sin \theta_f \cos \phi_f, \quad X_4 = \cos \theta_f, \quad X_6 = \sin \theta_f \sin \phi_f.$$
(25)

Due to the hypothesis of Sec. III, the solution of the optimal control problem corresponds to the one of the Grusin model on the sphere [3,26,37]. The Grusin model is a standard problem in optimal control and its solutions are recalled in the Appendix. Note that this model appears naturally when one considers a three-level system in quantum mechanics [15].

We consider four different qualitative cases of control. We recall that the initial state and the target state belong, respectively, to S_i and S_f .

Case (a). Passage from $X_3=1$ to $X_4=1$, i.e., from the state $|2\rangle$ to the state $i|2\rangle$ (modification of the phase of the state $|2\rangle$). The measurement operator is not fixed but allows passage from S_i to S_f .

Case (b). Passage from $X_3=1$ to $X_2=1$. We assume that the operator Q is of the form

$$Q = \frac{i}{\sqrt{3}} (\alpha |1\rangle \langle 1| + \beta |2\rangle \langle 2| + \gamma |3\rangle \langle 3|), \qquad (26)$$

where α , β , and γ are real constants.

Case (c). Passage from a state of S_i to the state $(\theta_f = \pi/2, \phi_f = \alpha)$ where $\alpha \in [0, 2\pi]$. The states associated to the measurement are given by $(\theta_f = \pi/4, \phi_f = 0)$, $(\theta_f = 3\pi/4, \phi_f)$



FIG. 1. Optimal synthesis for an initial state such that $\theta_i(0)=0$. θ and ϕ are two angles in radians.

=0), and $(\theta_f = \pi/2, \phi_f = \pi/2)$. The angle α is chosen such that the cost to reach the target state from one of the three states of the measured observable is the same. In this symmetric case, the optimal trajectory does not depend on the initial state.

Case (*d*). Passage from $|\psi_i\rangle = |1\rangle$ to $|\psi_f\rangle = e^{i\pi/4}/2|1\rangle + i\sqrt{2}|2\rangle + e^{-i\pi/4}/2|3\rangle$, i.e., $(\theta_f = \pi/4, \phi_f = \pi/4)$. The three states associated to the measurement are $(\theta_f = 0, \phi_f = 0)$, $(\theta_f = \pi/2, \phi_f = 0)$, and $(\theta_f = \pi/2, \phi_f = \pi/2)$.

B. Case (a)

We first solve the optimal control problem on S_i starting from $X_3=1$. This initial point is characterized by $\theta_0=0$. Using the results of the Appendix, one deduces that the extremal trajectories are associated to the value of the conserved integral of motion j=0. The case $\theta_0=0$ corresponds to a degenerate case which is not well defined if $j \neq 0$ [3,26]. From Eqs. (A14), it is then straightforward to see that the optimal trajectories are lines of equation $\phi_i=$ const. The optimal synthesis, i.e., all the extremals starting from the initial point, is represented in Fig. 1. Using Eqs. (A12), one can determine the corresponding control fields v_1 and v_2 which are given by

$$v_1 = 1, \quad v_2 = 0 \tag{27}$$

for the time-minimum problem and by

$$v_1 = \sqrt{2h_E}, \quad v_2 = 0,$$
 (28)

where $h_E > 0$ for the energy minimization problem. Let (θ_i, ϕ_i) be the coordinates of the final point on S_i . For the minimization of the time, since $\dot{\theta} = 1$, one deduces that $C_{T,0} = \theta_i$. For the energy case, we have

$$C_{E,0} = \int_0^T 2h_E dt = 2h_E T.$$
 (29)

But since $\theta_i = \sqrt{2h_E}T$, this leads to $C_{E,0} = \theta_i^2/T$.

