Role of controllability in optimizing quantum dynamics

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This paper reveals an important role that controllability plays in the complexity of optimizing quantum control dynamics. We show that the loss of controllability generally leads to multiple locally suboptimal controls when gate fidelity in a quantum control system is maximized, which does not happen if the system is controllable. Such local suboptimal controls may *attract* an optimization algorithm into a local trap when a global optimal solution is sought, even if the target gate can be perfectly realized. This conclusion results from an analysis of the critical topology of the corresponding quantum control landscape, which refers to the gate fidelity objective as a functional of the control fields. For uncontrollable systems, due to SU(2) and SU(3) dynamical symmetries, the control landscape corresponding to an implementable target gate is proven to possess multiple locally optimal critical points, and its ruggedness can be further increased if the target gate is not realizable. These results imply that the optimization of quantum dynamics can be seriously impeded when operating with local search algorithms under these conditions, and thus full controllability is demanded.

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I. INTRODUCTION

A quantum system is referred to as controllable if it can be transferred from an arbitrary state to another through engineering the dynamics. As a fundamental aspect of quantum control theory, controllability has been widely studied for various types of system including infinite-dimensional [1–3] and finite-dimensional [4–7] closed systems and Markovian open systems [8]. However, the practical necessity for controllability, which is not always available, is still unclear as it may not be required in many realistic applications. For example, the goal of realizing only a specific unitary transformation related to achieving a quantum computation algorithm, or of reaching particular excited states of a molecule, generally does not require full controllability. In most of the successfully achieved adaptive control experiments utilizing shaped laser pulses as the controls [9], there is no assessment of controllability and a simple yes-or-no controllability answer likely has little practical relevance. Hence, no apparent advantage can be seen to merely gaining additional controllability.

Here, this work is motivated by the quest to assess the practical impact of a loss of full controllability. We study this matter in the framework of the quantum control landscape [10], which was developed for understanding the complexity of optimizing quantum dynamics [9,11]. A quantum control landscape is formally defined as a target functional $J[\{\epsilon_k(\cdot)\}]$ to be maximized (minimized) over the set of implementable control fields $\{\epsilon_1(t),\ldots,\epsilon_m(t)\}$ that steer the following N-level quantum control system:

$$\frac{\partial U(t)}{\partial t}=(i\hbar)^{-1}\left\{H_0+\sum_{k=1}^{m}\epsilon_k(t)H_k\right\}U(t),U(0)=\mathbb{I},\qquad(1)$$

where $U(t)\in \mathrm{U}(N)$ is the system propagator at time t, H_0 is the internal Hamiltonian, and $\{H_1,\ldots,H_m\}$ are the control Hamiltonians.

A major goal of quantum control landscape theory is performance of a topological analysis of the critical points (i.e., the critical topology) from which insights can be gained about the complexity of optimizing quantum system dynamics. Consider the class of control landscapes in the form of $J=J(U(t_f))$, where the system propagator $U(t_f)$ at $t=t_f$ is an implicit functional of the control field through the Schrödinger equation (1). The control landscape can be displayed either on the space of the control fields (i.e., in the dynamical picture) or on the set of realizable propagators $U(t_f)$ (i.e., in the kinematic picture). The dynamical picture of control over Lie groups has been examined in other contexts [12–14], and some concepts central to the kinematic picture arose in other contexts [15,16] well before its applications to control-theoretic considerations were appreciated [10,17,18]. In prior studies [19,20], we have shown that the main topological characteristics of the critical points in the dynamical picture are preserved when mapped onto the critical points in the kinematic picture except for some singular critical points due to the singularity of the control-to-propagator mapping [20–22]. Such exceptional critical points appear to arise only under unusual conditions, and hence are expected to have little impact on the control landscape. Thus, almost all maxima, minima, and saddle points

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in the dynamical picture should correspond to the same type of critical points in the easier-to-analyze kinematic picture without distortion of the topological features.

