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Spheres and hemispheres as quantum state spaces

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Abstract

Spheres and hemispheres allow an interpretation as quantum state spaces quite similar as to projective spaces. Spheres describe systems with two levels of equal degeneracy. The geometric key lies in the relation between transition probability and geodesics.

There are isometric embeddings as geodesic submanifolds into the space of density operators assuming the latter is equipped with the Bures metric. Then parallel transporting is considered. Manageable expressions for parallel transport along geodesic arcs and polygons can be given.

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1. Introduction

One of my aims is to show the existence of a consistent interpretation of the n-sphere S^n as the space of (pure) states of certain quantum systems within the context of "orthodox" quantum theory. It is shown that n-spheres and $(n+1)$-hemispheres represent states, pure and mixed, respectively, of two level systems with equally degenerate levels. The basic concept is that of transition probability and its relation to the geodesics.

The observables can be shown to form a Jordan spin factor of type I_2 [26]. Representing it as a Jordan subalgebra of a matrix algebra, the spheres and hemispheres in question can be identified with submanifolds of density operators. By the introduction of the Bures metric [18] this identification becomes an isometric embedding onto geodesic submanifolds of the space of density operators.

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This enables an unambiguous way to introduce the parallel transport à la Berry [15] in its extension to density operators [37]. Explicit expressions for the parallel transport along geodesic arcs and polygons are derived, and possible implications for describing experiments are mentioned.

The remainder of this section is devoted to review and to arrange some facts in order to prepare the treatment of the spheres.

Let $\mathcal{H}$ denote a Hilbert space of complex dimension $m+1$, and let us recall that, allowing all hermitian operators to be observables, two of its vectors describe the same state iff they are linearly dependent. To get rid of this ambiguity the complex projective space $\mathbf{P}(\mathcal{H}) = \mathbb{C}\mathbf{P}^m$ of all complex one-dimensional subspaces of $\mathcal{H}$ can be introduced [30] the points of which correspond one-to-one to the pure states. Clearly, the possibility to handle all physical relevant questions of the theory within $\mathbb{C}\mathbf{P}^m$ is principally known since long. The renewed interest raised from insights in the geometric nature of the Berry phase [15,35,44,37,38], and from the interesting role of the Study Fubini metric [2,8,31].

Let $\Omega = \Omega(\mathcal{H})$ denote the convex (affine) set of all density operators. Let us identify every density operator ω with the state it defines, i.e. $A \to \omega(A) = \mathrm{tr}(A\omega)$. A point of Ω is called *pure* iff it is an extremal point of the state space Ω viewed as a convex set. The submanifold of extremal points of Ω is identified with $\mathbb{C}\mathbf{P}^m$ by identifying every one-dimensional subspace (or every ray) of $\mathcal{H}$ with the projection operator projecting $\mathcal{H}$ onto it.

Assume now the complex Hilbert space $\mathcal{H}$ is equipped with an antiunitary time reversal operator Θ [43]. Let a hermitian operator be called *observable* iff it commutes with Θ. With this restriction on the observables the states can be uniquely represented by the density operators commuting with Θ. Let Ω_Θ denote the new state space. The extremal points of Ω_Θ are by definition the pure states of the quantum system $\{\mathcal{H}, \Theta\}$. They can be described more directly. To do so we have to distinguish between the *Bose case* $\Theta^2 = \mathbf{1}$ and the *Fermi case* $\Theta^2 = -\mathbf{1}$.

In the *Bose* case the vectors ψ of $\mathcal{H}$ satisfying $\Theta\,\psi = \psi$ constitute a *real* Hilbert space of real dimension $m+1$, the real one-dimensional subspaces of which can be identified with the extremal points of Ω_Θ, and hence with the space of pure states. Thus the space of pure states in the Bose case is a real projective space $\mathbb{R}\mathbf{P}^m$.

In the *Fermi* case there are no Θ-invariant non-zero vectors contained in $\mathcal{H}$. Instead one has to consider its Θ-invariant projection operators of rank two, which, up to a normalizing factor $\frac{1}{2}$, are the extremal points of Ω_Θ. This reflects the well-known Kramer degeneracy [29] which will not be destroyed by Θ-invariant interactions and observations.

Now Θ anticommutes with the imaginary unit i. Thus by adjoining Θ to the complex numbers one gets the quaternions, and $\mathcal{H}$, equipped with these multipliers, becomes a quaternionic Hilbert space [25]. Two vectors differing by a quaternionic multiplier cannot be distinguished one from another by Θ-invariant observables. Therefore the space of pure states carries the structure of a quaternionic projective space $\mathbb{H}\mathbf{P}^k$ with $2k+1 = m$, while $m+1$ is the complex dimension of $\mathcal{H}$. See [13] for more details.

At this stage one may ask the following question: Let M be one of the Riemannian manifolds $\mathbb{R}\mathbf{P}^n$, $\mathbb{C}\mathbf{P}^n$, or $\mathbb{H}\mathbf{P}^n$, coming from Hopf bifurcating the real, complex, or quaternionic

Hilbert space and being equipped with the canonical Study Fubini metric. What geometric properties ensure the reconstruction of the observables and of the state spaces Ω, Ω_Θ, $\Theta^2 = \pm 1$? A key statement to this question reads: *Every geodesic of M closes with length π*, i.e. M is a C_π-manifold [16].

Let $x, y \in M$ be two points and $\mathrm{Dist}(x, y)$ their distance. If M is suitably embedded in an Euclidean space a given closed geodesic of M may be viewed as a circle of diameter one. The arc length between x and y then equals $\mathrm{Dist}(x, y)$.

