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Thomas rotation and the mixed state geometric phase

Péter Lévay

Department of Theoretical Physics, Institute of Physics, Technical University of Budapest, H-1521 Budapest, Hungary

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Abstract
It is shown that Uhlmann's parallel transport of purifications along a path of mixed states represented by 2×2 density matrices is just the path-ordered product of Thomas rotations. These rotations are invariant under hyperbolic translations inside the Bloch sphere that can be regarded as the Poincaré ball model of hyperbolic geometry. A general expression for the mixed state geometric phase for an *arbitrary* geodesic triangle in terms of the Bures fidelities is derived. The formula gives back the solid angle result well known from studies of the pure state geometric phase. It is also shown that this mixed state anholonomy can be reinterpreted as the pure state non-Abelian anholonomy of entangled states living in a suitable restriction of the quaternionic Hopf bundle. In this picture Uhlmann's parallel transport is just the Pancharatnam transport of quaternionic spinors.

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1. Introduction

Mixed state geometric phases as introduced by Uhlmann [1] provide a natural generalization of the well-known geometric phases [2] characterizing the geometric properties of unitarily or nonunitarily evolving pure states. Recently this idea of mixed state anholonomy was reconsidered within an interferometric approach [3,4], along with an alternative formulation of mixed state phases [5]. Possible experiments for confirming the appearance of such phases have been proposed and conducted (see, e.g., [6]), and their relevance in the evolution of systems subjected to decoherence through a quantum jump approach has been stressed [7].

The simplest example of an evolving one-qubit system giving rise to a path in the space of nondegenerate 2×2 density matrices was studied by many authors. Uhlmann himself established a formula for the geometric phase for geodesic triangles and quadrangles drawn on the surface of a sphere of *constant radius* inside the Bloch ball $\mathcal{B}$ [8]. An explicit formula for the anholonomy along an arbitrary geodesic segment in $\mathcal{B}$ with respect to the Bures metric was presented by Hübner [9]. In a recent paper for evolving systems giving rise to geodesic triangles defined by Bloch vectors in $\mathcal{B}$ of *fixed magnitude*, Slater [10] compared Uhlmann's geometric phase with the interferometric approach of [5]. The aim of the present paper is to point out for such systems an interesting connection between Uhlmann's parallel transport and the phenomenon of Thomas precession. Using this correspondence we present a formula valid for an *arbitrary* geodesic triangle inside $\mathcal{B}$. Our method is motivated by previous observations of Ungar [11] that hyperbolic geometry can be useful in describing the physical and mathematical phenomena associated with one-qubit density matrices.

The organization of the paper is as follows. In section 2, we briefly recall the background material needed for the definition of Uhlmann's anholonomy for mixed states. In section 3, using the hyperbolic parametrization of one-qubit density matrices, we show that Uhlmann's parallel transport can be expressed as the path-ordered product of suitably defined Thomas rotations arising from the multiplication of two hyperbolic rotations (Lorentz boosts). Here the invariance of these rotations under the so-called hyperbolic translates in the Poincaré ball model of hyperbolic geometry is also established. In section 4, we present our anholonomy formula valid for an arbitrary geodesic triangle in the space of nondegenerate one-qubit density matrices. Our result for the pure state limit gives back the solid angle rule well known from studies concerning the geometric phase [2, 5, 10]. Here an error of [10] is also pointed out. Section 5 is devoted to establishing a connection between our mixed state anholonomy and the pure state non-Abelian geometric phase. Section 6 is left for the comments and conclusions.

2. Mixed state anholonomy

According to Uhlmann [1], the mixed state anholonomy can be defined by lifting the curve $\rho(t)$ living in the space of strictly positive density operators to the space of its purifications such that the representative curve $W(t)$ of these purifications is parallel translated with respect to a suitable connection. W purifies ρ if we have $\rho = WW^\dagger$ and $\operatorname{Tr} WW^\dagger = 1$. W can be regarded as an element of the tensor product of the Hilbert space of a given fixed physical system with another Hilbert space representing a second system (the ancilla). In this picture $WW^\dagger$ corresponds to taking the partial trace over the ancilla. For the special case of purifications that are elements of $\mathcal{H} \otimes \mathcal{H}^*$ where $\mathcal{H}$ is a finite n-dimensional Hilbert space and give rise to strictly positive density matrices, we have $W \in GL(n, \mathbf{C})$. It is obvious that the process of purification is ambiguous, W and WU with $U \in U(n)$ gives rise to the same ρ. Hence we have a (trivial) principal bundle with total space $GL(n, \mathbf{C})$ base $\mathcal{D}_n^+ \equiv GL(n, \mathbf{C})/U(n)$ and fibre $U(n)$. According to the connection defined by Uhlmann, two purifications W_1 and W_2 giving rise to ρ_1 and ρ_2, respectively, are parallel iff

$$W_1^\dagger W_2 = W_2^\dagger W_1 > 0. \tag{1}$$

Using the polar decompositions $W_1 = \rho_1^{1/2} U_1$ and, $W_2 = \rho_2^{1/2} U_2$ that are arising as the right translates by $U(n)$ of the global section $\rho^{1/2}$, one can check that U_1 and U_2 related as

$$Y_{21} \equiv U_2 U_1^\dagger = \rho_2^{-1/2} \rho_1^{-1/2} \left(\rho_1^{1/2} \rho_2 \rho_1^{1/2}\right)^{1/2} \tag{2}$$

give rise to purifications satisfying (1). Dividing our path $\rho(t) \in \mathcal{D}_n^+$ with $0 \leqslant t \leqslant 1$ into small segments one gets

$$W_1 W_0^\dagger = \lim_{m\to\infty} X_{1s_1} X_{s_1 s_2} \ldots X_{s_m 0} \rho_0 \qquad X_{st} = \rho_t^{-1/2} \left(\rho_t^{1/2} \rho_s \rho_t^{1/2}\right)^{1/2} \rho_t^{-1/2} \tag{3}$$

where 'lim' indicates the process of going to finer and finer subdivisions producing a continuous path $C \in \mathcal{D}_n^+$. Although equation (3), with the basic building blocks being the X_{st}, was usually used in the literature, for later use we favour an alternative one expressed in terms of the Y_{st} defined by (2) as

$$W_1 W_0^\dagger = \lim_{m\to\infty} \rho_1^{1/2} Y_{1s_1} Y_{s_1 s_2} \ldots Y_{s_m 0} \rho_0^{1/2}. \tag{4}$$

This expression (the anholonomy of the curve C) will be our basic one for the description of parallel transport of purifications over a path $C \in \mathcal{D}_n^+$. For a closed path C we have $\rho_0 = \rho_1$ hence for the trace of this expression we get

$$\mathrm{Tr}\big(W_1 W_0^\dagger\big) = \lim_{m\to\infty} \mathrm{Tr}\big(Y_{1s_1} Y_{s_1 s_2} \dots Y_{s_m 0} \rho_0\big). \tag{5}$$

The quantity $\Phi_g = \arg \mathrm{Tr}\big(W_1 W_0^\dagger\big)$ is the generalization of the geometric phase for mixed states, and the magnitude $\nu \equiv \big|\mathrm{Tr}\big(W_1 W_0^\dagger\big)\big|$ is the visibility [5].

