# Comparing metrics for mixed quantum states: Sjöqvist and Bures

Paul M. Alsing<sup>1</sup>, Carlo Cafaro<sup>2</sup>, Orlando Luongo<sup>3,4,5</sup>, Cosmo

Lupo<sup>6</sup>, Stefano Mancini<sup>3,7</sup>, and Hernando Quevedo<sup>5,8,9</sup>

<sup>1</sup>Air Force Research Laboratory, Information Directorate, 13441 Rome, New York, USA

<sup>2</sup>SUNY Polytechnic Institute, 12203 Albany, New York, USA

<sup>3</sup>Università di Camerino, 62032 Camerino, Italy

<sup>4</sup>SUNY Polytechnic Institute, 13502 Utica, New York, USA

<sup>5</sup>Al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan

<sup>6</sup>Politecnico di Bari, 70126 Bari, Italy

<sup>7</sup>INFN, Sezione di Perugia, 06123 Perugia, Italy

<sup>8</sup>Universidad Nacional Autonoma de Mexico, 04510 Mexico D. F., Mexico and

<sup>9</sup>Università di Roma "La Sapienza", 00185 Roma, Italy

It is known that there are infinitely many distinguishability metrics for mixed quantum states. This freedom, in turn, leads to metric-dependent interpretations of physically meaningful geometric quantities such as complexity and volume of quantum states.

In this paper, we first present an explicit and unabridged mathematical discussion on the relation between the Sjöqvist metric and the Bures metric for arbitrary nondegenerate mixed quantum states, using the notion of decompositions of density operators by means of ensembles of pure quantum states. Then, to enhance our comprehension of the difference between these two metrics from a physics standpoint, we compare the formal expressions of these two metrics for arbitrary thermal quantum states specifying quantum systems in equilibrium with a reservoir at non-zero temperature. For illustrative purposes, we show the difference between these two metrics in the case of a simple physical system characterized by a spin-qubit in an arbitrarily oriented uniform and stationary external magnetic field in thermal equilibrium with a finite-temperature bath. Finally, we compare the Bures and Sjöqvist metrics in terms of their monotonicity property.

PACS numbers: Quantum Computation (03.67.Lx), Quantum Information (03.67.Ac), Riemannian Geometry (02.40.Ky).

### I. INTRODUCTION

The role played by geometric techniques in describing and, to a certain extent, comprehending interesting classical and quantum physical phenomena of relevance in Hamiltonian dynamics and statistical physics is becoming increasingly important [1, 2]. For instance, the concepts of complexity [3] and phase transition [4] are two illustrative examples of physical phenomena being intensively investigated with tools of information geometry [5], i.e. differential geometry combined with probability calculus. For example, the singularities of a metric tensor of a manifold of coupling constants that parametrize a quantum Hamiltonian can be shown to be linked to the quantum phase transitions specifying the corresponding physical system [6–8]. Moreover, the induced curvature of the parameter manifold constructed from the metric tensor can also be viewed to encode relevant information on peculiar characteristics of the system. Specifically, the change in sign of the curvature, its discontinuities and, finally, its possible divergences can be argued to be associated with different (critical) regions of the parameter manifold where the statistical properties of the physical system exhibit very distinctive behaviors [9–11].

In this paper we focus on the physics of quantum systems specified by mixed quantum states because there exist infinitely many distinguishability distances for mixed quantum states [12]. This freedom in the choice of the metric implies that these geometric investigations of physical phenomena are still open to metric-dependent interpretations since a unifying and complete conceptual understanding of these geometric tool (along with their connections to experimental observations) has yet to be achieved. In particular, given the non-uniqueness of such distinguishability distances, understanding the physical relevance of considering either metric remains a goal of great conceptual and practical interest [9–11]. Furthermore, for a chosen metric, comprehending the physical significance of its corresponding curvature is essential and deserves further investigation [7, 8, 13].

An information geometric theoretical construct has recently been discussed [14] to describe and, to a certain extent, comprehend the complex behavior of evolutions of quantum systems in pure and mixed states. The comparative study was probabilistic in nature, i.e., it involved a complexity measure [15, 16] based on a temporal averaging procedure along with a long-time limit, and it was limited to examining expected geodesic evolutions on the underlying manifolds. More specifically, the authors studied the complexity of geodesic paths on the manifolds of single-qubit pure and mixed quantum states equipped with the Fubini-Study [17–19] and the Sjöqvist metrics [20], respectively. They analytically showed that the evolution of mixed quantum states in the Bloch ball is more complex than the evolution of pure

states on the Bloch sphere. They also verified that the ranking based on their proposed measure of complexity, representing the asymptotic temporal behavior of an averaged volume of the region explored on the manifold during system evolutions, agreed with the geodesic length-based ranking. Finally, targeting geodesic lengths and curvature properties in manifolds of mixed quantum states, they observed a softening of the complexity on the Bures manifold (i.e., a manifold of density operators equipped with the Bures metric [21–23]) compared to the Sjöqvist manifold.

Motivated by the above-mentioned importance of choosing one metric over another one in such geometric characterizations of physical aspects of quantum systems and, in addition, intrigued by the different complexity behaviors recorded with the Sjöqvist and Bures metrics in Ref. [14], we report in this paper a complete and straightforward analysis of the link between the Sjöqvist metric and the Bures metric for arbitrary nondegenerate mixed quantum states. Our presentation draws its original motivation from the concise discussion presented by Sjöqvist himself in Ref. [20], and it relies heavily on the concept of decompositions of density operators by means of ensembles of pure quantum states [24]. To physically deepen our understanding about the discrepancy between these two metrics, we provide a comparison of the exact expressions of these two metrics for arbitrary thermal quantum states describing quantum systems in equilibrium with a bath at non-zero temperature. Finally, we clarify the difference between these two metrics for a simple physical system specified by a spin-qubit in an arbitrarily oriented uniform and stationary external magnetic field vector in thermal equilibrium with a finite-temperature environment.

The layout of the rest of the paper is as follows. In Section II, we revisit the Sjöqvist metric construction for nondegenerate spectrally decomposed mixed quantum states as originally presented in Ref. [20]. In Section III, inspired by the helpful remarks in Ref. [20], we make explicit the emergence of the Bures metric from the Sjöqvist metric construction extended to nondegenerate arbitrarily decomposed mixed quantum states. In Sections II and III, we especially stress the role played by the concept of geometric phase and the parallel transport condition for mixed states in deriving the Sjöqvist and Bures metrics, respectively. In Section IV, focusing on the physically relevant class of thermal quantum states and following the works by Hubner in Ref. [23] and Zanardi and collaborators in Ref. [8], we cast the Sjöqvist and Bures metrics in two forms suitable for an insightful geometric comparison between the metrics. We end Section IV with a discussion of an illustrative example. Specifically, we study the difference between the Sjöqvist and the Bures metrics in the case of a physical system defined by a spin-qubit in an arbitrarily oriented uniform and stationary external magnetic field in thermal equilibrium with a finite-temperature environment. In Section V, we discuss monotonicity aspects of the Sjöqvist metric. Our conclusive remarks along with a summary of our main findings appear in Section VI. Finally, for ease of reading, further technical details appear in Appendices A, B, and C.

# **II. THE SJÖQVIST METRIC CONSTRUCTION: SPECTRAL DECOMPOSITIONS**

In this section, we revisit the Sjöqvist metric construction for nondegenerate spectrally decomposed mixed quantum states as originally presented in Ref. [20]. Before starting, we remark that the Sjöqvist metric can be linked to observable quantities in suitably prepared interferometric measurements. For this reason, it is sometimes termed "interferometric" metric [9, 20].

Let us consider two neighboring rank-N nondegenerate density operators  $\rho(t)$  and  $\rho(t + dt)$  specified by the following ensembles of pure states,

$$\rho(t) \stackrel{\text{def}}{=} \left\{ \sqrt{p_k(t)} e^{if_k(t)} \left| n_k(t) \right\rangle \right\}, \text{ and } \rho(t+dt) \stackrel{\text{def}}{=} \left\{ \sqrt{p_k(t+dt)} e^{if_k(t+dt)} \left| n_k(t+dt) \right\rangle \right\}, \tag{1}$$

respectively, with  $1 \le k \le N$ . Assume that  $\langle n_k(t) | n_{k'}(t) \rangle = \delta_{kk'}$  and the phases  $f_k(t) \in \mathbb{R}$  for any  $1 \le k \le N$ . Using Eq. (1),  $\rho(t)$  and  $\rho(t+dt)$  can be recast in terms of their spectral decompositions as

$$\rho(t) = \sum_{k=1}^{N} p_k(t) |n_k(t)\rangle \langle n_k(t)|, \text{ and } \rho(t+dt) = \sum_{k=1}^{N} p_k(t+dt) |n_k(t+dt)\rangle \langle n_k(t+dt)|,$$
(2)

respectively. The Sjöqvist metric  $d_{Sjöqvist}^2(t, t + dt)$  between the two mixed quantum states  $\rho(t)$  and  $\rho(t + dt)$  in Eq. (1) is formally defined as [20],

$$d_{\text{Sjöqvist}}^{2}(t, t+dt) = \min_{\{f_{k}(t), f_{k}(t+dt)\}} \sum_{k=1}^{N} \left\| \sqrt{p_{k}(t)} e^{if_{k}(t)} \left| n_{k}(t) \right\rangle - \sqrt{p_{k}(t+dt)} e^{if_{k}(t+dt)} \left| n_{k}(t+dt) \right\rangle \right\|^{2}, \quad (3)$$

that is, after some algebra,

$$d_{\text{Sjöqvist}}^{2}(t, t+dt) = 2 - 2\sum_{k=1}^{N} \sqrt{p_{k}(t) p_{k}(t+dt)} \left| \langle n_{k}(t) | n_{k}(t+dt) \rangle \right|.$$
(4)

It is important to point out that in transitioning from Eq. (3) to Eq. (4), the minimum is obtained by choosing phases  $\{f_k(t), f_k(t+dt)\}$  such that

$$\dot{f}_k(t) dt + \arg \left[ 1 + \langle n_k(t) | \dot{n}_k(t) \rangle dt + O(dt^2) \right] = 0.$$
(5)

Recall that an arbitrary complex number z can be expressed as  $z = |z| e^{i \arg(z)}$ . Then, noting that  $e^{\langle n_k(t) | \dot{n}_k(t) \rangle dt} = 1 + \langle n_k(t) | \dot{n}_k(t) \rangle dt + O(dt^2)$  is such that  $\arg \left[ e^{\langle n_k(t) | \dot{n}_k(t) \rangle dt} \right] = -i \langle n_k(t) | \dot{n}_k(t) \rangle dt$ , Eq. (5) can be recast to the first order in dt as

$$\dot{f}_k(t) - i \langle n_k(t) | \dot{n}_k(t) \rangle = 0.$$
(6)

