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in quantum estimation theory**

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## Abstract

Two important classes of manifolds of quantum states, the locally quasi-classical manifold and the quasi-classical manifold, are introduced from the estimation theoretical viewpoint, and they are characterized geometrically by the vanishing conditions of the relative phase factor (RPF), implying the close tie between Uhlmann parallel transport and the quantum estimation theory.

## 1 Introduction, Uhlmann's parallelity, and SLD

Berry's phase, by far confirmed by several experiments, is a holonomy of a natural connection on the line bundle over the space of pure states [8][9]. In 1986, Uhlmann generalized the theory to include mixed states in the Hilbert space  $\mathcal{H}$  [10][11] [12]. Throughout this paper, for the sake of clarity,  $n \equiv \dim \mathcal{H}$  is assumed to be finite, and the density matrix is strictly positive, though Uhlmann's original theory is free of these assumptions.

Letting  $W$  be such a  $n$  by  $n$  matrix that  $\rho = \pi(W) \equiv WW^\dagger$ ,  $WU$  also satisfies  $\rho = \pi(WU)$  iff  $U$  is a unitary matrix. So, it is natural to see a space  $\mathcal{W} = \{W|W \in GL(n, \mathbf{C}), \text{Tr}WW^\dagger = 1\}$  as a fiber bundle over the space of strictly positive density matrices  $\mathcal{P}_n$  in  $\mathcal{H}$  with  $U(n)$ 's being its fiber. One possible physical interpretation of  $W$  is a representation of a state vector  $|\Phi\rangle$  in the bigger Hilbert space  $\mathcal{H} \otimes \mathcal{H}'$ . Here,  $\dim \mathcal{H}'$  is  $n$  and the operation  $\pi(*)$  corresponds to the partial trace of  $|\Phi\rangle\langle\Phi|$  over  $\mathcal{H}'$ .

To introduce a connection [13], or a concept of parallel transport along the curve  $C = \{\rho(t)|t \in \mathbf{R}\}$  in  $\mathcal{P}_n$ , a *horizontal lift*  $\{W(t)|t \in \mathbf{R}\} \in \mathcal{W}$  of  $C$  is defined so that  $\rho(t) =$

$\pi(W(t))$  and

$$\frac{dW(t)}{dt} = \frac{1}{2}L_t^S(t)W(t), \quad (1)$$

are satisfied, where  $L_t^S(t)$  is a Hermitian matrix is the root of the matrix equation  $d\rho(t)/dt = (1/2)(L_t^S(t)\rho(t) + \rho(t)L_t^S(t))$ .

Letting  $\{W(t)|t \in \mathbf{R}\}$  be a horizontal lift of  $C' = \{\rho(t)|0 \leq t \leq 1\}$ , the *relative phase factor* (RPF) between  $\rho_0$  and  $\rho_1$  along the curve  $C$  is the unitary matrix  $U$  defined by the equation  $W(1) = \hat{W}_1 U$ , where  $\hat{W}_1$  satisfies  $\rho(1) = \pi(\hat{W}_1)$  and  $\hat{W}_1^\dagger W(0) = W^\dagger(0)\hat{W}_1$ . RPF is said to vanish when it is equal to the identity.

Back in the 1968, Helstrom independently introduced the Hermitian matrix  $L_t^S(t)$ , which played a major role in the definition (1) of Uhlmann's parallelity, as a key concept of his statistical estimation theory of quantum states. He called the matrix  $L_t^S(t)$  *symmetrized logarithmic derivative* (SLD) because SLD is introduced as a quantum counterpart of a logarithmic derivative in the classical estimation theory (throughout this paper, the term 'classical estimation' means estimation of probability distributions) [1] [2]. Our starting point is the following queries: Why SLD plays such an important role both in the quantum estimation theory and in Uhlmann's parallelity? Is this just a coincidence?