3. Mixed state anholonomy as Thomas rotation

Now we start discussing our main concern here, namely mixed state anholonomy for a qubit system. For these systems ρ is an element of the interior of the usual Bloch ball $\mathcal{B}$. Moreover, the space of purifications for strictly positive 2×2 density matrices $\rho \in \mathcal{D}_2^+ \simeq \mathrm{Int}\,\mathcal{B}$ is $GL(2, \mathbf{C})$. Hence we have $\rho = WW^\dagger$ with $W \in GL(2, \mathbf{C})$. It is particularly instructive to regard this space as the space of normalized entangled states for a bipartite system, i.e. to have $\mathcal{H} \otimes \mathcal{H}^* \simeq \mathbf{C}^2 \otimes \mathbf{C}^2$, a description giving rise to our ρ upon taking the partial trace with respect to the second subsystem.

For this we write the entangled state $|\Psi\rangle \in \mathbf{C}^2 \otimes \mathbf{C}^2$ in the form

$$|\Psi\rangle = \sum_{j,k} W_{jk} |jk\rangle \qquad |j,k\rangle \equiv |j\rangle_1 \otimes |k\rangle_2 \qquad j,k = 0,1 \quad W_{jk} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{6}$$

The normalization condition $\langle\Psi|\Psi\rangle = 1$ in this picture corresponds to the constraint $\mathrm{Tr}(WW^\dagger) = 1$. Moreover, calculating the trace of the pure state density matrix $|\Psi\rangle\langle\Psi|$ with respect to the second subsystem yields our ρ, i.e. in the $|j\rangle_1$ base we have $\rho = \mathrm{Tr}_2|\Psi\rangle\langle\Psi| = WW^\dagger$. Since we are considering strictly positive density matrices we have the constraint $\mathrm{Det}\,\rho \neq 0$. In terms of the matrix elements of W it means $ad - bc \neq 0$, i.e. $W \in GL(2, \mathbf{C})$. It is well known that for this bipartite system the measure of entanglement is the *concurrence* $\mathcal{C}$ [12] which can be written as

$$0 \leqslant \mathcal{C} \equiv |ad - bc| \leqslant 1. \tag{7}$$

Separable states corresponding to reduced density matrices with a zero eigenvalue are precisely the ones with $\mathcal{C} = 0$.

Let us parametrize our density matrix as $\rho = \frac{1}{2}(I + \mathbf{u}\boldsymbol{\sigma}) = WW^\dagger$ with $|\mathbf{u}| < 1$. This means we have $2u_3 = |a|^2 + |b|^2 - |c|^2 - |d|^2$ and $u_1 + \mathrm{i}u_2 = \overline{a}c + \overline{b}d$, and it is easy to check that $\mathcal{C} = \sqrt{1 - |\mathbf{u}|^2} = 2\sqrt{\mathrm{Det}\,\rho}$. The four real numbers $-1 < u_1, u_2, u_3 < 1$ and $0 < u_4 \equiv \mathcal{C} \leqslant 1$ can be regarded as coordinates on the upper hemisphere of a three-dimensional sphere S^3 embedded in $\mathbf{R}^4$ homeomorphic to $\mathrm{Int}\,\mathcal{B}$.

In the following, it is convenient to introduce a new (hyperbolic) parametrization for ρ by introducing the rapidities [13, 14] θ as

$$|\mathbf{u}| = \tanh\theta_u \qquad 0 \leqslant \theta_u < \infty. \tag{8}$$

In this parametrization, the concurrence is related to the quantity $\gamma_u \equiv \cosh\theta_u$ of special relativity as $\mathcal{C} = \gamma_u^{-1}$. The reader can verify that in this case

$$\rho^{1/2} = \sqrt{\frac{\mathcal{C}}{2}} \left(\cosh\frac{\theta_u}{2} I + \sinh\frac{\theta_u}{2}\hat{\mathbf{u}}\boldsymbol{\sigma}\right) \equiv \sqrt{\frac{\mathcal{C}}{2}} L(\theta_u, \hat{\mathbf{u}}) \qquad \hat{\mathbf{u}} \equiv \frac{\mathbf{u}}{|\mathbf{u}|} \tag{9}$$

where $L(\theta_u, \hat{\mathbf{u}})$ is a Lorentz boost in the spinor representation.

Using the relation $M^2 - M\,\mathrm{Tr}\,\mathrm{M} + \mathrm{Det}\,M = 0$ (valid for 2×2 matrices) and its trace we have the formula

$$\sqrt{M} = \frac{M + \sqrt{\mathrm{Det}\,M}}{\sqrt{\mathrm{Tr}\,M + 2\sqrt{\mathrm{Det}\,M}}}. \tag{10}$$

Now we calculate the quantity Y_{uv} of (2) with the density matrices ρ_u and ρ_v. For this we insert $M \equiv \rho_v^{1/2}\rho_u\rho_v^{1/2}$ in equation (10). First we note that the square of the denominator of this equation has the form

$$\mathrm{Tr}(\rho_u\rho_v) + 2\sqrt{\mathrm{Det}(\rho_u\rho_v)} = \tfrac{1}{2}(1 + \mathbf{uv} + \mathcal{C}_u\mathcal{C}_v) = F(\mathbf{u},\mathbf{v}) \tag{11}$$

where $F(\mathbf{u},\mathbf{v})$ is the Bures fidelity. Moreover, by virtue of equation (9) its numerator multiplied by $\rho_u^{-1/2}\rho_v^{-1/2}$ has the form

$$\rho_u^{1/2}\rho_v^{1/2} + \frac{\mathcal{C}_u\mathcal{C}_v}{4}\rho_u^{-1/2}\rho_v^{-1/2} = \frac{1}{2}\sqrt{\mathcal{C}_u\mathcal{C}_v}\,(L(\theta_u,\hat{\mathbf{u}})L(\theta_v,\hat{\mathbf{v}}) + L(\theta_u,-\hat{\mathbf{u}})L(\theta_v,-\hat{\mathbf{v}}))\,. \tag{12}$$

Recalling that the composition of two boosts can be written as another boost times the Thomas rotation, the right-hand side of equation (12) can be written as

$$L(\theta_w,\hat{\mathbf{w}})R(\alpha,\hat{\mathbf{n}}) + L(\theta_w,-\hat{\mathbf{w}})R(\alpha,\mathbf{n}) = 2\cosh\frac{\theta_w}{2}R(\alpha,\hat{\mathbf{n}}) \tag{13}$$

where $R(\alpha,\hat{\mathbf{n}}) = \cos\frac{\alpha}{2}I + \mathrm{i}\sin\frac{\alpha}{2}\sigma\hat{\mathbf{n}}$ is the Thomas rotation matrix in the spinor representation. Note that the two different pairs of consecutive Lorentz transformations yield the same extra rotation and the Lorentz boost with the same rapidity but axis with its direction reversed. This can be proved by writing out explicitly the product of two boosts in the spinor representation establishing the dependence of the quantities α, θ_w, $\mathbf{w}$, $\mathbf{n}$ on the original ones θ_u, θ_v, $\mathbf{u}$ and $\mathbf{v}$ (see, e.g., [15] and references therein). In this way we get explicit expressions for $\hat{\mathbf{n}}$ and $\tan\frac{\alpha}{2}$ and none of them is sensitive to a sign change in $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$. (For an alternative understanding of this result see equation (18).) The sign change in the axis $\hat{\mathbf{w}}$ can be established similarly. Another formula of this kind we need is the hyperbolic law of cosines [13,15] which can be written as

$$\cosh\theta_w = \cosh\theta_u\cosh\theta_v + \sinh\theta_u\sinh\theta_v\hat{\mathbf{u}}\hat{\mathbf{v}} = \frac{1}{\mathcal{C}_u\mathcal{C}_v}(1 + \mathbf{uv}). \tag{14}$$