Eq. (6) is the parallel transport condition  $\left\langle \psi_k\left(t\right) \middle| \dot{\psi}_k\left(t\right) \right\rangle = 0$  with  $|\psi_k\left(t\right)\rangle \stackrel{\text{def}}{=} e^{if_k\left(t\right)} \left| n_k\left(t\right) \right\rangle$  associated with individual pure state paths in the given ensemble that specifies the mixed state  $\rho\left(t\right)$  [25]. For completeness, we recall here that a state  $\rho\left(t\right) = U\left(t\right)\rho\left(0\right)U\left(t\right)$  evolving in a unitary fashion is parallel transported along an arbitrary path when at each instant of time t the state  $\rho\left(t\right)$  is in phase with the state  $\rho\left(t+dt\right) = U\left(t+dt\right)U^{\dagger}\left(t\right)\rho\left(t\right)U(t)U^{\dagger}\left(t+dt\right)$  at an infinitesimal later time t+dt. Moreover, the parallel transport conditions for pure (with  $\rho\left(t\right) = |\psi\left(t\right)\rangle\langle\psi\left(t\right)|$ ) and mixed states evolving in a unitary way are given by  $\left\langle\psi\left(t\right)\middle|\dot{\psi}\left(t\right)\right\rangle = 0$  and  $\operatorname{tr}\left[\rho\left(t\right)\dot{U}(t)U^{\dagger}\left(t\right)\right] = 0$ , respectively [26]. For a discussion on the parallel transport condition for mixed quantum states evolving in a nonunitary manner, we refer to Ref. [27]. Interestingly, using clever algebraic manipulations and expanding to the lowest nontrivial order in dt,  $d_{\mathrm{Sj}\bar{c}qvist}^2\left(t, t+dt\right)$  in Eq. (4) can be rewritten as

$$d_{\rm Sjöqvist}^{2}(t, t+dt) = \frac{1}{4} \sum_{k=1}^{N} \frac{dp_{k}^{2}}{p_{k}} + \sum_{k=1}^{N} \langle \dot{n}_{k} | (\mathbf{I} - |n_{k}\rangle \langle n_{k}|) | \dot{n}_{k}\rangle dt^{2},$$
(7)

with I in Eq. (7) denoting the identity operator. It is worth observing that  $ds_k^2 \stackrel{\text{def}}{=} \langle \dot{n}_k | (\mathbf{I} - |n_k\rangle \langle n_k|) | \dot{n}_k\rangle dt^2$ in Eq. (7) can be expressed as  $ds_k^2 = \langle \nabla n_k | \nabla n_k \rangle$  where  $|\nabla n_k\rangle \stackrel{\text{def}}{=} \mathbf{P}_{\perp}^{(k)} | \dot{n}_k \rangle$  is the covariant derivative of  $|n_k\rangle$ and  $\mathbf{P}_{\perp}^{(k)} \stackrel{\text{def}}{=} \mathbf{I} - |n_k\rangle \langle n_k|$  is the projector onto states perpendicular to  $|n_k\rangle$ . Furthermore,  $\sum_k ds_k^2$  is the nonclassical contribution in  $d_{\text{Sjöqvist}}^2(t, t + dt)$  and represents a weighted average of pure state Fubini-Study metrics along directions defined by state vectors  $\{|n_k\rangle\}_{1\leq k\leq N}$ . This weighted average, in turn, can be regarded as a generalized version of the Provost-Vallee coherent sum procedure utilized to define a Riemannian metric on manifolds of pure quantum states in Ref. [17]. The derivation of Eq. (4) ends our revisitation of the original Sjöqvist metric construction for nondegenerate mixed quantum states. It is important to emphasize that  $d_{\text{Sjöqvist}}^2(t, t + dt)$  in Eq. (4) was obtained by using the spectral decompositions of the two neighboring mixed states  $\rho(t)$  and  $\rho(t + dt)$ . Therefore, the metric was calculated for a special decomposition of neighboring density operators expressed in terms of ensembles of pure states.

### III. THE SJÖQVIST METRIC CONSTRUCTION: ARBITRARY DECOMPOSITIONS

In this section, we make explicit the emergence of the Bures metric from the Sjöqvist metric construction (presented in Section II) extended to nondegenerate arbitrarily decomposed mixed quantum states. In particular, we emphasize the role played by the concept of geometric phase and the parallel transport condition for mixed states in this derivation of the Bures metrics. Our discussion is an extended version of the abridged presentation in Ref. [20].

## A. From spectral to arbitrary decompositions

It is well-known in quantum information and computation that a given density matrix can be expressed in terms of different ensembles of quantum states. In particular, the eigenvalues and eigenvectors of a density matrix just denote one of many possible ensembles that may generate a fixed density matrix. This flexibility leads to the so-called theorem on the unitary freedom in the ensembles for density matrices [28]. This theorem implies that  $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| = \sum_j q_j |\varphi_j\rangle \langle \varphi_j|$  for normalized states  $\{|\psi_i\rangle\}$  and  $\{|\varphi_j\rangle\}$  and probability distributions  $\{p_i\}$  and  $\{q_j\}$  if and only if  $\sqrt{p_i} |\psi_i\rangle = \sum_j u_{ij} |\varphi_j\rangle$  for some unitary matrix  $u_{ij}$ , and we may fill the smaller ensemble with zero-probability entries in order to get same-size ensembles. In what follows, we shall see the effect on metrics for mixed quantum states produced by this unitary freedom in the ensembles for density matrices.

Let us consider arbitrary decompositions of two rank-N neighboring density operators  $\rho(t)$  and  $\rho(t + dt)$  in terms of statistical ensembles of pure states. Let us start by defining the following set  $\{|s_k(t)\rangle\}_{1 \le k \le N}$  of quantum states

$$\left|s_{k}\left(t\right)\right\rangle \stackrel{\text{def}}{=} \sqrt{p_{k}\left(t\right)}\left|n_{k}\left(t\right)\right\rangle,\tag{8}$$

with  $\langle s_k(t) | s_k(t) \rangle = p_k(t)$  for any  $1 \le k \le N$ . Then, given  $\rho(t) \stackrel{\text{def}}{=} \{ e^{if_k(t)} | s_k(t) \rangle \}$ , the spectral decomposition of  $\rho(t)$  is

$$\rho(t) = \sum_{k=1}^{N} |s_k(t)\rangle \langle s_k(t)|.$$
(9)

Consider a unitary matrix V(t) satisfying the unitary condition  $V^{\dagger}(t) V(t) = V(t) V^{\dagger}(t) = I$ , with I being the  $N \times N$  identity matrix. In terms of complex matrix coefficients  $\{V_{hk}(t)\}_{1 \le h, k \le N}$ , the unitary condition can be expressed as

$$\sum_{h=1}^{N} V_{hk}(t) V_{hl}^{*}(t) = \delta_{kl}.$$
(10)

Using the set  $\{|s_k(t)\rangle\}_{1 \le k \le N}$  in Eq. (8) and the unitary matrix V(t), we define a new set of normalized state vectors  $\{|u_h(t)\rangle\}_{1 \le h \le N}$  as

$$\left|u_{h}\left(t\right)\right\rangle \stackrel{\text{def}}{=} \sum_{k=1}^{N} V_{hk}\left(t\right) \left|s_{k}\left(t\right)\right\rangle.$$

$$(11)$$

Given the set  $\{|u_h(t)\rangle\}_{1\leq h\leq N}$  with  $|u_h(t)\rangle$  in Eq. (11), we observe that we have constructed a set of unitarily equivalent representations of the mixed state  $\rho(t)$ . Indeed, we have

$$\sum_{h=1}^{N} |u_{h}(t)\rangle \langle u_{h}(t)| = \sum_{h,k,l=1}^{N} V_{hk}(t) V_{hl}^{*}(t) |s_{k}(t)\rangle \langle s_{l}(t)|$$

$$= \sum_{k,l=1}^{N} \left( \sum_{h=1}^{N} V_{hk}(t) V_{hl}^{*}(t) \right) |s_{k}(t)\rangle \langle s_{l}(t)|$$

$$= \sum_{k,l=1}^{N} |s_{k}(t)\rangle \langle s_{l}(t)| \delta_{kl}$$

$$= \sum_{k=1}^{N} |s_{k}(t)\rangle \langle s_{k}(t)|$$

$$= \sum_{k=1}^{N} p_{k}(t) |n_{k}(t)\rangle \langle n_{k}(t)|$$

$$= \rho(t)$$
(12)

that is,  $\rho(t)$  can be generally decomposed as

$$\rho(t) = \sum_{h=1}^{N} |u_h(t)\rangle \langle u_h(t)|.$$
(13)

Let us consider now two neighboring nondegenerate states  $\rho(t)$  and  $\rho(t + dt)$  specified by the following ensembles of pure states,

$$\rho\left(t\right) \stackrel{\text{def}}{=} \left\{ \sum_{k=1}^{N} V_{hk}\left(t\right) \sqrt{p_{k}\left(t\right)} \left| n_{k}\left(t\right) \right\rangle \right\} = \left\{ \left| u_{h}\left(t\right) \right\rangle \right\}$$
(14)

and,

$$\rho\left(t+dt\right) \stackrel{\text{def}}{=} \left\{ \sum_{k=1}^{N} V_{hk}\left(t+dt\right) \sqrt{p_k\left(t+dt\right)} \left| n_k\left(t+dt\right) \right\rangle \right\} = \left\{ \left| u_h\left(t+dt\right) \right\rangle \right\},\tag{15}$$

respectively. For completeness, we note that  $V_{hk}(t) = |V_{hk}(t)| e^{i \arg[V_{hk}(t)]} \in \mathbb{C}$  for any  $1 \le h, k \le N$ . In particular, one recovers the original construction proposed originally by Sjöqvist when

$$V_{hk}(t) = \delta_{hk} e^{if_k(t)}, \text{ and } |u_h(t)\rangle = \sqrt{p_h(t)} e^{if_h(t)} |n_h(t)\rangle.$$
(16)

Using the decompositions in Eqs. (14) and (15), the generalization  $\tilde{d}_{Sj\ddot{o}qvist}^2(t, t + dt)$  of  $d_{Sj\ddot{o}qvist}^2(t, t + dt)$  in Eq. (3) becomes

$$\tilde{d}_{\text{Sjöqvist}}^{2}\left(t,\,t+dt\right) \stackrel{\text{def}}{=} \min_{\{V(t),\,V(t+dt)\}} \sum_{h=1}^{N} \left\| \left| u_{h}\left(t\right) \right\rangle - \left| u_{h}\left(t+dt\right) \right\rangle \right\|^{2},\tag{17}$$

that is,

$$\tilde{d}_{\text{Sjöqvist}}^{2}(t, t+dt) = \sum_{h=1}^{N} \left\| \sum_{k=1}^{N} V_{hk}(t) \sqrt{p_{k}(t)} \left| n_{k}(t) \right\rangle - \sum_{k=1}^{N} V_{hk}(t+dt) \sqrt{p_{k}(t+dt)} \left| n_{k}(t+dt) \right\rangle \right\|^{2}.$$
(18)

To obtain a more compact expression of  $\tilde{d}_{Sj\"oqvist}^2(t, t+dt)$ , we note that

$$\sum_{h=1}^{N} \||u_{h}(t)\rangle - |u_{h}(t+dt)\rangle\|^{2} = 2 - 2 \operatorname{Re} \left[\sum_{h=1}^{N} \langle u_{h}(t) | u_{h}(t+dt) \rangle\right]$$
$$= 2 - 2 \operatorname{Re} \left[\sum_{h,k,k'} V_{hk}^{*}(t) \langle s_{k}(t) | s_{k'}(t+dt) \rangle V_{hk'}(t+dt)\right]$$
$$= 2 - 2 \operatorname{Re} \left[\sum_{h,k,k'} S_{kk'} V_{hk'}(t+dt) V_{hk}^{*}(t)\right]$$
$$= 2 - 2 \operatorname{Re} \operatorname{tr} \left[S_{t}(dt) V(t+dt) V^{\dagger}(t)\right],$$
(19)

that is,

$$\sum_{h=1}^{N} \||u_{h}(t)\rangle - |u_{h}(t+dt)\rangle\|^{2} = 2 - 2\operatorname{Re}\operatorname{tr}\left[S_{t}(dt)V(t+dt)V^{\dagger}(t)\right].$$
(20)

The matrix  $S_t(dt)$  in Eq. (20) is an overlap matrix with coefficients  $S_{kk'}$  defined as

$$S_{kk'} \stackrel{\text{def}}{=} \langle s_k(t) | s_{k'}(t+dt) \rangle = \sqrt{p_k(t) p_{k'}(t+dt)} \langle n_k(t) | n_{k'}(t+dt) \rangle.$$

$$(21)$$

Combining Eqs. (17) and (20), we finally get

$$\tilde{d}_{\text{Sjöqvist}}^{2}(t, t+dt) = \min_{\{V(t), V(t+dt)\}} \left\{ 2 - 2\operatorname{Re}\operatorname{tr}\left[S_{t}(dt)V(t+dt)V^{\dagger}(t)\right] \right\}.$$
(22)

In what follows, we shall see the emergence of the Bures metric by explicitly evaluating the *minimum* that specifies  $\tilde{d}_{Sj\ddot{o}qvist}^2(t, t + dt)$  in Eq. (22).

