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Quantum fidelity and relative entropy between unitary orbits

by

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Abstract

Fidelity and relative entropy are two significant quantities in quantum information theory. We study the quantum fidelity and relative entropy under unitary orbits. The maximal and minimal quantum fidelity and relative entropy between two unitary orbits are explicitly derived. The potential applications in quantum computation and information processing are discussed.

1 Introduction

There are many important quantities in characterizing a bipartite or multipartite quantum state, such as the mutual information, quantum correlation and entanglement etc. in quantum information theory. To investigate the variations of such quantities under *unitary dynamics* has practical applications. In [1, 2], by searching for the maximally and minimally correlated states on a unitary orbit, the authors studied the amount of correlations, quantified by the quantum mutual information, attainable between the components of a quantum system, when the system undergoes isolated, unitary dynamics. The correlations in a bipartite or multipartite state within the construction of unitary orbits have been also examined in [3].

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In fact, there are also many important quantities in characterizing the relations between two quantum states, such as the quantum fidelity and relative entropy. They give rise to the measures of a kind of distance between two quantum states. They can be also used to characterize the property of a given quantum state, for instance, to quantify the quantum entanglement between two parts of a state, which is the shortest distance between the state and the set of all separable states. Such distances between two quantum states have many applications in quantum information processing. In [4] it has been shown that the problem of deterministically quantum state discrimination is equivalent to that of embedding a simplex of points whose distances are maximal with respect to the Bures distance or trace distance of two quantum states.

In this paper, we study the quantum fidelity and relative entropy under arbitrary unitary dynamics. Under general unitary evolutions, every given quantum state belongs to a continuous orbit. We analyze the 'distance' between two quantum states under general unitary evolutions: the maximal and minimal quantum fidelity and relative entropy between two such unitary orbits, by using the combinatory techniques in majorization theory and operator monotones. It is also shown that they are intervals between these minimal and the maximal values.

The paper is organized as follows: In Sect. 2 we derive the maximal and minimal values of the quantum fidelity between the unitary orbits of two quantum states. Moreover, we prove that the values of the quantum fidelity fill out an interval. We also discuss the fidelity evolution generated by Hamiltonian. In Sect. 3 we consider the optimal problems for relative entropy and derive the maximal and minimal values of the relative entropy between the unitary orbits of two quantum states. We summarize and discuss in Sect. 4.

2   Quantum fidelity between unitary orbits

The *fidelity* between two $d \times d$ quantum states, represented by density operators ρ and σ, is defined as

$$\mathrm{F}(\rho, \sigma) = \mathrm{Tr} \left(\sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right) \equiv \mathrm{Tr} \left(|\sqrt{\rho} \sqrt{\sigma}| \right). \tag{2.1}$$

This is an extremely fundamental and useful quantity in quantum information theory. In quantum information processing, one wishes to transform a given quantum state to the final target state. For instance, in the quantum computation with qubits or qutrits, it is essential to estimate the "distance" between the desired target state and the approximate state that can be realized by projected Hamiltonian [5, 6]. Practically, due to the inevitable interaction between the quantum systems and its environment and possible experimental imperfectness, it is crucial to characterize quantitatively to what extent can an evolved quantum state be close to the target state. For this

purpose, the fidelity is often used as the measure of the distance between two quantum states. The squared fidelity above has been called *transition probability* [7, 8]. Operationally it is the maximal success probability of transforming a state to another one by measurements on a larger quantum system. The fidelity is also employed in a number of problems such as quantifying entanglement [9] and quantum error correction [10].

Let $\mathrm{U}\left(\mathcal{H}_d\right)$ denote the set of $d \times d$ unitary matrices on d-dimensional Hilbert space $\mathcal{H}_d$. For a given density matrix ρ, its *unitary orbit* is defined by

$$\mathcal{U}_\rho = \left\{ U\rho U^\dagger : U \in \mathrm{U}\left(\mathcal{H}_d\right) \right\}. \tag{2.2}$$

Clearly a density operator ρ whose evolution is governed by a von Neumann equation remains in a single orbit $\mathcal{U}_\rho$. The orbits $\mathcal{U}_\rho$ are in one-to-one correspondence with the possible spectra for density operators ρ.

