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Landscape of unitary transformations in controlled quantum dynamics

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We consider the control problem of generating unitary transformations, which is especially relevant to current research in quantum information processing and computing, in contrast to the usual state-to-state or the more general observable expectation value control problems. A previous analysis of optimal control landscapes for unitary transformations from a kinematic perspective in the finite-dimensional unitary matrices is extended to a dynamical one in the infinite-dimensional function space of the time-dependent external field. The underlying dynamical landscape is defined as the Frobenius square norm of the difference between the control unitary matrix and the target matrix. A nonsingular adaptation matrix is introduced to provide additional freedom for exploring and manipulating key features, specifically the slope and curvature, of the control landscapes. The dynamical analysis reveals many essential geometric features of optimal control landscapes for unitary transformations, including bounds on the local landscape slope and curvature. Close examination of the curvatures at the critical points shows that the unitary transformation control landscapes are free of local traps and proper choices of the adaptation matrix may facilitate the search for optimal control fields producing desired unitary transformations, in particular, in the neighborhood of the global extrema.

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I. INTRODUCTION

A potential application of quantum optimal control theory (OCT) [1–5] is to create specific unitary transformations [6] for realization of quantum information processing [7–30]. The efficiency and stability of generating unitary transformations rests on the topology and local structures of the underlying control landscape. This paper explores various aspects of a family of landscapes specified as a square norm of the difference between the controlled unitary transformation and the target one. Given an $N\times N$ target unitary transformation $\mathcal{W}$, any *kinematic* landscape [26,31]—which is defined as a smooth function on the unitary group $U(N)$ (the group of $N\times N$ unitary matrices, each composed of N^2 independent real variables)—with a global extremum at $\mathcal{W}$ can be considered a candidate landscape for generating $\mathcal{W}$. These candidate landscapes can vary widely in their detailed features. For example, some may have local extrama away from $\mathcal{W}$, others may not. In this paper, we examine a class of candidate landscapes for this problem (defined by a class of norms, parametrized by an arbitrary nonsingular "adaptation matrix" A), showing that they exhibit a wide range of geometrical features and critical topologies and that none of them contain any local extrema (i.e., traps).

The landscape properties of importance include the local magnitude of the slope and curvature, the existence and distribution of critical points where the slopes are zero, and the rank and signature of the curvature [Hessian, see Eq. (25)] at these critical points, especially at the global extrema (maximum and minimum). Significant insights have been gleaned in landscape studies of controlled population transfer [31–34], the control of general observables (Hermitian operators) in the context of the density matrix formulation [35–37], and the control of open quantum systems in the Kraus operator formulation [38]. A detailed *kinematic* study on one particular control landscape for generating quantum unitary transformations for N-level quantum systems has been performed [26,31], revealing the landscape topological features, including a lack of any local traps, which is of special relevance to the practical construction of unitary transformations. This paper extends the kinematic treatment, based on the unitary group, to a *dynamical* analysis, based on the control field $E(t)$, which brings in the time-dependent Schrödinger equation governing the quantum system evolution [39]. Here, the dynamical landscape is specifically defined as a *functional* of the control field $E(t)$ that belongs to the infinite-dimensional function space L_2 of square-integrable functions [40] in the time domain $0\leqslant t\leqslant T$. Whereas the kinematic landscape does not depend on how the quantum system evolves over the course of time (i.e., it is independent of the composition of the field-free Hamiltonian and the couplings between the quantum system and the time-dependent control fields), the dynamical landscape is directly related to how a specific quantum system evolves in the presence of an arbitrary time-dependent external field $E(t)$. Any constraint imposed on the control fields, for example the bandwidth, intensity, fluence, and pulse shape, will in general make the control landscape analysis difficult and the subject

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is beyond the scope of this paper. By imposing no constraint on the temporal behavior of the control field, many important generic features of the unitary transformation landscape, including no local traps, can be obtained analytically. To this end, fully controllable N-level quantum systems [41–48] are considered within the framework of the control field coupling into the Hamiltonian through the electric dipole interaction. Specifically, a quantum system is fully controllable at time $t=T>0$ if every unitary transformation $\mathcal{W}$ is dynamically accessible from the identity $\mathbf{I}$ in the group $U(N)$ via an evolution propagator $U(T,0)$ that satisfies the underlying time-dependent Schrödinger equation [46],

$$\imath\hbar\frac{\partial U(t,0)}{\partial t} = \{H_0 - \mu E(t)\}U(t,0), \quad U(0,0) = \mathbf{I}, \tag{1}$$

over the duration $[0,T]$, where H_0 is the field-free Hamiltonian, μ is the dipole moment operator, and $\mathbf{I}$ is the $N\times N$ identity matrix.

The paper is organized as follows. In Sec. II a generalized unitary transformation landscape for an N-level quantum system is defined in terms of the Frobenius square norm $\|(\mathcal{W}-\mathcal{U})A\|_F^2$ of the difference between the controlled unitary transformation $\mathcal{U}=U(T,0)$ and the target one $\mathcal{W}$, in conjunction with a nonsingular adaptation matrix A. Qualitative features, including bounds on the slope and curvature and the robustness of the control landscape, are analyzed in Sec. III. The landscape critical points, including the conditions for their existence and their multiplicity, are examined in Sec. IV. A qualitative description of the Hessian at the critical points is presented in Sec. V. A procedure based on quadratic forms is presented in Sec. VI for facilitating the analysis of the rank and signature of the Hessian matrices at the critical points. Finally, Sec. VII summarizes the findings. Appendix A describes a phase-independent unitary transformation landscape using a distance norm (to measure the fidelity between the controlled and target unitary matrices) defined up to an arbitrary global phase [16,17] (i.e., in contrast to the Frobenius norm that specifies the phase), and Appendix B addresses the optimal control robustness to control field noise for generic p-qubit quantum systems, drawing on the results from Appendix A.

II. DYNAMICAL LANDSCAPE OF UNITARY TRANSFORMATIONS

Consider a fully controllable N-level quantum system [41–48] and a preselected target unitary transformation $\mathcal{W}$. The underlying optimal control problem can be formally expressed as

$$\min_{E(t)} \mathcal{J}_F[E], \tag{2}$$

where the cost $\mathcal{J}_F[E]$, as a functional of the control field $E(t)$, may be specified as [22,26]

$$\mathcal{J}_F[E] = \|\mathcal{W}-\mathcal{U}\|_F^2, \tag{3}$$

which measures the magnitude and phase-specific difference of the target unitary transformation $\mathcal{W}$ and the system propagator

$$\mathcal{U} \equiv U(T,0), \tag{4}$$

at the end time T of the control pulse $E(t)$, $t\in[0,T]$. Here the notation

$$\|B\|_F^2 \equiv \sum_{i=1}^{N}\sum_{j=1}^{N}|b_{ij}|^2 = \mathrm{tr}(B^\dagger B) \tag{5}$$

denotes the Frobenius square norm of an arbitrary $N\times N$ square matrix B composed of the matrix elements b_{ij}, $1\leqslant i, j\leqslant N$. The optimal control field $E(t)$ belongs to the infinite-dimensional function space L_2 of square-integrable functions on the interval $[0,T]$, where T is a final time consistent with the dynamical capabilities of the physical system. In practice, the control fields $E(t)$ may be composed of a finite number of field components of different frequencies, amplitudes, and phases, thus spanning a finite-dimensional control field space. However, the control landscape is most revealing and the easiest to understand in the context of a single unconstrained time-dependent function $E(t)$. Moreover, the unitary matrix $\mathcal{W}$ may be block diagonal

$$\mathcal{W} = \mathcal{W}_n \oplus \emptyset_{N-n} + \emptyset_n \oplus \mathcal{Q}_{N-n} = \mathcal{W}_n \oplus \mathcal{Q}_{N-n}, \tag{6}$$

where the $n\times n$ matrix $\mathcal{W}_n$ is the relevant target unitary transformation operating on a subset of n chosen levels $(n\leqslant N)$, $\oplus$ denotes the direct sum (of lower dimensional matrices), $\emptyset_m$ $(m=N-n$ or $n)$ is a zero matrix of dimension m, and $\mathcal{Q}_{N-n}$ is an arbitrary $(N-n)\times(N-n)$ unitary matrix.

The condition defining the critical points of the control landscape $\mathcal{J}_F[E]$ is specified by the zero gradient [the first-order functional derivative with respect to the control field $E(t)$] [49]

$$\frac{\delta\mathcal{J}_F[E]}{\delta E(t)} = 0 \tag{7}$$

for all $t\in[0,T]$. The Hessian (the second-order functional derivatives) $\delta^2\mathcal{J}_F[E]/\delta E(t')\delta E(t)$, $t\geqslant t'$, at the critical points determines whether or not the control landscape $\mathcal{J}_F[E]$ possesses local traps. The expressions and bounds of the gradient and Hessian are given in Sec. III. The cost functional $\mathcal{J}_F[E]$ may be thought of as a composition of two maps. The first, denoted $V_T[E]$, takes in a control field $E(t)$ and produces the corresponding unitary propagator $\mathcal{U}=U(T,0)$. The second, $\hat{\mathcal{J}}_F(\mathcal{U})$, takes in a unitary propagator $\mathcal{U}$ and produces the real number $\hat{\mathcal{J}}_F(\mathcal{U})=\|(\mathcal{W}-\mathcal{U})\|_F^2$. Then $\mathcal{J}_F[E] = \hat{\mathcal{J}}_F(V_T[E])$ and

$$\frac{\delta\mathcal{J}_F}{\delta E(t)} = \left\langle \nabla\hat{\mathcal{J}}_F(\mathcal{U}), \frac{\delta V_T}{\delta E(t)}\right\rangle = \mathrm{Re}\left(\frac{\imath}{\hbar}\mathrm{tr}\{[\nabla\hat{\mathcal{J}}_F(\mathcal{U})]^\dagger\mathcal{U}\mu(t)\}\right), \tag{8}$$

where the notation $\langle\cdot,\cdot\rangle$ stands for the scalar product. A *regular* critical point of $\mathcal{J}_F[E]$ is one where the operator $\langle\cdot,\delta V_T/\delta E(t)\rangle$ is full rank and the gradient $\nabla\hat{\mathcal{J}}_F(\mathcal{U})=0$. A critical point of $\mathcal{J}_F[E]$ where $\delta V_T/\delta E(t)$ is rank deficient is called a *singular* point. Because V_T is a highly nonlinear map from an infinite-dimensional space to a finite-dimensional one, such singular points are expected to be rare and will not be considered here. It may be observed that the full rank condition on

$$\frac{\delta V_T}{\delta E(t)} = \frac{\imath}{\hbar}\mathcal{U}\mu(t), \tag{9}$$

where

$$\mu(t) = U^\dagger(t,0)\mu U(t,0), \tag{10}$$

is identical to the condition that

$$\{\mathrm{Re}[\langle i|\mu(t)|j\rangle], \quad \mathrm{Im}[\langle i|\mu(t)|j\rangle]: j \geqslant i = 1, \ldots, N\} \tag{11}$$

is a collection of N^2 linearly independent functions [50]. Consequently, it will always be assumed in this paper that these dipole functions are linearly independent at the critical points. Future work will seek to characterize the set of singular points and their role in quantum control.

To facilitate a full exploration of the optimal control landscape of unitary transformations, throughout the remaining derivations and discussions, we will consider the following generalized (A-adapted) cost functional

$$\begin{aligned}\mathcal{J}_F[E] &= \|(\mathcal{W}-\mathcal{U})A\|_F^2 = \mathrm{tr}\{[(\mathcal{W}-\mathcal{U})A]^\dagger(\mathcal{W}-\mathcal{U})A\}\\ &= 2\|A\|_F^2 - \mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\} - \mathrm{tr}\{\mathcal{U}^\dagger\mathcal{W}AA^\dagger\},\end{aligned} \tag{12}$$

where and henceforth, as in Eq. (3), the same notation $\mathcal{J}_F[E]$ for the A-adapted cost functional has been used for simplicity. The $N\times N$ landscape adaptation matrix A is an arbitrary nonsingular matrix that may be freely chosen for additional exploration of the control landscape properties. In general, each nonsingular adaptation matrix A (within a matrix similarity transformation) corresponds to a distinct control landscape, which can be characterized by the landscape gradient and Hessian, especially at the critical points. Specifically, we emphasize that the matrix A is mainly a mathematical device that can be arbitrarily chosen to manipulate unitary transformation control landscapes. The introduction of A allows us to simultaneously analyze an entire family of unitary transformation control landscapes (parametrized by A). We point out that the quantity $\|(\mathcal{W}-\mathcal{U})A\|_F^2$ is a measure of the fidelity of $\mathcal{U}$ where we are free to choose A. The situation in the laboratory calls for coming up with a means to determine $\mathcal{U}\equiv U(T,0)$ for offline use in the measure, which is a subject beyond the scope of this work.

For any nonsingular square matrix A, the product $AA^\dagger$ is Hermitian and positive definite (i.e., all its eigenvalues are real and positive) which aids in performing the landscape analysis. The matrix $AA^\dagger$ can be diagonalized via a unitary matrix D, $D^\dagger D = DD^\dagger = \mathbf{I}$,

$$D^\dagger(AA^\dagger)D = \Omega^2, \tag{13}$$

or equivalently [51],

$$AA^\dagger = D\Omega^2 D^\dagger, \tag{14}$$

where Ω^2 is a diagonal matrix

$$\Omega^2 = \mathrm{diag}\{\omega_1^2, \omega_2^2, \ldots, \omega_N^2\}, \tag{15}$$

consisting of real positive eigenvalues (singular values) $\omega_1^2 \geqslant \omega_2^2 \geqslant \ldots \omega_N^2 > 0$ of the matrix $AA^\dagger$ and the columns of D are the eigenvectors of $AA^\dagger$, i.e., $AA^\dagger D = D\Omega^2$.