## B. Emergence of the Bures metric

We begin by observing that the polar decomposition of  $S_t(dt)$  is given by [28],

$$S_t(dt) = |S_t(dt)| U_t(dt), \qquad (23)$$

where  $|S_t(dt)| \stackrel{\text{def}}{=} \sqrt{S_t(dt)S_t^{\dagger}(dt)}$  and  $U_t(dt)$  is a unitary matrix. Then, we note that minimizing  $2 - 2 \operatorname{Retr} \left[S_t(dt)V(t+dt)V^{\dagger}(t)\right]$  is equivalent to maximizing  $2 \operatorname{Retr} \left[S_t(dt)V(t+dt)V^{\dagger}(t)\right]$  with respect to  $\{V(t), V(t+dt)\}$ . Furthermore, we make two remarks. First of all,  $\operatorname{Re}(z) \leq |z|$  for any  $z \in \mathbb{C}$ . Second of all,  $\operatorname{tr}|A| \geq |\operatorname{tr}(AU_A)|$  for any operator A and unitary  $U_A$  with  $\max_{U_A} |\operatorname{tr}(AU_A)| = \operatorname{tr}|A|$  obtained by choosing  $U_A = V_A^{\dagger}$  where  $A = |A|V_A$  is the polar decomposition of A [28, 29]. Given this set of preliminary observations, we have that

$$\operatorname{Re}\operatorname{tr}\left[S_{t}(dt)V\left(t+dt\right)V^{\dagger}\left(t\right)\right] = \operatorname{Re}\operatorname{tr}\left[\left|S_{t}(dt)\right|U_{t}\left(dt\right)V\left(t+dt\right)V^{\dagger}\left(t\right)\right]$$
$$\leq \left|\operatorname{tr}\left[\left|S_{t}(dt)\right|U_{t}\left(dt\right)V\left(t+dt\right)V^{\dagger}\left(t\right)\right]\right|$$
$$\leq \operatorname{tr}\left|S_{t}(dt)\right|, \tag{24}$$

that is,

$$\max_{\{V(t), V(t+dt)\}} \operatorname{Re} \operatorname{tr} \left[ S_t(dt) V(t+dt) V^{\dagger}(t) \right] = \operatorname{tr} \left| S_t(dt) \right|$$
(25)

is obtained by choosing  $\{V(t), V(t+dt)\}$  such that the following condition is satisfied,

$$U_t \left( dt \right) V \left( t + dt \right) V^{\dagger} \left( t \right) = I.$$
<sup>(26)</sup>

Interestingly, we point out that the maximization procedure in Eq. (25) is similar to the use of the variational characterization of the trace norm that one employs to prove Uhlmann's theorem (see, for instance, Lemma 9.5 in Ref. [28] and Property 9.1.6 in Ref. [29]). We also remark that Eq. (26) is a constraint equation that can be regarded as the operator-analogue of the parallel transport condition in Eq. (6). For more details on this point, we refer to Appendix A. Finally, employing Eqs. (22) and (25), we get

$$\hat{d}_{\text{Sjöqvist}}^{2}(t, t+dt) = 2 - 2\text{tr} \left| S_{t}(dt) \right|.$$
(27)

We shall now show that  $\tilde{d}_{Sj \circ qvist}^2(t, t + dt)$  in Eq. (27) is indeed the Bures metric  $d_{Bures}^2(t, t + dt)$  defined as [12, 28],

$$d_{\text{Bures}}^{2}(t, t+dt) \stackrel{\text{def}}{=} 2 - 2\text{tr}\left[\sqrt{\rho^{1/2}(t)\rho(t+dt)\rho^{1/2}(t)}\right].$$
 (28)

Observe that  $|S_t(dt)|^2 = S_t(dt)S_t^{\dagger}(dt)$ , where

$$\left[S_t(dt)S_t^{\dagger}(dt)\right]_{kk''} = \sum_{k'=1}^N \left\langle s_k(t) \, | \, s_{k'}(t+dt) \right\rangle \left\langle s_{k'}(t+dt) \, | \, s_{k''}(t) \right\rangle.$$
(29)

After some algebra, we note that  $\rho^{1/2}(t) \rho(t+dt) \rho^{1/2}(t) = |S_t(dt)|^2$ . Indeed, we have

$$\begin{split} \rho^{1/2}(t) \,\rho\left(t+dt\right) \rho^{1/2}(t) &= \left(\sum_{k=1}^{N} \sqrt{p_{k}\left(t\right)} \left|n_{k}(t)\right\rangle \left\langle n_{k}(t)\right|\right) \left(\sum_{k'=1}^{N} p_{k'}\left(t+dt\right) \left|n_{k'}(t+dt)\right\rangle \left\langle n_{k'}(t+dt)\right|\right) \\ &= \left(\sum_{k,k',k''=1}^{N} \sqrt{p_{k''}\left(t\right)} \left|n_{k''}(t)\right\rangle \left\langle n_{k''}(t)\right|\right) \\ &= \sum_{k,k',k''=1}^{N} \left[\left(\frac{\left|n_{k}(t)\right\rangle \left(\sqrt{p_{k}\left(t\right)} p_{k'}\left(t+dt\right)}{\left(n_{k'}\left(t+dt\right)} \left|n_{k''}(t)\right\rangle\right)\right) \left\langle n_{k''}(t)\right|\right] \\ &= \sum_{k,k',k''=1}^{N} \left|n_{k}(t)\right\rangle \left(\left\langle s_{k}\left(t\right)\right| s_{k'}\left(t+dt\right)\right\rangle\right) \left(\left\langle s_{k'}\left(t+dt\right)\right| s_{k''}\left(t\right)\right)\right) \left\langle n_{k''}(t)\right| \\ &= \sum_{k,k''=1}^{N} \left|n_{k}(t)\right\rangle \left[\sum_{k=1}^{N} \left\langle s_{k}\left(t\right)\right| s_{k'}\left(t+dt\right)\right\rangle \left\langle s_{k'}\left(t+dt\right)\left|s_{k''}\left(t\right)\right\rangle\right] \left\langle n_{k''}(t)\right| \\ &= \sum_{k,k''=1}^{N} \left|n_{k}(t)\right\rangle \left[S_{t}\left(dt\right) S_{t}^{\dagger}\left(dt\right)\right]_{kk''} \left\langle n_{k''}(t)\right| \\ &= \sum_{k,k''=1}^{N} \left[S_{t}\left(dt\right) S_{t}^{\dagger}\left(dt\right)\right]_{kk''} \left|n_{k}(t)\right\rangle \left\langle n_{k''}(t)\right| \\ &= S_{t}\left(dt\right) S_{t}^{\dagger}\left(dt\right) \\ &= \left|S_{t}\left(dt\right)\right|^{2}. \end{split}$$

In conclusion, we arrive at the following relations

$$d_{\text{Bures}}^2\left(t, t+dt\right) = \tilde{d}_{\text{Sjöqvist}}^2\left(t, t+dt\right) \neq d_{\text{Sjöqvist}}^2\left(t, t+dt\right).$$
(31)

More specifically, we have  $\tilde{d}_{Sj\ddot{o}qvist}^2(t, t + dt) \leq d_{Sj\ddot{o}qvist}^2(t, t + dt)$  since the minimization procedure that specifies  $\tilde{d}_{Sj\ddot{o}qvist}^2(t, t + dt)$  is extended to arbitrary unitary  $\{V(t), V(t + dt)\}$  while, instead, the minimization procedure that specifies  $d_{Sj\ddot{o}qvist}^2(t, t + dt)$  is limited to unitary matrices of the form  $\{V(t), V(t + dt)\}$  with  $V_{hk}(t) = \delta_{hk}e^{if_k(t)}$ . With this last remark, we end our mathematical discussion on the emergence of the Bures metric from a generalized version of the Sjöqvist original metric construction. However, to better grasp the physical differences between the Sjöqvist and Bures metrics, we focus on thermal mixed states in the next section.

# IV. SJÖQVIST AND BURES METRICS FOR THERMAL STATES

In this section, we cast the Sjöqvist and the Bures metrics in two forms that are especially convenient for an insightful geometric comparison. In particular, we illustrate this comparison with an explicit example in which the physical system is specified by a spin-qubit in an arbitrarily oriented uniform and stationary magnetic field in thermal equilibrium with a finite-temperature reservoir.

### A. Suitable recast of metrics

We begin by observing that, in the Sjöqvist case (see Eq. (7)), the metric (infinitesimal line element) can be decomposed in terms of a classical and a nonclassical contribution,

$$ds_{\rm Sjöqvist}^2 = \left(ds_{\rm Sjöqvist}^2\right)^{\rm c} + \left(ds_{\rm Sjöqvist}^2\right)^{\rm nc}.$$
(32)

It happens that  $\left(ds_{\text{Sjöqvist}}^2\right)^{\text{c}}$  and  $\left(ds_{\text{Sjöqvist}}^2\right)^{\text{nc}}$  can be conveniently written as [20],

$$\left(ds_{\text{Sjöqvist}}^{2}\right)^{c} \stackrel{\text{def}}{=} \frac{1}{4} \sum_{n} \frac{dp_{n}^{2}}{p_{n}}, \text{ and } \left(ds_{\text{Sjöqvist}}^{2}\right)^{nc} \stackrel{\text{def}}{=} \sum_{n} p_{n} \left\langle dn | (\mathbf{I} - |n\rangle \left\langle n| \right) | dn \right\rangle,$$
(33)

Approved for Public Release; Distribution Unlimited: PA# AFRL 2023-1054

(30)

respectively. To recast  $(ds_{\text{Sjöqvist}}^2)^{\text{nc}}$  in Eq. (33) in a suitable manner for thermal states  $\rho \stackrel{\text{def}}{=} \sum_n p_n |n\rangle \langle n|$  where  $\{|n\rangle\}$  denotes the eigenbasis of  $\rho$  with eigenvalues  $\{p_n\}$  and  $1 \leq n \leq N$ , we note that

$$\langle dn | dn \rangle = \langle dn | n \rangle \langle n | dn \rangle + \sum_{k, \ k \neq n} \langle dn | k \rangle \langle k | dn \rangle.$$
(34)

Furthermore, assuming that the Hamiltonian operator H satisfies the relation  $H|n\rangle = E_n |n\rangle$  with  $\{E_n\}$  and  $\{|n\rangle\}$  being eigenvalues and eigenvectors of H, respectively, we find after some clever algebraic manipulations that

$$\langle k | dn \rangle \langle dn | k \rangle = \left| \frac{\langle k | dH | n \rangle}{E_n - E_k} \right|^2.$$
(35)

Then, exploiting Eqs. (34) and (35),  $\left(ds_{\text{Siöqvist}}^2\right)^{\text{nc}}$  in Eq. (33) can be finally expressed as

$$\left(ds_{\text{Sjöqvist}}^{2}\right)^{\text{nc}} = \sum_{n \neq k} \frac{e^{-\beta E_{n}} + e^{-\beta E_{k}}}{2\mathcal{Z}} \left|\frac{\langle n|dH|k\rangle}{E_{n} - E_{k}}\right|^{2}.$$
(36)

In Eq. (36),  $\mathcal{Z}_{=}^{\text{def}}$ tr  $(e^{-\beta H})$  is the partition function of the system,  $p_n \stackrel{\text{def}}{=} e^{-\beta E_n}/\mathcal{Z}$ ,  $\beta \stackrel{\text{def}}{=} (k_B T)^{-1}$ , and  $k_B$  is the Boltzmann constant. Eq. (36) is an interesting result of our work and denotes the suitable recast of  $(ds_{\text{Sjöqvist}}^2)^{\text{nc}}$  for thermal quantum states we were looking for. We need to find now the analog of Eq. (36) for the Bures case.