We investigate the bound of the quantum fidelity between the unitary orbits $\mathcal{U}_\rho$ and $\mathcal{U}_\sigma$ of two quantum states ρ and σ. Due to the unitary invariance of fidelity, the problem boils down to determining the following extremes: $\min_{U \in \mathrm{U}(\mathcal{H}_d)} \mathrm{F}(\rho, U\sigma U^\dagger)$ and $\max_{U \in \mathrm{U}(\mathcal{H}_d)} \mathrm{F}(\rho, U\sigma U^\dagger)$.

Let $\mathrm{F}(p,q) = \sum_j \sqrt{p_j q_j}$ denote the classical fidelity between two probability distributions $p = \{p_j\}$ and $q = \{q_j\}$.

Theorem 2.1. *The quantum fidelity between the unitary orbits $\mathcal{U}_\rho$ and $\mathcal{U}_\sigma$ satisfy the following relations;*

$$\max_{U \in \mathrm{U}(\mathcal{H}_d)} \mathrm{F}(\rho, U\sigma U^\dagger) = \mathrm{F}(\lambda^\downarrow(\rho), \lambda^\downarrow(\sigma)), \tag{2.3}$$

$$\min_{U \in \mathrm{U}(\mathcal{H}_d)} \mathrm{F}(\rho, U\sigma U^\dagger) = \mathrm{F}(\lambda^\downarrow(\rho), \lambda^\uparrow(\sigma)), \tag{2.4}$$

where $\lambda^\downarrow(\rho)$ (resp. $\lambda^\uparrow(\rho)$ is the probability vector consisted of the eigenvalues of ρ, listed in decreasing (resp. increasing) order.

Proof. We prove this Theorem for non-singular density matrices. The general case follows by continuity. Indeed, assume that the theorem is correct for non-singular density matrices. Let σ be singular. Then $\sigma + \varepsilon \mathbb{1}$ is non-singular. Since $\lim_{\varepsilon \to 0^+} \lambda^\downarrow(\sigma + \varepsilon \mathbb{1}) = \lambda^\downarrow(\sigma)$ and

$$\max_{U \in \mathrm{U}(\mathcal{H}_d)} \mathrm{F}(\rho, U(\sigma + \varepsilon \mathbb{1})U^\dagger) = \mathrm{F}(\lambda^\downarrow(\rho), \lambda^\downarrow(\sigma + \varepsilon \mathbb{1})),$$

by taking the limit $\varepsilon \to 0^+$, we have that the theorem will be also true for singular density matrices.

Since the eigenvectors of two density matrices can always be connected via a unitary, the problem is reduced to the case where $[\rho, \sigma] = 0$. Without loss of generality, we assume that ρ and

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σ have the following spectral decompositions:

$$\rho = \sum_{j=1}^{d} \lambda_j^{\downarrow}(\rho)|j\rangle\langle j| \quad \text{and} \quad \sigma = \sum_{j=1}^{d} \lambda_j^{\downarrow}(\sigma)|j\rangle\langle j|,$$

where $\lambda_j^{\downarrow}(\rho)$ and $\lambda_j^{\downarrow}(\sigma)$ are the eigenvalues of states ρ and σ respectively.

It has been shown that for any $n \times n$ Hermitian matrices A and B, there exist two unitary matrices V_1 and V_2 such that [11],

$$\exp(A/2)\exp(B)\exp(A/2) = \exp\left(V_1 A V_1^\dagger + V_2 B V_2^\dagger\right).$$

Hence for Hermitian matrices ρ and $U\sigma U^\dagger$, we have V_1 and $V_2 \in U(\mathcal{H}_d)$ such that

$$\sqrt{\rho} U\sigma U^\dagger \sqrt{\rho} = \exp\left(V_1 \log\rho V_1^\dagger + V_2 U \log\sigma U^\dagger V_2^\dagger\right). \tag{2.5}$$

Therefore

$$F(\rho, U\sigma U^\dagger) = \mathrm{Tr}\left(\sqrt{\sqrt{\rho}U\sigma U^\dagger\sqrt{\rho}}\right)$$

$$= \mathrm{Tr}\left(\exp\left(\frac{V_1 \log\rho V_1^\dagger + V_2 U \log\sigma U^\dagger V_2^\dagger}{2}\right)\right)$$

$$= \mathrm{Tr}\left(\exp\left(\frac{\log\rho + \widehat{U}\log\sigma\widehat{U}^\dagger}{2}\right)\right),$$

where $\widehat{U} = V_1^\dagger V_2 U$.