By invoking Eq. (14), Eq. (12) can be rewritten as

$$\begin{aligned}\mathcal{J}_F[E] &= \|D^\dagger(\mathcal{W}-\mathcal{U})D\Omega\|_F^2 = \|(\bar{\mathcal{W}}-\bar{\mathcal{U}})\Omega\|_F^2\\ &= 2\|\Omega\|_F^2 - \mathrm{tr}\{\Omega^2\bar{\mathcal{W}}^\dagger\bar{\mathcal{U}}\} - \mathrm{tr}\{\bar{\mathcal{U}}^\dagger\bar{\mathcal{W}}\Omega^2\}\\ &= 2\sum_{i=1}^N \omega_i^2 - \mathrm{tr}\{\Omega^2\bar{\mathcal{W}}^\dagger\bar{\mathcal{U}}\} - \mathrm{tr}\{\bar{\mathcal{U}}^\dagger\bar{\mathcal{W}}\Omega^2\},\end{aligned} \tag{16}$$

where $\bar{\mathcal{W}} = D^\dagger\mathcal{W}D$ and $\bar{\mathcal{U}} = D^\dagger\mathcal{U}D$. Here we have used the relation

$$\|A\|_F^2 = \|D\Omega D^\dagger\|_F^2 = \|\Omega\|_F^2 = \sum_{i=1}^N \omega_i^2. \tag{17}$$

Moreover, $\bar{\mathcal{U}} \equiv \bar{U}(T,0)$ where the rotated propagator $\bar{U}(t,0) \equiv D^\dagger U(t,0)D$ is governed by the equation

$$\imath\hbar\frac{\partial\bar{U}(t,0)}{\partial t} = \{D^\dagger H_0 D - D^\dagger\mu D E(t)\}\bar{U}(t,0), \qquad \bar{U}(0,0) = \mathbf{I}. \tag{18}$$

As a result, the control landscape $\mathcal{J}_F[E]$ depends on the unitary matrix D and the diagonal matrix Ω; both are arbitrary and, thus, at our disposal in the landscape analysis.

From Eq. (12), or equivalently Eq. (16), it is evident that the control landscape $\mathcal{J}_F[E]$ possesses one global minimum value and one global maximum value corresponding to the cases of $\mathcal{U}=\mathcal{W}$ and $\mathcal{U}=-\mathcal{W}$, respectively, independent of the specific choices of D and Ω (or equivalently that of A). However, the landscape details, including its local slopes and curvatures, and the number as well as the properties of the critical points depends on the choices of D and Ω. These various landscape features can significantly affect the process of identifying optimally shaped control fields. Although the limiting case of $AA^\dagger = \mathbf{I}$ (i.e., when A is unitary, including the identity matrix $\mathbf{I}$) is of special interest and has been studied extensively [21,22,25,26], other possibilities for A may also be exploited for altering the search for optimal control fields that generate the desired unitary transformation $\mathcal{W}$. For example, all singular values in the diagonal matrix Ω^2 may be distinct, i.e., $\omega_1^2 > \omega_2^2 > \ldots > \omega_N^2 > 0$, or they may be weighted in favor of the n eigenstates associated with $\mathcal{W}_n$ in Eq. (6), i.e., $\omega_1^2 \geqslant \omega_2^2 \geqslant \ldots \geqslant \omega_n^2 \geqslant \omega_{n+1}^2 \geqslant \ldots \geqslant \omega_N^2 > 0$.

In addition, the unitary matrix D may be determined such that the rotated unitary matrix $\bar{\mathcal{W}} = D^\dagger\mathcal{W}D$ is diagonal, or particularly in Eq. (6), D may be chosen as

$$D = D_n \oplus \varnothing_n + \varnothing_{N-n} \oplus \mathbf{I}_{N-n} = D_n \oplus \mathbf{I}_{N-n} \tag{19}$$

such that

$$\bar{\mathcal{W}}_n = D_n^\dagger \mathcal{W}_n D_n \tag{20}$$

is diagonal, where $\mathbf{I}_k$ $(k=n, N-n)$ is a $k\times k$ identity matrix and D_n is an $n\times n$ unitary matrix. In general, Ω^2 and D may be tailored to a specific quantum system of interest. Without specifically choosing A (or equivalently D and Ω), the focus of this paper will be on a detailed analysis of the generic properties of the control landscape $\mathcal{J}_F[E]$ in Eq. (12), based on Eq. (1) governing the propagator $U(t,0)$ of a controllable

N-level quantum system with the Hamiltonian $H(t)=H_0-\mu E(t)$.

Finally, in quantum information processing, the desired unitary transformation is a designated quantum logic gate $\mathcal{W}$, which is generally only defined within a global phase [16,17], i.e., $\mathcal{W}\leftarrow\mathcal{W}\exp(\imath\theta)$ where $0\leqslant\theta\leqslant 2\pi$. As a result, dependence on the global phase θ may be eliminated through a *phase-independent* control landscape [17,21]

$$\mathcal{J}_P[E]=|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\}|, \tag{21}$$

which is compared with the control landscape $\mathcal{J}_F[E]$ in Appendix A.

III. QUALITATIVE FEATURES OF THE A-ADAPTED $\mathcal{J}_F[E]$ LANDSCAPE

The topology of $\mathcal{J}_F[E]$ as a functional of the control field $E(t)$ will be described below in terms of the gradient $\delta\mathcal{J}_F[E]/\delta E(t)$ and Hessian $\delta^2\mathcal{J}_F[E]/\delta E(t')\delta E(t)$ [49].

A. Gradient and Hessian on the landscape

Within the electric dipole formulation of the Hamiltonian in Eq. (1), it can be shown that [35]

$$\frac{\delta U(t,0)}{\delta E(t')}=\frac{\imath}{\hbar}U(t,0)\mu(t'),\quad t\geqslant t', \tag{22}$$

and

$$\frac{\delta\mu(t)}{\delta E(t')}=\frac{\imath}{\hbar}[\mu(t),\mu(t')],\quad t\geqslant t'. \tag{23}$$

As a result, the gradient of $\mathcal{J}_F[E]$ can be expressed as

$$\begin{aligned}\frac{\delta\mathcal{J}_F[E]}{\delta E(t)}&=-\mathrm{tr}\left\{AA^\dagger\left[\mathcal{W}^\dagger\frac{\delta U(T,0)}{\delta E(t)}+\frac{\delta U^\dagger(T,0)}{\delta E(t)}\mathcal{W}\right]\right\}\\&=-\left(\frac{\imath}{\hbar}\right)\mathrm{tr}\{(AA^\dagger\mathcal{W}^\dagger\mathcal{U}-\mathcal{U}^\dagger\mathcal{W}AA^\dagger)\mu(t)\},\quad t\leqslant T,\end{aligned} \tag{24}$$

and the corresponding Hessian can be expressed as

$$\begin{aligned}\frac{\delta^2\mathcal{J}_F[E]}{\delta E(t')E(t)}&=-\frac{\imath}{\hbar}\mathrm{tr}\left[\left(AA^\dagger\mathcal{W}^\dagger\frac{\delta U(T,0)}{\delta E(t')}-\frac{\delta U^\dagger(T,0)}{\delta E(t')}\mathcal{W}AA^\dagger\right)\mu(t)\right.\\&\quad\left.+[AA^\dagger\mathcal{W}^\dagger U(T,0)-U^\dagger(T,0)\mathcal{W}AA^\dagger]\frac{\delta\mu(t)}{\delta E(t')}\right]\\&=\frac{1}{\hbar^2}\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\mu(t)\mu(t')+\mathcal{U}^\dagger\mathcal{W}AA^\dagger\mu(t')\mu(t)\},\\&\quad t\geqslant t'.\end{aligned} \tag{25}$$

For a fully controllable N-level quantum system, the gradient in Eq. (24) is essential for deriving the necessary and sufficient conditions for the existence of $\mathcal{J}_F[E]$ critical points, while the *rank* and *signature* (i.e., respectively, the sum and difference of the numbers of positive and negative eigenvalues) of the Hessian are needed to characterize each critical point [52]. Moreover, Eqs. (24) and (25) can be used to establish upper bounds on the gradient and Hessian, respectively. The magnitudes of these bounds are important for the efficiency and stability of control field searches to find effective unitary transformations. In particular, the Hessian properties at the global maximum determines the robustness of an optimal control field $E(t)$ subject to some small perturbation $\delta E(t)$ due to noise [53].

B. Bounds on the gradient and Hessian

The absolute magnitude of the gradient $\delta\mathcal{J}_F[E]/\delta E(t)$ can be expressed as

$$\left|\frac{\delta\mathcal{J}_F[E]}{\delta E(t)}\right|=\frac{1}{\hbar}|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\mu(t)\}-\mathrm{tr}\{\mathcal{U}^\dagger\mathcal{W}AA^\dagger\mu(t)\}|, \tag{26}$$

and by invoking the triangle inequality and the Cauchy-Schwarz inequality, we have

$$\begin{aligned}\left|\frac{\delta\mathcal{J}_F[E]}{\delta E(t)}\right|&\leqslant\frac{1}{\hbar}(|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\mu(t)\}|+|\mathrm{tr}\{\mathcal{U}^\dagger\mathcal{W}AA^\dagger\mu(t)\}|)\\&\leqslant\frac{2}{\hbar}\|AA^\dagger\|_F\|\mu\|_F.\end{aligned} \tag{27}$$

The bound of the gradient of $\mathcal{J}_F[E]$ is proportional to the product of the norm $\|\mu\|_F$ of the dipole moment operator μ and the norm

$$\|AA^\dagger\|_F=\sqrt{\sum_{i=1}^N\omega_i^4} \tag{28}$$

of the landscape adaptation matrix A. $\|AA^\dagger\|_F=\sqrt{N}$ when $AA^\dagger=\mathbf{I}$. Likewise, the bound of the Hessian $\delta^2\mathcal{J}_F[E]/\delta E(t')\delta E(t)$ becomes

$$\begin{aligned}\left|\frac{\delta^2\mathcal{J}_F[E]}{\delta E(t')\delta E(t)}\right|&=\frac{1}{\hbar^2}|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\mu(t)\mu(t')\\&\quad+\mathcal{U}^\dagger\mathcal{W}AA^\dagger\mu(t')\mu(t)\}|\\&\leqslant\frac{1}{\hbar^2}(|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\mu(t)\mu(t')\}|\\&\quad+|\mathrm{tr}\{\mathcal{U}^\dagger\mathcal{W}AA^\dagger\mu(t')\mu(t)\}|)\\&\leqslant\frac{2}{\hbar^2}\|AA^\dagger\|_F\|\mu(t)\mu(t')\|_F\\&\leqslant\frac{2}{\hbar^2}\|AA^\dagger\|_F\|\mu\|_F^2.\end{aligned} \tag{29}$$

It is evident that both the gradient and Hessian are finite and uniformly bounded, since the dipole moment norm $\|\mu\|_F$ of the quantum system is a bounded quantity for any N-level system. From Eqs. (27) and (29), it can be readily shown that the vector norm (i.e., two norm) of the gradient and the operator norm of the Hessian are bounded, respectively, by the relations

$$\left\| \frac{\delta \mathcal{J}_F}{\delta E(t)} \right\| = \left(\int_0^T \left| \frac{\delta \mathcal{J}_F}{\delta E(t)} \right|^2 dt \right)^{1/2} \leqslant \frac{2T^{1/2}}{\hbar} \|AA^\dagger\|_F \|\mu\|_F \tag{30}$$

and

$$\begin{aligned} \left\| \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \right\| &= \max_{\|f\|_2=1} \left(\int_0^T \left| \int_0^T \frac{\delta^2 \mathcal{J}_F}{\delta E(t')\delta E(t)} f(t') dt' \right|^2 dt \right)^{1/2} \\ &\leqslant \max_{\|f\|_2=1} \left[\int_0^T \left(\|f\|_2^2 \int_0^T \left| \frac{\delta^2 \mathcal{J}_F}{\delta E(t')\delta E(t)} \right|^2 dt' \right) dt \right]^{1/2} \\ &\leqslant \frac{2T}{\hbar^2} \|AA^\dagger\|_F \|\mu\|_F^2. \end{aligned} \tag{31}$$

These uniformly bounded norms are significant as they reveal the geometric picture of a regular and gently rolling landscape and they also are important for establishing the robustness of the optimal control field in the presence of field noises [54].