To summarize, the preceding computation gives the cost to reach a point of S_i from $X_3=1$. The next step is to apply a measurement to the system. The measurement is associated to the observable Q which reads

$$Q = \alpha |\phi_1\rangle \langle \phi_1| + \beta |\phi_2\rangle \langle \phi_2| + \gamma |\phi_3\rangle \langle \phi_3|.$$
(30)

We assume that the coordinates of the three states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ can be written, respectively, as (θ_m, ϕ_m) , $(\theta_m + \pi/2, \phi_m)$, and $(\pi/2, \phi_m - \pi/2)$ where (θ_m, ϕ_m) are coordinates on S_f . If C_i denotes the cost to reach $|\psi_f\rangle$ from $|\phi_i\rangle$ then one arrives after a simple computation at $C_1 = \theta_m$ (respectively, $C_1 = \theta_m^2/T$), $C_2 = \pi/2 + \theta_m$ [respectively, $C_2 = (\pi/2 + \theta_m)^2/T$] and $C_3 = \pi/2$ (respectively, $C_3 = \pi^2/4T$) for the time-minimum problem (respectively, energy minimum problem). Simple algebra leads to the total costs C_T and C_E which read

$$C_T = \theta_i + a \theta_m + b \left(\frac{\pi}{2} + \theta_m\right) + c \frac{\pi}{2}, \qquad (31)$$

and

$$C_E = \frac{1}{T} \left[\theta_i^2 + a \theta_m^2 + b \left(\frac{\pi}{2} + \theta_m \right)^2 + c \frac{\pi^2}{4} \right], \qquad (32)$$

where a, b, and c are given by

$$a = [\sin \theta_i \sin \theta_m \sin(\phi_m - \phi_i) + \cos \theta_i \cos \theta_m]^2,$$

$$b = [\sin \theta_i \cos \theta_m \sin(\phi_m - \phi_i) - \cos \theta_i \sin \theta_m]^2,$$

$$c = \sin^2 \theta_i \cos^2(\phi_m - \phi_i).$$
(33)

The last step of the optimization procedure is to minimize C_T and C_E as a function of (θ_i, ϕ_i) (i.e., the choice of the time of the measurement) and (θ_m, ϕ_m) (choice of the observable Q). Since $C_{T,E} \ge 0$, one sees that the optimal choice corresponds to $\theta_i = \theta_m = 0$ which leads to $C_{T,E} = 0$. To determine a solution which is not trivial, we fix the observable Q, i.e., the coordinates θ_m and ϕ_m , and we search for the values of θ_i and ϕ_i which minimize the cost. The two computations being similar, we only consider the time-minimum control problem. It can be shown that the minimum of C_T occurs for $\phi_m - \phi_i = \pi/2$ when $0 < \theta_m < \pi/2$ and for $\phi_m - \phi_i = 3\pi/2$ when $\pi/2 < \theta_m < \pi$. Analyzing the variations of C_T as a function of θ_i one deduces that the optimal value for θ_i is 0 if $\theta_m \le \arcsin(2/\pi)/2$ and $\theta_m \ge \pi - \arcsin(2/\pi)/2$. In the other cases, the minimum is reached for

$$\theta_i = \theta_m - \frac{1}{2} \arcsin\left(\frac{2}{\pi}\right) \tag{34}$$

when $\arcsin(2/\pi)/2 \le \theta_m \le \pi/2$ and

$$\theta_i = \pi - \theta_m - \frac{1}{2} \arcsin\left(\frac{2}{\pi}\right)$$
(35)

when $\pi/2 \le \theta_m \le \pi - \arcsin(2/\pi)/2$. Note that the maximum value that θ_i can attain is $\pi/2 - \arcsin(2/\pi)/2$.

C. Case (b)

We solve separately the control problems on S_i and S_f . Since the initial state is $X_3=1$, one deduces that $C_0^T = \theta_i$ and



FIG. 2. (a) Optimal trajectories for the time-minimum problem from $X_2=1$ to $X_6=1$. The upper and the lower extremals are associated, respectively, with $j=1/\sqrt{3}$, $h_T=1$, and $p_{\theta}=\pm\sqrt{h_T^2-j^2}$. The horizontal and vertical dashed lines are, respectively, for equations $\theta=\pi/2$ and $\phi=\pi/2$. (b) The optimal fields $u_1(t)$ and $u_2(t)$ corresponding to this trajectory are respectively represented in solid and dashed lines. u_1 , u_2 , and t are dimensionless.

