On Quantum Pure State Geometry

HIROSHI HASEGAWA
Institute of Quantum Science, College of Science and Technology
Nihon University, Chiyoda-ku, Tokyo 101-8308
JAFAN
h-hase@mx.jamshon.jp

Abstract: A Fréchet partial differential formula

\[
\frac{\partial \rho(\theta)}{\partial \theta_i}(A_i) = \frac{\partial^2 \rho(\theta)}{\partial \theta_i^2} A_i^2 + [\rho(\theta), \Delta A_i] \quad i = 1, 2, \ldots, m \leq n^2
\]

is shown to identify the \(m\) vectors \(\{\Delta_i\}\) with the set of operator covariance for parameter evolutions introduced by Anandan-Aharonov and Abe.

Key-words: positive-definite density matrix, pure state, projective Hilbert Space, Fubini-Study metric

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1 Introduction

Geometrical studies of phase in quantum wave functions were initiated by Berry [1], who pointed out that an adiabatic cyclic motion set up in the phase of an eigenfunction of a quantum system which makes its eigenstate property invariant still produces a nonvanishing excess phase factor \(\gamma(C)\) i.e.

\[
\psi \rightarrow \exp -i \int_0^T ds \exp -i \int_0^T E(s/T)ds i\gamma(C) \psi,
\]

where \(E(s/T)\) expresses the adiabatic change of the energy eigenvalue of \(\psi\) for a long time \(T\). The cited Berry's paper stimulated a number of geometrical investigations of quantum mechanics for example in relation to Aharonov-Bohm effect etc (3)-[6], which continued until the beginning of 1990 to clarify and to construct the framework of geometrical studies on parametric evolutions of wave functions in quantum systems. Some of important works there may be cited as follows.

1) Aharonov and Anandan(1987)[3] the first successful note of necessity that quantum state should be a ray (an equivalence class by which \(\psi\) and \(\lambda \psi\); \(\lambda \neq 0\) are regarded as equivalent). Consequently, any parametric evolution of state vector should be treated in the projective space of rays \(P\), not just in the starting Hilbert space \(H\).

2) Samuel and Bhandari(1988)[4]; Anandan and Aharonov(1988)[5] unneccessity to restrict the

adiabaticity and the cyclicity in the parametric motions of state vectors for which the dynamical phase may be written as

\[
\int_0^T \langle \psi(t)|H(t)|\psi(t)\rangle dt,
\]

where the time-evolution could be unrestricted to the Hamiltonian \(H(t)\).

3) Anandan and Aharonov(1990)[6] The above expression of evolution integral can be interpreted as the specific metric called Fubini-Study metric. Accordingly, a new interpretation of energy-time uncertainty \(\Delta E \Delta t \geq \frac{\hbar}{4}\) arises as the minimum distance between two different rays \(\psi_1\) and \(\psi_2\) corresponds to the geodesic connecting them.

4) Abe (1993)[7] In a parametric evolution of the state \(\psi\), the concept of “uncertainty” can be extended to any pair of the evolution generators by the use of the Fubini-Study metric defined from

\[
(ds)^2 = 1 - \frac{1}{2} |\langle \psi_0 | \psi_{\theta + \delta \theta} \rangle|^2
\]

\[= -2 Re \langle \psi_0 | iA \psi_0 \rangle + |\langle A^2 \psi_0 \rangle|^2 + O(\delta \theta)^3 \quad (1.3)\]

together with the evolution law (1.4) below

\[
\frac{\partial}{\partial \theta_j} \psi = i A_j \psi \quad j = 1, 2, \ldots, m, \quad (1.4)
\]
so that one can define a new Riemannian metric tensor

\[ g_{ij}(\{\theta_{ij}\}) = \langle \psi \frac{1}{2}(A_i A_j + A_j A_i) \psi \rangle - \langle \psi A_i \psi A_j \psi \rangle, \] (1.5)

where \( g_{ij}(\theta) \) can be interpreted as a covariance, or uncertainty between the pair of observables \( A_i \) and \( A_j \). Further, Abe[7] showed the Riemannian connection associated with the metric tensor \( g_{ij}(\theta) \) as a linear combination of three products of \( A_i \)s.

