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# Isometries of quantum states

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## Abstract

This paper treats the isometries of metric spaces of quantum states. In fact, we consider two metrics on the set of all quantum states, namely the Bures metric and that which comes from the trace-norm. We describe all the corresponding (nonlinear) isometries and also present similar results concerning the space of all (non-normalized) density operators.

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## 1. Introduction and statements of the results

The concepts of observables and states are of fundamental importance in quantum mechanics. In the Hilbert space formalism of the theory, the (bounded) observables are represented by the self-adjoint bounded linear operators of a Hilbert space  $H$  while the (normal) states are identified with the positive trace-class operators on  $H$  with trace 1. In the literature, one can find several metrics defined on the set of states which all come from different physical problems. A short summary of these problems and the corresponding metrics are given in the introduction of paper [1]. It turns out from the discussion there that all the metrics under consideration can be deduced from two fundamental distance functions which are the so-called Bures metric and the metric induced by the trace-norm.

Recently, Uhlmann, whose research work is closely connected with the study of Bures metric and transition probability (see, for example, [2–5]), has posed the following questions. Is it possible to describe all the transformations which preserve the Bures distance or, in other words, all the isometries of the space of all states (or the larger space of all density operators) equipped with the Bures metric? Moreover, in which connection are those isometries with the symmetry transformations? In this paper, we answer these questions by showing that every isometry under consideration is implemented by either a unitary or antiunitary operator on the underlying Hilbert space. Furthermore, we obtain results of the same spirit concerning

the other fundamental metric as well. We remark that interesting results and some physical applications can be found in [6] on linear but not necessarily surjective isometries with respect to this latter metric. In fact, in what follows we shall use two of the results in [6]. So, to sum up, as a consequence of our results, all the isometries with respect to all the metrics appearing in the introduction of [1] are determined.

Let us begin with the notation and the necessary definitions. Let  $H$  be a complex Hilbert space. We denote by  $B(H)$  the algebra of all bounded linear operators on  $H$ . The ideal of all trace-class operators, that is, those operators whose absolute value has finite trace, is denoted by  $C_1(H)$ . As usual,  $\text{tr}$  stands for the trace functional on  $C_1(H)$ . The positive operators in  $C_1(H)$  with trace 1 are called (normal) states and their collection is denoted by  $S(H)$ . This is a convex set whose extreme points are well known to be the rank-1 projections which are called pure states. Sometimes it is natural or just convenient to omit the normalizing condition  $\text{tr} A = 1$ . Accordingly,  $C_1^+(H)$  stands for the set of all positive trace-class operators (called density operators) on  $H$ .

For obvious reasons, we define our two basic metrics for the larger space  $C_1^+(H)$ . We begin with the Bures metric for which we need the concept of fidelity in the sense of Uhlmann [3, 7]. The fidelity  $F(A, B)$  of the operators  $A, B \in C_1^+(H)$  is defined by

$$F(A, B) = \text{tr}(A^{1/2}BA^{1/2})^{1/2}.$$

With the help of this, the Bures metric  $d_b$  on  $C_1^+(H)$  is expressed by the formula

$$d_b(A, B) = (\text{tr} A + \text{tr} B - 2F(A, B))^{1/2} \quad (A, B \in C_1^+(H)).$$

The other metric we are interested in comes from the trace-norm. If  $A \in C_1(H)$ , then its trace-norm (or, in other words, 1-norm) is

$$\|A\|_1 = \text{tr}|A|$$

where  $|A|$  stands for the absolute value of  $A$ . Our second metric denoted by  $d_1$  is defined by

$$d_1(A, B) = \|A - B\|_1 = \text{tr}|A - B| \quad (A, B \in C_1^+(H)).$$

As for the metrics on  $S(H)$ , they are just the restrictions of  $d_b, d_1$  onto  $S(H)$ .

Turning to the results of the paper, we note that they can be formulated in one single statement as follows. The isometries of both of the spaces  $S(H), C_1^+(H)$  with respect to both of the metrics  $d_b, d_1$  are induced by unitary or antiunitary operators of the underlying Hilbert space. However, in order that the proof is clear, well-sectioned and hence easy to follow, we divide this statement into parts as given below.

