Parallellity of mixed quantum ensembles

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A unifying framework for identifying distance and holonomy for decompositions of density operators is introduced. Parallellity between quantum ensembles is defined by minimizing this distance over allowed decompositions. The minimum is a property of a pair of states and coincides with the Bures distance. The parallellity condition imposes a connection (rule for parallel transport) that results in the Uhlmann holonomy for sequences of density operators. A distance and holonomy for spectral decompositions of density operators is identified as a sub-group restriction of the full decomposition freedom. These spectral concepts are gauge invariant (decomposition independent) properties of mixed quantum ensembles, as long as the corresponding density operators are non-degenerate. A gauge invariant spectral geometric phase for discrete sequences of mixed quantum states is obtained as the phase of the trace of the spectral holonomy. This geometric phase differs from the interferometric mixed state geometric phase in the continuous limit.

I. INTRODUCTION

In quantum information, quantum states act as resources for information processing, storage, and communication. This makes it important to quantify, by means of, e.g., coherence and correlations, the ability to perform such tasks. Geometry plays a central role in these quantification procedures [1]. This insight has triggered a revived interest in the geometry of quantum mechanical state spaces.

Mixed quantum states may describe situations where each particle of an ensemble in a quantum experiment is in a pure, but to us unknown state. A mixed quantum state can under these circumstances be viewed as a set of pure quantum states, and the relation between these states is determined by the density operator of the ensemble. The density operator is given by the projective map

$$\Pi : A_\rho \mapsto \rho.$$  

(1)

over the set of quantum states. The map entails that $A_\rho$ uniquely defines the state of the ensemble, while the converse is not true: there are infinitely many ways to prepare a given $\rho$. This defines a gauge structure, where gauge invariant quantities correspond to physical properties of mixed quantum ensembles.

Here, we examine geometrical aspects of the projective structure in Eq. (1). Specifically, we focus on the concept of parallellity associated with the projective map, and the resulting gauge invariant concepts of distance and holonomy along sequences of density operators.

Conceptually, the present approach is based on decompositions rather than purifications of density operators. While the purification-based framework views a quantum ensemble as a part of a larger system in a pure state, no extension of the system is needed in the present decomposition-based scheme. This difference has been summarized in terms of the concepts ‘improper’ and ‘proper’ mixed states, as introduced by d’Espagnat [2] (see also Ref. [3]). In this sense, the present approach can be regarded as a proper-mixed-state framework to quantum geometry, while a traditional approach, such as [4–7], takes the ensemble as an improper mixture of quantum states. A pertinent question in this context is whether the parallellity concepts associated with these ‘proper’ (decomposition-based) and ‘improper’ (purification-based) approaches mutually agree.

The paper is organized as follows. In the next section, parallellity of decompositions is introduced and the resulting distance and holonomy are derived. Their relations to the Bures distance and Uhlmann holonomy are delineated. Section III examines the geometry when the projective map is restricted to spectral decompositions of non-degenerate density operators. We introduce distance, holonomy, and geometric phase concepts associated with such restricted projective maps. The paper concludes with concluding remarks in Sec. IV.

II. PARALLEL DECOMPOSITIONS

Let us start by considering two quantum ensembles, one prepared by producing $K$ orthonormal pure states $\{|e_k\rangle\}$ with probabilities $\{p_k\}$, and the other prepared by producing $L$ (not necessarily orthogonal) normalized states $\{|\psi_l\rangle\}$ with probabilities $\{r_l\}$. These two ensembles are mixtures that correspond to the same quantum state if and only if there exists a unitary $L \times L$ matrix $V$ such that $\sum_k \sqrt{p_k} |e_k\rangle V |\psi_l\rangle = \sqrt{r_l} |\psi_l\rangle$. The sets $\{\sqrt{r_l} |\psi_l\rangle\}$ satisfying Eq. (2)

$$\sqrt{r_l} |\psi_l\rangle = \sum_k \sqrt{p_k} |e_k\rangle V |\psi_l\rangle.$$  

(2)

saturate the possible decompositions of the density operator $\rho = \sum_l \sqrt{r_l} |\psi_l\rangle \langle \psi_l|$. The sets