## 2 Quantum estimation theory

In this section, conventional theory of quantum estimation is reviewed briefly. In the quantum estimation theory, we try to know the density matrix of the given system from the data  $\xi \in \Xi$  produced from a measuring apparatus. For simplicity, it is assumed that the system belongs to a certain manifold  $\mathcal{M} = \{\rho(\theta)|\theta \in \Theta \subset \mathbf{R}^m\} \subset \mathcal{P}_n$ , and that the true value of the parameter  $\theta$  is not known. For example,  $\mathcal{M}$  is a set of spin states with given wave function part and unknown spin part. An estimate  $\hat{\theta}$  is obtained as a function  $\hat{\theta}(\xi)$  of data  $\xi \in \Xi$  to  $\mathbf{R}^m$ . The purpose of the theory is to obtain the best estimate and its accuracy. The optimization is done by the appropriate choice of the measuring apparatus and the function  $\hat{\theta}(\xi)$  from data to the estimate.

Whatever apparatus is used, the data  $\xi \in \Xi$  lie in a particular subset  $B$  of  $\Xi$  writes

$$\Pr\{\xi \in B|\theta\} = \text{Tr}\rho(\theta)M(B), \quad (2)$$

when the true value of the parameter is  $\theta$ . Here,  $M$ , which is called *measurement*, is a mapping from subsets  $B \subset \Xi$  to non-negative Hermitian matrices in  $\mathcal{H}$ , such that

$$\begin{aligned} M(\phi) &= O, M(\Xi) = I, \\ M\left(\bigcup_{i=1}^{\infty} B_i\right) &= \sum_{i=1}^{\infty} M(B_i) \quad (B_i \cap B_j = \phi, i \neq j), \end{aligned} \quad (3)$$

(see Ref.[2],p.53 and Ref.[3],p.50.). Conversely, some apparatus corresponds to any measurement  $M$  [6][5]. A pair  $(\hat{\theta}, M, \Xi)$  is called an *estimator*.

An estimator  $(\hat{\theta}, M, \Xi)$  is said to be *locally unbiased* at  $\theta$  if

$$\begin{aligned} E_{\theta}[\hat{\theta}(\xi)|M, \Xi] &= \theta, \\ \partial_i E_{\theta}[\theta^j(\xi)|M, \Xi] &= \delta_i^j \quad (i, j = 1, \dots, m), \end{aligned} \quad (4)$$

hold at  $\theta$ , where  $E_{\theta}[*|M, \Xi]$  is the expectation with respect to the probability measure (2), and  $\partial_i$  stands for  $\partial/\partial\theta^i$ . Only locally unbiased estimators are treated from now on.

In the classical estimation, the inverse of so-called Fisher information matrix provides the tight lower bound of covariance matrices of locally unbiased estimates, where local unbiasedness of the estimate is defined almost in the same way as in quantum estimation. Coming back to the quantum estimation,

$$V_{\theta}[\hat{\theta}(\xi)|M, \Xi] \geq (J^S(\theta))^{-1} \quad (5)$$

holds true, *i.e.*,  $V_{\theta}[\hat{\theta}(\xi)|M, \Xi] - (J^S(\theta))^{-1}$  is non-negative definite for any unbiased estimator  $(\hat{\theta}, M, \Xi)$  (see (5.4) in Ref.[3],p.276). Here,  $V_{\theta}[\hat{\theta}(\xi)|M, \Xi]$  is the covariance matrix of  $\hat{\theta} = \hat{\theta}(\xi)$  with respect to the probability measure (2), and  $J^S(\theta) = [J_{ij}^S(\theta)]$ , which is analogically called SLD Fisher information matrix, is defined by

$$J_{ij}^S(\theta) = \text{ReTr}\rho(\theta)L_i^S(\theta)L_j^S(\theta) \quad (i, j = 1, \dots, m), \quad (6)$$

where  $L_i^S(\theta)$  is the SLD of parameter  $\theta^i$ , *i.e.*,

$$\partial_i \rho(\theta) = \frac{1}{2}(L_i^S(\theta)\rho(\theta) + \rho(\theta)L_i^S(\theta)). \quad (7)$$

The bound  $(J^S(\theta))^{-1}$  is one of the bests, in the sense that any Hermitian matrix  $A$  such that  $A \geq (J^S(\theta))^{-1}$ , is no more a lower bound. However, different from the classical case, the equality in (5) is not attainable except for the case indicated by the following theorem, which is proved by Nagaoka [4].