We emphasize that the transformations in our results are not assumed to be linear in any sense.

**Theorem 1.** *Let  $\phi : C_1^+(H) \rightarrow C_1^+(H)$  be a bijective map which preserves the Bures distance, that is, suppose that*

$$d_b(\phi(A), \phi(B)) = d_b(A, B) \quad (A, B \in C_1^+(H)).$$

*Then there is either a unitary or antiunitary operator  $U$  on  $H$  such that  $\phi$  is of the form*

$$\phi(A) = UAU^* \quad (A \in C_1^+(H)). \quad (1)$$

**Theorem 2.** *Let  $\phi : S(H) \rightarrow S(H)$  be a bijective map which preserves the Bures distance. Then there is either a unitary or antiunitary operator  $U$  on  $H$  such that  $\phi$  is of the form*

$$\phi(A) = UAU^* \quad (A \in S(H)). \quad (2)$$

**Theorem 3.** *If  $\phi$  is a bijective map of  $C_1^+(H)$  which preserves the distance  $d_1$ , then there is either a unitary or antiunitary operator  $U$  on  $H$  such that  $\phi$  is of the form (1).*

**Theorem 4.** *If  $\phi : S(H) \rightarrow S(H)$  is a bijective map which preserves the distance  $d_1$ , then there is either a unitary or antiunitary operator  $U$  on  $H$  such that  $\phi$  is of the form (2).*

**2. Proofs**

As will be clear from the proofs below, the non-normalized cases (that is, when  $\phi$  is defined on  $C_1^+(H)$ ) are more complicated. In fact, concerning both metrics it is an essential part of our arguments to show that the corresponding isometries send 0 to 0. In order to see this, we have to characterize 0 in terms of the metric alone. As for the Bures metric this is done in our first lemma.

Let  $A \in C_1^+(H)$  and  $\epsilon > 0$ . Denote by  $B_\epsilon^b(A)$  (resp.  $B_\epsilon^1(A)$ ) the closed ball in  $C_1^+(H)$  equipped with the Bures metric  $d_b$  (resp. the metric  $d_1$ ) with centre  $A$  and radius  $\epsilon$ .

**Lemma 1.** *Let  $A \in C_1^+(H)$ . We have  $A = 0$  if and only if  $\text{diam } B_\epsilon^b(A) \leq \sqrt{2}\epsilon$  holds for every  $\epsilon > 0$ .*

**Proof.** First we prove that  $\text{diam } B_\epsilon^b(0) \leq \sqrt{2}\epsilon$ . Let  $\epsilon > 0$ . Pick arbitrary  $X, Y \in B_\epsilon^b(0)$ . We have

$$(\text{tr } X)^{1/2} = d_b(X, 0) \leq \epsilon$$

and the same inequality holds for  $Y$  as well. We compute

$$d_b(X, Y)^2 = \text{tr } X + \text{tr } Y - 2F(X, Y) \leq \text{tr } X + \text{tr } Y \leq 2\epsilon^2$$

and hence obtain the desired inequality for the diameter of  $B_\epsilon^b(0)$ .

We note that it is quite easy to see that if  $\dim H \geq 2$ , then  $\text{diam } B_\epsilon^b(0)$  is exactly  $\sqrt{2}\epsilon$  (just take two rank-1 projections  $P, Q$  which are orthogonal to each other and consider the operators  $X = \epsilon^2 P, Y = \epsilon^2 Q$ ), while in the case when  $\dim H = 1$  we have  $\text{diam } B_\epsilon^b(0) = \epsilon$ .

Now, let  $A \in C_1^+(H)$  be nonzero and define  $\epsilon = \sqrt{\text{tr } A}$ . It is easy to verify that  $0, 4A \in B_\epsilon^b(A)$  and  $d_b(0, 4A) = 2\epsilon$ , so we have  $\text{diam } B_\epsilon^b(A) = 2\epsilon > \sqrt{2}\epsilon$ . □

Using this metric characterization of 0, the proof of theorem 1 is easy. The main point is to show that our isometries preserve the fidelity.