C. Robustness of controlling unitary transformations

Expanding the cost functional $\mathcal{J}_F[E+\delta E]$ as

$$\mathcal{J}_F[E+\delta E] = \mathcal{J}_F[E] + \int_0^T \frac{\delta \mathcal{J}_F[E]}{\delta E(t)} \delta E(t) dt + \frac{1}{2} \int_0^T \int_0^T \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \delta E(t) \delta E(t') dt dt' + \cdots, \tag{32}$$

in terms of a perturbation $\delta E(t)$, $t \in [0,T]$ in the control field $E(t)$, and utilizing Eqs. (27) and (29) leads to

$$|\delta \mathcal{J}_F[E]| = |\mathcal{J}_F[E+\delta E] - \mathcal{J}_F[E]| \leqslant \left| \int_0^T \frac{\delta \mathcal{J}_F[E]}{\delta E(t)} \delta E(t) dt \right| + \left| \frac{1}{2} \int_0^T \int_0^T \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \delta E(t) \delta E(t') dt dt' \right|, \tag{33}$$

which is further bounded as

$$\begin{aligned} |\delta \mathcal{J}_F[E]| &\leqslant \max_{t\in[0,T]} \left(\left| \frac{\delta \mathcal{J}_F[E]}{\delta E(t)} \right| \right) \int_0^T |\delta E(t)| dt + \max_{t\in[0,T]} \\ &\quad \times \left(\left| \frac{1}{2} \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \right| \right) \int_0^T \int_0^T |\delta E(t) \delta E(t')| dt dt' \\ &\leqslant \|AA^\dagger\|_F \left\{ \frac{2}{\hbar} \|\mu\|_F \|\delta E\|_1 + \frac{1}{\hbar^2} \|\mu\|_F^2 \|\delta E\|_1^2 \right\}, \end{aligned} \tag{34}$$

where the one norm

$$\|\delta E\|_1 = \int_0^T |\delta E(t)| dt. \tag{35}$$

characterizes the control field variation (noise). At the critical points, including the global minimum and maximum, the linear term in $\|\delta E\|_1$ in Eq. (34) drops out since $\delta \mathcal{J}_F[E]/\delta E(t) = 0$, and we have the (normalized) error bound

$$\begin{aligned} \frac{|\delta \mathcal{J}_F[E]|}{\|AA^\dagger\|_F} &= \{ |\mathcal{J}_F[E+\delta E] - \mathcal{J}_F[E]| \} / \|AA^\dagger\|_F \\ &\leqslant \frac{\left| \frac{1}{2} \int_0^T \int_0^T \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \delta E(t) \delta E(t') dt dt' \right|}{\|AA^\dagger\|_F} \\ &\leqslant \frac{1}{\|AA^\dagger\|_F} \max_{t\in[0,T]} \left(\left| \frac{1}{2} \frac{\delta^2 \mathcal{J}_F[E]}{\delta E(t')\delta E(t)} \right| \right) \\ &\quad \times \left(\int_0^T |\delta E(t)| dt \right)^2 \\ &\leqslant \frac{1}{\hbar^2} \|\mu\|_F^2 \times \|\delta E\|_1^2. \end{aligned} \tag{36}$$

Equations (34) and (36) impose upper bounds for the control errors (i.e., the stability of $\mathcal{J}_F[E]$) in the presence of control field noise, implying that any generic N-level quantum unitary transformation control has an inherent degree of robustness in the presence of control field noise (i.e., insensitivity to field noise), assuming that the associated dipole moment norm $\|\mu\|_F$ is finite. Appendix B gives a similar robustness analysis in terms of the phase-independent cost functional $\mathcal{J}_P[E]$, Eq. (21), for the special case involving an ensemble of two-level quantum systems (i.e., qubits).

IV. KINEMATIC CRITICAL POINTS OF THE LANDSCAPE

Consider the critical point condition Eq. (7). In conjunction with Eq. (24), it becomes

$$\frac{\delta \mathcal{J}_F[E]}{\delta E(t)} = -\frac{\imath}{\hbar} \sum_i \sum_j \langle i | (AA^\dagger \mathcal{W}^\dagger \mathcal{U} - \mathcal{U}^\dagger \mathcal{W} AA^\dagger) | j \rangle \langle j | \mu(t) | i \rangle = 0, \tag{37}$$

which is satisfied if and only if

$$AA^\dagger \mathcal{W}^\dagger \mathcal{U} = \mathcal{U}^\dagger \mathcal{W} AA^\dagger, \tag{38}$$

under the assumption that the N^2 time-dependent functions $\langle i | \mu(t) | j \rangle$, $i,j = 1, \ldots, N$ are linearly independent, cf. Sec. II. To facilitate the analysis, define the unitary matrix

$$\mathcal{X} = \mathcal{W}^\dagger \mathcal{U}, \quad \mathcal{X}^\dagger \mathcal{X} = \mathbf{I}. \tag{39}$$

Using Eq. (13) in Eq. (38), we obtain

$$\mathcal{X} AA^\dagger \mathcal{X} = AA^\dagger = \mathcal{X}^\dagger AA^\dagger \mathcal{X}^\dagger = D\Omega^2 D^\dagger, \tag{40}$$

from which it can be shown that [55]

$$\mathcal{X}^\dagger = \mathcal{X}, \tag{41}$$

indicating that the matrix $\mathcal{X}$ is not only unitary, but also Hermitian. Moreover, from Eqs. (39) and (41), it is seen that $\mathcal{X}$ is a periodic matrix of second order satisfying the quadratic matrix equation:

$$\mathcal{X}^2 = \mathcal{X}^\dagger \mathcal{X} = \mathbf{I}, \tag{42}$$

whose solutions are the square roots of the identity matrix $\mathbf{I}$. Finally, from Eqs. (38) and (41), $\mathcal{X}$ and $AA^\dagger$ commute, i.e.,

$$[\mathcal{X}, AA^\dagger] = 0. \tag{43}$$

As a result, $\mathcal{X}$ and $AA^\dagger$ can be diagonalized by the same unitary transformation D, i.e.,

$$D^\dagger \mathcal{X} D = \Lambda, \tag{44}$$

where Λ is a real diagonal matrix, thus

$$\mathcal{X} = D\Lambda D^\dagger. \tag{45}$$

It can be shown that the diagonal matrix Λ is composed of real matrix elements

$$\lambda_i = \Lambda_{ii} = (-1)^{n_i}, \tag{46}$$

with n_i, $i=1,2\ldots,N$, being either even or odd integers, such that $\Lambda^2=\mathbf{I}$. The diagonal matrix Λ in Eq. (46) immediately satisfies Eq. (42), i.e., $\mathcal{X}^2=(D\Lambda D^\dagger)(D\Lambda D^\dagger)=D\Lambda^2 D^\dagger=DD^\dagger=\mathbf{I}$.

The number of solutions for the matrix $\mathcal{X}$, cf. Eq. (45), depends on whether the Hermitian matrix $AA^\dagger$ is degenerate or not. For example, only one $\mathcal{X}(=D\Lambda D^\dagger)$ solution exists (or, equivalently, only one $\mathcal{U}=\mathcal{W}\mathcal{X}=\mathcal{W}D\Lambda D^\dagger$ exists) when the matrix $AA^\dagger$ is completely nondegenerate (i.e., it possesses only distinct eigenvalues), since in this case each column of the unitary matrix D is uniquely defined within an overall phase factor (e.g., ϕ_k for the kth column of D such that the ith row and jth column of the matrix elements $\mathcal{X}_{ij}$ of the matrix $\mathcal{X}$ can be written as $\mathcal{X}_{ij}=\Sigma_k[D_{ik}\exp(\imath\phi_k)]\lambda_k[D^*_{jk}\exp(-\imath\phi_k]=\Sigma_k D_{ik}\lambda_k D^*_{jk}$, independent of the phases ϕ_k's). On the other hand, an infinite number of $\mathcal{X}$'s is allowed when $AA^\dagger$ is completely degenerate (e.g., $AA^\dagger=\mathbf{I}$, which can be diagonalized by any unitary matrix D). Explicitly, the degeneracy of the singular values $\omega_1^2 \geq \omega_2^2 \geq \ldots \geq \omega_N^2 > 0$ determines the properties of the local critical points. The signature of the Hessian at the critical points depends on the singular values of the matrix $AA^\dagger$, and the freedom of choosing the landscape adaptation matrix A may facilitate the search for optimal control fields. Finally, the results derived in Eqs. (41)–(46) are generic, independent of the number n of quantum states spanning the desired unitary transformation $\mathcal{W}_n$ and the exact content of the matrix $\mathcal{Q}_{N-n}$ in Eq. (6). The freedom of choosing the unitary matrix $\mathcal{Q}_{N-n}$ does not change the essential features of the underlying control landscape; however, it may be judiciously chosen to expedite the control processes.

From Eq. (12), the functional $\mathcal{J}_F[E]$ at the critical points may be expressed as

$$\begin{aligned}\mathcal{J}_F[E] &= 2\|A\|_F^2 - 2\,\mathrm{tr}\{AA^\dagger\mathcal{X}\} = 2\,\mathrm{tr}(D\Omega^2 D^\dagger) \\ &\quad - 2\,\mathrm{tr}\{D\Omega^2 D^\dagger D\Lambda D^\dagger\} = 2\,\mathrm{tr}(\Omega^2) - 2\,\mathrm{tr}\{\Omega^2\Lambda\} \\ &= 2\sum_{i=1}^{N}[1-(-1)^{n_i}]\omega_i^2 \geq 0,\end{aligned} \tag{47}$$

which possesses at most 2^N distinct values. These critical values may be grouped into $N+1$ classes, depending on the number k of n_i's in Eq. (47) that are odd integers: $\mathcal{J}_F[E]=0$ for $k=0$, $\mathcal{J}_F[E]=4\omega_i^2$, $i=1,\ldots,N$ for $k=1$, $\mathcal{J}_F[E]=4(\omega_i^2+\omega_j^2)$, $1\leq i\neq j\leq N$ for $k=2$, $\mathcal{J}_F[E]=4(\omega_i^2+\omega_j^2+\omega_k^2)$, $1\leq i\neq j\neq k\leq N$ for $k=3,\ldots$, and $\mathcal{J}_F[E]=4(\Sigma_{i=1}^N\omega_i^2)$ for $k=N$. The number of distinct critical $\mathcal{J}_F[E]$ values associated with each k is at most $\binom{N}{k}$, and the total number of the distinct critical values of $\mathcal{J}_F[E]$ is at most $\Sigma_{k=0}^N\binom{N}{k}=2^N$. Moreover, regardless of the exact nature of the landscape adaptation matrix A, there exist precisely one global minimum value $\mathcal{J}_F[E]=0$ and one global maximum value $\mathcal{J}_F[E]=4\Sigma_{i=1}^N\omega_i^2$, each associated with a unique unitary transformation matrix $\mathcal{U}$, i.e., there is a one-to-one relationship between the global extremal values and the global extrema, since $\Lambda=\mathbf{I}$, $\mathcal{X}=D\Lambda D^\dagger=\mathbf{I}$, and $\mathcal{U}=\mathcal{W}D\Lambda D^\dagger=\mathcal{W}$ at the global minimum at which all n_i are even integers whereas $\Lambda=-\mathbf{I}$, $\mathcal{X}=-\mathbf{I}$, and $\mathcal{U}=-\mathcal{W}$ at the global maximum at which all n_i are odd integers. However, there will be an infinite number of distinct control fields producing these unique extrema.

In the case that the matrix $AA^\dagger$ is nondegenerate, the corresponding $\mathcal{X}$ matrix is unique for a given Λ. Thus, the correspondence between local critical values and local critical points is one to one, each associated with a specific unitary transformation matrix $\mathcal{U}=\mathcal{W}D\Lambda D^\dagger$. However, in the case that $AA^\dagger$ is either partially or completely degenerate, an infinite number of $\mathcal{X}$'s always exist. Consequently, the correspondence between local critical values and local critical points is one to infinity, associated with an infinite number of distinct unitary transformations $\mathcal{U}=WD\Lambda D^\dagger$. In particular, in the completely degenerate case of $AA^\dagger=\mathbf{I}$, i.e., $\omega_i=1$, $\forall i=1,\ldots,N$, the cost functional is simply

$$\mathcal{J}_F[E] = 2N - 2\sum_{i=1}^{N}(-1)^{n_i}, \tag{48}$$

which possesses $N+1$ distinct critical values $0,4,\ldots,4N-4,4N$. Two of the critical values are $\mathcal{J}_F[E]=0$ at the global minimum and $\mathcal{J}_F[E]=4N$ at the global maximum. The other $N-1$ critical values take on the simple form $\mathcal{J}_F[E]=2N-2[(N-k)-k]=4k$, each characterized by a multiplicity equal to $\binom{N}{k}$ which depends on the index k [26].