 $C_0^E = \theta_i^2/T$ where θ_i is the coordinate of the state on which the measurement is performed. On S_f , we consider three different controls from, respectively, $X_2=1$, $X_4=1$, and $X_6=1$ to $X_2=1$. By construction, the first cost C_1 is zero. Using the results of case (a), one obtains that $C_2^T = \pi/2$ for the time minimum problem and $C_2^E = \pi^2/(4T)$ for the energy. The last optimal control is the most difficult to determine. We search for the trajectory which goes from $(\theta = \pi/2, \phi = 0)$ to $(\theta = \pi/2, \phi = \pi/2)$. For the time minimum, using Eq. (A18), one sees that the extremal $\phi(\theta)$ only depends, up to a sign, on the ratio h_T/j . From the analytical solution of Eq. (A18), it can be shown [15] that the optimal trajectory satisfies $h_T/j = \sqrt{3}$. This result is represented in Fig. 2 with the corresponding optimal fields u_1 and u_2 . Integrating the equation

$$\dot{\theta} = \pm \frac{\sqrt{h_T^2 - j^2 \cot^2 \theta}}{h_T},\tag{36}$$

one obtains that the travel time of this trajectory is $C_3^T = \pi \sqrt{3}/2$.

The total cost is then given by

$$C_T = \theta_i + C_1^T \sin^2 \theta_i \sin^2 \phi_i + C_2^T \cos^2 \theta_i + C_3^T \sin^2 \theta_i \cos^2 \phi_i,$$
(37)

which simplifies into

$$C_T = \theta_i + C_2^T \cos^2 \theta_i + C_3^T \sin^2 \theta_i \cos^2 \phi_i.$$
(38)

 C_T is minimum for $\phi_i = \pi/2$. We then have

$$C_T = \theta_i + C_2^T \cos^2 \theta_i, \qquad (39)$$

which is minimum for

$$\theta_i = \frac{1}{2} \arcsin\left(\frac{2}{\pi}\right). \tag{40}$$

For the energy, we have

$$C_E = \frac{\theta_i^2}{T} + C_2^E \cos^2 \theta_i + C_3^E \sin^2 \theta_i \cos^2 \phi_i, \qquad (41)$$

whose minimum can be determined as above.

D. Case (c)

To simplify the discussion, we limit here the study to the time-optimal control problem. As already mentioned above, we determine the target state and the angle α such that the travel time of the three extremal trajectories on S_f is the same. The optimal trajectories and the optimal fields for the extremal starting from $(\theta = \pi/2, \phi = \pi/2)$ are displayed in Fig. 3. When changing p_{θ} to $-p_{\theta}$ with the same value of j, we obtain two trajectories starting, respectively, from $(\theta = \pi/4, \phi=0)$ and $(\theta=3\pi/4, \phi=0)$ which are symmetric with respect to the axis $\theta = \pi/2$. These two extremals intersect on this axis at the same time.

We then determine the parameters of the trajectories initiated from $(\theta = \pi/2, \phi = \pi/2)$ and $(\theta = \pi/4, \phi = 0)$ such that they intersect on the axis $\theta = \pi/2$ at the same time. We have solved this problem numerically. We have obtained $p_{\theta}(0)$ $\simeq 0.6272$ and j=-1 for the first extremal and $p_{\theta}(0)$ $\simeq -0.9245$ and j=1 for the second one. The two extremals intersect in $\phi \simeq 1.091$ at time $t \simeq 1.668$. Let T_0 be the cost corresponding to these three trajectories. The total cost C_T is given by

$$C_T = C_0 + T_0. (42)$$

Since by definition $C_0 \ge 0$, the optimal solution is $C_0=0$, i.e., the measurement has to be performed at time t=0. The result is thus independent of the initial state of S_i . Note that the same work can be done for the minimization of the energy.

E. Case (d)

Here, again, we only consider the minimization of the time. Using Eq. (A21) of the Appendix, the time to go from $(\pi/2,0)$ to the state (θ_i, ϕ_i) where the measurement is performed is



FIG. 3. (a) Optimal trajectories for the time-minimum problem from the different states associated with the measurement to the target state. (b) The optimal fields $u_1(t)$ and $u_2(t)$ corresponding to the trajectory starting from $(\theta = \pi/2, \phi = \pi/2)$ are, respectively, represented in solid and dashed lines.