We note that in what follows whenever we speak about the preservation of an object or relation we always mean that it is preserved in both directions.

**Proof of theorem 1.** As  $\phi$  preserves the Bures distance, we obtain that

$$\text{diam } B_\epsilon^b(\phi(A)) = \text{diam } B_\epsilon^b(A).$$

Applying the characterization of 0 given in lemma 1, we easily deduce that  $\phi(0) = 0$ . Since

$$\text{tr } A = d_b(A, 0)^2 = d_b(\phi(A), \phi(0))^2 = d_b(\phi(A), 0)^2 = \text{tr } \phi(A)$$

we see that  $\phi$  preserves the trace. Considering the definition of the Bures distance, it is now obvious that  $\phi$  preserves the fidelity. The form of such transformations was described in our recent paper [8]. By [8, theorem 1] we have that  $\phi$  is of the form (1). □

**Proof of theorem 2.** In this case the proof is easier. Indeed, since  $\phi$  sends trace-1 operators to trace-1 operators, we see at once from the definition of  $d_b$  that  $\phi$  preserves the fidelity. Thus we can apply our corresponding result on the form of fidelity preserving maps on  $S(H)$  which is given in the concluding remarks of paper [8]. This completes the proof. □

We now turn to the description of the isometries with respect to the metric  $d_1$ . Just as in the case of the Bures metric, we shall need a characterization of 0 expressed by the metric  $d_1$  alone. This is the content of the next lemma.

**Lemma 2.** *Let  $A \in C_1^+(H)$ . Then  $A = 0$  if and only if for every  $\epsilon > 0$  and  $X, Y \in C_1^+(H)$  with the properties that*

$$d_1(X, A) = \epsilon \quad d_1(Y, A) = \epsilon \quad d_1(X, Y) = 2\epsilon$$

*we have*

$$B_\epsilon^1(X) \cap B_\epsilon^1(Y) \supseteq \{A\}.$$

**Proof.** First let  $A = 0$ . Let  $\epsilon > 0$  be arbitrary. Take  $X, Y \in C_1^+(H)$  such that  $\|X\|_1, \|Y\|_1 = \epsilon, \|X - Y\|_1 = 2\epsilon$ . Set  $Z = \frac{1}{2}(X + Y)$ . It is obvious that  $Z \in C_1^+(H)$  and

$$\|X - Z\|_1 = \frac{1}{2}\|X - Y\|_1 = \epsilon$$

and, similarly, we have  $\|Y - Z\|_1 = \epsilon$ . So,

$$Z \in B_\epsilon^1(X) \cap B_\epsilon^1(Y).$$

Moreover,  $Z \neq 0$  since in the opposite case (that is, when  $X + Y = 0$ ) by the positivity of  $X, Y$  we would get  $X = Y = 0$  and this is a contradiction. This proves the first part of our statement.

For the second part, let  $A$  be a nonzero element of  $C_1^+(H)$ . Clearly, there are a positive scalar  $\epsilon$  and a rank-1 projection  $P$  such that  $A + \epsilon P, A - \epsilon P \in C_1^+(H)$ . Define  $X = A + \epsilon P, Y = A - \epsilon P$ . We have  $d_1(X, A) = d_1(Y, A) = \epsilon$  and  $d_1(X, Y) = 2\epsilon$ . Let  $Z \in C_1^+(H)$  be such that  $d_1(X, Z), d_1(Y, Z) \leq \epsilon$ . Set  $T = X - Z$  and  $S = Z - Y$ . We clearly have

$$\|T\|_1, \|S\|_1 \leq \epsilon \tag{3}$$

and

$$\frac{1}{2}(T + S) = \frac{1}{2}(X - Y) = \epsilon P. \tag{4}$$

The result [9, theorem (3.1)] of Holub tells us that the extreme points of the unit ball of the normed linear space  $C_1(H)$  are exactly the rank-1 operators of norm 1. Therefore, using (3) and (4) we obtain that  $T = S = \epsilon P$ . This gives us that  $\epsilon P = T = X - Z = A + \epsilon P - Z$  which implies  $Z = A$ . Therefore, we have proved that

