The geometry of entanglement: metrics, connections and the geometric phase

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Abstract
Using the natural connection equivalent to the $SU(2)$ Yang–Mills instanton
on the quaternionic Hopf fibration of S^7 over the quaternionic projective space
$\mathbf{HP}^1 \simeq S^4$ with an $SU(2) \simeq S^3$ fibre, the geometry of entanglement for two
qubits is investigated. The relationship between base and fibre i.e. the twisting
of the bundle corresponds to the entanglement of the qubits. The measure of
entanglement can be related to the length of the shortest geodesic with respect
to the Mannoury–Fubini–Study metric on $\mathbf{HP}^1$ between an arbitrary entangled
state, and the separable state nearest to it. Using this result, an interpretation
of the standard Schmidt decomposition in geometric terms is given. Schmidt
states are the nearest and furthest separable ones obtained by parallel transport
along the geodesic passing through the entangled state. Some examples
showing the correspondence between the anholonomy of the connection and
entanglement via the geometric phase are shown. Connections with important
notions such as the Bures metric and Uhlmann's connection, the hyperbolic
structure for density matrices and anholonomic quantum computation are also
pointed out.

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1. Introduction

Since the advent of quantum computation, the importance of quantum entanglement cannot
be overestimated. Maximally entangled states have made their debut in physics via Bell-
type inequalities [1] exemplifying measurable differences between classical and quantum
predictions. Recently entangled states have become important via their basic use in quantum
computation processes [2], teleportation [3], dense coding [4] and quantum key distribution
[5]. In the light of such applications it has become evident that quantifying entanglement

and understanding its geometry is a problem of basic importance. Efforts have been made to quantify entanglement by introducing suitable measures for it [6, 7]. These approaches emphasize the difference between entangled and separable states by introducing measures usually related to the entropy of the states [8]. At the same time some authors have pointed out correspondences between the notion of entanglement and the basic geometry of the space of states . The space of states for spin-like systems with the composite Hilbert space $\mathcal{H} \simeq \mathbf{C}^n$ is $\mathbf{CP}^{n-1}$, the $n-1$ dimensional complex projective space. Here the slicing of the space of states for submanifolds of fixed entanglement was introduced and illustrated [9, 10]. It was also shown how algebraic geometric ideas can be used to study two qubit entanglement within the framework of geometric quantum mechanics [11]. Recently in an interesting paper Mosseri and Dandoloff [12] used the quaternionic Hopf fibration to take another look at the problem of characterizing the geometry of two-qubit entanglement. Their results have been generalized to three qubits by using the next Hopf fibration based on octonions [13].

This paper can be regarded as a further development in understanding entanglement in geometric terms. For illustrative purposes we take the simplest two-qubit case and use the convenient quaternionic representation [12] of two-qubit entanglement. In this picture the two-qubit Hilbert space is fibred over the 4-sphere S^4 which is isomorphic to $\mathbf{HP}^1$, the one dimensional quaternionic projective space. This 4-sphere is sliced to submanifolds of fixed entanglement. Our key idea is the observation that the quaternionic Hopf bundle can be equipped with a natural connection enabling a geometric method for comparing states belonging to submanifolds of different entanglement. This connection provides a splitting for vectors corresponding to entangled states to parts representing their horizontal and vertical components. Using this splitting a natural metric (the Mannoury–Fubini–Study metric) is induced on $\mathbf{HP}^1$ which is essentially the standard metric on the 4-sphere S^4 expressed in terms of stereographically projected coordinates. The geodesic distance with respect to this metric provides a natural tool for quantifying entanglement. This simple picture gives a further understanding of the results of Brody and Hughston [11] quantifying entanglement by the geodesic distance between the entangled state in question and the *nearest* separable state with respect to the standard Fubiny–Study metric on $\mathbf{CP}^3$. The important new ingredient of our paper is the possibility of using the non-Abelian geometric phase (the anholonomy of the natural connection) in obtaining a further insight into the geometry of two qubit entanglement. Our approach being interesting in its own right also gives an interesting application of the idea of holonomic quantum computation [14].

The organization of this paper is as follows. In section 2 we briefly summarize some basic background material concerning two-qubit entanglement. In section 3 we reformulate the results of Mosseri *et al* on the Hopf fibration of the two-qubit Hilbert space in a formalism convenient for our purposes. In section 4 we introduce our geometric structures, the connection and the metric. In section 5 using this formalism we show that the geodesic distance between an entangled state Ψ and the nearest separable state is a convenient quantity characterizing entanglement. In fact this quantity is expressed in terms of the concurrence of the entangled state in question. The nearest and furthest separable states obtained by parallel transport with respect to the instanton connection are those appearing in the Schmidt decomposition of Ψ. In section 6 some examples showing the correspondence between the anholonomy of the natural connection, anholonomic quantum computation and entanglement via the geometric phase is shown. In section 7 some connections with important notions such as the Bures metric and Uhlmann's connection for density matrices are also given. We also relate these notions to the hyperbolic structure of the space of reduced density matrices. The conclusions and some comments are given in section 8.

2. Two-qubit entanglement

In this section we summarize well-known results concerning two-particle pure-state entanglement. Although following formulae are valid for wavefunctions of both particles belonging to a finite N dimensional Hilbert space $\mathcal{H}^N$, we have in mind the $N = 2$ case i.e. two qubits. As a starting point we write the two-particle wave function as

$$|\Psi\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha,\beta=0}^{N-1} C_{\alpha\beta}|\alpha\beta\rangle \qquad |\alpha\beta\rangle \equiv |\alpha\rangle_1 \otimes |\beta\rangle_2 \qquad (1)$$

where $|\alpha\rangle_1$ and $|\beta\rangle_2$ are orthonormal bases for subsystems 1 and 2 and $\langle\Psi|\Psi\rangle = 1$. The pure-state density matrix of the total system is $\rho = |\Psi\rangle\langle\Psi|$. The reduced density matrices ρ_1 and ρ_2 characterizing the state of the system available to an observable capable of performing local manipulations merely on subsystem 1 respectively on subsystem 2 are given by the expressions

$$\rho_1 = \text{Tr}_2\rho = \frac{1}{N}CC^\dagger \qquad \rho_2 = \text{Tr}_1\rho = \frac{1}{N}\overline{C^\dagger C} \qquad (2)$$

where it is understood that ρ_1 and ρ_2 are $N \times N$ matrices expressed in the base $|\alpha\rangle_1$ and $|\beta\rangle_2$ respectively. The von Neumann entropy corresponding to the ith subsystem is defined as

$$S_i = -\text{Tr}\rho_i\log_2\rho_i = -\sum_{n,\lambda_n^{(i)}\neq 0} \lambda_n^{(i)}\log_2\lambda_n^{(i)} \qquad i = 1, 2. \qquad (3)$$

Using the fact that $CC^\dagger$ and $C^\dagger C$ are Hermitian matrices having the same real nonzero eigenvalues, one can see that $S_1 = S_2$.

For *maximally entangled states* we have $\rho_1 = \rho_2 = \frac{1}{N}I$ where I is the $N \times N$ identity matrix. In this case from (2) and (3) it follows that $C \in U(N)$ and $S = \log_2 N$, hence in particular for two qubits we have $C \in U(2)$ and $S = 1$. For *separable states* we have $C_{\alpha\beta} = X_\alpha Y_\beta$, hence in this case $|\Psi\rangle$ can be written in the product form $|\psi\rangle \otimes |\varphi\rangle$. One can readily show that $|\Psi\rangle$ is separable if and only if $S = 0$. Since for separable states the matrix C is a dyadic product of two vectors, the partially traced density matrices and C are all of rank 1. For the two-qubit $N = 2$ case it means that $|\Psi\rangle$ is separable if and only if $\det C = 0$. Separable and maximally entangled states are extremal in the sense that they give the minimum and maximum values for the von Neumann entropy. In between these cases lie states of intermediate entanglement characterized by the values $0 < S < \log_2 N$.

It is well known that an arbitrary state $|\Psi\rangle \in \mathcal{H}^N \otimes \mathcal{H}^N$ expressed as in (1) can be transformed to the Schmidt form [15]

$$|\Psi\rangle = \sum_{j=0}^{N-1} \sqrt{\lambda_j}|j\rangle_1 \otimes |j\rangle_2 \qquad (4)$$

by local unitary $U(N) \times U(N)$ transformations acting independently on the two subsystems. The non-negative real numbers λ_j are the eigenvalues of the reduced density matrices, hence they sum to one in accordance with the property $\text{Tr}\rho_{1,2} = 1$. The orthonormal states $|j\rangle_{1,2}$ can be obtained by finding the eigenvectors corresponding to the nonzero eigenvalues of the reduced density matrices $\rho_{1,2}$ whose squares are equal to -1.