Let us now turn to the development of quantum state geometry above history i.e. quantum geometry for positive definite states after 1991: this year is known as the first important step provided by Morozova and Chentsov to geometry of quantum states represented as positive-definite density matrices[8]. A major contribution to this development was made by Petz who established monotone metrics in terms of operator monotone functions [9] (See two papers presented at the Istanbul conference[10][11]). An important question here must be how this framework is related to the above-outlined pure state geometry.

In this paper, therefore, we aim to establish the completion of the work of Petz and Sudár, in particular, and, therefore, we aim to establish the completion of the work of Petz and Sudár, in particular, a logically consistent derivation of the parametric evolution of pure state in Fubini-Study geometry so far discussed in Refs.[3]-[7]. In Sec.2 we present a brief summary of the previous results on symmetric monotone metrics and connections with positive definite density matrices. In Sec.3 we discuss and simplify the Theorem of Petz and Sudár on reducibility of the monotone metrics with positive-definite density matrices to the Fubini-Study metric for pure states, and extend its application to the connection problem, where we show the usefulness of our tool i.e. the Fréchet partial differentiation formula[10].

where \( c(\lambda) = \frac{1}{\lambda} \) (Fisher term): \( c(\lambda, \mu) \) is called MC function. Also,

\[ K_\rho(A, B) = \langle A (R^{1/2} f(L_\rho R^{-1}) R^{1/2})^{-1} B \rangle, \] (2.2)

where \( L_\rho \) and \( R_\rho \) are called left and right multiplication operator satisfying

\[ L_\rho(A) \equiv \rho A, \quad R_\rho^{-1}(B) \equiv R_\rho^{-1}(B) = B \rho^{-1} \]

**Theorem of Petz** [9] (Theorem 3.2 in I)

There exists a one-to-one correspondence between the MC function \( c(\lambda, \mu) \) for a symmetric monotone metric \( K_\rho(A, B) \) and a metric characterizing function \( f(x); f(1) = 1 \) with monotonicity as follows.

\[ \begin{align*}
\text{(i)} f(x) &= \frac{1}{2} 
\text{(ii)} c(\lambda, \mu) = \frac{1}{f(\lambda/\mu)} 
\text{(iii)} c(\mu, \lambda) = c(\lambda, \mu) \iff x f(x^{-1}) = f(x), \quad \text{and}
\end{align*} \]

Every operator monotone function \( f \) lies in a narrow range between the two elementary functions

\[ f_{\min}(x) = \frac{1-x}{1+x} \quad \text{and} \quad f_{\max}(x) = \frac{2x}{1+x}, \quad \text{so that} \]

\[ f_{\max}(x) \geq f(x) \geq f_{\min}(x) \quad \text{holds.} \] (2.3)

\( f_{\max} \) and \( f_{\min} \) correspond to the minimum and the maximum metric, respectively, of all the symmetric monotone metrics (note that \( f \) is inversely proportional to the representing metric): the minimum metric is called the Bures metric which is known to provide the geodesic distance between any pair of mixed states.

Hasegawa[11] specified the inequalities (2.3) with a finer structure in terms of the Wigner-Yanase-Dyson(WYD) information(called WYD metric hereafter) and the power-mean metrics as

\[ f_{\max} = f_{\min} \geq f_{\text{power}} \geq f_{\text{power}} \]

\[ f_{\text{power}} \geq f_{\text{WYD}} \geq f_{\text{WYD}} \geq f_{\text{WYD}} = f_{\min}, \] (2.4)

(See Fig.1 in the Appendix) for an order of two parameter sets i.e.

\[ 1 \leq \nu_1 \leq \nu_2 \leq 2, 0 \leq |\alpha_1| \leq |\alpha_2| \leq 3. \]

This implies that the combination of the two subsets of symmetric operator monotone functions \( F_{\text{power}} \cup F_{\text{WYD}} \) is to form a linearly ordered subset with min-max bounds coincident to those of the entire set of symmetric monotone functions \( F = \{ f(x) \} \).
2.2 Affine connections associated with symmetric monotone metrics