Using this we have $2\cosh\frac{\theta_w}{2} = 2\sqrt{\frac{F(\mathbf{u},\mathbf{v})}{\mathcal{C}_u\mathcal{C}_v}}$. Putting this into equations (12), (13) and using equation (11), we obtain our result

$$Y_{uv} = \rho_u^{-1/2}\rho_v^{-1/2}\left(\rho_v^{1/2}\rho_u\rho_v^{1/2}\right)^{1/2} = R(\alpha,\hat{\mathbf{n}}). \tag{15}$$

Hence according to equation (4) Uhlmann's parallel transport can be understood as a sequence of Thomas rotations.

For an alternative calculation of the explicit form of $R(\alpha,\hat{\mathbf{n}})$, now we can use the left-hand side of equation (12) and the explicit forms of $\rho_u^{1/2}$ and $\rho_v^{1/2}$ obtained from equation (9) by expressing the hyperbolic functions in terms of $\mathcal{C}_u$, and $\mathcal{C}_v$,

$$\rho_u^{1/2} = \frac{1}{2\sqrt{1+\mathcal{C}_u}}(1 + \mathcal{C}_u + \mathbf{u}\boldsymbol{\sigma}) \qquad \rho_v^{1/2} = \frac{1}{2\sqrt{1+\mathcal{C}_v}}(1 + \mathcal{C}_v + \mathbf{v}\boldsymbol{\sigma}). \tag{16}$$

Collecting everything we get

$$Y_{uv} = R(\alpha,\hat{\mathbf{n}}) = \cos\frac{\alpha}{2}I + \mathrm{i}\sin\frac{\alpha}{2}\hat{\mathbf{n}}\boldsymbol{\sigma} = \frac{[(1+\mathcal{C}_u)(1+\mathcal{C}_v) + \mathbf{uv}]I + \mathrm{i}(\mathbf{u}\times\mathbf{v})\boldsymbol{\sigma}}{\sqrt{[(1+\mathcal{C}_u)(1+\mathcal{C}_v) + \mathbf{uv}]^2 + |\mathbf{u}\times\mathbf{v}|^2}}. \tag{17}$$

(Compare this explicit formula with the implicit one of equation (2) of [9].) From this

$$\tan\frac{\alpha}{2} = \frac{|\mathbf{u}\times\mathbf{v}|}{(1+\mathcal{C}_u)(1+\mathcal{C}_v) + \mathbf{uv}} \qquad \hat{\mathbf{n}} = \frac{\mathbf{u}\times\mathbf{v}}{|\mathbf{u}\times\mathbf{v}|} \tag{18}$$

also showing the independence of the rotation parameters on the direction of $\mathbf{u}$ and $\mathbf{v}$.

Let us now define the Bures distance of two density matrices as $d_B^2(\rho_1, \rho_2) = \inf\{\mathrm{Tr}(W_1 - W_2)(W_1 - W_2)^\dagger\}$, where the infimum is taken over all purifications W_1, W_2 of ρ_1 and ρ_2. Using the results of [9] it can be shown that d_B on $\mathcal{B}$ is related to the Bures fidelity of equation (11) by the formula $d_B^2(\rho_1, \rho_2) = 2 - 2\sqrt{F(\mathbf{u}_1, \mathbf{u}_2)}$, where $\mathbf{u}_{1,2}$ are the Bloch parameters of $\rho_{1,2}$. Moreover, according to [1, 9] Uhlmann's parallel transport is the one occurring along the shortest geodesic with respect to the Bures metric (the Riemannian metric corresponding to the Bures distance), between the two points $\mathbf{u}_1$ and $\mathbf{u}_2$ in the interior of the Bloch ball. Since every smooth curve can be approximated by a sequence of geodesic segments equation (4) can be regarded as such an approximation. According to equation (17) this parallel transport of purifications along a smooth curve in $\mathcal{B}$ can be represented as the path-ordered product of Thomas rotations.

Let us examine expression (17) for the anholonomy transformation matrix. First we introduce a new parametrization

$$\mathbf{a} \equiv \frac{\mathbf{u}}{1+\mathcal{C}_u} = \tanh\frac{\theta_u}{2}\hat{\mathbf{u}} \qquad \mathbf{b} \equiv \frac{\mathbf{v}}{1+\mathcal{C}_v} = \tanh\frac{\theta_v}{2}\hat{\mathbf{v}}. \tag{19}$$

It is clear that $\mathbf{a}$ and $\mathbf{b}$ are still elements of the Bloch ball, they are of the same direction as $\mathbf{u}$ and $\mathbf{v}$ but of different lengths. In terms of these new variables, $R(\alpha, \hat{\mathbf{n}})$ can be written as

$$R(\alpha, \hat{\mathbf{n}}) \equiv R(\mathbf{a}, \mathbf{b}) = \frac{(1+\mathbf{ab})I + \mathrm{i}(\mathbf{a}\times\mathbf{b})\boldsymbol{\sigma}}{\sqrt{1+2\mathbf{ab}+|\mathbf{a}|^2|\mathbf{b}|^2}} \in SU(2) \tag{20}$$

where we have used the formula $|\mathbf{a}\times\mathbf{b}|^2 = |\mathbf{a}|^2|\mathbf{b}|^2 - (\mathbf{ab})^2$. Note that in this notation the Bures fidelity is related to the square of the denominator of this formula via the identity

$$F(\mathbf{u}, \mathbf{v}) = \frac{1}{4}(1+\mathcal{C}_u)(1+\mathcal{C}_v)(1+2\mathbf{ab}+|\mathbf{a}|^2|\mathbf{b}|^2) = 1 - \frac{|\mathbf{a}-\mathbf{b}|^2}{(1+|\mathbf{a}|^2)(1+|\mathbf{b}|^2)}. \tag{21}$$

Here the second equality of equation (21) also reveals the relationship of $0 \leqslant F(\mathbf{u}, \mathbf{v}) < 1$ to the distance on the upper hemisphere of S^3, as can be checked by stereographic projection from the south pole of S^3 to $\mathbf{R}^3$ that maps the upper hemisphere of S^3 to $\mathcal{B}$. An alternative form of (21) is $F(\mathbf{u}, \mathbf{v}) = \cos^2\frac{\Delta}{2}$, where $0 \leqslant \Delta \leqslant \pi$ is the geodesic distance between $\mathbf{a}$ and $\mathbf{b}$ with respect to the metric on $\mathcal{B}$ arising via this stereographic projection.