$$B_\epsilon^1(X) \cap B_\epsilon^1(Y) = \{A\}.$$

The proof is complete. □

Now, we are in a position to prove theorem 3. In the proof, we use a nice result of Mankiewicz, namely, [10, theorem 5] (also see the remark after that theorem) which states that if we have a bijective isometry between convex sets in normed linear spaces with nonempty interiors, then this isometry can be uniquely extended to a bijective affine isometry between the whole spaces. Moreover, we also use a characterization of the orthogonality of the elements of  $C_1^+(H)$  which can be found in [6]. We say that the operators  $X, Y \in C_1^+(H)$  are orthogonal if  $XY = 0$ . By (2.2) in [6], for every  $X, Y \in C_1^+(H)$  we have

$$XY = 0 \iff \|X - Y\|_1 = \|X + Y\|_1. \tag{5}$$

**Proof of theorem 3.** By the metric characterization of 0 given in lemma 2, we obtain that  $\phi(0) = 0$ .

We assert that  $\phi$  preserves the orthogonality. In order to verify this, let  $X, Y \in C_1^+(H)$ . By the positivity of  $X, Y$  and  $X + Y$  we have

$$\|X + Y\|_1 = \text{tr}(X + Y) = \text{tr } X + \text{tr } Y = \|X\|_1 + \|Y\|_1.$$

It follows from the characterization (5) of the orthogonality that

$$XY = 0 \iff \|X - Y\|_1 = \|X\|_1 + \|Y\|_1 \iff d_1(X, Y) = d_1(X, 0) + d_1(Y, 0).$$

Since  $\phi$  preserves the distance  $d_1$  and sends 0 to 0, we obtain that  $\phi$  preserves the orthogonality.

For any set  $\mathcal{M} \subset C_1^+(H)$ , we denote by  $\mathcal{M}^\perp$  the set of all elements of  $C_1^+(H)$  which are orthogonal to every element of  $\mathcal{M}$ . It is easy to see that an operator  $A \in C_1^+(H)$  is of rank  $n$  if and only if the set  $\{A\}^{\perp\perp}$  contains  $n$  pairwise orthogonal nonzero elements and no more. As  $\phi$  preserves the orthogonality and sends 0 to 0, it is now clear that  $\phi$  preserves the rank of operators.

Let  $H_n$  be an arbitrary  $n$ -dimensional subspace of  $H$ . Pick an operator  $A \in C_1^+(H)$  whose range is  $H_n$  and let  $H'_n$  denote the range of  $\phi(A)$ . We know that  $\dim H'_n = n$ . We say that a self-adjoint operator  $T$  acts on the closed subspace  $H_0$  of  $H$  if  $T(H_0) \subset H_0$  and  $T(H_0^\perp) = \{0\}$ . It is then easy to see that those elements of  $C_1^+(H)$  which act on  $H_n$  are exactly the elements of  $\{A\}^{\perp\perp}$ . By the orthogonality preserving property of  $\phi$  we have

$$\phi(\{A\}^{\perp\perp}) = \{\phi(A)\}^{\perp\perp}.$$

Hence, we get that  $\phi$  maps isometrically the set of all elements of  $C_1^+(H)$  which act on  $H_n$  onto the set of all elements of  $C_1^+(H)$  which act on  $H'_n$ . In this way we can reduce the problem to the finite dimensional case.

It is obvious that in the finite dimensional case, the convex set of all density operators has nonempty interior in the normed linear spaces of all self-adjoint operators. (In fact, the interior of this set consists of all invertible positive operators.) Consequently, the result of Mankiewicz applies.