V. HESSIAN AT THE KINEMATIC CRITICAL POINTS

At the critical points, substituting the relation from Eq. (38) in Eq. (25), the Hessian $\mathcal{H}(t,t')\equiv\delta^2\mathcal{J}_F[E]/\delta E(t')\delta E(t)$ can be written as follows:

$$\mathcal{H}(t,t') = \frac{1}{\hbar^2}\mathrm{tr}\{AA^\dagger\mathcal{X}[\mu(t)\mu(t')+\mu(t')\mu(t)]\}. \tag{49}$$

By inserting the identity $D^\dagger D=\mathbf{I}$ and invoking the cyclic invariance property of the matrix trace, we have the following expansion

$$\begin{aligned}\mathcal{H}(t,t') &= \frac{1}{\hbar^2}\mathrm{tr}\{DD^\dagger AA^\dagger DD^\dagger\mathcal{X}DD^\dagger \\ &\quad\times[\mu(t)DD^\dagger\mu(t')+\mu(t')DD^\dagger\mu(t)]\} \\ &= \frac{1}{\hbar^2}\mathrm{tr}\{\Omega^2\Lambda D^\dagger[\mu(t)DD^\dagger\mu(t')+\mu(t')DD^\dagger\mu(t)]D\}\end{aligned}$$

$$= \frac{1}{\hbar^2}\sum_i (-1)^{n_i}\omega_i^2 \sum_j \{\langle i|\bar{\mu}(t)|j\rangle\langle j|\bar{\mu}(t')|i\rangle + \langle i|\bar{\mu}(t')|j\rangle \times \langle j|\bar{\mu}(t)|i\rangle\}, \tag{50}$$

where

$$\bar{\mu}(t) = D^\dagger \mu(t) D, \tag{51}$$

with the unitary matrix defined in Eq. (14). Here Eqs. (13), (44), and (46) have been used to derive Eq. (50). From Eq. (50), the Hessian trace at the critical points can be written as

$$\mathrm{tr}\mathcal{H} \equiv \int_0^T \mathcal{H}(t,t)dt = \frac{2}{\hbar^2}\int_0^T \sum_i (-1)^{n_i}\omega_i^2 \sum_j |\langle i|\bar{\mu}(t)|j\rangle|^2 dt, \tag{52}$$

which, by carrying out the integration over t and invoking the norm relation

$$\|\mu\|_F^2 = \|\bar{\mu}(t)\|_F^2 = \sum_i \sum_j |\langle i|\bar{\mu}(t)|j\rangle|^2, \tag{53}$$

yields the lower and upper bounds of the Hessian trace

$$-\frac{2}{\hbar^2}\|AA^\dagger\|_2\|\mu\|_F^2 \leqslant \frac{1}{T}\mathrm{tr}\mathcal{H} \leqslant \frac{2}{\hbar^2}\|AA^\dagger\|_2\|\mu\|_F^2 \leqslant \frac{2}{\hbar^2}\|AA^\dagger\|_F\|\mu\|_F^2, \tag{54}$$

where the two norm $\|AA^\dagger\|_2 = \max\{\omega_1^2, \ldots, \omega_N^2\}$, with the equalities at the global minimum (lower bound) when $\mathcal{U} = \mathcal{W}$ (corresponding to all even n_i integers) and at the global maximum (upper bound) when $\mathcal{U} = -\mathcal{W}$ (corresponding to all odd n_i integers). Note that (a) $\|AA^\dagger\|_2 \leqslant \|AA^\dagger\|_F \leqslant \sqrt{N}\|AA^\dagger\|_2$ and (b) $\|AA^\dagger\|_2 = 1$, $\|AA^\dagger\|_F = \sqrt{N}$ when $AA^\dagger = \mathbf{I}$.

By taking into account the Hermitian nature of the dipole moment operator $\bar{\mu}(t) = \bar{\mu}^\dagger(t)$, the Hessian $\mathcal{H}(t,t')$ at the critical points, Eq. (50), can be further written as

$$\begin{aligned}\mathcal{H}(t,t') = {} & \frac{2}{\hbar^2}\sum_i (-1)^{n_i}\omega_i^2 \langle i|\bar{\mu}(t)|i\rangle\langle i|\bar{\mu}(t')|i\rangle \\ & + \frac{2}{\hbar^2}\sum_i \sum_{j>i} \{(-1)^{n_i}\omega_i^2 + (-1)^{n_j}\omega_j^2\} \\ & \times \{\mathrm{Re}[\langle i|\bar{\mu}(t)|j\rangle]\mathrm{Re}[\langle i|\bar{\mu}(t')|j\rangle] \\ & + \mathrm{Im}[\langle i|\bar{\mu}(t)|j\rangle]\mathrm{Im}[\langle i|\bar{\mu}(t')|j\rangle]\}\end{aligned} \tag{55}$$

which is a separable and symmetric kernel spanned by N^2 linearly independent basis functions $\{\langle i|\bar{\mu}(t)|i\rangle, \mathrm{Re}(\langle i|\bar{\mu}(t)|j\rangle), \mathrm{Im}(\langle i|\bar{\mu}(t)|j\rangle), j > i = 1, \ldots, N\}$ of time $t \in [0,T]$, cf. Sec. II. The Hessian $\mathcal{H}(t,t')$ can be written in simple vector form

$$\mathcal{H}(t,t') = \boldsymbol{\mu}^{\mathrm{T}}(t)\Gamma\boldsymbol{\mu}(t') = \sum_{k=1}^{N^2} \gamma_k \mu_k(t)\mu_k(t'), \tag{56}$$

where

$$\begin{aligned}\boldsymbol{\mu}^{\mathrm{T}}(t) &= \Big(\underbrace{\mu_1(t), \mu_2(t), \ldots,}_{N+\frac{N(N-1)}{2}\ \text{terms}}\ \underbrace{\ldots, \mu_{N^2-1}(t), \mu_{N^2}(t)}_{\frac{N(N-1)}{2}\ \text{terms}}\Big) \\ &= \Big(\underbrace{\mathrm{Re}\,(\langle i|\bar{\mu}(t)|j\rangle)\,, 1 \le i, j \le N,}_{N+\frac{N(N-1)}{2}\ \text{terms}}\ \underbrace{\mathrm{Im}\,(\langle i|\bar{\mu}(t)|j\rangle)\,, 1 \le i < j \le N}_{\frac{N(N-1)}{2}\ \text{terms}}\Big)\end{aligned} \tag{57}$$

is the transpose (denoted as the superscript "T") of an N^2 dimensional column vector $\boldsymbol{\mu}(t)$ consisting of the N^2 linearly independent components of the dipole moment matrix $\bar{\mu}(t)$ and

$$\Gamma = \mathrm{diag}\Big\{\underbrace{\gamma_1, \gamma_2, \ldots, \gamma_N,}_{N\ \text{terms}}\ \underbrace{\gamma_{N+1}, \ldots,}_{\frac{N(N-1)}{2}\ \text{terms}}\ \underbrace{\ldots, \gamma_{N^2-1}, \gamma_{N^2}}_{\frac{N(N-1)}{2}\ \text{terms}}\Big\} \tag{58}$$

is a diagonal matrix which can be explicitly written as

$$\begin{aligned}\Gamma = \frac{2}{\hbar^2} \times \mathrm{diag}\Big\{ & \underbrace{(-1)^{n_1}\omega_1^2, \ldots, (-1)^{n_N}\omega_N^2,}_{N\ \text{terms}} \\ & \underbrace{\big[(-1)^{n_1}\omega_1^2 + (-1)^{n_2}\omega_2^2\big], \ldots, \big[(-1)^{n_{N-1}}\omega_{N-1}^2 + (-1)^{n_N}\omega_N^2\big],}_{\frac{N(N-1)}{2}\ \text{terms}} \\ & \underbrace{\big[(-1)^{n_1}\omega_1^2 + (-1)^{n_2}\omega_2^2\big], \ldots, \big[(-1)^{n_{N-1}}\omega_{N-1}^2 + (-1)^{n_N}\omega_N^2\big]}_{\frac{N(N-1)}{2}\ \text{terms}}\Big\},\end{aligned} \tag{59}$$

in terms of the eigenvalues of the matrix product $AA^\dagger$. Equations (56)–(59) indicate that the Hessian at a critical point possesses at most N^2 nonzero real eigenvalues, in addition to an infinite number of zero eigenvalues and their associated eigenfunctions.

Moreover, a proper choice the adaptation matrix A may mollify the magnitude of the gradient $\delta\mathcal{J}_F[E]/\delta E(t)$, cf. Eqs. (27) and (30), in such a way to improve the gradient-based search algorithms in the optimal control implementations. The situation where $AA^\dagger$ is completely nondegenerate is a special case in which each critical unitary matrix associated with the kinematic landscape $\hat{\mathcal{J}}_F[\mathcal{U}] = \|(\mathcal{W} - \mathcal{U})A\|_F^2$ is isolated. In addition, the Morse function $\hat{\mathcal{J}}_F[\mathcal{U}]$ has the fewest possible critical points, hence the fewest saddle points, among the Morse functions on U(N) (i.e., the function $\hat{\mathcal{J}}_F[\mathcal{U}]$ becomes a *perfect Morse function* [49]). Since the saddles may have the effect of increasing the computational complexity of the gradient descent optimization, such a perfect Morse function may be the most efficient landscape on which to perform a gradient descent. In particular, the Hessians in the neighborhood of the critical points may be approximated by Eq. (56) such that the corresponding gradients can be written as

$$\left.\frac{\delta \mathcal{J}_F[E]}{\delta E(t)}\right|_{E_0} \approx -\int_0^T \mathcal{H}(t,t')[E(t')-E_0(t')]dt' = -\boldsymbol{\mu}^{\mathrm{T}}(t)\Gamma\left(\int_0^T \boldsymbol{\mu}(t')[E(t')-E_0(t')]dt'\right), \tag{60}$$

where $E(t)$ and $E_0(t)$ are the control fields corresponding to a critical point and its neighborhood, respectively. By optimizing the basis functions $\mu_1(t),\ldots,\mu_{N^2}(t)$, cf. Eqs. (51) and (57), with proper choices of the adaptation matrix A, Eq. (60) may be solved [56] to greatly facilitate the search for optimal control fields $E(t)$, especially around the global extrema where the Hessian (equivalently the matrix Γ) is positive (minimum) or negative (maximum) definite.

VI. HESSIAN QUADRATIC FORMS, RANKS, AND SIGNATURES AT THE KINEMATIC CRITICAL POINTS

It may be shown [57] that every regular critical point of $\mathcal{J}_F[E]$ with Hessian rank R belongs to a critical submanifold of codimension R in the control space L_2 and that the null space of the Hessian is identical to the tangent space of this critical submanifold. The *rank* and *signature* of the Hessian $\mathcal{H}(t,t')$ are useful parameters to characterize the geometric properties of $\mathcal{J}_F[E]$ at the critical points. The rank can be directly deduced from Eq. (59). In this section, a more instructive and quantitative analysis is presented for revealing both the rank and signature by casting the Hessian into its various equivalent quadratic forms [52].

In terms of the N^2 linearly independent (usually nonorthogonal) basis functions $\mathrm{Re}(\langle i|\bar{\mu}(t)|j\rangle)$, $1\leqslant i\leqslant j\leqslant N$, and $\mathrm{Im}(\langle i|\bar{\mu}(t)|j\rangle)$, $1\leqslant i< j\leqslant N$, the rank-$N^2$ separable and symmetric Hessian $\mathcal{H}(t,t')$, Eq. (56), possesses a quadratic (bilinear) form

$$\langle v|\mathcal{H}|v\rangle = \int_0^T\int_0^T v(t)\mathcal{H}(t,t')v(t')dt'dt, \tag{61}$$

where $v(t)\in L_2$. The time-dependent function $v(t)$ can be expanded as

$$v(t) = \mathbf{c}^{\mathrm{T}}\boldsymbol{\mu}(t) + q(t) = \boldsymbol{\mu}^{\mathrm{T}}(t)\mathbf{c} + q(t) = \sum_{k=1}^{N^2} c_k\mu_k(t) + q(t), \tag{62}$$

where $q(t)\in(\mathrm{span}\{\mu_k(t):k=1,\ldots,N^2\})^{\perp}\subset L_2$ and

$$\mathbf{c}^{\mathrm{T}} = (c_1,c_2,\ldots,c_{N^2-1},c_{N^2}) \tag{63}$$

is the transpose of an N^2 dimensional vector $\mathbf{c}$ containing the unknown expansion coefficients $c_1,\ldots,c_{N^2}$. In the case that the matrix $AA^{\dagger}$ is nondegenerate, the quadratic form $\langle v|\mathcal{H}|v\rangle$ of the Hessian $\mathcal{H}(t,t')$ is of rank N^2 and diagonal in the (nonorthogonal) $\boldsymbol{\mu}$ representation, i.e.,

$$\langle v|\mathcal{H}|v\rangle = \mathbf{x}_{\mu}^{\mathrm{T}}\Gamma\mathbf{x}_{\mu}, \tag{64}$$

where the N^2-dimensional column vector $\mathbf{x}_{\mu}$ is given as

$$\mathbf{x}_{\mu} = \int_0^T \boldsymbol{\mu}(t)v(t)dt = \left\{\int_0^T \boldsymbol{\mu}(t)\boldsymbol{\mu}^{\mathrm{T}}(t)dt\right\}\mathbf{c}, \tag{65}$$

with its transpose $\mathbf{x}_{\mu}^{\mathrm{T}}=(x_{\mu}^1,\ldots,x_{\mu}^{N^2})$ composed of N^2 coordinates, since $\int_0^T\boldsymbol{\mu}(t)q(t)dt=0$.

Equations (59) and (64) show that the ranks of the Hessians at the global minimum and maximum are always N^2 for any nonsingular $N\times N$ matrix $AA^{\dagger}$ (or more precisely independent of the N nonzero singular values of $AA^{\dagger}$). However, the Hessian ranks and signatures at the saddle points depend on the different combinations of singular values, via the terms $(-1)^{n_i}\omega_i^2+(-1)^{n_j}\omega_j^2$, $i\neq j$, in Eq. (59), of the matrix $AA^{\dagger}$. For example, in the case of $AA^{\dagger}=\mathbf{I}$, the rank at the local critical points is $(N-k)^2+k^2=N^2-2k(N-k)$, with k being the number of n_i's that are odd integers: the Hessian ranks at both the global minimum and maximum (respectively, corresponding to $k=0$ and $k=N$) remain at N^2, while the counterparts (corresponding to $0<k<N$) at the saddle points are all less than N^2. In general, the matrix $AA^{\dagger}=D\Omega^2D^{\dagger}$, Eq. (14), can be constructed in terms of the diagonal matrix Ω^2 and the unitary matrix D to alter the relative magnitudes of $\omega_1^2,\omega_2^2,\ldots,\omega_N^2$ in Eq. (59) resulting in different Hessian ranks and signatures.