The *transition probability* $p(x, y)$ between the states represented by x and y in the cases mentioned above is given by

$$p(x, y) = \cos^2(\mathrm{Dist}(x, y)). \tag{1}$$

If $0 < p(x, y) < 1$ or, equivalently, $0 < \mathrm{Dist}(x, y) < \frac{1}{2}\pi$, there is exactly one curve joining x and y with length $\mathrm{Dist}(x, y)$, the geodesic arc joining them. If, however, the distance is maximal, namely $\frac{1}{2}\pi$, then $p(x, y) = 0$, the states are orthogonal, and y is a focal point of x.

For the usual pure states of quantum theory, parameterized by the projective manifolds, this and relation (1) is an *observation* [16,20,31,2,8]. It may serve as a *definition* for other C_π-manifolds, in particular for the spheres.

As seen above, the metrical distance allows to define the transition probability. The transition probabilities allow to characterize the *observables*. An observable is a real function on M the value of which at point x is its *expectation value* if the system is in the state represented by x. The set of observables is given by

$$\mathbf{O} = \mathbf{O}_M := \{A: x \to A(x) = \sum \mu_j \, p(x, y_j)\}, \tag{2}$$

where μ_k denotes real numbers and $y_1, y_2, \ldots$ a finite set of arbitrary points of M. The real linear space $\mathbf{O}$ is finite dimensional. An observable is a *positive* one iff it is non-negative as a function on M. The cone of positive observable is called $\mathbf{O}^+$. It contains the function 1_M which is constant and equal to one on M. Thus M together with its metric determines the system of observables

$$\{\mathbf{O}, \mathbf{O}^+, 1_M\}, \quad 1_M \in \mathbf{O}^+ \subset \mathbf{O}. \tag{3}$$

In the projective spaces every observable A allows for a decomposition (2) where all the points $y_1, y_2, \ldots$ are mutually orthogonal (spectral decomposition).

States and observables are dual objects: Defining one of these concepts, the definition of the other should follow unambiguously. In the treatment above at first the manifold M with its geometry has been defined to be the space of pure states, followed by the definition of observables. Hence the return to the states is programmed.

A *general state* ω with respect to a system (3) is a real linear form on $\mathbf{O}$ taking only non-negative values on $\mathbf{O}^+$, and which is normed by $\omega(1_M) = 1$. Let us call the set of all these states Ω_M. It is a convex subset of the linear space of all real linear forms on $\mathbf{O}$. Physically, as is well known, the convex structure reflects the possibility of performing Gibbsian mixtures.

In *this* context a state is called *pure* if and only if it is a point of the extreme boundary of the convex set of all states. In fact, for the real, complex, and projective spaces one knows

$$\Omega_M^{\text{pure}} := \text{extreme boundary of } \Omega_M \simeq M \tag{4}$$

topologically and as Riemannian manifolds.

Of course, all these statements apply to the n-spheres with n equal to 1, 2, 4, i.e. to the real, complex, and quaternionic projective lines (see [42,13] and, as will be shown, for the n-spheres).

2. The n-sphere as a space of pure states

Let $\mathbf{S}^n$ be an n-sphere embedded in $\mathbb{R}^{n+1}$ with radius $\frac{1}{2}$ such that

$$x_1^2 + \cdots + x_{n+1}^2 = \tfrac{1}{4}, \qquad \mathrm{d}s^2 = (\mathrm{d}x_1)^2 + \cdots + (\mathrm{d}x_{n+1})^2. \tag{5}$$

Consider two states $x, y \in \mathbf{S}^n$ seen under the angle α from the center. Their distance $\mathrm{Dist}(x, y)$ on the sphere, i.e. the minimal length of a curve on the sphere joining them, equals $\frac{1}{2}\alpha$. According to (1) their *transition probability* is necessarily defined by

$$p(x, y) := \cos^2(\tfrac{1}{2}\alpha) = \tfrac{1}{2}(1 + \cos\alpha) = \tfrac{1}{2}(1 + 4\,xy), \tag{6}$$

where x abbreviates $\{x_1, x_2, \ldots, x_{n+1}\}$. The *antipode* of x is denoted by $x^\perp$, i.e. it is $x^\perp = -x$. There is no other point than the antipode with distance $\frac{1}{2}\pi$ from x, and there is no other state than $x^\perp$ which is orthogonal to x. If y denotes a further point then $p(x, y) + p(x^\perp, y) = 1$. Indeed, $x, y, x^\perp$ form a rectangular triangle in $\mathbb{R}^{n+1}$ with base length one, and the squares of the Euclidean distances of $x^\perp, y$ and of y, x coincides with the transition probabilities $p(x, y)$ and $p(x^\perp, y)$ as seen from (6) and the Pythagorean theorem. Consequently, an observable, if not trivial, is necessarily an alternative, and the n-sphere behaves like a 2-level system: An *observable* $A = A^{x,\lambda,\mu}$, is given by a pair of orthogonal states x and $x^\perp = -x$ and by the values λ, μ which are attained by individual measurements according to whether x or $x^\perp$ is found. These data fix the *expectation value* of the observable at an arbitrary state y as follows:

$$y \mapsto A^{x;\lambda,\mu}(y) := \lambda p(y, x) + \mu p(y, x^\perp) = \tfrac{1}{2}(\lambda + \mu) + 2(\lambda - \mu)\,xy. \tag{7}$$

Thus the observables form an $(n + 2)$-dimensional real linear space $\mathbf{O} = \mathbf{O}^n = \mathbf{O}(\mathbf{S}^n)$. The same set of observables will be obtained by inserting into (2) the expression (6) for the transition probability.

In $\mathbf{O}$ there is a *unit element*, 1_n satisfying $1_n(y) = 1$ for all states y.