$$C_0 = \frac{-1}{\sqrt{1+m_i^2}} \arcsin(\sqrt{1+m_i^2} \cos \theta_i),$$
(43)

where $m_i = j/h_T$. To establish Eq. (43), we have assumed that the function $\theta(t)$ is an increasing function of time. In addition, we notice that the value ϕ_i depends on the constant m_i chosen. In other words, minimizing the cost with respect to (θ_i, ϕ_i) is equivalent to minimizing the cost with respect to θ_i and m_i . We next determine the cost to reach the target state from each state of the measured operator. From $(\theta_f=0, \phi_f=0)$, a result of case (a) leads to $C_1=\pi/4$. By symmetry, we also deduce that the cost from $(\theta_f=\pi/2, \phi_f=0)$ and $(\theta_f=\pi/2, \phi_f=\pi/2)$ is the same, i.e., $C_2=C_3=C$. We determine numerically this time. For the cost *C*, we have obtained m_f $\approx 1/1.126$ and a corresponding time *C* equal to 1.422. Using Eq. (A21), it can be shown that

$$C = \frac{2\pi}{2\sqrt{1+m_f^2}} - \frac{1}{\sqrt{1+m_f^2}} \operatorname{arcsin}\left(\frac{\sqrt{1+m_f^2}}{\sqrt{2}}\right).$$
(44)

To compute *C*, we have used the fact that for the extremal trajectory θ is not a monotonous function of time and that the



FIG. 4. Optimal trajectories for the time-minimum problem starting from the different states associated to the measurement.

minimum of θ is $\arccos(1/\sqrt{1+m_f^2})$. Figure 4 represents the three optimal trajectories reaching the target state.

A straightforward calculation then gives the total cost C_T which can be written as follows:

$$C_T = C_0 + \frac{\pi}{4} \cos^2 \theta_i + C(\sin^2 \theta_i \cos^2 \phi_i + \sin^2 \theta_i \sin^2 \phi_i),$$
(45)

$$=C_0 + \frac{\pi}{4}\cos^2\theta_i + C\sin^2\theta_i.$$
(46)

 C_T is then minimized with respect to θ_i and ϕ_i . We have checked numerically that the optimal solution corresponds to $C_0=0$. The total cost is given by $C_T=C$. We have also obtained the same result when the initial angle is different from $\pi/2$.

VI. CONCLUSION

We have investigated in this paper the control of a threelevel quantum system by laser fields and instantaneous selective measurements. We have considered only the case of a single measurement. We have defined a cost functional taking into account the measurements and we have applied the Pontryagin maximum principle to this case. For given initial and target states, we have optimized both the choice of the observable (and the time at which the measurement has to be performed) and the control field. In this paper, we have considered a simple model in order to highlight the geometrical structure of the control. The question which naturally arises is the generalization of this approach to more complex systems such as the nonisotropic three-level system (dipolar interaction with nonconstant terms) or systems having four or five levels. For instance, we could consider a N-level harmonic system associated to a constant dipolar interaction coupling only neighboring states. If N is odd then it can be shown that the dynamical Lie algebra of the system is so(N)[38] and that a von Neumann measurement can restore the complete controllability of the system [36]. Some progress in the geometrical description of these problems has recently been achieved [20,21] and could be used to determine the effect of von Neumann measurements. However, due to the number of degrees of freedom of such systems, the optimal control problem will be solved by numerical methods.

ACKNOWLEDGMENT

We acknowledge support from the Agence Nationale de la Recherche (ANR CoMoc).

APPENDIX: THE GRUSIN MODEL

In this section, we recall how to solve analytically the optimal control problem associated to the Grusin model on the sphere [3,26]. We consider the following control system of differential equations:

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = u_1 \begin{pmatrix} -y_2 \\ y_1 \\ 0 \end{pmatrix} + u_2 \begin{pmatrix} 0 \\ -y_3 \\ y_2 \end{pmatrix},$$
(A1)

where u_1 and u_2 are real controls. The coordinates (y_1, y_2, y_3) satisfy the relation $y_1^2 + y_2^2 + y_3^2 = 1$. This system can be written in a more compact form as

$$\dot{\mathbf{y}} = u_1 F_1 + u_2 F_2, \tag{A2}$$

where **y** is the vector of coordinates (y_1, y_2, y_3) and F_1 and F_2 are the following vector fields

$$F_1 = \begin{pmatrix} -y_2 \\ y_1 \\ 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 0 \\ -y_3 \\ y_2 \end{pmatrix}.$$
 (A3)

We introduce the spherical coordinates (θ, ϕ) defined by

$$y_1 = \cos \phi \sin \theta$$
, $y_2 = \cos \theta$, $y_3 = \sin \phi \sin \theta$. (A4)