The kinematic control landscape may be constructed from the (low-dimensional) set of realizable propagators. If the system is controllable, then the set of realizable propagators form the unitary group. This circumstance has been studied for practical optimization objectives (e.g., the state transfer probability [10], ensemble average [23], and gate fidelity [18]), which collectively show that none of these landscapes possess local suboptima that may impede the search for the ultimate global optima. This behavior provides a basis to explain the large and growing body of experimental quantum control successes, although in the laboratory many ancillary issues and constraints may be present.

Realistic quantum systems may not be always fully manipulable. A typical circumstance is when the system is under some dynamic symmetry that restricts the system's evolution, which indicates the degree of controllability of the underlying control system [6]. A classification scheme of such uncontrollable systems was proposed in [24] based on the Lie algebra g and their unitary irreducible representations (UIRs). Even if the system is not subject to a dynamic symmetry, the restrictions on available control resources (e.g., the amplitude, bandwidth, and center frequency of the applied field) can still cause a practical loss of full controllability, in which case movement over the landscape when searching for an optimal control can become limited on the otherwise trap-free landscape. Whether these uncontrollable systems still have a physically attractive landscape topology becomes practically important for assessing the complexity of the search for optimal controls, which is explored in this paper.

The loss of controllability poses restrictions on the set of reachable states, which impacts the kinematic analysis. It is generally very complex to identify the set of reachable states for control-restricted systems, while that for systems with dynamic symmetry may be simply revealed [e.g., as a Lie subgroup of $\mathrm{U}(N)$]. The landscape topology for systems with dynamic symmetry has been identified for gate fidelity under certain special symmetries [25,26], where no false traps were observed. However, as will be seen in this paper, false traps (i.e., yet appearing as real in practice) can occur in the landscape of symmetry-induced uncontrollable quantum systems. The paper will be organized as follows. Section II discusses the general conditions for the existence of critical points on such landscapes. Section III analyzes the case of the fidelity control landscape of transformations with $\mathrm{SU}(n)$ dynamic symmetry; where for $n = 2$ or 3 we derive the analytic structure for simple cases and graphically compare the landscapes for different symmetry types. Finally, conclusions are drawn in Sec. IV.

II. GENERAL CONDITIONS FOR CRITICAL POINTS ON A LANDSCAPE WITH DYNAMIC SYMMETRY

Let g be the Lie algebra spanned by $(i\hbar)^{-1}H_0,(i\hbar)^{-1}H_1,\ldots,(i\hbar)^{-1}H_m$, then the quantum propagator must evolve within the Lie group $G = \exp \mathrm{g}$ generated by g, which forms the dynamic symmetry of the system. If g forms a proper Lie subalgebra of $\mathrm{u}(N)$, the system must be uncontrollable. However, owing to the compactness of the unitary group, the set of realizable propagators can fill up the group G if the control is not limited and the evolution time is sufficiently long. Hence, in a kinematic analysis, one can suitably study the landscape of symmetry-induced uncontrollable quantum systems on the corresponding symmetry group.

The condition for $\tilde{U} \in G$ to be a landscape critical point can be derived through parametrizing its neighborhood in G as $\tilde{U}e^{A}$, where $A \in \mathrm{g}$ represents the local coordinates [27]. The variation of the landscape function with respect to A can then be written via the chain rule

$$\delta J_G = \langle \nabla J(\tilde{U}),\tilde{U}\delta A\rangle = \langle \tilde{U}^\dagger \nabla J(\tilde{U}),\delta A\rangle \equiv 0, \forall\, \delta A \in \mathrm{g}, \quad (2)$$

where $\nabla J(U)$ is the gradient function over $\mathrm{U}(N)$ and the matrix inner product $\langle X,Y\rangle = \mathrm{ReTr}(X^\dagger Y)$. Let $\mathbb{D}(\tilde{U}) = \tilde{U}^\dagger \nabla J(\tilde{U}) \in \mathrm{u}(N)$; then the condition for $\tilde{U} \in G$ to be critical is that

