

This is the accepted manuscript made available via CHORUS. The article has been published as:

Time-optimal synthesis of $SU(2)$ transformations for a spin- $1/2$ system

A. D. Boozer

Phys. Rev. A **85**, 012317 — Published 19 January 2012

DOI: [10.1103/PhysRevA.85.012317](https://doi.org/10.1103/PhysRevA.85.012317)

Time-optimal synthesis of $SU(2)$ transformations for a spin-1/2 system

A. D. Boozer*

Department of Physics, University of New Mexico Albuquerque, New Mexico 87131

We consider a quantum control problem involving a spin-1/2 particle in a magnetic field. The magnitude of the field is held constant, and the direction of the field, which is constrained to lie in the $x - y$ plane, serves as a control parameter that can be varied to govern the evolution of the system. We analytically solve for the time dependence of the control parameter that will synthesize a given target $SU(2)$ transformation in the least possible amount of time, and we show that the time-optimal solutions have a simple geometric interpretation in terms of the fiber bundle structure of $SU(2)$. We also generalize our time-optimal solutions to a control problem that includes a constant bias field along the \hat{z} axis, and to the case of inhomogeneous control, in which a single control parameter governs the evolution of an ensemble of spin-1/2 systems.

PACS numbers: 42.50.Dv, 02.30.Yy, 02.20.Sv

I. INTRODUCTION

Many applications rely on the ability to coherently control the state of a quantum system [1–6]. In particular, the current push to develop robust quantum information processors has led to the development of quantum control protocols for a diverse array of experimental platforms, including atomic, optical, and condensed matter systems [7–10]. In a typical control problem, the system in question is described by a Hamiltonian containing several control parameters that we are free to vary, and we would like to determine the time dependence of these parameters such that the evolution of the system implements a desired unitary transformation. This type of problem can be viewed as a quantum analog to motion planning in classical control theory, in which one would like to vary a set of control parameters so as to steer a classical dynamical system to a desired point in state space [11–13]. Control problems are generally highly nontrivial: they do not usually admit an analytic solution, and must be solved via numerical searches [14–21]. Analytic solutions can, however, sometimes be obtained for control problems involving low-dimensional systems. In particular, for control problems involving a spin-1/2 particle, analytic solutions have been obtained that minimize either an energy-type cost functional [22–24] or the total evolution time [25, 26].

Here we consider a model quantum control problem involving a spin-1/2 particle in a magnetic field. The magnitude of the field is held constant, and its direction, which is constrained to lie in the $x - y$ plane, serves as a control parameter that can be varied to govern the evolution of the system. The evolution can be described in terms of an $SU(2)$ evolution operator $U(t)$, such that if the state of the spin at time zero is $|\psi(0)\rangle$ then the state at time t is $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. Given an arbitrary

target $SU(2)$ transformation V , we analytically solve for the time dependence of the control parameter such that $U(t) = V$ and t is as small as possible. By viewing $SU(2)$ as a $U(1)$ fiber bundle over the two-dimensional sphere S^2 , we are able to give a simple geometric interpretation to these time-optimal solutions. We also generalize our time-optimal solutions to a control problem that includes a constant bias field along the \hat{z} axis.

An important development in the field of quantum control is the notion of inhomogeneous control, in which a single set of control parameters governs the evolution of an ensemble of systems subject to different Hamiltonians. The differences in the Hamiltonians may, for example, describe unwanted perturbations that give rise to decoherence. By choosing the control parameters properly, one can compensate for these perturbations so that the resulting system dynamics are insensitive to their presence [27, 28]. Alternatively, the differences in the Hamiltonians may be intentional, so as to provide a means of addressing individual systems in the ensemble [29–31].

We investigate inhomogeneous control in our model control problem by generalizing the problem to the case of an ensemble of N spin-1/2 systems. The magnetic fields of the different systems vary in magnitude but are all aligned along a common direction in the $x - y$ plane, and we take this common direction to be the control parameter that governs the evolution of the entire ensemble. We obtain a semi-analytic solution to this inhomogeneous control problem for the case $N = 2$, and we verify that our solution is time-optimal by comparing it with the results of a numerical search.

II. CONTROL PROBLEM

The system that we consider consists of a spin-1/2 particle in a magnetic field \mathbf{B} . We assume that the magnitude $B \equiv |\mathbf{B}|$ of the magnetic field is constant, and its direction $\hat{\mathbf{n}} \equiv \mathbf{B}/|\mathbf{B}|$ serves as a control parameter that can be varied to govern the evolution of the system. The

*Electronic address: boozer@unm.edu

Hamiltonian for the system is

$$H = -\mu B \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}, \quad (1)$$

where μ is the magnetic moment of the particle and σ_k are the Pauli spin matrices. For simplicity, we will choose units such that $\mu B = 1$. The system evolves in time according to the unitary transformation

$$U(t) = T \exp(-i \int_0^t H(t') dt'), \quad (2)$$

where T is a time-ordering operator that places operators at early times to the right of operators at later times. We note that U satisfies the Schrödinger equation

$$i\dot{U} = HU. \quad (3)$$

From Eq. (2), and the fact that H is traceless, it follows that $\det U = 1$, so U is an $SU(2)$ transformation.

We now consider a control problem in which we are given a target $SU(2)$ transformation V and are asked to determine the time dependence of the control parameter $\hat{\mathbf{n}}$ and the total evolution time t such that $U(t) = V$ and t is as small as possible. If $\hat{\mathbf{n}}$ is allowed to point in any direction, then the solution to the control problem is trivial: we write V in the form $V = e^{i\mathbf{r} \cdot \boldsymbol{\sigma}}$, where $|\mathbf{r}| \leq \pi$, and we take

$$\hat{\mathbf{n}} = \hat{\mathbf{r}}, \quad t = |\mathbf{r}|. \quad (4)$$

For example, for a target transformation $V = e^{i\eta\sigma_z/2}$ describing a spatial rotation with axis $\hat{\mathbf{z}}$ and angle η , we find that $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ and $t = \eta/2$.