Using the relations

$$\frac{\partial}{\partial y_1} = \cos \theta \cos \phi \frac{\partial}{\partial \theta} - \frac{\sin \phi}{\sin \theta} \frac{\partial}{\partial \phi}, \quad \frac{\partial}{\partial y_2} = -\sin \theta \frac{\partial}{\partial \theta},$$
$$\frac{\partial}{\partial y_3} = \cos \theta \sin \phi \frac{\partial}{\partial \theta} + \frac{\cos \phi}{\sin \theta} \frac{\partial}{\partial \phi}, \quad (A5)$$

one deduces that

$$F_1 = \begin{pmatrix} -\cos\phi\\\sin\phi\cot\theta \end{pmatrix}, \quad F_2 = \begin{pmatrix} \sin\phi\\\cos\phi\cot\theta \end{pmatrix}.$$
(A6)

In the coordinates (θ, ϕ) , the system (A1) reads

$$\begin{pmatrix} \dot{\theta} \\ \dot{\phi} \end{pmatrix} = u_1 \begin{pmatrix} -\cos\phi \\ \sin\phi\cot\theta \end{pmatrix} + u_2 \begin{pmatrix} \sin\phi \\ \cos\phi\cot\theta \end{pmatrix}.$$
 (A7)

The following rotation on the control:

$$v_1 = -\cos \phi u_1 + \sin \phi u_2, \quad v_2 = \sin \phi u_1 + \cos \phi u_2,$$
(A8)

which does not modify the cost, leads to



FIG. 5. Flow of the Hamiltonian H_T . Numerical values are taken to be $p_{\phi}(0)=2$, $\theta(0)=\pi/4$, and $\phi(0)=0$. $p_{\theta}(0)=\pm 5$ for the two trajectories in solid lines and $p_{\theta}(0)=0$ for the extremal in dashed lines.

$$\begin{pmatrix} \dot{\theta} \\ \dot{\phi} \end{pmatrix} = v_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + v_2 \begin{pmatrix} 0 \\ \cot \theta \end{pmatrix}.$$
 (A9)

The pseudo-Hamiltonians H_P associated to this system are, respectively, given by

$$H_P = v_1 p_{\theta} + v_2 p_{\phi} \cot \theta - \frac{1}{2} (v_1^2 + v_2^2), \qquad (A10)$$

for the energy minimization problem and by

$$H_P = v_1 p_\theta + v_2 p_\phi \cot \theta \tag{A11}$$

for the time-optimal control. In the first case, the constant p_0 of Eq. (15) has been normalized to -1/2 and in the second case, this constant has been subtracted in the definition of H_P . The application of the PMP gives the following extremal controls:

$$v_1 = \frac{p_\theta}{R}, \quad v_2 = \frac{p_\phi \cot \theta}{R},$$
 (A12)

where R=1 for the energy and $R=\sqrt{p_{\theta}^2+p_{\phi}^2\cot^2\theta}$ for the time-minimum problem. The extremal trajectories correspond to the flows of the Hamiltonians H_E (for the energy) and H_T (for the time minimum) given by

$$H_{E} = \frac{1}{2} (p_{\theta}^{2} + p_{\phi}^{2} \cot^{2} \theta), \quad H_{T} = \sqrt{p_{\theta}^{2} + p_{\phi}^{2} \cot^{2} \theta}.$$
(A13)

We then deduce that the extremal flows satisfy the following system given by Hamilton's equations associated to H_E and H_T :

$$\dot{\theta} = p_{\theta}/R, \quad \dot{\phi} = p_{\phi} \cot^2 \theta/R, \quad p_{\phi} = j,$$

 $\dot{p}_{\theta} = p_{\phi}^2 \cot \theta (1 + \cot^2 \theta)/R.$ (A14)

In the system of Eqs. (A14), p_{ϕ} is a constant of the motion denoted *j* which implies that H_E and H_T are integrable. One



FIG. 6. Symmetries of the flow of the Grusin model. Panel (a): Intersection on the antipodal parallel of equation $\theta = \pi - \theta(0)$ of two trajectories with the same cost. Panel (b): symmetry with respect to the axis $\phi = 0$ of the flow. Numerical values are taken to be in the two cases $p_{\phi}(0) = \pm 2$, $p_{\theta}(0) = \pm 5$, $\theta(0) = \pi/4$, and $\phi(0) = 0$.

of the consequences of this integrability is the fact that the trajectories can be calculated by quadratures as a function of the value of the Hamiltonian denoted h_E or h_T and of the value of the constant *j*.