Consider the Mirocova-Chentsov and Petz representation of the monotone metric with a paired form.

\[ K_\rho(A, B) = (A, D_\rho \varphi(\rho)D_\rho \chi(\rho)B). \]  

(2.5)

The affine connection associated with the metric (2.5) can be defined by the corresponding 2nd order Fréchet derivative, where 1st and 2nd order Fréchet derivatives can be conveniently written as the 1st and 2nd order divided difference, respectively, as follows:

\[ D_\rho \varphi(\rho)(A) = \sum_{i,j} \varphi^{[1]}(\lambda_i, \lambda_j) A_{ij} e_{ij} \]  

(2.6)

\[ D_\rho^2 \varphi(\rho)(A, C) = \sum_{i,j,k} \varphi^{[2]}(\lambda_i, \lambda_j, \lambda_k) \frac{1}{2} (A_{ij} C_{jk} + C_{ij} A_{jk}) e_{ik}. \]  

(2.7)

Accordingly, the corresponding connection, which can be seen to have a 2-fold structure called dual structure (Amari[16]), may be written as:

\[ \Gamma_\rho(A, C, B) = \sum_{i,j,k} \varphi^{[2]}(\lambda_i, \lambda_j, \lambda_k) \chi^{[1]}(\lambda_i, \lambda_k) \]  

\[ \times \frac{1}{2} (A_{ij} C_{jk} + C_{ij} A_{jk}) B^*_{ik}, \]  

(2.8)

and its dual form [14] for dual connection see Amari[16] i.e.

\[ \Gamma_\rho(A, C, B) = \sum_{i,j,k} \varphi^{[1]}(\lambda_i, \lambda_k) \chi^{[2]}(\lambda_i, \lambda_j, \lambda_k) \]  

\[ \times A_{ik} \frac{1}{2} (CB + BC)_{ik}. \]  

(2.9)

The quantity \( \varphi^{[1]}(\lambda_i, \lambda_j) \) and \( \varphi^{[2]}(\lambda_i, \lambda_j, \lambda_k) \) are the 1st order and 2nd order divided differences, respectively, [15] defined by:

\[ \varphi^{[1]}(\lambda_i, \lambda_j) \equiv \frac{\varphi(\lambda_i) - \varphi(\lambda_j)}{\lambda_i - \lambda_j} \]

\[ \varphi^{[2]}(\lambda_i, \lambda_j, \lambda_k) \equiv \frac{\varphi^{[1]}(\lambda_i, \lambda_j) - \varphi^{[1]}(\lambda_j, \lambda_k)}{\lambda_i - \lambda_k}. \]  

(2.10)

(For the special cases \( i = j, i = j = k \) etc. see Refs [14][15]; the parameters \( \lambda_i \) represent specific eigenvalues of the density matrix \( \rho \)).

Concrete Result for the WYD metrics

\[ \varphi(\rho) = \frac{2}{1-\alpha} - \frac{1+\alpha}{\rho^\alpha}; \quad \chi(\rho) = \frac{2}{1+\alpha} \rho^{1+\alpha} \]

which are denoted by \( \varphi_\alpha(\rho) \) and \( \varphi_-\alpha(\rho) \), respectively[10][11].

\[ \Gamma_\rho^\alpha(A, C, B) = \text{Tr} D_\rho^2 \varphi_\alpha(\rho)(A, C) D_\rho \varphi_-\alpha(\rho). \]