For a closer examination of the Hessian geometric properties at the critical points, it is useful to cast $\mathcal{H}(t,t')$ into the expansion

$$\mathcal{H}(t,t') = \sum_{k=1}^{N^2}\sigma_k u_k(t)u_k(t') = \mathbf{u}^{\mathrm{T}}(t)\Sigma\mathbf{u}(t'). \tag{66}$$

Here the diagonal matrix

$$\Sigma = \mathrm{diag}\{\sigma_1,\ldots,\sigma_{N^2}\} \tag{67}$$

consists of at most N^2 nonzero Hessian eigenvalues $\sigma_1,\ldots,\sigma_R$ (R the Hessian rank) and zero eigenvalues $\sigma_{R+1},\ldots,\sigma_{N^2}$ and the transpose $\mathbf{u}^{\mathrm{T}}(t)$ of the N^2-dimensional column vector $\mathbf{u}(t)$ is defined as

$$\mathbf{u}^{\mathrm{T}}(t) = [u_1(t),u_2(t),\ldots,u_{N^2-1}(t),u_{N^2}(t)], \tag{68}$$

which consists of the Hessian eigenfunctions $u_k(t)$ that satisfy the integral equation

$$\int_0^T \mathcal{H}(t,t')u_k(t')dt' = \sigma_k u_k(t) \quad ,k=1,\ldots,N^2. \tag{69}$$

The eigenfunctions $u_k(t)$'s are taken to be orthonormal

$$\int_0^T \mathbf{u}(t)\mathbf{u}^{\mathrm{T}}(t)dt = \mathbf{I} \tag{70}$$

and to span the same space as the functions $\{\mu_1(t),\ldots,\mu_{N^2}(t)\}$. It is seen from Eq. (66) that the quadratic form associated with $\mathcal{H}(t,t')$ in terms of the Hessian eigenfunctions is also a diagonal quadratic form in the (orthogonal) $\mathbf{u}$ representation,

$$\langle v|\mathcal{H}|v\rangle = \mathbf{x}_u^{\mathrm{T}}\Sigma\mathbf{x}_u, \tag{71}$$

where the N^2-dimensional column vector $\mathbf{x}_u$ is defined as

$$\mathbf{x}_u = \int_0^T \mathbf{u}(t)v(t)dt = \left\{\int_0^T \mathbf{u}(t)\boldsymbol{\mu}^{\mathrm{T}}(t)dt\right\}\mathbf{c}, \tag{72}$$

with its transpose $\mathbf{x}_u^{\mathrm{T}}=(x_u^1,\ldots,x_u^{N^2})$ composed of N^2 independent components (coordinates), since $\mathrm{span}\{u_k(t):k=1,\ldots,N^2\}=\mathrm{span}\{\mu_k(t):k=1,\ldots,N^2\}$, and therefore $\int_0^T\mathbf{u}(t)q(t)dt=0$. Combining Eqs. (64) and (71) results in

$$\mathbf{x}_u^{\mathrm{T}}\Sigma\mathbf{x}_u = \mathbf{x}_\mu^{\mathrm{T}}\Gamma\mathbf{x}_\mu. \tag{73}$$

By introducing the linear transformation $P\mathbf{u}(t)=\boldsymbol{\mu}(t)$ [or equivalently $P\mathbf{x}_u=\mathbf{x}_\mu$] in terms of the nonsingular matrix

$$P = \int_0^T \boldsymbol{\mu}(t)\mathbf{u}^{\mathrm{T}}(t)dt, \tag{74}$$

where both $\boldsymbol{\mu}(t)$ and $\mathbf{u}(t)$ are vectors of dimension N^2, we have $(\mathbf{x}_u^{\mathrm{T}}P^{\mathrm{T}})\Gamma(P\mathbf{x}_u)=\mathbf{x}_u^{\mathrm{T}}(P^{\mathrm{T}}\Gamma P)\mathbf{x}_u$, and thus Eq. (73) reduces to a simple relation

$$\Sigma = P^{\mathrm{T}}\Gamma P, \tag{75}$$

between the diagonal matrices Γ, given in Eq. (59), and Σ, given in Eq. (67).

Equation (73), or equivalently Eq. (75), indicates that the (diagonal) matrices Σ and Γ are congruent. Consequently, by invoking Sylvester's law of inertia for the equivalence of a symmetric matrix under a congruent transformation [52,58,59], it can be shown [60] that the numbers of positive, negative, and zero diagonal elements $\sigma^+>0$, $\sigma^-<0$, $\sigma^0=0$ of Σ, cf. Eq. (67), are, respectively, equal to those values $\gamma^+>0$, $\gamma^-<0$, $\gamma^0=0$ of Γ, cf. Eq. (59). For each distribution of even and odd integers n_i, $i=1,\ldots,N$, it is easy to enumerate the numbers of positive, negative, and zero diagonal elements in Γ. For example, it is readily seen that in the case that $AA^\dagger$ is nondegenerate, all of the γ_i's in Γ are nonzero regardless of any combination of even and odd n_i integers, $i=1,\ldots,N$. The rank of the corresponding Hessian is then equal to N^2 at any critical point. Moreover, except at the global minimum and maximum (respectively, corresponding to situations when all n_i's are even or odd integers), and independent of the degeneracy of $AA^\dagger$, there exists at least one negative and one positive γ_i value in Γ when the corresponding n_i's consist of mixed even and odd integers, indicating that *none of the local critical points are traps*.

In the special case of $AA^\dagger=\mathbf{I}$, the corresponding landscape can be summarized below: (1) at the global minimum (i.e., all n_i are even integers),

$$\frac{\hbar^2}{2}\Gamma^+ = \mathrm{diag}\{\underbrace{1,1,\ldots,1}_{N\text{ terms}},\underbrace{2,2,\ldots,2}_{N(N-1)\text{ terms}}\}, \tag{76}$$

(2) at the global maximum (i.e., all n_i are odd integers),

$$\frac{\hbar^2}{2}\Gamma^- = \mathrm{diag}\{\underbrace{-1,-1,\ldots,-1}_{N\text{ terms}},\underbrace{-2,-2,\ldots,-2}_{N(N-1)\text{ terms}}\}, \tag{77}$$

and (3) at a local critical point with $0<k<N$ odd integers (among all n_i's),

$$\frac{\hbar^2}{2}\Gamma^k = \mathrm{diag}\{\underbrace{1,1,\ldots,1}_{N-k\text{ terms}},\underbrace{2,2,\ldots,2}_{(N-k)(N-k-1)\text{ terms}},\underbrace{-1,-1,\ldots,-1}_{k\text{ terms}},\underbrace{-2,-2,\ldots,-2}_{k(k-1)\text{ terms}},\underbrace{0,0,\ldots,0}_{2(N-k)k\text{ terms}}\}. \tag{78}$$

As a result, we have, for $0\leqslant k\leqslant N$,

$$\Sigma^k = \mathrm{diag}\{\underbrace{\sigma_1^+,\ldots,\sigma_{(N-k)^2}^+}_{(N-k)^2\text{ terms}},\underbrace{\sigma_1^-,\ldots,\sigma_{k^2}^-}_{k^2\text{ terms}},\underbrace{0,0,\ldots,0}_{2(N-k)k\text{ terms}}\}. \tag{79}$$

The rank R_k and signature S_k of the Hessian $\mathcal{H}(t,t')$ at the critical points can be given in simple form: $R_k=N(N-2k)+2k^2$ and $S_k=N(N-2k)$, $k=0,1,\ldots,N$ ($k=0$ at the global minimum, $k=N$ at the global maximum, $0<k<N$ at all other critical points). Specifically, there are $(N-k)^2$ positive eigenvalues $\sigma_\ell^+>0$, $\ell=1,\ldots,(N-k)^2$, k^2 negative eigenvalues $\sigma_\ell^-<0$, $\ell=1,\ldots,k^2$, and $2(N-k)k$ additional zero eigenvalues. In addition, there are infinitely many zero eigenvalues due to the infinite dimensional continuous control field space in the temporal domain $[0,T]$. All of results obtained in this work based on the dynamical (control field) analysis are consistent to those obtained from the kinematic landscape (U matrix) analysis [26].

VII. SUMMARY

We have presented a detailed study of the control landscape of unitary transformations in the context of working with the infinite-dimensional function space L_2 of square-integrable control fields. Specifically, given a fully controllable N-level quantum system that evolves over time, governed by the unitary propagator $U(t,0)$, and a preselected unitary transformation $\mathcal{W}$, we explored the landscape structure and properties of the Frobenius matrix norm square

$\mathcal{J}_F[E]=\|(\mathcal{W}-\mathcal{U})A\|_F^2$ in the infinite-dimensional space L_2 of the control fields $E(t)$ in conjunction with a landscape adaptation matrix A, including a full analysis of the degenerate $AA^\dagger=\mathbf{I}$ case. The matrix $AA^\dagger=D\Omega^2D^\dagger$, Eq. (14), provides a flexible means for altering the dynamical control landscape $\mathcal{J}_F[E]$ by (i) changing the numbers of critical points, (ii) generating different Hessian ranks and signatures at the critical points, and (iii) optimizing the gradient $\delta\mathcal{J}_F[E]/\delta E(t)$, Eq. (24), with different choices of the diagonal matrix Ω^2 and the unitary matrix D. Proper choices of Ω^2 and D (i.e., $AA^\dagger$) may enable better implementations for seeking optimal controls of unitary transformations, especially, in the neighborhood of the global minimum and maximum.

Within the electric dipole formulation, upper bounds were obtained for both the slope (gradient) and curvature (Hessian) over the control field landscape, and accordingly a general assessment was made of robustness (i.e., error bounds in $\mathcal{J}_F[E]$ due to control field noise δE) when optimally controlling unitary transformations. It was found that for generic controllable N-level quantum systems, the corresponding error bound is proportional to the product of the square norm of the system's dipole moment and the square norm of the control field noise, implying that the underlying optimal control of the unitary transformation is inherently robust to the presence of control laser field noise of reasonable magnitude. We derived the necessary and sufficient conditions for the existence of the regular critical points, defined in Sec. II, and gave a thorough analysis of the qualitative properties of control landscape, based on the Hessian, at the corresponding critical points. It was found that there is only one global minimum and one global maximum value, corresponding to $\mathcal{U}=\mathcal{W}$ and $\mathcal{U}=-\mathcal{W}$, respectively. All other critical points are nontrapping saddles.

For a nonsingular landscape adaptation matrix A, at most 2^N distinct critical values of $\mathcal{J}_F[E]$ exist and every Hessian at the critical points, including both the global minimum and maximum and all local nontrapping saddles, has a rank of at most N^2. For the completely degenerate $AA^\dagger=\mathbf{I}$ case, in addition to the two values associated with the global minimum and maximum, there are $N-1$ local critical values of $\mathcal{J}_F[E]$. Moreover, when the matrix $\mathcal{W}^\dagger\mathcal{U}$ has exactly k negative eigenvalues, the rank and signature of the corresponding Hessian are, respectively, $(N-k)^2+k^2$ and $(N-k)^2-k^2$. In all cases, regardless of the exact nature of the nonsingular matrix A, all local critical points are nontrapping, which is consistent with a previous kinematic study of this special case [26].

For comparison, an alternative unitary transformation landscape was considered in Appendix A using the phase-independent functional $\mathcal{J}_P[E]=|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\}|$ to measure the fidelity between the controlled and target unitary matrices. The landscape $\mathcal{J}_P[E]$ depends on the target $\mathcal{W}$ up to an arbitrary global phase, in contrast to the Frobenius norm square $\mathcal{J}_F[E]$ that specifies the phase. It was found that (i) the Hessian at the $\mathcal{J}_P[E]$ critical points possess one additional zero eigenvalue beyond that of its $\mathcal{J}_F[E]$ counterpart due to the arbitrary global phase in the former, and (ii) both landscapes contain no false traps. In Appendix B, the issue of robustness for controlling quantum logic gates of a generic multiqubit (p-qubit) quantum system was addressed, based on the analysis of the $\mathcal{J}_P[E]$ landscape. An error bound of the unitary transformation fidelity $\mathcal{F}=|\mathrm{tr}\{\mathcal{W}^\dagger\mathcal{U}\}|/2^p$ for a coupled p-qubit system at the global maximum was found to scale approximately as $p^2 2^{p/2}$ in terms of the number p of the qubits and quadratically with the one norm $\|\delta E\|_1$ of the noise in the control field, implying that when the number of the qubits is large the unitary transformation involving fully coupled qubits may not be robust in the presence of control field noise, in agreement with the conclusion obtained from the analysis using the action matrix [61].

