Bang-Bang Control Design for Quantum State Transfer based on Hyperspherical Coordinates and Optimal Time-energy Control

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Abstract. We present a constructive control scheme for solving quantum state engineering problems based on a parametrization of the state vector in terms of complex hyperspherical coordinates. Unlike many control schemes based on factorization of unitary operators the scheme gives explicit expressions for all the Euler angles in terms of the hyperspherical coordinates of the initial and final state. The factorization, when applicable, has added benefits that phase rotations can be combined and performed concurrently. The control procedure can be realized using a simple bang-bang or square-wave-function controls. Optimal time-energy control is considered to find the optimal control amplitudes.

Keywords: quantum systems, Bang-Bang control, geometric parametrization, controllability, optimal control

1. Introduction

Control of quantum phenomena has been recognized as a crucial task for many years [1]. From early beginning in the 1980s [2, 3, 4], there has been considerable recent progress in both theory and experiment of quantum control [5, 6, 7]. Various techniques including feedback control [8, 9, 10, 11, 12, 13, 14], optimal control [15, 16, 17], Transfer Functions [18, 19], constructive control based Lie-group docompositions [20, 21, 22], Lyapunov control [23, 24, 25], and other methods [26, 27, 28, 29, 30, 31], have been proposed to control quantum systems.

Although optimal control using shaped pulses is a very important area that holds considerable promise of enabling global control of complex systems with only a few local actuators, improving control performance for imperfect systems, etc, the implementation of complex control pulses remains challenging in many cases. Controls with complex temporal and spectral profiles may be difficult to implement, for instance, in solid-state quantum dot systems controlled by voltages applied to gate

electrodes. For these reasons constructive control schemes that rely on simple pulses such as approximately piecewise-constant functions remain useful and popular.

In this article we revisit the problem of bang-bang-type control for state-transfer tasks. We show that parametrization of the initial and target states in hyperspherical coordinates [32] yields a simple constructive control scheme for state-transfer tasks that requires no complex calculations of the control parameters, i.e., all control parameters are given in terms of simple functions of the initial and final state coordinates. The scheme has some additional advantages over alternative geometric schemes in that many operations can be performed either sequentially or in parallel. We further explore the trade-off between time and energy optimal control using time-energy performance index $J = \int_0^{t_f} [\lambda + E(t)]dt$ where $E(t)$ is energy cost of Bang-Bang control at t, t_f is terminal time, and λ is the ratio factor of time and energy. It is shown that the product of the terminal time t_f^* and the energy cost E^* for optimal bounded or unbounded piecewise constant controls only depends on the geometric parameters of the initial and target states and is independent of λ but λ determines the optimal field strength of the controls, $L_* = \sqrt{\lambda}$.

2. Pure-state Transfer by Bang-Bang Control

Pure-states $|\psi\rangle$ of a quantum system defined on a complex Hilbert space $\mathcal{H}$ with $\dim \mathcal{H} = N < \infty$ can be represented by complex vectors $\vec{c} \in \mathbb{C}^N$ by choosing a suitable basis $\{|n\rangle\}_{n=1}^N$ for $\mathcal{H}$,

$$|\psi\rangle = \sum_{n=1}^{N} c_n |n\rangle. \tag{1}$$

The modulus squared $|c_n|^2$ of the coordinates can be interpreted in terms of probabilities provided $\vec{c}$ is a unit vector. For most applications the global phase of the state is irrelevant, i.e., we can further identify $|\psi\rangle \sim e^{i\phi}|\psi\rangle$. Given these considerations, physically distinguishable pure states can be uniquely identified with elements in the complex projective space $\mathbb{CP}^{N-1} = S^{2N-1}/S_1$, and we can uniquely represent pure states by unit vectors in $\mathbb{C}^N$ if we fix the complex phase of one coordinate.