$$\sum_k \sqrt{p_k} |e_k\rangle V |\psi_l\rangle = \sqrt{r_l} |\psi_l\rangle,$$  

(3)

are the parallel decompositions associated with the projective map $\Pi : A_\rho \mapsto \rho$. When the density operator $\rho$ is a proper decomposition of a pure state, the projective map $\Pi$ is restricted to spectral decompositions. The parallellity condition $\Pi : A_\rho \mapsto \rho$ is defined by minimizing this distance over allowed decompositions. The minimum is a property of a pair of states and coincides with the Bures distance. The parallellity condition imposes a connection (rule for parallel transport) that results in the Uhlmann holonomy for sequences of density operators. A distance and holonomy for spectral decompositions of density operators is identified as a sub-group restriction of the full decomposition freedom. These spectral concepts are gauge invariant (decomposition independent) properties of mixed quantum ensembles, as long as the corresponding density operators are non-degenerate. A gauge invariant spectral geometric phase for discrete sequences of mixed quantum states is obtained as the phase of the trace of the spectral holonomy. This geometric phase differs from the interferometric mixed state geometric phase in the continuous limit.

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\( \sum_k p_k |e_k \rangle \langle e_k | \) representing the quantum state. The decompositions are empirically equivalent as they produce the same set of expectation values and probabilities for all possible measurements on the ensemble.

In general, one may have \( L > K \). In such cases, only a \( K \times L \) sub-matrix of \( V \) is used, while the remaining \( L-K \) rows are arbitrary up to the condition that \( V \) should be unitary. In order to simplify the analysis, we shall in the following assume that \( L = K \). In other words, it is assumed throughout that the number of states in the decompositions always coincides with the rank of the density operator. In order to simplify further, we shall assume that we compare density operators having the same rank \([11]\).

The following definition captures a notion of distance between pairs of decompositions:

**Definition.** Let \( A_\rho = \{ \sqrt{\pi_l} | \psi_l \rangle \} \) and \( A_\sigma = \{ \sqrt{\pi_l} | \phi_l \rangle \} \) be decompositions of two rank-\( K \) density operators \( \rho \) and \( \sigma \). The distance between this pair of decompositions is defined as

\[
D(A_\rho, A_\sigma) = \left( \sum_l \| \sqrt{\pi_l} | \phi_l \rangle - \sqrt{\pi_l} | \psi_l \rangle \|^2 \right)^{\frac{1}{2}}.
\]

Based on this distance measure, we now introduce the concept of parallelity. To understand the idea, we note that the relevant geometrical structure is a fibre bundle for which decompositions form the total space, the density operators form the base space, the projection is the map \( \Pi \) in Eq. (1), and the fibre is the set of unitary \( K \times K \) matrices.

The following definition of parallelity captures the horizontal lift of this bundle:

**Definition.** The decompositions \( A_\rho \) and \( A_\sigma \) are said to be parallel if they satisfy

\[
\sqrt{\pi_l} | \psi_l \rangle = \sum_k \sqrt{p_k} | e_k \rangle V_{kl},
\]

\[
\sqrt{\pi_l} | \phi_l \rangle = \sum_{k,m} \sqrt{q_k} | f_k \rangle W_{km} V_{ml},
\]

\( W \) being the unitary part of the overlap matrix

\[
M_{kl} = \sqrt{q_k} \langle f_k | e_l \rangle \sqrt{\pi_l}
\]

of the sub-normalized eigenvectors \( \sqrt{\pi_l} | e_l \rangle \) and \( \sqrt{\sqrt{p_k}} | f_k \rangle \) of \( \rho \) and \( \sigma \), respectively.

We use the left polar form \( M = |M| W \) in the definition of \( |M| \geq 0 \). Provided \( |M|^{-1} \) exists, which is equivalent to the stronger condition \( |M| > 0 \), \( W \) is uniquely given by \( |M|^{-1} M \)[12].

In the following two subsections, we address the question whether the above parallelity concept agrees with the traditional purification-based approach. The latter is known to lead to the Bures distance and Uhlmann holonomy for sequences of density operators. In order to establish the relation between the decomposition- and purification-based approaches, we thus check explicitly how our parallelity concept relates to the Bures distance and Uhlmann holonomy.