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APPENDIX A: PHASE-INDEPENDENT LANDSCAPE OF $\mathcal{J}_P[E]=|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\}|$

Consider a fully controllable N-level quantum system, $N\geqslant 2$, where the goal is to find a control field $E(t)$, $t\in[0,T]$ that can generate a target $\mathcal{W}$ unitary transformation, within a globally unspecified phase θ. The associated optimal control problem may be posed as the following maximization problem [17,21,22,25]

$$\max_{E(t)} \mathcal{J}_P[E], \tag{A1}$$

where the cost functional $\mathcal{J}_P[E]$ defining the landscape is

$$\mathcal{J}_P[E]=|\mathrm{tr}\{AA^\dagger\mathcal{W}^\dagger\mathcal{U}\}|>0. \tag{A2}$$

The cost functional $\mathcal{J}_P[E]$ measures the fidelity between the unitary transformation $\mathcal{U}=U(T,0)$, associated with a control field $E(t)$, and the designated unitary transformation $\mathcal{W}$ within a globally arbitrary phase. The functional derivative $\delta\mathcal{J}_P[E]/\delta E(t)$ of $\mathcal{J}_P[E]$ with respect to $E(t)$ is not defined at the global minimum when $\mathcal{J}_P[E]=0$ (see below), thus we only consider the landscape of $\mathcal{J}_P[E]>0$, cf. Eq. (A2), in this appendix. An arbitrary nonsingular adaptation matrix A has been introduced to enable additional manipulation of the $\mathcal{J}_P[E]$ landscape in the control field function space, thereby facilitating the search for optimal control fields. The special case of $AA^\dagger=\mathbf{I}$ has been the subject of many recent studies, especially in quantum information processing [16–22,27,61]. In this case, the unitary transformation $\mathcal{W}$ is related to a quantum logic gate associated with a p-qubit ($p\geqslant 1$) quantum system containing $N=2^p$ quantum states and the cost functional $\mathcal{J}_P[E]$ serves as a measure of the fidelity of the optimal unitary transformation $\mathcal{U}$ with respect to $\mathcal{W}$. The robustness for controlling a p-qubit quantum logic gate is presented in Appendix B.

To simplify the formulation, Eq. (A2) is rewritten as

$$\mathcal{J}_P[E]=\tfrac{1}{2}\{\mathrm{tr}(AA^\dagger\mathcal{W}^\dagger\mathcal{U})\alpha^*+\mathrm{tr}(\mathcal{U}^\dagger\mathcal{W}AA^\dagger)\alpha\}, \tag{A3}$$

where the complex global phase parameter $\alpha\equiv\exp(\imath\theta)$ is

$$\alpha = \frac{\mathrm{tr}\{AA^\dagger \mathcal{W}^\dagger \mathcal{U}\}}{|\mathrm{tr}\{AA^\dagger \mathcal{W}^\dagger \mathcal{U}\}|} \tag{A4}$$

in terms of A, $\mathcal{W}$, and $\mathcal{U}$. The phase parameter α is of unit modulus, i.e., $|\alpha|=1$. Moreover, $\alpha\alpha^*=1$ and $\alpha^*=\alpha^{-1}$. The phase parameter α is ill defined when $\mathcal{J}_P[E]=|\mathrm{tr}\{AA^\dagger \mathcal{W}^\dagger \mathcal{U}\}|=0$. From Eq. (A3), the first-order functional derivative $\delta\mathcal{J}_P[E]/\delta E(t)$ can be expressed as

$$\frac{\delta \mathcal{J}_P[E]}{\delta E(t)} = \frac{\imath}{2\hbar}\mathrm{tr}\{(\alpha^* AA^\dagger \mathcal{X} - \alpha \mathcal{X}^\dagger AA^\dagger)\mu(t)\}, \tag{A5}$$

where $\mu(t)=U(t,0)^\dagger \mu U(t,0)$ and $\mathcal{X}=\mathcal{W}^\dagger\mathcal{U}$. The functional derivative $\delta\mathcal{J}_P[E]/\delta E(t)$ in Eq. (A5) is not defined when $\mathcal{J}_P[E]=0$ due to the ill-defined phase parameter α, cf. Eq. (A4). Likewise, the corresponding second-order functional derivative $\delta^2\mathcal{J}_P[E]/\delta E(t')\delta E(t)$ can be written as

$$\begin{aligned}\frac{\delta^2 \mathcal{J}_P[E]}{\delta E(t')\delta E(t)} = {}& \frac{\imath}{2\hbar}\left(\frac{\delta\alpha^*}{\delta E(t')}\mathrm{tr}\{AA^\dagger \mathcal{X}\mu(t)\}\right.\\ &\left. - \frac{\delta\alpha}{\delta E(t')}\mathrm{tr}\{\mathcal{X}^\dagger AA^\dagger \mu(t)\}\right)\\ &- \frac{1}{2\hbar^2}(\alpha^*\,\mathrm{tr}\{AA^\dagger\mathcal{X}\mu(t')\mu(t)\}\\ &+ \alpha\,\mathrm{tr}\{\mathcal{X}^\dagger AA^\dagger \mu(t)\mu(t')\}) - \frac{1}{2\hbar^2}\mathrm{tr}\{(\alpha^* AA^\dagger\mathcal{X}\\ &- \alpha\mathcal{X}^\dagger AA^\dagger)[\mu(t),\mu(t')]\},\end{aligned} \tag{A6}$$

where

$$\frac{\delta\alpha}{\delta E(t)} = \frac{1}{\mathcal{J}_P[E]}\frac{\imath\alpha}{2\hbar}(\alpha^*\,\mathrm{tr}\{AA^\dagger\mathcal{X}\mu(t)\} + \alpha\,\mathrm{tr}\{\mathcal{X}^\dagger AA^\dagger\mu(t)\}). \tag{A7}$$

At the critical points where $\delta\mathcal{J}_P[E]/\delta E(t)=0$, it can be shown that the equality (the critical point condition)

$$AA^\dagger\tilde{\mathcal{X}} = \tilde{\mathcal{X}}^\dagger AA^\dagger \tag{A8}$$

holds for a fully controllable N-level quantum system, as shown in Secs. II and IV. In Eq. (A8), we have introduced the notation

$$\tilde{\mathcal{X}} = \alpha^*\mathcal{X} = \alpha^*\mathcal{W}^\dagger\mathcal{U}. \tag{A9}$$

Multiplying Eq. (A8) with $\tilde{\mathcal{X}}$ on the left-hand side and $\tilde{\mathcal{X}}^\dagger$ on the right-hand side produces the relation

$$\tilde{\mathcal{X}}AA^\dagger\tilde{\mathcal{X}} = AA^\dagger = \tilde{\mathcal{X}}^\dagger AA^\dagger\tilde{\mathcal{X}}^\dagger. \tag{A10}$$

It can then be shown [55] that Eq. (A10) leads to

$$\tilde{\mathcal{X}}^\dagger = \tilde{\mathcal{X}} \tag{A11}$$

for $\tilde{\mathcal{X}}$ and the commutation relation

$$[AA^\dagger, \tilde{\mathcal{X}}] = 0 \tag{A12}$$

between $AA^\dagger$ and $\tilde{\mathcal{X}}$. Note that $\tilde{\mathcal{X}}^\dagger\tilde{\mathcal{X}}=\mathcal{X}^\dagger\mathcal{X}=\mathbf{I}$, i.e., $\tilde{\mathcal{X}}$ is also unitary, recalling that $\mathcal{X}\equiv\mathcal{W}^\dagger\mathcal{U}$ and $\mathcal{X}^\dagger\mathcal{X}=\mathbf{I}$. Thus, $\tilde{\mathcal{X}}$ satisfies the quadratic matrix equation

$$\tilde{\mathcal{X}}^2 = \tilde{\mathcal{X}}^\dagger\tilde{\mathcal{X}} = \mathbf{I}, \tag{A13}$$

whose solutions are the square roots of the identity $\mathbf{I}$.

Due to the commutation relation Eq. (A12), the matrices $AA^\dagger$ and $\tilde{\mathcal{X}}$ can be simultaneously diagonalized by the same unitary matrix D, $D^\dagger D=\mathbf{I}$, such that

$$D^\dagger(AA^\dagger)D = \Omega^2 \tag{A14}$$

and

$$D^\dagger\tilde{\mathcal{X}}D = \Lambda, \tag{A15}$$

where Ω^2 and Λ are both diagonal square matrices whose diagonal matrix elements are, respectively, given by

$$\omega_i^2 = \Omega_{ii}^2 > 0 \tag{A16}$$

and

$$\lambda_i \equiv \Lambda_{ii} = (-1)^{n_i} \quad (n_i \text{ even or odd integers}). \tag{A17}$$

From Eqs. (A14)–(A17), we can show that at the critical points

$$\mathcal{J}_P[E] = \mathrm{tr}\{AA^\dagger\tilde{\mathcal{X}}\} = \sum_i (-1)^{n_i}\omega_i^2, \tag{A18}$$

$$|\mathrm{tr}\{AA^\dagger\mathcal{X}\}| = |\mathrm{tr}\{AA^\dagger\tilde{\mathcal{X}}\}| = \left|\sum_i (-1)^{n_i}\omega_i^2\right|, \tag{A19}$$

and

$$\alpha^*\alpha = \frac{\mathrm{tr}\{AA^\dagger\tilde{\mathcal{X}}\}}{|\mathrm{tr}\{AA^\dagger\tilde{\mathcal{X}}\}|} = \frac{\sum_i (-1)^{n_i}\omega_i^2}{|\sum_i (-1)^{n_i}\omega_i^2|} = 1, \tag{A20}$$

leading to the condition

$$\mathcal{J}_P^c = \sum_i (-1)^{n_i}\omega_i^2 = \left|\sum_i (-1)^{n_i}\omega_i^2\right| > 0 \tag{A21}$$

that the integers $\{n_i\}$ must fulfill in characterizing the eigenvalues $\{\lambda_i\}$ of $\tilde{\mathcal{X}}$, as given in Eq. (A17). As a result, at the critical points, the cost functional $\mathcal{J}_P[E]$ can be easily computed using the simple expression

$$\mathcal{J}_P[E] = \mathcal{J}_P^c = \left|\sum_{i=1}^N (-1)^{n_i}\omega_i^2\right| > 0, \quad N \geqslant 2, \tag{A22}$$

independent of the global phase parameter α, but subject to the condition, Eq. (A21). From Eqs. (A21) and (A22), it is found that $\mathcal{J}_P[E]$ is a maximum, with magnitude $\sum_{i=1}^N\omega_i^2$, when $\{n_i\}$ are all even integers. In the case that $AA^\dagger$ is completely nondegenerate, i.e., $\omega_1^2 \neq \omega_2^2 \neq \ldots \neq \omega_N^2$, the number of allowed values of $\mathcal{J}_P[E]$ at the critical points is at most 2^{N-1}, as opposed to 2^N for the Frobenius cost functional

$\mathcal{J}_F[E]$, cf. Eq. (47). Moreover, in the special case of $AA^\dagger = \mathbf{I}$, since $\omega_1^2 = \omega_2^2 = \ldots = \omega_N^2 = 1$, the number of odd integers among all n_i's must be less than that of even ones due to the constraint Eq. (A21). Thus, when $AA^\dagger = \mathbf{I}$, the allowed (positive) values of $\mathcal{J}_P[E]$ at the critical points are $N-2k$ with $k = 0, 1, \ldots, [N/2]$ being the allowed numbers of odd integers among all n_i's, where $[N/2] = (N-2)/2$ when N is an even number and $[N/2] = (N-1)/2$ when N is an odd number, cf. Eq. (48).

Using Eq. (A8) in Eq. (A6), the Hessian $\mathcal{H}(t,t') \equiv \delta^2 \mathcal{J}_P[E]/\delta E(t')\delta E(t)$ at a critical point can be succinctly written as

$$\mathcal{H}(t,t') = -\frac{1}{\hbar^2 \mathcal{J}_P^c}(\mathcal{J}_P^c \mathrm{tr}\{\tilde{\mathcal{Y}}\mu(t')\mu(t)\} - \mathrm{tr}\{\tilde{\mathcal{Y}}\mu(t')\}\mathrm{tr}\{\tilde{\mathcal{Y}}\mu(t)\}), \tag{A23}$$

where the matrix $\tilde{\mathcal{Y}}$ is given by

$$\tilde{\mathcal{Y}} = \alpha^* AA^\dagger \mathcal{W}^\dagger \mathcal{U} = AA^\dagger \tilde{\mathcal{X}} = \tilde{\mathcal{X}} AA^\dagger. \tag{A24}$$

The Hermitian matrix $\tilde{\mathcal{Y}}$ can be diagonalized as follows:

$$\tilde{\Lambda} = D^\dagger \tilde{\mathcal{Y}} D = D^\dagger AA^\dagger DD^\dagger \tilde{\mathcal{X}} D = \Omega^2 \Lambda, \tag{A25}$$

with diagonal matrix $\tilde{\Lambda}$ composed of elements

$$\tilde{\lambda}_i = \tilde{\Lambda}_{ii} = (-1)^{n_i}\omega_i^2. \tag{A26}$$

From Eqs. (A23)–(A25), the Hessian $\mathcal{H}(t,t')$ can be further expressed as

$$\mathcal{H}(t,t') = -\frac{1}{\hbar^2}\sum_i (-1)^{n_i}\omega_i^2\left(\sum_j \langle i|\bar{\mu}(t')|j\rangle\langle j|\bar{\mu}(t)|i\rangle\right) + \frac{1}{\hbar^2 \mathcal{J}_P^c}\left(\sum_i (-1)^{n_i}\omega_i^2 \langle i|\bar{\mu}(t')|i\rangle\right) \times \left(\sum_i (-1)^{n_i}\omega_i^2\langle i|\bar{\mu}(t)|i\rangle\right), \tag{A27}$$

where $\bar{\mu}(t) = D^\dagger \mu(t) D$. Equation (A27) can be rearranged to yield

$$\mathcal{H}(t,t') = -\frac{1}{\hbar^2 \mathcal{J}_P^c}\sum_i \Bigg\{ (\mathcal{J}_P^c - (-1)^{n_i}\omega_i^2)(-1)^{n_i}\omega_i^2 \langle i|\bar{\mu}(t')|i\rangle \times \langle i|\bar{\mu}(t)|i\rangle - \sum_{j\neq i}(-1)^{n_i+n_j}\omega_i^2\omega_j^2 \langle i|\bar{\mu}(t')|i\rangle\langle j|\bar{\mu}(t)|j\rangle \Bigg\} - \frac{1}{\hbar^2}\sum_i (-1)^{n_i}\omega_i^2 \sum_{j\neq i}\langle i|\bar{\mu}(t')|j\rangle\langle j|\bar{\mu}(t)|i\rangle. \tag{A28}$$