The idea is to eliminate the time parametrization and to introduce functions $\theta \rightarrow \phi(\theta)$ in the coordinates (ϕ, θ) . In both cases, we have

$$\frac{\dot{\theta}}{\dot{\phi}} = \frac{d\theta}{d\phi} = \frac{p_{\theta}}{j \cot^2 \theta}.$$
 (A15)

Using Eqs. (A13), a simple computation leads to

$$p_{\theta} = \pm \sqrt{2h_E - j^2 \cot^2 \theta}$$
 (A16)

for the energy minimum and

$$p_{\theta} = \pm \sqrt{h_T^2 - j^2 \cot^2 \theta}.$$
 (A17)

for the time minimum. One finally arrives at

OPTIMAL CONTROL OF A THREE-LEVEL QUANTUM ...

$$\frac{d\theta}{d\phi} = \pm \frac{\sqrt{2h_E - j^2 \cot^2 \theta}}{j \cot^2 \theta}, \quad \frac{d\theta}{d\phi} = \pm \frac{\sqrt{h_T^2 - j^2 \cot^2 \theta}}{j \cot^2 \theta}$$
(A18)

for the two cases.

The Hamiltonian equations can be integrated to determine θ and ϕ as a function of time. We start from the equation

$$\dot{\theta}^2 = 1 - m^2 \cot^2 \theta, \tag{A19}$$

where $m=j/h_T$ for the time minimum problem and m=j with $h_E=1/2$ for the minimization of the energy. Equation (A19) can be straightforwardly obtained from Eqs. (A14), (A16), and (A17). Simple algebra leads to

$$\dot{\theta}^2 = \frac{1 - (m^2 + 1)\cos^2\theta}{\sin^2\theta}.$$
 (A20)

We obtain for the positive branch that

$$T = \int_{\theta_0}^{\theta_1} \frac{\sin \,\theta d\,\theta}{\sqrt{1 - (1 + m^2)\cos^2 \,\theta}},\tag{A21}$$

where θ_0 and θ_1 are the initial and final values of θ . Using the fact that

$$\int \frac{\sin \theta d\theta}{\sqrt{1 - a \cos^2 \theta}} = -\frac{1}{\sqrt{a}} \arcsin(\sqrt{a} \cos \theta), \quad (A22)$$

one arrives at

- L. S. Pontryagin, *The Mathematical Theory of the Optimal Process* (Wiley-Interscience, New York, 1962).
- [2] V. Jurdjevic, Geometric Control Theory (Cambridge University Press, Cambridge, England, 1996).
- [3] B. Bonnard and D. Sugny (unpublished).
- [4] B. Bonnard and M. Chyba, Singular Trajectories and their Role in Control Theory (Springer, New York, 2003), Vol. 40.
- [5] U. Boscain and B. Picolli, Optimal Syntheses for Control Systems on 2-D Manifolds (Springer, New York, 2004), Vol. 43.
- [6] W. Zhu and H. Rabitz, J. Chem. Phys. 110, 7142 (1999).
- [7] W. Zhu and H. Rabitz, J. Chem. Phys. 109, 385 (1998).
- [8] Y. Maday and G. Turinici, J. Chem. Phys. 118, 8191 (2003).
- [9] Y. Ohtsuki, W. Zhu, and H. Rabitz, J. Chem. Phys. 110, 9825 (1999).
- [10] Y. Ohtsuki, G. Turinici, and H. Rabitz, J. Chem. Phys. 120, 5509 (2004).
- [11] H. Jirari and W. Potz, Phys. Rev. A 72, 013409 (2005).
- [12] D. Sugny, C. Kontz, M. Ndong, Y. Justum, G. Dive, and M. Desouter-Lecomte, Phys. Rev. A 74, 043419 (2006).
- [13] D. Sugny, M. Ndong, D. Lauvergnat, Y. Justum, and M. Desouter-Lecomte, J. Photochem. Photobiol. Chem. 190, 359 (2007).
- [14] M. Ndong, L. Bomble, D. Sugny, Y. Justum, and M. Desouter-Lecomte, Phys. Rev. A 76, 043424 (2007).
- [15] U. Boscain, G. Charlot, J.-P. Gauthier, S. Guérin, and H. R.

$$T = \frac{1}{\sqrt{1+m^2}} [\arcsin(\sqrt{1+m^2}\cos\theta_0) - \arcsin(\sqrt{1+m^2}\cos\theta_1)].$$
(A23)

The inversion of this relation gives

$$\theta(t) = \frac{\pi}{2} + \arcsin\left[\frac{1}{\sqrt{1+m^2}}\sin(\sqrt{1+m^2}t + K)\right],$$
(A24)

in the case where θ is an increasing function of *t*. *K* is a constant which can be determined from $\theta(0)$. The evolution of ϕ is obtained from the differential equation

$$\dot{\phi} = m \cot^2 \theta \tag{A25}$$

and Eq. (A24).