### A. Relation to Bures distance

The meaning of the parallelity condition in Eq. (4) is to minimize the distance between decompositions in Eq. (3). By inserting Eq. (4) into Eq. (3), one obtains the minimal distance \([14]\)

\[
D_{\text{min}} = \min_{A_\rho, A_\sigma} D(A_\rho, A_\sigma) = \left( 2 - 2 \text{Tr} |M| \right)^{\frac{1}{2}}.
\]

This can be put on a familiar form by using the orthonormality of \( |f_k \rangle \). We have

\[
\sqrt{\sigma} \rho \sqrt{\sigma} = \sum_{k,l} | f_k \rangle |M|_{kl}^2 \langle f_l |,
\]

\[
= \left( \sum_{k,m} | f_k \rangle |M|_{km} \langle f_m | \right) \times \left( \sum_{n,l} | f_n \rangle |M|_{nl} \langle f_l | \right),
\]

from which follows

\[
\left( \sqrt{\sigma} \rho \sqrt{\sigma} \right)^{\frac{1}{2}} = \sum_{k,l} | f_k \rangle |M|_{kl} \langle f_l |.
\]

We thus obtain the fidelity \([5]\)

\[
\text{Tr} \left( \sqrt{\sigma} \rho \sqrt{\sigma} \right)^{\frac{1}{2}} = \sum_{k,l} \delta_{kl} |M|_{kl} = \text{Tr} |M|.
\]

Equations (6) and (9) yield

\[
D_{\text{min}} = \left[ 2 - 2 \text{Tr} \left( \sqrt{\sigma} \rho \sqrt{\sigma} \right)^{\frac{1}{2}} \right]^{\frac{1}{2}},
\]

which is the Bures distance \( d_B(\rho, \sigma) \)[15][17]. This proves that \( D_{\text{min}} \) and the purification-based distance coincide.

### B. Relation to the Uhlmann holonomy

The parallelity condition in Eq. (4) defines a connection (rule for parallel transport) over the set of quantum states. It gives rise to a holonomy when applied to decompositions \( \{ \sqrt{\pi_{l1}} | \psi_{l1} \rangle, \ldots, \sqrt{\pi_{la}} | \psi_{la} \rangle \} \) of an ordered sequence \( S \) of rank-\( K \) density operators \( \rho_1, \ldots, \rho_n \). We further assume the overlap matrices \( M^{(a+1,a)} \) for nearby decompositions satisfy \( |M^{(a+1,a)}| > 0 \), which
guarantee that all $\mathcal{W}^{(a+1,a)}$ are uniquely defined. The corresponding unitary $V_a$ (cf. Eq. (2)) is the ‘phase’ of the decomposition. This phase can be transported in a parallel fashion by requiring that all nearby $V_a$ and $V_{a+1}$ are related according to the connection, i.e.,

$$V_{a+1} = \mathcal{W}^{(a+1,a)}V_a.$$  

Iterating over the whole sequence uniquely determines the Pancharatnam-like ‘relative phase’ [13] between the decompositions of the final and first density operators

$$V_nV_1^{-1} = \mathcal{W}^{(n,n-1)} \ldots \mathcal{W}^{(2,1)}.$$  

We can put this relative phase on more familiar form by introducing orthonormal eigenvectors $|e_{a;k}\rangle$ of $\rho_a$ and by observing that

$$\sqrt{\rho_{a+1}} \sqrt{\rho_{a}} = \left( \sum_{k,m} |e_{a+1;k}\rangle \mathcal{W}^{(a+1,a)}_{kl} |e_{a+1;m}\rangle \right)\left( \sum_{n,l} |e_{a+1;n}\rangle \mathcal{W}^{(a+1,a)}_{nl} |e_{a;l}\rangle \right)$$

$$= \left( \sqrt{\rho_a} \sqrt{\rho_{a+1}} \right)^{1/2} \left( \sum_{n,l} |e_{a+1;n}\rangle \mathcal{W}^{(a+1,a)}_{nl} |e_{a;l}\rangle \right),$$  