Pure-state transfer, also known as quantum state engineering, is the task of transforming a given pure quantum state $|\psi^{(0)}\rangle$ to a desired pure quantum state $|\psi^{(s)}\rangle$. It is one of the most fundamental tasks in control of quantum systems. Many of the control strategies mentioned in the introduction have been applied to this problem, including constructive control schemes based on Lie group decompositions. Indeed, it is quite straightforward to see how to solve the state transfer problem for an N-level system in principle, if we are able to implement unitary gates on a sequence of connected two-level subspaces [36]. Assume, e.g., that we can implement $\mathbf{SU}(2)$ operations on the subspaces spanned by $\{|1\rangle, |2\rangle\}$, $\{|2\rangle, |3\rangle\}$, ..., $\{|N-1\rangle, |N\rangle\}$. We can decompose any unitary operator in $\mathbf{SU}(N)$ into a sequence of $\mathbf{SU}(2)$ rotations on these two-dimensional (2D) subspaces. We can further decompose any unitary operator in $\mathbf{SU}(2)$ into a sequence of three rotations about two orthogonal axes using the Euler decomposition. It therefore suffices if we can implement rotations about two fixed orthogonal axes on each of the 2D subspaces. Applied to the problem of quantum state transfer, it is not difficult to see that we can transform any complex unit vector $\vec{c}^{(0)}$ into any other complex unit vector $\vec{c}^{(s)}$ by a sequence of $N-1$ rotations on the

2D subspaces defined above

$$\vec{c}^{(s)} = U^{(N-1,N)} \dots U^{(2,3)} U^{(1,2)} \vec{c}^{(0)} \tag{2}$$

where $U^{(n,n+1)}$ indicates a complex rotation on the subspace spanned by $\{|n\rangle, |n+1\rangle\}$. Decomposing each $U^{(n,n+1)}$ further into three rotations about two fixed orthogonal axes, $U_1^{(n,n+1)}(\alpha)$ and $U_2^{(n,n+1)}(\beta)$, by suitable angles γ_k,

$$U^{(n,n+1)} = U_1^{(n,n+1)}(\gamma_3) U_2^{(n,n+1)}(\gamma_2) U_1^{(n,n+1)}(\gamma_1), \tag{3}$$

shows that in general $3(N-1)$ such rotations are required to transform a given initial state to a target state using a sequence of elementary unitary transformations,

$$\begin{aligned} \vec{c}^{(s)} = U_1^{(N-1,N)}(\gamma_{3N-3}) U_2^{(N-1,N)}(\gamma_{3N-4}) U_1^{(N-1,N)}(\gamma_{3N-5}) \times \dots \\ \times U_1^{(1,2)}(\gamma_3) U_2^{(1,2)}(\gamma_2) U_1^{(1,2)}(\gamma_1) \vec{c}^{(0)}. \end{aligned} \tag{4}$$

Thus it easy to see how to transform pure states in principle, but it is not obvious how to derive the correct rotation angles γ_k in the sequence, which is what matters in practice. Although it is possible to constructively compute the γ_k, the dependence of γ_k on the state vectors $\vec{c}^{(0)}$ and $\vec{c}^{(s)}$ is complicated.

3. Bang-Bang Control Scheme based on Hyperspherical Parametrization

3.1. Complex hyperspherical coordinates

We now show that the problem of obtaining a geometric control sequence with explicit expression for the rotation angles γ_k can easily be solved by parametrizing the initial and target states in terms of complex hyperspherical coordinates. Any complex unit vector $\vec{c}$ can be parametrized in terms of complex hyperspherical coordinates $(\vec{\theta}, \vec{\phi})$,

$$\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N-1} \\ c_N \end{pmatrix} = e^{i\phi_0} \begin{pmatrix} \cos\theta_1 \\ e^{i\phi_1} \sin\theta_1 \cos\theta_2 \\ \vdots \\ e^{i\phi_{N-2}} \sin\theta_1 \dots \sin\theta_{N-2} \cos\theta_{N-1} \\ e^{i\phi_{N-1}} \sin\theta_1 \dots \sin\theta_{N-1} \end{pmatrix} \tag{5}$$

where $\vec{\theta}$ and $\vec{\phi}$ are vectors in $\mathbb{R}^{N-1}$ with $0 \le \theta_n \le \frac{\pi}{2}$ and $-\pi \le \phi_n \le \pi$, and $e^{i\phi_0}$ is a global phase factor, which is usually negligible. Thus, assuming normalization and neglecting global phases, any pure state is uniquely determined by its complex hyperspherical coordinates $(\vec{\theta}, \vec{\phi})$. Calculating hyperspherical coordinates is very easy as shown in Algorithm 1.