As for arbitrary Hermitian matrices A and B, one has the *Golden-Thompson's inequality*:

$$\mathrm{Tr}\left(e^{A+B}\right) \leqslant \mathrm{Tr}\left(e^A e^B\right),$$

in which the equality holds if and only if $[A, B] = 0$ [12, 13], we have

$$\mathrm{Tr}\left(\exp\left(\frac{\log\rho + \widehat{U}\log\sigma\widehat{U}^\dagger}{2}\right)\right) \leqslant \mathrm{Tr}\left(\sqrt{\rho}\widehat{U}\sqrt{\sigma}\widehat{U}^\dagger\right) \leqslant F(\rho, \widehat{U}\sigma\widehat{U}^\dagger). \tag{2.6}$$

Since the unitary group $U(\mathcal{H}_d)$ is compact, the supremum is actually attained on some unitary. Let $U_0 \in U(\mathcal{H}_d)$ be such that

$$\max_U F(\rho, U\sigma U^\dagger) = F(\rho, U_0\sigma U_0^\dagger) = \mathrm{Tr}\left(\exp\left(\frac{\log\rho + \widehat{U}_0\log\sigma\widehat{U}_0^\dagger}{2}\right)\right).$$

We see that $F(\rho, U_0\sigma U_0^\dagger) = F(\rho, \widehat{U}_0\sigma\widehat{U}_0^\dagger)$, namely, the inequality (2.6) must be an equality. Hence $\left[\rho, \widehat{U}_0\sigma\widehat{U}_0^\dagger\right] = 0$, and $\widehat{U}_0$ is just a permutation operator since $[\rho, \sigma] = 0$.

We have shown that if $[\rho, \sigma] = 0$, then there exists a permutation matrix P such that

$$\max_U F(\rho, U\sigma U^\dagger) = F(\rho, P\sigma P^\dagger).$$

Obviously the maximum is attained when the permutation P is the identity operator $\mathbb{1}_d$. That is, if $[\rho, \sigma] = 0$, then

$$\max_U F(\rho, U\sigma U^\dagger) = F(\rho, \sigma) = \sum_{j=1}^d \sqrt{\lambda_j^\downarrow(\rho)\lambda_j^\downarrow(\sigma)},$$

which proves (2.3).

On the other hand, we have

$$F(\rho, U\sigma U^\dagger) \;=\; \mathrm{Tr}\left(\left|\sqrt{\rho}U\sqrt{\sigma}U^\dagger\right|\right) \geqslant \mathrm{Tr}\left(\sqrt{\rho}U\sqrt{\sigma}U^\dagger\right).$$

Since for Hermitian matrices A and B [14],

$$\langle \lambda^\downarrow(A), \lambda^\uparrow(B)\rangle \leqslant \mathrm{Tr}\,(AB) \leqslant \langle \lambda^\downarrow(A), \lambda^\downarrow(B)\rangle, \tag{2.7}$$

where $\langle u, v\rangle := \sum_j \bar{u}_j v_j$, we obtain

$$\min_U F(\rho, U\sigma U^\dagger) \;\geqslant\; \min_U \mathrm{Tr}\left(\sqrt{\rho}U\sqrt{\sigma}U^\dagger\right) = \sum_{j=1}^d \sqrt{\lambda_j^\downarrow(\rho)\lambda_j^\uparrow(\sigma)}. \tag{2.8}$$

The above inequality becomes an equality for $U \in U(\mathcal{H}_d)$ such that $U|j\rangle = |d - j + 1\rangle$, which proves (2.4). $\qquad\square$

Theorem 2.1 gives a easy way to estimate the maximal and minimal values of the quantum fidelity between the unitary orbits of two quantum states. They are simply given by the eigenvalues of the density matrices.