$$\langle \mathbb{D}(\tilde{U}),\mathrm{g}\rangle = 0, \quad (3)$$

which requires that the vector $\mathbb{D}(\tilde{U}) \in \mathrm{u}(N)$ be orthogonal to the subspace g. For example, $\mathbb{D}(U) = [U\rho U^\dagger,\theta]$ corresponds to the ensemble control landscape $J = \mathrm{Tr}(U\rho U^\dagger \theta)$ and $\mathbb{D}(U) = W^\dagger U - U^\dagger W$ corresponds to the gate fidelity control landscape $J = \mathrm{ReTr}(W^\dagger U)$. The set of critical points with G dynamic symmetry can then be expressed as

$$\mathcal{M}_G = \{U \in G : \langle \mathbb{D}(U),\mathrm{g}\rangle = 0\}.$$

The condition (3) provides a clear geometric picture for the critical points; however, it is difficult to use for directly determining the critical topology with an arbitrary dynamic symmetry, except in the extreme case that the system is controllable [i.e., $\mathrm{g} = \mathrm{u}(N)$], where the condition can be simplified to $\mathbb{D}(\tilde{U}) = 0$ on $\mathrm{U}(N)$. It is also possible, as will be shown below, to simplify the analysis by making use of the symmetric form of the landscape function, from which we can either solve for the critical topology or easily visualize it for low-dimensional symmetries.

III. QUANTUM GATE FIDELITY CONTROL LANDSCAPE WITH SU(n) DYNAMIC SYMMETRY

The quantum gate fidelity landscape is defined as

$$J(U) = N^{-1}|\mathrm{Tr}(W^\dagger U)| \quad (4)$$

where N is the dimension of the system and $W \in \mathrm{U}(N)$ is the target unitary transformation. This function is similar to but distinct from the one studied in [18]. We use the present one to avoid the influence of the trivial global phase. One can prove that, although more complicated, the landscape for J in Eq. (4) is still trap-free for controllable systems [28]. If the target transformation W is realizable, i.e., $W \in G$, then we can use the transformation $\tilde{U} = W^\dagger U$ to change the landscape function into a canonical form $J_G(\tilde{U}) = N^{-1}|\mathrm{Tr}(\tilde{U})|$.

From group representation theory, a dynamic symmetry group $G \subset \mathrm{U}(N)$ can be taken as an N-dimensional unitary representation of the abstract Lie group G, which thereby can be decomposed into smaller unitary irreducible representations, i.e., one can always find a constant unitary similarity transformation in G that turns each $U \in G$ into a block diagonal form:

$$U = \begin{pmatrix} U^{(1)} & & \\ & \ddots & \\ & & U^{(r)} \end{pmatrix},$$

where $U^{(j)} \in \mathrm{U}(N_j), N_1 + \cdots + N_r = N$, and each sub-block $U^{(j)}$ cannot be decomposed into smaller ones. For the gate fidelity control landscape, the landscape function with G carrying a reducible representation can be written as the sum of the landscape function values evaluated on its irreducible components. Hence, it is convenient to start with the case that G is a unitary irreducible representation of some abstract Lie group in $\mathrm{U}(N)$.

Here we consider the class of $\mathrm{SU}(n)$ dynamic symmetry (i.e., the group of $n \times n$ unit trace unitary matrices). For example, the SU(2) dynamic symmetry may arise when the free and control Hamiltonians of spin-j particles (or a rigid rotor whose angular momentum is j^2) in a magnetic field are linear combinations of the spin operators J_x, J_y, and J_z that possess an ($N = 2j + 1$)-dimensional UIR (denoted by D_j). Similarly, two noninteracting spin particles with spin j_1 and spin j_2 in a magnetic field (e.g., two electrons in a multielectron molecular system) possess a tensor product of SU(2) UIRs $D = D_{j_1} \otimes D_{j_2}$, which can be decomposed into the direct sum of smaller UIRs of SU(2).

