Environment-invariant measure of distance between evolutions of an open quantum system

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Abstract. The problem of quantifying the difference between evolutions of an open quantum system (in particular, between the actual evolution of an open system and the ideal target operation on the corresponding closed system) is important in quantum control, especially in control of quantum information processing. Motivated by this problem, we develop a measure for evaluating the distance between unitary evolution operators of a composite quantum system that consists of a sub-system of interest (e.g. a quantum information processor) and environment. The main characteristic of this measure is the invariance with respect to the effect of the evolution operator on the environment, which follows from an equivalence relation that exists between unitary operators acting on the composite system, when the effect on only the sub-system of interest is considered. The invariance to the environment’s transformation makes it possible to quantitatively compare the evolution of an open quantum system and its closed counterpart. The distance measure also determines the fidelity bounds of a general quantum channel (a completely positive and trace-preserving map acting on the sub-system of interest) with respect to a unitary target transformation. This measure is also independent of the initial state of the system and straightforward to numerically calculate. As an example, the measure is used in numerical

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simulations to evaluate fidelities of optimally controlled quantum gate operations (for one- and two-qubit systems), in the presence of a decohering environment. This example illustrates the utility of this measure for optimal control of quantum operations in the realistic case of open-system dynamics.

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1. Introduction

Control and optimization of open quantum systems are a rapidly growing area of theoretical [1]–[15] and experimental [16]–[23] research. This research is connected, to a considerable degree, to a large body of work that has been recently devoted to integrating concepts and methods of optimal quantum control [24]–[27] into the fields of quantum information and quantum computation (QC) [28]. In particular, optimal control theory was used to design external control fields for generating quantum-gate operations in the presence of an environment [29]–[36]. In this context, an important problem is to evaluate the distance between different quantum operations, especially between actual and ideal processes [28], [37]–[43]. One obstacle in the comparison of such processes is the reliance of many existing distance and
fidelity measures on the initial state of the system or, to a lesser extent, on an integration or optimization over all possible states. Another difficulty arises when we consider the evolution of the quantum system of interest, in this case, a quantum information processor (QIP) that is coupled to a (finite-dimensional) environment. The main obstacle is that the unitary time-evolution operator for the composite system (consisting of the QIP and environment) and the target unitary operator for the QIP have different dimensions.

In this work, we develop a measure (originally proposed in [44]) that quantifies the distance between evolutions of a composite (bipartite) quantum system in such a way that only the effect of the evolution operator on one component (the sub-system of interest) is relevant in the measure, while the effect on the other component (the environment) can be arbitrary. Due to the invariance to the transformation on the environment, it is possible to evaluate the difference between unitary evolutions of the composite system (including the environment) and the sub-system of interest alone (excluding the environment), i.e. between unitary quantum operations of different dimensions. Therefore, the proposed measure enables us to compare unitary quantum operations (or, more generally, quantum channels [28]) corresponding to dynamics of ideal (i.e. closed) and real (i.e. open) systems. When the sub-system of interest is not coupled to an environment, the proposed distance measure reduces to a form that was previously used to evaluate the fidelity of closed-system unitary operations (see, e.g. [45]–[47]). Another important advantage of this distance measure is that it is independent of the initial state of the system. This property is important, since the fundamental objective of QC is to generate a specified target transformation for any initial state.

The development of an appropriate objective functional is a crucial issue for control and optimization (for both classical and quantum systems) [48]. Since maxima or minima of the objective functional determine control optimality, the selection of the objective is just as important as that of the physical model and optimization algorithm. Therefore, constructing an objective functional that represents control goals in the best possible way is one of the first tasks in any application of optimal control. In addition, the emerging studies of quantum control landscapes [49], for state-preparation control [50, 51], observable control [52]–[54], and unitary-transformation control [55]–[57], emphasize the profound effects that the choice of the objective functional has on the optimization (the control landscape is defined by the objective as a function of control variables, $J = J(C)$). In particular, the relationship between the control landscape structure and optimization search efforts was recently analyzed [58, 59]. The measure we present here is well suited for directly evaluating distances between general operations resulting from control of open quantum systems. The utility of this distance measure for optimal control of quantum gates in the presence of an environment is illustrated with a detailed numerical example.

This paper is organized as follows. Section 2 presents an equivalence relation between unitary evolution operators acting on a composite (bipartite) quantum system. This relation is based on the effect of these operators on the sub-system of interest, while the effect on the other sub-system (representing the environment) is not taken into account and thus can be arbitrary. The equivalence relation produces a quotient space that is a homogeneous manifold of the original space of unitary operators. In section 3, a quotient metric is defined on this space, resulting in a generalized expression of the distance measure. This measure can be used to quantitatively compare unitary evolutions of the entire composite system and one of its components (the sub-system of interest), e.g. unitary operations of different dimensions. Particular forms of the general distance measure can be obtained using different matrix norms.
In section 4, the distance measure is computed explicitly using the Hilbert–Schmidt norm, producing an analytical expression that is calculated directly from the unitary operator of the composite system. In addition, several properties of this specific measure are discussed. Section 5 develops the distance measure using the induced two-norm (i.e. the maximum singular value). In section 6, we relate the distance measure developed in section 4 to a few typical fidelity measures defined for a general quantum channel (acting on the sub-system of interest) with respect to a target unitary transformation. It is shown that the distance measure and an average channel fidelity both depend on the trace norm of the same matrix (as the matrix norm increases, distance decreases and fidelity increases), and that the distance measure sets the lower and upper bounds of this fidelity. Section 7 illustrates, using a numerical example, how the distance measure developed here can be directly incorporated into the optimal control of quantum operations in the presence of a decohering environment. In this application, the actual unitary evolution operator for the composite system (consisting of a QIP and its environment) is compared to the target unitary operator for the QIP alone, which is of a smaller dimension. This example demonstrates the utility of the distance measure in optimal control of unitary quantum gates for QC. Lastly, section 8 concludes the paper with a summary of the results and a brief discussion of future directions. For the continuity of the presentation, some mathematical details and most proofs are relegated to appendices.

2. Equivalence classes of unitary evolution operators

Consider a finite-dimensional, closed, bipartite quantum system with a Hamiltonian (possibly time-dependent) of the form

\[ H := H_s + H_e + H_{\text{int}}, \]  

where \( H_s \) and \( H_e \) represent the Hamiltonians for the system \( S \) (e.g. a QIP) and environment \( E \), respectively, and \( H_{\text{int}} \) represents the system–environment interaction. Let \( \mathcal{H}_s \) and \( \mathcal{H}_e \) denote the respective Hilbert spaces of the system and environment, where \( n_s := \dim(\mathcal{H}_s) \) and \( n_e := \dim(\mathcal{H}_e) \). Thus, the Hilbert space of the composite system \( \mathcal{C} \) is \( \mathcal{H}_c := \mathcal{H}_s \otimes \mathcal{H}_e \) and \( n := \dim(\mathcal{H}_c) = n_sn_e \). Let \( \{|i\rangle\}, \{|v\rangle\} \) and \( \{|i\rangle \otimes |v\rangle\} \) be orthonormal bases that span the Hilbert spaces \( \mathcal{H}_s, \mathcal{H}_e \) and \( \mathcal{H}_c \), respectively.

For a given Hilbert space \( \mathcal{H} \), the set of admissible states, represented as density matrices on \( \mathcal{H} \), is denoted by \( \mathcal{D}(\mathcal{H}) \). As such, a density matrix \( \rho \in \mathcal{D}(\mathcal{H}) \) is a positive operator of trace one, i.e. \( \rho \succeq 0 \) and \( \text{Tr}(\rho) = 1 \). Elements of \( \mathcal{D}(\mathcal{H}) \) correspond to either pure \( [\text{Tr}(\rho^2) = 1] \) or mixed \( [\text{Tr}(\rho^2) < 1] \) states. Density matrices for pure states can also be expressed as \( |\psi\rangle\langle\psi| \), where \( |\psi\rangle \) represents a normalized vector in \( \mathcal{H} \) (i.e. \( \langle\psi|\psi\rangle = 1 \)). The group of all unitary operators on \( \mathcal{H} \) is denoted by \( U(\mathcal{H}) \).

Let \( U(t) \in U(\mathcal{H}_c) \) denote the unitary time-evolution operator of the composite system \( \mathcal{C} \), whose evolution is governed by the Schrödinger equation \( (\hbar = 1) \):

\[ \frac{dU(t)}{dt} = -iH(t)U(t), \] 

with the initial condition \( U(t = 0) = 1_c \), the identity operator on \( \mathcal{H}_c \). Given an initial density matrix \( \rho(t = 0) \in \mathcal{D}(\mathcal{H}_c) \), this state evolves in time as

\[ \rho(t) = U(t)\rho(0)U^\dagger(t). \]
For any state \( \rho \in \mathcal{D}(\mathcal{H}_c) \), the state of the system \( \mathcal{S} \), with which system observables are calculated, is described by the reduced density matrix \( \rho_s := \text{Tr}_c(\rho) \), where \( \text{Tr}_c \) denotes the partial trace over \( \mathcal{H}_c \). Thus, from (3), \( \rho_s \) evolves as
\[
\rho_s(t) = \text{Tr}_c[U(t)\rho(0)U^\dagger(t)].
\] (4)

If two composite unitary operators \( U, V \in U(\mathcal{H}_c) \) are such that
\[
\text{Tr}_c(U\rho U^\dagger) = \text{Tr}_c(V\rho V^\dagger), \quad \forall \rho \in \mathcal{D}(\mathcal{H}_c),
\] (5)
then they will produce identical evolutions of the reduced density matrix \( \rho_s \). In this situation, \( U \) and \( V \) are said to be system- or \( S \)-equivalent, a relationship expressed as \( U \sim V \). The condition described by (5) defines an equivalence relation [60] (in addition to being symmetric and reflexive, \( S \)-equivalence is also transitive, i.e. if \( U_1 \sim U_2 \) and \( U_2 \sim U_3 \), then \( U_1 \sim U_3 \)). The necessary and sufficient condition for \( S \)-equivalence is stated in the following theorem.

**Theorem 1.** Let \( U, V \in U(\mathcal{H}_c) \). Then \( \text{Tr}_c(U\rho U^\dagger) = \text{Tr}_c(V\rho V^\dagger) \) for all density matrices \( \rho \in \mathcal{D}(\mathcal{H}_c) \) if and only if \( U = (\mathbb{1}_s \otimes \Phi)V \) for some \( \Phi \in U(\mathcal{H}_c) \).

**Proof.** See appendix A. \( \square \)

This theorem is related to a unitary invariance of Kraus maps [28, 61], which is described further in section 6.

For any \( U \in U(\mathcal{H}_c) \), let \([U] \) denote the equivalence class of \( U \), i.e. \([U] = \{(\mathbb{1}_s \otimes \Phi)U : \Phi \in U(\mathcal{H}_c)\} \). As a consequence of theorem 1, every equivalence class is isomorphic to the closed subgroup \( \mathbb{1}_s \otimes U(\mathcal{H}_c) = \{\mathbb{1}_s \otimes \Phi : \Phi \in U(\mathcal{H}_c)\} \), i.e. \([U] \) is just a right-translation of \( \mathbb{1}_s \otimes U(\mathcal{H}_c) \) by \( U \). Therefore, if only the evolution of \( S \) is relevant, then just the space of \( S \)-equivalence classes, i.e. the quotient space \( \mathcal{Q} := U(\mathcal{H}_c)/\mathbb{1}_s \otimes U(\mathcal{H}_c) \) needs to be considered, rather than the space of all unitary operators \( U(\mathcal{H}_c) \). While \( \mathcal{Q} \) is not a Lie group like \( U(\mathcal{H}_c) \), it is a smooth (right) homogeneous manifold of dimension \((n_s^2 - 1)n_s^2 \) [62]. Although not explored here, the fact that \( \mathcal{Q} \) has the additional structure of a homogeneous manifold may be useful for further analysis (e.g. explorations of the landscape topology [57]) of the distance measure.

### 3. Properties of metrics on the quotient space of equivalent operators

A metric space consists of a pair of objects: a set \( \Omega \) and a real-valued metric or distance measure \( \Delta \). The ordered pair \((\Omega, \Delta)\) is a metric space if the following conditions are satisfied for any \( x, y, z \in \Omega \) [60]:

(i) Non-negativity: \( \Delta(x, y) \geq 0 \).

(ii) Strict positivity: \( \Delta(x, y) = 0 \) if and only if \( x = y \).

(iii) Symmetry: \( \Delta(x, y) = \Delta(y, x) \).

(iv) Triangle inequality: \( \Delta(x, z) \leq \Delta(x, y) + \Delta(y, z) \).

In this work, \( \Omega \) is the quotient space \( \mathcal{Q} \) developed in section 2; elements of this space are the equivalence classes \([U]\). Let \( \Delta \) be any metric on \( U(\mathcal{H}_c) \), then the corresponding quotient metric \( \tilde{\Delta} \) on \( \mathcal{Q} \) is
\[
\tilde{\Delta}([U], [V]) := \min_{\Phi_1, \Phi_2} \Delta((\mathbb{1}_s \otimes \Phi_1)U, (\mathbb{1}_s \otimes \Phi_2)V).
\] (6)
This expression can be used to obtain the quotient metric for various choices of \( \Delta \), for example, when \( \Delta \) is the Hilbert–Schmidt norm distance, the induced two-norm distance, the geodesic distance with respect to some Riemannian metric, etc [63]–[65].

The quotient metric (6) does not involve the partial trace over the environment, which is implicit in other distance (and fidelity) measures that use the operator-sum representation [28], [38]–[43]. Moreover, the quotient metric is independent of any particular initial state, which is a very useful practical feature in applications to QC. In contrast to other measures of quantum gate fidelity, e.g. some of those in [28], [38]–[43], \( \tilde{\Delta}(\{U\}, \{V\}) \) is directly evaluated by propagating the evolution operator \( U(t) \) in (2), without making any assumptions about the initial state of the composite system \( C \). This property allows one to consistently quantify the distance between unitary quantum operations (e.g. the actual and the ideal operation) for any initial state.