Theorem 2.2. *The set* $\left\{F(\rho, U\sigma U^\dagger) : U \in U(\mathcal{H}_d)\right\}$ *is identical to the interval*

$$\left[F(\lambda^\downarrow(\rho), \lambda^\uparrow(\sigma)), F(\lambda^\downarrow(\rho), \lambda^\downarrow(\sigma))\right]. \tag{2.9}$$

Proof. Note that any unitary matrix U can be parameterized as $U = \exp(tK)$ for some skew-Hermitian matrix K. In order to prove the set $\left\{F(\rho, U\sigma U^\dagger) : U \in U(\mathcal{H}_d)\right\}$ is an interval, we denote

$$g(t) = F(\rho, U_t\sigma U_t^\dagger) = \mathrm{Tr}\left(\sqrt{\sqrt{\rho}U_t\sigma U_t^\dagger\sqrt{\rho}}\right), \tag{2.10}$$

where $U_t = \exp(tK)$ for some skew-Hermitian matrix K. Here $t \mapsto U_t$ is a path in the unitary matrix space.

We need an integral representation of operator monotone function:

$$a^r = \frac{\sin(r\pi)}{\pi} \int_0^{+\infty} \frac{a}{a+x} x^{r-1} dx,$$

where $0 < r < 1$, $a > 0$). For convenience, let $\mu(x) = x^r$. Then we have

$$a^r = \frac{\sin(r\pi)}{r\pi} \int_0^{+\infty} \frac{a}{a+x} d\mu(x),$$

where $r \in (0,1)$, $a \in (0,+\infty)$).

Assume that all the operations are taken on the support of operators. Given a nonnegative operator A, we have:

$$A^r = \frac{\sin(r\pi)}{r\pi} \int_0^{+\infty} A(A+x)^{-1} d\mu(x), \quad r \in (0,1).$$

In particular, for $r = \frac{1}{2}$, we have

$$\sqrt{A} = \frac{2}{\pi} \int_0^{+\infty} A(A+x)^{-1} d\mu(x), \tag{2.11}$$

which gives rise to

$$
\begin{aligned}
\frac{d\sqrt{A}}{dt} &= \frac{2}{\pi} \int_0^{+\infty} \left[\frac{dA}{dt}(A+x)^{-1} + A\frac{d(A+x)^{-1}}{dt} \right] d\mu(x) \\
&= \frac{2}{\pi} \int_0^{+\infty} (A+x)^{-1}\frac{dA}{dt}(A+x)^{-1} x\, d\mu(x),
\end{aligned}
$$

and

$$
\begin{aligned}
\mathrm{Tr}\left(\frac{d\sqrt{A}}{dt} \right) &= \frac{2}{\pi} \int_0^{+\infty} \mathrm{Tr}\left((A+x)^{-2}\frac{dA}{dt} \right) x\, d\mu(x) \\
&= \frac{2}{\pi} \mathrm{Tr}\left(\left[\int_0^{+\infty} (A+x)^{-2} x\, d\mu(x) \right] \frac{dA}{dt} \right) \\
&= \frac{2}{\pi} \mathrm{Tr}\left(\varphi(A)\frac{dA}{dt} \right),
\end{aligned}
$$

where

$$\varphi(A) := \int_0^{+\infty} (A+x)^{-2} x\, d\mu(x) = \frac{\pi}{4} A^{-1/2}. \tag{2.12}$$

Set $A_t = \sqrt{\rho} U_t \sigma U_t^\dagger \sqrt{\rho}$. One has

$$\frac{dA_t}{dt} = \sqrt{\rho} U_t [K, \sigma] U_t^\dagger \sqrt{\rho}. \tag{2.13}$$

Replacing A with A_t in (2.12), we get

$$
\begin{aligned}
\frac{dg(t)}{dt} &= \frac{d\,\mathrm{Tr}\left(\sqrt{A_t}\right)}{dt} = \mathrm{Tr}\left(\frac{d\sqrt{A_t}}{dt}\right) \\
&= \frac{1}{2}\mathrm{Tr}\left(A_t^{-1/2}\frac{dA_t}{dt}\right) \\
&= \frac{1}{2}\mathrm{Tr}\left(U_t^\dagger\sqrt{\rho}A_t^{-1/2}\sqrt{\rho}U_t[K,\sigma]\right).
\end{aligned}
$$

From Theorem 2.1 the maximal and minimal values of $F(\rho, U\sigma U^\dagger)$ are attained for some U such that $[\rho, U\sigma U^\dagger] = 0$. Hence $g(t) = F(\rho, U_t\sigma U_t^\dagger)$, where $U_t = exp(tK)$, achieves its maximal values at $t = 0$. An extremal point of $g(t)$ is then given by

$$
0 = \frac{d\,g(t)}{dt}\Big|_{t=0} = \frac{1}{2}\mathrm{Tr}\left(K[\sigma, \sqrt{\rho}A_0^{-1/2}\sqrt{\rho}]\right) \tag{2.14}
$$

for all skew-Hermitian matrices K. Thus $[\sigma, \sqrt{\rho}A_0^{-1/2}\sqrt{\rho}] = 0$, which is compatible with $[\rho, \sigma] = 0$.