Let us give explicit expressions for the $N = 2$ case. We write

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle) \qquad \text{i.e.} \quad C_{\alpha\beta} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \qquad (5)$$

Let us define the complex numbers

$$z \equiv \bar{a}c + \bar{b}d \qquad w \equiv ad - bc \qquad \zeta \equiv \bar{a}b + \bar{c}d. \qquad (6)$$

Then the reduced density matrices are

$$\rho_1 = \frac{1}{2}\begin{pmatrix} |a|^2 + |b|^2 & \bar{z} \\ z & |c|^2 + |d|^2 \end{pmatrix} \qquad \rho_2 = \frac{1}{2}\begin{pmatrix} |a|^2 + |c|^2 & \bar{\zeta} \\ \zeta & |b|^2 + |d|^2 \end{pmatrix}. \tag{7}$$

Due to the normalization condition $\langle\Psi|\Psi\rangle = 1$, we have $\mathrm{Tr}\rho_{1,2} = 1$; moreover, by virtue of (2) $\det\rho_{1,2} = \frac{1}{4}|\det C|^2 = \frac{1}{4}|w|^2$. The magnitude of w is the *concurrence* satisfying the relation $0 \leqslant \mathcal{C} \equiv |w| \leqslant 1$ [7]. It is obvious that for separable states one has $\mathcal{C} = 0$. For maximally entangled states $C \in U(2) \simeq U(1) \times SU(2)$ hence $\mathcal{C} = |\det C| = 1$. The eigenvalues of the reduced density matrices in terms of the concurrence read

$$\lambda_\pm = \tfrac{1}{2}\left(1 \pm \sqrt{1 - \mathcal{C}^2}\right). \tag{8}$$

Using this result it is reasonable to define the entanglement of a two-qubit pure state $|\Psi\rangle$ as its von Neumann entropy [16] i.e.

$$E(\Psi) = -\mathrm{Tr}\rho_1\log_2\rho_1 = -\mathrm{Tr}\rho_2\log_2\rho_2 = -\lambda_+\log_2\lambda_+ - \lambda_-\log_2\lambda_-. \tag{9}$$

Since $\mathcal{C}$ has the same range for its values and is monotonically related to $E(\Psi)$, the concurrence can be regarded as a measure of entanglement in its own right.

Employing *local* $U(2) \times U(2)$ rotations our $|\Psi\rangle$ can be transformed to the Schmidt form (4); i.e. we have

$$|\Psi\rangle = \sum_{j,\alpha,\beta=0,1} \sqrt{\lambda_j}|\alpha\rangle_1 U_{\alpha j} \otimes |\beta\rangle_2 V_{\beta j} \qquad U^\dagger U = V^\dagger V = I \tag{10}$$

where $\lambda_{0,1} = \lambda_{+,-}$. Using this expression one can check that (see also [9])

$$\frac{1}{\sqrt{2}}C = UDV^T \qquad \rho_1 = UD^2U^\dagger \qquad \rho_2 = VD^2V^\dagger \tag{11}$$

where D is the diagonal matrix containing the square root of the eigenvalues $\lambda_\pm$ in its diagonal. Taking the magnitude of the determinant of the expression for C in equation (11) shows that local transformations preserve the concurrence, hence they do not change the degree of entanglement. This observation fulfils our expectations that entanglement can be changed only by *global* (i.e. $U(4)$ transformations).

3. Entanglement and the quaternionic Hopf fibration

According to equation (5) the set of normalized states characterized by the constraint $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 2$ (recall our convention of pulling out a factor of $\frac{1}{\sqrt{2}}$ from the expansion coefficients of $|\Psi\rangle$) is the 7-sphere S^7. The basic observation of [12] is that for understanding the geometry of two-qubit entanglement it is useful to fibre S^7 over the four dimensional sphere S^4 by employing the second Hopf fibration. Moreover, it is convenient to introduce quaternionic notation for our basic quantities since the geometry of this fibration is then easily described. Let us represent an element of S^7 by the quaternionic spinor, i.e. let

$$\frac{1}{\sqrt{2}}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \mapsto \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} \equiv \frac{1}{\sqrt{2}}\begin{pmatrix} a + b\mathbf{j} \\ c + d\mathbf{j} \end{pmatrix}. \tag{12}$$

The quaternionic units $\mathbf{i}, \mathbf{j}$ and $\mathbf{k}$ with squares equal to -1 satisfy the usual relations $\mathbf{ij} = -\mathbf{ji} = \mathbf{k}$ and similar ones obtained by employing cyclic permutations of the symbols $\mathbf{ijk}$. In this way an arbitrary quaternion $q \in \mathbf{H}$ can be expressed as a pair of complex numbers $q = (q_1 + q_2\mathbf{i}) + (q_3 + q_4\mathbf{i})\mathbf{j}$, where the components q_l, $l = 1, 2, 3, 4$, are real numbers. The

conjugate quaternion $\bar{q}$ is obtained by changing the signs in front of the terms containing **i**, **j** and **k**, $\bar{q} = (q_0 - q_1\mathbf{i}) - (q_2 + q_3\mathbf{i})\mathbf{j}$. Recall also that due to the noncommutativity of quaternionic multiplication, we have $\overline{qp} = (\bar{p})(\bar{q})$, and the norm squared of a quaternion q is defined as the real number $|q|^2 = \bar{q}q$. Now we are ready to define the second Hopf fibration by the map π as follows:

$$\pi : S^7 \to S^4 \qquad \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} \mapsto (2u_1\overline{u_0}, |u_0|^2 - |u_1|^2) \equiv (\xi, \xi_0) \qquad (13)$$

where $\xi = (\xi_1 + \xi_2\mathbf{i}) + (\xi_3 + \xi_4\mathbf{i})\mathbf{j}, \xi_\mu\xi_\mu = \xi_0^2 + \bar{\xi}\xi = 1, \mu = 0, 1, \ldots, 4$, are Cartesian coordinates for S^4 (summation for repeated indices is understood). Since $2u_1\bar{u}_0 = (c + d\mathbf{j})\overline{(a + b\mathbf{j})} = (c + d\mathbf{j})(\bar{a} - \mathbf{j}\bar{b}) = z + w\mathbf{j}$, the Cartesian coordinates for S^4 can be expressed in terms of the quantities defined in (6) characterizing two-qubit entanglement, i.e. we have

$$\xi_0 = \pm\sqrt{1 - |z|^2 - |w|^2} \qquad \xi_1 + \xi_2\mathbf{i} = z \qquad \xi_3 + \xi_4\mathbf{i} = w. \qquad (14)$$

The basic result of [12] was that the mapping π is entanglement sensitive. In this formalism this result is easily reproduced by noting that submanifolds of fixed entanglement are characterized by fixed values for the concurrence $\mathcal{C} \equiv \sqrt{|\xi_3|^2 + |\xi_4|^2}$. Hence separable states are mapped to points of S^4 with vanishing values for the coordinates ξ_3 and ξ_4, i.e they are on the 2-sphere $S^2 \subset S^4$ described by the constraint $\xi_0^2 + \xi_1^2 + \xi_2^2 = 1$. For maximally entangled states we have $\mathcal{C} = 1$, then for these states we have $\xi_0 = \xi_1 = \xi_2 = 0$. These states are parametrized by a great circle of the 'equator' (which is a 3-sphere S^3) of S^4.

It is clear from equation (13) that multiplication of the quaternionic spinor from the right by a *unit quaternion q* (i.e. a quaternion with unit norm $|q|^2 \equiv \bar{q}q = 1$) leaves the coordinates ξ_μ invariant. Since quaternions of unit norm ('quaternionic phases') form the group $Sp(1) \simeq SU(2)$, entangled states related by an $SU(2)$ rotation project to states of the same concurrence. This gauge degree of freedom corresponds to the fibre of the second Hopf fibration. Since $SU(2) \simeq S^3$ the fibration π is one with total space S^7, base space S^4 and fibre S^3. The important result of the present paper is that the local gauge transformations of the Hopf fibration associated with this $Sp(1) \simeq SU(2)$ degree of freedom give rise to a geometric interpretation that *local* transformations in the *second* subsystem do not change the entanglement properties of our two-qubit system. The information available for the observer of the *first* subsystem is parametrized by the base space S^4 of the fibration as can be seen from the form (7) of the reduced density matrix ρ_1. By exchanging the parameters b and c in the definition (12), we obtain another representation of the Hopf fibration with Cartesian coordinates η_μ for the corresponding 4-sphere S^4. The assignment in this case reads $\eta = \zeta + w\mathbf{j}$ with ζ defined by equation (6). In this case, as explained in [12], the roles of the two qubits are exchanged.

The relationship between base and fibre (i.e. the twisting of the bundle) is the entanglement of the two qubits. A natural way of describing this twisting is by introducing a connection on our bundle. Luckily for the second Hopf fibration, we have a canonical connection the properties of which have been described in many instances (see e.g. [17, 18]). This connection is equivalent to the instanton connection well known to physicists. Moreover, it can be related to a metric on $\mathbf{HP}^1 \simeq S^4$ which is the quaternionic counterpart of the complex Fubini–Study metric on $\mathbf{CP}^1 \simeq S^2$. Our next task is to describe these quantities, and relate them to our basic quantities in section 2 describing the phenomenon of two-qubit entanglement.