Let us suppose, however, that the control parameter $\hat{\mathbf{n}}$ is constrained to lie in the $x - y$ plane. The control problem is still solvable, but the solution is no longer trivial. We can verify that the control problem is solvable by presenting a solution that is not time-optimal. Let us write the target transformation V in terms of Euler angles ψ , θ , and ϕ :

$$V = e^{i\psi\sigma_x/2} e^{i\theta\sigma_y/2} e^{i\phi\sigma_x/2}. \quad (5)$$

From Eq. (5), it follows that V can be synthesized by taking

$$\hat{\mathbf{n}}(\tau) = \begin{cases} \hat{\mathbf{x}} & \text{for } 0 < \tau < |\phi/2|, \\ \hat{\mathbf{y}} & \text{for } |\phi/2| < \tau < |\phi/2| + |\theta/2|, \\ \hat{\mathbf{x}} & \text{for } |\phi/2| + |\theta/2| < \tau < t, \end{cases} \quad (6)$$

$$t = |\psi/2| + |\theta/2| + |\phi/2|. \quad (7)$$

For example, consider again a target transformation $V = e^{i\eta\sigma_z/2}$ describing a spatial rotation with axis $\hat{\mathbf{z}}$ and angle η . We find that $V = e^{-i\pi\sigma_x/4} e^{i\eta\sigma_y/2} e^{i\pi\sigma_x/4}$, so $\phi = -\psi = \pi/2$, $\theta = \eta$, and $t = \pi/2 + \eta/2$. For comparison, recall that $t = \eta/2$ for the unconstrained control problem in which $\hat{\mathbf{n}}$ is allowed to point in any direction.

III. TIME-OPTIMAL SOLUTION

We now present a time-optimal solution to the constrained control problem. We begin by describing two methods for assigning coordinates to an $SU(2)$ transformation U . For the first method, we assign real-valued coordinates $\mathbf{r} = (w, x, y, z)$ to U by expanding U in the Pauli spin matrices:

$$U = w + ix\sigma_x + iy\sigma_y + iz\sigma_z. \quad (8)$$

We call these coordinates embedding coordinates, because they describe an embedding of $SU(2)$ into \mathbb{R}^4 . For the second method, we assign complex-valued coordinates (z_1, z_2) to U by expressing U in the form

$$U = \begin{pmatrix} z_1 & z_2 \\ -z_2^* & z_1^* \end{pmatrix}. \quad (9)$$

We call these coordinates complex coordinates. From Eqs. (8) and (9), it follows that the two sets of coordinates are related by $(z_1, z_2) = (w + iz, y + ix)$.

The Lie group $SU(2)$ is three-dimensional, but both sets of coordinates label $SU(2)$ transformations using four real parameters. So for both sets of coordinates there are more coordinate degrees of freedom than physical degrees of freedom, and only some of the points in the coordinate space actually correspond to $SU(2)$ transformations. From Eqs. (8) and (9), it follows that such points satisfy the constraint

$$|\mathbf{r}|^2 = |z_1|^2 + |z_2|^2 = 1. \quad (10)$$

The locus of points \mathbf{r} that satisfy Eq. (10) is a three-dimensional sphere S^3 embedded in \mathbb{R}^4 , and the mapping $U \mapsto \mathbf{r}$ is a diffeomorphism from $SU(2)$ to S^3 .

It is useful to express the Schrödinger equation (3) in terms of both sets of coordinates. We first consider the embedding coordinates. We substitute the definition of the embedding coordinates given in Eq. (8) into the Schrödinger equation (3) to obtain an equation of motion for \mathbf{r} :

$$\dot{\mathbf{r}} = n_x \mathbf{L}_x(\mathbf{r}) + n_y \mathbf{L}_y(\mathbf{r}) + n_z \mathbf{L}_z(\mathbf{r}), \quad (11)$$

where

$$\mathbf{L}_x(\mathbf{r}) = w\hat{\mathbf{x}} - x\hat{\mathbf{w}} + z\hat{\mathbf{y}} - y\hat{\mathbf{z}}, \quad (12)$$

$$\mathbf{L}_y(\mathbf{r}) = w\hat{\mathbf{y}} - y\hat{\mathbf{w}} + x\hat{\mathbf{z}} - z\hat{\mathbf{x}}, \quad (13)$$

$$\mathbf{L}_z(\mathbf{r}) = w\hat{\mathbf{z}} - z\hat{\mathbf{w}} + y\hat{\mathbf{x}} - x\hat{\mathbf{y}}, \quad (14)$$

are orthonormal vectors that span the tangent space of S^3 at the point \mathbf{r} . As \mathbf{r} evolves in time, it traces out a path in S^3 whose tangent vector is $\dot{\mathbf{r}}$. From Eq. (11) it follows that the length of the tangent vector is $|\dot{\mathbf{r}}| = 1$, so time corresponds to arc length along the path. The time evolution of \mathbf{r} is governed by the control parameter $\hat{\mathbf{n}}$, which dictates the projection of the tangent vector $\dot{\mathbf{r}}$

along the basis vectors $\mathbf{L}_k(\mathbf{r})$:

$$\mathbf{L}_x(\mathbf{r}) \cdot \dot{\mathbf{r}} = n_x, \quad (15)$$

$$\mathbf{L}_y(\mathbf{r}) \cdot \dot{\mathbf{r}} = n_y, \quad (16)$$

$$\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = n_z. \quad (17)$$

For the constrained control problem $\hat{\mathbf{n}} = \cos \phi \hat{\mathbf{x}} + \sin \phi \hat{\mathbf{y}}$ for some angle ϕ , so

$$\mathbf{L}_x(\mathbf{r}) \cdot \dot{\mathbf{r}} = \cos \phi, \quad (18)$$

$$\mathbf{L}_y(\mathbf{r}) \cdot \dot{\mathbf{r}} = \sin \phi, \quad (19)$$

$$\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0. \quad (20)$$

It is also useful to express the Schrödinger equation (3) in terms of the complex coordinates. We substitute the definition of the complex coordinates given in Eq. (9) into Eq. (3) to obtain equations of motion for z_1 and z_2 :

$$\dot{z}_1 = -ie^{-i\phi} z_2^*, \quad (21)$$

$$\dot{z}_2 = ie^{-i\phi} z_1^*. \quad (22)$$

If we differentiate Eqs. (21) and (22) with respect to t and then substitute for \dot{z}_1 and \dot{z}_2 using the original equations, we obtain the decoupled equations

$$\ddot{z}_1 + i\dot{\phi}\dot{z}_1 + z_1 = 0, \quad (23)$$

$$\ddot{z}_2 + i\dot{\phi}\dot{z}_2 + z_2 = 0. \quad (24)$$

Using Eqs. (21) and (22), it is straightforward to derive the identities

$$\dot{z}_1 z_1^* + \dot{z}_2 z_2^* = 0, \quad (25)$$

$$\dot{z}_2 z_1 - \dot{z}_1 z_2 = ie^{-i\phi}. \quad (26)$$

We can understand the meaning of these identities by transforming from complex coordinates to embedding coordinates:

$$\dot{z}_1 z_1^* + \dot{z}_2 z_2^* = \mathbf{r} \cdot \dot{\mathbf{r}} + i\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}}, \quad (27)$$

$$\dot{z}_2 z_1 - \dot{z}_1 z_2 = \mathbf{L}_y(\mathbf{r}) \cdot \dot{\mathbf{r}} + i\mathbf{L}_x(\mathbf{r}) \cdot \dot{\mathbf{r}}. \quad (28)$$

So Eqs. (25) and (26) follow from Eqs. (10) and (18)–(20).