**Theorem 1** *The equality in (5) is attainable at  $\theta$  iff  $[L_i^S(\theta), L_j^S(\theta)] = 0$  for any  $i, j$ . Letting  $|\xi\rangle$  be a simultaneous eigenvector of the matrices  $\{L_j^S(\theta)|j = 1, \dots, m\}$  and  $\lambda_i(\xi)$  be the eigenvalue of  $L_i^S(\theta)$  corresponding to  $|\xi\rangle$ , the equality is attained by the estimator  $(\hat{\theta}_{(\theta)}, M_{(\theta)}, \Xi)$  such that*

$$\begin{aligned}\Xi &= \{\xi|\xi = 1, \dots, n\}, \\ M_{(\theta)}(\xi) &= |\xi\rangle\langle\xi|, \\ \hat{\theta}_{(\theta)}^j(\xi) &= \theta^j + \sum_{k=1}^n [(J^S)^{-1}]^{jk} \lambda_k(\xi).\end{aligned}\tag{8}$$

*Remark* In this paper, we focus on the lower bound (5), and are not concerned with the lower bound of  $\text{TrGV}[M]$ , which is treated in Refs. [2]-[3].

The manifold  $\mathcal{M}$  is said to be *locally quasi-classical* at  $\theta$  iff  $L_i^S(\theta)$  and  $L_j^S(\theta)$  commute for any  $i, j$ . In this case, the bound (5) becomes tight as its classical counterpart is and the analogy of classical estimation seemingly works well. However, this analogy fails in that the measurement  $M_{(\theta)}$  in (8) is dependent on the true value of the parameter, which is unknown before the estimation. Hence, we need to adopt the measurement through the process of estimation using the knowledge about the parameter obtained so far [4].

Let us move to the easier case, in which  $L_i^S(\theta)$  and  $L_j^S(\theta')$  commute for any  $\theta \neq \theta'$ , in addition to being locally quasi-classical at any  $\theta \in \Theta$ . Here, the measurement  $M_{(\theta)}$  in (8), denoted by  $M_{best}$  hereafter, is independent of theta and is uniformly optimal for all  $\theta$  (so is the corresponding apparatus). We say such a manifold is *quasi-classical* [7], because given the optimal apparatus, the quantum estimation reduces to the classical estimation.

### 3 Vanishing conditions for RPF

So far, we have reviewed the conventional theory of quantum estimation and Uhlmann's parallelity. In this section, we derive conditions for RPF to vanish, which is used to characterize the classes of manifold defined in the previous section. For notational simplicity, the argument  $\theta$  is omitted, as long as the omission is not misleading.

The RPF for the infinitesimal loop

$$\begin{aligned} \theta &= (\theta^1, \theta^2, \dots, \theta^m) \rightarrow (\theta^1 + d\theta^1, \theta^2, \dots, \theta^m) \rightarrow (\theta^1 + d\theta^1, \theta^2 + d\theta^2, \dots, \theta^m) \\ &\rightarrow (\theta^1, \theta^2 + d\theta^2, \dots, \theta^m) \rightarrow (\theta^1, \theta^2, \dots, \theta^m) = \theta, \end{aligned}$$

is calculated up to the second order of  $d\theta$  by expanding the solution of the equation (1) to that order:

$$\begin{aligned} I + \frac{1}{2}W^{-1}F_{12}W d\theta^1 d\theta^2 + o(d\theta)^2, \\ F_{ij} = (\partial_i L_j^S - \partial_j L_i^S) - \frac{1}{2}[L_i^S, L_j^S]. \end{aligned} \quad (9)$$

Note that  $F_{ij}$  is a ‘representation’ of the curvature form, and that RPF for any closed loop vanishes iff  $F_{ij}$  is zero at any point in  $\mathcal{M}$ .

**Theorem 2** *RPF for any closed loop vanishes iff  $[L_i^S(\theta), L_j^S(\theta)] = 0$  for any  $\theta \in \Theta$ . In other words,*

$$F_{ij}(\theta) = 0 \iff [L_i^S(\theta), L_j^S(\theta)] = 0. \quad (10)$$

**Proof** If  $F_{ij}$  equals zero, then both of the two terms in the left-hand side of (9) must vanish, because the first term is Hermitian and the second term is skew-Hermitian. Hence, if  $F_{ij} = 0$ ,  $[L_i^S, L_j^S]$  vanishes.