If \( \Delta \) is a left-invariant metric on \( U(H_c) \) (i.e. \( \Delta(WU, WV) = \Delta(U, V) \) for any \( U, V, W \in U(H_c) \)), then (6) becomes

\[
\tilde{\Delta}(\{U\}, \{V\}) = \min_{\Phi} \Delta(U, (1_s \otimes \Phi)V).
\]

In the context of a norm distance, equation (7) can also be expressed as

\[
\tilde{\Delta}(\{U\}, \{V\}) = \lambda \min_{\Phi} \|U - (1_s \otimes \Phi)V\|,
\]

where \( \lambda \) is a specified normalization factor and \( \| \cdot \| \) is any left-invariant matrix norm on the space of \( n \times n \) complex matrices, denoted as \( \mathcal{M}_n(\mathbb{C}) \).

In the following sections, we introduce some useful properties of unitarily invariant quotient metrics on the homogeneous space \( Q \).

### 3.1. Closed-system target transformations

A very typical situation in QC occurs when the target unitary transformation is specified for an ideal closed system (i.e. for \( S \) alone, excluding coupling to the environment). Let \( U \) denote the actual evolution operator for the composite system \( C \) and \( V \) denote the target quantum operation. If the target is defined for the closed system, then \( V \) is decoupled: \( V = V_s \otimes V_e \), where \( V_s \in U(H_s) \) is the specified target unitary transformation for \( S \) and \( V_e \in U(H_e) \) is arbitrary. Because \( V_e \) is an arbitrary operation on \( E \), it can be incorporated into \( \Phi_2 \) in (6):

\[
\min_{\Phi_1, \Phi_2} \Delta((1_s \otimes \Phi_1)U, (1_s \otimes \Phi_2)(V_s \otimes V_e)) = \min_{\Phi_1, \Phi_2} \Delta((1_s \otimes \Phi_1)U, (1_s \otimes \Phi_2)(V_s \otimes 1_e)).
\]

Similarly, \( V_e \) can be incorporated into \( \Phi \) in (7) and (8). Therefore, for the closed-system target \( V_s \), expressions (6)–(8) of the quotient metric are reformulated as

\[
\tilde{\Delta}(\{U\}, \{V_s \otimes 1_e\}) = \min_{\Phi_1, \Phi_2} \Delta((1_s \otimes \Phi_1)U, (V_s \otimes \Phi_2)),
\]

\[
\tilde{\Delta}(\{U\}, \{V_s \otimes 1_e\}) = \min_{\Phi} \Delta(U, (V_s \otimes \Phi))
\]

and

\[
\tilde{\Delta}(\{U\}, \{V_s \otimes 1_e\}) = \lambda \min_{\Phi} \|U - (V_s \otimes \Phi)\|,
\]

respectively. From a practical point of view, these results mean that we can use the distance measure \( \tilde{\Delta}(\{U\}, \{V_s \otimes 1_e\}) \) to quantitatively compare the actual evolution operator \( U \in U(H_c) \) of the composite system \( C \) (of dimension \( n \)) and the target transformation \( V_s \in U(H_s) \) specified for the sub-system \( S \) (of a smaller dimension \( n_s \)).
3.2. Chaining of unitary operations

Consider a physical process composed of several components, such as the application of a sequence of $n$ unitary operations, $U_n \ldots U_2 U_1$, acting on the composite system, compared to the corresponding sequence of target unitary operations, $V_n \ldots V_2 V_1$, where $U_i, V_i \in \mathcal{U}(\mathcal{H}_c)$. In this context, a metric or distance measure is said to possess the chaining criterion [42] if

$$
\Delta(U_m \ldots U_2 U_1, V_m \ldots V_2 V_1) \leq \Delta(U_1, V_1) + \Delta(U_2, V_2) + \cdots + \Delta(U_m, V_m).
$$

(10)

Thus, the total error of the process is bounded from above by the sum of the individual errors $\Delta(U_i, V_i)$. This property is useful for analyzing the overall fidelity of a quantum algorithm, consisting of, e.g. a sequence of one- and two-qubit operations [28, 42].

**Theorem 2.** If $\Delta$ is a bi-invariant metric on $\mathcal{U}(\mathcal{H}_c)$ (i.e. $\Delta(W_1 U W_2, W_1 V W_2) = \Delta(U, V)$ for any $U, V, W_1, W_2 \in \mathcal{U}(\mathcal{H}_c)$), then the chaining criterion (10) holds for any $U_1, U_2, \ldots, U_m \in \mathcal{U}(\mathcal{H}_c)$ and $V_1, V_2, \ldots, V_m \in \mathcal{U}(\mathcal{H}_c) \otimes \mathcal{U}(\mathcal{H}_c)$.  

**Proof.** See appendix B.

From this result, the chaining property holds for $V_i \in \mathcal{U}(\mathcal{H}_c) \otimes \mathcal{U}(\mathcal{H}_c)$, i.e. the set of all decoupled or factorizable unitary operators in $\mathcal{U}(\mathcal{H}_c)$. This condition is satisfied by any $V_i$ that preserves the isolation of the system $S$ from the environment $E$, a ubiquitous objective in QC.

3.3. Convexity

Performing the minimization in (6) over $\Phi_1, \Phi_2 \in \mathcal{U}(\mathcal{H}_c)$ to compute $\tilde{\Delta}([U], [V])$ may be difficult and expensive in general. However, when the distance measure is determined by a left-invariant norm (7), the minimization can be recast as a convex optimization problem [66]. Relaxing the condition on $\Phi$ from $\Phi^\dagger \Phi = \mathbb{1}_c$ to $\Phi^\dagger \Phi \leq \mathbb{1}_c$ produces such a problem since (i) any norm is a convex function, (ii) the argument in the norm is affine in the optimization variable $\Phi$ and (iii) the set of matrices that satisfies $\Phi^\dagger \Phi \leq \mathbb{1}_c$ is a convex set in $\Phi$. To show this, note that the set of matrices that satisfies $\Phi^\dagger \Phi \leq \mathbb{1}_c$ is equal to the set that satisfies $\|\Phi\|_2 \leq 1$, where $\|\cdot\|_2$ is the induced two-norm described in section 5. Thus, $\|\theta \Phi_1 + (1-\theta) \Phi_2\|_2 \leq \theta \|\Phi_1\|_2 + (1-\theta) \|\Phi_2\|_2 \leq 1$ for all $0 \leq \theta \leq 1$, which follows from the triangle inequality. Expressing (7) (or (8)) as a convex optimization problem is desirable, provided the solution is on the boundary of $\Phi^\dagger \Phi \leq \mathbb{1}_c$ (i.e. $\Phi \in \mathcal{U}(\mathcal{H}_c)$), because if a local minimum exists in a convex set, it is also a global minimum [66].

3.4. Stability

Another important metric property is stability [42]. A metric is said to be stable if

$$
\Delta([U] \otimes \Xi, [V] \otimes \Xi) = \Delta([U], [V]),
$$

(11)

for any unitary operator $\Xi$ of any given dimension. Stability means that operations on an ancillary system that is not coupled to the original composite system do not affect the value of $\Delta$, and hence $\tilde{\Delta}$ [42]. We do not prove stability for the general form of the distance measure in (6) or (8), but demonstrate it for the Hilbert–Schmidt norm distance in the following section.
4. Computing the distance measure with the Hilbert–Schmidt norm

In this section, the distance measure presented in section 3 is evaluated with the Hilbert–Schmidt norm (also referred to as the Frobenius norm), which is defined as [64]

$$\|M\|_{\text{HS}} := \sqrt{\text{Tr}(M^\dagger M)} = \left[ \sum_{i=1}^{n} \sigma_i^2(M) \right]^{1/2}, \quad \forall M \in \mathcal{M}_n(\mathbb{C}),$$

(12)

where $\sigma_i(M)$ is the $i$th singular value of $M$. The $i$th singular value, $\sigma_i(M)$, is the square root of the $i$th eigenvalue of the positive square matrix $M^\dagger M$, where the singular values appear in descending order: $\sigma_i(M) \geq \sigma_{i+1}(M)$ for all $i$.

The general form of the Hilbert–Schmidt norm distance is, according to (8),

$$\tilde{\Delta}_{\text{HS}}([U], [V]) := \lambda_n \min_{\Phi} \{\|U - (\mathbb{1}_s \otimes \Phi)V\|_{\text{HS}} : \Phi \in \mathcal{U}(\mathcal{H}_s)\}.$$  

(13)

Using (12) in (13) and $\lambda_n = (2n)^{-1/2}$, the minimization over $\Phi$ can be carried out analytically and, as shown below, we obtain:

$$\tilde{\Delta}_{\text{HS}}([U], [V]) = \sqrt{1 - \frac{1}{n} \|\Gamma\|_{\text{Tr}}},$$

(14)

where $\Gamma \in \mathcal{M}_{n_t}(\mathbb{C})$ is

$$\Gamma := \text{Tr}_s(UV^\dagger),$$

(15)

and $\|\cdot\|_{\text{Tr}}$ in (14) is the trace norm [64]:

$$\|M\|_{\text{Tr}} := \text{Tr}\left(\sqrt{M^\dagger M}\right) = \sum_{i=1}^{n} \sigma_i(M), \quad \forall M \in \mathcal{M}_n(\mathbb{C}).$$

(16)

Note that in (15), $\text{Tr}_s(\cdot)$ denotes the partial trace over the system space $\mathcal{H}_s$.

**Proof.** The derivation of (14) begins with some algebraic rearrangement of (13), initially yielding

$$\tilde{\Delta}_{\text{HS}}([U], [V]) = \min_{\Phi} \sqrt{1 - \frac{1}{n} \text{Re}\{\text{Tr}[UV^\dagger(\mathbb{1}_s \otimes \Phi^\dagger)]\}},$$

(17a)

$$= \min_{\Phi} \sqrt{1 - \frac{1}{n} \text{Re}\{\text{Tr}_s[\Phi^\dagger \times \text{Tr}_s(UV^\dagger)]\}},$$

(17b)

$$= \min_{\Phi} \sqrt{1 - \frac{1}{n} \text{Re}\{\text{Tr}(\Gamma \Phi^\dagger)\}}.$$  

(17c)

Computing the singular value decomposition (SVD) of $\Gamma$ yields $\Gamma = W \Sigma X^\dagger$, where $W, X \in \mathcal{U}(\mathcal{H}_s)$ and $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n) \in \mathcal{M}_{n_t}(\mathbb{R})$, with $\sigma_i \geq \sigma_{i+1} \geq 0$, for all $i$. Thus,

$$\text{Tr}(\Gamma \Phi^\dagger) = \text{Tr}(W \Sigma X^\dagger \Phi^\dagger) = \text{Tr}(\Sigma X^\dagger \Phi^\dagger W) = \text{Tr}(\Sigma Y),$$

(18)

where $Y = X^\dagger \Phi^\dagger W \in \mathcal{U}(\mathcal{H}_s)$. Hence,

$$\text{Re}\{\text{Tr}(\Gamma \Phi^\dagger)\} = \text{Re}\{\text{Tr}(\Sigma Y)\} = \sum_{i=1}^{n_t} \sigma_i \text{Re}(Y_{ii}),$$

(19)
which, because \( Y \) is unitary, achieves the maximum of \( \text{Tr}(\Sigma) \) when \( Y = \mathbb{1}_e \). For a unitary matrix \( Y \), as a result of orthonormality, \( \sum_j |y_{ij}|^2 = 1 \) for all \( i \). Hence, \( 0 \leq |y_{ij}| \leq 1 \) for all \( i, j \), and in particular \( 0 \leq |y_{ij}| \leq 1 \) for all \( i \). Since \( \Sigma \) is diagonal and positive (with matrix elements \( \sigma_i \)), \( \text{Re}[\text{Tr}(\Sigma Y)] = \sum_i \sigma_i \text{Re}(y_{ii}) \leq \sum_i \sigma_i |y_{ii}| \leq \sum_i \sigma_i = \text{Tr}(\Sigma) \). Thus, the maximum of \( \text{Re}[\text{Tr}(\Sigma Y)] \) is attained when \( Y = \mathbb{1}_e \).

To show that \( \text{Tr}(\Sigma) = \|\Gamma\|_{\text{Tr}} \), consider \( \Sigma = W^\dagger \Gamma X = X^\dagger \Gamma^\dagger W \), which implies that \( \Sigma^2 = X^\dagger \Gamma^\dagger \Gamma X \). Because \( \Sigma \) is diagonal, the matrix \( \Sigma^2 \) is also diagonal, and \( X \) is the unitary matrix that diagonalizes the positive matrix \( \Gamma^\dagger \Gamma \). Therefore, it follows that \( \sqrt{\Sigma^2} = \Sigma = X^\dagger \sqrt{\Gamma^\dagger \Gamma} X \).

Thus,

\[
\max_{\Phi} [\text{Re}[\text{Tr}(\Gamma \Phi^\dagger)]] = \text{Tr}(\Sigma) = \|\Gamma\|_{\text{Tr}},
\]

and (14) results. \( \square \)

From this proof it follows that

\[
\min_{\Phi} \|U - (\mathbb{1}_s \otimes \Phi)V\|_{\text{HS}} : \Phi^\dagger \Phi \equiv \mathbb{1}_e = \min_{\Phi} \|U - (\mathbb{1}_s \otimes \Phi)V\|_{\text{HS}} : \Phi^\dagger \Phi \leq \mathbb{1}_e,
\]

and the minimum occurs on the boundary of the set \( \Phi^\dagger \Phi \leq \mathbb{1}_e \), i.e. \( \Phi = WX^\dagger \in \mathcal{U}(\mathcal{H}_e) \), where \( X \) and \( W \) are the unitary matrices from the SVD of \( \Gamma \).

For the case where the target unitary transformation \( V_s \in \mathcal{U}(\mathcal{H}_e) \) is specified for a closed system, results of section 3.1 can be used to obtain:

\[
\tilde{\Delta}_{\text{HS}}([U], [V_s \otimes \mathbb{1}_e]) = \sqrt{1 - \frac{1}{n} \|\Gamma\|_{\text{Tr}}}, \quad \text{where} \quad \Gamma = \text{Tr}_s[U(V_s^\dagger \otimes \mathbb{1}_e)].
\]

4.1. Stability of the Hilbert–Schmidt norm

Consider the stability [42] of the Hilbert–Schmidt norm, as expressed in (11):

\[
\tilde{\Delta}_{\text{HS}}([U] \otimes \Xi, [V] \otimes \Xi) = \lambda_{n_{\Xi}} \min_{\Phi} \|[U - (\mathbb{1}_s \otimes \Phi)V] \otimes \Xi\|_{\text{HS}} : \Phi \in \mathcal{U}(\mathcal{H}_e)),
\]

where \( \Xi \) is any unitary operator and \( n_{\Xi} = \dim[\Xi] \). For this norm, a tensor product of operators factors into the corresponding product of the norms of those operators:

\[
\tilde{\Delta}_{\text{HS}}([U] \otimes \Xi, [V] \otimes \Xi)) = \lambda_n \min_{\Phi} \|[U - (\mathbb{1}_s \otimes \Phi)V]\|_{\text{HS}} \times \|\Xi\|_{\text{HS}} / \sqrt{n_{\Xi}},
\]

\[
= \lambda_n \min_{\Phi} \|[U - (\mathbb{1}_s \otimes \Phi)V]\|_{\text{HS}},
\]

\[
= \tilde{\Delta}_{\text{HS}}([U], [V]).
\]

Therefore, with the appropriate normalization factor, \( \tilde{\Delta}_{\text{HS}} \) is stable.