Let us now return to the embedding coordinates and consider the problem of finding a minimum-length path in S^3 that satisfies the constraint $\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0$. Such a path can be obtained by minimizing the action

$$S = \int (|\mathbf{r}'| + \gamma(|\mathbf{r}|^2 - 1) + \lambda \mathbf{L}_z(\mathbf{r}) \cdot \mathbf{r}') du. \quad (29)$$

Here u is an arbitrary parameterization of the path, $\mathbf{r}' \equiv d\mathbf{r}/du$, and γ and λ are Lagrange multipliers. The first term of the integrand gives the length of the path, the second term imposes the constraint $|\mathbf{r}|^2 = 1$, which restricts the path to S^3 , and the third term imposes the constraint $\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0$, which expresses the fact that the control parameter $\hat{\mathbf{n}}$ must lie in the x – y plane. Note that

$\mathbf{r}' \equiv d\mathbf{r}/du = (dt/du)\dot{\mathbf{r}}$ and $|\dot{\mathbf{r}}| = 1$, so the parameter u is related to the time t by

$$dt/du = |\mathbf{r}'|. \quad (30)$$

We write down the Euler-Lagrange equations corresponding to the action given in Eq. (29), use Eq. (30) to replace u with t , and transform from embedding coordinates to complex coordinates to obtain

$$\ddot{z}_1 + 2i\lambda\dot{z}_1 + (i\dot{\lambda} - 2\gamma)z_1 = 0, \quad (31)$$

$$\ddot{z}_2 + 2i\lambda\dot{z}_2 + (i\dot{\lambda} - 2\gamma)z_2 = 0. \quad (32)$$

A time-optimal solution to the constrained control problem must satisfy the Schrödinger equations (23) and (24) as well as the Euler-Lagrange equations (31) and (32). We subtract Eq. (23) from (31) and Eq. (24) from (32) to obtain

$$i(2\lambda - \dot{\phi})\dot{z}_1 + (i\dot{\lambda} - 2\gamma - 1)z_1 = 0, \quad (33)$$

$$i(2\lambda - \dot{\phi})\dot{z}_2 + (i\dot{\lambda} - 2\gamma - 1)z_2 = 0. \quad (34)$$

Using the identities given in Eqs. (25) and (26), we can eliminate the coordinates z_1 and z_2 from Eq. (33) and (34) and obtain equations that involve only the parameters γ , λ , and ϕ :

$$\dot{\phi} = 2\lambda, \quad i\dot{\lambda} = 2\gamma + 1. \quad (35)$$

The solution to these equations is

$$\gamma = -1/2, \quad \lambda = \omega/2, \quad \phi = \phi_0 + \omega t, \quad (36)$$

where ϕ_0 and ω are integration constants. So an $SU(2)$ transformation can be synthesized in a time-optimal fashion by varying the control parameter ϕ as described by Eq. (36).

We would now like to calculate the evolution operator U that results when the control parameter ϕ is varied in the time-optimal fashion described by Eq. (36). We first note that $U(0)$ is the identity transformation, which has complex coordinates $(z_1, z_2) = (1, 0)$. We substitute Eq. (36) for ϕ into the Schrödinger equations (21) and (22) and solve them subject to these initial conditions to obtain

$$z_1 = (2\alpha)^{-1}(\beta_+ e^{i\beta_- t} + \beta_- e^{-i\beta_+ t}), \quad (37)$$

$$z_2 = (2\alpha)^{-1}e^{-i\phi_0}(e^{i\beta_- t} - e^{-i\beta_+ t}), \quad (38)$$

where

$$\alpha \equiv (1 + \omega^2/4)^{1/2}, \quad \beta_{\pm} \equiv \alpha \pm \omega/2. \quad (39)$$

It is useful to view the parameters (ϕ_0, ω, t) as defining a third set of coordinates for U . We call these coordinates time-optimal coordinates. Eqs. (37) and (38) can then be viewed as describing a coordinate transformation from time-optimal coordinates to complex coordinates.

Suppose we are given a target $SU(2)$ transformation V . We can synthesize V in a time-optimal fashion by

determining its complex coordinates (z_1, z_2) and then inverting Eqs. (37) and (38) to obtain its time-optimal coordinates (ϕ_0, ω, t) . The parameters ϕ_0 and ω tell us the time dependence of the control parameter ϕ , and the parameter t tells us the total evolution time.

Let us now consider some specific examples. First we consider a target transformation $V = e^{i\eta\hat{e}_\theta \cdot \boldsymbol{\sigma}/2}$ that describes a spatial rotation with axis $\hat{e}_\theta \equiv \cos\theta \hat{x} + \sin\theta \hat{y}$ and angle η . The complex coordinates of V are $(z_1, z_2) = (\cos\eta/2, ie^{-i\theta}\sin\eta/2)$. We invert Eqs. (37) and (38) to obtain the time-optimal coordinates:

$$\phi_0 = \theta, \quad \omega = 0, \quad t = \eta/2. \quad (40)$$

This solution is identical to the time-optimal solution for the unconstrained control problem described in Eq. (4). This is to be expected, since the time-optimal solution for the unconstrained control problem satisfies the constraint that \hat{n} must lie in the $x-y$ plane.