Let us define the hyperbolic translation [16] of the vector $\mathbf{b}$ by the vector $\mathbf{a}$ as

$$\tau_{\mathbf{a}}(\mathbf{b}) \equiv \frac{(1-|\mathbf{a}|^2)\mathbf{b} + (1+2\mathbf{ab}+|\mathbf{b}|^2)\mathbf{a}}{1+2\mathbf{ab}+|\mathbf{a}|^2|\mathbf{b}|^2}. \tag{22}$$

$\tau_{\mathbf{a}}$ is the composite of two reflections in planes orthogonal to the line $\left(-\frac{\mathbf{a}}{|\mathbf{a}|}, \frac{\mathbf{a}}{|\mathbf{a}|}\right)$. Obviously $\tau_{\mathbf{a}}(\mathbf{0}) = \mathbf{a}$ for all $\mathbf{a} \in \mathcal{B}$, moreover one can show that $\tau_{\mathbf{a}}$ acts as a translation along the aforementioned line [16]. Denoting $\mathbf{a}' \equiv \tau_{\mathbf{a}}(\mathbf{b})$ one can show that $|\mathbf{a}'|^2 = |\mathbf{a}+\mathbf{b}|^2/(1+2\mathbf{ab}+|\mathbf{a}|^2|\mathbf{b}|^2) \leqslant 1$, i.e. this transformation maps $\mathcal{B}$ onto itself. Using this we get $(1+2\mathbf{a}'\mathbf{b}+|\mathbf{a}'|^2|\mathbf{b}|^2)(1+2\mathbf{ab}+|\mathbf{a}|^2|\mathbf{b}|^2) = (1+2\mathbf{ab}+|\mathbf{b}|^2)^2$. Now it is easy to establish the formula

$$R(\mathbf{a}, \mathbf{b}) = R(\tau_{\mathbf{a}}(\mathbf{b}), \mathbf{b}) = R(\mathbf{a}, \tau_{\mathbf{b}}(\mathbf{a})). \tag{23}$$

Equation (23) states the important result that the anholonomy for Uhlmann's parallel transport is invariant with respect to hyperbolic translations of the Bloch ball regarded as the Poincaré ball model of hyperbolic geometry. These properties were called by Ungar [11] 'left-loop' and 'right-loop' properties in his study of density matrices and gyrovector spaces. In this way we established an implementation of his abstract setting up on Uhlmann's parallel transport of purifications. We note in closing that properties (23) can be used to find deformations of curves consisting of geodesic segments having the same anholonomy, a property that can be useful for the experimental verification of Uhlmann parallelism in this most general set-up.

4. Geodesic triangles

In this section we use the results of the previous section to derive an explicit formula for the anholonomy of a special closed path: the geodesic triangle. Note that this problem has already been considered in [8] and [10] for the three points of the triangle lying on a spherical shell of $\mathcal{B}$ of *fixed concurrence*. Here we consider the general case and chose three *arbitrary* points $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ in the interior of the Bloch ball. The corresponding concurrences are $\mathcal{C}_u, \mathcal{C}_v$ and $\mathcal{C}_w$. We renormalize our vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ as in equation (19), the resulting vectors still belonging to $\mathrm{Int}\,\mathcal{B}$ are $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. According to equations (4), (17) and (20) in order to calculate the anholonomy we have to evaluate the quantity

$$\mathcal{R}(\mathbf{a},\mathbf{b},\mathbf{c}) \equiv R(\mathbf{a},\mathbf{c})R(\mathbf{c},\mathbf{b})R(\mathbf{b},\mathbf{a}) = \cos\frac{\delta}{2} + \mathrm{i}\sin\frac{\delta}{2}\mathbf{m}\boldsymbol{\sigma} \tag{24}$$

where the last equality expresses the fact that the resulting matrix should also have an $SU(2)$ form.

By virtue of equations (20), (21) we can extract a factor from $\mathcal{R}(\mathbf{a},\mathbf{b},\mathbf{c})$ of the form $\frac{1}{8}(1+\mathcal{C}_u)(1+\mathcal{C}_v)(1+\mathcal{C}_w)/\sqrt{F(\mathbf{u},\mathbf{v})F(\mathbf{w},\mathbf{v})F(\mathbf{v},\mathbf{u})}$. Hence we merely have to evaluate the matrix

$$J \equiv (I + a\cdot c)(I + c\cdot b)(I + b\cdot a) \qquad \text{where} \quad a\cdot c \equiv (\mathbf{a}\boldsymbol{\sigma})(\mathbf{c}\boldsymbol{\sigma}) = (\mathbf{ac})I + \mathrm{i}(\mathbf{a}\times\mathbf{c})\boldsymbol{\sigma} \quad \text{etc.} \tag{25}$$

A straightforward calculation yields the result

$$\begin{aligned} J = {} & (1 + a^2b^2c^2 + (1+a^2)(\mathbf{bc}) + (1+b^2)(\mathbf{ca}) + (1+c^2)(\mathbf{ab}))I + [c - (\mathbf{ca})a, b - (\mathbf{ab})a] \\ & + \tfrac{1}{2}((1-a^2)[b,c] - (1-b^2)[c,a] - (1-c^2)[a,b]) \end{aligned} \tag{26}$$

where $a \equiv (\mathbf{a}\boldsymbol{\sigma}), a^2 \equiv |\mathbf{a}|^2$ etc, and $[a, c]$ denotes the commutator of the corresponding matrices. By virtue of the relations $a^2 = (1-\mathcal{C}_u)/(1+\mathcal{C}_u)$ etc and definition (11) of the Bures fidelity, we obtain for that part of $\mathcal{R}(\mathbf{a},\mathbf{b},\mathbf{c})$ which is proportional to the identity matrix the formula

$$\cos\frac{\delta}{2} = \frac{F(\mathbf{u},\mathbf{w}) + F(\mathbf{w},\mathbf{v}) + F(\mathbf{v},\mathbf{u}) - 1}{2\sqrt{F(\mathbf{u},\mathbf{w})F(\mathbf{w},\mathbf{v})F(\mathbf{v},\mathbf{u})}}. \tag{27}$$

In order to also find the axis of rotation we introduce the vectors

$$\mathbf{p} \equiv \frac{(1+a^2)\mathbf{c} - (1+2\mathbf{ac} - c^2)\mathbf{a}}{1+2\mathbf{ac}+a^2c^2} \qquad \mathbf{q} \equiv \frac{(1+a^2)\mathbf{b} - (1+2\mathbf{ab} - b^2)\mathbf{a}}{1+2\mathbf{ab}+a^2b^2}. \tag{28}$$

With these vectors it is straightforward to check that

$$\mathcal{R}(\mathbf{a},\mathbf{b},\mathbf{c}) = \frac{(1+\mathbf{pq})I + \mathrm{i}(\mathbf{p}\times\mathbf{q})\boldsymbol{\sigma}}{\sqrt{1+2\mathbf{pq}+p^2q^2}} \tag{29}$$

hence the angle δ and axis $\mathbf{m}$ of the resulting Thomas rotation are given by the expressions

$$\tan\frac{\delta}{2} = \frac{|\mathbf{p}\times\mathbf{q}|}{(1+\mathbf{pq})} \qquad \mathbf{m} = \frac{\mathbf{p}\times\mathbf{q}}{|\mathbf{p}\times\mathbf{q}|}. \tag{30}$$

A comparison of equations (28) and (22) shows that formulae for $\mathbf{p}$ and $\mathbf{q}$ up to some crucial sign changes look like the hyperbolic translates. $\mathbf{p}$ and $\mathbf{q}$ are 'translates' by $-\mathbf{a}$ of $\mathbf{c}$ and $\mathbf{b}$. However, by virtue of the relations $p^2 = |\mathbf{a}-\mathbf{c}|^2/(1+2\mathbf{ac}+a^2c^2)$ and $q^2 = |\mathbf{a}-\mathbf{b}|^2/(1+2\mathbf{ab}+a^2b^2)$, one can see that these 'spherical translates' are not mapping $\mathcal{B}$ (homeomorphic to the upper half of S^3) onto itself. These are rather isometries of the *full* S^3 with its metric given by equation (21).

