Quantum Statistical Manifolds: The Finite-Dimensional Case

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Abstract. Quantum information geometry studies families of quantum states by means of differential geometry. A new approach is followed. The emphasis is shifted from a manifold of strictly positive density matrices to a manifold $\mathbb{M}$ of faithful quantum states on a von Neumann algebra of bounded linear operators working on a Hilbert space. In order to avoid technicalities the theory is developed for the algebra of n-by-n matrices. A chart is introduced which is centered at a given faithful state ω_ρ. It maps the manifold $\mathbb{M}$ onto a real Banach space of self-adjoint operators belonging to the commutant algebra. The operator labeling any state ω_σ of $\mathbb{M}$ also determines a tangent vector in the point ω_ρ along the exponential geodesic in the direction of ω_σ. A link with the theory of the modular automorphism group is worked out. Explicit expressions for the chart can be derived in terms of the modular conjugation and the relative modular operators.

Keywords: Information geometry · Quantum statistical manifolds · Quantum exponential family · Modular automorphism group · Relative modular operator

1 Introduction

In quantum information theory [1] the state of the system is described either by a wave function, which is a normalized element of a Hilbert space, or, more generally, by a density matrix. Density matrices are also used in quantum statistical physics. The equilibrium state of a quantum system at the inverse temperature β is given by the density matrix

$$\rho_\beta = \frac{1}{Z(\beta)} \exp(-\beta H).$$

Here, H is a Hermitian matrix, called the Hamiltonian, and $Z(\beta) = \mathrm{Tr}\, \exp(-\beta H)$ is the normalizing factor and is called the partition sum. The expression is the quantum analogue of a Boltzmann-Gibbs distribution. It is the prototype of a model belonging to the quantum exponential family.

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Information geometry deals with the application of differential geometry to statistical models. A quantum version of Amari's dually flat geometry [2] was studied by Hasegawa [3,4], Jenčová [5] and others. The approach of Pistone and Sempi [6] was transferred to the quantum setting by Streater [7,8].

In [9], the present author proposes to shift the emphasis from manifolds of density matrices to manifolds of states on a von Neumann algebra. The intention of this move is to get rid of tracial states and, by doing so, to facilitate further generalizations. However, both [9] and the present work are limited to the case of a finite-dimensional Hilbert space in order to avoid technicalities. A first attempt to advance with the general case is found in [10].

The next three sections review the mathematical formalism, the notion of a manifold of quantum states and some elements of the theory of the modular automorphism group. Section 5 derives an explicit expression for the positive operators wich belong to the commutant algebra and characterize the states of the manifold. In Sect. 6 the vectors tangent to an exponential geodesic are characterized. The paper finishes with a short discussion in Sect. 7.

2 The GNS Representation

The space of n-by-n matrices forms a Hilbert space $\mathcal{H}^{\text{HS}}$ for the Hilbert-Schmidt inner product

$$\langle A, B\rangle^{\text{HS}} = \operatorname{Tr} B^* A.$$

Here, B^* is the adjoint matrix, i.e. the Hermitian conjugate of the matrix B. Operators on $\mathcal{H}^{\text{HS}}$ are sometimes called *superoperators* because the matrices are themselves already operators on the Hilbert space $\mathbb{C}^n$. An alternative view is offered by the Gelfand-Naimark-Segal (GNS) representation. It is more powerful and very general. The starting point is the remark that the Hilbert-Schmidt inner product can be written as

$$\langle A, B\rangle^{\text{HS}} = n \operatorname{Tr} \rho_0 B^* A,$$

where the *density matrix* ρ_0 is the identity matrix $\mathbb{I}$ divided by n.

By definition, a density matrix ρ is positive and has trace equal to one: $\operatorname{Tr}\rho = 1$. By the GNS theorem there exists a Hilbert space $\mathcal{H}$, a vector Ω_ρ in $\mathcal{H}$ and a *-representation of the algebra $\mathcal{A}$ of n-by-n matrices as operators on $\mathcal{H}$ such that

$$\operatorname{Tr}\rho A = (A\Omega_\rho, \Omega_\rho) \quad \text{for all } A \in \mathcal{A}.$$

The map $A \mapsto \omega_\rho(A) = (A\Omega_\rho, \Omega_\rho)$ belongs to the dual $\mathcal{A}^*$ of $\mathcal{A}$ and is called a *state*. Its defining properties are that $\omega_\rho(A^*A) \geq 0$ for all A (positivity) and $\omega_\rho(\mathbb{I}) = 1$ (normalization). The state is said to be *faithful* if $\omega_\rho(A^*A) = 0$ implies $A = 0$. This is the case if the density matrix ρ is non-degenerate.