Next we consider a target transformation $V = e^{i\eta\sigma_z/2}$ that describes a spatial rotation with axis \hat{z} and angle η . The complex coordinates of V are $(z_1, z_2) = (e^{i\eta/2}, 0)$. We invert Eqs. (37) and (38) to obtain the time-optimal coordinates:

$$\omega = 2\nu(1 - \nu^2)^{-1/2}, \quad t = \pi(1 - \nu^2)^{1/2}, \quad (41)$$

where $\nu \equiv 1 - \eta/2\pi$. The parameter ϕ_0 is undetermined by the inversion, and any value can be used to perform a time-optimal synthesis of V . Mathematically, ϕ_0 is undetermined because V is located at a coordinate singularity of the time-optimal coordinate system; physically, it is because V is invariant under similarity transformations involving arbitrary rotations about the \hat{z} axis. In Fig. 1 we compare the time-optimal solution described in Eq. (41) with the Euler solution described in Eqs. (6)–(7) and the time-optimal solution for the unconstrained control problem described in Eq. (4).

Let us now consider the trajectory of the spin on the Bloch sphere as it evolves along a time-optimal path. If the state of the spin at time zero is $|\psi(0)\rangle$, then the state at time t is $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. We can represent the state of the spin at time t as a point $\hat{s}(t) = \langle\psi(t)|\boldsymbol{\sigma}|\psi(t)\rangle$ on the Bloch sphere. In Fig. 2 we plot the trajectory of the spin on the Bloch sphere for the time-optimal synthesis of a $\pi/2$ -rotation about the \hat{z} axis ($V = e^{i\pi\sigma_z/4}$), where the spin is initially aligned along the \hat{z} axis for Fig. 2(a) and the $-\hat{y}$ axis for Fig. 2(b). For both curves we take $\phi_0 = 0$.

IV. PROPERTIES OF THE TIME-OPTIMAL SOLUTIONS

We can visualize the time-optimal solutions by representing $SU(2)$ transformations as points on the two-dimensional sphere S^2 . Given an $SU(2)$ transformation U , we define $\hat{\mathbf{p}}(U)$ to be the point on S^2 corresponding

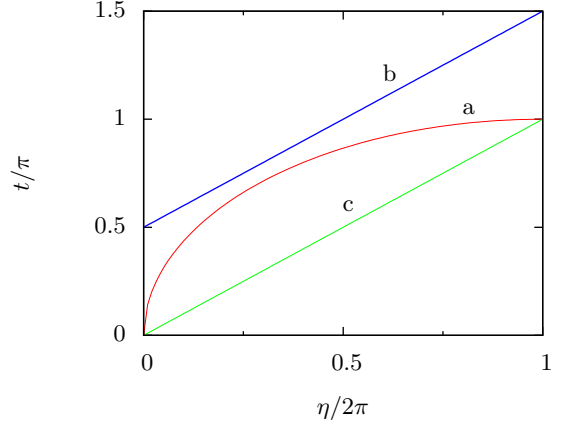


FIG. 1: (Color online) Time t needed to synthesize the transformation $V = e^{i\eta\sigma_z/2}$ versus η . (a) Time-optimal solution for the constrained control problem. (b) Euler solution for the constrained control problem. (c) Time-optimal solution for the unconstrained control problem.

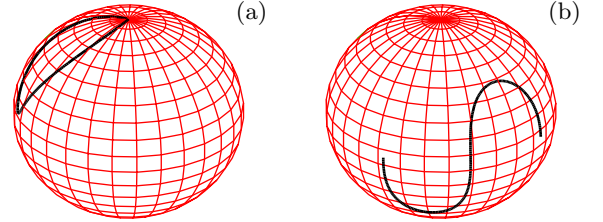


FIG. 2: (Color online) Trajectory of the spin on the Bloch sphere for the time-optimal synthesis of the transformation $V = e^{i\pi\sigma_z/4}$, which describes $\pi/2$ -rotation about the \hat{z} axis. (a) Spin initially aligned along the \hat{z} axis. (b) Spin initially aligned along the $-\hat{y}$ axis.

to the state $U^\dagger|\uparrow\rangle$:

$$\hat{\mathbf{p}}(U) = \langle\uparrow|U\boldsymbol{\sigma}U^\dagger|\uparrow\rangle. \quad (42)$$

We note that $\hat{\mathbf{p}}(U) = \hat{\mathbf{p}}(e^{i\theta\sigma_z}U)$ for any value of θ . This property of $\hat{\mathbf{p}}$ allows us to view $SU(2)$ as a fiber bundle, where S^2 is the base manifold, $U(1)$ is the fiber, and $\hat{\mathbf{p}} : SU(2) \rightarrow S^2$ is the projection function.

We will now show that the time-optimal solutions project to circles on S^2 . Let us identify the plane that bisects S^2 at the equator with the complex plane. We can map points $\hat{\mathbf{p}}$ on S^2 to complex numbers $\zeta(\hat{\mathbf{p}})$ on the complex plane by stereographically projecting from the south pole:

$$\zeta(\hat{\mathbf{p}}) = \frac{p_x + ip_y}{1 + p_z}. \quad (43)$$

Let (z_1, z_2) denote the complex coordinates of an arbitrary $SU(2)$ transformation U . From Eqs. (9), (42), and (43), it follows that

$$\zeta(\hat{\mathbf{p}}(U)) = z_1/z_2. \quad (44)$$

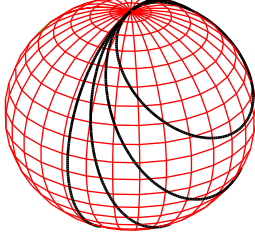


FIG. 3: (Color online) Paths on the two-dimensional sphere S^2 for the time-optimal synthesis of the transformation $V = e^{i\eta\sigma_z/2}$, where $\eta = \pi/2, \pi, 3\pi/2, 2\pi$. Longer paths correspond to larger values of η .

For a time-optimal solution, z_1 and z_2 are given by Eqs. (37) and (38). We substitute these expressions into Eq. (44) to obtain $\zeta(t) = f(e^{2i\alpha t})$, where

$$f(z) \equiv \frac{e^{-i\phi_0}(z-1)}{\beta_+ z + \beta_-}. \quad (45)$$

The function $f(z)$ is a Möbius transformation. Since $e^{2i\alpha t}$ describes a circle in the complex plane, and both stereographic projection and Möbius transformations preserve circles, it follows that the time-optimal solutions project to circular paths on S^2 . In Fig. 3 we plot example paths for the time-optimal synthesis of the transformation $V = e^{i\eta\sigma_z/2}$, which describes a spatial rotation with axis \hat{z} and angle η . The paths begin and end at the north pole. For the paths shown we take $\phi_0 = 0$; alternative paths that also synthesize V can be obtained by taking different values of ϕ_0 , and for such paths Fig. 3 is rotated about the \hat{z} axis through an angle ϕ_0 . Under the fiber bundle interpretation, the time-optimal solutions can be obtained by lifting the circular paths from S^2 to $SU(2)$, where the lifts are performed relative to the connection induced by the constraint $\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0$. Another way to visualize the time-optimal solutions is to stereographically project from the north pole, in which case the time-optimal solutions map to straight lines on the complex plane.