In order to gain some more insight into the geometric meaning of the (28) 'spherical translate' we note that

$$\frac{\mathbf{p}}{|\mathbf{p}|^2} = \mathbf{a} + \frac{(1+a^2)}{|\mathbf{c}-\mathbf{a}|^2}(\mathbf{c}-\mathbf{a}). \tag{31}$$

Now recall [16] the definition of the transformation $\sigma^r_{\mathbf{a}} : \mathbf{R}^3 \to \mathbf{R}^3$

$$\sigma^r_{\mathbf{a}}(\mathbf{x}) \equiv \mathbf{a} + \frac{r^2}{|\mathbf{x}-\mathbf{a}|^2}(\mathbf{x}-\mathbf{a}) \tag{32}$$

which is the inversion with respect to a sphere S^2 in $\mathbf{R}^3$ centred at $\mathbf{a}$ with radius r. It is now obvious that (31) is an inversion of $\mathbf{c}$ with respect to a sphere centred at $\mathbf{a}$ with radius $r^2 = 1 + a^2$. Moreover, since the transformation $\mathbf{p} \to \mathbf{p}/p^2$ is also an inversion with respect to the sphere centred at the origin with radius 1, we obtain the following result. $\mathbf{p}$ (resp. $\mathbf{q}$) is the result of two inversions applied to the point $\mathbf{c}$ (resp. $\mathbf{b}$). One of the inversions is defined by the point $\mathbf{a}$, the point we have chosen as the starting one for the traversal of the geodesic triangle.

Now let us calculate the geometric phase corresponding to our geodesic triangle! First we note that

$$1 + 2\mathbf{pq} + p^2q^2 = (1+a^2)^2 \frac{1 + 2\mathbf{bc} + b^2c^2}{(1 + 2\mathbf{ab} + a^2b^2)(1 + 2\mathbf{ac} + a^2c^2)}. \tag{33}$$

From equations (5) and (24) we get $\mathrm{Tr}(\mathcal{R}(\mathbf{u}, \mathbf{v}, \mathbf{w})\rho_u) = \cos\frac{\delta}{2} + \mathrm{i}\sin\frac{\delta}{2}(\mathbf{um})$ hence after recalling equations (19), (21), (27)–(30) and (33) straightforward calculation yields the result

$$\nu\,\mathrm{e}^{\mathrm{i}\Phi_g} \equiv \mathrm{Tr}(\mathcal{R}\rho_u) = \frac{F(\mathbf{u}, \mathbf{v}) + F(\mathbf{v}, \mathbf{w}) + F(\mathbf{w}, \mathbf{u}) - 1 - \frac{\mathrm{i}}{2}\mathbf{u}(\mathbf{v}\times\mathbf{w})}{2\sqrt{F(\mathbf{u}, \mathbf{v})F(\mathbf{v}, \mathbf{w})F(\mathbf{w}, \mathbf{u})}}. \tag{34}$$

Hence our formula for the mixed state geometric phase takes the form

$$\tan\Phi_g = -\frac{\frac{1}{2}\mathbf{u}(\mathbf{v}\times\mathbf{w})}{F(\mathbf{u}, \mathbf{v}) + F(\mathbf{v}, \mathbf{w}) + F(\mathbf{w}, \mathbf{u}) - 1}. \tag{35}$$

In the pure state limit we have $\mathcal{C}_u = \mathcal{C}_v = \mathcal{C}_w = 0$. Since the vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ are of unit norm we denote them in this special case as $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{n}_3$. Recalling equation (11) for the Bures fidelity from (35) we obtain the result

$$\tan\Phi_g = -\tan\frac{\Omega}{2} = -\frac{\mathbf{n}_1(\mathbf{n}_2\times\mathbf{n}_3)}{1 + \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 + \mathbf{n}_3\mathbf{n}_1} \tag{36}$$

which is the formula for the tangent of minus half the solid angle [17] corresponding to the geodesic triangle on the surface of the unit sphere S^2, i.e. we have $\Phi_g = -\frac{\Omega}{2}$. Note that a more familiar form for $\frac{\Omega}{2}$ is given by [17]

$$\cos\frac{\Omega}{2} = \frac{\cos^2\frac{\theta_{12}}{2} + \cos^2\frac{\theta_{23}}{2} + \cos^2\frac{\theta_{31}}{2} - 1}{2\frac{\cos\theta_{12}}{2}\frac{\cos\theta_{23}}{2}\frac{\cos\theta_{31}}{2}} = \frac{1 + \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 + \mathbf{n}_3\mathbf{n}_1}{\sqrt{2(1+\mathbf{n}_1\mathbf{n}_2)(1+\mathbf{n}_2\mathbf{n}_3)(1+\mathbf{n}_3\mathbf{n}_1)}} \tag{37}$$

with $\mathbf{n}_i\mathbf{n}_j \equiv \cos\theta_{ij}$. Comparing this with the pure state limit of equation (27) we see that in this case the Thomas rotation angle is just the solid angle, i.e. $\delta = \Omega$. Hence for pure states we get back to the well known results from studies concerning the ordinary geometric phase.

Equation (34) is the most general formula that defines the visibility ν and the Uhlmann mixed state geometric phase Φ_g valid for an *arbitrary* geodesic triangle defined by the points $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ inside the Bloch ball $\mathcal{B}$. The usual geometric phase is obtained in the limiting case of sending all of the points to the boundary of $\mathcal{B}$ representing pure states. As a further investigation of formula (34) let us now consider the important special case studied by

Slater [10] when $|\mathbf{u}| = |\mathbf{v}| = |\mathbf{w}| = r = \text{const}$! Let $\mathbf{u} \equiv r\mathbf{n}_1, \mathbf{v} \equiv r\mathbf{n}_2$ and $\mathbf{w} = r\mathbf{n}_3$, then $F(\mathbf{u}, \mathbf{v}) = 1 + \frac{1}{2}r^2(\mathbf{n}_1\mathbf{n}_2 - 1)$ etc. By virtue of (35), we have the result

$$\tan\Phi_g = -\frac{r^3\mathbf{n}_1(\mathbf{n}_2 \times \mathbf{n}_3)}{4(1-r^2) + r^2(1 + \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 + \mathbf{n}_3\mathbf{n}_1)} = -\frac{r^3\mu}{4(1-r^2) + r^2\mu}\tan\frac{\Omega}{2} \tag{38}$$

where $\mu \equiv 1 + \mathbf{n}_1\mathbf{n}_2 + \mathbf{n}_2\mathbf{n}_3 + \mathbf{n}_3\mathbf{n}_1$, a notation used in [10]. This result is in contrast with the claim of Slater (see, equation, (18) of [10])

$$\tan\Phi_g^{\text{Slater}} = -\frac{r^3\mu}{4 + (\mu - 10)r^2 + 6r^4}\tan\frac{\Omega}{2}. \tag{39}$$

Note that after the replacement $6r^4 \rightarrow 6r^2$ his result would reproduce the correct one of equation (38).