4.2. Unitary operators that are exact tensor products

Suppose that \( U \) and \( V \), the actual and target operators, respectively, are exact tensor products, i.e.

\[
U = U_s \otimes U_e \quad \text{and} \quad V = V_s \otimes V_e,
\]

where \( U_s \) and \( V_s \) are unitary operators on \( s \)-dimensional systems, and \( U_e \) and \( V_e \) are unitary operators on \( e \)-dimensional systems. Then, we have:

\[
U = U_s \otimes U_e \quad \text{and} \quad V = V_s \otimes V_e,
\]

which implies that:

\[
\text{Tr}(U) = \text{Tr}(U_s) \ast \text{Tr}(U_e) \quad \text{and} \quad \text{Tr}(V) = \text{Tr}(V_s) \ast \text{Tr}(V_e),
\]

where \( \ast \) denotes the Kronecker product. Therefore, for any unitary operator \( W \), we have:

\[
\text{Tr}(W) = \text{Tr}(W_s) \ast \text{Tr}(W_e),
\]

where \( W_s \) and \( W_e \) are unitary operators on \( s \)-dimensional and \( e \)-dimensional systems, respectively.

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where $U_s, V_s \in \mathbb{U} \mathcal{H}_s$ and $U_e, V_e \in \mathbb{U} \mathcal{H}_e$. Such a situation would occur if, e.g. there is no system–environment interaction ($H_{\text{int}} = 0$) or the system and environment are decoupled at a final time $t = t_f$. Then, from (15),
\[
\Gamma = \text{Tr}(U_s V_s^\dagger) U_e V_e^\dagger
\]
and
\[
\|\Gamma\|_\text{Tr} = |\text{Tr}(U_s V_s^\dagger)| \text{Tr}\left(\sqrt{V_e U_e^\dagger U_e V_e}\right) = n_e |\text{Tr}(U_s V_s^\dagger)|.
\]

The distance measure now becomes
\[
\tilde{\Delta}_\text{HS}([U_s \otimes U_e], [V_s \otimes V_e]) = \sqrt{1 - \frac{1}{n_s} |\text{Tr}(U_s V_s^\dagger)|},
\]
which is, as one would expect, completely independent of $U_e$ and $V_e$. Indeed, as discussed in section 3.1, $U_e$ and $V_e$ can be incorporated into $\Phi$ in the quotient metric in (8) and thus simply replaced by $\mathbb{1}_e$. Therefore, the matrix $\Gamma$ in (26) can be replaced by $\Gamma = \text{Tr}(U_s V_s^\dagger) \mathbb{1}_e$ (immediately leading to (27)), and the distance measure in (28) can be expressed as $\tilde{\Delta}_\text{HS}([U_s \otimes \mathbb{1}_e], [V_s \otimes \mathbb{1}_e])$.

The distance measure in (28) is related to other distance and fidelity measures used in previous works for optimal control of unitary operations [45]–[47] and analysis of the unitary control landscape [55]–[57] in closed quantum systems. For control landscapes, the analysis of critical points of $\tilde{\Delta}_\text{HS}([U_s \otimes \mathbb{1}_e], [V_s \otimes \mathbb{1}_e])$ with respect to the control field is especially important.

Note that the distance in (28) is zero if and only if $U_s$ and $V_s$ differ only by a global phase, i.e. $U_s = \exp(i\phi)V_s$ for any real $\phi$. Therefore, this distance can be considered as a phase-independent generalization of
\[
\frac{1}{\sqrt{2n_s}}\|U_s - V_s\|_{\text{HS}} = \sqrt{1 - \frac{1}{n_s} \text{Re}\left[\text{Tr}(U_s V_s^\dagger)\right]},
\]
a frequently used distance [57] that is zero if and only if $U_s = V_s$.

5. Computing the distance measure with the maximum singular value

Suppose a (possibly entangled) normalized pure state $|\psi\rangle$ of the composite system $\mathcal{C}$ is acted upon by a unitary operator $U$. The output of this action, $U|\psi\rangle$, can be compared to the output of the target action, $V|\psi\rangle$ (modulo $\mathbb{1}_s \otimes \Phi$). The output state error $\varepsilon$ is
\[
\varepsilon := [U - (\mathbb{1}_s \otimes \Phi)] V |\psi\rangle.
\]
The maximum (over all normalized pure states) norm of the error is
\[
\max_\psi \varepsilon^\dagger \varepsilon = \|U - (\mathbb{1}_s \otimes \Phi)V\|_2^2,
\]
where $\|\cdot\|_2$ is the induced two-norm of a matrix [64], i.e. the maximum singular value of the matrix argument.\(^6\) Now consider the distance measure based on the induced two-norm:
\[
\tilde{\Delta}_2([U], [V]) = \lambda_2 \min_\Phi \{\|U - (\mathbb{1}_s \otimes \Phi)V\|_2 \mid \Phi \in \mathbb{U}(\mathcal{H}_s)\},
\]
\(^6\) Equation (31) may also be expressed in terms of the operator norm [64]: $\|U - (\mathbb{1}_s \otimes \Phi)V\|_\infty := \sup_\psi \|U - (\mathbb{1}_s \otimes \Phi)V\|_2 |\psi\rangle$, where $\langle \psi | \psi \rangle = 1$. In this context, $\|\cdot\|_2$ is the standard vector two-norm.
where $\lambda_2 = 2^{-1}$. Although an explicit solution for $\tilde{\Delta}_2([U], [V])$ is not presented in this work, we establish the following bounds:

$$\lambda_2 \| U - (\mathbb{1}_s \otimes \Phi)V \|_2 \leq \tilde{\Delta}_2([U], [V]) \leq \lambda_2 \| U - (\mathbb{1}_s \otimes \Phi)V \|_2,$$

(33)

where $\Phi$ is the solution to the following optimization problem:

$$\Phi := \arg \min_{\Phi} \{ \| U - (\mathbb{1}_s \otimes \Phi)V \|_2 : \Phi^\dagger \Phi \leq \mathbb{1}_c \}. \quad (34)$$

Here, $\Phi^\dagger \Phi \leq \mathbb{1}_c$ indicates that $\Phi^\dagger \Phi$ is a positive Hermitian matrix whose eigenvalues are at most 1. The optimization in (34) is convex for the same reasons as those discussed in section 3.3. However, there is no guarantee that the resulting optimizer $\Phi$ is unitary. Since $\Phi$ in (34) is less constrained than in (32), it follows that the lower bound in (33) applies. The operator $\tilde{\Phi}$ is obtained from the SVD of $\Phi$:

$$\tilde{\Phi} = W S X^\dagger \rightarrow \tilde{\Phi} = WX^\dagger.$$

Thus, $\tilde{\Phi}$ is a unitary approximation to $\Phi$, and since it is not necessarily the optimal solution to (32), the upper bound in (33) follows. The lower and upper bounds in (33) will be close to each other if the singular values of $\Phi$ are close to unity, i.e. if $\Phi$ is close to a unitary matrix.

For any matrix $M \in \mathcal{M}_n(\mathbb{C})$, the induced two-norm is bounded from above by the Hilbert–Schmidt norm [64]: $\| M \|_2 \leq \| M \|_{HS}$. Comparing the distance measure with these norms yields a similar relationship. Given $U, V \in U(\mathcal{H}_c)$, let $\Phi_{HS}$ be minimizer of $\tilde{\Delta}_{HS}([U], [V])$. It follows that

$$\lambda_2^{-1} \tilde{\Delta}_2([U], [V]) \leq \| U - (\mathbb{1}_s \otimes \Phi_{HS})V \|_2 \leq \| U - (\mathbb{1}_s \otimes \Phi_{HS})V \|_{HS} = \lambda_2^{-1} \tilde{\Delta}_{HS}([U], [V]),$$

(36)

i.e. $\tilde{\Delta}_2([U], [V])$ is bounded from above by $(n/2)^{1/2} \tilde{\Delta}_{HS}([U], [V])$.

6. Relating the distance measure to quantum channel fidelity

Quantum operations, for example, a free or controlled time evolution (possibly in the presence of decoherence) or a transmission of information (possibly via a noisy connection), are generally described by quantum channels [28, 67]. In this section, we consider a common situation in QC, where the target quantum channel is a unitary transformation specified for a closed system (i.e. for $S$ alone). We denote this target unitary transformation as $V_s \in U(\mathcal{H}_s)$ (cf sections 3.1 and 4.2), and the Hilbert–Schmidt norm distance $\tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_c])$ corresponding to the closed-system target is given by (22). We demonstrate that the distance measure $\tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_c])$ and a typical measure of quantum channel fidelity both depend on the matrix norm of $\Gamma = \text{Tr}_e[U(V_s^\dagger \otimes \mathbb{1}_c)]$ from (22).

There are several ways to define the fidelity of a quantum channel with respect to the target unitary transformation [28], [37]–[43]. For example, the Uhlmann state fidelity, defined as [37, 38]

$$F_u(\rho_1, \rho_2) := \| \sqrt{\rho_1} \sqrt{\rho_2} \|_{Tr}^2 = \left\{ \text{Tr} \left[ (\sqrt{\rho_1} \rho_2 \sqrt{\rho_1})^{1/2} \right] \right\}^2,$$

(37)

where $\rho_1, \rho_2 \in \mathcal{D}(\mathcal{H})$, can be used to measure the effect of quantum channels on states. The Kolmogorov distance between two density matrices is [40]

$$D_k(\rho_1, \rho_2) := \frac{1}{2} \| \rho_1 - \rho_2 \|_{Tr},$$

(38)
which bounds the Uhlmann state fidelity \[ F \]:
\[
[1 - D_\Delta(\rho_1, \rho_2)]^2 \leq \mathcal{F}_u(\rho_1, \rho_2) \leq 1 - D_H^2(\rho_1, \rho_2).
\] (39)

In this section, we develop a direct measure of fidelity for quantum channels based on \( \mathcal{F}_u \) in (37), and establish bounds analogous to those in (39) with the distance measure \( \Delta_{\text{HS}} \).

Let \( \mathcal{K} \) denote a completely positive and trace-preserving quantum channel [28], mapping the state \( \rho_s \) to \( \tilde{\rho}_s \), where \( \rho_s, \tilde{\rho}_s \in \mathcal{D}(\mathcal{H}_s) \), with the following operator-sum representation (also known as the Kraus map [61]):
\[
\tilde{\rho}_s = \mathcal{K}[\rho_s] := \sum_i K_i \rho_s K_i^\dagger,
\] (40a)
such that
\[
\sum_i K_i^\dagger K_i = \mathbb{1}_s, \quad \text{where } K_i \in \mathcal{M}_n(\mathbb{C}).
\] (40b)

The target quantum channel is the unitary transformation \( V_s \) that maps \( \rho_s \) to \( V_s \rho_s V_s^\dagger \).

We can compare the actual and target quantum channels, \( \mathcal{K} \) and \( V_s \), respectively, using the Uhlmann fidelity of (37):
\[
\mathcal{F}_u(V_s | \rho_s | V_s^\dagger, \tilde{\rho}_s) = \left\{ \text{Tr}\left[ (V_s \sqrt{\tilde{\rho}_s} V_s^\dagger \rho_s \sqrt{\tilde{\rho}_s} V_s^\dagger)^{1/2} \right] \right\}^2.
\] (41)

When the input state \( \rho_s \) is pure, it can be expressed as \( \rho_s = |\psi_s\rangle \langle \psi_s| \); then (41) yields
\[
\mathcal{F}_u(V_s | \psi_s | V_s^\dagger, \tilde{\rho}_s) = \langle \psi_s | V_s^\dagger \tilde{\rho}_s V_s | \psi_s \rangle = \sum_i |\langle \psi_s | V_s^\dagger K_i | \psi_s \rangle|^2.
\] (42)

To evaluate the proximity of the quantum channel \( \mathcal{K} \) to the target transformation \( V_s \), it is convenient to use a measure that is independent of the input state. One such measure is the minimum pure-state fidelity \( \mathcal{F}_p(\mathcal{K}, V_s) \) [28], which is obtained by minimizing the form (42) of the Uhlmann fidelity over the set of all pure input states:
\[
\mathcal{F}_p(\mathcal{K}, V_s) := \min_{|\psi_s\rangle} \mathcal{F}_u(V_s | \psi_s | V_s^\dagger, \tilde{\rho}_s) = \min_{|\psi_s\rangle} \sum_i |\langle \psi_s | V_s^\dagger K_i | \psi_s \rangle|^2.
\] (43)

Calculating \( \mathcal{F}_p(\mathcal{K}, V_s) \) is not easy, in general, because the minimization in (43) is not convex. However, this problem can be related to a convex optimization, producing the following lower bound:
\[
\mathcal{F}(\mathcal{K}, V_s) \leq \mathcal{F}_p(\mathcal{K}, V_s),
\] (44a)

where
\[
\mathcal{F}(\mathcal{K}, V_s) := \min_{\rho_s} \sum_i \left| \text{Tr}(V_s^\dagger K_i \rho_s) \right|^2.
\] (44b)

Both fidelities are contained in the interval \([0, 1]\) and equal to one if and only if \( \mathcal{K}[\rho_s] = V_s \rho_s V_s^\dagger \) for all density matrices \( \rho_s \in \mathcal{D}(\mathcal{H}_s) \), i.e. if \( K_i = \alpha_i V_s \) for all \( i \) and \( \sum_i |\alpha_i|^2 = 1 \). For a given \( \mathcal{K} \), \( \mathcal{F}(\mathcal{K}, V_s) \) is found via a convex optimization over all states \( \rho_s \in \mathcal{D}(\mathcal{H}_s) \), and hence, it can be efficiently obtained numerically. It is shown in [28] that \( \mathcal{F}(\mathcal{K}, V_s) \) and \( \mathcal{F}_p(\mathcal{K}, V_s) \) have the same pure-state minimum, but since the set of all density matrices is convex, while the set of all pure states is not, finding \( \mathcal{F}(\mathcal{K}, V_s) \) is an easier optimization problem.
If, instead of minimizing over all possible density matrices, \( \rho \) in \( \mathcal{F}(\mathcal{K}, V_s) \) is simply the so-called maximally mixed system state \( \rho_{m,s} := \frac{1}{n_s} \), this results in another variant of quantum channel fidelity, \( \mathcal{F}_{m,s}(\mathcal{K}, V_s) \) [28, 41, 67]:

\[
\mathcal{F}_{m,s}(\mathcal{K}, V_s) := \frac{1}{n_s} \sum_i |\text{Tr}(V_s^\dagger K_i)|^2. \tag{45}
\]

This fidelity also evaluates the proximity of the quantum channel \( \mathcal{K} \) to the target transformation \( V_s \) [28], but without state optimization. Interestingly, \( \rho_{m,s} \) has the unique property of being the density matrix with the ‘shortest’ maximum distance, under the Hilbert–Schmidt norm, to any other density matrix:

\[
\rho_{m,s} = \text{arg min}_{\rho_2} \left( \max_{\rho_1} \frac{1}{n_s} \sum_i |\text{Tr}(V_s^\dagger K_i)|^2 \right), \quad \forall \rho_1, \rho_2 \in \mathcal{D}(\mathcal{H}), \tag{46a}
\]

where

\[
\min_{\rho_2} \left( \max_{\rho_1} \frac{1}{n_s} \sum_i |\text{Tr}(V_s^\dagger K_i)|^2 \right) = \frac{n_s - 1}{n_s}. \tag{46b}
\]

This result suggests that \( \rho_{m,s} \) is ‘centrally located’ within the space of density matrices in the Hilbert–Schmidt geometry.