where we have used Eq. (8) in the last equality. By using Eqs. (12) and (13), we can express the Uhlmann holonomy [14] as

$$U_{\text{Uhl}} = \left( \sqrt{\rho_n} \sqrt{\rho_{n-1}} \cdots \sqrt{\rho_2} \sqrt{\rho_1} \right)^{-1/2} \left( \sqrt{\rho_n} \sqrt{\rho_{n-1}} \cdots \sqrt{\rho_2} \sqrt{\rho_1} \right)$$

$$= \sum_{k_1,k_n} |e_{n;k_n}\rangle \mathcal{W}^{(n,n-1)} \cdots \mathcal{W}^{(2,1)}_{k_1k_n} |e_{1;k_1}\rangle$$

$$= \sum_{k_1,k_n} |e_{n;k_n}\rangle \mathcal{W}_{n1}^{1} \mathcal{W}^{(1)}_{k_nk_1} |e_{1;k_1}\rangle.$$  

Thus, our notion of parallelity in Eq. (4) is able to realize the Uhlmann holonomy for sequences of quantum states, again proving that the proper and improper approaches mutually agree.

### III. PARALLELITY OF SPECTRAL DECOMPOSITIONS

As can be seen in Eq. (2), the equivalence of decompositions is tested relative the spectral decomposition. In this sense, the spectral decomposition plays a special role for mixed ensembles. This motivates us to consider the above distance and holonomy concepts when we restrict to the freedom left in the spectral decompositions of density operators. This is basically the freedom of permuting the eigenstates and the phase of the corresponding eigenvectors. In other words, we look at phases of the form

$$\mathcal{V}_{kl} = e^{i\theta_{kl}},$$  

$\hat{Q}_{kl}$ being permutation matrices of $K$ elements. These matrices represent the symmetric group $S_K$. Note that $\{\mathcal{V}\}$ form a sub-group of $U(K)$. We shall call the distance and holonomy emerging from $\mathcal{V}$ the spectral distance and spectral holonomy, respectively.

#### A. Spectral parallelity and distance

Assume $\{|e_k\rangle\}$ and $\{|f_k\rangle\}$ are two orthonormal sets of $K$ unit vectors and consider two non-degenerate rank-$K$ density operators $\rho = \sum_k p_k |e_k\rangle \langle e_k|$ and $\sigma = \sum_k q_k |f_k\rangle \langle f_k|$. Given a spectral decomposition $B_{\rho} = \{\sqrt{H} |\psi_i\rangle = \sqrt{p_i} |e_i\rangle e^{i\theta_i} \}$ of $\rho$, we look for the parallel spectral decomposition $B_{\sigma} = \{\sqrt{H} |\phi_i\rangle = \sum_k \sqrt{q_k} |f_k\rangle e^{i\theta_i} \hat{Q}_{kl} |\psi_i\rangle \}$ of $\sigma$. By varying over the permutations and phases of the spectral decomposition of $\sigma$, one finds the minimal distance

$$d_{\text{min}} = \left( 2 - 2 \sum_{k,l} \sqrt{q_k p_l} \langle |f_k |e_l\rangle |\hat{Q}_{kl}\rangle^{1/2} \right),$$  

where the permutation $\hat{Q}$ satisfies

$$\sum_{k,l} \sqrt{q_k p_l} \langle |f_k |e_l\rangle |\hat{Q}_{kl}\rangle \leq \sum_{k,l} \sqrt{q_k p_l} \langle |f_k |e_l\rangle |\hat{Q}_{kl}\rangle$$

for all $\hat{Q} \in S_K$. In this way, parallelity of the spectral decompositions can be defined as follows:

**Definition.** For non-degenerate $\rho$ and $\sigma$ [15], $B_{\rho}$ and $B_{\sigma}$ are said to be parallel if they satisfy

$$|\psi_i\rangle = |e_i\rangle e^{i\theta_i},$$

$$|\phi_i\rangle = \sum_k |f_k\rangle \hat{Q}_{kl} e^{i\theta_i + i \arg(f_k |e_l\rangle)}$$

with $\hat{Q}$ given by Eq. (17).