Using ideas of interferometry an alternative definition (different from the one as given by Uhlmann) for the mixed state geometric phase appeared in [5]. In this approach the result for the situation studied above is [5]

$$\tan\Phi_g^{\text{int}} = -r\tan\frac{\Omega}{2}. \tag{40}$$

From equations (38) and (40) we see that the ratio $\tan\Phi_g/\tan\Phi_g^{\text{int}}$ is $r^2\mu/r^2\mu + 4(1-r^2)$ hence the two different types of mixed state phases are equal merely in the pure state ($r = 1$) case. (In [10] it was claimed that the two phases are equal also for the nontrivial case with $r = \sqrt{2/3}$, a possibility clearly follows from the erroneous result of equation (39).) The fact that the two approaches give different results for the mixed state anholonomy was first stressed in [10] and [4].

Before closing this section we check that the formula for the visibility (i.e. the magnitude of the rhs of equation (34)) gives the result $\nu = 1$ in the pure state limit. The visibility is

$$\nu = \sqrt{\frac{(F(\mathbf{u},\mathbf{v}) + F(\mathbf{v},\mathbf{w}) + F(\mathbf{w},\mathbf{u}) - 1)^2 + \frac{1}{4}V^2}{4F(\mathbf{u},\mathbf{v})F(\mathbf{v},\mathbf{w})F(\mathbf{w},\mathbf{u})}} \tag{41}$$

where $V = \mathbf{u}(\mathbf{v} \times \mathbf{w})$ is the volume of the parallelepiped spanned by the triple $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$. In the pure state limit we get

$$\nu = \sqrt{\frac{\mu^2 + V^2}{2(1 + \mathbf{n}_1\mathbf{n}_2)(1 + \mathbf{n}_2\mathbf{n}_3)(1 + \mathbf{n}_3\mathbf{n}_1)}}. \tag{42}$$

Using the first law of cosines [16] $\cos\theta_{12} - \cos\theta_{23}\cos\theta_{31} = \sin\theta_{23}\sin\theta_{31}\cos\gamma$ of spherical trigonometry, where γ is the angle of the spherical triangle at the point defined by $\mathbf{n}_3$, and the relations $\mathbf{n}_i\mathbf{n}_j = \cos\theta_{ij}$ and $\sin\theta_{23}\sin\theta_{31}\sin\gamma = V$, a straightforward calculation yields the expected result $\nu = 1$. Hence, for the mixed state case δ is different from Ω and $\nu \neq 1$ ($\mathbf{um} \neq 1$) properties also shown by analysing the alternative formula $\nu = \sqrt{\cos^2\delta/2 + \sin^2\delta/2(\mathbf{um})^2}$ to be compared for $r =$ constant with formula (26) of [5].

5. Mixed state anholonomy and quaternionic phases

Representing the space of purifications as the space of normalized entangled states in $\mathbf{C}^2 \otimes \mathbf{C}^2$ (see equation (6)), we have the possibility to build up a dictionary between the nomenclatures of the mixed and the pure state anholonomies. In order to do this recall that due to the constraint $\langle\Psi|\Psi\rangle = \operatorname{Tr} WW^\dagger = 1$, the space of such purifications is the seven sphere S^7. Let us parametrize the matrix W of (6) as

$$W = \frac{1}{\sqrt{2}}(Q_0 + \mathrm{i}Q_1) \qquad Q_0 = \alpha_0 I - \mathrm{i}\alpha_j\sigma_j \qquad Q_1 \equiv \beta_0 I - \mathrm{i}\beta_j\sigma_j. \tag{43}$$

(Summation over repeated indices is understood, and $\sigma_j \, j = 1, 2, 3$ are the Pauli matrices.) Note that equation (43) amounts to a change of parametrization from the *four complex* numbers a, b, c, d of equation (6) to the *eight real* ones α_μ and $\beta_\mu \mu = 0, 1, 2, 3$. Explicitly we have

$$a = (\alpha_0 + \beta_3) + \mathrm{i}(\beta_0 - \alpha_3) \qquad b = (\beta_1 - \alpha_2) - \mathrm{i}(\alpha_1 + \beta_2)$$
$$c = (\beta_1 + \alpha_2) - \mathrm{i}(\alpha_1 - \beta_2) \qquad d = (\alpha_0 - \beta_3) + \mathrm{i}(\beta_0 + \alpha_3) \tag{44}$$

and

$$2\alpha_0 = \mathrm{Re}\, a + \mathrm{Re}\, d \quad 2\alpha_1 = -\mathrm{Im}\, b - \mathrm{Im}\, c \qquad 2\alpha_2 = \mathrm{Re}\, c - \mathrm{Re}\, b \quad 2\alpha_3 = \mathrm{Im}\, d - \mathrm{Im}\, a$$
$$2\beta_0 = \mathrm{Im}\, a + \mathrm{Im}\, d \quad 2\beta_1 = \mathrm{Re}\, b + \mathrm{Re}\, c \qquad 2\beta_2 = \mathrm{Im}\, c - \mathrm{Im}\, b \quad 2\beta_3 = \mathrm{Re}\, a - \mathrm{Re}\, d \tag{45}$$

where Re and Im refer to the real and imaginary parts of the corresponding complex numbers. Note moreover that the correspondence

$$\mathbf{i} \leftrightarrow -\mathrm{i}\sigma_1 \qquad \mathbf{j} \leftrightarrow -\mathrm{i}\sigma_2 \qquad \mathbf{k} \leftrightarrow -\mathrm{i}\sigma_3 \tag{46}$$

defines a mapping between a $W \in GL(2, \mathbf{C})$ and a *quaternionic spinor* $(q_0, q_1)^T \in \mathbf{H}^2$, i.e. we have the correspondence

$$W \mapsto \begin{pmatrix} q_0 \\ q_1 \end{pmatrix} \qquad q_0 = \alpha_0 + \alpha_1\mathbf{i} + \alpha_2\mathbf{j} + \alpha_3\mathbf{k} \qquad q_1 = \beta_0 + \beta_1\mathbf{i} + \beta_2\mathbf{j} + \beta_3\mathbf{k}. \tag{47}$$

On the space of two component quaternionic spinors we can define an inner product $\langle | \rangle : \mathbf{H}^2 \times \mathbf{H}^2 \to \mathbf{H}$ as $\langle q|p\rangle \equiv \overline{q_0} p_0 + \overline{q_1} p_1$, i.e. we have quaternionic conjugation in the first factor. From the normalization condition $\mathrm{Tr}\, WW^\dagger = 1$, it follows that $\alpha_\mu\alpha_\mu + \beta_\mu\beta_\mu = 1$, i.e. the spinor $(q_0, q_1)^T$ is normalized, $\|q\|^2 \equiv \langle q|q\rangle = 1$. It means that α_μ and β_μ are Cartesian coordinates for the 7-sphere S^7.