The above discussion also indicates that the real function $g(t)$ is differentiable at each point over $\mathbb{R}$ for all skew-Hermitian K. That is, $g(t)$ is a continuous function because the unitary matrix group is path-connected. Therefore

$$
g(\mathbb{R}) = \left[F(\lambda^\downarrow(\rho), \lambda^\uparrow(\sigma)), F(\lambda^\downarrow(\rho), \lambda^\downarrow(\sigma))\right],
$$

where we are implicitly taking the union over all the images of g for all skew-hermitian K. And the set $\{F(\rho, U\sigma U^\dagger) : U \in U(\mathcal{H}_d)\}$ is identical to the interval $\left[F(\lambda^\downarrow(\rho), \lambda^\uparrow(\sigma)), F(\lambda^\downarrow(\rho), \lambda^\downarrow(\sigma))\right]$.
$\square$

Remark 2.3. A quantum system usually evolves unitarily with $\{U_t = \exp(-itH) : t \in \mathbb{R}\}$ according to certain Hamiltonian H, rather than the whole unitary group. The problem is then reduced to determine the optimized values: $\min_{t\in\mathbb{R}} F(\rho, U_t\sigma U_t^\dagger)$ and $\max_{t\in\mathbb{R}} F(\rho, U_t\sigma U_t^\dagger)$ for given density operators ρ and σ. Note that every matrix Lie group is a smooth manifold. Thus the unitary matrix group $U(\mathcal{H}_d)$, a compact group, is connected if and only if it is path-connected [15]. It is seen that any unitary matrix is path-connected with $\mathbb{1}_d$ via a path $U_t = \exp(tK)$ for some skew-Hermitian matrix K, i.e. $K^\dagger = -K$. Indeed since any unitary matrix U can be parameterized in this way for both unitary matrix U and V, there exists a skew-Hermitian matrix K such that $UV^{-1} = \exp(K)$. Let $U_t = \exp(tK)V$. Then $U_0 = V$ and $U_t = U$. That is, $U_t, t \in [0, 1]$ is a path between U and V.

Hence if $[H, \rho] = 0$ or $[H, \sigma] = 0$, then

$$
\max_{t\in\mathbb{R}} F(\rho, U_t\sigma U_t^\dagger) = \min_{t\in\mathbb{R}} F(\rho, U_t\sigma U_t^\dagger) = F(\rho, \sigma).
$$

Assume that $[H, \rho] \neq 0$ and $[H, \sigma] \neq 0$, and denote

$$g(t) := \mathrm{F}(\rho, U_t \sigma U_t^\dagger). \tag{2.15}$$

Clearly since $g(t)$ is a continuous function and the unitary group $\mathrm{U}(\mathcal{H}_d)$ is compact, the extreme values of $g(t)$ over $\mathbb{R}$ do exist. Thus the range of $g(t)$ is a closed interval. But determining the extreme values is very complicated and difficult. We leave this open question in the future research.

3 Relative entropy between unitary orbits

We have studied the quantum fidelity between unitary orbits. One may also consider other measures of 'distance' instead of quantum fidelity. In this section we consider the relative entropy between unitary orbits of two quantum states. We first give a Lemma about vectors and stochastic matrices.