Suppose that G carries an N-dimensional UIR of $\mathrm{SU}(n)$; then there must be a homeomorphic mapping $\mathcal{R}$ that transforms any unitary matrix $U \in G \subset \mathrm{U}(N)$ to an $n \times n$ unitary matrix $U' \in \mathrm{SU}(n)$ such that $U = \mathcal{R}(U')$. Let the complex numbers $\epsilon_1, \ldots, \epsilon_n$ be the eigenvalues of U' corresponding to U, which satisfy $|\epsilon_1| = \cdots = |\epsilon_n| = 1 = \epsilon_1 \cdots \epsilon_n$; then according to the well-known Weyl formula [29], the UIRs of $\mathrm{SU}(n)$ are labeled by a group of integers $r_1 > \cdots > r_{n-1}$ [29], and the trace of U can be expressed as the following character function:

$$\begin{aligned}\mathrm{Tr}(U) &= \chi_{r_1,\ldots,r_{n-1}}(\epsilon_1, \ldots, \epsilon_n) \\ &= |\epsilon^{r_1}, \ldots, \epsilon^{r_{n-1}}, 1| / |\epsilon^{n-1}, \ldots, \epsilon, 1|, \end{aligned} \quad (5)$$

where

$$|\epsilon^{r_1}, \ldots, \epsilon^{r_{n-1}}, 1| = \det \begin{pmatrix} \epsilon_1^{r_1} & \cdots & \epsilon_1^{r_{n-1}} & 1 \\ \epsilon_2^{r_1} & \cdots & \epsilon_2^{r_{n-1}} & 1 \\ \vdots & \ddots & \vdots & 1 \\ \epsilon_n^{r_1} & \cdots & \epsilon_n^{r_{n-1}} & 1 \end{pmatrix}.$$

This formula shows that the original landscape function on an $(N^2 - 1)$-dimensional group manifold G can be reduced to a function of $n - 1$ independent variables $(\epsilon_1, \ldots, \epsilon_{n-1})$ on the $(n - 1)$-tori T^{n-1}; thereby all $U \in G$ corresponding to a critical point $(\epsilon_1, \ldots, \epsilon_{n-1}) \in T^{n-1}$ form a subset of the critical submanifold with the same J value.

As a direct application of the above formula, the case of SU(2) can be computed. Suppose that G carries a UIR D_j of SU(2); then the landscape function is

$$J_{D_j}(\epsilon_1, \epsilon_2) = (2j + 1)^{-1} \frac{\epsilon_1^{2j+1} - \epsilon_2^{2j+1}}{\epsilon_1 - \epsilon_2} \quad (6)$$

according to (5). Let $\epsilon_1 = e^{i\beta}$ and $\epsilon_2 = e^{-i\beta}$, where $\beta \in [0, 2\pi)$; then (6) can be reduced to a single variable function

$$J_{D_j}(\beta) = \left| \frac{\sin[(2j + 1)\beta]}{(2j + 1)\sin\beta} \right|, \quad (7)$$

whose critical points $\beta_1, \beta_2, \ldots$ characterize the critical topology.

In addition to SU(2), the SU(3) case is relatively simple, but a universal solution is still not available for the critical topology of all its UIRs. However, as the corresponding character formula involves only two independent variables, it is possible to solve for the critical topology of low-dimensional UIRs, and, numerically, it is easy to visualize the landscape in a three-dimensional (3D) image for any individual UIR (labeled by two integers $r_1 > r_2$). The dimension of the (r_1, r_2) UIR is given by $N_{r_1, r_2} = \frac{r_1 r_2 (r_1 - r_2)}{2}$. In the following, we will use SU(2) and SU(3) examples to study the impact of the symmetry group and the UIR dimensionality and the influence of realizability of the target gate upon the landscape topology. The case $\mathrm{SU}(n)$ for $n > 3$ will not be discussed in this paper.