In the Bures case, the metric (infinitesimal line element) can be decomposed in terms of a classical and a nonclassical contribution,

$$ds_{\rm Bures}^2 = \left(ds_{\rm Bures}^2\right)^{\rm c} + \left(ds_{\rm Bures}^2\right)^{\rm nc}.$$
(37)

Focusing on thermal quantum states  $\rho \stackrel{\text{def}}{=} \sum_{n} p_n |n\rangle \langle n|$  as pointed out earlier, it can be shown that  $(ds_{\text{Bures}}^2)^c = (ds_{\text{Sjöqvist}}^2)^c$  in Eq. (33) and  $(ds_{\text{Bures}}^2)^{\text{nc}}$  can be expressed as [8, 23],

$$\left(ds_{\rm Bures}^2\right)^{\rm nc} = \sum_{n \neq k} \frac{e^{-\beta E_n} + e^{-\beta E_k}}{2\mathcal{Z}} \left(\frac{e^{-\beta E_n} - e^{-\beta E_k}}{e^{-\beta E_n} + e^{-\beta E_k}}\right)^2 \left|\frac{\langle n|dH|k\rangle}{E_n - E_k}\right|^2.$$
(38)

For completeness, note that a general expression of  $ds_{\text{Bures}}^2$  in Eq. (37) can be obtained by replacing  $e^{-\beta E_n}/\mathcal{Z}$  with an arbitrary  $p_n$  as remarked in Ref. [8]. We observe that Eq. (38) is, modulo a clever rewriting that suits our comparative discussion between the Sjöqvist and the Bures metrics here, equivalent to Eq. (6) in Ref. [8]. The difference between the Sjöqvist and the Bures metrics  $ds_{\text{Sjöqvist}}^2$  and  $ds_{\text{Bures}}^2$  appears in their non-classical metric components  $g_{\text{Sjöqvist}}^{nc}$  and  $g_{\text{Bures}}^{nc}$ . In particular, focusing on Eqs. (36) and (38), the difference between these components, in turn, tends to vanish when the minimum separation between the modulus of two distinct quantum-mechanical energy levels  $E_n$  and  $E_k$  of the system is much greater than the characteristic thermal energy  $k_BT$ , i.e.

$$\min_{n \to k} |E_n - E_k| \gg k_B T. \tag{39}$$

Clearly, Eq. (39) is satisfied when the temperature T approaches zero (i.e., asymptotic limit of  $\beta$  approaching infinity) with  $|E_n - E_k|$  finite (and nonzero) for any  $n \neq k$ . In this case, mixed quantum states tend to become pure states and, in particular, both metrics (i.e., Sjöqvist and Bures) reduce to the Fubini-Study metric.

### B. Illustrative example

To better grasp the difference between these two metrics as reported in Eqs. (36) and (38), we discuss an explicit example. Let us take into consideration a spin-1/2 particle specified by an electron of m, charge -e with  $e \ge 0$  immersed in an external magnetic field  $\vec{B}(t)$ . The Hamiltonian of this system can be quantum-mechanically specified by the Hermitian operator  $\mathbf{H}(t) \stackrel{\text{def}}{=} -\vec{\mu} \cdot \vec{B}(t)$ , where  $\vec{\mu} \stackrel{\text{def}}{=} - (e/m)\vec{s}$  is the electron magnetic moment operator and  $\vec{s} \stackrel{\text{def}}{=} (\hbar/2)\vec{\sigma}$  is the spin operator. Naturally,  $\hbar \stackrel{\text{def}}{=} h/(2\pi)$  denotes the reduced Planck constant and  $\vec{\sigma} \stackrel{\text{def}}{=} (\sigma_x, \sigma_y, \sigma_z)$  represents the Pauli spin vector operator. If we consider a time-independent, uniform, and arbitrarily magnetic field given by

 $\vec{B} \stackrel{\text{def}}{=} B_x \hat{x} + B_y \hat{y} + B_z \hat{z}$  and introduce the frequency vector  $\vec{\omega} \stackrel{\text{def}}{=} (\omega_x, \omega_y, \omega_z) = ((e/m)B_x, (e/m)B_y, (e/m)B_z)$ , the spin-1/2 qubit (SQ) Hamiltonian becomes

$$\mathbf{H}_{\mathrm{SQ}}\left(\vec{\omega}\right) \stackrel{\mathrm{def}}{=} \frac{\hbar}{2} \left(\vec{\omega} \cdot \vec{\sigma}\right). \tag{40}$$

Note that with the sign convention used for  $H_{SQ}(\vec{\omega})$  in Eq. (40), when  $\vec{\omega} = \omega_z \hat{z}$  with  $\omega_z > 0$ , we have that  $|1\rangle$ ( $|0\rangle$ ) represents the ground (excited) state of the system with energy  $-\hbar\omega_z/2$  ( $+\hbar\omega_z/2$ ). Furthermore, let us suppose that the system specified by the Hamiltonian  $H_{SQ}$  in Eq. (40) is in thermal equilibrium with a reservoir at non-zero temperature T. Then, quantum statistical mechanics [30] specifies that the system has temperature T and its state is characterized by a thermal state [31] specified by a density matrix  $\rho$  given by

$$\rho_{\rm SQ}\left(\beta,\,\vec{\omega}\right) \stackrel{\rm def}{=} \frac{e^{-\beta H_{\rm SQ}\left(\vec{\omega}\right)}}{\operatorname{tr}\left(e^{-\beta H_{\rm SQ}\left(\vec{\omega}\right)}\right)}.\tag{41}$$

In Eq. (41),  $\beta \stackrel{\text{def}}{=} (k_B T)^{-1}$  is the so-called inverse temperature, while  $k_B$  denotes the Boltzmann constant. Using Eqs. (40) and (41), one obtains after some algebra that the formal expression of the thermal state  $\rho_{\text{SQ}}(\beta, \vec{\omega})$  is given by

$$\rho_{\rm SQ}\left(\beta,\,\vec{\omega}\right) = \frac{1}{2} \left[ I - \tanh\left(\beta\frac{\hbar\omega}{2}\right)\frac{\vec{\omega}\cdot\vec{\sigma}}{\omega} \right],\tag{42}$$

with  $\omega \stackrel{\text{def}}{=} \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$  denoting the magnitude of the frequency vector  $\vec{\omega}$  and I in Eq. (42) being the identify operator. Finally, assuming to keep  $\omega_x$ -fixed  $\neq 0$ ,  $\omega_y$ -fixed  $\neq 0$  and, at the same time, tuning only the two parameters  $\beta$  and  $\omega_z$ , the Sjöqvist and the Bures metrics specifying the distance between the two neighboring mixed states  $\rho_{SQ}$ and  $\rho_{SQ} + d\rho_{SQ}$  can be analytically shown to be equal to

$$g_{ij}^{\text{Sjöqvist}}\left(\beta,\,\omega_{z}\right) = \frac{\hbar^{2}}{16} \left[1 - \tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right)\right] \left(\begin{array}{cc}\omega^{2} & \beta\omega_{z}\\\beta\omega_{z} & \beta^{2}\left(\frac{\omega_{z}}{\omega}\right)^{2} + \frac{4}{\hbar^{2}}\frac{\omega_{x}^{2} + \omega_{y}^{2}}{\omega^{4}}\frac{1}{1 - \tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right)}\end{array}\right),\tag{43}$$

and

$$g_{ij}^{\text{Bures}}\left(\beta,\,\omega_{z}\right) = \frac{\hbar^{2}}{16} \left[1 - \tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right)\right] \left(\begin{array}{cc}\omega^{2} & \beta\omega_{z}\\\beta\omega_{z} & \beta^{2}\left(\frac{\omega_{z}}{\omega}\right)^{2} + \frac{4}{\hbar^{2}}\frac{\omega_{x}^{2} + \omega_{y}^{2}}{\omega^{4}}\frac{\tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right)}{1 - \tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right)}\right),\tag{44}$$

respectively, with  $1 \leq i, j \leq 2$  (where  $1 \leftrightarrow \beta$  and  $2 \leftrightarrow \omega_z$ ). For explicit technical details on how to analytically calculate the Sjöqvist and the Bures metrics, we refer to Ref. [32]. From Eqs. (43) and (44), it is clear that the Sjöqvist and the Bures metrics only differ in the non-classical contribution  $[g_{22}(\beta, \omega_z)]_{\rm nc}$  of their  $g_{22}(\beta, \omega_z)$  metric component. Specifically, we observe that

$$0 \le \left[g_{22}^{\text{Bures}}\left(\beta,\,\omega_{z}\right)\right]_{\text{nc}} / \left[g_{22}^{\text{Sjöqvist}}\left(\beta,\,\omega_{z}\right)\right]_{\text{nc}} = \tanh^{2}\left(\beta\frac{\hbar\omega}{2}\right) \le 1.$$
(45)

Interestingly, for a two-level system with  $E_1 = \hbar\omega/2$  and  $E_2 = -\hbar\omega/2$ , the factor  $\left[\left(e^{-\beta E_1} - e^{-\beta E_2}\right) / \left(e^{-\beta E_1} + e^{-\beta E_2}\right)\right]^2$  in Eq. (38) becomes exactly  $\tanh^2 \left[\beta \left(\hbar\omega/2\right)\right]$  (i.e., the ratio in Eq. (45)).

We note that, in the limiting case in which  $\vec{\omega} = (0, 0, \omega_z)$ , setting  $k_B = 1, \beta = t^{-1}$ , and  $\omega_z = t$ , our Eq. (44) reduces to the last relation found by Zanardi and collaborators in Ref. [8]. In Ref. [8], the limiting scenario considered by Zanardi and collaborators corresponds to the case of a one-dimensional quantum Ising model in a transverse magnetic field  $h \equiv B_z$  with  $|h| \gg 1$ . When  $|h| \gg 1$ , the lowest order approximation of the quantum Ising Hamiltonian is  $H = h \sum_i \sigma_i^z$ . In this approximation, the Bures metric between two neighboring thermal states parametrized by  $\{\beta, h\}$  and emerging from this approximated Hamiltonian vanishes. In our analysis, the degeneracy of the Bures metric appears when the spin-qubit is immersed in a magnetic field oriented along the z-axis. In particular, the metric has in this case only one nonvanishing eigenvalue, its determinant vanishes, and no definition of connection and curvature exists. In summary, no Riemannian structure survives at all when the metric is degenerate. In Ref. [8], the degeneration of the metric can be removed by considering higher order approximations of the quantum Ising Hamiltonian. In our case, instead, the degeneracy of the Bures metric can be removed by considering more general orientations of the external magnetic field. Interestingly, the degenerate scenario can be given a clear interpretation, despite the absence of any Riemannian structure. Indeed, given that the eigenvectors of the Bures metric tensor define the directions of maximal and minimal growth of the line element  $ds_{\text{Bures}}^2$  [8], the eigenvector of the metric related to the highest eigenvalue defines at each point of the two-dimensional parametric plane the direction along which the Uhlmann fidelity between two nearby states decreases most quickly, i. e., the direction of highest distinguishability between two neighboring thermal states. Therefore, when proceeding along the direction specified by an eigenvector corresponding to the vanishing eigenvalue, one can conclude that no change in the state of the system takes place.