For a given d-dimensional real vector $u = [u_1, u_2, \cdots, u_d]^\mathsf{T} \in \mathbb{R}^d$, we denote

$$u^\downarrow = [u_1^\downarrow, u_2^\downarrow, \ldots, u_d^\downarrow]^\mathsf{T}$$

the rearrangement of u in decreasing order, $\{u_i^\downarrow\}$ is a permutation of $\{u_i\}$ and $u_1^\downarrow \geqslant u_2^\downarrow \geqslant \cdots \geqslant u_d^\downarrow$. Similarly, we denote

$$u^\uparrow = [u_1^\uparrow, u_2^\uparrow, \cdots, u_d^\uparrow]^\mathsf{T}$$

the rearrangement of u in increasing order. A real vector u is *majorized* by v, $u \prec v$, if $\sum_{i=1}^k u_i^\downarrow \leqslant \sum_{i=1}^k v_i^\downarrow$ for each $k = 1, \ldots, d$ and $\sum_{i=1}^d u_i^\downarrow = \sum_{i=1}^d v_i^\downarrow$. A matrix $B = [b_{ij}]$ is called *bi-stochastic* if $b_{ij} \geqslant 0$, $\sum_{i=1}^d b_{ij} = \sum_{j=1}^d b_{ij} = 1$ [16]. A real vector u is majorized by v if and only if $u = Bv$ for some $d \times d$ bi-stochastic matrix B [17].

Denote by $\mathbf{B}_d$ the set of all $d \times d$ bi-stochastic matrices. A *unistochastic* matrix D is a bi-stochastic matrix satisfying $D = U \circ \overline{U}$, where $\circ$ is the *Schur product*, defined between two matrices as $A \circ B = [a_{ij}b_{ij}]$ for $A = [a_{ij}]$ and $B = [b_{ij}]$; U is a unitary matrix and $\overline{U}$ is the complex conjugation of U. We denote $\mathbf{B}_d^u$ the set of all $d \times d$ unistochastic matrices.

Let $\mathcal{S}_d$ be the permutation group on the set $\{1, 2, \cdots, d\}$. For each $\pi \in \mathcal{S}_d$, we define a $d \times d$ matrix $P_\pi = [\delta_{i\pi(j)}]$, $P_\pi u = [u_{\pi(1)}, \cdots, u_{\pi(d)}]^\mathsf{T}$. P_π is bi-stochastic and the set of bi-stochastic matrices is a convex set. The *Birkhoff-von Neumann theorem* states that the bi-stochastic matrices are given by the convex hull of the permutation matrices [18]: A $d \times d$ real matrix B is bi-stochastic if and only if there exists a probability distribution λ on $\mathcal{S}_d$ such that $B = \sum_{\pi \in \mathcal{S}_d} \lambda_\pi P_\pi$.

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Lemma 3.1. *For any two real vectors $u, v \in \mathbb{R}^d$, we have*

$$\{\langle u, Bv \rangle : B \in \mathbf{B}_d^u\} = \{\langle u, Bv \rangle : B \in \mathbf{B}_d\}, \tag{3.1}$$

which in turn is identical to the interval $\left[\langle u^\downarrow, v^\uparrow \rangle, \langle u^\downarrow, v^\downarrow \rangle\right]$.

Proof. Firstly, we show that

$$\{\langle u, Bv \rangle : B \in \mathbf{B}_d\} = [\langle u^\downarrow, v^\uparrow \rangle, \langle u^\downarrow, v^\downarrow \rangle]. \tag{3.2}$$

From the Birkhoff-von Neumann theorem, we see that each $B \in \mathbf{B}_d$ can be written as a convex combination of permutation matrices:

$$B = \sum_{\pi \in \mathcal{S}_d} \lambda_\pi P_\pi, \quad \forall \pi \in \mathcal{S}_d : \lambda_\pi \geqslant 0, \sum_{\pi \in \mathcal{S}_d} \lambda_\pi = 1.$$

Thus $\langle u, Bv \rangle = \sum_{\pi \in \mathcal{S}_d} \lambda_\pi \langle u^\downarrow, P_\pi v^\downarrow \rangle$. Since for any real numbers $x_1 \leqslant \cdots \leqslant x_d$ and $y_1 \leqslant \cdots \leqslant y_d$, one has

$$\sum_{i=1}^d x_i y_{d+1-i} \leqslant \sum_{i=1}^d x_1 y_{\pi(i)} \leqslant \sum_{i=1}^d x_i y_i$$

under any permutation π, it is seen that

$$\langle u^\downarrow, v^\uparrow \rangle \leqslant \langle u^\downarrow, P_\pi v^\downarrow \rangle \leqslant \langle u^\downarrow, v^\downarrow \rangle, \quad \forall \pi \in \mathcal{S}_d. \tag{3.3}$$

As the set $\{\langle u^\downarrow, P_\pi v^\downarrow \rangle : \pi \in \mathcal{S}_d\}$ is discrete and finite, it follows that the convex hull of this set is a one-dimensional simplex with their boundary points $\langle u^\downarrow, v^\uparrow \rangle$ and $\langle u^\downarrow, v^\downarrow \rangle$. Therefore (3.2) holds.