If all the expectation values of an observable are non-negative, the observable is called *positive*. For the observable (7) this just means $\lambda \geq 0, \mu \geq O$. The positive observables form a cone $\mathbf{O}^+$ containing 1_n. Hence we meet exactly the situation (3), and we have to consider the positive normed linear functionals to get all states, pure and mixed ones.

Denoting the convex set of general states by

$$\Omega_n = \Omega(\mathbf{S}^n) = \{\omega \in \mathbf{O}^*\colon \omega(A) \geq 0 \text{ for all } A \in \mathbf{O}^+, \omega(1_n) = 1\}, \tag{8}$$

it is to show that Ω_n can be identified with the convex hull of the n-sphere. This implies the validity of (4) because the boundary of the n-ball coincides with the extreme boundary, and this is the n-sphere. Indeed, let us see that the general states are parameterized by the points of the ball

$$\Omega_n \simeq \{\mathbf{E}^n\colon y_1^2 + \cdots + y_{n+1}^2 \leq \tfrac{1}{4}\} \tag{9}$$

in the following manner: To every state ω there is one and only one point y of the ball (9) such that for all observables

$$\omega = \omega_y, \quad \omega_y(A^{x;\lambda,\mu}) = \tfrac{1}{2}(\lambda + \mu) + 2(\lambda - \mu)\, xy. \tag{10}$$

In fact, with no restriction on y the right-hand side can represent every real and normed linear form on $\mathbf{O}$. But such a form is non-negative for all positive observables if and only if y is a point of the ball with diameter one.

The symmetry group is the orthogonal group $O(n+1)$. If $n > 2$ its generators cannot be identified with observables, a fact shared by the real and quaternionic projective spaces. A generator X defines a Killing vector field of the ball (9). Hence $\dot{x} = Xx$ can be regarded as an evolution equation. If $n = 2$ this is a rewriting of a von Neumann equation, see [2,31,17] for more details. Converting the equation to the observables one obtains a Heisenberg like equation

$$\omega\left(\frac{\mathrm{d}A}{\mathrm{d}t}\right) := \frac{\mathrm{d}\omega}{\mathrm{d}t}(A), \quad \text{hence} \quad \frac{\mathrm{d}A^{x;\lambda,\mu}}{\mathrm{d}t}(y) = 2(\lambda - \mu)\, \dot{x} y. \tag{11}$$

There is yet another important parameterization of the state space in the case at hand: By introducing a new variable $\tilde{y}$ the inequality (9) can be made an equality. The states can be described by the points

$$\Omega_n \simeq \{\mathbf{S}_+^{n+1}\colon y_1^2 + \cdots + y_{n+1}^2 + \tilde{y}^2 = \tfrac{1}{4}, \tilde{y} \geq 0\}, \tag{12}$$

which is a deformation of the ball (9) to a *hemisphere* of dimension $n+1$. In the interior of the ball the metric has been changed. The new metric reflects partly the superposition principle. Below we shall see its close relation to the *Bures distance* [18].

The metric (12) indicates an extension of the notation of transition probability as introduced by (6):

$$p(x, y) = p(\omega_x, \omega_y) := \tfrac{1}{2}(1 + 4xy + 4\tilde{x}\tilde{y}), \quad x, y \in \mathbf{E}^n, \tag{13}$$

so that the mixed states appear embedded within the pure states of an $(n+1)$-sphere: they are *purified*. The purification can be achieved by allowing the points y_j in (2) to be chosen from the hemisphere (12), and by using (13) to define the transition probability. This enlarges the set of observables $\mathbf{O}^n$ of (7), and one gets $\mathbf{O}^{n+1}$.

As a first indication that things go together with the definition (13) we compare it with the transition probability in the state space of unital $*$-algebras, [19,36]. (The rather different definitions in these references turned out to coincide for unital C^*-algebras, [33,11].) For two states, ϱ_1, ϱ_2 of a unital C^*-algebra $\mathcal{A}$ one knows [3]

$$p(\omega_1, \omega_2) = \inf \omega_1(A)\, \omega_2(A^{-1}), \quad A > 0,\ A, A^{-1} \in \mathcal{A}. \tag{14}$$

A similar relation is true with (13). At first, a power $A^{(k)}$ of an observable $A = A^{x;\lambda,\mu}$ is defined by the substitutions $x \mapsto x$, $\lambda \mapsto (\lambda)^k$ and $\mu \mapsto (\mu)^k$. Here k is a natural number and, if λ and μ both are different from zero, k may be an arbitrary integer. We call $A^{(k)}$ the kth *Jordan* power, and we write $A^{(k)}$ to distinguish it from the k-power of A as a function on the sphere. An observable A is positive, $A \in \mathbf{O}^+$, iff it is a Jordan square, $A = B^{(2)}$. Now for x, y within the unit ball it is

$$(\tfrac{1}{2} + 2\,xy + 2\,\tilde{x}\tilde{y}) = \inf \omega_x(A)\, \omega_y(A^{(-1)}), \quad A > 0. \tag{15}$$

That the assertion is true can be shown either by explicit computation or, as seen below, by embedding arguments.

3. The Jordan structure

The powers $A^{(k)}$ introduced above serve to define the *Jordan product*

$$A \circ B := \tfrac{1}{4}(A + B)^{(2)} - \tfrac{1}{4}(A - B)^{(2)}. \tag{16}$$

By this definition $\mathbf{O}$ becomes a *real Jordan algebra*. It is a *Jordan spin factor* (of type I_2) [26].