For completeness, we reiterate that in this paper we limited our theoretical discussions to nondegenerate density matrices for which Sjöqvist's original metric is nonsingular. In particular, our explicit illustrative example was specified by an Hamiltonian with nondegenerate eigenvalues yielding nondegenerate density operators. However, degenerate thermal states that emerge from degenerate-spectrum Hamiltonians are pervasive in physics [33]. In these latter scenarios, insights on the physics of quantum systems can be generally obtained by studying the geometry of thermal state manifolds equipped with a generalized version of Sjöqvist's original metric. This generalized metric is also suitable for degenerate mixed quantum states and was proposed by Silva and collaborators in Ref. [9].

In conclusion, we point out that for pure quantum states  $(\rho = \rho^2)$  and for mixed quantum states  $(\rho \neq \rho^2)$  for which the non-commutative probabilistic structure underlying quantum theory is invisible (i.e., in the classical scenario with  $[\rho, \rho + d\rho] = 0$ ), the Bures and the Sjöqvist metrics are essentially the same. Indeed, in the former and latter cases, they reduce to the Fubini-Study and Fisher-Rao information metrics, respectively. Instead, when considering mixed quantum states for which the non-commutative probabilistic structure of quantum mechanics is visible (i.e., in the non-classical scenario with  $[\rho, \rho + d\rho] \neq 0$ ), the Bures and the Sjöqvist metrics are generally different. This latter scenario has been explicitly illustrated in our proposed example.

In the next section, we shall investigate the monotonicity aspects of the Sjöqvist metric for mixed states.

# V. MONOTONICITY OF THE SJÖQVIST METRIC

In this section, we discuss the monotonicity of the Sjöqvist metric in the single-qubit case. Unlike the Bures metric, we shall see that the Sjöqvist metric is not specified by a proper Morozova-Chentsov function and is not a monotone metric. For some technical details on the monotonicity of the Bures metric, see Appendix B.

### A. Preliminaries

If a distance between classical probability distributions or quantum density matrices expresses statistical distinguishability, then this distance must not increase under coarse-graining. In particular, a metric that does not grow under the action of a stochastic map is called monotone [12]. In the classical setting, the Fisher-Rao information metric is the unique [34, 35], except for a constant scale factor, Riemannian metric that is invariant under Markov embeddings (i.e., stochastic maps). In the quantum setting, instead, there are infinitely many monotone Riemannian metrics on the space of quantum states [12]. In the quantum case, quantum stochastic maps are represented by completely positive and trace preserving (CPTP) maps. If  $D_{\rm mon}(\rho, \sigma)$  represents the distance between density matrices  $\rho$  and  $\sigma$  that originates from a monotone metric, it must be

$$D_{\mathrm{mon}}\left(\Lambda\left(\rho\right),\Lambda\left(\sigma\right)\right) \le D_{\mathrm{mon}}\left(\rho,\sigma\right),\tag{46}$$

for any CPTP map  $\Lambda$ . Morozova and Chentsov originally considered the problem of finding monotone Riemannian metrics on the space of density matrices [36]. However, although they proposed several candidates, they did not present a single explicit example of a monotone metric. It was Petz, building on the work of Morozova and Chentsov, who showed the abundance of monotone metrics by exploiting the concept of operator monotone function in Ref. [37]. A scalar function  $f: I \to \mathbb{R}$  is said to be matrix (or, operator) monotone (increasing) on an interval  $I \subset D_f \subset \mathbb{R}$ , with  $D_f$  denoting the domain of definition of f, if for all Hermitian matrices A and B of all orders whose eigenvalues lie in  $I, A \geq B \Rightarrow f(A) \geq f(B)$ . Observe that  $A \geq B$  if and only if A - B is a positive matrix. We point of that the concept of an operator monotone function can be subtle. For instance, there are examples of monotone functions that are not operator monotone (for instance [12],  $f(t) = t^2$ ). For more details on the notion of operator monotone functions along with suitable techniques to construct them, we refer to Refs. [38–43]. The key contribution by Petz in Ref. [37] was that of using operator monotone functions to construct explicit examples of monotone metrics. The joint work of Morozova-Chentsov-Petz (MCP) led to the much appreciated MCP theorem [36, 37]. Roughly speaking, this theorem states that every monotone metric on the space of density matrices can be recast in a suitable form specified by a so-called Morozova-Chentsov (MC) function. A scalar function  $f: \mathbb{R}_+ \to \mathbb{R}_+$  is called Morozova-Chentsov if it satisfies three conditions: (i) f is operator monotone; (ii) f is self inversive, that is f(1/t) = f(t)/t for any  $t \in \mathbb{R}_+$ ; and (iii) f(1) = 1. Condition (ii) is necessary to have a symmetric mean A#B between two Hermitian operators A and B [12]. Recall that  $A\#B \stackrel{\text{def}}{=} \sqrt{A} f\left(\frac{1}{\sqrt{A}}B\frac{1}{\sqrt{A}}\right)\sqrt{A}$ , where A > 0 and f is an operator monotone function on  $[0, \infty)$  with f(1) = 1. Finally, condition (iii) is a normalization condition which helps to avoid a conical singularity of the metric at the maximally mixed state.

In the next subsection, we do not discuss the non-monotonicity of the Sjöqvist metric by providing the existence of a CPTP map that violates the inequality in Eq. (46). Rather, we argue that the Sjöqvist metric is not a monotone metric because it violates the MCP theorem since it is not specified by a proper Morozova-Chentsov function.

### B. Discussion

Consider two neighboring single-qubit density matrices  $\rho$  and  $\rho + d\rho$  in the Bloch ball, with  $\rho$  given by

$$\rho = \frac{\hat{1} + \vec{r} \cdot \vec{\sigma}}{2} = \frac{1}{2} \begin{pmatrix} 1 + r\cos\left(\theta\right) & r\sin\left(\theta\right)e^{-i\varphi} \\ r\sin\left(\theta\right)e^{i\varphi} & 1 - r\cos\left(\theta\right) \end{pmatrix},\tag{47}$$

and a diagonal form specified by  $\rho_{\text{diag}} = (1/2) \operatorname{diag} (1+r, 1-r)$ . In Eq. (47),  $\vec{r}$  denotes the polarization vector given by  $\vec{r} \stackrel{\text{def}}{=} r\hat{n}$  with  $\hat{n} \stackrel{\text{def}}{=} (\sin(\theta) \cos(\varphi), \sin(\theta) \sin(\varphi), \cos(\theta))$ . Observe that for mixed quantum states,  $0 \le r < 1$  and det  $(\rho) = (1/2) (1 - \vec{r}^2) \ge 0$  because of the positiveness of  $\rho$ . For pure quantum states, instead, we have r = 1 and det  $(\rho) = 0$ . According to the MCP theorem, any Riemannian monotone metric between  $\rho$  and  $\rho + d\rho$  in the Bloch ball with  $\rho$  in Eq. (47) can be recast as [12]

$$ds^{2} = \frac{1}{4} \left[ \frac{dr^{2}}{1 - r^{2}} + \frac{1}{f\left(\frac{1 - r}{1 + r}\right)} \frac{r^{2}}{1 + r} d\Omega^{2} \right],$$
(48)

with 0 < r < 1. In Eq. (48),  $d\Omega^2 \stackrel{\text{def}}{=} d\theta^2 + \sin^2(\theta) d\varphi^2$  specifies the metric on the unit 2-sphere while  $f : \mathbb{R}_+ \to \mathbb{R}_+$  is the so-called Morozova-Chentsov function f = f(t). Note that at the maximally mixed state where r = 0, t is defined as  $t(r) \stackrel{\text{def}}{=} (1-r) / (1+r) \in [0, 1]$  and becomes t(0) = 1. Therefore, the constraint (iii) (i.e.,  $f(1) = 1 \neq 0$ ) is necessary to bypass a conical singularity in the metric. In the case of the Bures metric,

$$ds_{\rm Bures}^2 = \frac{1}{4} \left[ \frac{dr^2}{1 - r^2} + r^2 d\Omega^2 \right].$$
 (49)

From Eqs. (48) and (49),

$$\frac{1}{f_{\text{Bures}}\left(\frac{1-r}{1+r}\right)}\frac{r^2}{1+r} = r^2.$$
(50)

Then, recalling that  $r(t) \stackrel{\text{def}}{=} (1-t)/(1+t)$ , we find from Eq. (50) that that

$$f_{\text{Bures}}\left(t\right) \stackrel{\text{def}}{=} \frac{1+t}{2}.$$
(51)

Clearly,  $f_{\text{Bures}}(t)$  satisfies conditions (i), (ii), and (iii) [12]. In the case of the Sjöqvist metric, we have

$$ds_{\rm Sjöqvist}^{2} = \frac{1}{4} \left[ \frac{dr^{2}}{1 - r^{2}} + d\Omega^{2} \right].$$
 (52)

From Eqs. (48) and (52), we find that [14]

$$f_{\rm Sj\"oqvist}(t) \stackrel{\rm def}{=} \frac{1}{2} \frac{(1-t)^2}{1+t}.$$
 (53)

For a brief comparative discussion on Eqs. (49) and (52) along with remarks on finite lengths of geodesics connecting mixed quantum states in the Bures and Sjöqvist geometries, we refer to Appendix C. We observe now that although  $f_{\text{Sjöqvist}}(t)$  is self inversive since  $f_{\text{Sjöqvist}}(1/t) = f_{\text{Sjöqvist}}(t)/t$ ,  $f_{\text{Sjöqvist}}(1) = 0 \neq 1$ . Therefore, as pointed out in Ref.

[20], the Sjöqvist metric in Eq. (52) is singular at the origin of the Bloch ball where r = 0 (i.e.,  $t \equiv t(0) = 1$ ) and the angular components of the metric tensor diverge because  $f_{\text{Sjöqvist}}(1) = 0$ . For this reason, the original Sjöqvist metric is limited to non-degenerate mixed quantum states. Alternatively, the emergence of the singular behavior of the Sjöqvist metric expressed in the form of Eq. (48) can be understood by noting that  $1/f_{\text{Sjöqvist}}\left(\frac{1-r}{1+r}\right) = (1+r)/r^2$ diverges as r approaches zero. To properly understand the monotonicity property of the Sjöqvist metric, we need to also check if  $f_{\text{Sjöqvist}}(t)$  in Eq. (53) is an operator monotone function.