The extremal trajectories, which are the same for H_E and H_T , are represented in Fig. 5 for a given value of j and different values of h. These trajectories have three symmetries.

The figure is first symmetric with respect to translation in ϕ . In addition, two trajectories corresponding, respectively, to p_{ϕ} and $-p_{\phi}$ are symmetric with respect to the meridian ϕ =const. Finally two extremals starting from the same point $(\phi(0), \theta(0))$ but with opposite initial values of $p_{\theta}(0)$ intersect on the antipodal parallel $\theta = \pi - \theta(0)$ with the same value of the cost. As shown in Fig. 5, we notice that the trajectory with $p_{\theta}(0)=0$ is tangent to the antipodal parallel. Figure 6 illustrates these two symmetries.

Jauslin, J. Math. Phys. 43, 2107 (2002).

- [16] N. Khaneja, R. Brockett, and S. J. Glaser, Phys. Rev. A 63, 032308 (2001).
- [17] N. Khaneja, S. J. Glaser, and R. Brockett, Phys. Rev. A 65, 032301 (2002).
- [18] H. Yuan and N. Khaneja, Phys. Rev. A 72, 040301(R) (2005).
- [19] U. Boscain and P. Mason, J. Math. Phys. 47, 062101 (2006).
- [20] U. Boscain, T. Chambrion, and G. Charlot, Discrete Contin. Dyn. Syst., Ser. B 5, 957 (2005).
- [21] U. Boscain and G. Charlot, ESAIM :Control, Optimisation and Calculus of Variations (COCV), Vol. 10, pp. 593–614 (2004).
- [22] D. Sugny, A. Keller, O. Atabek, D. Daems, C. M. Dion, S. Guérin, and H. R. Jauslin, Phys. Rev. A 71, 063402 (2005).
- [23] D. Sugny, A. Keller, O. Atabek, D. Daems, C. M. Dion, S. Guérin, and H. R. Jauslin, Phys. Rev. A 72, 032704 (2005).
- [24] D. Sugny, C. Kontz, and H. R. Jauslin, Phys. Rev. A 74, 053411 (2006).
- [25] D. Sugny, C. Kontz, and H. R. Jauslin, Phys. Rev. A 76, 023419 (2007).
- [26] B. Bonnard and D. Sugny, SIAM J. Control Opt. (to be published).
- [27] U. Boscain, T. Chambrion, and J.-P. Gauthier, J. Dyn. Contr. Syst. 8, 547 (2002).
- [28] J. von Neumann, Mathematical Foundations of Quantum Mechanics (Princeton University Press, Princeton, 1955).

- [29] A. Pechen, N. Il'in, F. Shuang, and H. Rabitz, Phys. Rev. A 74, 052102 (2006).
- [30] J. Gong and S. A. Rice, J. Chem. Phys. 120, 9984 (2004).
- [31] L. Roa and G. A. Olivares-Renteria, Phys. Rev. A 73, 062327 (2006).
- [32] L. Roa, A. Delgado, M. L. Ladron de Guevara, and A. B. Klimov, Phys. Rev. A 73, 012322 (2006).
- [33] M. Sugawara, J. Chem. Phys. 123, 204115 (2005).
- [34] F. Shuang, A. Pechen, T.-S. Ho, and H. Rabitz, J. Chem. Phys. 126, 134303 (2007).
- [35] S. Schirmer, J. Phys. A 37, 1389 (2004).
- [36] R. Vilela Mendes and V. I. Man'ko, Phys. Rev. A 67, 053404 (2003).
- [37] A. Agrachev, U. Boscain, and M. Sigalotti, Discrete Contin. Dyn. Syst. 20, 801 (2008).
- [38] S. Schirmer, J. Phys. A 35, 2327 (2002).