**Proof.** See appendix D.

Relating \( U \) (the composite-system evolution operator) to \( \mathcal{K} \) (the quantum channel for the system \( S \)) requires the specification of an initial state of the composite system \( C \). For simplicity, assume that this initial state is an uncorrelated tensor-product state:

\[
\rho = \rho_s \otimes \rho_e = \rho_s \otimes \sum_{v=1}^{n_e} \zeta_v |v\rangle\langle v|, \tag{47}
\]

where, as before, \( \rho \in \mathcal{D}(\mathcal{H}_e), \rho \geq 0 \) and \( \text{Tr}(\rho) = 1 \). The reduced dynamics of the system \( S \) can be represented by the mapping in (40), where the Kraus operators \( K_{\nu\nu'} \) are

\[
K_{\nu\nu'} := \sqrt{\zeta_{\nu'}} \text{Tr}_e(\mathbb{1}_s \otimes |\nu\rangle\langle \nu| U) = \sqrt{\zeta_{\nu'}} \sum_{i, i'=1}^{n_s} U_{\nu\nu'}^{i,i'} |i\rangle\langle i'|, \tag{48}
\]

with the unitary operator \( U \) expanded as

\[
U = \sum_{i, i'=1}^{n_s} \sum_{\nu, \nu'=1}^{n_e} U_{\nu\nu'}^{i,i'} |i\rangle\langle i'| \otimes |\nu\rangle\langle \nu'|. \tag{49}
\]

There exist infinitely many different sets of Kraus operators, \( \{K_j\} \), that represent the same map \( \mathcal{K} \) (i.e. they evolve the system state \( \rho_s \) in exactly the same way) [61]. This is related to the equivalence relation defined in section 2, namely that \( U \) and \( (\mathbb{1}_s \otimes \Phi)U \) produce the same system evolution and hence, the same Kraus map. Moreover, any Kraus map for a \( k \)-level system can be represented by a set of at most \( k^2 \) Kraus operators.

The mapping from \( U \) and \( \rho \) to \( \mathcal{K} \) described above illustrates the dependence of the quantum channel \( \mathcal{K} \) (and hence of the corresponding fidelities) on the initial state of the environment. Note that the exact treatment of the dynamics requires the propagation of the evolution operator for the composite system \( C \), which is also required for computing \( \tilde{\Delta}(\{U\}, \{V_s \otimes \mathbb{1}_e\}) \).
Although approximations may simplify the calculation of $\mathcal{K}$, they may eliminate certain physical processes, e.g. the Markovian approximation limits the memory of the environment, preventing possible coherence revivals. However, even when no approximations are made, measures of fidelity for a quantum channel $\mathcal{K}$ require (for the mapping from $U$ to $\mathcal{K}$) the specification of the environment’s initial state and thus are less general than the distance measure $\Delta([U], [V_s \otimes \mathbb{1}_e])$.

With (48), the fidelity $\mathcal{F}_{m,s}(\mathcal{K}, V_s)$ in (45) becomes

$$\mathcal{F}_{m,s}(\mathcal{K}, V_s) = \frac{1}{n_s^2} \sum n_s \xi_{v,v'} |\Gamma_{v,v'}|^2 = \frac{1}{n_s^2} \|\Gamma \sqrt{\rho_e}\|_{HS}^2,$$

where $\rho_e \in \mathcal{D}(\mathcal{H}_e)$ is the initial state of the environment, $\rho_e = \sum_{v=1}^{n_e} \xi_v |v\rangle \langle v|$. Also, we see that both the distance measure $\tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_e])$ and quantum channel fidelity $\mathcal{F}_{m,s}(\mathcal{K}, V_s)$ depend on the matrix $\Gamma$ defined in (22). Specifically, increasing the norm of $\Gamma$ will increase fidelity and decrease distance. As a concluding example, suppose that $\rho_e$ is the maximally mixed environment state, i.e. $\rho_{m,e} := \mathbb{1}_e/n_e$. In this case, the quantum channel fidelity $\mathcal{F}_{m,c}(\mathcal{K}, V_s)$ becomes

$$\mathcal{F}_{m,c}(\mathcal{K}, V_s) := \frac{1}{n_s n} \sum \xi_{v,v'} |\Gamma_{v,v'}|^2 = \frac{1}{n_s n} \|\Gamma \|_{HS}^2,$$

further emphasizing the dependence of fidelity on the norm of $\Gamma$.

We show that the inequality relation between the distance and fidelity of quantum states presented in (39) [40] also applies to the distance and fidelity of quantum operations given by $\tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_e])$ and $\mathcal{F}_{m,c}(\mathcal{K}, V_s)$, respectively. Specifically, we obtain the following lower and upper bounds of $\mathcal{F}_{m,c}(\mathcal{K}, V_s)$:

$$[1 - \tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_e])]^2 \leq \mathcal{F}_{m,c}(\mathcal{K}, V_s) \leq 1 - \tilde{\Delta}_{HS}^2([U], [V_s \otimes \mathbb{1}_e]).$$

**Proof.** See appendix E. \(\square\)

7. Applications: optimal control of quantum gates

7.1. Model open system

In this section, we illustrate the use of the distance measure $\tilde{\Delta}_{HS}([U], [V_s \otimes \mathbb{1}_e])$ in the optimal control of one- and two-qubit gates relevant for QC. Specifically, this measure is used in numerical calculations to evaluate the distance between quantum operations generated in the framework of optimal control theory [25, 27] for a system coupled to a decohering environment [32, 33], and a target unitary transformation. We use a model of interacting two-level particles, which are divided into a QIP, composed of $q$ qubits, and an environment, composed of $e$ two-level particles. The qubits are directly coupled to a time-dependent external control field, while the environment is not directly controlled and is thereby managed only through its interaction with the qubits. The Hamiltonian for the composite system $\mathcal{C}$, abbreviated as $H = H_0 + H_{c(t)} + H_{int}$,\(^7\) has the explicit form

$$H = \sum_{i=1}^{q+e} \omega_i S_{iz} - \sum_{i=1}^{q} \mu_i C(t) S_{ix} - \sum_{j=i+1}^{q+e} \sum_{i=1}^{q+e} \gamma_{ij} S_i \cdot S_j.$$

\(^7\) Compare this expression to the abbreviated Hamiltonian in (1): $H_0 + H_{c(t)} = H_c + H_e$. 

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Here, $\mathbf{S}_i = (S_{ix}, S_{iy}, S_{iz})$ is the spin operator for the $i$th particle ($\mathbf{S}_i = \frac{1}{2}\sigma_i$, in terms of the Pauli matrices), $H_0$ is the sum over the free Hamiltonians $\omega_i S_{iz}$ for all $q + e$ particles ($\omega_i$ is the transition angular frequency for the $i$th particle), $H_{ct}(t)$ specifies the coupling between the $q$ qubits and the time-dependent control field $C(t)$ ($\mu_i$ are the corresponding dipole moments) and $H_{\text{int}}$ represents the Heisenberg exchange interaction between the particles ($\gamma_{ij}$ is the coupling parameter for the $i$th and $j$th particles). Hamiltonians of the form in (53) are often referred to as effective or spin Hamiltonians [68].

The evolution of the composite system $C$ is calculated in an exact quantum-mechanical manner, by propagating the Schrödinger equation (2) for the Hamiltonian in (53), without either approximating the dynamics by a master equation or using a perturbative analysis based on a weak coupling assumption. This calculation produces the final-time evolution operator $U_{\text{e}} \in \mathbb{U}(\mathcal{H}_c)$ (an $n \times n$ unitary matrix), which is compared to the target gate operation $V_s \in \mathbb{U}(\mathcal{H}_q)$ (an $n_s \times n_s$ unitary matrix) via $\Delta_{\text{HS}}([U_{\text{e}}], [V_s \otimes \mathbb{1}_e])$. Note that $n_s = 2^q$, $n_e = 2^e$ and $n = 2^{(q+e)}$.

For our examples, we consider two different composite systems. In the first example, one qubit is coupled to a two-particle environment ($q = 1$ and $e = 2$), which can be modeled by a linear chain of particles with the qubit $q_1$ at the center, equally coupled to both environment particles $e_2$ and $e_3$:

$$ e_2 \xleftarrow{\gamma_{12}} q_1 \xrightarrow{\gamma_{13}} e_3, \quad (54) $$

where $\gamma_{12} = \gamma_{13} = \gamma$. Assuming only nearest-neighbor coupling in this configuration, we set $\gamma_{23} = 0$. In the second example, two qubits are equally coupled to a one-particle environment ($q = 2$ and $e = 1$). This is modeled as a triangular cluster:

$$ \begin{align*}
&\gamma_{13} \quad e_3 \\
&\gamma_{23} \\
q_1 \xleftrightarrow{\gamma_{21}} q_2
\end{align*}, \quad (55) $$

where the two qubits are denoted as $q_1$ and $q_2$, the environment particle as $e_3$, and $\gamma_{13} = \gamma_{23} = \gamma$. Other system–environment configurations and corresponding optimal control results, using $\Delta_{\text{HS}}([U_{\text{e}}], [V_s \otimes \mathbb{1}_e])$, are presented in [32, 33].

Parameters of the composite system are selected to ensure complex dynamics and strong decoherence: values of $\gamma/\omega$ are up to 0.02 and frequencies $\omega_i$ are close, but not equal, to enhance the system–environment interaction (see [32] for more details). In addition to setting $\hbar = 1$, we introduce a natural system of units by setting $\mu_i = 1$ for all $i$ and the qubit frequency $\omega_1 = 1$, implying that one period of free evolution is $2\pi$.\(^8\)

### 7.2. Optimal control algorithm

The ultimate control goal is to decouple the system $S$ from the environment $E$ at a time $t = t_f$ and simultaneously produce the target unitary operation $V_s \in \mathbb{U}(\mathcal{H}_q)$ for $S$. Target quantum gates for the one- and two-qubit systems are the Hadamard gate $H_q$ and controlled-not gate CNOT, respectively (both of these gates are elements of a universal set of logical operations.

\[8\] For one-qubit coupled to a two-particle environment, the frequencies of the environment particles are: $\omega_2 \approx 0.99841$ and $\omega_3 \approx 1.00159$. For two qubits coupled to a one-particle environment, the frequencies of $q_2$ and $e_3$ are: $\omega_2 \approx 1.09159$ and $\omega_3 \approx 0.99841$, respectively.

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for QC [28]):

\[ H_g := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad \text{and} \quad \text{CNOT} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \quad (56) \]

A hybrid optimization method incorporating genetic and gradient algorithms [69] is employed to minimize the distance measure \( \tilde{\Delta}_{HS}(|U_t\rangle, [V_s \otimes \mathbb{1}_c]) \) with respect to the control field \( C(t) \). After an initial optimization with a genetic algorithm, we remove the constraints imposed by the parameterized form of the control field to provide the potential for more flexible and effective control. An optimal control field is then found by minimizing the objective functional \( J_t^{[V]} \), given by

\[ J_t^{[V]}(C) := \tilde{\Delta}_{HS}([U_t(C)], [V_s \otimes \mathbb{1}_c]) + \frac{\alpha}{2} \|C\|^2_{K_{t}}, \quad (57) \]

using a gradient algorithm (see [32, 46] for details of the gradient-based optimization). Here, \( K_{t} \) denotes a particular closed subspace of \( L^2([0, t_f]; \mathbb{R}) \) (see appendix F for details), and for the time-dependent Hamiltonian in (53), \( U_{t_f} : K_{t_f} \to U(H_c) \) denotes the map, defined implicitly through the Schrödinger equation (2), that takes a control field \( C(t) \in K_{t_f} \) to the unitary time-evolution operator \( U_{t_f} \in U(H_c) \). Thus, \( K_{t_f} \) is a Hilbert space of admissible controls, on which \( U(t; C) \) exists for all \( t \in [0, t_f] \) and all \( C \in K_{t_f} \) [70]. As such, \( J_t^{[V]} : K_{t_f} \to \mathbb{R} \) is the ‘dynamical’ version of the distance measure \( \tilde{\Delta}_{HS} \), with an additional cost on the control field fluence, where \( \alpha > 0 \) is the weight parameter for this cost. The gradient of \( J_t^{[V]} \) is derived in appendix F.