A. The dimensionality of UIR

Consider the SU(2) case with W being realizable. Figure 1 shows two examples with $j = 3$ and $7/2$ for $\beta \in [0, \frac{\pi}{2}]$ (the remaining part $\beta \in [\frac{\pi}{2}, 2\pi]$ is repeating and thus omitted) according to the formula (7), respectively corresponding to dimensions $N = 7$ and 8. Both landscapes possess four local maxima, and their local minima are all of value zero. No saddle points are found. There are three traps on the landscape, and the results obtained from the two examples can be generalized as follows:

Theorem 1. Denote $\lfloor j \rfloor$ as the largest integer that is no greater than j. The control landscape J_{D_j} has $\lfloor j \rfloor$ local suboptima.

The systems that carry higher-dimensional UIRs (i.e., with a larger j in D_j) are less controllable because the number of degrees of freedom is always 3 [versus the total number $(2j + 1)^2$ in $\mathrm{U}(2j + 1)$]. Thus, we can see from the theorem that the search for an optimal control is more likely to be

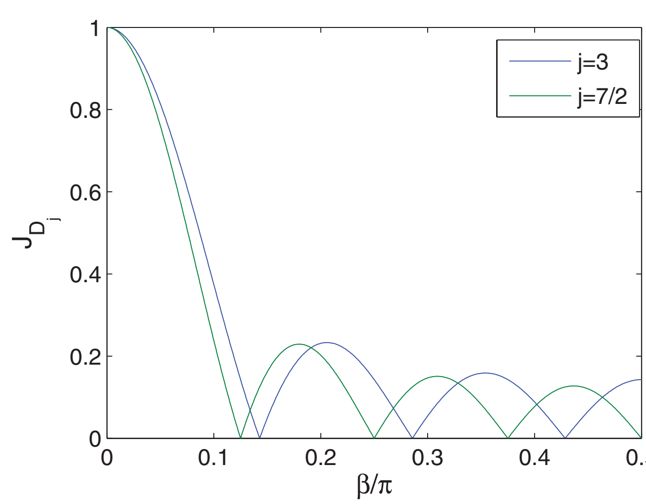

FIG. 1. (Color online) The character functions for D_3 and $D_{7/2}$ UIRs.

trapped on such landscapes because there tends to be a larger number of traps. Moreover, the convergence region of the global optimum $U = \mathbb{I}$ can be identified as $\beta \in [0, \frac{\pi}{2j+1}]$ according to (7), which also shrinks when j increases, leaving the system more likely to be trapped by some of the $\lfloor j \rfloor - 1$ local suboptima outside the region. Therefore, the loss of controllability leads to an increase of the ruggedness of the landscape.

B. The realizability of the target transformation

Consider again the dynamic symmetry SU(2). If the target gate is not realizable, i.e., $W \notin G$, then the dynamic symmetry group G is not invariant under the transformation $\tilde{U} = W^\dagger U$, and hence the approach used above for realizable W is no longer applicable. In this case, the landscape function cannot be reduced to having a single characterizing parameter, and we have to analyze it on the original three-dimensional group manifold. Here we adopt the well-known Euler decomposition

$$U(\psi_1,\theta,\psi_2) = e^{\psi_1 L_z} e^{\theta L_x} e^{\psi_2 L_z},$$

which parametrizes the landscape function by (θ,ψ_1,ψ_2). To facilitate visualization of the results, we consider the special case that the target gate W commutes with L_z, i.e., $[W,L_z] = 0$, for which the landscape function reduces to the following two-variable form:

$$\begin{aligned} J(U) &= N^{-1}|\mathrm{Tr}\{W^\dagger e^{\psi_1 L_z} e^{\theta L_x} e^{\psi_2 L_z}\}| \\ &= N^{-1}|\mathrm{Tr}\{W^\dagger e^{(\psi_1+\psi_2) L_z} e^{\theta L_x}\}| \triangleq J(\theta,\phi), \end{aligned}$$