4. Sections, connections and metrics

First for two quaternionic spinors $|v\rangle$ and $|u\rangle$, we introduce the scalar product $\langle v|u\rangle \equiv \bar{v}^\alpha u_\alpha = \bar{v}_0 u_0 + \bar{v}_1 u_1$. Note that *right* multiplication of our spinors with the nonzero quaternion q yields the expression $\langle vq|uq\rangle = \bar{q}\langle v|u\rangle q$. The vector space $\mathbf{H}^2$ of quaternionic spinors with this scalar product is an example of a *quaternionic Hilbert space* (see [18] and references therein). States in quaternionic quantum mechanics based on the space $\mathbf{H}^N$ are represented by points of the quaternionic space of rays which is $\mathbf{HP}^{N-1}$, the $N-1$ dimensional quaternionic projective space. It is amusing to see that the $N = 2$ case of interest for us yields the space $\mathbf{HP}^1 \simeq S^4$, which is the quaternionic analogue of the usual Bloch sphere representation of *complex* spinors, i.e. we have $\mathbf{CP}^1 \simeq S^2$. The complex Bloch sphere is of basic importance for the geometric description of complex superposition, likewise the 'quaternionic Bloch sphere' plays a similar role for the geometrical description of quantum entanglement. Though this correspondence between entanglement and quaternionic quantum mechanics is an interesting idea to follow in its own right, here we work out merely the simplest $N = 2$ case and regard the quaternionic Hilbert space formalism merely as a comfortable representation.

What is interesting for us is that two important geometric quantities can be defined on the space of normalized quaternionic spinors S^7 which pull back naturally to the base space $\mathbf{HP}^1 \simeq S^4$, a metric and a connection. The first of these is related to the transition probability $|\langle v|u\rangle|^2$ and the second is related to the transition amplitude $\langle v|u\rangle$ [18]. Indeed a distance

$$\cos^2 \frac{\Delta_{vu}}{2} = |\langle v|u\rangle|^2 \qquad 0 < \Delta < \pi \tag{15}$$

between two nonidentical, nonorthogonal quaternionic spinors representing entangled states can be defined. It is related to the distance along the geodesic connecting the points $\pi(|v\rangle)$ and $\pi(|u\rangle)$, representing the corresponding states in $\mathbf{HP}^1$, with respect to the metric which is the obvious quaternionic generalization of the well-known Fubini–Study metric. By using local coordinates $x_k, k = 1, 2, 3, 4$, on an open set $\mathcal{U} \subset \mathbf{HP}^1$ parametrizing our spinor $|u\rangle$ and putting $\mathrm{d}l = \Delta$, it is defined by the relation

$$\mathrm{d}l^2 = g_{km}\, \mathrm{d}x^k \otimes \mathrm{d}x^m = 4(1 - |\langle u + \mathrm{d}u|u\rangle|^2). \tag{16}$$

Here it is understood that this equality is valid only up to terms higher than second order in the change of local coordinates.

Moreover, since our entangled states are defined up to right multiplication with a unit quaternion, it would be desirable to define a method for comparing the 'quaternionic phases' of states of different entanglement. For the rule of comparing 'phases' we adopt the definition that two such states are 'in phase' if $\langle u + \mathrm{d}u|u\rangle = 1$ up to second order terms in $\mathrm{d}u$ (the quaternionic analogue of the so-called Pancharatnam connection [18]). By introducing the quantity

$$\Gamma = 1 - \langle u + \mathrm{d}u|u\rangle \tag{17}$$

to be used later, this rule can be restated as $\Gamma = 0$ up to a second order term.

In order to enable an explicit construction we have to choose a section for our bundle. This means that we have to adopt a choice for $|u\rangle \in S^7$ parametrized by points of S^4. If the bundle is nontrivial the best we can do is choose *local sections*. We choose the section

$$|u\rangle = \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \frac{1}{\sqrt{1 + |x|^2}} \begin{pmatrix} 1 \\ x \end{pmatrix} q \tag{18}$$

with $\bar{q}q = 1$. In this parametrization we have $x = u_1(u_0)^{-1}$, hence it is valid on the coordinate patch $\mathcal{U}$ characterized by the constraint $u_0 \neq 0$. Using this section we can pull back the metric (15) and connection (16) to the base space $\mathbf{HP}^1$ yielding the formulae

$$dl^2 = \frac{4 d\bar{x} \, dx}{(1 + |x|^2)^2} \tag{19}$$

$$\Gamma = \bar{q} \left(\frac{\mathrm{Im}\bar{x} \, dx}{1 + |x|^2} \right) q + \bar{q} \, dq. \tag{20}$$

Here $\mathrm{Im}\, q = \frac{1}{2}(q - \bar{q})$ is the imaginary part of an arbitrary quaternion q. (Similarly the real part of q is defined by $\mathrm{Re}\, q = \frac{1}{2}(q + \bar{q})$.) The quantity $A = \mathrm{Im} \frac{\bar{x} dx}{1 + |x|^2}$ is an $sp(1) \simeq su(2)$ valued 1-form (non-Abelian gauge-field) equivalent to the standard $SU(2)$ instanton with self-dual curvature and second Chern number $C_2 = 1$ [17, 18]. Note that according to equation (17), Pancharatnam connection ($\Gamma = 0$) yields a condition for parallel translation of quaternionic phases. Indeed, using equation (20) with a suitable boundary condition we obtain the usual differential equation of parallel transport. For a curve $\mathcal{C}$ lying entirely in $\mathcal{U}$ with initial and end points being $q(0) = 1$ and $q(\tau)$, respectively, we obtain the standard path ordered solution

$$q(\tau) = \mathbf{P} \exp \left(- \int_{\mathcal{C}} A \right). \tag{21}$$

Observe that our coordinates $x = x_1 + x_2 \mathbf{i} + x_3 \mathbf{j} + x_4 \mathbf{k}$ used in section (18) are related to the Cartesian coordinates $\xi = \xi_1 + \xi_2 \mathbf{i} + \xi_2 \mathbf{j} + \xi_4 \mathbf{k}$ and ξ_0 by stereographic projection of the sphere S^4 from its south pole to $\mathbf{R}^4 \cup \{\infty\}$ [18]. It is straightforward to check in these coordinates that $dl^2 = d\xi_0^2 + d\xi_1^2 + d\xi_2^2 + d\xi_3^2 + d\xi_4^2$ is (19). Let us define $R^2 = \xi_0^2 + \xi_1^2 + \xi_2^2$, then we have the relation $0 \leqslant \mathcal{C}^2 = 1 - R^2 \leqslant 1$ where $\mathcal{C}$ is the concurrence. Using R and the polar coordinates (R, Θ, Φ) on the unit ball $\mathbf{B}^3$, originally parametrized by the coordinates (ξ_0, ξ_1, ξ_2), we have

$$dl^2 = \frac{d\mathcal{C}^2}{1 - \mathcal{C}^2} + \mathcal{C}^2 \, d\chi^2 + (1 - \mathcal{C}^2) \, d\Omega = \frac{dR^2}{1 - R^2} + (1 - R^2) \, d\chi^2 + R^2 \, d\Omega^2 \tag{22}$$

where $w = |w| \, e^{\mathrm{i}\arg w} = \mathcal{C} \, e^{\mathrm{i}\chi}$, and $d\Omega = d\Theta^2 + \sin^2 \Theta \, d\Phi^2$. For separable states we have $\mathcal{C} = 0$, hence this line element is reduced to $d\Omega$ the one for the 2-sphere S^2 corresponding to one of our separate qubits in the base. For maximally entangled states we have $R = 0$, then the line element characterizing our base qubit reduces to that of a circle i.e. $dl^2 = d\chi^2$. The other qubit in all cases is associated with the fibre of unit quaternions. The relationship between the two qubits associated with the base and fibre in all cases can be described by parallel transport with respect to the connection Γ. To gain some insight into this relationship as a first step, we have to express the pull-back one form A in terms of our complex coordinates z and w.