In the case of a non-degenerate density matrix ρ the GNS representation can be made explicit as follows. The Hilbert space $\mathcal{H}$ is the tensor product $\mathbb{C}^n \otimes \mathbb{C}^n$. Each matrix A is replaced by the matrix $A \otimes \mathbb{I}$, which has dimension n^2-by-n^2.

Choose an orthonormal basis ψ_j, $j = 1, 2, \cdots, n$ of eigenvectors of ρ. One has $\rho\psi_j = p_j\psi_j$ with eigenvalues $p_j > 0$. Let

$$\Omega_\rho = \sum_j \sqrt{p_j}\psi_j \otimes \psi_j.$$

A short calculation then shows that for any n-by-n matrix A one has $\omega_\rho(A) = \mathrm{Tr}\,\rho A = (A\Omega_\rho, \Omega_\rho)$.

The main advantage of this representation of the state ω is that the commutant $\mathcal{A}'$ of the algebra $\mathcal{A}$ is explicitly present. It consists of all matrices of the form $\mathbb{I} \otimes A$. They clearly commute with all matrices of the form $A \otimes \mathbb{I}$. In particular, with any density matrix σ there corresponds a unique positive operator X_σ in the commutant $\mathcal{A}'$ such that

$$\omega_\sigma(A) \equiv \mathrm{Tr}\,\sigma A = (AX_\sigma^{1/2}\Omega_\rho, X_\sigma^{1/2}\Omega_\rho) \quad \text{for all } A \in \mathcal{A}. \tag{1}$$

3 The Manifold

The manifold $\mathbb{M}$ consists of all states ω_σ on the von Neumann algebra $\mathcal{A}$, where σ is any non-degenerate density matrix of dimension n-by-n. Guided by recent works of Pistone et al. [11,12] a chart χ_ρ is introduced which is centered at a state ω_ρ, corresponding with an arbitrary chosen but fixed non-degenerate density matrix ρ. For any state ω_σ in $\mathbb{M}$ the chart defines an element $\chi_\rho(\omega_\sigma)$ of the commutant $\mathcal{A}'$. Its construction follows later on in Sect. 6.

If $t \mapsto \omega_t \in \mathbb{M}$ is a smooth curve then tangent vectors f_t are defined by

$$f_t(A) = \frac{\mathrm{d}}{\mathrm{d}t}\omega_t(A), \quad A \in \mathcal{A}. \tag{2}$$

They belong to the dual $\mathcal{A}^*$ of the algebra $\mathcal{A}$ and satisfy $f_t(\mathbb{I}) = 0$ and $f_t(A^*) = \overline{f_t(A)}$. The tangent plane at the point ω_ρ is denoted $T_\rho\mathbb{M}$ and consists of all linear functionals f_K of the form

$$f_K(A) = (A\Omega_\rho, K\Omega_\rho), \qquad A \in \mathcal{A},$$

where K belongs to the Banach space $\mathcal{B}_x$ of all self-adjoint elements of the commutant algebra $\mathcal{A}'$ and satisfies $(\Omega_\rho, K\Omega_\rho) = 0$.

The metric chosen on the tangent plane is that of Bogoliubov (see for instance [1,2,13,14]). It can be derived from Umegaki's relative entropy [15]

$$D(\sigma||\tau) = \mathrm{Tr}\,\sigma\,[\log\sigma - \log\tau]\,.$$

by taking twice a derivative. The metric is not discussed in the present paper. Details can be found in [9].

A geodesic corresponding to the exponential connection and connecting the state $\omega_\sigma \in \mathbb{M}$ to the state ω_ρ at the center is of the form $t \mapsto \omega_{\sigma,t}$, where

$$\begin{aligned}
\omega_{\sigma,t}(A) &= \mathrm{Tr}\,\sigma_t A, \quad A \in \mathcal{A}, \qquad \text{with}\\
\log\sigma_t &= \log\rho + tH_\sigma - \zeta(tH_\sigma)\\
H_\sigma &= \log\sigma - \log\rho,\\
\zeta(tH_\sigma) &= \log\,\mathrm{Tr}\,\exp(\log\rho + tH_\sigma).
\end{aligned} \tag{3}$$

The chart χ_ρ is constructed in such a way that the tangent in the point ω_ρ equals the linear functional f_K with $K = \chi_\rho(\omega_\sigma)$.