where $\phi = \psi_1 + \psi_2$. For example, suppose that L_z is diagonal under some chosen UIR basis; then the landscape function can be reduced to a two-variable function if the target gate is a diagonal N-dimensional unitary matrix, whose diagonal elements affect the landscape topology. For such a class of unrealizable target gates, one can easily depict the two-dimensional landscape topology as exemplified in Fig. 2. Compared to the case of a realizable W, the landscape height (i.e., the maximal fidelity) decreases to $J_{\max} = 0.8$ due to the inability of perfectly realizing the gate W. In addition, the landscape with realizable W possesses three critical submanifolds (owing to the intrinsic dependence upon a single variable), while the landscape with an unreachable W is much more rugged, implying that having an unattainable target state not only degrades the maximal achievable fidelity but also increases the complexity of the landscape topology. Consequently, local search algorithms (e.g., gradient-based methods) on such a control landscape likely will be less effective.

C. Comparison between different dynamic symmetry groups

To compare the influence of different dynamic symmetry groups, we choose the (5,2) and (6,1) UIRs of SU(3) and the UIR D_7 of SU(2), whose dimensions are all 15 (i.e., corresponding to different dynamic symmetries in the same physical system). We directly show the 3D landscape profiles in Fig. 3. The landscape topology is less rugged for the SU(3) case, as all critical points are isolated. Moreover, the region of attraction for the global maximum is rather large, while that of the SU(2) symmetry is small, making its peak very sharp. This shows from another perspective that the enhanced controllability (corresponding to a larger dynamic symmetry group) helps to improve the search efficiency for global optimal controls by smoothing the landscape topology. It is also interesting that the landscapes of different UIRs of the SU(3) symmetry group can be distinct [i.e., the UIR (5,2) landscape is less rugged] even when their dimensions are identical.

IV. DISCUSSION

The present study on the landscape of uncontrollable systems with SU(2) and SU(3) dynamic symmetries shows that controllability plays an important role in facilitating the search for optimal controls that maximize unitary gate fidelity, *whether or not the desired target is attainable*. The loss of controllability can lead to false traps over the corresponding restricted kinematic control landscape on the dynamic

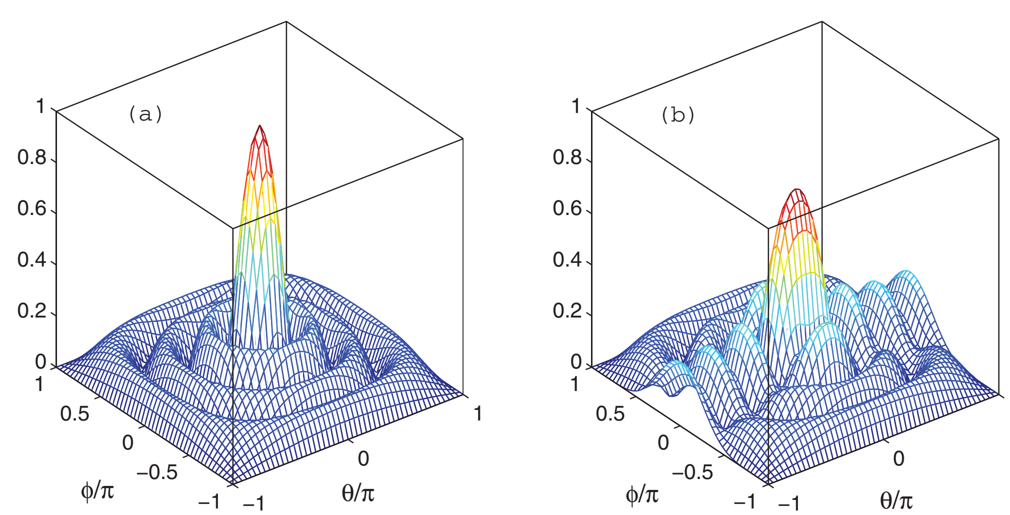

FIG. 2. (Color online) Two-dimensional illustration of the landscape topology of $J(U) = N^{-1}|\mathrm{Tr}(W^\dagger U)|$ with (a) $W = \mathbb{I}_8 \in \mathrm{SU}(2)$; (b) $W = \mathrm{diag}\{-1,1,\ldots,1\} \notin \mathrm{SU}(2)$.