7.3. Results

Because 0 \( \leq \tilde{\Delta}_{HS} \leq 1 \) in general, it is convenient to define gate fidelities based on the respective lower and upper bounds of \( F_{m,c}(K, V_s) \) in (52):

\[ F_{HS}^l([U_t], [V_s \otimes \mathbb{1}_c]) := \left[ 1 - \Delta_{HS}([U_t], [V_s \otimes \mathbb{1}_c]) \right]^2 \quad (58a) \]

and

\[ F_{HS}^u([U_t], [V_s \otimes \mathbb{1}_c]) := 1 - \Delta_{HS}^2([U_t], [V_s \otimes \mathbb{1}_c]). \quad (58b) \]

Both fidelities are independent of the initial state and are evaluated directly from the evolution operator \( U_{t_f} \) of the composite system. These fidelities, computed for the one-qubit Hadamard gate, optimally controlled in the presence of a two-particle environment, are presented in figure 1 for various values of the qubit–environment coupling parameter \( \gamma \). For comparison, a fidelity based on the upper bound of the induced two-norm distance (as defined in (33)) is also presented:

\[ F_2([U_t], [V_s \otimes \mathbb{1}_c]) := \left[ 1 - \lambda_2 \|U_t - (V_s \otimes \hat{\Phi})\|_2 \right]^2, \quad (59) \]

where \( \hat{\Phi} \) is defined in (33)–(35). This fidelity was cast as a semidefinite program [66] and calculated from the final-time evolution operator \( U_{t_f} \) using the SDPT3 solver [71] and the YALMIP toolbox [72] in MATLAB. Since the evolution operators \( U_{t_f} \) produced via optimal control in this example are very close to the target equivalence class, the upper and lower
Figure 1. Gate fidelities $F_{\text{HS}}^u$ (circles, also shown at a different scale in the inset), $F_{\text{HS}}^l$ (squares) and $F_2$ (triangles) versus the coupling parameter $\gamma$, for the optimally controlled one-qubit Hadamard gate $H_g$. The qubit is equally coupled to a two-particle environment ($q = 1, e = 2$). Values of $\gamma$ range from 0 to 0.02 in increments of 0.001.

bounds on the induced two-norm distance are nearly indistinguishable, although this is not true in general.

For the one-qubit system with no coupling to the environment ($\gamma = 0$), the optimal control field produces the Hadamard gate with the following values of the distance and fidelities: $\Delta_{\text{HS}} \approx 10^{-6}$, $F_{\text{HS}}^u \approx 1 - 10^{-12}$ and $F_{\text{HS}}^l \approx 1 - 2 \times 10^{-6}$. For the maximum coupling to the environment ($\gamma = 0.02$), we obtain for the optimally controlled Hadamard gate: $\Delta_{\text{HS}} \approx 0.0035$, $F_{\text{HS}}^u \approx 1 - 10^{-5}$ and $F_{\text{HS}}^l \approx 0.993$. For the two-qubit system with no coupling to the environment ($\gamma = 0$), the optimal control field produces the CNOT gate with the following values of the distance and fidelities: $\Delta_{\text{HS}} \approx 10^{-4}$, $F_{\text{HS}}^u \approx 1 - 10^{-8}$ and $F_{\text{HS}}^l \approx 0.9998$. For the maximum coupling to the environment ($\gamma = 0.01$), we obtain for the optimally controlled CNOT gate: $\Delta_{\text{HS}} \approx 0.02$, $F_{\text{HS}}^u \approx 0.9996$ and $F_{\text{HS}}^l \approx 0.96$.

More significant than the actual fidelity values obtained in this example is the demonstrated ability of the distance measure $\Delta_{\text{HS}}([U_{\text{t}}], [V_s \otimes 1_e])$ to quantitatively compare the evolution of a realistic open system to a target unitary transformation specified for an ideal closed system. Thus, the use of the distance $\Delta_{\text{HS}}([U_{\text{t}}], [V_s \otimes 1_e])$ allows for the direct optimization of quantum operations in the presence of an environment, without specifying any part of the composite-system state.

For randomly selected unitary operators in $U(\mathcal{H}_c)$, the bounds in (33) are well separated and the minimizer $\Phi$ defined in (34) is not unitary.
8. Conclusions

We presented the novel and useful distance measure $\Delta([[U], [V]])$ for the quantitative comparison of unitary quantum operations acting on a composite quantum system, where the effect on only one sub-system (e.g. a QIP) is important, while the effect on the rest of the system (e.g. an environment) can be arbitrary. In practically important situations, where the target operation is specified only for the sub-system of interest, the corresponding measure $\Delta([[U], [V_s \otimes I_e]])$ can evaluate the distance between the evolution of the entire composite system and the target transformation (i.e. effectively compare unitary operations of different dimensions). This capability is especially desirable for measuring the distance between the actual controlled quantum process in a realistic open system and the target unitary transformation in its ideal closed counterpart. The measure developed in this paper does not require the specification of the initial state of any component of the system, is straightforward to calculate with the Hilbert–Schmidt norm, and can be used to define relevant state-independent fidelity measures. A fidelity measure independent of the initial state is extremely valuable for optimal control of quantum gates, which is a crucially important task in realistic QC.

The quotient metric developed here is also applicable to other proposals for design and control of quantum operations. For example, it can be used for evaluating the fidelity of quantum gates in situations where multilevel encoding (MLE) of quantum logical states is employed (i.e. where each logical basis state of a qubit is encoded by multiple physical levels of a quantum system) [73]. Target unitary operations for a QIP equipped with MLE have a tensor-product structure similar to that in (25), and the logical equivalence can exist between different physical operations (i.e. different physical processes can result in the same quantum logical operation on the QIP). However, the environment is not explicitly included in the MLE formalism.

Future research arising from the present work will involve the analysis of quantum control landscapes [55]–[57], [74]–[78] for objective functionals based on various forms of the distance measure $\Delta([[U], [V]])$, in particular, on the Hilbert–Schmidt norm distance $\Delta_{HS}([[U_{tf}(C)], [V_s \otimes I_e]])$. It would be interesting to investigate the structure of these control landscapes and systematically search for robust control solutions that incorporate requirements on realistic physical resources. This search can be performed using a method called diffeomorphic modulation under observable-response-preserving homotopy (D-MORPH) [74]–[77]. This method provides an accurate numerical tool for finding optimal controls. In particular, D-MORPH applied to closed quantum systems is able to identify optimal controls generating a target unitary transformation up to machine precision [77]. Extending the applicability of this approach to open quantum systems is an important goal, currently under development. Implementing efficient numerical algorithms to calculate unitary time-evolution operators for larger composite systems is essential for practical optimal control simulations. Recent work has shown that such unitary maps can be efficiently constructed from appropriately designed state-to-state maps [79], utilizing the favorable state-control landscape structure [50, 55]. The possibility of expanding the method developed in [79] to the optimal control of open quantum systems is being explored.

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Appendix A. Equivalence of unitary operations

The theorem from section 2 is repeated here for convenience.

**Theorem 1.** Let \( U, V \in U(\mathcal{H}) \). Then \( \text{Tr}_e(U \rho U^\dagger) = \text{Tr}_e(V \rho V^\dagger) \) for all density matrices \( \rho \in \mathcal{D}(\mathcal{H}) \) if and only if \( U = (\mathbb{1}_s \otimes \Phi)V \) for some \( \Phi \in U(\mathcal{H}) \).

**Proof.** First, if \( U = (\mathbb{1}_s \otimes \Phi)V \), then \( \text{Tr}_e(U \rho U^\dagger) = \text{Tr}_e[(\mathbb{1}_s \otimes \Phi) \rho (\mathbb{1}_s \otimes \Phi^\dagger)] = \text{Tr}_e(\rho V^\dagger V) \), so the ‘if’ implication is proved. Next, to show the ‘only if’ implication, suppose that \( \text{Tr}_e(U \rho U^\dagger) = \text{Tr}_e(V \rho V^\dagger) \) for all density matrices \( \rho \). By complex linearity, \( \text{Tr}_e(U AV^\dagger) = \text{Tr}_e(V AV^\dagger) \) for all complex matrices \( A \in \mathcal{M}_n(\mathbb{C}) \). Therefore, \( \langle B, \text{Tr}_e(U AV^\dagger) \rangle = \langle B, \text{Tr}_e(V AV^\dagger) \rangle \) for all \( A \in \mathcal{M}_n(\mathbb{C}) \) and all \( B \in \mathcal{M}_n(\mathbb{C}) \), where

\[
\langle B_1, B_2 \rangle = \text{Re}[\text{Tr}(B_1^\dagger B_2)], \quad \forall B_1, B_2 \in \mathcal{M}_n(\mathbb{C}),
\]

is the real Hilbert–Schmidt inner product on \( \mathcal{M}_n(\mathbb{C}) \) (analogously for \( \mathcal{M}_p(\mathbb{C}) \)). If

\[
\langle B, \text{Tr}_e(U AV^\dagger) \rangle = \langle B, \text{Tr}_e(V AV^\dagger) \rangle, \quad \forall A \in \mathcal{M}_n(\mathbb{C}) \text{ and } B \in \mathcal{M}_n(\mathbb{C}),
\]

then

\[
\langle \text{Tr}_e^\dagger(B), U AV^\dagger \rangle = \langle \text{Tr}_e^\dagger(B), V AV^\dagger \rangle, \quad \forall A \in \mathcal{M}_n(\mathbb{C}) \text{ and } B \in \mathcal{M}_n(\mathbb{C}),
\]

where \( \text{Tr}_e^\dagger(\cdot) \) is the operator adjoint of \( \text{Tr}_e(\cdot) \). Starting from \( \langle B, \text{Tr}_e(A) \rangle = \langle \text{Tr}_e^\dagger(B), A \rangle \), for all \( B \in \mathcal{M}_n(\mathbb{C}) \) and \( A \in \mathcal{M}_n(\mathbb{C}) \), we show that \( \text{Tr}_e^\dagger(B) = B \otimes \mathbb{1}_c \):

\[
\langle B, \text{Tr}_e(A) \rangle = \sum_{i,k=1}^{n} \sum_{j=1}^{n} (B^\dagger)_{ki} A_{ijk},
\]

\[
= \sum_{i,k=1}^{n} \sum_{j,k=1}^{n} (B^\dagger \otimes \mathbb{1}_c)_{kiij} A_{ijkl},
\]

\[
= \langle \text{Tr}_e^\dagger(B), A \rangle \implies \text{Tr}_e^\dagger(B) = (B \otimes \mathbb{1}_c).
\]

As such, for all \( A \in \mathcal{M}_n(\mathbb{C}) \) and \( B \in \mathcal{M}_n(\mathbb{C}) \),

\[
\langle B \otimes \mathbb{1}_c, U AV^\dagger \rangle = \langle B \otimes \mathbb{1}_c, V AV^\dagger \rangle,
\]

\[
\implies \langle U^\dagger(B \otimes \mathbb{1}_c)U, A \rangle = \langle V^\dagger(B \otimes \mathbb{1}_c)V, A \rangle.
\]

Since (A.4b) is true for all \( A \in \mathcal{M}_n(\mathbb{C}) \) and \( B \in \mathcal{M}_n(\mathbb{C}) \), then

\[
U^\dagger(B \otimes \mathbb{1}_c)U = V^\dagger(B \otimes \mathbb{1}_c)V,
\]

\[
\implies (B \otimes \mathbb{1}_c)(U V^\dagger) = (U V^\dagger)(B \otimes \mathbb{1}_c).
\]

Finally, because (A.4d) is true for all \( B \in \mathcal{M}_n(\mathbb{C}) \), it holds for all \( W \in U(\mathcal{H}) \):

\[
(W \otimes \mathbb{1}_c)(U V^\dagger) = (U V^\dagger)(W \otimes \mathbb{1}_c),
\]
i.e. $UV^\dagger$ commutes with $W \otimes 1_e$, for all $W$. As such, $UV^\dagger$ is an element of the centralizer of $U(H_\mathcal{e}) \otimes 1_e$ (i.e. the subgroup of $U(H_\mathcal{e})$ that commutes with $U(H_\mathcal{e}) \otimes 1_e$, also formally defined in appendix C), denoted as $C_{U(H_\mathcal{e})}(U(H_\mathcal{e}) \otimes 1_e)$ [80, 81]. In appendix C, we show that the centralizer of $U(H_\mathcal{e}) \otimes 1_e$ is $1_e \otimes U(H_\mathcal{e})$. Thus,

$$ U V^\dagger = 1_e \otimes \Phi \in 1_e \otimes U(H_\mathcal{e}). $$

(A.5)

So, we conclude that $U = (1_e \otimes \Phi)V$ for some $\Phi \in U(H_\mathcal{e})$. □

**Appendix B. Chaining of unitary operations**

After defining and establishing some mathematical objects and terms necessary for our work, we show that the chaining property from (10) holds for a unitarily bi-invariant quotient metric on the homogeneous space $Q$.

**Definition 1.** Let $G$ be a group and $H$ be a subgroup of $G$. The normalizer of $H$ in $G$, $N_G[H] = \{g \in G : gHg^{-1} = H\}$, is the largest subgroup of $G$ such that $H$ is a normal subgroup of $N_G[H]$.

**Lemma 1.** The normalizer of $U(H_\mathcal{e}) \otimes 1_e$ in $U(H_\mathcal{e})$ is $U(H_\mathcal{e}) \otimes U(H_\mathcal{e}) := \{\Psi \otimes \Phi : \Psi \in U(H_\mathcal{e}) \text{ and } \Phi \in U(H_\mathcal{e})\}$. Likewise, the normalizer of $1_e \otimes U(H_\mathcal{e})$ in $U(H_\mathcal{e})$ is $U(H_\mathcal{e}) \otimes U(H_\mathcal{e})$.

**Definition 2.** The centralizer of $H$ in $G$, $C_G[H] = \{g \in G : ghg^{-1} = h, \forall h \in H\}$, is the subgroup of all elements in $G$ that commute with all elements of $H$. Thus, $C_G[H]$ is a subgroup of $N_G[H]$ [80, 81].

**Lemma 2.** The centralizer of $U(H_\mathcal{e}) \otimes 1_e$ in $U(H_\mathcal{e})$ is $1_e \otimes U(H_\mathcal{e}) := \{1_e \otimes \Phi : \Phi \in U(H_\mathcal{e})\}$. Likewise, the centralizer of $1_e \otimes U(H_\mathcal{e})$ in $U(H_\mathcal{e})$ is $U(H_\mathcal{e}) \otimes 1_e$.

Proofs of these lemmas are provided in appendix C. The theorem from section 3 is repeated here for convenience.