4 Relative Modular Operators

In [9] the chart χ_ρ is constructed in an indirect manner. A more direct construction is given below in Sect. 6. It is based on Araki's notion of *relative modular operators* [16,17].

Let S denote the *modular conjugation operator* [18] determined by the vector Ω_ρ. It is the anti-linear operator defined by $SA\Omega_\rho = A^*\Omega_\rho$ for all A in $\mathcal{A}$. The *modular operator* Δ equals S^*S and does not depend on the specific choice of the vector Ω_ρ representing the state ω_ρ. The polar decomposition of S reads $S = J\Delta^{1/2}$. The operator J satisfies $J^* = J$, $J^2 = \mathbb{I}$. An important result of Tomita-Takesaki theory, needed further on, states that JAJ belongs to the commutant algebra $\mathcal{A}'$ if and only if A belongs to $\mathcal{A}$.

Given any vector Ξ in the Hilbert space $\mathcal{H}$ the *relative modular conjugation operator* S_{Ξ,Ω_ρ} is defined by

$$S_{\Xi,\Omega_\rho} A\Omega_\rho = A^*\Xi, \qquad A \in \mathcal{A}.$$

For convenience, let us introduce the notation $S_\sigma \equiv S_{\Xi,\Omega_\rho}$ when $\Xi = X_\sigma^{1/2}\Omega_\rho$. The *relative modular operator* Δ_σ is then given by

$$\Delta_\sigma = S_\sigma^* S_\sigma = S^* X_\sigma S = \Delta\rho^{-1}\sigma.$$

Consider now the geodesic $t \mapsto \omega_{\sigma,t}$ given by (3). Because $\Delta\rho^{-1}$ commutes with σ_t it follows from $\Delta_{\sigma,t} = \Delta\rho^{-1}\sigma_t$ that

$$\begin{aligned} \log \Delta_{\sigma,t} &= \log \Delta\rho^{-1} + \log \rho + tH_\sigma - \zeta(tH_\sigma) \\ &= \log \Delta + tH_\sigma - \zeta(tH_\sigma). \end{aligned} \tag{4}$$

One concludes that the operator H_σ which generates the exponential geodesic also describes the relative modular operator $\Delta_{\sigma,t}$ for all states $\omega_{\sigma,t}$ along the geodesic.

5 Explicit Expressions

In [9] the operator X_σ, which characterizes the state ω_σ via (1) is defined in an indirect manner by requiring that

$$X_\sigma\Omega_\rho = \sigma\rho^{-1}\Omega_\rho.$$

An explicit expression is given by the following proposition.

Proposition 1. *The operator X_σ satisfies $X_\sigma = S\rho^{-1}\sigma S$. The relative modular operator Δ_σ satisfies*

$$\Delta_\sigma = S^* X_\sigma S \quad \textit{and} \quad \Delta_\sigma^{1/2} = (\rho^{-1}\Delta)^{1/2}\sigma^{1/2}.$$

Proof. One has for all A in $\mathcal{A}$

$$X_\sigma A\Omega_\rho = AX_\sigma\Omega_\rho = A\sigma\rho^{-1}\Omega_\rho = S\rho^{-1}\sigma SA\Omega_\rho$$

Because Ω_ρ is cyclic for $\mathcal{A}$ this implies that $X_\sigma = S\rho^{-1}\sigma S$. Next use that $\rho^{-1}\Delta = \Delta\rho^{-1}$ belongs to the commutant $\mathcal{A}'$ to obtain

$$X_\sigma = J\Delta^{1/2}\rho^{-1}\sigma S = J\Delta^{-1/2}[\Delta\rho^{-1}]\sigma S = S^*\left([\Delta\rho^{-1}]^{1/2}\sigma^{1/2}\right)^2 S.$$

Finally, one has for all A in $\mathcal{A}$

$$S_\sigma A\Omega_\rho = A^* X_\sigma^{1/2}\Omega_\rho = X_\sigma^{1/2}A^*\Omega_\rho = X_\sigma^{1/2}SA\Omega_\rho.$$

This implies $S_\sigma = X_\sigma^{1/2}S$ and hence

$$\Delta_\sigma = S_\sigma^* S_\sigma = S^* X_\sigma S = \left([\Delta\rho^{-1}]^{1/2}\sigma^{1/2}\right)^2.$$