A straightforward calculation yields

$$A^{x;1,-1} \circ A^{y;1,-1} = \cos\alpha\, 1_n = 4\,xy\, 1_n, \tag{17}$$

where $\cos\alpha$ is given by (6), and, for arbitrary A and B, it is, abbreviating

$$A := A^{x;a,c} = \tfrac{1}{2}(a + c)\, 1_n + \tfrac{1}{2}(a - c) A^{x;1-1} \quad \text{and} \quad B := A^{y;b,d}, \tag{18}$$

$$\begin{aligned} A \circ B = {} & \tfrac{1}{2}(b + d)A + \tfrac{1}{2}(a + c)B \\ & - \tfrac{1}{2}\{(ab + cd)\sin^2(\tfrac{1}{2}\alpha) + (ad + cb)\cos^2(\tfrac{1}{2}\alpha)\} 1_n \end{aligned} \tag{19}$$

thus obtaining the multiplication law of a Jordan spin factor.

On the other hand, $\mathbf{O}$ admits a distinguished linear form, called *trace*:

$$\operatorname{Tr} A^{x,\lambda,\mu} := \lambda + \mu. \tag{20}$$

The Jordan product enables one to define a positive definite scalar product on $\mathbf{O}$:

$$(A, B) := \operatorname{Tr} A \circ B, \tag{21}$$

which is uniquely associated to the Jordan structure.

Every real linear form ω on $\mathbf{O}$ allows for a unique representation by

$$\omega(A) = \operatorname{Tr} A \circ D. \tag{22}$$

D is positive iff ω is positive. Namely, with respect to the scalar product (21) the cone $\mathbf{O}^+$ becomes self-dual. Clearly, D has trace one iff $\omega(1_n) = 1$.

A (general) state of $\mathbf{O}$ appeared now as a positive and normed real linear form on the Jordan algebra $\mathbf{O}$. Then D of (22) is called its density operator.

It is a known fact that n-balls (respectively) n-spheres are the (pure) state spaces of Jordan spin factors [6].

4. Isometric embedding of $\Omega(\mathbf{S}^n)$ into $\Omega(\mathcal{H})$

Let $\mathcal{H}$ be a complex Hilbert space of *even* complex dimension m with $m \geq n$. A unital Jordan isomorphism of the Jordan algebra $\mathbf{O}(\mathbf{S}^n)$ to a Jordan subalgebra of $\mathbf{B}(\mathcal{H})$ can be constructed. $\mathcal{H}$ carries a Clifford base $E_1, \ldots, E_{n+1}$ of operators fulfilling

$$E_j E_k + E_k E_j = 2\delta_{jk} I, \quad E_j = E_j^* = E_j^{-1}, \tag{23}$$

$I = I_m$ denotes the identity operator. The real linear and unital map

$$\iota : A^{x;\lambda,\mu} \mapsto \tfrac{1}{2}(\lambda + \mu) I + (\lambda - \mu) \sum x_j E_j, \qquad 1_n \mapsto I \tag{24}$$

is a Jordan isomorphism into the hermitian operators. To see this, it suffices to look at the anticommutator

$$\tfrac{1}{2}\{\iota(A^{x;1,-1}), \iota(A^{y;1,-1})\} = 2 \sum x_k y_j \{E_k, E_j\} = 4xyI, \tag{25}$$

which is $\iota(A^{x;1,-1} \circ A^{y;1,-1})$ according to (17). Remark that λ and μ are the eigenvalues of $\iota(A^{x;\lambda,\mu})$. Their degeneracy is $\frac{1}{2}m$. Now $\mathbf{O}^n$ can be identified with the real unital Jordan subalgebra of $\mathbf{B}(\mathcal{H})$ generated by $E_1, \ldots, E_{n+1}$ and the identity operator I.

Being a positive and unital mapping its dual ι^* maps $\Omega(\mathcal{H})$ onto $\Omega(\mathbf{S}^n)$. There is a map κ from $\Omega(\mathbf{S}^n)$ into $\Omega(\mathcal{H})$ such that $\tau = \iota^* \kappa$ is the identity map of $\Omega(\mathbf{S}^n)$.

To construct κ one associates to every point $y = \{y_1, \ldots, y_{n+1}\}$ of the ball (9) the density operator

$$y \mapsto D^y := \frac{1}{m} I + \frac{2}{m} \sum_{1}^{n+1} y_j E_j. \tag{26}$$

Then

$$\kappa(\omega_y) = \omega^y, \qquad \omega^y(B) := \operatorname{tr}(B D^y), \quad B \in \mathbf{B}(\mathcal{H}), \tag{27}$$

where "tr" is the trace on $\mathcal{H}$. This is justified by

$$\omega_y(A^{x;\lambda,\mu}) = A^{x;\lambda,\mu}(y) = \operatorname{tr}\big(\iota(A^{x;\lambda,\mu})\, D^y\big) = \omega^y(\iota(A^{x;\lambda,\mu})). \tag{28}$$

We now identify $\Omega(\mathbf{S}^n)$ with $\kappa(\Omega(\mathbf{S}^n))$. Then the map τ can be expressed by

$$\tau(\omega) = \omega^y, \qquad y_j = 2\,\omega(E_j), \quad j = 1, 2, \dots, n+1 \tag{29}$$

and becomes an affine map from $\Omega(\mathcal{H})$ onto its fix-point set, the fix-point set being the embedded state space of the embedded Jordan algebra. The next aim is to compare and to compute some transition probabilities. Let ω and ϱ be two states of $\Omega := \Omega(\mathcal{H})$. Their transition probability can be expressed by their density operators D_ω and D_ϱ [10,36],

$$p(\omega, \varrho)^{1/2} = \operatorname{tr} \sqrt{(D_\omega^{1/2} D_\varrho D_\omega^{1/2})}. \tag{30}$$

A nice way to describe this is by the help of an operator version of the non-commutative geometrical mean [32]

$$S\#R := R^{1/2}\big(R^{-1/2} S R^{-1/2}\big)^{1/2} R^{1/2}, \quad R > 0, S > 0. \tag{31}$$

Then, assuming ϱ and ω faithful, consider the operators

$$A := D_\varrho \# D_\omega^{-1}, \qquad A^{-1} = D_\omega \# D_\varrho^{-1}. \tag{32}$$

They have the property

$$p(\omega_\omega, \omega_\varrho)^{1/2} = \omega(D_\varrho \# D_\omega^{-1}) = \varrho(D_\omega \# D_\varrho^{-1}), \tag{33}$$

so that with this choice of A the infimum of (14) will be attained.