Since the special term (iii) gives \( \varphi^{[1]}(\lambda, \lambda, \lambda) = \frac{1}{2} \varphi''(\lambda) \) [14],

\[ \Gamma_\rho^\alpha(A, C, B) = \sum_i -\frac{(1+\alpha)}{4} \frac{1}{\lambda_i^2} A_{ii} C_{ii} B_{ii} \]

and

\[ \sum_{i \neq j} \frac{1}{\lambda_1^{1/2} + \lambda_j^{1/2}} (A_{ij} C_{jik} + C_{ij} A_{jik}) B^*_{ik} \]

which is simplified as

\[ -\sum_{i \neq k} \frac{1}{\lambda_1^{1/2} + \lambda_k^{1/2}} (A_{ik} C_{kk} + C_{ik} A_{ii}) B_{ki} \]

\[ -\frac{d}{d\lambda_k} \left( \frac{1}{\lambda_1^{1/2} + \lambda_k^{1/2}} \right)^2 (A_{ik} C_{kk} + C_{ik} A_{kk}) B_{ki} \]

so that

\[ \Gamma_\rho^{\alpha=0}(A, C, B) = \sum_i -\frac{1}{4\lambda_i^2} (A^c C^c B^c)_{ii} \]

(2.12)

This property of the special subseries \( j = k \) can be extended to Cases for \( \alpha \neq 0 \) by using the Hansen’s formula (See [14] Appendix B)

\[ \varphi^{[2]}(\lambda_i, \lambda_j, \lambda_k) = \left( \frac{d}{d\lambda_k} \varphi^{[1]}(\lambda_i, \lambda_k) \right) \]  

(2.13)

thus,

\[ \Gamma_\rho^{\alpha=0}(A, C, B) = \sum_i -\frac{1}{4\lambda_i^2} (A^c C^c B^c)_{ii} \]
\[- \sum_{i,j,k} \left( \frac{d}{d\lambda_k} \varphi_{\lambda}^{[i]}(\lambda_i, \lambda_k) \right) \varphi_{-\lambda}^{[i]}(\lambda_i, \lambda_k) \times \frac{1}{2} (A_{ik}C_{kk} + C_{ik}A_{kk}) B_{ki}. \tag{2.14} \]

We shall see that this series plays an essential role in the formation of connection on pure states (Sec.3.4).

**Concrete result for the power-mean metrics**

Petz’s function \( f \) and Morozova-Chentsov function \( c \) for this class are given by

\[ f_\nu(x) = \left( 1 + x^{1/\nu} \right)^\nu \quad 1 \leq \nu \leq 2; \]

\[ c_\nu^{\text{power}}(\lambda, \mu) = \frac{1}{f_\nu(\lambda/\mu)} \left( \frac{2}{\lambda^{1/\nu} + \mu^{1/\nu}} \right)^\nu, \]

so that

\[ \Gamma_\nu^{\text{power}}(A, C, B) = \sum_i \left( \frac{d}{d\lambda_k} c_\nu^{\text{power}}(\lambda_i, \lambda_k) \right) \frac{1}{2} (A_{ik}C_{kk} + C_{ik}A_{kk}) B_{ki}. \]

The expression for \( c_\nu^{\text{power}}(\lambda, \mu) \) satisfies

\[ \frac{\partial}{\partial \mu} c_\nu^{\text{power}}(\lambda, \mu) = -\mu^{1/\nu-1}2^\nu(\lambda^{1/\nu} + \mu^{1/\nu})^{-\nu-1}; \tag{2.15} \]

specifically,

\[ -\frac{2}{(\lambda + \mu)^2} \quad \text{for } \nu = 1 \quad \text{Bures and} \]

\[ -\frac{4\mu^{-1/2}}{(\lambda^{1/\nu} + \mu^{1/\nu})^3} \quad \text{for } \nu = 2 \quad \text{WYD(\( \alpha = 0 \)).} \]

In general, by using the relation between the MC function and the Petz’s \( f \) function i.e.

\[ c(\lambda, \mu) = \frac{1}{f(\lambda/\mu)} \quad \text{(ii)in Petz theorem} \]

\[ \frac{\partial}{\partial \lambda} c(\lambda, \mu) = -f'(\lambda/\mu) \left( \frac{1}{f(\lambda/\mu)} \right)^2, \]

we can get a general formula of connection in case of the \( j = k \) subseries i.e.

\[ \Gamma_\nu^{\text{j=k series}}(A, C, B) = \sum_i \left( \frac{d}{d\lambda_k} \right) \frac{1}{2} (A_{ik}C_{kk} + C_{ik}A_{kk}) B_{ki}. \]