Note that $d_{\text{min}} \geq D_{\text{min}}$ with equality for commuting density operators [20] or pure ensembles ($K = 1$). $d_{\text{min}}$ is the spectral distance between $\rho$ and $\sigma$.

#### B. Spectral holonomy

The parallelity of spectral decomposition defines the connection

$$\mathcal{V}_{a+1} = \hat{Q}_{kl}^{(a+1,a)} e^{i \arg(e_{a+1,k} |e_{a,l}\rangle)} \mathcal{V}_a,$$  

(19)
being a discrete version of the connection underlying the interferometric mixed state geometric phase (GP) proposed in Refs. [21][22]. Equation (19) describes a non-Abelian $S_K \times U(1)^{\otimes K}$ bundle over the space of density matrices. It yields the holonomy
\[
U = \sum_{k_1,k_n} |e_{n,k_n} \rangle \langle e_{1,k_1}| \quad \text{for} \quad \langle e_{1,k_1}| e_{n,k_n} \rangle = \delta_{kn}.
\]
Equation (20) describes the spectral distance and holonomy
\[
\langle e_{a,k}| e_{a,l} \rangle = \delta_{kl}. \quad \text{The symmetric group } S_2 \text{ consists of two elements:}
\]
\[
I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]
holds for any pair $a, a'$ of qubit ensembles.

Let us first consider the spectral distance between $\rho_a$ and $\rho_{a'}$. We choose the corresponding eigenvectors to be
\[
\{|a\rangle, |a'\rangle\} = \left\{ \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right\},
\]
where $a \in [0, 1]$, $\beta = \sqrt{1 - \alpha^2}$, and $\varphi \in [0, \pi]$. These two eigenbases are mutually unbiased [23] for $\alpha = 0$ and for $\alpha = \frac{1}{2}$, $\varphi = \frac{\pi}{2}$; they are identical for $\alpha = \frac{1}{2}$, $\varphi = 0$. To capture this, we introduce the parameter
\[
\eta = 2\alpha\beta \cos \varphi,
\]
where $|\eta|$ being a natural measure of ‘mutual unbiasedness’. By using Eqs. (17) and (25), we see that $Q^{(a',a)} = \mathbb{I}$ if
\[
|\langle e_{a',0}| e_{a,0} \rangle|^2 < 4p(1-p) |\langle e_{a',1}| e_{a,0} \rangle|^2
\]
\[
1 + \eta < 4p(1-p)(1-\eta)
\]
and $Q^{(a',a)} = X$ if
\[
|\langle e_{a',0}| e_{a,0} \rangle|^2 > 4p(1-p) |\langle e_{a',1}| e_{a,0} \rangle|^2
\]
\[
1 + \eta < 4p(1-p)(1-\eta).
\]
Since $4p(1-p) \in [0, 1)$ for non-degenerate (p ≠ 1/2) density operators, Eq. (28) holds for $\eta \geq 0$ and $Q^{(a',a)} = \mathbb{I}$ in this case. For $\eta < 0$, we find that $Q^{(a',a)} = X$ if
\[
\frac{1}{2} \left( 1 - \sqrt{\frac{2|\eta|}{1+|\eta|}} \right) < p < \frac{1}{2} \left( 1 + \sqrt{\frac{2|\eta|}{1+|\eta|}} \right)
\]
while $Q^{(a',a)} = \mathbb{I}$ otherwise. We thus see that $Q^{(a',a)} = X$ is only possible if $\eta < 0$, i.e., if $\varphi \in \left( \frac{\pi}{2}, \pi \right)$. For $p \neq \frac{1}{2}$, we therefore find the minimal distance
\[
d_{\min} = \left( 2 - 2\sqrt{2p(1-p)} \sqrt{1-\eta} \right)^{\frac{1}{2}}
\]
for $p$ satisfying Eq. (30), and
\[
d_{\min} = \left( 2 - \sqrt{2} \sqrt{1+\eta} \right)^{\frac{1}{2}}
\]
C. Qubit example