Now let us return to the embedded states of the sphere, i.e. to density operators of the form (26). For them

$$(D^y)^2 - \frac{2}{m} D^y + \frac{4}{m^2} \tilde{y}^2 I = 0, \quad m = \dim \mathcal{H} \tag{34}$$

is valid. This enables a direct calculation of the operators (32). One obtains

$$D^x \# (D^y)^{-1} = \frac{m^2 D^x + 4\tilde{x}\tilde{y}(D^y)^{-1}}{2m\sqrt{\frac{1}{2} + 2xy + 2\tilde{x}\tilde{y}}} \tag{35}$$

or

$$D^x \# (D^y)^{-1} = \frac{\frac{1}{2}(\tilde{x} + \tilde{y})I + \sum(\tilde{y}x_j - \tilde{x}y_j)E_j}{\tilde{y}\sqrt{\frac{1}{2} + 2xy + 2\tilde{x}\tilde{y}}}. \tag{36}$$

Inserting this into (33) yields

$$p(\omega^x, \omega^y)^{1/2} = \omega^y(D^x \# (D^y)^{-1}) = \sqrt{\tfrac{1}{2} + 2\sum x_j y_j + 2\tilde{x}\tilde{y}}, \tag{37}$$

which again justifies the setting (13), see also [27,40].

This short discussion of transition probabilities will be finished by the following general remark. The definition given in [36] can be converted in one which uses only the Jordan product $A \circ B = \frac{1}{2}(AB + BA)$ in $\mathbf{B}(\mathcal{H})$: Consider all hermitian functionals ν satisfying for all hermitian operators of the algebra

$$|\mu(A \circ B)|^2 \le \omega(A^2)\,\varrho(B^2). \tag{38}$$

Then one gets

$$p(\omega, \varrho) = \sup |\mu(I)|^2. \tag{39}$$

Let us now relate the discussion above to the Bures *distance* [18] and to the Riemann metric associated to it. The distance of Bures between two states reads

$$\mathrm{dist}^B(\omega, \varrho) = \sqrt{2 - 2\sqrt{p(\omega, \varrho)}} = \inf \sqrt{(\xi - \eta, \xi - \eta)}, \tag{40}$$

where ξ, η run through all the possibilities to represent the given states simultaneously as vector states. Restricting to states the vectors ξ and η are points of the unit sphere in the representation space. The length of a geodesic arc between them equals $\arccos |\langle \xi_1, \xi_2 \rangle|$. Thus it seems more appropriate to use this length than the Hilbert distance as in (40). It is therefore natural to define, literally as in (1),

$$\cos^2 \mathrm{Dist}^B(\omega_1, \omega_2) = p(\omega_1, \omega_2), \quad 0 \le \mathrm{Dist}^B \le \tfrac{1}{2}\pi. \tag{41}$$

This arc length can be restricted to $\frac{1}{2}\pi$ because ξ and $-\xi$ yield the same state. Comparing the metric on the semisphere (12) with Dist^B using (37) the proposition follows.

Proposition 1. *The $(n+1)$-semisphere* (12), *$\Omega(\mathbf{S}^n)$, is isometrically embedded by κ within $\Omega(\mathcal{H})$ if the latter is equipped with the (modified) distance of Bures*, Dist^B, *of* (41).

Proposition 2. *$\Omega(\mathbf{S}^n)$ is a* geodesic *subset (a geodesic submanifold with boundary) of $\Omega(\mathcal{H})$.*

Proposition 3. *τ is a Dist^B-contraction of $\Omega(\mathcal{H})$ onto $\Omega(\mathbf{S}^n)$. Being the fix-points of τ, the set $\Omega(\mathbf{S}^n)$ is a retract of $\Omega(\mathcal{H})$.*

Proposition 1 is already proved. Proposition 3 follows from the fact [4] that transition probabilities never decrease under the action of affine maps of $\Omega(\mathcal{H})$ into itself. Hence Dist^B (as well as dist^B) never increase and those mappings are metrically contracting. This applies in particular to τ, and proves Proposition 3. But now Proposition 2 is almost evident. A metrical contraction maps geodesics onto curves (or onto points) with smaller length. If, therefore, two points of the geodesic do not change the arc connecting them remains a geodesic after a metrical contraction. Considering τ, the mapped geodesic belongs to the retract $\Omega(\mathbf{S}^n)$.

There is a remarkable Riemann metric $\mathrm{d}s_B$ on the state space $\Omega(\mathcal{H})$ [38] induced by either the Bures distance dist^B or Dist^B. Both distances give the same Riemann line element [40,41]. With the solution G of [21]

$$\frac{\mathrm{d}}{\mathrm{d}t} D_\omega = G D_\omega + D_\omega G, \tag{42}$$

one gets along a curve with parameter t

$$ds_B = \sqrt{\operatorname{tr}(G^2 D_\omega)}\,dt = \sqrt{\operatorname{tr}(\tfrac{1}{2} G \dot{D}_\omega)}\,dt = \sqrt{\omega(G^2)}\,dt = \sqrt{\tfrac{1}{2}\dot{\omega}(G)}\,dt. \tag{43}$$

In quite another context the Riemannian metric belonging to the Bures distance has been considered in [45].