Secondly, we show that $\{\langle u, Bv \rangle : B \in \mathbf{B}_d^u\} = \{\langle u, Bv \rangle : B \in \mathbf{B}_d\}$. Indeed, since $\mathbf{B}_d^u$ is a proper subset of $\mathbf{B}_d$, one has $\{\langle u, Bv \rangle : B \in \mathbf{B}_d^u\} \subset \{\langle u, Bv \rangle : B \in \mathbf{B}_d\}$. Now for arbitrary $D \in \mathbf{B}_d$, clearly $Dv \prec v$, there exists a unistochastic matrices $D' \in \mathbf{B}_d^u$ such that $Dv = D'v$ [18, Thm.11.2.]. This implies that $\langle u, Dv \rangle = \langle u, D'v \rangle$ in $\{\langle u, Dv \rangle : D \in \mathbf{B}_d^u\}$. That is

$$\{\langle u, Bv \rangle : B \in \mathbf{B}_d^u\} \supset \{\langle u, Bv \rangle : B \in \mathbf{B}_d\}.$$

Finally, they are identically to an interval $\left[\langle u^\downarrow, v^\uparrow \rangle, \langle u^\downarrow, v^\downarrow \rangle\right]$. $\qquad \square$

In fact, the following consequence can be derived directly from (2.7) and the Lemma above,

$$\langle \lambda^\downarrow(A), \lambda^\uparrow(B) \rangle \leqslant \mathrm{Tr}\left(AUBU^\dagger\right) \leqslant \langle \lambda^\downarrow(A), \lambda^\downarrow(B) \rangle \tag{3.4}$$

for arbitrary $U \in \mathrm{U}(\mathcal{H}_d)$. Moreover, since

$$\mathrm{Tr}\left(AUBU^\dagger\right) = \sum_{i,j} \lambda_i^\downarrow(A) \lambda_j^\downarrow(B) \left| \langle a_i | U | b_j \rangle \right|^2 = \langle \lambda^\downarrow(A), D_U \lambda^\downarrow(B) \rangle,$$

where $D_U = \left[|\langle a_i | U | b_j \rangle|^2 \right] \in \mathbf{B}_d^u$, one has

$$\left\{ \mathrm{Tr} \left(A U B U^\dagger \right) : U \in \mathrm{U} \left(\mathcal{H}_d \right) \right\} = \left\{ \langle \lambda^\downarrow(A), D_U \lambda^\downarrow(B) \rangle : D_U \in \mathbf{B}_d^u \right\} \tag{3.5}$$

$$= \left[\langle \lambda^\downarrow(A), \lambda^\uparrow(B) \rangle, \langle \lambda^\downarrow(A), \lambda^\downarrow(B) \rangle \right]. \tag{3.6}$$

Therefore the set $\left\{ \mathrm{Tr} \left(A U B U^\dagger \right) : U \in \mathrm{U} \left(\mathcal{H}_d \right) \right\}$ is an interval:

$$\left\{ \mathrm{Tr} \left(A U B U^\dagger \right) : U \in \mathrm{U} \left(\mathcal{H}_d \right) \right\} = \left[\langle \lambda^\downarrow(A), \lambda^\uparrow(B) \rangle, \langle \lambda^\downarrow(A), \lambda^\downarrow(B) \rangle \right].$$

The relative entropy of two quantum states ρ and σ is defined by

$$S(\rho||\sigma) = \mathrm{Tr} \left(\rho(\log \rho - \log \sigma) \right) \tag{3.7}$$

if $\mathrm{supp}(\rho) \subseteq \mathrm{supp}(\sigma)$, where $\mathrm{supp}(\rho)$ is the support of ρ defined as the span of the eigenvectors with the corresponding eigenvalues great than zero. Let $\mathrm{H}(p||q)$ denote the classical relative entropy of two probability distributions $p = \{p_j\}$ and $q = \{q_j\}$,

$$\mathrm{H}(p||q) = \begin{cases} \displaystyle\sum_j p_j(\log p_j - \log q_j), & \text{if } \mathrm{supp}(p) \subseteq \mathrm{supp}(q), \\ +\infty, & \text{otherwise.} \end{cases}$$