□

6 The Chart

In [9] the operator $\chi_\rho(\omega_\sigma)$ belonging to the commutant $\mathcal{A}'$ is defined by the relation

$$\chi_\rho(\omega_\sigma)\Omega_\rho = \int_0^1 \mathrm{d}u\, \rho^u \left[\log\sigma - \log\rho + D(\rho||\sigma)\right]\rho^{-u}\Omega_\rho. \tag{5}$$

Its main property is that, given an exponential geodesic $t \mapsto \omega_{\sigma,t}$ of the form (3), the tangent vector at $t = 0$ satisfies

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \omega_{\sigma,t}(A) = \left(A\Omega_\rho, \chi_\rho(\omega_\sigma)\Omega_\rho\right), \qquad A \in \mathcal{A}. \tag{6}$$

There is a one-to-one correspondence between the tangent vectors of $T_\rho\mathbb{M}$ and the elements of the Banach space $\mathcal{B}_x$.

Alternative proof of (6)

Starting point is the following relation between any state ω_σ in the manifold $\mathbb{M}$ and the corresponding relative modular operator Δ_σ

$$\omega_\sigma(A) = (A\Omega_\rho, X_\sigma\Omega_\rho) = (A\Omega_\rho, S^*\Delta_\sigma S\Omega_\rho), \qquad A \in \mathcal{A}. \tag{7}$$

Consider a geodesic $t \mapsto \omega_{\sigma,t}$ of the form (3). The relative modular operator $\Delta_{\sigma,t}$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta_{\sigma,t} = \frac{\mathrm{d}}{\mathrm{d}t}\exp\left(\log\Delta + tH_\sigma - \zeta(tH_\sigma)\right).$$

Use the identity

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} e^{AH+tH} = \int_0^1 \mathrm{d}u\, e^{uA} H e^{(1-u)A}$$

to obtain

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Delta_{\sigma,t} &= \int_0^1 \mathrm{d}u\, \Delta^u \left(H_\sigma - \left.\frac{\mathrm{d}}{\mathrm{d}t}\zeta(tH_\sigma)\right|_{t=0} \right) \Delta^{1-u} \\ &= \left[\int_0^1 \mathrm{d}u\, \rho^u H_\sigma \rho^{-u} - \left.\frac{\mathrm{d}}{\mathrm{d}t}\zeta(tH_\sigma)\right|_{t=0} \right] \Delta. \end{aligned} \tag{8}$$

From (5) one obtains

$$\chi_\rho(\omega_\sigma) = S \left(\int_0^1 \mathrm{d}u\, \rho^u \left[H + D(\rho||\sigma) \right] \rho^{-u} \right)^* S.$$

Combine this with

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \zeta(tH_\sigma) = -D(\rho||\sigma).$$

and (8) to obtain

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Delta_{\sigma,t} = S^* \chi_\rho(\omega_\sigma) S. \tag{9}$$

Putting the pieces together one obtains (6) from (7) and (9)

7 Discussion

The manifold $\mathbb{M}$ of faithful states on the von Neumann algebra $\mathcal{A}$ of n-by-n matrices is studied. An arbitrary state ω_ρ in $\mathbb{M}$ is selected as the reference state. Other states in $\mathbb{M}$ are labeled with operators in the commutant of the G.N.S.-representation of the selected state. Tangent vectors are linear functionals on the von Neumann algebra. They are also labeled with operators belonging to the commutant algebra. In particular, the vectors tangent to an exponential geodesic are characterized. By the use of the theory of the modular automorphism group [18] and the relative modular operators [16,17] explicit expressions are obtained for operators which were introduced already in a previous paper [9]. The explicit expressions should help in generalizing the present approach to manifolds of states on arbitrary σ-finite von Neumann algebras.

The expression (4) for the logarithm of the relative modular operator is affine along the exponential geodesic, up to a scalar function which is due to normalization. It resembles the similar expression (3) for the density matrix. Both use the operator $H_\sigma = \log\sigma - \log\rho$ as the generator of the geodesic connecting the state ω_σ to the state ω_ρ. The map $\omega_\sigma \mapsto H_\sigma$ labels the states of the manifold with operators belonging to the algebra $\mathcal{A}$. On the other hand, the chart χ_ρ, defined in Sect. 6, uses operators belonging to the commutant algebra $\mathcal{A}'$. This chart determines in a direct manner the vectors tangent to the exponential geodesics at the state ω_ρ.

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