To address this point, we start by recalling that in spherical coordinates the normalized volume element on the manifold of single-qubit mixed states equipped with the most general Riemannian monotone metric is given by [12, 44]

$$dV \stackrel{\text{def}}{=} p(r, \theta, \varphi) \, dr d\theta d\varphi = \mathcal{N} \frac{r^2 \sin(\theta)}{f\left(\frac{1-r}{1+r}\right) \left(1-r^2\right)^{1/2} \left(1+r\right)} dr d\theta d\varphi,\tag{54}$$

where  $\mathcal{N}$  is a constant such that the probability density function (pdf)  $p(r, \theta, \varphi)$  in Eq. (54) is normalized to unity. For instance, in the Bures and Sjöqvist metric cases, we have

$$p_{\text{Bures}}(r,\,\theta,\,\varphi) \stackrel{\text{def}}{=} \frac{1}{\pi^2} \frac{r^2 \sin\left(\theta\right)}{\sqrt{1-r^2}}, \text{ and } p_{\text{Sjöqvist}}\left(r,\,\theta,\,\varphi\right) \stackrel{\text{def}}{=} \frac{1}{2\pi^2} \frac{\sin\left(\theta\right)}{\sqrt{1-r^2}},$$
(55)

respectively. Note that from Eqs. (54) and (55),  $\mathcal{N}_{\text{Bures}} \stackrel{\text{def}}{=} 1/\pi^2$  and  $\mathcal{N}_{\text{Sjöqvist}} \stackrel{\text{def}}{=} 1/(2\pi^2)$ . In Ref. [45], Zyczkowski-Horodecki-Sanpera-Lewenstein (ZHSL) introduced a "natural measure" in the space of density matrices specifying N-dimensional quantum systems to compute the volume of separable and entangled states. The probability measure  $\mu_{\text{unitary}}$  used by ZHLS to describe the manner in which  $N \times N$  random density matrices  $\rho$  that describe N-dimensional quantum systems are drawn, is specified by means of a product  $\mu_{\text{unitary}} = \Delta_1 \times \nu_{\text{Haar}}$ . The quantity  $\nu_{\text{Haar}}$  denotes the Haar measure in the space of unitary matrices U(N) [46–49], while  $\Delta_1$  is the uniform measure on the (N-1)dimensional simplex defined by the constraint  $\sum_{i=1}^{N} d_i = 1$  (where  $\{d_i\}_{1 \leq i \leq N}$  are the N positive eigenvalues of  $\rho$ ) [50]. ZHLS proposed the product  $\mu_{\text{unitary}} = \Delta_1 \times \nu_{\text{Haar}}$  motivated by the rotational invariance of both terms  $\Delta_1$ and  $\nu_{\text{Haar}}$ . In Ref. [51], Zyczkowski discussed the measure-dependence of questions concerning the separability of randomly chosen mixed quantum states expressed as a mixture of pure states in an N-dimensional Hilbert space. In Ref. [52], focusing on the two-dimensional case with N = 2, Slater showed that the pdf that characterizes the ZHSL volume element equals

$$p_{\text{ZHSL}}\left(r,\,\theta,\,\varphi\right) \stackrel{\text{def}}{=} \frac{\Gamma\left(\frac{1}{2}+\nu\right)}{2\pi^{3/2}\Gamma\left(\nu\right)} \left(1-r^2\right)^{\nu-1}\sin\left(\theta\right),\tag{56}$$

where  $\Gamma(\nu)$  is the Euler gamma function and  $\nu > 0$  is the usual concentration parameter that appears in probability theory [53]. Recasting  $dV_{\text{ZHSL}} \stackrel{\text{def}}{=} p_{\text{ZHSL}}(r, \theta, \varphi) dr d\theta d\varphi$  as in Eq. (54) and following Slater's work, we get

$$f_{\rm ZHSL}(t;\nu) \stackrel{\rm def}{=} \mathcal{N}_{\rm ZHSL}(\nu) \cdot \frac{2\pi^{3/2}\Gamma(\nu)}{\Gamma(\frac{1}{2}+\nu)} \cdot \frac{1}{2}\frac{(1-t)^2}{1+t} \cdot \left(\frac{4t}{(1+t)^2}\right)^{\frac{1}{2}-\nu}.$$
(57)

In Ref. [52], Slater noticed that the one-parameter family of functions  $f_{\text{ZHSL}}(t; \nu)$  in Eq. (57) are such that

 $f_{\text{ZHSL}}(1; \nu) = 0 \neq 1$ , for any  $\nu > 0$ . Therefore, these functions are not normalizable as required by a proper Morozova-Chentsov function. However, since  $f_{\text{ZHSL}}(1/t; \nu) = f_{\text{ZHSL}}(t; \nu)/t$ ,  $f_{\text{ZHSL}}(t; \nu)$  is self inversive. Furthermore, although  $f_{\text{ZHSL}}(t; \nu)$  is monotone decreasing for  $t \in [0, 1]$  and monotone increasing for t > 1, they are not operator monotone [52]. Thus,  $dV_{\text{ZHSL}}$  is not proportional to the volume element of a monotonic metric. As a consequence, any metric associated with the ZHSL measure would lack the statistically meaningful feature of decreasing under the action of stochastic mappings [52, 54]. Comparing Eqs. (53) and (57), for  $\nu = 1/2$  we have

$$f_{\rm ZHSL}\left(t;\,1/2\right) = f_{\rm Sj\"oqvist}\left(t\right),\tag{58}$$

where  $\mathcal{N}_{\text{ZHSL}}(1/2) = 1/(2\pi^2) = \mathcal{N}_{\text{Sjöqvist}}$ . Thus, exploiting the finding of Slater in Refs. [52, 54], we conclude that for N = 2 the Sjöqvist metric is not a monotone metric (unlike the Bures metric). For completeness, we point out that one can explicitly verify that  $f_{\text{Sjöqvist}}(t)$  in Eq. (53) on [0, 1] is not operator monotone since there exist positive matrices A, B such that B - A is positive but  $f_{\text{Sjöqvist}}(B) - f_{\text{Sjöqvist}}(A)$  is not. To see this, take B = I and A = I/2with I being the 2 × 2 identity matrix. The discovery of the link in Eq. (58) between the family of ZHSL metrics and the Sjöqvist metric is intriguing in its own right and, we believe, goes beyond the monotonicity aspects being discussed here. We are now ready for our summary and concluding remarks.

### VI. CONCLUSION

In this paper, we presented an explicit mathematical discussion on the link between the Sjöqvist metric and the Bures metric for arbitrary nondegenerate mixed quantum states in terms of decompositions of density operators via ensembles of pure quantum states. Furthermore, to deepen our physical understanding of the difference between these two metrics, we found and compared the formal expressions of these two metrics for arbitrary thermal quantum states describing quantum systems in equilibrium with an environment at non-zero temperature (Eqs. (36) and (38)). Finally, we illustrated the discrepancy (Eq. (45)) between these two metrics (Eqs. (43) and (44)) in the case of a simple physical system defined by a spin-qubit in an arbitrarily oriented uniform and stationary magnetic field in thermal equilibrium with a finite-temperature reservoir. Our main conclusive remarks can be summarized as follows:

- [i] Motivated by the original considerations presented in Ref. [20], we have explicitly clarified that the Sjöqvist metric  $d_{\text{Sjöqvist}}^2(t, t + dt)$  in Eq. (4) is generally different from the Bures metric  $d_{\text{Bures}}^2(t, t + dt)$  in Eq. (28).
- [ii] Building on the quantitative analysis that appeared in Ref. [20], we have explicitly verified that the generalized Sjöqvist metric  $\tilde{d}_{\text{Siöqvist}}^2(t, t + dt)$  in Eq. (27) coincides with the Bures metric  $d_{\text{Bures}}^2(t, t + dt)$  in Eq. (28).
- [iii] We have explicitly stated that  $d_{\text{Bures}}^2(t, t + dt) = \tilde{d}_{\text{Sjöqvist}}^2(t, t + dt) \leq d_{\text{Sjöqvist}}^2(t, t + dt)$ . This inequality is a consequence of the fact that in the generalized Sjöqvist metric construction, the minimization procedure occurs in a larger space of unitary matrices (Eq. (17)) that includes the smaller space of unitary matrices (Eq. (3)) explored in the original Sjöqvist construction.
- [iv] Inspired by the work in Ref. [20], we have explicitly point out that either  $d_{Sj\ddot{o}qvist}^2(t, t + dt)$  or  $\tilde{d}_{Sj\ddot{o}qvist}^2(t, t + dt)$  can be obtained starting from a common general minimization procedure. However, these two metrics are generally different since they correspond to different minima (i.e., different choices of the unitary matrix  $V(t) \leftrightarrow [V_{hk}(t)]_{1 \le h,k \le N}$  with  $V_{hk}(t) \in \mathbb{C}$  introduced in Eq. (14)).
- [v] For the class of thermal states in an arbitrary finite-dimensional setting, we stressed the difference between the Sjöqvist and the Bures metrics in terms of their non-classical metric components (Eqs. (36) and (38)).
- [vi] For single-qubit mixed states, we argued that unlike the Bures metric (with the MC function in Eq. (51)), the Sjöqvist metric (with the MC-like function in Eq. (53)) is not a monotone metric.

For the set of pure states there is no room for ambiguity and the (unitary-invariant) Fubini–Study metric leads to the only natural choice for a measure that defines "random states". For mixed-state density matrices, instead, the geometric structure of the state space is more intricate [12, 55]. There is a variety of different metrics that can be employed, each of them with a different physical justification, advantages, and drawbacks that can depend on the specific application one might examine. In particular, both basic geometric quantities (i.e., path, path length, volume, and curvature) and more involved geometric concepts built out of these basic entities (i.e., complexity) happen to depend on the measure chosen on the space of mixed quantum states that specify the physical system being studied [14, 51]. For these reasons, our work carried out in this paper can be especially relevant in providing a clearer comparative analysis between the (younger) Sjöqvist interferometric geometry and the (older) Bures geometry for mixed quantum states. Interestingly, the relevance of this type of comparative analysis was recently remarked in Refs. [11] and [14] as well.

It would be interesting to investigate the monotonicity of the Sjöqvist metric for N > 2. In particular, keeping N = 2, it would be intriguing to identify an explicit counterexample of a CPTP map for single-qubits for which the Sjöqvist distance does not decrease under its action (see, for instance, Ref. [56] for the existence of an explicit counterexample exhibiting the non-monotonicity of the Hilbert-Schmidt distance). Finally, thanks to Eq. (58), we found for N = 2 and  $\nu = 1/2$  that the metric associated with the ZHSL measure is equal to the Sjöqvist metric in Eq. (52). This connection deserves further investigation, we believe. For the time being, we leave a deeper quantitative understanding of these lines of investigation to forthcoming scientific efforts.

Despite its relative simplicity, we hope this work will inspire other scientists to strengthen our mathematical and physical comprehension of this intriguing link among geometry, statistical mechanics, and quantum physics.

### Acknowledgments

P.M.A. acknowledges support from the Air Force Office of Scientific Research (AFOSR). C.C. is grateful to the United States Air Force Research Laboratory (AFRL) Summer Faculty Fellowship Program for providing support for this work. Any opinions, findings and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Air Force Research Laboratory (AFRL). O.L. is grateful to the Department of Physics of the Al-Farabi University for hospitality during the period in which this manuscript was written. C.L. and S.M. acknowledge financial support from "PNRR MUR project PE0000023-NQSTI". Finally, the work of H.Q. was supported partially by PAPIIT-DGAPA-UNAM, Grant No. 114520, and Conacyt-Mexico, Grant No. A1-S-31269.