**Theorem 2.** If $\Delta$ is bi-invariant on $U(H_\mathcal{e})$, then

$$ \Delta(U_m, U_2 U_1, V_m, V_2 V_1) \leq \Delta(U_1, V_1) + \Delta(U_2, V_2) + \cdots + \Delta(U_m, V_m) $$

(B.1)

holds for any $U_1, U_2, \ldots, U_m \in U(H_\mathcal{e})$ and $V_1, V_2, \ldots, V_m \in U(H_\mathcal{e}) \otimes U(H_\mathcal{e})$.

**Proof.** We demonstrate that (B.1) holds for $m = 2$. This result can be generalized to arbitrary values of $m$. If $\Delta$ is bi-invariant on $U(H_\mathcal{e})$, i.e. for any $U, V, W_1, W_2 \in U(H_\mathcal{e})$,

$$ \Delta(W_1 U W_2, W_1 V W_2) = \Delta(U, V) $$

then, for any $U_1, U_2, V_1, V_2 \in U(H_\mathcal{e})$,

$$ \tilde{\Delta}([U_2 U_1], [V_2 V_1]) = \min_{\Phi} \{ \Delta[U_2 U_1, (1_e \otimes \Phi)V_2 V_1] \}, \quad (B.2a) $$

\[ \leq \min_{\Phi} \{ \Delta[U_2 U_1, U_2 \otimes 1_e] + \Delta(U_2, (1_e \otimes \Phi)V_2 V_1) \}, \quad (B.2b) \]

\[ = \Delta[U_1, (1_e \otimes \Phi)V_1] + \min_{\Phi} \{ \Delta[U_2, (1_e \otimes \Phi)V_2 (1_e \otimes \Phi V_1)] \}, \quad (B.2c) \]

\[ \leq \Delta[U_1, (1_e \otimes \Phi)V_1] + \min_{\Phi} \{ \Delta[U_2, (1_e \otimes \Phi) V_2] + \Delta((1_e \otimes \Phi) V_2, V_2 (1_e \otimes \Phi V_2)] \}. \quad (B.2d) \]

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The final result of (B.2) is obtained through repeated usage of the bi-invariance of $\Delta$ and the triangle inequality. Because this inequality holds for all $\Phi_1, \Phi_2 \in U(H_e)$, it holds for the $\Phi_1$ that minimizes $\Delta[U_1, (1_e \otimes \Phi_1)V_1]$. Now, if $V_2 \in \mathcal{N}_{U(H_e)}[1_e \otimes U(H_e)]$, i.e. $V_2$ is an element of the normalizer of $1_e \otimes U(H_e)$ in $U(H_e)$, then for each $\Phi_1 \in U(H_e)$ there exists a $\Phi_2 \in U(H_e)$ such that $\Delta[(1_e \otimes \Phi_2)V_2, V_2(1_e \otimes \Phi_1)] = 0$. In particular, such a $\Phi_2$ exists for the minimizing operator $\Phi_1$. Therefore, under these conditions,

$$\Delta([U_2U_1], [V_2V_1]) \leq \min_{\Phi_1} \left\{ \Delta[U_1, (1_e \otimes \Phi_1)V_1] \right\} + \min_{\Phi_2} \left\{ \Delta[U_2, (1_e \otimes \Phi_2)V_2] \right\},$$

$$= \Delta([U_1], [V_1]) + \Delta([U_2], [V_2]).$$

From this result, the chaining property holds when $V_2 \in \mathcal{N}_{U(H_e)}[1_e \otimes U(H_e)] = U(H_s) \otimes U(H_e)$, i.e. the set of all decoupled or factorizable unitary operators in $U(H_e)$. This condition is satisfied by any $V_2$ that preserves the isolation of the system $S$ from the environment $E$, a crucial target in QC.

Appendix C. The normalizer and centralizer of $U(H_s) \otimes 1_e$ in $U(H_e)$

The lemmas from appendix B are repeated here for convenience.

**Lemma 1.** The normalizer of $U(H_s) \otimes 1_e$ in $U(H_e)$ is $U(H_s) \otimes U(H_e) := \{ \Psi \otimes \Phi : \Psi \in U(H_s) \text{ and } \Phi \in U(H_e) \}$. The normalizer of $1_e \otimes U(H_e)$ in $U(H_e)$ is also $U(H_s) \otimes U(H_e)$.

**Proof.** We determine the structure of the normalizer of $U(H_s) \otimes 1_e$ in $U(H_e)$; the structure of the normalizer of $1_s \otimes U(H_e)$ follows from the symmetry of the tensor product. First, we define a fixed non-degenerate diagonal unitary matrix $\Lambda \in U(H_s)$. Note that if $U \in \mathcal{N}_{U(H_s)}[1_e \otimes U(H_e)]$, then in particular, $U(\Lambda \otimes 1_e)^\dagger \in U(H_s) \otimes 1_e$. For simplicity, let $U(\Lambda \otimes 1_e)^\dagger = V \otimes 1_e$, where $V \in U(H_s)$. Because $U$ is unitary, $V \otimes 1_e$ and $\Lambda \otimes 1_e$ have the same eigenvalues (they are related by a similarity transformation), hence $V$ and $\Lambda$ must have the same eigenvalues, so there exists an $\Omega \in U(H_s)$ such that $\Omega V \Omega^\dagger = \Lambda$. Therefore,

$$\Omega \otimes 1_e)(\Lambda \otimes 1_e)(\Omega \otimes 1_e)^\dagger = \Lambda \otimes 1_e,$$

(C.1)

demonstrating that $(\Omega \otimes 1_e)U$ is an element of the stabilizer subgroup of $\Lambda \otimes 1_e$ with respect to the group action of conjugation. Hence,

$$(\Omega \otimes 1_e)U \in \underbrace{U(H_e) \oplus \cdots \oplus U(H_e)}_{n_e \text{ times}},$$

(C.2)

i.e. $(\Omega \otimes 1_e)U$ is block diagonal with $n_e$ blocks, each of which are $n_e \times n_e$ unitary matrices. So we have shown that any $U$ in the normalizer can be written as $U = (\Omega \otimes 1_e) V$ for some $\Omega \in U(H_s)$ and $V \in U(H_e)$. We can write

$$V = \begin{pmatrix} V_1 & \cdots & V_{n_e} \\ V_2 & \cdots & \vdots \\ \vdots & \ddots & \vdots \\ V_{n_e} & \cdots & V_1 \end{pmatrix},$$

(C.3)

where each $V_i \in U(H_e)$ for all $i$. 

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In order for $U$ to be in the normalizer subgroup, it must be true that for each $W \in \mathcal{U} \subseteq \mathcal{U}_c$, there exists an $X \in \mathcal{U} \otimes \mathcal{V}$ such that $U(W \otimes 1_e) = (X \otimes 1_e)U$. If $U = (\Omega_r \otimes 1_e)\rho_1$, we must have $V(W \otimes 1_e) = (\Omega_r X \Omega_r \otimes 1_e)V$. This condition implies that $w_{ij}V = (\Omega_r X \Omega_r)_{ij}V$ for all $1 \leq i, j \leq r$. Because $W$ is arbitrary, for each $i$ consider the case where $w_{1i} = 1$ (and $w_{ij} = 0$ for $j \neq i$), implying that $V_i$ is a scalar times $V_i$. Hence, $V = \text{diag}[\exp(i\delta_1), \ldots, \exp(i\delta_n)] \otimes \Phi \in \mathcal{U} \otimes \mathcal{V}$. Therefore, we conclude that $U = (\Omega_r \otimes 1_e)V \in \mathcal{U}_c \otimes \mathcal{U}_c$ and $\mathcal{N}_U(\mathcal{U}_c \otimes 1_e) \subseteq \mathcal{U}_c \otimes \mathcal{U}_c$.

For any $U = \Psi \otimes \Phi \in \mathcal{U}_c \otimes \mathcal{U}_c$, $U(U(c) \otimes 1_e)U^\dagger = \Psi U(c) \Psi^\dagger \otimes 1_e = U(c) \otimes 1_e$, so that $\mathcal{N}_U(\mathcal{U}_c \otimes 1_e) \subseteq \mathcal{U}_c \otimes \mathcal{U}_c$. Therefore, $\mathcal{N}_U(\mathcal{U}_c \otimes 1_e) = \mathcal{U}_c \otimes \mathcal{U}_c$.

**Lemma 2.** The centralizer of $\mathcal{U}(\mathcal{H}_c) \otimes 1_e$ in $\mathcal{U}_c$ is $1_e \otimes \mathcal{U}_c$. Likewise, the centralizer of $1_e \otimes \mathcal{U}_c$ in $\mathcal{U}_c$ is $\mathcal{U}_c \otimes 1_e$.

**Proof.** We consider the centralizer of $\mathcal{U}(\mathcal{H}_c) \otimes 1_e$ in $\mathcal{U}_c$, since the centralizer of $1_e \otimes \mathcal{U}_c$ in $\mathcal{U}_c$ follows from the symmetry of the tensor product. Because the centralizer must be a subset of the normalizer subgroup, each $U \in \mathcal{C}_U(\mathcal{U}(\mathcal{H}_c) \otimes 1_e)$ must be of the form $U = \Psi \otimes \Phi$ where $\Psi \in \mathcal{U}(\mathcal{H}_c)$ and $\Phi \in \mathcal{U}_c$. So,

$$\mathcal{C}_U(\mathcal{U}(\mathcal{H}_c) \otimes 1_e) = \{\Psi \otimes \Phi : \Psi \in \mathcal{U}_c, \Phi \in \mathcal{U}_c\}.$$  \hspace{1cm} (C.4)

Now, $(\Psi \otimes \Phi)(V \otimes 1_e)(\Psi \otimes \Phi)^\dagger = (\Psi \Psi^\dagger) \otimes 1_e$, so the only condition on $\Psi$ and $\Phi$ is that $\Psi$ must lie in the center of $\mathcal{U}_c$, i.e. $\Psi = \exp(i\theta) \otimes 1_e$ and $\Phi \in \mathcal{U}_c$. Then, $\Psi \otimes \Phi = \exp(i\theta) \otimes 1_e = \otimes (\exp(i\theta)) \in 1_e \otimes \mathcal{U}_c$. Therefore, $\mathcal{C}_U(\mathcal{U}(\mathcal{H}_c) \otimes 1_e) \subseteq 1_e \otimes \mathcal{U}_c$. Because every element of $1_e \otimes \mathcal{U}_c$ clearly commutes with $1_e \otimes \mathcal{U}_c$, we conclude that $\mathcal{C}_U(\mathcal{U}(\mathcal{H}_c) \otimes 1_e) = 1_e \otimes \mathcal{U}_c$.

**Appendix D. Centrality of the maximally mixed state**

We show that $\rho_{m,s} := 1_s/n_s$ is the density matrix with the ‘shortest’ maximum distance, under the Hilbert–Schmidt norm, to all other density matrices, i.e.

$$\rho_{m,s} = \arg \min_{\rho_1} \left( \max_{\rho_1} \left\| \rho_1 - \rho_{m,s} \right\|_2^2 \right) \hspace{1cm} (D.1a)$$

where

$$\min_{\rho_1} \left( \max_{\rho_1} \left\| \rho_1 - \rho_{m,s} \right\|_2^2 \right) = \frac{n_s - 1}{n_s}. \hspace{1cm} (D.1b)$$

**Proof.** Let $\rho_2 = \sum_i \xi_i |i\rangle \langle i|$ with $0 \leq \xi_1 \leq \cdots \leq \xi_n \leq 1$, and define the Hilbert–Schmidt distance as

$$f(\rho_1) := \| \rho_2 - \rho_1 \|_2^2 = \| \rho_2 \|_2^2 + \| \rho_1 \|_2^2 - 2 \text{Tr}(\rho_2 \rho_1). \hspace{1cm} (D.2)$$

If $\rho_1 = |1\rangle \langle 1|$, then $f(\rho_1) = \| \rho_2 \|_2^2 + 1 - 2\xi_1$. Thus, $\max_{\rho_1} f(\rho_1) \geq \| \rho_2 \|_2^2 + 1 - 2\xi_1$. Now, $\text{Tr}(\rho_2 \rho_1) = \sum_i \xi_i |i\rangle \langle i| \rho_1 |i\rangle$ for all $\rho_1$, where $\sum_i |i\rangle \langle i| = \text{Tr}(\rho_1) = 1$, so $\text{Tr}(\rho_2 \rho_1) \geq \xi_1$. Also, $\| \rho_1 \|_2 \leq 1$ in general, which implies that $f(\rho_1) \leq \| \rho_2 \|_2^2 + 1 - 2\xi_1$ for all $\rho_1$. Therefore,

$$\max_{\rho_1} \| \rho_2 - \rho_1 \|_2^2 = \| \rho_2 \|_2^2 + 1 - 2\xi_1. \hspace{1cm} (D.3)$$
To minimize this expression over $\rho_2$, we want to minimize $\|\rho_2\|_{\text{HS}}^2$ and maximize $\zeta_1$. Because $\zeta_1$ is the minimum eigenvalue of $\rho_2$, its maximum value of $1/n_s$ occurs when $\rho_2 = \mathbb{1}_s/n_s$. Likewise, $\|\rho_2\|_{\text{HS}}^2$ takes its minimum value $1/n_s$ at $\rho_2 = \mathbb{1}_s/n_s$. So, indeed the argument of $\min_{\rho_2} \max_{\rho_1} \|\rho_2 - \rho_1\|_{\text{HS}}$ is $\rho_{m,s} = \mathbb{1}_s/n_s$ and its value is $(n_s - 1)/n_s$. □

### Appendix E. Relating the distance measure to fidelity

We demonstrate that the inequality relation between the distance and fidelity of quantum states presented in (39) [40] also applies to the distance and fidelity of quantum operations given by $\Delta_{\text{HS}}([U], [V_s \otimes \mathbb{1}_c])$ in (22) and $\mathcal{F}_{m,c}(\mathcal{K}, V_s)$ in (51):

$$\left[1 - \tilde{\Delta}_{\text{HS}}([U], [V_s \otimes \mathbb{1}_c])\right]^2 \leq \mathcal{F}_{m,c}(\mathcal{K}, V_s) \leq 1 - \Delta_{\text{HS}}([U], [V_s \otimes \mathbb{1}_c])^2. \quad (E.1)$$

**Proof.** We first show that the bounds on $\mathcal{F}_{m,c}(\mathcal{K}, V_s)$ follow from $\|\Gamma\|_2 = \max_i \sigma_i \leq n_s$, where $\sigma_i$ is the $i$th singular value of $\Gamma$. Then we show that $\|\Gamma\|_2 \leq n_s$ holds.