Denote by  $C_1(H)_s$  the real linear space of all self-adjoint operators in  $C_1(H)$ . Define the map  $\psi : C_1(H)_s \rightarrow C_1(H)_s$  by

$$\psi(T) = \phi(T_+) - \phi(T_-) \quad (T \in C_1(H)_s).$$

Here  $T_+, T_-$  denote the positive and negative parts of  $T \in C_1(H)_s$ , respectively, that is, we have

$$T_+ = \frac{1}{2}(|T| + T) \quad T_- = \frac{1}{2}(|T| - T).$$

Using Mankiewicz's result and what we have proved above, we see that  $\psi$ , when restricted to the set of all self-adjoint operators which act on  $H_n$ , equals the Mankiewicz extension of  $\phi$  and hence it is a linear isometry onto the set of all self-adjoint operators which act on  $H'_n$ . We recall that  $H_n$  was an arbitrary finite dimensional subspace of  $H$ . Therefore, we deduce that  $\psi$  is a linear isometry from the space of all self-adjoint finite rank operators on  $H$  onto itself. But this set is dense in  $C_1(H)_s$  and  $\psi$  is continuous on  $C_1(H)_s$ . In fact, this follows from the continuity of  $\phi$  and from the continuity of the absolute value in  $C_1(H)$  (see [11, example 1, p 42]). It is now obvious that  $\psi$  is a surjective linear isometry of  $C_1(H)_s$ . Even more is true. In fact, as  $\phi$  is an isometry and sends 0 to 0, it is clear that  $\psi$  sends positive operators to positive operators and preserves the trace. In the terminology of paper [6], we can say that  $\psi$  is a surjective stochastic isometry. According to the result [6, proposition 3.1],  $\psi$  is implemented by a unitary-antiunitary operator and this completes the proof.  $\square$

Finally, we prove our last result.

**Proof of theorem 4.** Let  $\phi : S(H) \rightarrow S(H)$  be a bijective map which preserves the distance  $d_1$ .

Let  $X, Y \in S(H)$ . Since  $\|X\|_1 = \|Y\|_1 = 1$  and

$$\|X + Y\|_1 = \operatorname{tr}(X + Y) = \operatorname{tr} X + \operatorname{tr} Y = 2$$

using (5) we infer that

$$XY = 0 \iff \|X - Y\|_1 = 2 \iff d_1(X, Y) = 2.$$

Therefore, we obtain that  $\phi$  preserves the orthogonality.

Now, we can borrow some steps from the proof of theorem 3. Indeed, using the argument presented there we can prove that  $\phi$  preserves the rank. Next we can show that for an arbitrary  $n$ -dimensional subspace  $H_n$  of  $H$ , there exists an  $n$ -dimensional subspace  $H'_n$  of  $H$  with the property that  $A \in S(H)$  acts on  $H_n$  if and only if  $\phi(A)$  acts on  $H'_n$ . Hence, just as in the proof of theorem 3, we can reduce the problem to the finite dimensional case.

Let us see what we can do if  $H$  is finite dimensional. Denote by  $T_0(H)$  the linear space of all trace-zero self-adjoint operators on  $H$ . Clearly,  $T_0(H)$  is a normed linear space under the norm  $\|\cdot\|_1$ . Let  $n = \dim H$ . We assert that the convex subset  $K(H) = S(H) - \frac{I}{n}$  of  $T_0(H)$  has nonempty interior. In fact, this is because the elements of that set can be characterized as those trace-zero self-adjoint operators on  $H$  whose eigenvalues lie in the interval  $[-\frac{1}{n}, 1 - \frac{1}{n}]$ . Now, one can verify that the interior of  $K(H)$  consists of those trace-zero self-adjoint operators whose eigenvalues lie in  $]-\frac{1}{n}, 1 - \frac{1}{n}[$ . Consider the map

$$A \mapsto \phi \left( A + \frac{I}{n} \right) - \frac{I}{n}.$$

It is clear that this is a bijective isometry of the convex set  $K(H)$ . Hence, Mankiewicz's result applies and we get that this map is affine. Obviously, we obtain that  $\phi$  is also affine. This was about the finite dimensional case.

In the general case, similarly to the corresponding part of the proof of theorem 3 we can deduce that  $\phi$  is an affine bijection of the subset of all finite rank elements in  $S(H)$ . But this set is dense in  $S(H)$  and  $\phi$  is an isometry. Hence we infer that  $\phi$  is a bijective affine map on  $S(H)$ , that is, a so-called affine automorphism of  $S(H)$ . These transformations are well known to be of the form (2) (see, for example, [12]) and this completes the proof.  $\square$

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