For this we combine equations (14) and stereographic projection [18] to see that the quaternionic phase of x (i.e. the unit quaternion $p \equiv \frac{x}{|x|}$) can be expressed as

$$p \equiv \frac{x}{|x|} = \frac{z + w\mathbf{j}}{\sqrt{|z|^2 + |w|^2}} \in Sp(1) \simeq SU(2). \tag{23}$$

Moreover, since the sum of the squared magnitudes of ξ and ξ_0 is equals 1, it is useful to represent them as $\xi = \sin\theta p, \xi_0 = \cos\theta, 0 \leqslant \theta < \pi$. However unlike for the usual parametrization we favour z and w more than θ, hence we express it in terms of these quantities as $\theta = \arcsin\left(\sqrt{|z|^2 + |w|^2}\right)$. In this parametrization the section of equation (18) reads

$$|u\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} p \end{pmatrix} q = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1 \pm \sqrt{1 - |z|^2 - |w|^2}} \\ \sqrt{1 \mp \sqrt{1 - |z|^2 - |w|^2}} \frac{z + w\mathbf{j}}{\sqrt{|z|^2 + |w|^2}} \end{pmatrix} q \tag{24}$$

where $\pm$ ($\mp$) corresponds to sections over the northern or southern hemispheres. Since $p, q \in Sp(1)$ i.e. they are quaternionic phases, the parametrization in terms of θ and the pair (p, q) is

of the same form as the well-known parametrization of a complex spinor associated with the Bloch sphere. However, the second equality also shows the meaning of these parameters in terms of the entanglement parameters. Comparing equation (24) with equation (12) we realize that on the open set $\mathcal{U}$ we can always choose a section for which our parameter b is equals to zero. For later use here we also remark that in this ($b = 0$) parametrization a formula between our complex parameters z, w and ζ of equation (6) holds:

$$\zeta = \frac{1}{2}\left(1 \mp \sqrt{1 - |z|^2 - |w|^2}\right)\frac{w/z}{1 + |w/z|^2} \equiv \sin^2\theta/2 \frac{r}{1 + |r|^2} \qquad r \equiv w/z. \tag{25}$$

Expressing our instanton gauge potential in terms of the complex coordinates z and w, we obtain on $\mathcal{U}$ the expression

$$A = \frac{1}{2}(1 - \cos\theta)\mathrm{Im}(\bar{p}\,\mathrm{d}p) = \frac{\mathrm{Im}(\bar{z}\,\mathrm{d}z + \bar{w}\,\mathrm{d}w + (\bar{z}\,\mathrm{d}w - w\,\mathrm{d}\bar{z})\mathbf{j})}{2\sqrt{1 \pm \sqrt{1 - |z|^2 - |w|^2}}}. \tag{26}$$

We note that for another coordinate patch $\mathcal{V}$ with $u_1 \neq 0$ we would obtain an $Sp(1)$ gauge-transformed expression for A [18]. From equation (26) we see that for separable states ($w = 0$) A defined on the submanifold S^2 (the boundary of the unit ball $\mathbf{B}^3$) of S^4 has the form $A = \frac{1}{2}(1 - \cos\Theta)\,\mathrm{d}\Phi$ where $\Phi \equiv \arg z$, $\cos\Theta = \pm\sqrt{1 - |z|^2}$ which is the $U(1)$ gauge potential of a magnetic monopole with pole strength $\frac{1}{2}$. Hence we see that when moving entirely in the $S^2 \simeq \partial\mathbf{B}^3$ submanifold of separable states, the relationship between the qubit in the base and that in the fibre is characterized merely by the possible occurrence of a $U(1)$ anholonomy factor. For maximally entangled states we have $|w| = 1$ i.e. $w = \mathrm{e}^{\mathrm{i}\chi}$ and $|z| = 0$, hence in this case we have the 1-form $A = -\frac{1}{2}\mathrm{Im}\left(\frac{\mathrm{d}w}{w}\right) = -\frac{1}{2}\mathrm{d}\chi$ living on the great circle of the equator S^3 of S^4. States parametrized by the points of this circle belong to the $Sp(1) \simeq S^3$ fibre. Parallel transporting an element $q \in Sp(1)$ along this circle with respect to this 1-form A yields an anholonomy factor of -1 or $+1$ depending on the winding number of traversals being even or odd. In this way we have obtained an alternative proof of the well-known fact that the manifold of maximally entangled states in $\mathbf{CP}^3$ is $Sp(1)/\mathbf{Z}_2 \simeq S^3/\mathbf{Z}_2$. ($S^7$ is also fibred over $\mathbf{CP}^3$ with the $U(1) \simeq S^1$ fibre corresponding now corresponding to our circle parametrized by the angle χ.) For states of intermediate entanglement labelled by the values of θ in the interval $0 < \theta < \frac{\pi}{2}$ from equation (26) we have a mixing between the complex coordinates z and w. This will result in a more complicated pattern for the anholonomy properties, reflecting the richness of the entanglement possibilities for the qubits. An explicit example for this phenomenon will be given in section 6.

5. The geometrical meaning of the Schmidt decomposition

According to equations (19) and (20) a line element and the pull-back of a connection can be induced on our space S^4 which can be sliced to submanifolds of fixed entanglement. Now we make use of these facts to give geometrical interpretation to the Schmidt decomposition for two qubits. In order to do this we have to characterize a special subclass of geodesics in S^7 that projects to geodesics on S^4. For this we consider a curve $C = |u(s)\rangle \subset S^7$. Using equation (16) for this curve we have $\mathrm{d}l^2 = 4(1 - |\langle u(s + \mathrm{d}s)|u(s)\rangle|^2)$ up to terms second order in $\mathrm{d}s$. Taylor expanding this expression a formula for $\mathrm{d}l^2$ is obtained,

$$\mathrm{d}l^2 = 4\|Q(s)\dot{u}(s)\|^2\,\mathrm{d}s^2 \qquad Q(s) = I - P(s) \quad P(s) = |u(s)\rangle\langle u(s)| \tag{27}$$

where $|\dot{u}(s)\rangle \equiv \frac{\mathrm{d}}{\mathrm{d}s}|u(s)\rangle$. Right multiplication by a unit quaternion $q(s)$ leaves invariant the projector $Q(s)$, but $|\dot{u}(s)\rangle$ transforms to $|\dot{u}(s)\rangle q(s) + |u(s)\rangle\dot{q}(s)$. However, since $Q(s)|u(s)\rangle = 0$ we see that $\mathrm{d}l^2$ is gauge invariant, hence it can be used to define the length of

the 'shadow' curve $\pi(C)$ in S^4 of an arbitrary curve $C \subset S^7$. Moreover, note that expression (27) is also reparametrization invariant. Now we can characterize geodesics in S^4 in the following way. Geodesics in S^4 are those curves $\pi(C)$ through $\pi(|u(s_1)\rangle)$ and $\pi(|u(s_2)\rangle)$ for which the following reparametrization and gauge invariant functional

$$L[C] = 2 \int_{s_1}^{s_2} ds \, \| Q(s)\dot{u}(s) \| \qquad C \subset S^7 \tag{28}$$

is stationary. The variation of a similar functional for the complex case and the derivation of the geodesics was already given in [20]. For the quaternionic case the same steps have to be taken with the important difference that quaternions do not commute, so we have to be careful in grouping terms. However, since the variation $\delta L[C]$ is a real number it can be represented as the integral of the real part of a quaternion depending on s. Luckily we can cyclically permute the quaternionic entries under the operation of taking the real part (it is the operation of taking the trace when we interpret the quaternions as two-by-two matrices) so the derivation is a straightforward exercise of following the steps described in [20, pp 220–3]. The result is the following. Using gauge invariance we can find a solution $|u(s)\rangle$ with initial vector $|u_i\rangle = |u(0)\rangle$ to the geodesic equation on S^7 which is *horizontal* i.e. parallel transported along the geodesic $\pi(|u(s)\rangle)$ with initial point $\pi(|u_i\rangle)$ in S^4. Moreover, exploiting the reparametrization invariance it is *affinely parametrized* i.e. $\|\dot{u}(s)\|$ is constant along $C \subset S^7$. Such affine parametrizations are unique up to linear inhomogeneous changes in s, for convenience we choose the parametrization for which $\| |\dot{u}(s)\rangle \| = \frac{1}{4}$. In particular a geodesic C starting from $|v\rangle$ which is the horizontal lift of the shadow geodesic $\pi(C)$ connecting $\pi(|v\rangle)$ and an other point $\pi(|u\rangle)$ is of the form

$$|u(s)\rangle = \cos\frac{s}{2}|\phi_1\rangle + \sin\frac{s}{2}|\phi_2\rangle \qquad \langle\phi_i|\phi_j\rangle = \delta_{ij} \quad i, j = 1, 2 \tag{29}$$

where

$$|\phi_1\rangle = |v\rangle \qquad |\phi_2\rangle = \left(|u\rangle \frac{\langle u|v\rangle}{|\langle u|v\rangle|} - \cos\frac{\Delta}{2}|v\rangle \right) \Big/ \sin\frac{\Delta}{2} \qquad |\langle u|v\rangle| = \cos\frac{\Delta}{2}. \tag{30}$$

It is now understood that as was claimed in equation (15) Δ is the geodesic distance between the points $\pi(|v\rangle)$ and $\pi(|u\rangle)$.