Equation (A28) can be written as an equivalent quadratic form

$$\langle v|\mathcal{H}|v\rangle = \mathbf{x}_\mu^{\mathrm{T}} \tilde{\Gamma} \mathbf{x}_\mu \tag{A29}$$

in terms of an N^2-dimensional column vector $\mathbf{x}_\mu = \int_0^T \boldsymbol{\mu}(t) v(t) dt$ containing as components the real and imaginary parts of the integrals over the products of the matrix elements of $\mu(t)$ and an arbitrary function $v(t)$, c.f., Eqs. (55)–(57) and Eqs. (64) and (65). By invoking Sylvester's law of inertia [52,58,59], it can be concluded that at the critical points both the Hessian $\mathcal{H}(t,t')$ and $\tilde{\Gamma}$ possess the same rank and signature in terms of the distribution of their respective positive, negative, and zero eigenvalues. The Hessian at the global maximum of the landscape $\mathcal{J}_P[E]$ is of rank N^2-1, in comparison with the rank, which is N^2, of the Hessian associated with the landscape $\mathcal{J}_F[E]$ in Eq. (12). This can be shown as follows.

The $N^2 \times N^2$ real symmetric matrix $\tilde{\Gamma}$ can be written in block-diagonal form

$$\tilde{\Gamma} = \tilde{\Gamma}' \oplus \tilde{\Gamma}'', \tag{A30}$$

where the $N \times N$ real symmetric matrix $\tilde{\Gamma}'$ is composed of the nonvanishing matrix elements

$$\tilde{\Gamma}'_{ii} = -\frac{1}{\hbar^2 \mathcal{J}_P^c}[\mathcal{J}_P^c - (-1)^{n_i}\omega_i^2](-1)^{n_i}\omega_i^2, \quad i = 1, \ldots, N, \tag{A31}$$

$$\tilde{\Gamma}'_{ij} = +\frac{1}{\hbar^2 \mathcal{J}_P^c}(-1)^{n_i+n_j}\omega_i^2\omega_j^2, \quad 1 \leq i \neq j \leq N \tag{A32}$$

and the $N(N-1)\times N(N-1)$ real symmetric matrix $\tilde{\Gamma}''$ is diagonal with the following $N(N-1)$ elements

$$\tilde{\Gamma}''_{J_{ij}J_{ij}} = -\frac{1}{\hbar^2}[(-1)^{n_i}\omega_i^2 + (-1)^{n_j}\omega_j^2], \quad 1 \leq i < j \leq N, \tag{A33}$$

$$\tilde{\Gamma}''_{K_{ij}K_{ij}} = -\frac{1}{\hbar^2}[(-1)^{n_i}\omega_i^2 + (-1)^{n_j}\omega_j^2], \quad 1 \leq i < j \leq N, \tag{A34}$$

with the indexes $J_{ij} = (i-1)N - i(i+1)/2 + j$ and $K_{ij} = N(N-1)/2 + J_{ij}$. It is important to reveal the eigenvalues, including their signs, of the Hessians at the critical points, equivalently those of the matrix $\tilde{\Gamma}$ given in Eq. (A30), in order to characterize the associated dynamical control landscape $\mathcal{J}_P[E]$. To this end, it is expected that all eigenvalues of the matrix $\tilde{\Gamma}$ in Eq. (A30) are less than or equal to zero at the global maximum of the landscape $\mathcal{J}_P[E]$.

For example, in the special case of $AA^\dagger = \mathbf{I}$, i.e., $\omega_1^2 = \omega_2^2 = \ldots = \omega_N^2 = 1$, the matrix $\tilde{\Gamma}$ at the global maximum, i.e., $\mathcal{J}_P[E] = N$, contains the following nonzero elements:

$$\tilde{\Gamma}_{ii} = -\frac{1}{N\hbar^2}(N-1), \quad i = 1, \ldots, N, \tag{A35}$$

$$\tilde{\Gamma}_{ij} = +\frac{1}{N\hbar^2}, \quad 1 \leq i \neq j \leq N, \tag{A36}$$

$$\tilde{\Gamma}_{ii} = -\frac{2}{\hbar^2}, \quad N+1 \leq i \leq N^2, \tag{A37}$$

from which the characteristic polynomial may be written as [62,63]

$$\det[\tilde{\gamma}\mathbf{I}-\tilde{\Gamma}]=\tilde{\gamma}\left(\tilde{\gamma}+\frac{1}{\hbar^2}\right)^{N-1}\left(\tilde{\gamma}+\frac{2}{\hbar^2}\right)^{N(N-1)}=0. \tag{A38}$$

Thus, we have

$$-\frac{1}{\hbar^2}\{0,\ \underbrace{1,\ldots,1}_{N-1\text{ terms}},\ \underbrace{2,2,\ldots,2}_{N(N-1)\text{ terms}}\}, \tag{A39}$$

as the eigenvalues of the matrix $\tilde{\Gamma}$, compared to its counterpart

$$\frac{2}{\hbar^2}\{\underbrace{\pm 1,\pm 1,\ldots,\pm 1}_{N\text{ terms}},\ \underbrace{\pm 2,\pm 2,\ldots,\pm 2}_{N(N-1)\text{ terms}}\}, \tag{A40}$$

for the matrix Γ, cf., Eqs. (76) and (77), corresponding to the global minimum and maximum of the landscape $\mathcal{J}_F[E]$. It is interesting to see that regardless of the number N of quantum levels, the corresponding Hessian possesses an extra zero eigenvalue (on the top of infinitely many zero eigenvalues that already exist due to the infinite dimensionality of the control field function space), $N-1$ negative eigenvalues $-\frac{1}{\hbar^2}$ and $N(N-1)$ negative eigenvalues $-\frac{2}{\hbar^2}$ for the matrix $\tilde{\Gamma}$ at the global maximum. The Hessian rank of $\mathcal{J}_P[E]$ being smaller than that of $\mathcal{J}_F[E]$ by one is consistent with the fact that the $\mathcal{J}_P[E]$ landscape is independent of the global phase of the designated unitary transformation $\mathcal{W}$. In the remaining section we present an analysis of the eigenvalues of the matrix $\tilde{\Gamma}$ of Eq. (A30), therefore of the Hessian of $\mathcal{J}_P[E]$. In particular it will be shown that for $1\leqslant n\leqslant N$, $\tilde{\Gamma}$ always possesses at least one positive and at least on negative eigenvalue. From this result, it may be concluded that the landscape $\mathcal{J}_P[E]$ has no false traps.

Many of the eigenvalues of the matrix $\tilde{\Gamma}$ Eq. (A30) can be directly read off from the diagonal matrix $\tilde{\Gamma}''$, which is an $N(N-1)\times N(N-1)$ diagonal matrix, characterized by $N(N-1)/2$ duplicate entries (eigenvalues), cf. Eqs. (A33) and (A34). It is seen that all eigenvalues (i.e., the elements) of the diagonal matrix $\tilde{\Gamma}''$ are negative at the global maximum where all n_i's are even integers. Moreover, the eigenvalues of $\tilde{\Gamma}''$ are always mixtures of both positive and negative values as long as the number k of odd integers among n_i's is greater than one. In general, the number of positive eigenvalues (implying no false local traps) that the matrix $\tilde{\Gamma}''$ may possess increases with the number k. The matrix Γ'' possesses at least $k(k-1)/2$ duplicate positive eigenvalues, or equivalently at most $(N-k)(N+k-1)/2$ duplicate negative eigenvalues, when $k\geqslant 2$. In the special case that the index n_N (corresponding to the smallest singular value ω_N^2 of the matrix $A^{\dagger}A$) is the only odd integer (i.e., all other $n_1,n_2,\ldots,n_{N-1}$ are even integers), the matrix $\tilde{\Gamma}''$ possesses only negative eigenvalues [as well as $2(m-1)$ zeros when the smallest eigenvalue of $AA^{\dagger}$ is m-fold degenerate, i.e., $\omega_1^2>\ldots>\omega_{N-m}^2=\ldots=\omega_N^2>0$]. However, it can be shown in the following that in this special $k=1$ case the corresponding matrix $\tilde{\Gamma}'$ possesses at least one positive eigenvalue.

The eigenvalue problem involving the $N\times N$ real symmetric submatrix $\tilde{\Gamma}'$ [c.f. Eqs. (A31) and (A32)], is in general difficult to solve since it is a full matrix, except at the global maximum for the special case of $AA^{\dagger}=\mathbf{I}$ in which all $n_1,\ldots,n_N$ are even integers, see Eqs. (A35)–(A39). Nevertheless, because of the special structure of the matrix $\tilde{\Gamma}'$, it can be shown that, in general, the determinant of the matrix $\tilde{\gamma}'\mathbf{I}-\tilde{\Gamma}'$ can be written in closed form [62]

$$\det[\tilde{\gamma}'\mathbf{I}-\tilde{\Gamma}']=\left(1-\frac{1}{\hbar^2\mathcal{J}_P^c}\sum_{i=1}^{N}\frac{\omega_i^4}{\tilde{\gamma}'+(-1)^{n_i}\omega_i^2/\hbar^2}\right)\times\prod_{i=1}^{N}\left(\tilde{\gamma}'+\frac{1}{\hbar^2}(-1)^{n_i}\omega_i^2\right). \tag{A41}$$

It can then be shown that the characteristic polynomial of the matrix $\tilde{\Gamma}'$ is [cf. Eq. (A41)]

$$\det\left[\tilde{\gamma}'\mathbf{I}-\tilde{\Gamma}'\right]=\tilde{\gamma}'\times\underbrace{\left(\tilde{\gamma}'-\tilde{\gamma}_2'\right)\times\ldots\times\left(\tilde{\gamma}'-\tilde{\gamma}_N'\right)}_{N-1\text{ terms}}=0, \tag{A42}$$

where $\tilde{\gamma}_2'\times\cdots\times\tilde{\gamma}_N'\neq 0$. As a result, the matrix $\tilde{\Gamma}'$ possesses exactly one zero eigenvalue, say $\tilde{\gamma}_1'=0$, at all critical points, a manifestation of the global phase of the unitary matrix $\mathcal{W}$ being unspecified in the cost functional $\mathcal{J}_P[E]$. From Eqs. (A41) and (A42), we can readily derive the equality

$$c_N=\underbrace{\tilde{\gamma}_2'\ldots\tilde{\gamma}_N'}_{N-1\text{ terms}}=N\left(\frac{-1}{\hbar^2}\right)^{N-1}\prod_{i=1}^{N}(-1)^{n_i}\omega_i^2\Big/\sum_{i=1}^{N}(-1)^{n_i}\omega_i^2\neq 0, \tag{A43}$$

which is a product of $N-1$ eigenvalues $\tilde{\gamma}_2'\ldots\tilde{\gamma}_N'$ and holds for arbitrary $N\geqslant 2$. It is seen from examining the right-hand side of Eq. (A43), and invoking Eqs. (A21) and (A22), that (i) $c_N<0$ if N and k are both even integers or are both odd integers and (ii) $c_N>0$ if N is an even integer and k is an odd one or vice versa, since the denominator $\sum_{i=1}^{N}(-1)^{n_i}\omega_i^2$ is always positive, cf. Eq. (A21). As a result, in the case of $k=1$ (i.e., only one odd integer among all n_i's), the corresponding $N-1$ nonzero eigenvalues $\tilde{\gamma}_2',\ldots,\tilde{\gamma}_N'$ of $\tilde{\Gamma}'$ cannot all be negative, i.e., the matrix $\tilde{\Gamma}'$ always possesses at least one positive eigenvalue regardless of whether N is an even or odd number. In the case of $k\geqslant 2$ (i.e., two or more negative integers among all n_i's), the matrix $\tilde{\Gamma}''$, Eqs. (A33) and (A34), is endowed with at least one duplicate positive eigenvalue. As a result, the matrix $\tilde{\Gamma}=\tilde{\Gamma}'\oplus\tilde{\Gamma}''$ possesses at least one duplicate positive eigenvalue. It can therefore be concluded that the landscape $\mathcal{J}_P[E]$, similar to that of $\mathcal{J}_F[E]$, also contains no local false traps (i.e., all saddles) regardless of the number N of levels.