Although there are many equivalent parameterizations of pure state vectors, the beauty of complex hyperspherical coordinates is that we can easily give an explicit constructive bang-bang control scheme for state transfer $|\psi_0\rangle \mapsto |\psi_s\rangle$ such that all control pulses are determined directly by the coordinates of the initial and final state $(\vec{\theta}^{(0)}, \vec{\phi}^{(0)}, \vec{\theta}^{(s)}, \vec{\phi}^{(s)})$.

$(\theta, \phi) \leftarrow$ HYPERCOORD (c)
Compute complex hyperspherical coordinates

In: c complex vector/pure state
Out: θ, ϕ hyper-spherical coordinates

$N \leftarrow$ LENGTH(c)
$c \leftarrow c/$NORM(c)
$c \leftarrow \exp(-i *$ ANGLE$(c_1)) * c$
$\phi \leftarrow$ ANGLE$(c_{2:N})$
$a \leftarrow$ ABS(c)
$\theta_1 \leftarrow \arccos(a_1)$
$s_1 \leftarrow \sin(\theta_1)$
for $n \leftarrow 2, \ldots, N-1$
  $\theta_n \leftarrow \arccos(a_n/s_{n-1})$
  $s_n \leftarrow s_{n-1}\sin(\theta_n)$

Algorithm 1: Computation of complex hyperspherical coordinates

3.2. Control Assumptions

The following scheme is based on the assumption that (a) we can neglect free evolution, $H_0 = 0$; (b) we have local phase control, i.e., can implement control operators that introduce a local phase shift,

$$Z_n = \Pi_n, \quad n = 2, \ldots, N \tag{6}$$

where I_N is the identity on $\mathcal{H}$ and Π_n is the projector onto the subspace of $\mathcal{H}$ spanned by the basis state $|n\rangle$, and (c) can individually control transitions between adjacent energy levels, i.e., that we can realize control Hamiltonians of the form X_n or Y_n,

$$X_n = (|n+1\rangle\langle n| + |n\rangle\langle n+1|), \quad n = 1, \ldots, N-1.$$
$$Y_n = i(|n+1\rangle\langle n| - |n\rangle\langle n+1|), \quad n = 1, \ldots, N-1.$$

The evolution of the system under any Hamiltonian H is governed by the Schrodinger equation

$$i\hbar\dot{U}(t) = HU(t), \quad U(0) = I_N, \tag{8}$$

and we choose units such that the Planck constant $\hbar = 1$. This shows that the evolution under the control Hamiltonian $H \in \{LX_n, LY_n, LZ_n\}$ is given by the one-parameter groups $\exp(-iLtX_n)$, $\exp(-iLtY_n)$ and $\exp(-iLtZ_n)$, respectively. The evolution is unitary as the operators X_n, Z_n and Y_n are Hermitian. In particular, this means that we can implement the complex rotations

$$U_n^X(\alpha) = \exp(-i\alpha X_n), \quad U_n^Y(\alpha) = \exp(-i\alpha Y_n), \quad U_n^Z(\alpha) = \exp(-i\alpha Z_n), \tag{9}$$

by applying the control Hamiltonians LX_n, LY_n or LZ_n for some time $t = \alpha/L$. In the following we only require two types of control operations $\{X_n, Z_n\}$ or $\{Y_n, Z_n\}$.

The assumptions on the control Hamiltonian are somewhat demanding, although no more so than the control requirements for the standard geometric decomposition (4). While these requirements cannot always be satisfied, there are systems for which these control operations are quite natural such as a charge trapped in a multi-well potential created and controlled by surface control electrodes as shown in Fig. 1.

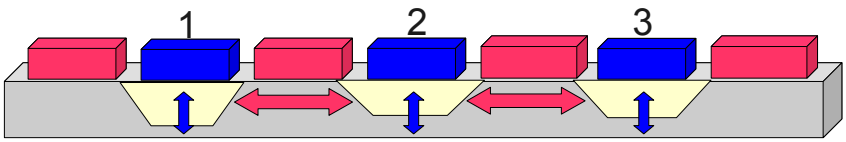

Figure 1. Charged particle trapped in a multi-well potential created by control electrodes. Red electrodes allow control of potential barriers and thus tunnelling rates, while blue electrodes control depths of the wells, and thus energy levels. We can choose default voltage settings such that all wells have the same depth and there is no tunnelling, so that we effectively have $H_0 = 0$.