Having the geodesic distance at our disposal, let us now define the measure of entanglement as the distance between an arbitrary entangled state and the *separable state nearest to it*. This idea has already been proposed and illustrated in [11] and [19]. In [19] for an N dimensional Hilbert space though the maximal violation of generalized Bell inequalities is equal to the Euclidean distance on a suitable real N^2 dimensional Hilbert space between the entangled state and the set of separable states, in this picture no bundle description emerged. We are currently not aware whether a convenient fibre bundle picture can be developed also for this approach. As far as [11] is concerned $\mathbf{CP}^3$ was regarded as the base for an *Abelian* $U(1)$ fibration of S^7, hence this approach provides an alternative parametrization for submanifolds of fixed entanglement, but without any hint where the qubits reside. Here in contrast to [11], we use the Hopf fibration of S^7 with the fibre being the *non-Abelian* group $Sp(1)$ of quaternionic phases making it possible for the two qubits to reside in different spaces, the base and the fibre respectively.

It is instructive to see by giving an alternative proof, how this measure of entanglement is encoded into the structure of the Hopf bundle. In order to do this we choose a representative $|u\rangle$ of our entangled state in the form (24) with $q = 1$ and for the unknown separable state as

$$|v\rangle = \begin{pmatrix} \cos\frac{\sigma}{2} \\ \sin\frac{\sigma}{2}\, e^{i\varphi} \end{pmatrix}. \tag{31}$$

This representative has $b = d = 0$, hence $\mathcal{C} = 0$;, moreover, it is already of the form of our standard section valid on $\mathcal{U}$. We have to find the nearest separable state to $|u\rangle$, which means we have to determine σ and φ as a function of the entanglement coordinates z and w. To achieve this we have to maximize the expression $\cos^2 \Delta_{vu}/2 = |\langle v|u\rangle|^2$. A short calculation yields for this quantity the expression

$$|\langle v|u\rangle|^2 = \cos^2\frac{\Delta}{2} = \cos^2\frac{\sigma}{2}\cos^2\frac{\theta}{2} + \sin^2\frac{\sigma}{2}\sin^2\frac{\theta}{2} + \frac{1}{2}\sin\sigma\,\mathrm{Re}(\mathrm{e}^{-\mathrm{i}\varphi}(z + w\mathbf{j})). \tag{32}$$

Since our sections are merely local ones living on $\mathcal{U}$ we should exclude the south pole ($\sigma = \theta = \pi$), hence we have $0 < \theta < \pi$ and $0 < \sigma < \pi$. For these values (32) is maximal if $\varphi = \arg z$. In this case we are left with the expression $\cos^2\frac{\sigma}{2}\cos^2\frac{\theta}{2} + \sin^2\frac{\sigma}{2}\sin^2\frac{\theta}{2} + \frac{1}{2}|z|\sin\sigma$ to be maximized with respect to changes in σ. As one can check this quantity is maximal provided $\tan\sigma = \frac{|z|}{\cos\theta}$. Hence separable states $|v\rangle$ nearest to our entangled state $|u\rangle$ labelled by the complex numbers z and w are characterized by the angles

$$\cos\sigma = \pm\sqrt{1 - \frac{|z|^2}{1 - |w|^2}} \qquad \varphi = \arg z. \tag{33}$$

Using these angles in equation (32) we obtain for the distance Δ_{uv} the important formula

$$\cos^2\frac{\Delta_{uv}}{2} = \frac{1}{2}\left(1 + \sqrt{1 - \mathcal{C}^2}\right). \tag{34}$$

Comparing our result with equation (8) we see that the value appearing in (34) is precisely the eigenvalue λ_+ of the reduced density matrix also appearing in the Schmidt decomposition. Moreover, it is easy to see that the distance of our $|u\rangle$ from the state $|v'\rangle$ orthogonal to $|v\rangle$ (this state is antipodal to $|v\rangle$ in S^4) is related to the other eigenvalue λ_-. Hence the (9) von Neumann entropy as a measure of entanglement is a special combination of lengths for the shorter and the longer segments of the geodesic linking our entangled state $\pi(|u\rangle)$ to the surface $S^2 \subset S^4$ of separable states.

What is the meaning of the separable state $|v\rangle$ nearest to the entangled state $|u\rangle$? It is the quaternionic representative of one of the states $|j\rangle_1$ ($j = 0, 1$) in the Schmidt decomposition (10). For proof we have to diagonalize the reduced density matrices ρ_1 and ρ_2 of equation (7). We write these matrices in the form $\rho_1 = \frac{1}{2}(I + \mathbf{v}\boldsymbol{\sigma})$ and $\rho_2 = \frac{1}{2}(I + \mathbf{t}\boldsymbol{\sigma})$ where

$$\mathbf{v} = \begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \end{pmatrix} = |\mathbf{v}| \begin{pmatrix} \cos\sigma \\ \sin\sigma\cos\varphi \\ \sin\sigma\sin\varphi \end{pmatrix} \qquad \mathbf{t} = \begin{pmatrix} \eta_0 \\ \eta_1 \\ \eta_2 \end{pmatrix} = |\mathbf{t}| \begin{pmatrix} \cos\tau \\ \sin\tau\cos\epsilon \\ \sin\tau\sin\epsilon \end{pmatrix}. \tag{35}$$

σ and φ turn out to be precisely the quantities of (33), and τ and ϵ are defined by replacing in (33) the coordinate z by ζ of equation (6). To check this note that $\mathbf{v}$ and $\mathbf{t}$ are elements of the unit ball $\mathbf{B}^3$ i.e. we have $|\mathbf{v}| = |\mathbf{t}| = \sqrt{1 - |w|^2} \leqslant 1$, and $\xi_0 = \cos\theta = \pm\sqrt{1 - |z|^2 - |w|^2}$. In order to diagonalize the reduced density matrices we have to diagonalize $\mathbf{v}\boldsymbol{\sigma}$ and $\mathbf{t}\boldsymbol{\sigma}$. It is well known that there is no global only local diagonalization of this problem over $\mathbf{B}^3$. The reason for this is the fact that the eigenstates of these operators form a nontrivial fibration over $\mathbf{B}^3$ related to the first (complex) Hopf fibration. Eigensections of ρ_1 and ρ_2 corresponding to the eigenvalue λ_+ of (8) that are singular on the $-\xi_0$ and $-\eta_0$ axes are of the form

$$|\mathbf{v}\rangle = \begin{pmatrix} \cos\frac{\sigma}{2} \\ \sin\frac{\sigma}{2}\,\mathrm{e}^{\mathrm{i}\varphi} \end{pmatrix} \qquad |\mathbf{t}\rangle = \begin{pmatrix} \cos\frac{\tau}{2} \\ \sin\frac{\tau}{2}\,\mathrm{e}^{\mathrm{i}\epsilon} \end{pmatrix}. \tag{36}$$

For the eigensections belonging to the eigenvalue λ_-, we have

$$|\mathbf{v}^\perp\rangle = \begin{pmatrix} -\sin\frac{\sigma}{2}\,\mathrm{e}^{-\mathrm{i}\varphi} \\ \cos\frac{\sigma}{2} \end{pmatrix} \qquad |\mathbf{t}^\perp\rangle = \begin{pmatrix} -\sin\frac{\tau}{2}\,\mathrm{e}^{-\mathrm{i}\varphi} \\ \cos\frac{\tau}{2} \end{pmatrix}. \tag{37}$$

Looking at equation (36) we immediately see that the first vector $|\mathbf{v}\rangle$ regarded as a quaternion is precisely $|v\rangle$ nearest to $|u\rangle$.

What is the meaning of $|\mathbf{t}\rangle$ the Schmidt vector representing one of the orthonormal vectors $|j\rangle_2$ ($j = 0, 1$) used for the other qubit? In the quaternionic notation we know that this vector resides in the fibre of the Hopf fibration, hence we should be able to recover it from the holonomy of our connection. In the following we will show that the representative of $|\mathbf{t}\rangle$ is the unit quaternion Q obtained by parallel transporting our entangled vector $|u\rangle \in S^7$ with respect to the instanton connection along the geodesic segment between $\pi(|u\rangle)$ and $\pi(|v\rangle)$ representing the closest separable state.

In order to verify this we represent our entangled state in the form (24) with $q = 1$, hence its matrix $\frac{C}{\sqrt{2}}$ and the diagonal matrix D of equation (11) have the following form:

$$\frac{C}{\sqrt{2}} = \begin{pmatrix} \cos \frac{\theta}{2} & 0 \\ \sin \frac{\theta}{2} \frac{z}{\sqrt{|z|^2+|w|^2}} & \sin \frac{\theta}{2} \frac{w}{\sqrt{|z|^2+|w|^2}} \end{pmatrix} \qquad D = \begin{pmatrix} \cos \frac{\Delta}{2} & 0 \\ 0 & \sin \frac{\Delta}{2} \end{pmatrix}. \tag{38}$$

Likewise using the unitary matrices U and V diagonalizing on $\mathcal{U}$, the reduced density matrices ρ_1 and ρ_2 are obtained by putting the orthogonal pairs of vectors of equations (36) and (37) columnwise in two 2×2 matrices. Putting these matrices in the first of equation (11), we obtain the relations

$$\sin \frac{\tau}{2} e^{i\epsilon} = \frac{\sin \frac{\sigma}{2} \sin \frac{\theta}{2}}{\cos \frac{\Delta}{2}} \frac{|w/z|}{\sqrt{1+|w/z|^2}} e^{\arg w/z} \tag{39}$$

and

$$\cos \frac{\tau}{2} = \frac{\cos \frac{\sigma}{2} \cos \frac{\theta}{2}}{\cos \frac{\Delta}{2}} + \frac{\sin \frac{\sigma}{2} \sin \frac{\theta}{2}}{\cos \frac{\Delta}{2}} \frac{1}{\sqrt{1+|w/z|^2}}. \tag{40}$$

to be used later. A quick check for the phase of (39) is given by relation (25) giving $\epsilon \equiv \arg \zeta = \arg w/z$.