On the other hand, the identity  $\partial_i \partial_j \rho - \partial_j \partial_i \rho = 0$ , or its equivalence

$$(\partial_i L_j^S - \partial_j L_i^S - \frac{1}{2}[L_i^S, L_j^S])\rho + \rho(\partial_i L_j^S - \partial_j L_i^S + \frac{1}{2}[L_i^S, L_j^S]) = 0,$$

implies that  $\partial_i L_j^S - \partial_j L_i^S$  vanishes if  $[L_i^S, L_j^S] = 0$ , because  $\partial_i L_j^S - \partial_j L_i^S$  is Hermitian and  $\rho$  is positive definite. Thus we see  $F_{ij} = 0$  if  $L_i^S$  and  $L_j^S$  commute.  $\square$

A manifold  $\mathcal{M}$  is said to be *parallel* when the RPF between any two points along any curve vanishes. From the definition, if  $\mathcal{M}$  is parallel, RPF along any closed loop vanishes, but the reverse is not necessarily true. The following theorem is a generalization of Uhlmann’s theory of  $\Omega$ -horizontal real plane [12].

**Theorem 3** *The following three conditions are equivalent.*

(1)  $\mathcal{M}$  is parallel.

(2) Any element  $\rho(\theta)$  of  $\mathcal{M}$  writes  $M(\theta)\rho_0M(\theta)$ , where  $M(\theta)$  is Hermitian and  $M(\theta_0)M(\theta_1) = M(\theta_1)M(\theta_0)$  for any  $\theta_0, \theta_1 \in \Theta$ .

(3)  $\forall i, j, \forall \theta_0, \theta_1 \in \Theta, [L_i^S(\theta_0), L_j^S(\theta_1)] = 0$ .

Proof Let  $W(\theta_t) = M(\theta_t)W_0$  be a horizontal lift of  $\{\rho(\theta_t), t \in \mathbf{R}\} \subset \mathcal{M}$ . Then,  $W_0^\dagger W(\theta_t) = W^\dagger(\theta_t)W_0$  implies  $M(\theta_t) = M^\dagger(\theta_t)$ , and  $W^\dagger(\theta_{t_0})W(\theta_{t_1}) = W^\dagger(\theta_{t_1})W(\theta_{t_0})$  implies  $M(\theta_{t_0})M(\theta_{t_1}) = M(\theta_{t_1})M(\theta_{t_0})$ . Thus we get (1)  $\Rightarrow$  (2). Obviously, the reverse also holds true. For the proof of (2)  $\Leftrightarrow$  (3), see Ref. [7], pp.31-33.  $\square$

## 4 Uhlmann's parallelity in quantum estimation theory

In this section, geometrical structure of  $\mathcal{W}$  is related to the quantum estimation theory. First, we imply the statistical significance of natural metric  $\text{Tr}\dot{W}\dot{W}^\dagger$  in the space  $\mathcal{W}$ . When  $\dim\mathcal{M} = 1$ , the equality in (5) is always attainable (see Refs. [1]-[3]). By virtue of the geometrical identity

$$J_t^S(t) = \min_{W(t) \in \pi^{-1}(\rho(t))} 4\text{Tr} \frac{dW(t)}{dt} \frac{dW^\dagger(t)}{dt} \quad (11)$$

(see Refs. [11]-[12]), the inequality (5) in the case of  $\dim\mathcal{M} = 1$ , allows natural geometrical interpretation: the closer two fibers  $\pi^{-1}(\rho(t))$  and  $\pi^{-1}(\rho(t + dt))$  are, the harder it is to distinguish  $\rho(t)$  from  $\rho(t + dt)$ .

To conclude the paper, we present the theorems which geometrically characterize the locally quasi-classical manifold and quasi-classical manifold, described statistically so far, by the vanishing conditions of RPF, implying the close tie between Uhlmann parallel transport and the quantum estimation theory. They are straightforward consequences of the definitions of the terminologies and theorems 1 -3.

**Theorem 4**  $\mathcal{M}$  is locally quasi-classical at  $\theta$  iff  $F_{ij}(\theta) = 0$  for any  $i, j$ .  $\mathcal{M}$  is locally quasi-classical at any  $\theta \in \Theta$  iff the RPF for any loop vanishes.

**Theorem 5**  $\mathcal{M}$  is quasi-classical iff  $\mathcal{M}$  is parallel.

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