On $\Omega(\mathbf{S}^n)$ a manageable solution of (42) can be gained:

$$G = g\left(\tfrac{1}{2} - \sum y_j E_j\right) + \tfrac{d}{dt} \sum y_j E_j, \tag{44}$$

where

$$g = \frac{d}{dt} \ln \tilde{y} \quad \text{if } \tilde{y} \neq 0, \tag{45}$$

while g remains undetermined if $\tilde{y} = 0$. Inserting into (43) results always in

$$(ds_B)^2 = d\tilde{y}^2 + \sum dy_j^2. \tag{46}$$

5. Geometric phases

Having transition probabilities at our disposal one may ask for transition amplitudes

$$(\text{transition amplitude}) \sim \sqrt{\text{transition probability}} \cdot (\text{relative phase}). \tag{47}$$

For a state $\omega \in \Omega(\mathcal{H})$ we start with an ansatz

$$\omega \to D_\omega = W W^*, \qquad W = \sqrt{D_\omega}\, V \tag{48}$$

and call W an *amplitude* and V a *phase* of ω. The phases commute with the observables so that only relative phases can become physically relevant.

At this point we do *not* fix the support of $V V^*$ to be that of D_ω but require only that V is an isometry. Within this restriction the phases posed by (48) should be arbitrary.

For faithful states in finite dimensions the ambiguity of W (and of V) is a gauge transformation by unitaries

$$W \mapsto W U, \qquad U \in \mathbf{U}(\mathcal{H}), \tag{49}$$

so that for a given curve γ of states there are many lifts to curves of amplitudes:

$$W_t = \sqrt{D_{\omega_t}}\, U_t, \quad \text{if } \gamma : t \mapsto \omega_t,\ 0 \le t \le 1. \tag{50}$$

Following [37] one can fix the amplitude along a smooth curve γ with smoothly changing supports by the *parallelity condition*

$$\frac{dW^*}{dt} W = W^* \frac{dW}{dt} \tag{51}$$

up to a global, t-independent gauge. (For the existence and properties of parallelity in the state space of W^*- and C^*-algebras, see [5].) For a *parallel* curve of amplitudes the operator

$$W_1 W_0^* = \sqrt{D_1}\, U_1 U_0^* \sqrt{D_0}, \quad V_\gamma := U_1 U_0^* \tag{52}$$

is a gauge invariant quantity. The same is true with that part of the relative phase V_γ which is fixed by the supports of the initial and final density operators involved in (52). The relative phase should be called *geometric* as it depends only on the curve γ. On the observables one may introduce the linear functional

$$\nu_\gamma(A) := \operatorname{tr}(A W_1 W_0^*) = \operatorname{tr}(\sqrt{D_0} A \sqrt{D_1} V_\gamma) \tag{53}$$

measuring the interference of ω_0 and ω_1 if ω_0 is parallel transported along γ to ω_1.

In the following we are mainly concerned with parallel transport along geodesics. But it had to be remarked that the transport along circles on the 3-hemisphere [22] and most of the calculations [23,24], of the associated gauge potential [39] can be extended to the n-(hemi)spheres.

One observes that the parallelity condition (51) implies

$$\mathrm{d}_B s = \sqrt{\operatorname{tr} \frac{\mathrm{d}W^*}{\mathrm{d}t} \frac{\mathrm{d}W}{\mathrm{d}t}}\, \mathrm{d}t \quad \text{along } \gamma \tag{54}$$

and, indeed, the necessary integrations to compute ν_γ can be carried out if γ is a geodesic arc connecting ω_0 with ω_1.

Lemma 4. *Let W_0 and W_1 be amplitudes of the states ω_0 and ω_1, and*

$$W_0^* W_1 \geq 0. \tag{55}$$

Then there is in the state space one and only one oriented smooth geodesic arc γ starting at ω_0 and terminating at ω_1, such that:

no proper subarc of the considered arc already connects ω_0 with ω_1 and

W_1 is the result of transporting W_0 along a parallel lift of γ.

Corollary 5.

(1) *γ is of constant support at its inner points.*

(2) *The Bures length of γ does not exceed $\frac{1}{2}\pi$.*

(3) *If γ is part of a closed geodesic, its complement transports W_0 to $-W_1$.*

Abbreviating

$$\alpha := \operatorname{Dist}^B(\omega_0, \omega_1), \quad 0 < \alpha \leq \tfrac{1}{2}\pi, \tag{56}$$

let us construct γ. Because of (55) every curve contained in the real linear space X spanned by W_0 and W_1 fulfills the parallelity condition (51). Now

$$(W, W') = \operatorname{tr} W^* W' \tag{57}$$

is a real scalar product on X, and there is exactly one $W_0^\perp$ in X with

$$(W_0^\perp, W_0^\perp) = 1, \qquad (W_0, W_0^\perp) = 0, \qquad (W_1, W_0^\perp) > 0, \tag{58}$$

namely

$$W_0^\perp = \frac{W_1 - \cos\alpha\, W_0}{\sin\alpha}. \tag{59}$$

(It is $\sin\alpha > 0$ and $\cos\alpha \geq 0$ for $0 < \alpha \leq \frac{1}{2}\pi$.) Now

$$W(\phi) := W_0 \cos\phi + W_0^{\perp} \sin\phi \tag{60}$$

is a parallel curve of amplitudes where ϕ measures its Bures length

$$\mathrm{tr}\, \frac{\mathrm{d}W^*}{\mathrm{d}\phi} \frac{\mathrm{d}W}{\mathrm{d}\phi} = 1, \qquad \mathrm{d}_B s = \mathrm{d}\phi. \tag{61}$$