Since $S(U \rho U^\dagger || \sigma) = -S(\rho) - \mathrm{Tr} \left(U \rho U^\dagger \log \sigma \right)$, from (2.7) and the analysis above, we have the following results for relative entropy:

Theorem 3.2. *For arbitrary given two quantum states $\rho, \sigma \in \mathrm{D} \left(\mathcal{H}_d \right)$, with σ full-ranked,*

$$\min_{U \in \mathrm{U}(\mathcal{H}_d)} S(U \rho U^\dagger || \sigma) = \mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\downarrow(\sigma)), \tag{3.8}$$

$$\max_{U \in \mathrm{U}(\mathcal{H}_d)} S(U \rho U^\dagger || \sigma) = \mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\uparrow(\sigma)). \tag{3.9}$$

Moreover, the set $\left\{ S(U \rho U^\dagger || \sigma) : U \in \mathrm{U} \left(\mathcal{H}_d \right) \right\}$ is an interval,

$$\left\{ S(U \rho U^\dagger || \sigma) : U \in \mathrm{U} \left(\mathcal{H}_d \right) \right\} = \left[\mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\downarrow(\sigma)), \mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\uparrow(\sigma)) \right].$$

Theorem 3.2 shows that the maximal and minimal values of the relative entropy between the unitary orbits of two quantum states are determined by the classical relative entropy of probability distributions given by the eigenvalues of two density matrices. In addition, one can show that Theorem 3.2 also gives rise to the following inequality:

$$\mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\downarrow(\sigma)) \leqslant S(\rho||\sigma) \leqslant \mathrm{H}(\lambda^\downarrow(\rho) || \lambda^\uparrow(\sigma)). \tag{3.10}$$

4 Discussions

We have solved the problem of evaluating the fidelity between unitary orbits of quantum states. The analytical formulas for the minimal and maximal values have been obtained. It has been also proved that the fidelity goes through the whole interval between the minimal and the maximal values.

As a "measure of the distance" between the fixed state and the evolved one, we have used the fidelity $\mathrm{F}(\rho, \sigma(t))$, where $\sigma(t) = e^{-itH}\sigma e^{itH}$. The analysis can be also analogously used for other kinds of measures, for instance, the constrained optimization problem for the relative entropy:

$$\max_{t \in \mathbb{R}} \mathrm{S}(U_t \rho U_t^\dagger || \sigma) \quad \text{and} \quad \min_{t \in \mathbb{R}} \mathrm{S}(U_t \rho U_t^\dagger || \sigma), \tag{4.1}$$

where $U_t = e^{-itH}$ is the unitary dynamics generated by a Hamiltonian H. The above constrained optimization problems are related with the speed of quantum dynamical evolution [19, 20].

Our results can be also applied to other subjects in quantum computation and quantum information processing, such as optimal quantum control, in which the state $\rho(0)$ at time zero evolves into the state $\rho(t)$ at time t, $\rho(t) = U(t)\rho(0)U^\dagger(t)$ for some unitary operator $U(t)$. The unitary operator $U(t)$ is determined by the Hamiltonian of the system $H(t)$ satisfying the time-dependent Schrödinger equation, $\dot{U}(t) = -iH(t)U(t)$, with $U(0) = \mathbb{1}$ the identity operator. $H(t)$ is a Hermitian matrix of the form, $H(t) = H_d + \sum_{i=1}^{m} v_i(t) H_i$, where H_d is called the drift Hamiltonian which is internal to the system, and $\sum_{i=1}^{m} v_i(t) H_i$ is the control Hamiltonian such that the coefficients $v_i(t)$ can be externally manipulated [21, 22]. If the target state is not in the scope of the states that can be generated be the given Hamiltonian. Then one has to find a "best" unitary operator to reach a final state such that the best fidelity between the target state and the final state is attained.

The results obtained in this context can be also used to study the modified version of super-additivity of relative entropy and that of sub-multiplicativity of fidelity in [23]. In fact, the concerned problems have a surprisingly rich mathematical structure and need to be investigated further.

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