We have shown that time-optimal solutions project to circular paths on S^2 . We will now show that the length of the path on S^2 is equal to twice the amount of time needed to synthesize the corresponding transformation. We first assign coordinates (ψ, θ, ϕ) to an arbitrary $SU(2)$ transformation U by performing an Euler-angle decomposition:

$$U = e^{i\psi\sigma_z/2} e^{i\theta\sigma_y/2} e^{i\phi\sigma_z/2}. \quad (46)$$

We call these coordinates Euler coordinates. Note that

$$\hat{\mathbf{p}}(U) = \sin\theta \cos\phi \hat{\mathbf{x}} + \sin\theta \sin\phi \hat{\mathbf{y}} + \cos\theta \hat{\mathbf{z}}, \quad (47)$$

so the coordinates (θ, ϕ) are the spherical-polar coordinates of the point $\hat{\mathbf{p}}(U)$ on S^2 . From Eqs. (8), (9) and (46), it follows that the Euler coordinates are related to

the complex coordinates (z_1, z_2) and the embedding coordinates $\mathbf{r} = (w, x, y, z)$ by

$$z_1 = w + iz = e^{i(\psi+\phi)/2} \cos\theta/2, \quad (48)$$

$$z_2 = y + ix = e^{i(\psi-\phi)/2} \sin\theta/2. \quad (49)$$

Let us consider a small segment $[t, t+dt]$ of a time-optimal path on S^3 . From Eq. (48), it follows that the arc length dt of the segment is given by

$$\begin{aligned} dt &= (d\mathbf{r} \cdot d\mathbf{r})^{1/2} \\ &= (1/2)(d\theta^2 + d\phi^2 + d\psi^2 + 2\cos\theta d\phi d\psi)^{1/2}. \end{aligned} \quad (50)$$

Recall that time-optimal paths satisfy the constraint $\mathbf{L}_z(\mathbf{r}) \cdot \dot{\mathbf{r}} = 0$. From Eqs. (14) and (48), it follows that in Euler coordinates this constraint takes the form

$$d\psi + \cos\theta d\phi = 0. \quad (51)$$

We substitute Eq. (51) into Eq. (50) to obtain

$$dt^2 = (1/4)(d\theta^2 + \sin^2\theta d\phi^2) = (1/4)ds^2, \quad (52)$$

where ds^2 is the standard metric on S^2 , which is induced by the Euclidean metric on \mathbb{R}^3 via the embedding of S^2 into \mathbb{R}^3 . From Eq. (52), it follows that the time needed to synthesize an $SU(2)$ transformation is equal to half the length of the corresponding path in S^2 .

V. BIAS FIELD

Let us now generalize the control problem described in Sec. II by adding a constant bias magnetic field along the \hat{z} axis. The Hamiltonian for the system is now given by

$$H = -\boldsymbol{\sigma} \cdot \hat{\mathbf{n}} + b\sigma_z, \quad (53)$$

where b characterizes the strength of the bias field. As before, we assume that $\hat{\mathbf{n}}$ is constrained to lie in the $x-y$ plane and thus has the form $\hat{\mathbf{n}} = \cos\phi \hat{\mathbf{x}} + \sin\phi \hat{\mathbf{y}}$. We assume that we are given a target $SU(2)$ transformation V and bias field value b , and we would like to determine the time dependence of ϕ and total evolution time t so as to synthesize V in a time-optimal fashion.

It is convenient to work in the interaction picture. We express the Hamiltonian as $H = H_0 + H_i$, where $H_0 = b\sigma_z$ is the bare Hamiltonian and $H_i = -\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}$ is the interaction Hamiltonian, and we define $U_i = e^{iH_0 t} U$ to be the interaction-picture evolution operator. The operator U_i satisfies the Schrödinger equation

$$i\dot{U}_i = H_i U_i, \quad (54)$$

where

$$H_i = e^{iH_0 t} H_i e^{-iH_0 t} = -\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}_I, \quad (55)$$

$$\hat{\mathbf{n}}_I = \hat{\mathbf{x}} \cos\phi_I + \hat{\mathbf{y}} \sin\phi_I, \quad (56)$$

$$\phi_I = \phi + 2bt. \quad (57)$$

From the results of Sec. III, it follows that the time-optimal solution for ϕ_I is given by $\phi_I = \phi_0 + \omega t$, where ϕ_0 and ω are constants, and the complex coordinates $(z_1(U_i), z_2(U_i))$ of U_i are given by Eqs. (37) and (38). Since $U = e^{-iH_0 t} U_i$, it follows that the complex coordinates $(z_1(U), z_2(U))$ of U are given by

$$z_1(U) = (2\alpha)^{-1} e^{-ibt} (\beta_+ e^{i\beta_- t} + \beta_- e^{-i\beta_+ t}), \quad (58)$$

$$z_2(U) = (2\alpha)^{-1} e^{-i(\phi_0 + bt)} (e^{i\beta_- t} - e^{-i\beta_+ t}), \quad (59)$$

where α and β_{\pm} are given by Eq. (39). Given the complex coordinates of the target transformation V , we can invert Eqs. (58) and (59) to determine the parameters needed to synthesize V in a time-optimal fashion.

VI. INHOMOGENEOUS CONTROL

We will now generalize the control problem described in Sec. II to the case of inhomogeneous control. We consider an ensemble of N spin-1/2 particles, where particle i is in a magnetic field $\mathbf{B}_i = B_i \hat{\mathbf{n}}$ with magnitude B_i and direction $\hat{\mathbf{n}}$. The Hamiltonian for particle i is

$$H_i = -\chi_i \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}, \quad (60)$$

where $\chi_i \equiv \mu B_i$. As before, we assume that $\hat{\mathbf{n}}$ is constrained to lie in the $x-y$ plane and thus has the form $\hat{\mathbf{n}} = \cos \phi \hat{\mathbf{x}} + \sin \phi \hat{\mathbf{y}}$. We note that the single control parameter ϕ governs the evolution of all N particles. If we evolve the ensemble for a time t while varying the control parameter ϕ , we obtain $SU(2)$ evolution operators $\{U_1(t), \dots, U_N(t)\}$, where $U_i(t)$ is the evolution operator for particle i . We assume that we are given a list of target $SU(2)$ transformations $\{V_1, \dots, V_N\}$ and a list of field values $\{\chi_1, \dots, \chi_N\}$. We would like to determine the time dependence of ϕ and total evolution time t such that $U_i(t) = V_i$ for $i = 1, \dots, N$, and t is as small as possible.