Inserting (59) into (60) shows

$$W(0) = W_0, \qquad W(\alpha) = W_1, \qquad \int_0^{\alpha} \mathrm{d}_B s = \mathrm{Dist}^{\mathrm{B}}(\omega_0, \omega_1) \tag{62}$$

and

$$\phi \to W(\phi) W(\phi)^*, \quad 0 \leq \phi \leq \alpha \tag{63}$$

is an oriented curve which connects ω_0 with ω_1. It is of the shortest possible length: On the unit sphere of the W-space the length of parallel curves coincides with their Hilbert length, and a geodesic arc has to be a part of a large circle. The latter is defined by the unique real plane X containing W_0 and W_1. (In W-space W_0 and W_1 cannot be real linearly dependent if $\omega_0 \neq \omega_1$.) Remark that the complement part goes from $\phi = 0$ to $\phi = \frac{1}{2}\pi - \alpha$ and transports the amplitude to $-W_1$ according to (55). One observes further

$$W(\phi)^* W(\phi') \geq 0 \quad \text{if } 0 \leq \phi, \ \phi' \leq \alpha. \tag{64}$$

Hence the support of $W(\phi)^* W(\phi')$ cannot change on the interior of the allowed parameter interval. Otherwise there would be a change on the sign of at least one eigenvalue on the left-hand side of (64) contradicting its semipositiveness.

The lemma and the corollary are now established.

Next we try to calculate (52) and (53) for geodesic arcs. According to (55)

$$W_0^* W_1 = \sqrt{(W_0^* W_1)(W_1^* W_0)} = U_0^* (D_0^{1/2} D_1 D_0^{1/2})^{1/2} U_0. \tag{65}$$

The support of this expression is contained in the left support of W_0. Restricting operation on this support we are allowed to write

$$P_0 W_1 W_0^* = (W_0^*)^{-1} W_0^* W_1 (W_0^*), \quad P_0 = U_0 U_0^*, \tag{66}$$

so that we obtain

$$P_0 W_1 W_0^* = D_0^{-1/2} P_0 (D_0^{1/2} D_1 D_0^{1/2})^{1/2} D_0^{1/2} \tag{67}$$

and we obviously need the condition

$$\mathrm{supp}(\omega_0) \subseteq \mathrm{supp}(\omega_1), \quad \text{or equivalently,} \quad \mathrm{supp}(D_0) \subseteq \mathrm{supp}(D_1) \tag{68}$$

to get the invariant (52) and the linear form ν_γ. With this support property we are allowed to abandon the projection P_0. Recalling (31) and (33) one can state:

If (68) is fulfilled then

$$W_1 W_0^* = D_0^{-1/2}(D_0^{1/2} D_1 D_0^{1/2})^{1/2} D_0^{1/2} = (D_1 \# D_0^{-1}) D_0, \tag{69}$$

$$\nu_\gamma(A) = \omega_0(A(D_1 \# D_0^{-1})). \tag{70}$$

We need the even stronger assumption of equal supports of D_0 and D_1 to rewrite (52) by inserting (69):

$$V_\gamma = U_1 U_0^* = D_1^{-1/2} D_0^{-1/2} (D_0^{1/2} D_1 D_0^{1/2})^{1/2}. \tag{71}$$

Denoting by P the assumed common support of the density operators involved, and taking care of the operational definitions, one observes

$$V_\gamma V_\gamma^* = V_\gamma^* V_\gamma = P. \tag{72}$$

The equal support condition is fulfilled for two parameter values in the interior of the geodesic arc γ. So we can try to define in the general case

$$V_\gamma := \lim V_\delta, \quad \delta \mapsto \gamma,\ \delta \subset \text{interior}(\gamma), \tag{73}$$

so that in concrete cases one has to examine whether the lim is unique or not, and, in the bad case, whether the arbitrariness cancels in certain expressions. If P is the projection onto the support on the inner part of the geodesic, P_0 and P_1 the projectors belonging to the starting and of the terminating point of the arc, then $P_0 \le P$ and $P_1 \le P$. The rank of the density operators can possibly decrease at the end points of the arc. They can then cut some part of the relative geometric phase. An example is the transport:

$$W_0 = D_0^{1/2} U_0 \quad \to \quad W_1 = D_1^{1/2} V_\gamma U_0. \tag{74}$$

Let us return to the hemisphere $\omega(\mathbf{S}^n)$ embedded within $\Omega(\mathcal{H})$, and let us set $\omega_1 = \omega^x$ with density matrix D_1, and $\omega_0 = \omega^y$ with density matrix D_0. Eq. (36) then shows that $D_1 \# D_0^{-1}$ is continuous in D_1, so that (74) exists with respect to the end point of the geodesic arc. The arbitrariness is hence at most in the starting point of the arc.

Using $W_0 = (D_0)^{1/2}$ as starting amplitude, one gets from (35)

$$W_1 = \frac{m^2 D_1 D_0^{1/2} + 4\tilde{x}\tilde{y} D_0^{-1/2}}{2m\sqrt{\frac{1}{2} + 2xy + 2\tilde{x}\tilde{y}}} \tag{75}$$

as the transported amplitude. With the projection operator P^y onto the support of $D_0 = D^y$ one gets from the characteristic equation

$$\tilde{y}(D^y)^{-1/2} = (1/m)(\text{tr}(D^y)^{1/2}) P^y - (D^y)^{1/2}. \tag{76}$$

Therefore W_1 depends smoothly also on the starting point of the geodesic.

Hence the transport of the amplitude along a geodesic arc within $\Omega(\mathbf{S}^n)$ depends smoothly on the geodesic arc, even if the supports at its starting and (or) terminating point do not coincide with the support of its inner points.

Similar is the situation with respect to the relative geometric phase. A short calculation, again based on (35) or (36) yields

$$V_\gamma = (2m)^{-1} p(\omega_0, \omega_1)^{-1/2} \left(m^2 D_1^{1/2} D_0^{1/2} + 4\tilde{x}\tilde{y} D_1^{-1/2} D_0^{-1/2}\right) \quad (77)$$

if γ is the geodesic arc transporting ω_0 to ω_1. It can be seen that (76) guarantees:

The relative geometric phase depends continuously on the starting and on the terminating state for all short geodesic arcs on the hemisphere.