### 3 Reduction of positive-definite states to a pure state in geometry

#### 3.1 Theorem of Petz and Sudár (1996)

Consider the representation of monotone metrics on \( n \times n \) matrix spaces with a positive-definite density matrix \( \rho \in \mathcal{R}_n^+ \) whose eigenvalues are nondegenerate:

\[ K_\rho(A, B) = \sum_{i,j} c(\lambda_i, \lambda_j) A_{ij} B_{ij} \quad \text{(Morozova-Chentsov)} \]

\[ = \text{Tr} A f(I_{\rho} R_{\rho}^{-1})^{-1} R_{\rho}^{-1} B \quad \text{(Petz).} \tag{3.1} \]

The Petz-Sudár theorem which provides the condition of reducibility of a symmetric monotone metric to the Fubini-Study metric can be stated as follows.

**Given a positive definite density matrix \( \rho \in \mathcal{R}_n^+ \) with which a symmetric monotone metric is written as in eq.(3.1)** Suppose that the density matrix depends smoothly on a parameter \( t \in [0, \infty) \) such that

\[ \rho(t) = \sum_{i=1}^{n} \lambda_i(t) e_i e_i^T \]

\[ \lambda_1(t) \geq \lambda_2(t) \geq \ldots \geq \lambda_n(t); \]

\[ \lim_{t \to \infty} \lambda_1(t) = 1 \quad \lim_{t \to \infty} \lambda_i(t) = 0 \quad i = 2, 3, \ldots, n. \tag{3.2} \]

Then, a smooth reduction \( c \) of the symmetric monotone metric to the Fubini-Study metric is possible, if and only if \( f(0) > 0 \), where the latter metric is given by

\[ \pi : K_\rho(A, B) \to C_f(\psi_A \cdot \psi_B), \]

\[ \text{with } C_f = \frac{1}{2f(0)}. \tag{3.3} \]

This implies that the reduction of the symmetric monotone metric to the Fubini-Study metric by the limiting process \( t \to \infty \) can be looked as the equivalent projection map \( \pi \) on the fiber space \( \mathcal{R}_n^+ \) conditioned by \( f(0) > 0 \). Also, it can be seen from the result in Sec. 2.2 the possible allowed range \( f(0) > 0 \) can be fixed for the combined set \( \mathcal{F}_\nu^{\text{power}} \cup \mathcal{F}_{\text{WYD}} \) so that, in terms of \( C_f = 1/2f(0) \)

\[ 1 = C_{\text{Bures}} \leq C_{\text{power}, \nu} \leq C_{\text{power}, \nu=2} = C_{\text{WYD}, \alpha=1} < C_{\text{WYD}, \alpha=1} = 1. \tag{3.4} \]

This series of inequalities shows that the reducibility holds for the class of power-mean metrics, but only for a part of the class of Wigner-Yanase-Dyson metrics, namely for those indexed by \( -1 < \alpha < 1 \). Thus, the important example of the Bogolubov-Kubo-Merri(KBM) metric, \( f_{\text{WYD}, \alpha=1}(0) = 0 \), cannot be reduced to the Fubini-Study metric (see Fig.1 in the Appendix).
3.2 Fréchet partial differential on parameter spaces

We now present a formulation of the pure-state parametric evolution discussed by Anandan-Aharanov[6] and Abe[7]: its derivation from a noncommutative manifold of generally mixes density matrix

\[ \rho(\theta); \quad \theta = (\theta_1, \theta_2, \ldots, \theta_m) \]

\[ m \text{-dimensional smooth manifold } (3.5) \]

by means of a type of the Fréchet partial differentiations, which we have discussed previously[10]. Namely,

\[ \partial_i \varphi(\rho(\theta)) = D_{\theta_i} \varphi(\rho(\theta))(A_i) \]

\[ = \frac{\partial \varphi}{\partial \theta_i} A_i^\dagger + [\varphi(\rho), \Delta A_i], \]

and \( \varphi \) is set equal to 1. This is relevant for the present purpose of the subject of reduction to pure states: there

\[ \partial_i \rho(\theta) = D_{\theta_i} \rho(\theta)(A_i) = \frac{\partial \rho}{\partial \theta_i} A_i^\dagger + [\rho, \Delta A_i]. \quad (3.6) \]