We begin by adapting the formalism developed in Sec. III to the case of the Hamiltonian H_i given in Eq. (60). We denote the embedding coordinates of U_i by \mathbf{r}_i and the complex coordinates of U_i by (z_{1i}, z_{2i}) . The Schrödinger equation in embedding coordinates is

$$\dot{\mathbf{r}}_i = \chi_i (n_x \mathbf{L}_x(\mathbf{r}_i) + n_y \mathbf{L}_y(\mathbf{r}_i) + n_z \mathbf{L}_z(\mathbf{r}_i)), \quad (61)$$

From Eq. (61) and the orthonormality of the vector fields \mathbf{L}_k , it follows that the magnitude of the tangent vector $\dot{\mathbf{r}}_i$ is $|\dot{\mathbf{r}}_i| = \chi_i$, so the arc length s of the path traced out by \mathbf{r}_i in S^3 is related to the time t by $s = \chi_i t$. The Schrödinger equation in complex coordinates is

$$\dot{z}_{1i} = -i\chi_i e^{-i\phi} z_{2i}^*, \quad (62)$$

$$\dot{z}_{2i} = i\chi_i e^{-i\phi} z_{1i}^*. \quad (63)$$

From Eqs. (62) and (63) we obtain the decoupled equations of motion

$$\ddot{z}_{1i} + i\dot{\phi} \dot{z}_{1i} + \chi_i^2 z_{1i} = 0, \quad (64)$$

$$\ddot{z}_{2i} + i\dot{\phi} \dot{z}_{2i} + \chi_i^2 z_{2i} = 0, \quad (65)$$

and the identities

$$\dot{z}_{1i} z_{1i}^* + \dot{z}_{2i} z_{2i}^* = 0, \quad (66)$$

$$\dot{z}_{2i} z_{1i} - \dot{z}_{1i} z_{2i} = i\chi_i e^{-i\phi}. \quad (67)$$

We can obtain a time-optimal solution to the control problem by minimizing the action

$$S = \sum_i A_i + \sum_{i \neq j} (B_{ij} + C_{ij}), \quad (68)$$

where

$$A_i = \chi_i \int (|\mathbf{r}'_i| + \gamma_i (|\mathbf{r}_i|^2 - 1) + \lambda_i \mathbf{L}_z(\mathbf{r}_i) \cdot \mathbf{r}'_i) du, \quad (69)$$

$$B_{ij} = b_{ij} \int (\mathbf{L}_x(\mathbf{r}_i) \cdot \mathbf{r}'_i - \mathbf{L}_x(\mathbf{r}_j) \cdot \mathbf{r}'_j) du, \quad (70)$$

$$C_{ij} = c_{ij} \int (\mathbf{L}_y(\mathbf{r}_i) \cdot \mathbf{r}'_i - \mathbf{L}_y(\mathbf{r}_j) \cdot \mathbf{r}'_j) du, \quad (71)$$

and γ_i , λ_i , b_{ij} , and c_{ij} are Lagrange multipliers. The terms A_i are straightforward generalizations of the action (29) for the original control problem; the prefactor χ_i accounts for the fact that the arc length s of a path in S^3 is related to the time t by $s = \chi_i t$. The terms B_{ij} and C_{ij} impose the constraints $\mathbf{L}_x(\mathbf{r}_i) \cdot \dot{\mathbf{r}}_i = \mathbf{L}_x(\mathbf{r}_j) \cdot \dot{\mathbf{r}}_j$ and $\mathbf{L}_y(\mathbf{r}_i) \cdot \dot{\mathbf{r}}_i = \mathbf{L}_y(\mathbf{r}_j) \cdot \dot{\mathbf{r}}_j$; from Eqs. (18) and (19), we see that these constraints account for the fact that the same control parameter ϕ governs the evolution of all N evolution operators $\{U_1, \dots, U_N\}$.

We now follow the same procedure described in Sec. III: we write down the Euler-Lagrange equations for S , subtract the decoupled Schrödinger equation (62) and (63), and use the identities (66) and (67) to obtain equations that involve only the Lagrange multipliers and the control parameter ϕ . We find that

$$\chi_i^2 (2\lambda_i - \dot{\phi}) = e^{i\phi} \sum_{ij} (\dot{w}_{ij} - \dot{w}_{ji}), \quad (72)$$

$$i\dot{\lambda}_i - 2\gamma_i - \chi_i^2 = -2ie^{i\phi} \sum_{ij} (w_{ij} - w_{ji}), \quad (73)$$

where $w_{ij} \equiv b_{ij} + ic_{ij}$.

For the case $N = 2$ we can solve Eqs. (72) and (73) to obtain an equation of motion for ϕ . From Eqs. (72) it follows that

$$\lambda_1 = (1/2)(\dot{\phi} + \alpha/\chi_1^2), \quad (74)$$

$$\lambda_2 = (1/2)(\dot{\phi} - \alpha/\chi_2^2), \quad (75)$$

where

$$\alpha \equiv \dot{w} e^{i\phi} \quad (76)$$

and $w \equiv w_{12} - w_{21}$. From Eqs. (73) it follows that

$$\dot{\lambda}_1 + \dot{\lambda}_2 = 0, \quad (77)$$

$$w = -(1/4)(\dot{\lambda}_1 - \dot{\lambda}_2 + 2i\beta) e^{-i\phi}, \quad (78)$$

where $\beta = 2\gamma_1 + \chi_1^2 = -(2\gamma_2 + \chi_2^2)$. We integrate Eq. (77) to obtain

$$\lambda_1 + \lambda_2 = A, \quad (79)$$

where A is an integration constant. We solve Eqs. (74), (75), and (79) for λ_1 , λ_2 , and α in terms of $\dot{\phi}$ and A :

$$\lambda_1 = (\chi/2)\dot{\phi} - (\chi'/2\chi_1^2)A, \quad (80)$$

$$\lambda_2 = -(\chi/2)\dot{\phi} + (\chi'/2\chi_2^2)A, \quad (81)$$

$$\alpha = \chi'(\dot{\phi} - A), \quad (82)$$

where

$$\chi \equiv \frac{\chi_1^2 + \chi_2^2}{\chi_1^2 - \chi_2^2}, \quad \chi' \equiv \frac{2\chi_1^2\chi_2^2}{\chi_1^2 - \chi_2^2}. \quad (83)$$