The upper bound holds if and only if $\|\Gamma\|_{\text{HS}}^2 \leq n_s \|\Gamma\|_{\text{Tr}}$, or equivalently, $\sum_i \sigma_i^2 \leq n_s \sum_i \sigma_i$. Assuming that $\max_i \sigma_i \leq n_s$, it immediately follows that $\sum_i \sigma_i^2 \leq n_s \sum_i \sigma_i$, which establishes the upper bound.

With some algebraic rearrangement, the lower bound becomes $\|\Gamma\|_{\text{Tr}} + (1/n_s)\|\Gamma\|_{\text{HS}}^2 \leq 2\sqrt{n_s}\|\Gamma\|_{\text{HS}}$. If $\|\Gamma\|_2 \leq n_s$, which implies that $\|\Gamma\|_{\text{HS}}^2 \leq n_s \|\Gamma\|_{\text{Tr}}$ and $\|\Gamma\|_{\text{Tr}} + 1/n_s\|\Gamma\|_{\text{HS}}^2 \leq 2\|\Gamma\|_{\text{Tr}}$, the lower bound holds if $\|\Gamma\|_{\text{Tr}} \leq \sqrt{n_s}\|\Gamma\|_{\text{HS}}$. This is a known inequality for any matrix and thus establishing the lower bound. To prove this inequality, let $\vec{\sigma}$ and $\vec{\tau}$ be two $k$-dimensional vectors (where $k \leq n_c$) with entries $\sigma_i$, which are the singular values of $\Gamma$, and $\tau_i = 1$ for all $i$, respectively. It follows from the Cauchy–Schwarz inequality that $\|\vec{\sigma}\|_2 = \sum_i \sigma_i^2 = \|\vec{\sigma}\|_1 = \langle \vec{\sigma}, \vec{\tau} \rangle \leq \|\vec{\sigma}\|_2 \|\vec{\tau}\|_2 = \sqrt{k}\|\vec{\sigma}\|_2 = \sqrt{k}\|\Gamma\|_{\text{HS}} \leq \sqrt{n_c}\|\Gamma\|_{\text{HS}}$, where, for a vector, $\|\cdot\|_2$ is the Euclidean norm (also referred to as the $\ell_2$ norm):

$$\|\vec{\sigma}\|_2 := \left(\sum_{i=1}^k \sigma_i^2\right)^{\frac{1}{2}}. \quad (E.2)$$

To show that $\sigma_i \leq n_s$, consider

$$\|\Gamma\psi\|_2 = \|\text{Tr}_s[U(V_{\psi}^\dagger \otimes \mathbb{1}_c)]\psi\|_2, \quad (E.3a)$$

$$= \|\text{Tr}_s[U(V_{\psi}^\dagger \otimes \mathbb{1}_c)(\mathbb{1}_s \otimes |\psi\rangle)]\|_2, \quad (E.3b)$$

where $\dim\{|\psi\rangle\} = n_c$ and $\langle\psi|\psi\rangle = 1$. Applying the Cauchy–Schwarz inequality [64] to the argument of (E.3b) yields

$$\|\Gamma\psi\|_2 \leq \sqrt{n_c}\|U(V_{\psi}^\dagger \otimes \mathbb{1}_c)(\mathbb{1}_s \otimes |\psi\rangle)\|_2. \quad (E.3c)$$

Because the two-norm is bounded from above by the Hilbert–Schmidt norm [64],

$$\|\Gamma\psi\|_2 \leq \sqrt{n_c}\|U(V_{\psi}^\dagger \otimes \mathbb{1}_c)(\mathbb{1}_s \otimes |\psi\rangle)\|_{\text{HS}}, \quad (E.3d)$$

$$= \sqrt{n_c}\|\mathbb{1}_s \otimes |\psi\rangle\|_{\text{HS}}, \quad (E.3e)$$

$$= n_s \langle\psi|\psi\rangle = n_s. \quad (E.3f)$$

Since $\|\Gamma\psi\|_2 \leq n_s$ is true for all normalized $|\psi\rangle$, it follows that $\|\Gamma\|_2 \leq n_s$. □
Appendix F. Optimal control objective functional: $\mathcal{J}_n^{[V]}$

In section 7.2, we use the objective functional $\mathcal{J}_n^{[V]}$ in (57), which corresponds to a special situation (although ubiquitous in QC), where the target unitary transformation $V_e \in U(H_c)$ is specified for a closed system (i.e. for the system $S$). As discussed in section 3.1, in this situation the target unitary operator $V \in U(H_c)$ should be replaced by the tensor product $V_e \otimes \mathbb{1}_e$ in the quotient metric, leading to the Hilbert–Schmidt norm distance $\tilde{\Delta}_{HS}([U], [V_e \otimes \mathbb{1}_e])$ of (22). However, in this appendix, we consider a more general case: an arbitrary target unitary operator $V \in U(H_c)$, not necessarily the tensor-product one. The corresponding objective functional $\mathcal{J}_n^{[V]}$ is

$$\mathcal{J}_n^{[V]}(C) := \tilde{\Delta}_{HS}([U_n(C)], [V]) + \frac{\alpha}{2} ||C||^2_{HS},$$

(F.1)

where the Hilbert–Schmidt norm distance $\tilde{\Delta}_{HS}([U], [V])$ is defined by (14) and (15).

F.1. Computing $\text{grad}\, \tilde{\Delta}([U], [V])_{HS}$

Let $H_n$ denote the space of $n \times n$ Hermitian matrices, i.e. $H_n = \{A \in M_n(\mathbb{C}) : A^\dagger = A\}$. We endow the linear spaces $H_n$ and $M_n(\mathbb{C})$ with the real Hilbert–Schmidt inner product in (A.1), and $U(H_c)$ is given the Riemannian metric induced by this inner product. Define maps $y, Z$ and $\Gamma_V$ by

$$y : H_n \rightarrow \mathbb{R}, \quad y(Z) := \sqrt{1-n^{-1}} \text{Tr}(Z),$$

$$Z : M_n(\mathbb{C}) \rightarrow H_n, \quad Z(\Gamma) := \sqrt{\Gamma^\dagger \Gamma},$$

$$\Gamma_V : U(H_c) \rightarrow M_n(\mathbb{C}), \quad \Gamma_V(U) := \text{Tr}_e[U V^\dagger].$$

(F.2)

For any fixed equivalence class $[V] \in \mathcal{Q}$, let $\Delta_{HS}^{[V]} : U(H_c) \rightarrow \mathbb{R}$ be defined by $\Delta_{HS}^{[V]}(U) := \tilde{\Delta}_{HS}([U], [V])$. Then $\Delta_{HS}^{[V]}(U) = y \circ Z \circ \Gamma_V(U)$, and the differential of $\Delta_{HS}^{[V]}$ at the point $U \in U(H_c)$ in the direction $\delta U \in T_U U(H_c)$ is given by the chain rule:

$$d_U \Delta_{HS}^{[V]}(\delta U) = d_Z(\Gamma_V(U)) y \circ d_{\Gamma_V(U)} Z \circ d_U \Gamma_V(\delta U).$$

(F.3)

The differential and the gradient are related through the Riemannian metric by $d_U \Delta_{HS}^{[V]}(\delta U) = \langle \text{grad} \, \Delta_{HS}^{[V]}(U), \delta U \rangle$ for all $\delta U \in T_U U(H_c)$ [65]. Using (F.3), we can also write

$$d_U \Delta_{HS}^{[V]}(\delta U) = \langle \text{grad} \, y[Z[\Gamma_V(U)]], d_{\Gamma_V(U)} Z \circ d_U \Gamma_V(\delta U) \rangle,$$

$$= \langle (d_U \Gamma_V)^* \circ (d_{\Gamma_V(U)} Z)^*(\text{grad} \, y[Z[\Gamma_V(U)]]), \delta U \rangle,$$

(F.4a)

where $\text{grad} \, y[Z[\Gamma_V(U)]]$ denotes the gradient of $y$ at the point $Z[\Gamma_V(U)]$ and $^*$ denotes the operator adjoint. So, we can compute the desired gradient as

$$\text{grad} \, \Delta_{HS}^{[V]}(U) = (d_U \Gamma_V)^* \left\{ (d_{\Gamma_V(U)} Z)^* \text{grad} \, y[Z[\Gamma_V(U)]] \right\}.$$  

(F.4b)

To do this, we must find expressions for the gradient and two adjoint operators on the right-hand side of (5). We develop each of these differentials separately.

We begin by first computing $\text{grad} \, y$. For $y(Z) = \sqrt{1-n^{-1}} \text{Tr}(Z)$, the argument of the square root is an affine scalar function of $Z$, so $d_Z y(\delta Z) = -\text{Tr}(\delta Z)/[2n \, y(Z)]$. The gradient
is then given by \( d_Z \, y(\delta Z) = \langle \text{grad} \, y(Z), \delta Z \rangle = \text{Re}[\text{Tr}(\text{grad} \, y(Z) \delta Z)] = \text{Tr}[\text{grad} \, y(Z) \delta Z] \). Hence,

\[
\text{grad} \, y(Z) = -\frac{1}{[2n \, y(Z)]}.
\]  

(F.6)

We now turn to the problem of differentiating \( Z \). Differentiating a square root in a commutative setting is straightforward; we used this fact to differentiate \( y \). But for matrices, non-commutativity may cause trouble. So, we begin by rewriting the definition of \( Z \) as \( Z^2 = \Gamma^\dagger \Gamma \), and differentiating both sides:

\[
Z \frac{d}{d\Gamma} Z(\delta \Gamma) + \frac{d}{d\Gamma} Z(\delta \Gamma) Z = \delta \Gamma^\dagger \Gamma + \Gamma^\dagger \delta \Gamma.
\]  

(F.7)

Define \( \nu : \mathcal{M}_{n_n}(\mathbb{C}) \to \mathbb{C}^{n^2} \) to be the linear operator that stacks the columns of a square matrix to create a vector. If we let \( \mathcal{M}_{n_n}(\mathbb{C}) \) and \( \mathbb{C}^{n^2} \) both be real Hilbert spaces with respective inner products \( \langle A, B \rangle = \text{Re}[\text{Tr}(A^\dagger B)] \) and \( \langle x, y \rangle = \text{Re}(x^\dagger y) \), then \( \nu \) is a linear isometry [60] between these two spaces:

\[
\langle A, B \rangle = \sum_{i,j} \text{Re}(A_{ij}) \text{Re}(B_{ij}) + \text{Im}(A_{ij}) \text{Im}(B_{ij}) = \langle \nu(A), \nu(B) \rangle,
\]

(F.8)

for all \( A, B \in \mathcal{M}_{n_n}(\mathbb{C}) \). Hence \( \nu^* = \nu^{-1} \) is the ‘matrix-ization’ operator that returns a square matrix.

From the discussion of matrix equations and the Kronecker product in [82], we can rewrite (F.7) as

\[
\left[ Z^T \otimes 1 + 1 \otimes Z \right] \nu \left[ \frac{d}{d\Gamma} Z(\delta \Gamma) \right] = \nu(\delta \Gamma^\dagger \Gamma + \Gamma^\dagger \delta \Gamma).
\]

(F.9)

By construction, \( Z \) will be Hermitian and positive semi-definite; the transpose \( Z^T \) will also be Hermitian and will have the same eigenvalue decomposition as \( Z \). Because of this, we know that \( Z^T \otimes 1 + 1 \otimes Z \) will also be Hermitian and positive semi-definite (the eigenvalues of the Kronecker sum are just the set of all pairwise sums of the eigenvalues of \( Z \)). If we assume that \( Z \) is positive definite, then \( Z^T \otimes 1 + 1 \otimes Z \) will also be positive definite and this linear system will have a unique solution:

\[
\frac{d}{d\Gamma} Z(\delta \Gamma) = \nu^*[\left(Z^T \otimes 1 + 1 \otimes Z\right)^{-1} \nu(\delta \Gamma^\dagger \Gamma + \Gamma^\dagger \delta \Gamma)].
\]

(F.10)

Let \( \mathcal{L}_\Gamma : \mathcal{M}_{n_n}(\mathbb{C}) \to \mathcal{M}_{n_n}(\mathbb{C}) \) be given by \( \mathcal{L}_\Gamma(A) = A^\dagger \Gamma + \Gamma^\dagger A \). Then, considering \( \mathcal{M}_{n_n}(\mathbb{C}) \) to be a real Hilbert space with the real Hilbert–Schmidt inner product, \( \mathcal{L}_\Gamma \) is a linear operator, and we can find its adjoint:

\[
\langle A, \mathcal{L}_\Gamma^* (B) \rangle = \langle \mathcal{L}_\Gamma (A), B \rangle = \langle A^\dagger \Gamma + \Gamma^\dagger A, B \rangle,
\]

(F.11a)

\[
= \text{Re}[\text{Tr}(\Gamma^\dagger AB + A^\dagger \Gamma B)],
\]

(F.11b)

\[
= \text{Re}[\text{Tr}((\Gamma B)^\dagger A + (\Gamma B)^\dagger A)] = \langle A, \Gamma (B + B^\dagger) \rangle,
\]

(F.11c)

for a given \( B \in \mathcal{M}_{n_n}(\mathbb{C}) \) and all \( A \in \mathcal{M}_{n_n}(\mathbb{C}) \). Hence, \( \mathcal{L}_\Gamma^* (B) = \Gamma (B + B^\dagger) \). Then,

\[
\frac{d}{d\Gamma} Z = \nu^* \circ \left(Z^T \otimes 1 + 1 \otimes Z\right)^{-1} \circ \nu \circ \mathcal{L}_\Gamma
\]

(F.12a)

and

\[
\frac{d}{d\Gamma} Z^* = \mathcal{L}_\Gamma^* \circ \nu^* \circ \left(Z^T \otimes 1 + 1 \otimes Z\right)^{-1} \circ \nu.
\]

(F.12b)
Using \( \text{grad} \ y(Z) = -1/[2n \, y(Z)] \) derived previously yields

\[
\frac{1}{2n \, y(Z)} \mathcal{L}_R^{\star} \circ v^\star \circ (Z \otimes 1 + 1 \otimes Z)^{-1} \circ v(1). \tag{F.13}
\]