Let $|v\rangle$ be the (31) separable state a representative of the states over $\pi(|v\rangle)$! We know that the point $\pi(|v\rangle)$ is the nearest to $\pi(|u\rangle)$. Consider now the unique horizontal geodesic (29) passing through the antipodal separable states $|v\rangle$ and $|v'\rangle$ where the states $|\Phi_1\rangle = |v\rangle$ and $|\Phi_2\rangle = |v'\rangle$ are defined by equation (30). This horizontal geodesic in S^7 also passes through the state $|u\rangle \frac{\langle u|v\rangle}{|\langle u|v\rangle|}$ which, apart from a quaternionic phase, is our entangled state we have started with. Explicitly we have the relation

$$|u\rangle \frac{\langle u|v\rangle}{|\langle u|v\rangle|} = \cos \frac{\Delta}{2} |v\rangle + \sin \frac{\Delta}{2} |v'\rangle. \tag{41}$$

Multiplying this equation from the right by the quaternionic phase $\frac{\langle v|u\rangle}{|\langle v|u\rangle|}$, and noting that $\cos \frac{\Delta}{2}$ and $\sin \frac{\Delta}{2}$ are the square roots of the eigenvalues of the reduced density matrices, we obtain a form which looks like the quaternionic version of the Schmidt decomposition

$$|u\rangle = \sqrt{\lambda_+} |v\rangle Q + \sqrt{\lambda_-} |v^\perp\rangle P \qquad Q \equiv \frac{\langle v|u\rangle}{|\langle v|u\rangle|} \tag{42}$$

where P is the quaternionic phase transforming $|v'\rangle$ to $|v^\perp\rangle$ having the standard form (37). In order to show that it is indeed the Schmidt decomposition we have to show that the quaternionic phase Q somehow represents the other qubit in the Schmidt decomposition belonging to the fibre. In other words we have to show that the vector $|\mathbf{t}\rangle$ of (36) corresponds to Q. Using the definition (42) for Q, sections (24) and (31) with $q = 1$ and relations (39) and (40), one readily obtains

$$Q = \frac{\cos \frac{\sigma}{2} \cos \frac{\theta}{2}}{\cos \frac{\Delta}{2}} + \frac{\sin \frac{\sigma}{2} \sin \frac{\theta}{2}}{\cos \frac{\Delta}{2}} \frac{1 + (w/z)\mathbf{j}}{\sqrt{1+|w/z|^2}} = \cos \frac{\tau}{2} + \sin \frac{\tau}{2} e^{i\epsilon} \mathbf{j}. \tag{43}$$

Since according to [12] a generic state $|\psi_Q\rangle$ in the fibre is defined as $Q \equiv |\psi_Q\rangle = c_0|0\rangle_Q + c_1|1\rangle_Q$ where the orthogonal states $|0\rangle_Q$ and $|1\rangle_Q$ are related to the choice $Q = 1$ and $Q = \mathbf{j}$ respectively, the correspondence between Q and $|\mathbf{t}\rangle$ is established. Alternatively the reader can check by calculating $|v\rangle Q$ and then identifying the parameters a, b, c, d using (12) and (5) that this quaternionic spinor represents the separable state $|\mathbf{v}\rangle \otimes |\mathbf{t}\rangle$.

Based on these considerations we have the following geometrical representation of the Schmidt decomposition for two qubits. Choose first a special entangled state represented by a quaternionic spinor in the standard form (i.e. by putting $q = 1$ in equation (24) and call this $|u\rangle$. This state is represented by a point $\hat{u} \equiv \pi(|u\rangle)$ in $\mathbf{HP}^1 \sim S^4$. Find the point $\hat{v}$ in the separable submanifold $S^2 \subset S^4$ nearest to $\hat{u}$ connected by the unique geodesic segment. (If $|u\rangle$ is not maximally entangled then we have a unique solution.) As a next step parallel transport $|u\rangle$ along this geodesic with respect to the instanton connection to the fibre over $\hat{v}$. Then one pair from the biorthogonal Schmidt states is recovered as the standard (i.e. of the (31) form) section $|v\rangle$ over $\hat{v}$ and as the quaternionic phase Q between this section and the state obtained by parallel transport. The real expansion coefficient multiplying this pair forming the separable state $|v\rangle Q$ is $\cos \frac{\Delta}{2}$ where Δ is the geodesic distance between $\hat{u}$ and $\hat{v}$. Repeat the same process for the antipodal point $\hat{v}^\perp$ of $\hat{v}$ in S^4 to obtain the the other pair of Schmidt states with expansion coefficient being the corresponding geodesic distance.

If we use the Hopf fibration with the first qubit belonging to the base and the second belonging to the fibre the gauge degree of freedom is manifested in the freedom for the choice of the unitary matrix V in equation (11). This corresponds to a different choice for the local base belonging to the second qubit. In our representation for an *arbitrary* entangled state, this means that we have a quaternionic spinor $|u\rangle$ this time with some fixed $q \neq 1$. Of course this new choice will not change our geometric interpretation of the Schmidt decomposition. It is easy to see that the new state representing the first qubit in the Schmidt decomposition is the same, and the second is obtained from Q by right multiplication by q. Hence we have proved that the Schmidt decomposition for two qubits is amenable for a nice geometric interpretation in terms of the anholonomy of the canonical connection on the Hopf fibration. Instantons were originally introduced as classical solutions of $SU(2)$ gauge theories in Wick rotated space time. They also play an important role in quantum field theories describing tunnelling between different vacua. It is amusing to find them here as the basic entities describing a fundamental aspect of quantum theory—two qubit entanglement.

6. Geometric phases

We have seen that the instanton connection on the Hopf fibration plays a vital role for the geometrical description of entanglement for two qubits. A further interesting possibility for exploring is to look at the non-Abelian (an)holonomy of the instanton connection, and reinterpret the results in the language of entanglement. For this purpose we have to somehow generate closed curves in the base manifold S^4 and calculate the quaternionic phases picked up by an initial quaternionic spinor after completing a circuit. Reinterpreting these spinors as entangled states the result of this non-Abelian parallel transport will be some final entangled state with very different form but *the same concurrence*. For different loops we obtain different anholonomy matrices, that can serve as quantum gates. This process is called anholonomic quantum computation [14].

However, S^4 is sliced to submanifolds of fixed entanglement, and we know that for separable states the anholonomy of the connection is Abelian. Therefore interesting curves generating non-Abelian anholonomy are those not restricted to the S^2 submanifold with concurrence $\mathcal{C} = 0$. Moreover, form expression (26) of A we see that the states characterized

by the condition $|z| = 0$ describe another 2-sphere $S^2 \subset S^4$, with another monopole-like gauge field on it. According to [12] states with $|z| = 0$ are those with trivial Schmidt decomposition. For curves lying in the submanifold of these states the holonomy is again Abelian.

Let us suppose then that we have a curve C lying entirely in $\mathcal{U} \subset S^4$ not belonging to any of the submanifolds described above. In this case we have to calculate the quaternionic phase $q[C]$ as given by the formula

$$q[C] = \mathbf{P} \, e^{-\oint_C \mathcal{A}}. \tag{44}$$

A more manageable form for $q[C]$ can be given by dividing the loop C into N segments characterized by the N points $\xi_0, \xi_1, \ldots, \xi_N = \xi_0 \in \mathcal{U} \subset S^4$. Each of these points represents a whole family of gauge equivalent entangled states. Let $P_n \equiv P(\xi_n) = |u(\xi_n)\rangle\langle u(\xi_n)|$ be the projectors corresponding to the spinors $|u_n\rangle \equiv |u(\xi_n)\rangle$. By using $\langle u(\xi_{n+1})|u(\xi_n)\rangle \sim I - A(\xi_n) + \cdots$ one can show that [21]

$$|u(\xi_0)\rangle \mathbf{P} \, e^{-\oint_C A} = \lim_{N \to \infty} P(\xi_N) P(\xi_{N-1}) \cdots P(\xi_1) |u(\xi_0)\rangle. \tag{45}$$

Now in order to describe curves in S^4 we have to characterize a one-parameter family of rank 1 quaternionic projectors $P(t)$. These are 2×2 quaternion-Hermitian matrices consisting of a single dyadic product of quaternionic spinors. It is easy to see that such projectors are of the form

$$P(t) = \tfrac{1}{2}(I + \Gamma_\mu \xi_\mu(t)) \tag{46}$$

where $\xi_\mu \in S^4$ and the 2×2 quaternion-Hermitian matrices Γ_μ, $\mu = 0, \ldots, 4$, are defined as

$$\Gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \Gamma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \Gamma_{2,3,4} = \begin{pmatrix} 0 & -\mathbf{i}, \mathbf{j}, \mathbf{k} \\ \mathbf{i}, \mathbf{j}, \mathbf{k} & 0 \end{pmatrix}. \tag{47}$$

To see this note that $\{\Gamma_\mu, \Gamma_\nu\} = 2I\delta_{\mu\nu}$, hence $P^2 = P$ and then check that $\langle u|\Gamma_\mu|u\rangle = \xi_\mu$ which is another way of describing the quaternionic Hopf fibration (13).