We substitute Eqs. (80) and (81) for λ_1 and λ_2 into Eq. (78) to obtain

$$w = -(1/4)(\chi\ddot{\phi} + 2i\beta)e^{-i\phi}. \quad (84)$$

We differentiate Eq. (84) with respect to time and substitute the resulting expression for \dot{w} into Eq. (76) to obtain

$$\alpha = -(1/4)(\chi\ddot{\phi} + 2i\dot{\beta} - i\dot{\phi}(\chi\ddot{\phi} + 2i\beta)). \quad (85)$$

Taking the real and imaginary parts of Eq. (85), we find that

$$\alpha = -(1/4)(\chi\ddot{\phi} + 2\beta\dot{\phi}), \quad (86)$$

$$0 = -(1/4)(2\dot{\beta} - \chi\ddot{\phi}). \quad (87)$$

We integrate Eq. (87) to obtain

$$\beta = (\chi/4)\dot{\phi}^2 + B, \quad (88)$$

where B is an integration constant. Substituting Eqs. (85) for α and (88) for β into Eq. (86), we find that

$$\ddot{\phi} + \dot{\phi}^3/2 + (2B/\chi)\dot{\phi} + (4\chi'/\chi)(\dot{\phi} - A) = 0. \quad (89)$$

So the control parameter ϕ satisfies the equation of motion

$$\ddot{\phi} + \dot{\phi}^3/2 + b\dot{\phi} + a = 0, \quad (90)$$

where $a \equiv -(4\chi'/\chi)A$ and $b \equiv (2/\chi)B - 4\chi'/\chi$. We note that since the integration constants A and B can take any values, the parameters a and b can also take any values, and are thus not constrained by the values of χ_1 and χ_2 .

Given initial conditions $(\phi_0, \dot{\phi}_0, \ddot{\phi}_0)$ and parameters (a, b) , we can integrate Eq. (90) to obtain a time-optimal solution for ϕ . Given this time-optimal solution, we can integrate the Schrödinger equations (64) and (65) subject to the initial conditions $(z_{1i}, z_{2i}) = (1, 0)$ to obtain the complex coordinates of a pair of evolution operators $\{U_1, U_2\}$. It is useful to view the parameters

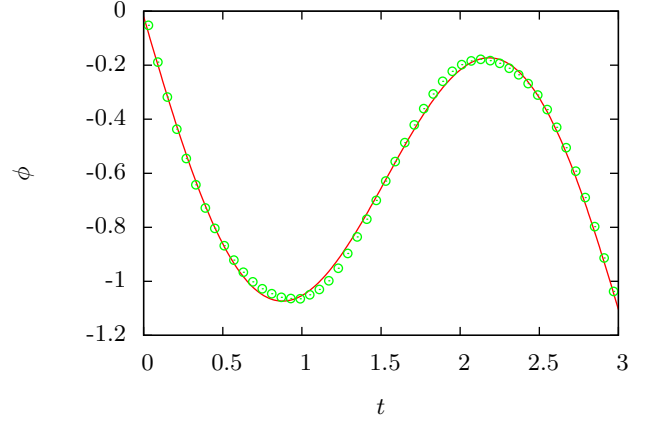


FIG. 4: (Color online) Control parameter ϕ versus time t . The solid curve is obtained by numerically integrating Eq. (90); the points are obtained from a numerical gradient-ascent search with $t = 3$ and $R = 50$.

$(\phi_0, \dot{\phi}_0, \ddot{\phi}_0, a, b, t)$ as a generalization of the time-optimal coordinates described in Sec. III. The two integrations then define a coordinate transformation from the time-optimal coordinates to the complex coordinates of the pair of evolution operators $\{U_1, U_2\}$. Given target $SU(2)$ transformations $\{V_1, V_2\}$ and field values $\{\chi_1, \chi_2\}$, we can write down the complex coordinates of $\{V_1, V_2\}$ and then invert this coordinate transformation to determine the time dependence of the control parameter ϕ and the total evolution time t needed to synthesize V_1 and V_2 in a time-optimal fashion. We have thus formally solved the inhomogeneous control problem for the case $N = 2$.

We note that the parameters $(\phi_0, \dot{\phi}_0, \ddot{\phi}_0, a, b)$ determine a time-optimal evolution for the control parameter ϕ , and this evolution, together with the parameters (t, χ_1, χ_2) , determine a pair of evolution operators $\{U_1, U_2\}$. It is interesting that the time-optimality of ϕ does not depend on the field values χ_1 and χ_2 . That is, if we hold the time dependence of ϕ and the total evolution time t fixed, and vary χ_1 and χ_2 , we will synthesize different evolution operators U_1 and U_2 , but it will always be the case that the synthesis of these operators is time-optimal.

Let us now consider a specific example. We will take the field values to be $\chi_1 = 1/2$ and $\chi_2 = 3/2$, and consider the pair of transformations $\{V_1, V_2\}$ whose time optimal coordinates are $\phi_0 = 0$, $\dot{\phi}_0 = -2$, $\ddot{\phi}_0 = 0$, $a = 2$, $b = 3$, $t = 3$. We numerically integrate the equation of motion (90) to determine the time evolution of the control parameter ϕ that synthesizes $V_1 = U_1(t)$ and $V_2 = U_2(t)$ in a time-optimal fashion, and we numerically integrate the Schrödinger equations (62) and (63) to determine the complex coordinates of the pair $\{V_1, V_2\}$. In Fig. 4 we plot the resulting time-optimal evolution of ϕ .