3.3. Explicit Control Sequence

To illustrate the constructive procedure, let us consider the case $N = 3$ with Y, Z controls. In this case the control operators take the explicit form

$$Z_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Z_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad Y_1 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Y_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

and the corresponding evolution operators are

$$U_2^Z(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-i\alpha} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad U_2^Z(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\alpha} \end{pmatrix},$$

$$U_1^Y(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad U_2^Y(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix},$$

etc. Given these control operators and the hyperspherical coordinate representation of the initial and target states, it is now very easy to see how to steer an arbitrary initial state to an arbitrary target state in the following seven steps:

Step 1. $(\theta_1^{(0)}, \theta_2^{(0)}; \phi_1^{(0)}, \phi_2^{(0)}) \to (\theta_1^{(0)}, \theta_2^{(0)}; \phi_1^{(0)}, 0)$: Apply phase rotation $U_3^Z(\phi_2^{(0)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\phi_2^{(0)}} \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(0)} \\ e^{i\phi_1^{(0)}} \sin\theta_1^{(0)} \cos\theta_2^{(0)} \\ e^{i\phi_2^{(0)}} \sin\theta_1^{(0)} \sin\theta_2^{(0)} \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(0)} \\ e^{i\phi_1^{(0)}} \sin\theta_1^{(0)} \cos\theta_2^{(0)} \\ \sin\theta_1^{(0)} \sin\theta_2^{(0)} \end{pmatrix}.$$

Step 2. $(\theta_1^{(0)}, \theta_2^{(0)}; \phi_1^{(0)}, 0) \to (\theta_1^{(0)}, \theta_2^{(0)}; 0, 0)$: Apply phase rotation $U_2^Z(\phi_1^{(0)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-i\phi_1^{(0)}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(0)} \\ e^{i\phi_1^{(0)}} \sin\theta_1^{(0)} \cos\theta_2^{(0)} \\ \sin\theta_1^{(0)} \sin\theta_2^{(0)} \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(0)} \\ \sin\theta_1^{(0)} \cos\theta_2^{(0)} \\ \sin\theta_1^{(0)} \sin\theta_2^{(0)} \end{pmatrix}$$

Step 3. $(\theta_1^{(0)}, \theta_2^{(0)}; 0, 0) \to (\theta_1^{(0)}, 0; 0, 0)$: Apply population rotation $U_2^Y(-\theta_2^{(0)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_2^{(0)} & \sin\theta_2^{(0)} \\ 0 & -\sin\theta_2^{(0)} & \cos\theta_2^{(0)} \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(0)} \\ \sin\theta_1^{(0)} \cos\theta_2^{(0)} \\ \sin\theta_1^{(0)} \sin\theta_2^{(0)} \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(0)} \\ \sin\theta_1^{(0)} \\ 0 \end{pmatrix}$$

Step 4. $(\theta_1^{(0)},0;0,0) \to (\theta_1^{(s)},,0;0,0)$: Apply population rotation $U_1^Y(\theta_1^{(s)}-\theta_1^{(0)})$

$$\begin{pmatrix} \cos(\theta_1^{(s)}-\theta_1^{(0)}) & -\sin(\theta_1^{(s)}-\theta_1^{(0)}) & 0 \\ \sin(\theta_1^{(s)}-\theta_1^{(0)}) & \cos(\theta_1^{(s)}-\theta_1^{(0)}) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(0)} \\ \sin\theta_1^{(0)} \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(s)} \\ \sin\theta_1^{(s)} \\ 0 \end{pmatrix}$$