- [1] M. Pettini, Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics, Springer-Verlag New York (2007).
- [2] C. Cafaro, O. Luongo, S. Mancini, and H. Quevedo, Thermodynamic length, geometric efficiency and Legendre invariance, Physica A590, 126740 (2022).
- [3] D. Felice, C. Cafaro, and S. Mancini, Information geometric methods for complexity, Chaos 28, 032101 (2018).
- [4] A. Carollo, D. Valenti, and B. Spagnolo, Geometry of quantum phase transitions, Phys. Rep. 838, 1 (2020).
- [5] S. Amari and H. Nagaoka, Methods of Information Geometry, Oxford University Press (2000).
- [6] P. Zanardi and N. Paunkovic, Ground state overlap and quantum phase transitions, Phys. Rev. E74, 031123 (2006).
- [7] P. Zanardi, P. Giorda, and M. Cozzini, Information-theoretic differential geometry of quantum phase transitions, Phys. Rev. Lett. 99, 100603 (2007).
- [8] P. Zanardi, L. Campos Venuti, and P. Giorda, Bures metric over thermal state manifolds and quantum criticality, Phys. Rev. A76, 062318 (2007).
- H. Silva, B. Mera, and N. Paunkovic, Interferometric geometry from symmetry-broken Uhlmann gauge group with applications to topological phase transitions, Phys. Rev. B103, 085127 (2021).
- [10] H. V. da Silva, Quantum information geometry and applications, MS Thesis in Engineering Physics, IT Lisboa (2021).
- [11] B. Mera, N. Paunkovic, S. T. Amin, and V. R. Vieira, Information geometry of quantum critical submanifolds: Relevant, marginal, and irrelevant operators, Phys. Rev. B106, 155101 (2022).
- [12] I. Bengtsson and K. Zyczkowski, Geometry of Quantum States, Cambridge University Press (2006).
- [13] P. Pessoa and C. Cafaro, Information geometry for Fermi-Dirac and Bose-Einstein quantum statistics, Physica A576, 126061 (2021).
- [14] C. Cafaro and P. M. Alsing, Complexity of pure and mixed qubit geodesic paths on curved manifolds, Phys. Rev. D106, 096004 (2022).
- [15] C. Cafaro, The Information Geometry of Chaos, PhD Thesis, State University of New York at Albany, Albany-NY, USA (2008). Available online at arXiv: math-ph/1601.07935 (2016).
- [16] C. Cafaro, Works on an information geometrodynamical approach to chaos, Chaos, Solitons & Fractals 41, 886 (2009).
- [17] J. P. Provost and G. Vallee, Riemannian structure on manifolds of quantum states, Commun. Math. Phys. 76, 289 (1980).
- [18] W. K. Wootters, Statistical distance and Hilbert space, Phys. Rev. D23, 357 (1981).
- [19] S. L. Braunstein and C. M. Caves, Statistical distance and the geometry of quantum states, Phys. Rev. Lett. 72, 3439 (1994).
- [20] E. Sjöqvist, Geometry along evolution of mixed quantum states, Phys. Rev. Research 2, 013344 (2020).
- [21] D. Bures, An extension of Kakutani's theorem on infinite product measures to the tensor product of semifinite  $\omega^*$ -algebras, Trans. Amer. Math. Soc. **135**, 199 (1969).
- [22] A. Uhlmann, The "transition probability" in the state space of a \*-algebra, Rep. Math. Phys. 9, 273 (1976).
- [23] M. Hübner, Explicit computation of the Bures distance for density matrices, Phys. Lett. A163, 239 (1992).
- [24] L. P. Hughston, R. Jozsa, and W. K. Wootters, A complete classification of quantum ensembles having a given density matrix, Phys. Lett. A183, 14 (1993).
- [25] Y. Aharonov and J. Anandan, Phase change during a cyclic quantum evolution, Phys. Rev. Lett. 58, 1593 (1987).
- [26] E. Sjöqvist, A. K. Pati, A. Eckert, J. S. Anandan, M. Ericsson, D. K. L. Oi, and V. Vedral, Geometric phases for mixed states in interferometry, Phys. Rev. Lett. 85, 2845 (2000).
- [27] D. M. Tong, E. Sjöqvist, L. C. Kwek, and C. H. Oh, *Kinematic approach to the mixed state geometry phase in nonunitary* evolution, Phys. Rev. Lett. **93**, 080405 (2004).
- [28] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press (2000).
- [29] M. M. Wilde, *Quantum Information Theory*, Cambridge University Press (2013).
- [30] K. Huang, Statistical Mechanics, John Wiley & Sons, Inc. (1987).
- [31] F. Strocchi, *Thermal states*, Lect. Notes Phys. 732, 139 (2008).
- [32] C. Cafaro and P. M. Alsing, Bures and Sjöqvist metrics over thermal state manifolds for spin qubits and superconducting flux qubits, arXiv:quant-ph/2303.01680 (2023).
- [33] S. S. Gubser and R. K. Bradley, Degenerate eigenvalues for Hamiltonians with no obvious symmetries, Adv. Theor. Math. Phys. 9, 593 (2005).
- [34] N. N. Cencov, Statistical decision rules and optimal inference, Transl. Math. Monographs, vol. 53, Amer. Math. Soc., Providence-RI (1981).
- [35] L. L. Campbell, An extended Cencov characterization of the information metric, Proc. Am. Math. Soc. 98, 135 (1986).
- [36] E. A. Morozova and N. N. Chentsov, Markov invariant geometry on manifolds of states, Journal of Soviet Mathematics 56, 2648 (1991).

- [37] D. Petz, Monotone metrics on matrix spaces, Lin. Algebra Appl. 244, 81 (1996).
- [38] K. Löwner, Über monotone matrixfunktionen, Mathematishe Zeitschrift 38, 177 (1934).
- [39] R. Bhatia, Matrix Analysis, Springer-Verlag (1997).
- [40] M. K. Kwong, Some results on matrix monotone functions, Lin. Algebra Appl. 118, 129 (1989).
- [41] T. Furuta, Concrete examples of operator monotone functions obtained by an elementary method without appealing to Löwner integral representation, Lin. Algebra Appl. 429, 972 (2008).
- [42] P. Gibilisco, F. Hansen, and T. Isola, On a correspondence between regular and non-regular operator monotone functions, Lin. Algebra Appl. 430, 2225 (2009).
- [43] B. Simon, Loewner's Theorem on Monotone Matrix Functions, Springer Nature Switzerland AG (2019).
- [44] D. Petz and C. Sudar, Geometries of quantum states, J. Math. Phys. 37, 2662 (1996).
- [45] K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Volume of the set of separable states, Phys. Rev. A58, 883 (1998).
- [46] M S Marinov, Invariant volumes of compact groups, J. Phys. A13: Math. Gen., 3357 (1980).
- [47] T. Maekava, Explicit form of the Haar measure of U(N) and differential forms, J. Math. Phys. 26, 1902 (1985).
- [48] L. J. Boya, E. C. G. Sudarshan, and T. Tilma, Volumes of compact manifolds, Rep. Math. Phys. 52, 401 (2003).
- [49] P. M. Alsing, C. C. Tison, J. Schneeloch, R. J. Birrittella, and M. L. Fanto, Distribution of density matrices at fixed purity for arbitrary dimensions, Phys. Rev. Research 4, 043114 (2022).
- [50] S. Chatterjee, A note about uniform distribution on the intersection of a simplex and a sphere, Journal of Topology and Analysis 9, 717 (2017).
- [51] K. Zyczkowski, Volume of the set of separable states. II, Phys, Rev. A60, 3496 (1999).
- [52] P. B. Slater, Monotonicity properties of certain measures over the two-level quantum systems, Lett. Math. Phys. **52**, 343 (2000).
- [53] D. S. Sivia, Data Analysis: A Bayesian Tutorial, Oxford University Press (1996).
- [54] P. B. Slater, A priori probabilities of separable quantum states, J. Phys. A32: Math. Gen., 5261 (1999).
- [55] D. C. Brody and B. Longstaff, Evolution speed of open quantum dynamics, Phys. Rev. Research 1, 033127 (2019).
- [56] M. Ozawa, Entanglement measures and the Hilbert-Schmidt distance, Phys. Lett. A268, 158 (2000).
- [57] A. Uhlmann, Parallel transport and "quantum holonomy" along density operators, Rep. Math. Phys. 24, 229 (1986).
- [58] A. Uhlmann, A gauge field governing parallel transport along mixed states, Lett. Math. Phys. 21, 229 (1991).
- [59] A. Uhlmann, The metric of Bures and the geometric phase. In: R. Gielerak, J. Lukierski, and Z. Popowicz (Eds.), Groups and Related Topics, Mathematical Physics Studies, vol. 13, pp. 267-274, Springer, Dordrecht (1992).
- [60] A. Uhlmann, Geometric phases and related structures, Rep. Math. Phys. 36, 461 (1995).
- [61] H. Barnum, C. M. Caves, C. A. Fuchs, R. Jozsa, and B. Schumacher, Noncommuting mixed states cannot be broadcast, Phys. Rev. Lett. 76, 2818 (1996).
- [62] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, Quantifying entanglement, Phys. Rev. Lett. 78, 2275 (1997).
- [63] V. Vedral and M. B. Plenio, Entanglement measures and purification procedures, Phys. Rev. A57, 1619 (1998).
- [64] C. Cafaro and P. M. Alsing, Qubit geodesics on the Bloch sphere from optimal-speed Hamiltonian evolutions, Class. Quantum Grav. 40, 115005 (2023).

### Appendix A: Parallel transport condition for mixed quantum states

In Appendix A, to better grasp the significance of the relation  $U_t(dt) V(t+dt) V^{\dagger}(t) = I$  in Eq. (26), we recall the concept of parallel transport for pure [25] and mixed [26, 27] quantum states.

Remember that a unitarily evolving mixed quantum state  $\rho(t) \stackrel{\text{def}}{=} U(t) \rho(0) U^{\dagger}(t)$  is said to gain a geometric phase with respect to  $\rho(0)$  if  $\arg\{\operatorname{tr}[\rho(0) U(t)]\}$  is nonzero [26]. Then, the parallel transport condition of  $\rho(t)$ along an arbitrary path is specified by the condition that the state  $\rho(t)$  must be, at each temporal interval, in phase with the state  $\rho(t+dt) \stackrel{\text{def}}{=} U(t+dt) \rho(0) U^{\dagger}(t+dt) = U(t+dt) U^{\dagger}(t) \rho(t) U(t) U^{\dagger}(t+dt)$ . Being in phase requires, in turn, that  $\arg\left\{\operatorname{tr}\left[\rho(t) U(t+dt) U^{\dagger}(t)\right]\right\}$  must vanish, that is,  $\operatorname{tr}\left[\rho(t) U(t+dt) U^{\dagger}(t)\right]$  must be *real* and positive. However, noting that  $U(d + dt) = U(t) + \dot{U}(t) dt + O(dt^2)$ , the parallel transport condition can be recast as  $\arg \left\{ \operatorname{tr} \left[ \rho(t) \dot{U}(t) U^{\dagger}(t) \right] \right\} = 0$ . Finally, since  $\rho(t) \dot{U}(t) U^{\dagger}(t)$  is a purely imaginary number since  $\rho = \rho^{\dagger}$ (Hermiticity) and  $UU^{\dagger} = U^{\dagger}U = I$  (unitarity), the parallel transport condition reduces to tr  $\left[\rho(t)\dot{U}(t)U^{\dagger}(t)\right] = U^{\dagger}U^{\dagger}$ 0. For a characterization of the mixed state geometric phase in the case of nonunitary evolutions, we refer to Ref. [27]. For a pure state density operator  $\rho(t) \stackrel{\text{def}}{=} |\psi(t)\rangle \langle \psi(t)|$ , the parallel transport condition is given by  $\langle \psi(t) | \dot{\psi}(t) \rangle = 0$  [25]. Therefore, setting for example  $|\psi(t)\rangle \stackrel{\text{def}}{=} e^{if_k(t)} |n_k(t)\rangle$ , the condition  $\langle \psi(t) | \dot{\psi}(t) \rangle = 0$ yields the scalar constraint  $\dot{f}_k(t) - i \langle n_k(t) | \dot{n}_k(t) \rangle = 0$  which was obtained by Sjöqvist in his original derivation of the metric tensor for mixed quantum states. Given this background information, we point out that the relation  $U_t(dt)V(t+dt)V^{\dagger}(t) = I$  in Eq. (26) is a constraint equation that can be regarded as the operator-analogue of the parallel transport condition  $f_k(t) - i \langle n_k(t) | \dot{n}_k(t) \rangle = 0$ . In particular, it is straightforward to check that when the polar decomposition of the overlap matrix  $M_t(dt)$  is given by  $|M_t(dt)| U_t(dt)$  with matrix coefficients  $[M_t(dt)]_{kl} \stackrel{\text{def}}{=} \sqrt{p_k(t) p_l(t)} \langle n_k(t) | n_l(t+dt) \rangle$  that are diagonalizable with *real* and *positive* eigenvalues, the relation  $U_t(dt)V(t+dt)V^{\dagger}(t) = I$  leads to the constraint tr $\left[\rho(t)\dot{V}(t)V^{\dagger}(t)\right] = 0$ . This latter relation can be explicitly verified by exploiting the fact that  $tr[\rho(t)] = 1$  and, in addition, the unitary matrix V(t) satisfies the relation  $V(t+dt) = V(t) + \dot{V}(t) dt + O(dt^2)$ . For a rigorous mathematical discussion on the notion of parallel transport along density operators, we suggest Refs. [22, 57–60].