We know that the anholonomy of the instanton connection representing the parallel transport of entangled states is described by equation (45) with $P(\xi)$ given by (46). However, it is desirable to simplify (45) by restricting our attention to a subclass of curves of the form $P(t) = U(t)PU^\dagger(t)$, where P is a fixed projector representing the initial entangled state in S^4. $U(t)$ is a one-parameter family of 2×2 quaternion unitary matrices, i.e. $U(t) \in Sp(2) \simeq Spin(5)$ ($Spin(5)/\mathbf{Z}_2 \sim SO(5)$). Such matrices are generated by quaternion skew-Hermitian matrices S in the form $U(t) = e^{tS}$, where S can be expressed in terms of the generators of $Spin(5)$ as $S = \alpha_{\mu\nu} S_{\mu\nu}$ with $S_{\mu\nu} = \tfrac{1}{4}[\Gamma_\mu, \Gamma_\nu]$ and $\alpha_{\mu\nu} = -\alpha_{\nu\mu}$ are real parameters. For a closed loop we should have $P(2\pi) = P(0)$.

Now suppose we have an initial entangled state $|u\rangle \in S^7$ corresponding to the projector $P = |u\rangle\langle u|$ and a closed loop $P(t) = U(t)PU^\dagger(t)$ satisfying $P(2\pi) = P(0) = P$. This loop is defined by some choice for the real parameters $\alpha_{\mu\nu}$. Then we have the formula (proposition 7.4 of [22])

$$\lim_{N \to \infty} P(\xi_N) P(\xi_{N-1}) \cdots P(\xi_1) P = e^{tS} \left(\cos(t\|PSP\|) P - \frac{\sin(t\|PSP\|)}{\|PSP\|} PSP \right) \tag{48}$$

where $P = P(\xi_0)$, and the quaternionic matrix norm is $\|B\|^2 = \mathrm{Tr}_{\mathbf{H}}(B^\dagger B)$. Using this result we obtain our final formula

$$|u\rangle \mathbf{P} \, e^{-\oint_C A} = e^{tS} \left(\cos(t\|PSP\|) - \frac{\sin(t\|PSP\|)}{\|PSP\|} PS \right) |u\rangle \tag{49}$$

where $|u\rangle \equiv |u(\xi_0)\rangle$ is the quaternionic spinor representing our initial entangled state.

As an explicit example, we take

$$S = \tfrac{1}{2}\Gamma_1(\cos\kappa\,\Gamma_3 - \sin\kappa\,\Gamma_4) = \tfrac{1}{4}\alpha_{\mu\nu}[\Gamma_\mu, \Gamma_\nu] \qquad 0 \leqslant \kappa \leqslant 2\pi \tag{50}$$

which means the real parameters are chosen as $\alpha_{13} = \cos\kappa$ and $\alpha_{14} = -\sin\kappa$. One can check that $4S^2 = -I$, hence $U(t) = e^{tS} = \cos(t/2) + \sin(t/2)2S$. Using this we have $U(2\pi) = -I$ which means $P(2\pi) = P(0)$ for any initial projector. Hence for changing values for κ we obtain a parametrized family of loops C_κ.

Let us choose the initial state to be the maximally entangled Bell state,

$$|u\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathbf{j} \end{pmatrix} \mapsto |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |0\rangle_2 + |1\rangle_1 \otimes |1\rangle_2\right). \tag{51}$$

Since this vector is the eigenvector of the matrix Γ_3, the initial projector is $P = P(\xi_0) = \tfrac{1}{2}(I + \Gamma_3)$. This means that the initial vector $\xi_0 \in S^4$ for our loop C_κ has components $\xi_{0\mu} = (0, 0, 0, 1, 0)$. Straightforward calculation shows that

$$PSP = -\frac{1}{4}\sin\kappa\begin{pmatrix} \mathbf{k} & \mathbf{i} \\ \mathbf{i} & -\mathbf{k} \end{pmatrix} \qquad \|PSP\| = \frac{1}{2}\sin\kappa. \tag{52}$$

Putting these results into equation (49), we get the result

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathbf{j} \end{pmatrix}\mathbf{P}\,e^{-\oint_C A} = -\begin{pmatrix} \cos(\pi\sin\kappa) & \mathbf{i}\sin(\pi\sin\kappa) \\ \mathbf{i}\sin(\pi\sin\kappa) & \cos(\pi\sin\kappa) \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathbf{j} \end{pmatrix}. \tag{53}$$

Hence after parallel transporting the Bell state $|u\rangle$ along C, it will pick up a quaternionic phase of the form

$$q[C] = \mathbf{P}\,e^{-\oint_C A} = -\cos(\pi\sin\kappa) - \sin(\pi\sin\kappa)\mathbf{k}. \tag{54}$$

From this equation and definition (12) one can read off the complex coefficients identifying the new entangled state. These are $a = d = -\cos(\pi\sin\kappa)$ and $b = c = -\mathrm{i}\sin(\pi\sin\kappa)$. Since $\mathcal{C} = |ad - bc| = 1$ we see that the anholonomy for our families of closed loops C_κ does not change the degree of entanglement. This is not surprising since, as the reader can check, the $SU(2) \sim Sp(1)$ anholonomy transformations associated with an arbitrary loop C belong to the local transformations manipulating only the second qubit. For the choice $\kappa = \frac{\pi}{6}$ we have $q[C] = -\mathbf{k}$. In this case the new state is

$$|u\rangle q[C] = -\frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{k} \\ \mathbf{i} \end{pmatrix} \mapsto |\psi'\rangle = -\frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |1\rangle_2 + |1\rangle_1 \otimes |0\rangle_2\right) \tag{55}$$

hence for the loop $C_{\pi/6}$ we obtain another Bell state up to a sign.

We have not clarified the nature of our loops C_κ, $0 \leqslant \kappa \leqslant 2\pi$, yet. Using the explicit form of our $U(t)$ straightforward calculation shows that the family of curves C_κ in S^4 is given by

$$\xi_\mu(t; \kappa) = \begin{pmatrix} 0 \\ \sin t \cos\kappa \\ 0 \\ \cos^2\frac{t}{2} - \sin^2\frac{t}{2}\cos 2\kappa \\ \sin^2\frac{t}{2}\sin 2\kappa \end{pmatrix}. \tag{56}$$

Noting that $\xi_0 = 0$ we see that our family of loops lies in the equator of S^4 which is a 3-sphere S^3. Moreover, recalling equation (14) we see that $z(t; \kappa) = \sin t \cos\kappa$ and $w(t; \kappa) = \cos^2\frac{t}{2} - \sin^2\frac{t}{2}e^{-2\mathrm{i}\kappa}$. Using $\mathcal{C} = |w|$ the concurrence as a function of t and κ can be determined,

$$\mathcal{C} = \sqrt{\tfrac{1}{2}(1 + \cos^2 t - \sin^2 t \cos 2\kappa)}. \tag{57}$$

We see that the loops visit submanifolds of different entanglement, except for the case $\kappa = \frac{\pi}{2}$, $z = 0$ when the loop degenerates to the starting point. It can be understood as follows. Our $U(t)$ is an element of the subgroup $Spin(4) \subset Spin(5) \simeq Sp(2)$. $Spin(4)/\mathbf{Z}_2 \simeq SO(4)$ is the four dimensional rotation group. The terms $\Gamma_1\Gamma_3$ and $\Gamma_1\Gamma_4$ in (50) generate $SO(4)$ rotations in the 13 and 14 planes respectively. Clearly for $\kappa = \frac{\pi}{2}$ we have merely 14 rotations that do not change the $\xi_3 = w = 1$ constraint characterizing our initial Bell state. On the other hand for $\kappa = 0$ we have 13 rotations. In this case we have $z(t) = \sin t$ and $w(t) = \cos t$, hence $\mathcal{C} = |\cos t|$. This loop starting from the maximally entangled submanifold then crosses the separable surface at $t = \frac{\pi}{2}$ meeting the maximally entangled surface again at $t = \pi$ and gets back to the separable surface at $t = \frac{3\pi}{2}$ and then to the initial state at $t = 2\pi$. The anholonomy matrix for this curve from (53) is $-I$ reproducing the sign change of quaternionic spinors under a 2π rotation. For the case $\kappa = \frac{\pi}{6}$ studied in equation (55) we get for the concurrence $\mathcal{C} = \frac{1}{2}\sqrt{3 + \cos^2 t}$ along the loop.