Step 5. $(\theta_1^{(s)},0;0,0) \to (\theta_1^{(s)},\theta_2^{(s)};0,0)$: Apply population rotation $U_2^Y(\theta_2^{(s)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_2^{(s)} & -\sin\theta_2^{(s)} \\ 0 & \sin\theta_2^{(s)} & \cos\theta_2^{(s)} \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(s)} \\ \sin\theta_1^{(s)} \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(s)} \\ \sin\theta_1^{(s)}\cos\theta_2^{(s)} \\ \sin\theta_1^{(s)}\sin\theta_2^{(s)} \end{pmatrix}$$

Step 6. $(\theta_1^{(s)},\theta_2^{(s)};0,0) \to (\theta_1^{(s)},\theta_2^{(s)};\phi_1^{(s)},0)$: Apply phase rotation $U_2^Z(-\phi_1^{(s)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\phi_1^{(s)}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(s)} \\ \sin\theta_1^{(s)}\cos\theta_2^{(s)} \\ \sin\theta_1^{(s)}\sin\theta_2^{(s)} \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(s)} \\ e^{i\phi_1^{(s)}}\sin\theta_1^{(s)}\cos\theta_2^{(s)} \\ \sin\theta_1^{(s)}\sin\theta_2^{(s)} \end{pmatrix}$$

Step 7. $(\theta_1^{(s)},\theta_2^{(s)};\phi_1^{(s)},0) \to (\theta_1^{(s)},\theta_2^{(s)};\phi_1^{(s)},\phi_2^{(s)})$: Apply phase rotation $U_1^Z(-\phi_2^{(s)})$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\phi_2^{(s)}} \end{pmatrix} \begin{pmatrix} \cos\theta_1^{(s)} \\ e^{i\phi_1^{(s)}}\sin\theta_1^{(s)}\cos\theta_2^{(s)} \\ \sin\theta_1^{(s)}\sin\theta_2^{(s)} \end{pmatrix} = \begin{pmatrix} \cos\theta_1^{(s)} \\ e^{i\phi_1^{(s)}}\sin\theta_1^{(s)}\cos\theta_2^{(s)} \\ e^{i\phi_2^{(s)}}\sin\theta_1^{(s)}\sin\theta_2^{(s)} \end{pmatrix}$$

The generalization to $N > 3$ is straightforward, as shown in algorithm 2. Given a Hamiltonian of the form

$$H = \sum_{m=1}^{2N-1} u_m(t) H_m \tag{10}$$

with $H_{2n-1} = Z_{n+1}$ and $H_{2n} = Y_n$, where $u_m(t)$ are controls (e.g., voltages) we can implement the bang-bang control sequence given by Algorithm 2 in a straightforward manner by applying $4N-5$ control pulses. At the kth step we apply a constant control field $u_{S(k)} = L_k$ for time $t_k = \gamma_k/L_k$, while all other controls at set to 0 (or the voltages are set to their default values). Notice that in practice we cannot apply fields for negative times, thus the sign of L_k must match that of γ_k. However, if γ_k is negative and $L_k > 0$, we can also apply a field $f_{S(k)} = L_k$ for time $t_k = (\gamma_k + 2\pi)/L_k$ as $\gamma_k + 2\pi > 0$ and effects the same rotation.

If we have X_n control Hamiltonians instead of Y_n control Hamiltonians the algorithm needs to be slightly modified to correct for phase factors of i^{n-1} being created in the nth coordinate by the population rotations. We can achieve this by adding $\frac{\pi}{2}(n \mod 4)$ from the phase angles ϕ_n, noting that $e^{i\pi/2(n \mod 4)} = i^n$ and the phase factor of the nth coordinate is $e^{i\phi_{n-1}}$.

Besides giving explicit expressions for the rotation angles in the decomposition, the scheme has an additional advantage compared the the standard decomposition (4) considered earlier: While the rotations in the standard factorization do not commute, the first $N-1$ and final $N-1$ phase rotations in the decomposition based on complex hyperspherical coordinates are represented by diagonal matrices which commute. This means that these operations can be applied concurrently rather than sequentially, leading to a potentially considerable reduction in the total length of the control sequence.