We illustrate the spectral distance and holonomy in the case of non-degenerate isospectral qubit density operators $\rho_a$ with spectral decompositions $\mathcal{E}_a = \{ \sqrt{p} |e_{a,0}\rangle, \sqrt{1-p} |e_{a,1}\rangle \}$, $p \in [0, 1]$, $p \neq \frac{1}{2}$, and
otherwise, $d_{\text{min}}^{(\alpha', \alpha)}$ is shown in Fig. 1. The non-smooth behavior is due to the abrupt change of the permutation of the eigenvectors that may occur for negative $\eta$, as described above. Note that for $p = \frac{1}{2}$ the two density operators coincide, i.e., by using the technique in Ref. [19], we may take $\alpha\beta = \frac{1}{2}, \varphi = 0$. This in turn implies that only $\eta = 1$ is allowed. In other words, the spectral distance is singular for degenerate eigenvalues.

Let us now turn to the holonomy $U$ of the sequence $B_1 \rightarrow \ldots \rightarrow B_n$, $n \geq 3$. We need the pure state GPs $\gamma_{k_1, \ldots, k_n} = \arg \Delta^{(n)}(e_{1,k_1}, \ldots, e_{n,k_n})$, $k_1, \ldots, k_n = 0, 1$. These phases satisfy the symmetry relation

$$\gamma_{k_1 \oplus 1, \ldots, k_n \oplus 1} = -\gamma_{k_1, \ldots, k_n}$$

with $\oplus$ addition modulo 2. This implies

$$\text{Tr}U = 2 |\langle e_{1,0}|e_{n,0} \rangle| \cos \gamma_{k_1, \ldots, k_n},$$

(34)

where we have used Eq. (25). Here, $l = 0$ and $l = 1$ correspond to $Q_{k_1, \ldots, k_n} = I$ and $X$, respectively. The sequence $k_1, \ldots, k_n$ is determined by minimizing the distance between nearby states. We thus see that $\Phi_0$ can only be $0, \pi$, or undefined. These cases correspond to $\text{Tr}U > 0$, $\text{Tr}U < 0$, and $\text{Tr}U = 0$, respectively, or equivalently to whether the relevant $|\gamma|$ is smaller than, greater than, or equal to $\frac{\pi}{2}$. We note that this is generic in the qubit case and essentially means that a non-trivial spectral GP is obtained only if $|\Omega| > \pi$, $\Omega$ being the enclosed solid angle of the polygon on the Bloch sphere with vertices at $e_{1,k_1}, \ldots, e_{n,k_n}$. In higher Hilbert space dimensions, the spectral GPs may take any value since Eqs. (25) and (33) no longer hold.

IV. CONCLUSIONS

The decomposition freedom of a quantum state defines a projective map from the set of decompositions to the corresponding density operator. For pairs of states, this projective structure defines a natural notion of parallelity between decompositions over the states: parallel decompositions minimize the distance between the corresponding sub-normalized vectors.

By allowing for all possible decompositions, the parallelity condition yields the Bures distance and Uhlmann connection. Thus, the parallelity between decompositions and purifications of density operators mutually agree.

A restriction to spectral decompositions gives rise to a distance as well as a discrete version of the connection on which the interferometric mixed state GP in [21, 22] is based. By iteration, the connection yields a spectral holonomy for discrete sequences of quantum ensembles. In this way, a spectral GP is obtained as the phase of the trace of the spectral holonomy. As the spectral connection treats equally all density operators along the sequence, including its end-points, this GP does not tend to the standard interferometric mixed state GP in the continuous limit, as the latter explicitly involves the spectral weights of the initial and final states along the path.

We end by suggesting a possible application of the proposed spectral GP and distance. It has been argued by Reuter et al. [24] that a discretized version of the Berry phase can be used to examine quantum critical phenomena in interacting spin systems in an experimentally accessible manner. This suggests that the proposed spectral GP and pair-distance for sets of thermal density operators could be useful to study phase transitions in spin systems at finite temperature.

Acknowledgments

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$$\sum_{k,l} \sqrt{q_k p_l} \langle f_k | e_l \rangle \Omega_{kl} = \sum_k \sqrt{q_k p_k}.$$  

This is the classical fidelity, which is known (see, e.g., Ref. [6]) to coincide with the quantum fidelity given by Eq. (9) in this particular case.

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