Note that \( v^\star \circ (Z^T \otimes 1 + 1 \otimes Z)^{-1} \circ v(1) \) is just the matrix solution to the problem \( ZA + AZ = 1 \), and therefore is \( A = \frac{1}{2}Z^{-1} \), since we are assuming \( Z \) is not just positive semi-definite, but positive definite. Then,

\[
d_R \, Z^* [\text{grad} \ y(Z)] = -\frac{1}{4n \, y(Z)} \mathcal{L}_R^{\star} (Z^{-1})
= -\frac{1}{4n \, y(Z)} \Gamma Z^{-1}. \tag{F.14}
\]

For the differential of \( \Gamma_V \), we can extend \( \Gamma_V \) to \( \tilde{\Gamma}_V : \mathcal{M}_n(\mathbb{C}) \to \mathcal{M}_n(\mathbb{C}) \), by letting \( \tilde{\Gamma}_V(A) = \text{Tr}_s(AV^\top) \). Then, \( \tilde{\Gamma}_V \) is a linear map, so the differential of \( \tilde{\Gamma}_V \) is just itself, i.e.

\[
d_{A} \tilde{\Gamma}_V(\delta A) = \tilde{\Gamma}_V(\delta A).
\]

For any \( \delta U \in T_U \mathcal{U}(\mathcal{H}_c) \), \( d_{U} \tilde{\Gamma}_V(\delta U) = d_{U} \tilde{\Gamma}_V(\delta U) = \tilde{\Gamma}_V(\delta U) \). We can find the adjoint of \( d_{U} \tilde{\Gamma}_V \) by

\[
\langle [d_{U} \tilde{\Gamma}_V]^* (B), \delta U \rangle = \langle B, d_{U} \tilde{\Gamma}_V(\delta U) \rangle = \text{Re} \{ \text{Tr} [B^\top d_{U} \tilde{\Gamma}_V(\delta U)] \}, \tag{F.15a}
\]

\[
= \text{Re} \{ \text{Tr} [B^\top \text{Tr}_s(\delta U \, V^\top)] \}, \tag{F.15b}
\]

\[
= \text{Re} \{ \text{Tr} [\delta U \, V^\top (1 \otimes B^\top)] \}, \tag{F.15c}
\]

\[
= \frac{1}{2} \langle (1 \otimes B) \, V - UV^\top (1 \otimes B^\top) \, U, \delta U \rangle, \tag{F.15d}
\]

where the last step involves projecting \((1 \otimes B) \, V \) onto \( T_U \mathcal{U}(\mathcal{H}_c) \). Hence, \( (d_{U} \tilde{\Gamma}_V)^* (B) = \frac{1}{2} [(1 \otimes B) \, V - UV^\top (1 \otimes B^\top) \, U] \) for any \( B \in \mathcal{M}_n(\mathbb{C}) \).

Combining these components, we find that

\[
\text{grad} \ \Delta_{HS}^{\gamma}(U) = (d_{U} \tilde{\Gamma}_V)^* \left[ (d_{U} \tilde{\Gamma}_V) Z^* \left( \text{grad} \ y(Z) \, [\Gamma_V(U)] \right) \right]. \tag{F.16a}
\]

\[
= -\frac{1}{4n \, \Delta_{HS}^{\gamma}(U)} \langle R - UR^\top U, \rangle \tag{F.16b}
\]

where \( R = (1 \otimes \{ \Gamma_V(U) \, Z^{-1} [\Gamma_V(U)] \}) \, V = [1 \otimes (\Omega W^\top)] \, V \) and \( \Gamma_V(U) = \Omega SW^\top \) is the SVD of \( \Gamma_V(U) \). Since \( V \in \mathcal{U}(\mathcal{H}_c) \) and \( \Omega W^\top \in \mathcal{U}(\mathcal{H}_c) \), we have \( R \in \mathcal{U}(\mathcal{H}_c) \). Note that \( R \) is the element of the equivalence class \([V]\) that is closest to \( U \) under the Hilbert–Schmidt distance, i.e.

\[
R = (1_s \otimes \Phi) \, V, \text{ where } \Phi := \arg \min_{\Phi} \{ \| U - (1_s \otimes \Phi) \, V \|_{HS} \}.
\]

**F.2. Explicitly coupling the Schrödinger equation to the objective functional**

In this section, we consider the problem of coupling the Schrödinger equation to the kinematic cost function \( \Delta_{HS}^{\gamma}(U) \) to arrive at a gradient flow through the space of controls \( \mathbb{K}_t \) leading to an optimal control. To do this, we need to clarify the definition and geometry of \( \mathbb{K}_t \).

Let \( \eta : [0, t_e] \to \mathbb{R} \), the ‘shape function’, be positive almost everywhere and continuous (and therefore bounded). Define the inner product on \( \mathbb{K}_t \) as

\[
(f, g)_{\mathbb{K}_t} := \int_0^{t_e} \frac{f(t)g(t)}{\eta(t)} \, dt, \tag{F.17}
\]

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where $\mathbb{K}_{t}$ is the set of (equivalence classes of) functions $f \in L^2([0, t_i]; \mathbb{R})$ such that $\|f\|_{\mathbb{K}_{t_i}} < \infty$. Bilinearity, symmetry and non-negativity of the inner product $\langle \cdot, \cdot \rangle_{\mathbb{K}_{t_i}}$ are clear from the definition. When $\eta(t) \equiv 1$, $\mathbb{K}_{t}$ is $L^2([0, t_i]; \mathbb{R})$ with the standard inner product. Other choices of $\eta(t)$ change the standard geometry, moving undesirably shaped functions far away from the origin, or out to infinity, where they are less likely to be the targets of an optimization on $\mathbb{K}_{t}$. This point is discussed in more detail throughout this section. For the optimizations performed in this work, $\eta(t) = \sin(\pi t / t_1)$.

To make this approach (and geometric interpretation) rigorous, we need to verify that $\mathbb{K}_{t}$ is indeed a Hilbert space under the inner product $\langle \cdot, \cdot \rangle_{\mathbb{K}_{t}}$ in (F.17). Suppose $f$ is a measurable function such that $\|f\|_{\mathbb{K}_{t}} < \infty$. Because $\eta$ is positive almost everywhere and bounded above, $1/\eta$ is positive everywhere and bounded below by some $\beta > 0$. Then,

$$\|f\|_{\mathbb{K}_{t}}^2 = \int_0^{t_i} \frac{f^2(t)}{\eta(t)} \, dt > \beta \|f\|_{L^2}^2 := \beta \int_0^{t_i} f^2(t) \, dt. \quad \text{(F.18)}$$

Hence, $\|f\|_{L^2} < \infty$, so that $f \in L^2([0, t_i]; \mathbb{R})$, where $\|\cdot\|_{L^2}$ denotes the $L^2$ norm on $[0, t_i]$. If $f(t) \neq 0$ on a set of nonzero measure, then $f^2(t) > 0$ on a set of nonzero measure (analogously for $\eta(t)$ and $f^2(t)/\eta(t)$). Hence, $\|f\|_{\mathbb{K}_{t}} > 0$, so we have non-degeneracy, and $\mathbb{K}_{t}$ is thus an inner product space.

Suppose that $\{f_k\}$ is a Cauchy sequence in $\mathbb{K}_{t}$ [60]. Then $g_k := f_k / \sqrt{\eta}$ is a Cauchy sequence in $L^2$, i.e. $\|g_k - g_{k'}\|_{L^2} = \|f_k - f_{k'}\|_{\mathbb{K}_{t}} \to 0$. Since $L^2([0, t_i]; \mathbb{R})$ is complete, this implies that $g_k \to g \in L^2([0, t_i]; \mathbb{R})$. Let $f := g / \sqrt{\eta}$, thus,

$$\|f\|_{\mathbb{K}_{t}}^2 = \int_0^{t_i} \frac{f^2(t) / \eta(t)}{g^2(t)} \, dt = \int_0^{t_i} \frac{f^2(t)}{\eta(t)} \, dt = \|g\|_{L^2}^2 < \infty \quad \text{(F.19a)}$$

and

$$\|f_k - f\|_{\mathbb{K}_{t}}^2 = \int_0^{t_i} \frac{\left[f_k(t) - f(t)\right]^2}{\eta(t)} \, dt, \quad \text{(F.19b)}$$

$$= \int_0^{t_i} \left[g_k(t) - g(t)\right]^2 \, dt = \|g_k - g\|_{L^2}^2 \to 0, \quad \text{(F.19c)}$$

so that $f \in \mathbb{K}_{t}$ and $f_k \to f$ in the topology induced by $\langle \cdot, \cdot \rangle_{\mathbb{K}_{t}}$. Hence, $\mathbb{K}_{t}$ with $\langle \cdot, \cdot \rangle_{\mathbb{K}_{t}}$ is a complete inner product space, i.e. a Hilbert space. We have not simply effected a change in geometry, but we also have restricted the domain to a linear subspace of $L^2([0, t_i]; \mathbb{R})$. If $C \in L^2([0, t_i]; \mathbb{R})/\mathbb{K}_{t}$, then $\mathcal{J}_{t}^{[\psi]} = \infty$, so that $C$ is not a viable solution. This new geometry puts desirable functions near the origin and undesirable functions out near infinity, which makes this optimization different from the unshaped version.

Now, consider the mapping $U_{t_i}: \mathbb{K}_{t} \to \mathcal{U}(\mathcal{H}_c)$ introduced in section 7.2. The differential of the final-time evolution operator $U_{t_i}$ with respect to the control field depends on evolution operators at all times in $[0, t_i]$. It is shown in [77] that

$$d_C U_{t_i}(\delta C) = iU_{t_i}(C) \int_0^{t_i} U^\dagger(t; C) \mu U(t; C) \delta C(t) \, dt, \quad \text{(F.20)}$$

where $\mu$ is the dipole moment operator (e.g. $\mu = \sum_i \mu_i S_i$ in (53)). With the usual Hilbert–Schmidt inner product as the Riemannian metric on $\mathcal{U}(\mathcal{H}_c)$, we can find the adjoint
of this differential: for any \( A \in T_{U(t)}(\mathcal{K}) \) and all \( \delta C \in T_C \mathcal{K} \simeq \mathcal{K} \),
\[
\{(d_C U_t)'^*(A), \delta C\}_{\mathcal{K}} = \{A, d_C U_t(\delta C)\}_{T_{U(t)}(\mathcal{K})}, \tag{F.21a}
\]
\[
= \text{Re} \left\{ \text{Tr} \left[ i A^T U_t(C) \int_0^t U^\dagger(t; C) \mu U(t; C) \delta C(t) \ d t \right] \right\}, \tag{F.21b}
\]
\[
= \int_0^t \text{Re} \{ \text{Tr} [i A^T U_t(C) U^\dagger(t; C) \mu U(t; C)] \delta C(t) \ d t \}, \tag{F.21c}
\]
\[
= \{ \eta \text{Re} \{ \text{Tr} [i A^T U_t(C) U^\dagger(t; C) \mu U(t; C)] \}, \delta C\}_{\mathcal{K}}. \tag{F.21d}
\]
So that
\[
[(d_C U_t)'^*(A)](t) = -\eta(t) \text{Im} \{ \text{Tr} [A^T U_t(C) U^\dagger(t; C) \mu U(t; C)] \}. \tag{F.22}
\]

With \( J_{\mu}^{[V]}(C) \) in (1), using previous arguments regarding the chain rule on gradients, we obtain
\[
(\text{grad} J_{\mu}^{[V]}(C))(t) = [(d_C U_t)^*(\text{grad} \Delta_{\mu}^{[V]}[U_t(C)])](t) + \alpha C(t), \tag{F.23a}
\]
\[
= \frac{\eta(t)}{4 n \Delta_{\mu}^{[V]}[U_t(C)]} \text{Im} \{ \text{Tr} \left\{ [R^T - U^\dagger(t; C) R U^\dagger(t; C)] U_t(C) U^\dagger(t; C) \mu U(t; C) \right\} + \alpha C(t), \tag{F.23b}
\]
\[
= \frac{\eta(t)}{4 n \Delta_{\mu}^{[V]}[U_t(C)]} \text{Im} \{ \text{Tr} \left\{ [R^T U_t(C) - U^\dagger(t; C) R] U^\dagger(t; C) \mu U(t; C) \right\} + \alpha C(t). \tag{F.23c}
\]

Observe that \( \tilde{\Delta}_{\mu} \) is continuous on \( U(\mathcal{K}) \), and therefore bounded. It is shown in [77] that \( \| (d_C U_t)^* \| \) is uniformly bounded for all \( C \in \mathcal{K} \). In fact, \( \| (d_C U_t)^* \|_{\infty} \leq \| \mu \|_{\mu} \| \eta \|_{L^1}^{1/2} \), where \( \| \cdot \|_{L^1} \) denotes the \( L^1 \) norm.\(^{10}\) Therefore, there exists a \( \kappa > 0 \) such that
\[
\left\| (d_C U_t)^*(\text{grad} \Delta_{\mu}^{[V]}[U_t(C)]) \right\| \leq \kappa \tag{F.24}
\]
for all \( C \in \mathcal{K} \). Then, since
\[
C(t) = -\frac{\eta(t)}{4 n \Delta_{\mu}^{[V]}[U_t(C)]} \text{Im} \{ \text{Tr} \left\{ [R^T U_t(C) - U^\dagger(t; C) R] U^\dagger(t; C) \mu U(t; C) \right\} \}, \tag{F.25}
\]
at a local extremum of \( J_{\mu}^{[V]} \), all local extrema of \( J_{\mu}^{[V]} \) must lie within the hypersphere \( \| C \| \leq \kappa / \alpha \). From this perspective, the role of the shape function can be interpreted as moving undesirably shaped controls outside of this hypersphere, to the region where they can no longer act as local extrema of \( J_{\mu}^{[V]} \). Note that both the space \( K_{\mu} \) and the control objective \( J_{\mu}^{[V]} \) depend on the shape function \( \eta(t) \). When a shape function is used in an iterative optimization routine via (F.23), this results in the minimization of a different (though conceptually related) objective on a different space than when \( \eta(t) \equiv 1 \).

\(^{10}\) Here, \( \| (d_C U_t)^* \|_{\infty} \) denotes the operator norm [64]: \( \| (d_C U_t)^* \|_{\infty} := \sup_{U(t) \in \mathcal{K} \setminus \{0\}} \frac{\| (d_C U_t)^*(\delta U) \|_{\mathcal{K}}}{\| \delta U \|_{\mathcal{K}}} \).
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