$(S, \gamma) \leftarrow$ StateTransfer $(c^{(0)}, c^{(s)})$
Compute sequence of rotations required for state transfer

In: $c^{(0)}, c^{(s)}$ initial and target state vectors
Out: S, γ Bang-bang control sequence

$(\theta^{(0)}, \phi^{(0)}) \leftarrow$ HyperCoord$(c^{(0)})$
$(\theta^{(s)}, \phi^{(s)}) \leftarrow$ HyperCoord$(c^{(s)})$
for $n \leftarrow N-1, \ldots, 1$
    Append S by $2n-1$, γ by $\phi_n^{(0)}$ // *Apply Phase Rotation* $U_{n+1}^Z(\phi_n^{(0)})$
for $n \leftarrow N-1, \ldots, 2$
    Append S by $2n$, γ by $-\theta_n^{(0)}$ // *Apply Population Rotation* $U_n^Y(-\theta_n^{(0)})$
Append S by 2, γ by $\theta_1^{(s)} - \theta_1^{(0)}$ // *Apply Population Rotation* $U_1^Y(\theta_1^{(s)} - \theta_1^{(0)})$
for $n \leftarrow 2, \ldots, N-1$
    Append S by $2n$, γ by $\theta_n^{(s)}$ // *Apply Population Rotation* $U_n^Y(\theta_n^{(s)})$
for $n \leftarrow 1, \ldots, N-1$
    Append S by $2n-1$, γ by $-\phi_n^{(s)}$ // *Apply Phase Rotation* $U_{n+1}^Z(-\phi_n^{(s)})$

Algorithm 2: Control Scheme to achieve state transfer $\vec{c}^{(0)} \mapsto \vec{c}^{(s)}$ in $4N-5$ steps using bang-bang control, based on hyperspherical coordinate parametrization. $\vec{S}$ and $\vec{\gamma}$ are vectors of length $4N-5$, whose elements are integer labels indicating the control Hamiltonian ($m = 1, \ldots, 2N-2$) and rotation angle γ_k, respectively.

4. Optimal piecewise-constant Control and Time-energy Performance

The bang-bang control sequence given by algorithm 2 leaves us considerable freedom of choice for the controls. Choosing large control amplitudes will result in short pulse durations, thus optimizing the transfer time t_f . However, large control amplitudes may not be feasible and have undesirable side effects in terms of transfering too much energy to the system. We can try to optimize the field amplitude by stipulating that the state transfer is to be achieved while minimizing a time-energy performance index

$$J = \int_0^{t_f} [\lambda + \sum_{m=1}^{2N-2} |u_m(t)|^2] \, dt \tag{11}$$

with the ratio factor of time and energy $\lambda > 0$. Larger values of λ indicate a stronger emphasis on time-cost, while smaller values of λ give more weight to the energy cost of the controls.

If the controls can take values $f_m(t) \in \{0, \pm L\}$ and the pulses are applied strictly sequentially then the total length t_f of the control sequence is

$$\begin{aligned} t_f &= \frac{1}{L}\left[\sum_{n=1}^{N-1} |\phi_n^{(0)}| + |\phi_n^{(s)}| + \sum_{n=2}^{N-1} (\theta_n^{(0)} + \theta_n^{(s)}) + |\theta_1^{(s)} - \theta_1^{(0)}|\right] \\ &\leq \frac{1}{L}\left[2(N-1)\pi + 2(N-2)\frac{\pi}{2} + \frac{\pi}{2}\right] = \frac{(6N-7)\pi}{2L} \end{aligned} \tag{12}$$

noting that $0 \leq \theta_n \leq \frac{\pi}{2}$ and $0 \leq |\phi_n| \leq \pi$. Noting that $a^2 + b^2 \geq 2ab$, with equality

exactly if $a = b$, we have

$$J = \sum_{k=1}^{K} (\lambda + L_k^2) t_k \leq \sum_{k=1}^{K} 2\sqrt{\lambda} L_k t_k \leq 2\sqrt{\lambda} t_f \max_k L_k \tag{13}$$

with equality if and only if $L_k = \sqrt{\lambda}$. This shows that the optimal choice of the field amplitudes is $L_k = \sqrt{\lambda}$, for which we have

$$t_f^* \leq \frac{(6N-7)\pi}{2\sqrt{\lambda}}, \quad J_* = \min J = 2\lambda t_f^* \leq \sqrt{\lambda}(6N-7)\pi \tag{14}$$