APPENDIX B: ROBUSTNESS FOR CONTROL OF A *p*-QUBIT QUANTUM LOGIC GATE

In this appendix, we specifically consider the phase-independent unitary transformation fidelity defined as [16,61]

$$\mathcal{F} = \frac{1}{N}|\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\}|, \tag{B1}$$

for an ensemble of p qubits, where $N=2^p$. Given a perfect (noiseless) control field $E(t)$ maximizing $\mathcal{F}$, $t\in[0,T]$, for a target quantum logic gate $\mathcal{W}$, the matrix $\mathcal{U}=U(T,0)$ is the unitary transformation $\mathcal{W}$ at the time T, within a global phase. Note that $\mathcal{F}=\mathcal{J}_P[E]/N$ with $AA^{\dagger}=\mathbf{I}$ in Eq. (A2) in Appendix A. In quantum information science applications, it is important to know the error $\delta\mathcal{F}$ in the cost functional $\mathcal{F}$ due to the control field noise $\delta E(t)$, particularly at the global maximum of the landscape $\mathcal{F}$, namely,

$$\begin{aligned}\delta\mathcal{F} &= \mathcal{F}[E(t)+\delta E(t)] - \mathcal{F}[E(t)]\\ &\approx \frac{1}{2}\int_0^T\int_0^T \mathcal{H}_{\mathcal{F}}(t,t')\delta E(t)\delta E(t')dtdt',\end{aligned} \tag{B2}$$

where, from Appendix A, the corresponding Hessian can be written as

$$\begin{aligned}\mathcal{H}_{\mathcal{F}}(t,t') = \frac{\delta^2\mathcal{F}}{\delta E(t')\delta E(t)} &= \frac{1}{\hbar^2}\frac{1}{N^2}[\mathrm{tr}\{\alpha^*\mathcal{W}^{\dagger}\mathcal{U}\mu(t')\}]\\ &\times[\mathrm{tr}\{\alpha^*\mathcal{W}^{\dagger}\mathcal{U}\mu(t)\}] - \frac{1}{\hbar^2}\frac{1}{N}\mathrm{tr}\{\alpha^*\mathcal{W}^{\dagger}\mathcal{U}\mu(t')\mu(t)\}\end{aligned} \tag{B3}$$

with the phase parameter $\alpha=\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\}/|\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\}|$. The Hessian at the global maximum of $\mathcal{F}$ is bounded by the relation

$$\begin{aligned}|\mathcal{H}_{\mathcal{F}}(t,t')| &\leqslant \frac{1}{\hbar^2}\frac{1}{N^2}|(\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\mu(t')\})(\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\mu(t)\})|\\ &\quad+\frac{1}{\hbar^2}\frac{1}{N}|\mathrm{tr}\{\mathcal{W}^{\dagger}\mathcal{U}\mu(t')\mu(t)\}|\\ &\leqslant \frac{1}{\hbar^2}\frac{1}{N^2}N\|\mu\|_F^2 + \frac{1}{\hbar^2}\frac{1}{N}N^{1/2}\|\mu\|_F^2\\ &= \frac{1}{\hbar^2}\frac{1}{N}(1+N^{1/2})\|\mu\|_F^2,\end{aligned} \tag{B4}$$

thus resulting in an error bound (up to second order) for the underlying fidelity

$$\begin{aligned}|\delta\mathcal{F}| &\leqslant \frac{1}{2}\int_0^T\int_0^T|\mathcal{H}_{\mathcal{F}}(t,t')\delta E(t)\delta E(t')|dtdt' \leqslant \frac{1}{2}\frac{1}{\hbar^2}\frac{1}{N}(1\\ &\quad+N^{1/2})\|\mu\|_F^2\left(\int_0^T|\delta E(t)|dt\right)^2 = \frac{1}{\hbar^2}\frac{1}{2^{p+1}}(1+2^{p/2})\|\mu\|_F^2\\ &\quad\times\|\delta E\|_1^2.\end{aligned} \tag{B5}$$

Here we have remarked that the norm $\|\mathcal{W}^{\dagger}\mathcal{U}\|=N^{1/2}=2^{p/2}$ for a p-qubit system.

The Hamiltonian of a p-qubit system in the presence of a control field $E(t)$ may be modeled as [27]

$$\begin{aligned}H(t) = \frac{1}{2}\Bigg\{&\sum_{i=1}^{p}\epsilon_i\boldsymbol{\sigma}_{iz} - \sum_{i=1}^{p-1}\sum_{j>i}^{p}\gamma_{ij}(\boldsymbol{\sigma}_{ix}\otimes\boldsymbol{\sigma}_{jx} + \boldsymbol{\sigma}_{iy}\otimes\boldsymbol{\sigma}_{jy}\\ &+\boldsymbol{\sigma}_{iz}\otimes\boldsymbol{\sigma}_{jz})\Bigg\} - \frac{1}{2}\sum_{i=1}^{p}\mu_i E(t)\boldsymbol{\sigma}_{ix},\end{aligned} \tag{B6}$$

where ϵ_i and μ_i are, respectively, the energy spacing and internal coupling constant of the ith qubit, and $\gamma_{ij}(\geqslant 0)$ is the coupling constant between the ith and jth qubits. The 2×2 matrices $\boldsymbol{\sigma}_{ix}$, $\boldsymbol{\sigma}_{iy}$, $\boldsymbol{\sigma}_{iz}$ are, respectively, defined as the tensor products

$$\boldsymbol{\sigma}_{ix} \equiv \underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{i-1\text{ terms}}\otimes\boldsymbol{\sigma}_x\otimes\underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{p-i\text{ terms}}, \tag{B7}$$

$$\boldsymbol{\sigma}_{iy} \equiv \underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{i-1\text{ terms}}\otimes\boldsymbol{\sigma}_y\otimes\underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{p-i\text{ terms}}, \tag{B8}$$

$$\boldsymbol{\sigma}_{iz} \equiv \underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{i-1\text{ terms}}\otimes\boldsymbol{\sigma}_z\otimes\underbrace{\mathbf{I}_2\otimes\ldots\otimes\mathbf{I}_2}_{p-i\text{ terms}}, \tag{B9}$$

in terms of the 2×2 identity matrix $\mathbf{I}_2$ and the 2×2 Pauli matrices $\boldsymbol{\sigma}_x$, $\boldsymbol{\sigma}_y$, $\boldsymbol{\sigma}_z$, with the subscript i designating the ith qubit. As a result, we have $\|\boldsymbol{\sigma}_{ix}\|_F=\|\boldsymbol{\sigma}_{iy}\|_F=\|\boldsymbol{\sigma}_{iz}\|_F=2^{p/2}$, independent of the index i, since $\|\mathbf{I}_2\|_F=\|\boldsymbol{\sigma}_x\|_F=\|\boldsymbol{\sigma}_y\|_F=\|\boldsymbol{\sigma}_z\|_F=2^{1/2}$ and $\|\boldsymbol{\sigma}_{ix,y,z}\|_F=\|\mathbf{I}_2\|_F^{i-1}\times\|\boldsymbol{\sigma}_{x,y,z}\|_F\times\|\mathbf{I}_2\|_F^{p-i}$. It can be easily shown that for p qubits the corresponding Frobenius norm $\|\mu\|_F$ of the operator μ may be estimated as

$$\begin{aligned}\|\mu\|_F = \left\|\frac{1}{2}\sum_{i=1}^{p}\mu_i\boldsymbol{\sigma}_{ix}\right\|_F &\leqslant \frac{1}{2}\sum_{i=1}^{p}|\mu_i|\times\|\boldsymbol{\sigma}_{ix}\|_F\\ &= \frac{1}{2}2^{p/2}\sum_{i=1}^{p}|\mu_i| \approx \frac{p}{2}2^{p/2}\mu_0,\end{aligned} \tag{B10}$$

assuming that $|\mu_i|\approx\mu_0$ for all i. Substituting Eq. (B10) in Eq. (B5) yields an approximated error bound for the fidelity the p-qubit system

$$|\delta\mathcal{F}| \leqslant \frac{1}{\hbar^2}\frac{p^2}{2^3}(1+2^{p/2})\mu_0^2\|\delta E\|_1^2 \overset{p\gg 1}{\rightarrow} \frac{1}{\hbar^2}\frac{p^2}{2^3}2^{p/2}\mu_0^2\|\delta E\|_1^2. \tag{B11}$$

The estimated error bound for the unitary transformation fidelity of a coupled p-qubit system scales as $p^2 2^{p/2}$ in terms of the number p of the qubits and quadratically with the one norm $\|\delta E\|_1$ of the noise in the control field, implying that when p is large the unitary transformation involving fully coupled p qubits may not be robust in the presence of control field noise. These findings are generally in agreement with the conclusion obtained from the analysis using the action matrix [61].

In summary, a detailed analysis has been performed in the Appendixes A and B for the maximization of the cost functional $\mathcal{J}_P[E]=|\mathrm{tr}\{AA^{\dagger}\mathcal{W}^{\dagger}U(T,0)\}|$. It is found that the landscapes of $\mathcal{J}_P[E]$ and $\mathcal{J}_F[E]$ are essentially the same, with the difference being attributed to the additional, indefinite global phase, producing an extra null-space dimension at the global maximum of $\mathcal{J}_P[E]$. The issue of robustness for controlling quantum logic gates of a generic p-qubit quantum system was also addressed.

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$\langle i|\mu(t)|j\rangle=\Sigma_{k=1}^{N}\Sigma_{\ell=1}^{N}\langle i|U_I^\dagger(t)|k\rangle\langle k|\mu|\ell\rangle\langle \ell|U_I(t)|j\rangle\exp(\imath\omega_{k\ell}t)$, where $1\leqslant i,\ j\leqslant N$, $U_I(t,0)$ is the evolution operator in the interaction picture $U_I(t,0)=\exp(\imath H_0 t/\hbar)U(t,0)$ and $\omega_{k\ell}$ is the transition frequency from the level ℓ to the level k. The above expansion is in general an arbitrary superposition of N^2 linearly independent functions of time t, with the possible exception of the constant field case in which at most N^2-N+1 linearly independent functions exist in the expansion.

[51] In terms of a singular value decomposition [58], given any nonsingular $N\times N$ landscape adaptation matrix A there always exist $N\times N$ unitary matrices D and $\tilde{D}$ such that $D^\dagger A\tilde{D}=\mathrm{diag}(\omega_1,\omega_2,\ldots,\omega_N)$ where $\omega_1\geqslant\omega_2\geqslant\ldots\geqslant\omega_N(>0)$. As a result, we have $AA^\dagger=(D\Omega\tilde{D}^\dagger)(\tilde{D}\Omega D^\dagger)=D\Omega^2D^\dagger$, c.f., Eq. (14).

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[55] Consider the equality $\mathcal{X}AA^\dagger\mathcal{X}=AA^\dagger=\mathcal{X}^\dagger AA^\dagger\mathcal{X}^\dagger$, where $\mathcal{X}$ is an $N\times N$ unitary matrix, $\mathcal{X}^\dagger\mathcal{X}=\mathbf{I}$, and A is a nonsingular $N\times N$ matrix, $AA^\dagger=(AA^\dagger)^\dagger$. Let $C=D^\dagger\mathcal{X}D$ and $D^\dagger AA^\dagger D=\Omega^2$, where D is a unitary matrix and $\Omega^2=\mathrm{diag}(\omega_1^2>0,\ldots,\omega_N^2>0)$. Then $C^\dagger=(D^\dagger\mathcal{X}D)^\dagger=D^\dagger\mathcal{X}^\dagger D$, $C^\dagger C=\mathbf{I}$. Moreover, $\Omega^2=D^\dagger\mathcal{X}AA^\dagger\mathcal{X}D=D^\dagger\mathcal{X}D\Omega^2D^\dagger\mathcal{X}D=C\Omega^2C$ and $\Omega^2=C^\dagger\Omega^2C^\dagger$. Thus $C\Omega^2=\Omega^2C^\dagger$ and $\Omega^4C=C\Omega^4$, indicating that $C_{ij}\omega_j^2=\omega_i^2C_{ji}^*$ and $(\omega_i^4-\omega_j^4)C_{ij}=0\ \forall i,j=1,\ldots,N$. So, $C_{ij}=C_{ji}^*$ if $\omega_i^2=\omega_j^2$ and $C_{ij}=0$ if $\omega_i^2\neq\omega_j^2$, i.e., the matrix C must be unitary, Hermitian, and block diagonal regardless of the degeneracy of Ω^2. As a result, $\mathcal{X}^\dagger=DC^\dagger D^\dagger=DCD^\dagger=\mathcal{X}$, $\mathcal{X}^2=\mathcal{X}^\dagger\mathcal{X}=\mathbf{I}$, and $AA^\dagger\mathcal{X}=(\mathcal{X}AA^\dagger\mathcal{X})\mathcal{X}=\mathcal{X}AA^\dagger$.

[56] A general solution of Eq. (60) may be written as $E(t)=E_0(t)-\boldsymbol{\mu}^{\mathrm{T}}(t)(G\Gamma G)^{-1}\mathbf{y}+q(t)$, where $G=\int_0^T\boldsymbol{\mu}(t)\boldsymbol{\mu}^{\mathrm{T}}(t)dt$, $\mathbf{y}=\int_0^T\boldsymbol{\mu}(t)\{\,\delta\mathcal{J}_F[E]/\,\delta E(t)|_{E_0}\}dt$, and $q(t)$ is an arbitrary funtion of t that is orthogonal to $\boldsymbol{\mu}(t)$.

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