We verify that the synthesis of V_1 and V_2 is time optimal as follows. Given arbitrary $SU(2)$ transformations A_1 and A_2 , we define the fidelity with which A_1 and A_2

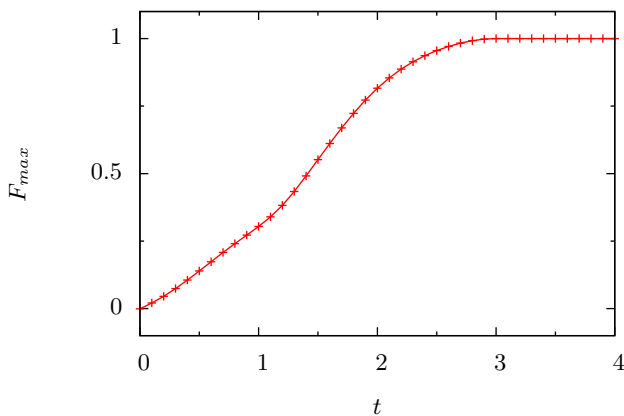


FIG. 5: (Color online) Maximum fidelity F_{max} versus time t , as determined by a gradient-ascent search with $R = 50$.

approximate V_1 and V_2 to be

$$F = (1/4)(\text{Tr}[V_1^\dagger A_1] + \text{Tr}[V_2^\dagger A_2]). \quad (91)$$

The fidelity ranges from -1 to 1 , where $F = 1$ if $A_1 = V_1$ and $A_2 = V_2$, and F decreases as the deviation of A_1 and A_2 from V_1 and V_2 increases. We fix the total evolution time t , and we discretize the time evolution of the control parameter by dividing t into R timesteps of duration $\delta t = t/R$. We define $\phi_r = \phi(r\delta t)$ to be the value of the control field at timestep r . We then take $A_1 = U_1(t)$ and $A_2 = U_2(t)$, and perform a numerical gradient-ascent search to maximize F with respect to the discretized control parameter values $\{\phi_0, \dots, \phi_{R-1}\}$. In Fig. 5 we plot the numerically-determined maximum fidelity F_{max} as a function of t for $R = 50$. Since F_{max} first reaches 1 at $t = 3$, we see that the evolution described above is indeed

time-optimal. In Fig. 4, we plot the time-optimal evolution of ϕ for $t = 3$, as determined by the gradient-ascent search. We find good agreement with the time-optimal evolution of ϕ obtained by integrating the equation of motion (90).

VII. SUMMARY

We have considered a quantum control problem involving a spin-1/2 particle in a magnetic field. We have analytically solved for the time dependence of the control parameter needed to synthesize an arbitrary $SU(2)$ transformation in a time-optimal fashion, and we have generalized our solution to the case of an inhomogeneous control problem involving an ensemble of spin-1/2 systems. It is interesting to consider how our results might be extended to other control problems. The formalism we have developed relies heavily on the fact that $SU(2)$ is diffeomorphic to the three-dimensional sphere S^3 ; since no $SU(d)$ for $d > 2$ is diffeomorphic to an n -dimensional sphere, our formalism cannot be directly extended to higher-dimensional systems. Our formalism could, however, be used to describe $SU(2)$ control problems involving a different choice of control fields, and it would be interesting to see if such problems are also analytically solvable.

VIII. ACKNOWLEDGEMENTS

The author would like to thank Ivan Deutsch for valuable discussions and suggestions. This research was supported by NSF Grant No. PHY-0903953.

-
- [1] M. Shapiro and P. Brumer, J. Chem. Phys. **84**, 4103 (1986).
 - [2] R. S. Judson and H. Rabitz, Phys. Rev. Lett. **68**, 1500 (1992).
 - [3] P.W. Brumer and M. Shapiro, *Principles of the Quantum Control of Molecular Processes* (Wiley InterScience, Hoboken, NJ, 2003).
 - [4] H. Rabitz *et al.*, Science **288**, 824 (2000).
 - [5] N. Khaneja, R. Brockett, and S. J. Glaser, Phys. Rev. A **63**, 032308 (2001).
 - [6] C. Ramanathan *et al.*, Quantum Inf. Process. **3**, 15 (2004).
 - [7] L. Viola, S. Lloyd, and E. Knill, Phys. Rev. Lett. **83**, 4888 (1999).
 - [8] M. Grace *et al.*, J. Phys. B **40**, S103 (2007).
 - [9] G. De Chiara *et al.*, Phys. Rev. A **77**, 052333 (2008).
 - [10] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
 - [11] A. M. Bloch, *Nonholonomic Mechanics and Control* (Springer-Verlag, New York, 2003).
 - [12] Baillieul, J. and J. C. Willems (eds.), *Mathematical control theory* (Springer-Verlag, New York, 1999).
 - [13] Li, Z. and J. Canny, *Nonholonomic Motion Planning* (Kluwer, New York, 1993).
 - [14] A. P. Peirce, M. A. Dahleh, and H. Rabitz, Phys. Rev. A, **37**, 4950–4964 (1988).
 - [15] H. A. Rabitz, M. M. Hsieh, and C. M. Rosenthal, Science **303**, 1998 (2004).
 - [16] Z. Shen, M. Hsieh, and H. Rabitz, J. Chem. Phys. **124**, 204106 (2006).
 - [17] M. Hsieh and H. Rabitz, Phys. Rev. A **77**, 042306 (2008).
 - [18] K. Moore, M. Hsieh, and H. Rabitz, J. Chem. Phys. **128**, 154117 (2008).
 - [19] I. Walmsley and H. Rabitz, Phys. Today **56**, No. 8, 43 (2003).
 - [20] C. M. Tesch and R. de Vivie-Riedle, Phys. Rev. Lett. **89**, 157901 (2002).
 - [21] J. P. Palao and R. Kosloff, Phys. Rev. A **68**, 062308 (2003).

- [22] U. Boscain *et al.*, J. Math. Phys. **43**, 2107 (2002).
- [23] D. D'Alessandro and M. Dahleh, Proceedings of the American Control Conference **6**, 3893 (2000).
- [24] D. D'Alessandro and M. Dahleh, IEEE Transactions on Automatic Control **46**, 866 (2001).
- [25] N. Khaneja, R. Brockett, and S. J. Glaser, Phys. Rev. A **63**, 032308 (2001).
- [26] U. Boscain, P. Mason, J. Math. Phys. **47**, 062101 (2006).
- [27] L. M. K. Vandersypen and I. L. Chuang, Rev. Mod. Phys. **76**, 1037 (2005).
- [28] H. K. Cummins, G. Llewellyn, and J. A. Jones, Phys. Rev. A **67**, 042308 (2003).
- [29] J. S. Li and N. Khaneja, Phys. Rev. A **73**, 030302 (2006).
- [30] K. Kobzar *et al.*, J. Magn. Reson. **173**, 229 (2005).
- [31] N. Khaneja *et al.*, J. Magn. Reson. **172**, 296 (2005).