and the corresponding optimal energy cost is $E^* = J^* - \lambda t_f^* \leq \frac{1}{2}\sqrt{\lambda}(6N-7)\pi$. As expected, as λ goes to 0, t_f^* becomes infinite and E^* goes to 0, but their product remains constant

$$t_f^* \cdot E^* = \left[\sum_{n=1}^{N-1} |\phi_n^{(0)}| + |\phi_n^{(s)}| + \sum_{n=2}^{N-1} (\theta_n^{(0)} + \theta_n^{(s)}) + |\theta_1^{(s)} - \theta_1^{(0)}| \right]^2 \leq \tfrac{(6N-7)^2\pi^2}{4} \tag{15}$$

and depends only on the geometric parameters of the initial state and target states.

If first and last $N-1$ phase rotations are applied concurrently the transfer time is reduced

$$\begin{aligned} t_f' &= \frac{1}{L} \left[\max_n |\phi_n^{(0)}| + \max_n |\phi_n^{(s)}| + \sum_{n=2}^{N-1} (\theta_n^{(0)} + \theta_n^{(s)}) + |\theta_1^{(s)} - \theta_1^{(0)}| \right] \\ &\leq \frac{1}{L} \left[2\pi + 2(N-2)\frac{\pi}{2} + \frac{\pi}{2} \right] = \frac{(2N+3)\pi}{2L}. \end{aligned} \tag{16}$$

Setting $\phi_{\max}^{(0)} = \max_n |\phi_n^{(0)}|$ and $\phi_{\max}^{(s)} = \max_n |\phi_n^{(s)}|$, shows that we have $t_1 = \phi_{\max}^{(0)}/L$ and $t_K = \phi_{\max}^{(s)}/L$, and thus we must choose $L_n \geq \phi_n^{(0)}/t_1$ and $L_n = \phi_n^{(s)}/t_K$, respectively for the control amplitude of the first and last $N-1$ concurrent pulses to be able to implement all $N-1$ phase rotations concurrently in time t_1 or t_K, respectively. Furthermore the performance index changes

$$J \leq 2t_f' \sqrt{\lambda} \max_{N \leq k \leq K+1-N} L_k + \sum_{k=1}^{N-1} L_k^2 + \sum_{k=K-N+2}^{K} L_k^2, \tag{17}$$

which suggests that we can improve the performance index and reduce the energy cost by choosing the amplitudes of the first and last $N-1$ concurrent pulses to be as small as possible, i.e., $L_n = \phi_n^{(0)}/t_1$ and $L_n = \phi_n^{(s)}/t_K$, and $L_k = \sqrt{\lambda}$ for all other amplitudes.

5. Discussions and Conclusion

We have presented an explicit geometric control scheme for quantum state transfer problems based on a parametrization of the pure state vectors in terms of complex hyperspherical coordinates. Although it is not difficult to find constructive control schemes for state transfer based on Lie group decompositions, most schemes do not give explicit expressions for the rotation angles ("generalized Euler angles") in the factorization, and thus the rotation angles usually have to computed numerically. By

parametrizing the initial and the target state in terms of hyperspherical coordinates, we obtain a factorization where all generalized Euler angles are given explicitly in terms of the hyperspherical coordinates of the initial and target states, eliminating the need for numerical calculation of the generalized Euler angles, aside from computation of the hyperspherical coordinates, which is trivial in terms of computational overhead.

The factorization is applicable given controls capable of implementing phase rotations and population rotations (of either X or Y type) on a collection of two-dimensional subspaces, similar to the general requirements for constructive geometric control schemes. Compared to control schemes based on the standard factorization, the factorization based on hyperpherical coordinates has the additional advantage that all initial and final phase rotations can be combined in a single step and executed concurrently, reducing the time required to achieve the state transfer. As with all bang-bang control schemes based on Lie group decompositions, the factorization only determines the sequence in which the controls are applied and the pulse area (rotation angle) of the control pulses, leaving us with considerable freedom to choose the pulse shapes and amplitudes, which can be used to further optimize a performance index. Here we have considered optimization of the pulse amplitudes for piecewise constant controls such as to minimize a time-energy performance index that takes into account the competing goals of trying to minimize the transfer time and energy cost of the controls.

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