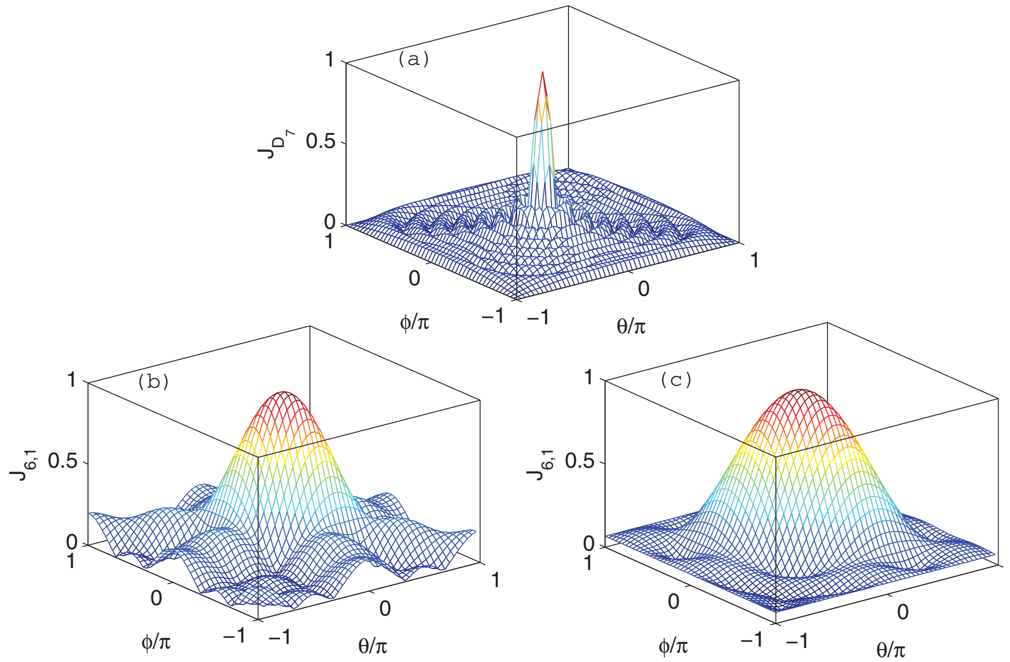

FIG. 3. (Color online) The gate fidelity landscape topology for 15-dimensional systems under SU(2) and SU(3) dynamic symmetries: (a) the landscape with SU(2) symmetry with UIR D_7; (b) the landscape with SU(3) symmetry with UIR labeled by (6,1); (c) the landscape with SU(3) symmetry with UIR labeled by (5,2). Their landscape ruggedness is in decreasing order.

symmetry group, which is distinct from the trap-free landscape of controllable systems. The landscape ruggedness generally increases when controllability is weakened, i.e., either with a smaller dynamic symmetry group or an unattainable target unitary transformation, making the search for global optimal controls much more difficult.

The details of the landscape topology depend on the particular structure of the dynamic symmetry group and the unitary representation it carries (see [24] for a classification of such systems). Uncontrollable systems with dynamic symmetry generally possess rugged control landscapes, but this may not always be the case. For example, the gate fidelity landscape with W realizable and the following reachable sets in U(N) were found (or can be easily proved) to be devoid of local suboptima:

(1) Symmetry matrices in U(N) [26].

(2) Self-dual matrices in U(N) [26].

(3) Symplectic matrices (symplectic group) [25].

(4) Real orthogonal matrices (orthogonal group) in U(N).

The landscape structure for the observable control problem [18] also becomes rugged when the system is under dynamic symmetry. The corresponding critical topology structure is dependent on the spectra of the system density matrix and the observable, and will be more complicated than in the case of a unitary fidelity landscape. This important problem will be explored in future studies.

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