Let us express our reduced density matrix $\rho = \mathrm{Tr}_2|\Psi\rangle\langle\Psi| = WW^\dagger$ in terms of the matrices Q_0 and Q_1 corresponding to the quaternions q_0 and q_1! By virtue of (43) we have

$$\rho = \tfrac{1}{2}\big(Q_0 Q_0^\dagger + Q_1 Q_1^\dagger + \mathrm{i}\big(Q_1 Q_0^\dagger - Q_0 Q_1^\dagger\big)\big) = \tfrac{1}{2}(I + \mathbf{u}\boldsymbol{\sigma}) \tag{48}$$

where we have used the normalization condition and the fact that the matrix $Q_1 Q_0^\dagger - Q_0 Q_1^\dagger$ is an anti-Hermitian 2×2 one, hence it can be expanded as $-\mathrm{i}\sigma_j u_j$, $j = 1, 2, 3$ with u_1, u_2, u_3 are *real* parameters of the one-qubit density matrix. For later use we also define the quantity $u_0 \equiv Q_1 Q_0^\dagger + Q_0 Q_1^\dagger$ which is two times the Hermitian part of $Q_1 Q_0^\dagger$. The Hermitian and anti-Hermitian parts of the matrix $Q_1 Q_0^\dagger$ correspond to the *real* and *imaginary* parts of the corresponding quaternion $q_1\overline{q}_0$ hence we can define the quaternion

$$u \equiv u_0 + u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k} = 2q_1\overline{q_0} \qquad \mathrm{Re}(u) = \tfrac{1}{2}(u + \overline{u}) = u_0 \qquad \mathrm{Im}(u) = \tfrac{1}{2}(u - \overline{u}). \tag{49}$$

Let us define one more quantity

$$u_4 \equiv |q_0|^2 - |q_1|^2 = Q_0 Q_0^\dagger - Q_1 Q_1^\dagger. \tag{50}$$

Recall also from section 3 that the coordinates $u_{\hat\mu}\ \hat\mu = 0, 1, 2, 3, 4$, are related to the complex numbers a, b, c, d as $u_4 + \mathrm{i}u_0 = ad - bc$, $u_1 + \mathrm{i}u_2 = \overline{a}c + \overline{b}d$ and $2u_3 = |a|^2 + |b|^2 - |c|^2 - |d|^2$. Hence the concurrence is just $\mathcal{C} = \sqrt{u_4^2 + u_0^2}$. It is straightforward to check that $\overline{u}u + u_4^2 = u_{\hat{\mu}}u_{\hat{\mu}} = 1$, hence $u_{\hat{\mu}} \in S^4$, i.e. it is an element of the *four-dimensional* sphere. As a result of equations (49), (50) one can define a map $\pi : S^7 \to S^4$. Note that according to the explicit form of this map, the transformation (*right* multiplication of the quaternionic spinor with a *unit* quaternion)

$$\begin{pmatrix} q_0 \\ q_1 \end{pmatrix} \to \begin{pmatrix} q_0 \\ q_1 \end{pmatrix} s \qquad \text{where} \quad \overline{s}s = 1 \tag{51}$$

leaves the coordinates $u_{\hat{\mu}}$ invariant. Since unit quaternions correspond to elements of $SU(2) \sim S^3$ the projection π defines a fibration (the second Hopf fibration [18]) of S^7 with base S^4 and fibre S^3. Reinterpreting our quaternionic spinors as entangled states, it is straightforward to show that this $SU(2)$ fibre degree of freedom corresponds to the possibility of making local unitary transformations $I \otimes S$, $S \in SU(2)$ in the *second* subsystem. This idea of representing entanglement via the twisting of a nontrivial fibre bundle was initiated in [19] and further developed in [20] and [21]. Here we merely need one result from [20]: an element $|q\rangle \in S^7$ can be parametrized by a pair $(|u\rangle, s)$ where $|u\rangle \in S^4$-SP and $s \in S^3$, as

$$|q\rangle = \begin{pmatrix} q_0 \\ q_1 \end{pmatrix} = \frac{1}{\sqrt{2(1+u_4)}} \begin{pmatrix} 1+u_4 \\ u \end{pmatrix} s \equiv |u\rangle s \qquad \overline{s}s = 1 \qquad u_{\hat{\mu}} \in S^4 - \{\mathrm{SP}\}. \tag{52}$$

Here SP refers to the south pole of S^4, hence for a fixed s equation (52) defines a local section of our bundle. There are no global sections (i.e. expressions such as (52) nonsingular over all of S^4) which is just another way of saying that the Hopf bundle is nontrivial, i.e. $S^7 \neq S^4 \times S^3$. Of course, we can define alternative sections that are singular at different points, (52) choice is dictated by convenience.

Consider now three quaternionic spinors $|q\rangle = |u\rangle s$, $|p\rangle = |v\rangle x$ and $|r\rangle = |w\rangle y$, $s, x, y \in SU(2)$ representing entangled states $|\Psi\rangle$, $|\Phi\rangle$ and $|\chi\rangle$! Note that the notation indicates that the corresponding quaternionic spinors are parametrized by the vectors $u_{\hat{\mu}}$, $v_{\hat{\mu}}$ and $w_{\hat{\mu}}$ which are elements of the open neighbourhood $S^4 - \{\mathrm{SP}\}$.

As a next step we consider the trivial subbundle $\mathcal{E}$ of the Hopf bundle defined by the conditions $u_0 = 0$, and $u_4 = \mathcal{C} > 0$. $\mathcal{E}$ is a fibre bundle with an S^3 fibre over the submanifold $\mathcal{M}$ of the upper half hemisphere of S^4 defined by the aforementioned constraints. It is easy to see that $\mathcal{M}$ is topologically the upper half hemisphere of a 3-sphere defined by the coordinates $\mathcal{C}, u_1, u_2, u_3$ and can be identified with the interior of the Bloch ball of reduced density matrices $\mathrm{Int}\,\mathcal{B}$. For more details on the structure of the bundle $\mathcal{E}$ that has already been studied in the context of Uhlmann's connection see [22]. Let us suppose that our spinors $|q\rangle$, $|p\rangle$ and $|r\rangle$ are fixed elements of $\mathcal{E}$. This means that we can set the parameter values $u_0 = v_0 = w_0$ in expressions such as equation (52) to zero, and the ones u_4, v_4, w_4 to $\mathcal{C}_u, \mathcal{C}_v$ and $\mathcal{C}_w$.

It is now straightforward to check that the unit quaternion $\langle v|u\rangle/|\langle v|u\rangle|$ is just Y_{vu} of equation (17). Moreover employing the notation of equation (19), equation (24) can be written in the following form:

$$\mathcal{R}(\mathbf{u}, \mathbf{v}, \mathbf{w}) = s \frac{\langle q|r\rangle}{|\langle q|r\rangle|} \frac{\langle r|p\rangle}{|\langle r|p\rangle|} \frac{\langle p|q\rangle}{|\langle p|q\rangle|} \overline{s} \tag{53}$$

where it is now understood that the left-hand side is also regarded as a unit quaternion.

Note now that equation (52) is just the quaternionic analogue of the polar decomposition. Indeed according to equation (16), the spinor $|u\rangle$ corresponds to the matrix $\rho_u^{1/2}$, and the unit quaternion s to the $SU(2)$ part of the $U(2)$ matrix S of the polar decomposition $W_0 = \rho_u^{1/2} S$. Since $U(2)$ is isomorphic to $U(1) \times SU(2)$ we only have to account for a complex phase, but this is fixed by our choice $u_0 = 0$ when restricting to the subbundle $\mathcal{E}$. (Note that according to equations (6), (7) $u_4 + \mathrm{i}u_0 \equiv \mathcal{C}\mathrm{e}^{\mathrm{i}\kappa} = 2\mathrm{Det}\,W$, where $\tan\kappa = u_0/u_4$. Hence the $u_0 \neq 0$ case amounts to multiplying our (6) entangled state by a $U(1)$ phase.)