Whether this behavior can be proved for $\Omega(\mathcal{H})$ remains to be seen. The problem is the uniqueness of the limit in coming from the interior to the boundary. Due to the complicated boundary of $\Omega(\mathcal{H})$ (see [1] for $n = 4$) this is not evident.

6. Comment on cyclic processes

For the spheres and hemispheres we are now in a position to calculate holonomy invariants of closed curves which consists of short geodesic arcs. This seems to be sufficient to discuss the outcome of some (possible or gedanken) experiments with mirrors as described in [28] or by the help of filters [7,34,14], see also [9]: Whether the *pure* state is rapidly changed by devices like mirrors or by filtering measurements, the phase change resulting from such "quantum jumps" can be described by parallel transporting the wave function along the shortest path connecting the corresponding points in the projective Hilbert space.

In these experiments an isoenergetic (monochromatic) beam of particles (photons) goes in a cyclic process through some devices and the outcome is superposed with a split part of the original beam. (Or, more generally, every part of a split beam undergoes a cyclic evolution.) By varying the devices the dynamical phase will (ideally) not alter, and the change in the interference pattern shows the appearance of the geometrical phase.

However, there is no reason within Quantum Theory that prevents the scheme to work also with beams starting with a definite degree of polarization (mixedness) and (or) with devices altering the mixedness. In mirror-like devices the intensity of the beam will be unchanged. In a filter-like device that converts a state ω into a state ϱ the intensity loss is at least by a factor $p(\omega, \varrho)$ according to (30) and (13)

$$\text{Intensity}_{\text{out}} \le p(\omega, \varrho)\, \text{Intensity}_{\text{in}}. \quad (78)$$

Equality in good approximation would indicate an ideal filtering device. Whether this can be reached if both states are mixed ones has to be seen.

Let us assume

$$\omega_1 \mapsto \omega_2 \mapsto \cdots \mapsto \omega_k \mapsto \omega_{k+1} = \omega_1 \quad (79)$$

is a cyclic process as described above where no pair of consecutive states is orthogonal. Then there is a unique shortest geodesic arc, $\gamma_{j,j+1}$ connecting ω_j with ω_{j+1}, and these arcs close to a geodesic polygon. We have to adjust for every j an amplitude W_j of ω_j in such a way that W_{j+1} is the result of the parallel transport along $\gamma_{j,j+1}$ with initial amplitude W_j:

$$W_1 \mapsto W_2 \mapsto \cdots \mapsto W_{k+1} = W_1 V_{\rm cycl}, \tag{80}$$

where $V_{\rm cycl}$ is the geometric phase that accompanies the cyclic process.

In superposing the cyclic transported and the original initial state ω_1 one has to respect a possible dynamical phase ϵ which, for isoenergetic processes, is a complex number of modulus one depending on the geometry of the experimental equipment and (almost) not on the action of the devices which change the state. The reason is that in going from one device to another, the particle remains in one and the same eigenstate of the Hamiltonian. It "rests a while at a corner of the geodesic polygon in state space", getting there a dynamical phase factor. The dynamical phase factors emerging from all the corners (i.e. from the path between the devices in real space) will be multiplied to $\epsilon_{\rm cycl}$ and compared with that one ϵ_0 coming from the other, unchanged part of the split beam. This gives the relative dynamical phase $\epsilon = \bar{\epsilon}_0 \epsilon_{\rm cycl}$ which contributes to the observable relative phase.

Hence the final amplitude and intensity of the cyclic transported beam will be proportional to

$$W_{\rm superposed} = W_1 + W_1 V_{\rm cycl}\, \epsilon \quad \text{and} \quad 1 + \tfrac{1}{2} {\rm tr}\, D_1 (\epsilon V_{\rm cycl} + V_{\rm cycl}^* \bar{\epsilon}), \tag{81}$$

where D_1 is the density operator of ω_1.

Substitute in (77) ω_j for ω^y and ω_{j+1} for ω^x and call the resulting phase $V_{j+1,j}$. Repeated application of (74) results in

$$W_j = D_j^{1/2} V_{j,j-1} V_{j-1,j-2} \cdots V_{2,1} U_1, \qquad W_1 = D_1^{1/2} U_1. \tag{82}$$

The cyclic geometric phase and the holonomy invariant (52) can be written as

$$V_{\rm cycl} = V_{1,k} V_{k-1,k-2} \cdots V_{2,1}, \tag{83}$$

$$W_{k+1} W_1^* = D_1^{1/2} V_{\rm cycl} D_1^{1/2}. \tag{84}$$

If the supports are changing in the course of the cyclic process we nevertheless stay slightly inside the hemisphere, performing only at the last moment the limit to the boundary.

In the interesting case where we stay always in the interior of the state space, not touching its boundary, the general recipe (79) shows

$$W_{k+1} = (D_1 \# D_k^{-1})(D_k \# D_{k-1}^{-1}) \cdots (D_2 \# D_1^{-1}) W_1, \tag{85}$$

where one may insert the expressions (35) or (36).

This can be further simplified if the degree of polarization (the degree of mixedness) is not changed during the cyclic process. Because, then

$$D_{j+1} \# D_j^{-1} = \frac{2I + m(D_{j+1} - D_j)}{2\sqrt{p(D_j, D_{j+1})}} \tag{86}$$

which is easier to handle. It allows for a reformulation in terms of suitably weighted parallel transports of the eigenstates of the density operators along all closed and oriented subpolygons of the given one. A more detailed explanation is in preparation.

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