#### Appendix B: Monotonicity of the Bures metric

In this appendix, we report some details on the monotonicity property satisfied by the Bures metric viewed as a Riemannian metric.

We recall that there exist infinitely many monotone Riemannian metrics on the space of mixed quantum states [12]. In particular, the monotonicity of the Bures metric  $d_{\text{Bures}}^2(t, t + dt)$  under stochastic quantum maps { $\Phi$ } (i.e., completely positive trace preserving (CPTP) maps) is a consequence of the monotonicity of the Bures distance  $D_{\text{Bures}}^2(\rho_1, \rho_2)$  [12],

$$D_{\text{Bures}}^{2}(\rho_{1}, \rho_{2}) \stackrel{\text{def}}{=} \operatorname{tr}(\rho_{1}) + \operatorname{tr}(\rho_{2}) - 2\operatorname{tr}(\sqrt{\rho_{2}^{1/2}\rho_{1}\rho_{2}^{1/2}}), \tag{B1}$$

as a function of the fidelity  $\operatorname{tr}(\sqrt{\rho_2^{1/2}\rho_1\rho_2^{1/2}})$ . No physical operation expressed in terms of a CPTP map  $\Phi$  can increase  $D_{\text{Bures}}^2(\rho_1, \rho_2)$ ,

$$D_{\text{Bures}}^2\left(\Phi\rho_1, \, \Phi\rho_2\right) \le D_{\text{Bures}}^2\left(\rho_1, \, \rho_2\right). \tag{B2}$$

To avoid confusion, we point out that the quantity  $\operatorname{tr}(\sqrt{\rho_2^{1/2}\rho_1\rho_2^{1/2}})$  is denoted with  $\sqrt{F}(\rho_1, \rho_2)$  and called root fidelity in Ref. [12] (see Eq. (9.33). Instead,  $\operatorname{tr}(\sqrt{\rho_2^{1/2}\rho_1\rho_2^{1/2}})$  is denoted with  $F(\rho_1, \rho_2)$  and called fidelity in Ref. [28] (see Eq. (9.53). Interestingly, the fidelity  $F(\rho_1, \rho_2)$  can be used to define the so-called Bures angle  $D_A^{\text{Bures}}(\rho_1, \rho_2)$  as

$$D_A^{\text{Bures}}(\rho_1, \rho_2) \stackrel{\text{def}}{=} \arccos\left[ \text{tr}(\sqrt{\rho_2^{1/2} \rho_1 \rho_2^{1/2}}) \right].$$
(B3)

The Bures angle  $D_A^{\text{Bures}}(\rho_1, \rho_2)$  in Eq. (B3) is a metric [28] that, similarly to the Bures distance  $D_{\text{Bures}}^2(\rho_1, \rho_2)$  in Eq. (B1), satisfies the contractivity property given by

$$D_A^{\text{Bures}}\left(\Phi\rho_1, \, \Phi\rho_2\right) \le D_A^{\text{Bures}}\left(\rho_1, \, \rho_2\right),\tag{B4}$$

for any CPTP map  $\Phi$  [12]. Eq. (B4) is a consequence of two facts: i)  $D_A^{\text{Bures}}(\rho_1, \rho_2)$  in Eq. (B3) is a monotone decreasing function of the fidelity  $\sqrt{\rho_2^{1/2}\rho_1\rho_2^{1/2}}$ ; ii) the fidelity  $F(\rho_1, \rho_2)$ , expressed as  $\sqrt{\rho_2^{1/2}\rho_1\rho_2^{1/2}}$  and thanks to Uhlmann's theorem, can be shown to fulfill the monotonicity property

$$F\left(\Phi\rho_{1}, \Phi\rho_{2}\right) \geq F\left(\rho_{1}, \rho_{2}\right),\tag{B5}$$

for any CPTP map  $\Phi$  [28]. For proof that fidelity does not decrease under local general measurements (LGMs) and classical communication (CC), we refer to Ref. [61]. Finally, for an interesting discussion on the relevance of the contractivity property for distances used to properly quantify entanglement in quantum information science, we refer to Refs. [62, 63].

## Appendix C: Finite lengths of geodesic paths

We begin Appendix C by pointing out that in order to better understand from an intuitive standpoint the difference between the Bures and the Sjöqvist metrics, in addition to the expressions of their infinitesimal line elements in Eqs. (49) and (52), respectively, it would be convenient to also have an explicit formula for the finite distance between two arbitrary qubit mixed states. However, before addressing the problem of finding the finite length of a geodesic path of suitably parametrized density operators connecting an initial and a final mixed state, we present some preliminary remarks. First, considering a change of variables defined by  $r \stackrel{\text{def}}{=} \sin(\alpha_r)$  with  $0 \leq \alpha_r \leq \pi/2$ , we obtain that  $4ds_{\text{Sjöqvist}}^2 = d\alpha_r^2 + d\Omega_{\text{sphere}}^2$  and  $4ds_{\text{Bures}}^2 = d\alpha_r^2 + \sin^2(\alpha_r) d\Omega_{\text{sphere}}^2$  with  $d\Omega_{\text{sphere}}^2 \stackrel{\text{def}}{=} d\theta^2 + \sin^2(\theta) d\varphi^2$ . Recalling that the line element in the standard cylindrical coordinates  $(\rho, \varphi, z)$  is given by  $ds_{\text{cylinder}}^2 = dz^2 + d\Omega_{\text{cylinder}}^2$  with  $d\Omega_{\text{cylinder}}^2 \stackrel{\text{def}}{=} d\rho^2 + \rho^2 d\varphi^2$ , one observes that the structure of the Sjöqvist line element rewritten in this alternative form is evocative of the structure of a line element in the standard cylindrical coordinates once one associates the pair  $(\alpha_r, d\Omega_{\text{sphere}})$  with the pair  $(\rho, d\Omega_{\text{cylinder}})$ . Second, after considering this change of variables, one can connect a cylinder with a constant (varying) radius to the Sjöqvist (Bures) geometry, respectively. In particular, one observes that the varying radius in the Bures case is upper bounded by the constant value that defines the radius in the Sjöqvist geometry. These geometric insights would lead one to intuitively expect different lengths of geodesic paths in the two cases, with the Sjöqvist geometry yielding longer lengths eventually [14]. Returning to the issue of finite lengths, we consider for illustrative purposes two mixed states  $\rho_A$  and  $\rho_B$  specified by Bloch vectors  $\vec{a} = r_a \hat{n}_a$  and  $\vec{b} = r_b \hat{n}_b$  with  $\hat{n}_a \stackrel{\text{def}}{=} (0, 0, 1)$  and  $\hat{n}_b \stackrel{\text{def}}{=} (\sin(\theta_b), 0, \cos(\theta_b))$ , respectively. In other words,  $\rho_A$  and  $\rho_B$  are points in the Bloch sphere given in spherical coordinates by  $P_A = (r_a, \theta_a, \varphi_a) \stackrel{\text{def}}{=} (r_a, 0, 0)$  and  $P_B = (r_b, \theta_b, \varphi_b) \stackrel{\text{def}}{=} (r_b, \theta_b, 0)$ , respectively. Therefore,  $\rho_A$  and  $\rho_B$  are assumed to be points that lie on the *xz*-plane since  $\varphi_a = \varphi_b = 0$ . A relatively straightforward calculation yields expressions of the finite lengths evaluated along the geodesic paths connecting  $\rho_A$ and  $\rho_B$  in the Bures and Sjöqvist cases, respectively. The lengths are given by

$$\mathcal{L}_{\text{Bures}}(r_a, r_b, \theta_b) = \left[ 2 \left\{ 1 - \sqrt{2 \left[ \frac{1 + r_a r_b \cos(\theta_b)}{4} + \sqrt{\frac{1 - r_a^2}{4} \cdot \frac{1 - r_b^2}{4}} \right]} \right\} \right]^{1/2}, \tag{C1}$$

and [20],

$$\mathcal{L}_{\text{Sjöqvist}}\left(r_{a}, r_{b}, \theta_{b}\right) = \frac{1}{2}\sqrt{\theta_{b}^{2} + \left[\arcsin\left(r_{b}\right) - \arcsin\left(r_{a}\right)\right]},\tag{C2}$$

respectively. To further grasp insights into our discussion and, in addition, to cross-check the consistency of our calculations with what is expected to happen in the case of neighboring pure quantum states, we set  $r_a = r_b = 1$ . Then, Eqs. (C1) and (C2) reduce to

$$\mathcal{L}_{\text{Bures}}\left(\theta_{b}\right) = \left[2\left(1 - \sqrt{\frac{1 + \cos\left(\theta_{b}\right)}{2}}\right)\right]^{1/2}, \text{ and } \mathcal{L}_{\text{Sjöqvist}}\left(\theta_{b}\right) = \frac{\theta_{b}}{2}, \tag{C3}$$

respectively. From Eq. (C3) we observe that  $0 \leq \mathcal{L}_{\text{Bures}}(\theta_b) \leq \mathcal{L}_{\text{Sjöqvist}}(\theta_b)$  for any  $0 \leq \theta_b \leq \pi$ . Moreover, for neighboring quantum states with  $\theta_b \ll 1$ , the second order Taylor expansions in  $\theta_b$  of  $\mathcal{L}_{\text{Bures}}(\theta_b)$ ,  $\mathcal{L}_{\text{Sjöqvist}}(\theta_b)$ , and  $\mathcal{L}_{\text{Fubini-Study}}(\theta_b) \stackrel{\text{def}}{=} (1/2)d_{\text{Fubini-Study}}(\theta_b)$  with  $d_{\text{Fubini-Study}}(\theta_b) \stackrel{\text{def}}{=} 2\left[1 - \cos^2(\theta_b/2)\right]^{1/2}$  being the Fubini-Study distance [64], coincide. Indeed, when the Wootters angle  $\theta_b \ll 1$ , one finds  $\mathcal{L}_{\text{Bures}}(\theta_b) \approx \mathcal{L}_{\text{Sjöqvist}}(\theta_b) \approx \mathcal{L}_{\text{Fubini-Study}}(\theta_b) \approx \theta_b/2$ .

18

We defer a more in-depth quantitative comparison between the Sjöqvist and Bures geometries based upon the difference between the finite lengths of geodesics connecting arbitrary mixed quantum states to a future scientific endeavor.