Now let us write equation (4) for the geodesic triangle in the following form:

$$W_1 \equiv \Lambda W_0 = \rho_u^{1/2} \mathcal{R}(\mathbf{u}, \mathbf{v}, \mathbf{w}) \rho_u^{-1/2} W_0 \qquad \text{where} \quad \rho_u = W_0 W_0^\dagger. \tag{54}$$

Since the polar decomposition $W_0 = \rho_u^{1/2} S$ corresponds to section (52) of the bundle $\mathcal{E}$, we can write

$$W_1 = \Lambda \rho_u^{1/2} S = \rho_u^{1/2} S S^\dagger \mathcal{R}(\mathbf{u}, \mathbf{v}, \mathbf{w}) S. \tag{55}$$

Using the notation $|q'\rangle$ for the quaternionic representative of W_1, we see that the quaternionic version of equation (55) is $|q'\rangle = |q\rangle \overline{s} \mathcal{R} s$. By virtue of equation (53) Uhlmann's parallel transport in $\mathcal{E}$ in the quaternionic representation can be written as

$$|q'\rangle = |q\rangle \frac{\langle q|r\rangle}{|\langle q|r\rangle|} \frac{\langle r|p\rangle}{|\langle r|p\rangle|} \frac{\langle p|q\rangle}{|\langle p|q\rangle|}. \tag{56}$$

It is clear that for an arbitrary geodesic polygon equation (56) has to be multiplied from the right by extra quaternionic phase factors corresponding to transitions to the new points of the polygon. The geodesic rule obtained in this way is the non-Abelian analogue of the well-known one obtained for filtering measurements in the context of the usual geometric phase [23, 24]. In this picture each polygon Γ is decomposed into a sequence of geodesic triangles. Each triangle Δ_j gives rise to the Thomas rotation of form (24) with angle δ_j and axis $\mathbf{m}_j$. Since Γ in general is not a planar curve the rotations corresponding to different triangles have different axes. As a result the total rotation angle is not the sum of the component rotations as was in the Abelian case corresponding to the ordinary geometric phase. In this more general case we have to combine rotations with different axis resulting in the appearance of a path-ordered product. Going to finer and finer subdivisions any smooth closed curve C can be approximated by a suitable polygon Γ. The resulting quaternionic phase can be written as the path-ordered exponent $\mathcal{P}\,\mathrm{e}^{-\oint_C A}$ where the $su(2)$-valued gauge-field can be written as

$$A = \mathrm{Im}\langle u|du\rangle = \frac{1}{2}\,\mathrm{Im}\,\frac{\overline{u}du}{1+u_4} \qquad u = u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k} \qquad u_4 \equiv \mathcal{C}_u. \tag{57}$$

As was remarked in [20, 22] A is just the pull-back of the restriction of the canonical (instanton) connection on the quaternionic Hopf bundle to the bundle $\mathcal{E}$ with respect to the section $s = 1$ (see equation (52)).

6. Conclusions

In this paper we investigated Uhlmann's parallel transport as applied to a qubit system. In spite of being the simplest and hence best studied example this system still shows nice geometric properties that have not fully been appreciated by the physics community. Our paper was intended to fill in this gap by explicitly working out these missing interesting details. First we have shown that the very special features of the qubit system enable one to reinterpret Uhlmann's parallel transport as a sequence of Thomas rotations. We have also shown some interesting connections with hyperbolic geometry. In particular we proved that the finite Thomas rotations are invariant with respect to hyperbolic translates of the interior of the Bloch ball regarded as the Poincaré model of hyperbolic geometry (see equation (23)). These observations should not come as a surprise since Uhlmann's parallel transport has its origin in the underlying Bures geometry [1] of the Bloch ball $\mathcal{B}$, that has already been related to the Poncaré metric in hyperbolic geometry [13, 20]; moreover it is easy to see [20] that the Bures metric is conformally equivalent to the standard Poincaré one.

In section 4, we derived an explicit formula for the $SU(2)$ anholonomy matrix in the case of a geodesic triangle (equations (28)–(30)). From this, an expression in terms of the Bures fidelities for the mixed state geometric phase and the visibility was derived (equations (35) and (41)). These general results were shown to give back in the pure state limit the corresponding ones known from studies concerning the usual geometric phase. As far as the author knows these formulae in their full generality have not appeared in the literature yet. The geometric significance of these expressions was elaborated, and an error that appeared in [10] was corrected.

In section 5 we managed to reformulate our results concerning the mixed state anholonomy in terms of the pure state *non-Abelian* one. The idea was to reinterpret the space of purifications as the Hilbert space for an entangled two-qubit system. This trick enabled us to recast Uhlmann's parallel transport in yet another form, i.e. in one of a sequence of quaternionic filtering measurements (equation (56)). By going to finer and finer subdivisions we have recovered Uhlmann's parallelism as the Wilson loop over a gauge field which is a suitable restriction of the well-known instanton connection.

The advantage of this quaternionic formalism is clear: Uhlmann's parallel transport for one-qubit density matrices in this representation is just the quaternionic analogue of the usual Pancharatnam transport extensively used in studies concerning the geometric phase [2, 25]. In this language two entangled states $|\Psi\rangle$ and $|\Phi\rangle$ regarded as purifications for one-qubit density matrices are 'in phase' iff their quaternionic representatives $|q\rangle$ and $|p\rangle$ satisfy the constraint: $\langle p|q\rangle$ is real and positive. It is easy to check that this constraint is equivalent to the one as given by equation (1). Moreover, this rule provides a nice way of defining the difference of these entangled states in their local unitary transformations corresponding to the second subsystem. Indeed, consider $|\Psi\rangle$ and $|\Phi\rangle$ as above and define their relative $U(1)$ phase to be the usual Pancharatnam phase factor $\frac{\langle\Phi|\Psi\rangle}{|\langle\Phi|\Psi\rangle|} \in U(1)$. Now define their *relative* $SU(2)$ '(quaternionic) phase' as $\frac{\langle p|q\rangle}{|\langle p|q\rangle|}$. Since $U(2)$ is isomorphic to $U(1) \times SU(2)$ this convention defines a relative $U(2)$ 'phase' for our entangled states. When the entangled states in question have the same reduced density matrices, this $U(2)$ transformation corresponds to the possibility of the observer in the second subsystem to rotate the shared state $|\Psi\rangle$ to $|\Phi\rangle$, via his freedom to employ local unitary transformations. In the general case using this definition we can compare the local unitary transformations (corresponding to the second subsystem) of two entangled states with different reduced density matrices.

It is clear that these results imply many interesting applications. Apart from studying the generalization of our results for nonsingular $n \times n$ density matrices via the use of the anholonomy defined by Uhlmann's connection on the trivial bundle $GL(n, \mathbf{C})/U(n)$, there is also the interesting possibility of studying quantum gates defined by anholonomy transformations over the stratification manifold of entangled qudit systems. Though some of these issues have already been partly discussed [20, 22] we hope to report some new results in a subsequent publication.

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