As in the starting general formulation (see [10] 1), there exists for a tangent manifold \( T \) at \( \rho \) a set of \( m \) linearly independent hermitians

\[ (i\Delta A_1, i\Delta A_2, \ldots, i\Delta A_m) \quad (3.7) \]

which we will show that it plays the role of generators for parametric evolutions in pure states assumed previously[6][7]. Let us reconsider the expression (3.10) for the noncommutative part of the \( (\varphi, \chi) \) paired metric, first single parameter case \( m = 1 \).

\[
\begin{align*}
\lim_{t \to \infty} \text{Tr}[\varphi(\rho), \Delta A]\chi(\rho), \Delta B] &= \\
\text{Tr}[\varphi(\rho)\Delta A^\dagger(\rho)\Delta B + \varphi(\rho)\Delta B^\dagger(\rho)\Delta A] \\
&= \frac{2}{f(0)} (\langle \psi, AB \psi \rangle - \langle \psi, A \psi \rangle \langle \psi, B \psi \rangle)
\end{align*}
\]

where

\[
\{AB\} = \frac{AB + BA}{2}. \quad (3.11)
\]

In particular, for \( A = B \),

\[
\begin{align*}
\lim_{t \to \infty} \text{Tr}[\varphi(\rho), \Delta A]\chi(\rho), \Delta A] &= \\
\frac{2}{f(0)} (\langle \psi, A^2 \psi \rangle - \langle \psi, A \psi \rangle^2)
\end{align*}
\]

in agreement with the expression given by Abe[7] who called it "uncertainty". It can be generalized easily for several parameter case (1.5). Namely,

\[
\begin{align*}
\lim_{t \to \infty} \text{Tr}[\varrho(\theta), \Delta A_i]\chi(\rho), \Delta A_j] = \\
\langle \psi, A_i A_j \psi \rangle - \langle \psi, A_i \psi \rangle \langle \psi, A_j \psi \rangle.
\end{align*}
\]

As for the connections, the present scheme of partial Fréchet derivatives yield, consistently with [7],

\[
\begin{align*}
\lim_{t \to \infty} \text{Tr} &\{\left[\left(\frac{1}{2}[[\varphi(\rho), \Delta A_i], \Delta A_j] + i \leftrightarrow j\right) \\
&= \left(\frac{2}{f(0)}\right) \right. \}
\end{align*}
\]

where

\[
\langle \psi(\cdot) \psi = \langle \psi(\{A_iA_j\}), A_k - A_k \{A_iA_j\} \rangle \psi \rangle
\]

with \( B_i \equiv A_i - \langle \psi, A_i \psi \rangle. \quad (3.14) \]

4. Conclusion

From the foregoing analysis and results, it can be said that symmetric monotone metrics of Merloza-Chentsov and Petz defined on positive definite density operators can be reduced in a smooth way to the Fubini-Study metric, the smooth reduction being facilitated by means of Fréchet differentiations.

In particular, the Fréchet partial derivatives defined on parametrized matrix manifolds with \( m \) linearly independent commutators

\[
[\rho(\theta_i)]; \quad \sqrt{-1}A_i \quad i = 1, \ldots, m \quad (4.1)
\]

play the role of parameter evolution in the pure state geometry, where the \( m \) hermitians \{\( A_i \)\} identify precisely the generators assumed by Anandan-Aharanov and Abe in their studies of pure state geometry.
Appendix

Fig. 1
Order structure of monotone metrics on matrix spaces in terms of the Petz $f$ functions. The reducibility to pure states is restricted by the condition $f(0) > 0$ (Petz and Sudár) which is satisfied by all the power-mean metrics (left side) and the WYD metrics with $-1 < \alpha < 1$ (right side).

References