Since $S^4 \simeq SO(5)/SO(4)$ (i.e. $SO(5)$ acts transitively on S^4) we can also consider more general loops generated by $SO(5)$ rotations. Such loops are generated by an S also containing terms of the form $\alpha_{0l}\Gamma_0\Gamma_k$, $k = 1, 2, 3, 4$. There is also the possibility of considering loops generated by ordinary $SO(3)$ rotations. However, the structure of $SO(3)$ orbits on S^4 is more complicated. For the details of these orbits see [23]. It is now clear that using an explicit form for S and employing formula (48) one can calculate the anholonomy of an arbitrary entangled state represented by a fixed projector P for loops regarded as $SO(n)$ orbits ($n = 3, 4, 5$) of the form $P(t) = U(t)PU^\dagger(t)$.

It is obvious that if we have a way of generating a prescribed set of closed loops on $\mathbf{HP}^1 \simeq S^4$ through an entangled state of fixed concurrence, we can associate with this loop an $SU(2)$ anholonomy matrix. Moreover, this correspondence between loops and anholonomy matrices can be useful in building one-qubit gates in the spirit of anholonomic quantum computation [14]. Due to the geometric nature of these gates, quantum information processing is expected to be fault tolerant. With this possibility in sight the question arises: how to generate loops on $\mathbf{HP}^1$? The first possibility is the case of adiabatic evolution. For this, one can consider the parametrized family of 2×2 quaternion-Hermitian Hamiltonians $H(\xi) = \Gamma_\mu\xi_\mu$ reinterpreted as 4×4 complex-Hermitian Hamiltonians with two Kramers degenerate doublets [24]. Note, however, that unlike in [24] now we have to regard $H(\xi)$ as a parametrized family of Hamiltonians coupling two qubits. In this picture we can view the entangled states as a parametrized family of eigenstates (eigensections) of these Hamiltonians.

In order to be more explicit we write $H(\xi)$ in the form

$$H(X) = X_{mn}J_mJ_n = \Gamma_\mu\xi_\mu \qquad \mu = 0, 1, \ldots, 4 \quad m, n = 1, 2, 3 \tag{58}$$

where

$$X_{mn} = \frac{1}{\sqrt{3}}\begin{pmatrix} -\xi_1 + \frac{1}{\sqrt{3}}\xi_0 & -\xi_2 & -\xi_3 \\ -\xi_2 & \xi_1 + \frac{1}{\sqrt{3}}\xi_0 & \xi_4 \\ -\xi_3 & \xi_4 & -\frac{2}{\sqrt{3}}\xi_0 \end{pmatrix} \tag{59}$$

and J_m are generators of an $so(3)$ algebra. In this way we have made a mapping from S^4 to the space of real traceless symmetric 3×3 matrices satisfying $\frac{3}{2}\mathrm{Tr}X^2 = 1$ i.e. to the space of unit quadrupoles. $H(X)$ are precisely the quadrupole Hamiltonians studied by Avron *et al* in [24]. However, now these Hamiltonians have a different interpretation. We are not regarding these operators as describing a spin $\frac{3}{2}$ particle in an adiabatically changing quadrupole electric field with the underlying Hilbert space being $\mathbf{C}^4$. We rather regard them as a parametrized set of coupling Hamiltonians for two qubits with Hilbert space $\mathbf{C}^2 \times \mathbf{C}^2$. This correspondence provides a nice formalism to label entangled states with the eigenstates

of quadrupole Hamiltonians. For example separable states ($\xi_3 = \xi_4 = 0$) are represented with a block diagonal quadrupole. Maximally entangled states are those with a complementary structure for X_{mn}, i.e. $\xi_0 = \xi_1 = \xi_2 = 0$. The Bell state of (51) is represented by the quadrupole with the only nonvanishing components $X_{13} = X_{31} = -1/\sqrt{3}$.

Now we fix a unit quadrupole representing an entangled state. Changing the quadrupole components (i.e. the coupling between the two subsystems) we adiabatically trace out a loop C in S^4. Thanks to the adiabatic theorem [22] the time dependent Schrödinger equation maps an initial eigenstate onto an instantaneous eigenstate of the quadrupole Hamiltonian, hence this state evolves along an open curve in S^7 whose shadow in S^4 is C. The difference between the initial and final states in S^7 is an $SU(2)$ matrix (an $Sp(1)$ quaternionic phase) containing a dynamic and a geometric part. The geometric part in this case can be separated—it is precisely the anholonomy matrix corresponding to the operation of our quantum gate. In this way we have implemented quantum computation via quantum adiabatic evolution in the slowly changing environment of unit quadrupoles.

The other possibility for realizing closed curves on $\mathbf{HP}^1$ is by the non-Abelian version of the Aharonov–Anandan phase [25]. In this case the assumption of adiabaticity is relaxed, by introducing cyclic solutions of the time dependent Schrödinger equation. These are such solutions of the Schrödinger equation in S^7 whose shadow curves are closed in $\mathbf{HP}^1$. (In this case the solution curve is *not* an eigenstate of the instantaneous Hamiltonian.) In order to obtain an example of a cyclic evolution process in the quaternionic representation we have to find a 2×2 quaternion unitary matrix $U(t)$ and a $T \in \mathbf{R}$ for which we have $U(T)|u(0)\rangle = |u(0)\rangle p$, $p \in Sp(1)$. We can specify such a $U(t)$ by giving its quaternion skew-Hermitian generator S. A nice example of this kind is given by the choice

$$S(t) = \tfrac{1}{4}[H(X(t)), H(\dot{X}(t))] = \tfrac{1}{4}[H(\eta(t)), H(\dot{\eta}(t))] = \tfrac{1}{4}[\Gamma_\mu, \Gamma_\nu]\eta_\mu(t)\dot{\eta}_\nu(t) \qquad (60)$$

for an $\eta_\mu(t)$ defining a closed loop ($\eta_\mu(T) = \eta_\mu(0)$) in *another 4 sphere* S^4_η. Hence $U(t)$ is a $Sp(2) \simeq Spin(5)$ rotation of the form $U(t) = e^{S(t)}$ with $\alpha_{\mu\nu}(t) \equiv \eta_{[\mu}(t)\dot{\eta}_{\nu]}(t)$. It is important not to mix the 4-sphere S^4_η defining the parameters of the $Spin(5)$ rotation with the other 4-sphere $\mathbf{HP}^1 \simeq S^4$ the 'space of states' for the entangled two qubits stratified into submanifolds of fixed entanglement. We can of course identify the parameters of S^4_η with the space of unit quadrupoles (this is reflected in the first equality in (60)), but then the relationship between the quadrupole components and the coordinates of $\mathbf{HP}^1$ is not canonical as was in the case of adiabatic evolution.

It is easy to show that the time evolution operator along the curve C' in S^7 is precisely the operator of parallel transport along $\pi(C') = C \subset \mathcal{U} \subset \mathbf{HP}^1$ i.e. we have [18]

$$\mathbf{P}\,e^{-\int_{C'} S(t)dt}|u(0)\rangle = \lim_{n \to \infty} P(T)P\left(\frac{n-1}{n}T\right)\cdots P\left(\frac{2}{n}T\right)P\left(\frac{1}{n}T\right)|u(0)\rangle \qquad (61)$$

where $P(t)$ is the projector belonging to the quadrupole operator $H(\eta(t)) = H(X(t)) = \Gamma_\mu\eta_\mu(t)$ (the relationship between X_{mn} and η_μ is of the same form as in (59)). Note, however, that unlike in the adiabatic case $|u(0)\rangle$ is *not* an eigenvector of the instantaneous Hamiltonian corresponding to $S(t)$. The evolution is nonadiabatic and cyclic. Since the dynamical phase [18] is the integral of $\langle u(t)|S(t)|u(t)\rangle \equiv 0$ where $|u(t)\rangle$ are the instantaneous eigenstates of $H(t)$, the anholonomy of the evolution is purely geometric. Hence we see that quadrupole-like Hamiltonians are capable of generating closed curves via the standard Schrödinger type of evolution (both adiabatic and nonadiabatic) in the stratification manifold of two qubits, enabling an implementation for anholonomic quantum computation. In this picture the quantum gates of this computation are represented by anholonomy transformations of the instanton connection our basic entity governing the entanglement properties of two qubits.

7. Density matrices

We have seen that the base space of our fibration is S^4 which is parametrized by the reduced density matrix ρ_1 of equation (7). In this section we want to make this statement more precise. As is well known, the space of density matrices is the three dimensional unit ball $\mathbf{B}^3$. The relationship between $\mathbf{B}^3$ and S^4 is clarified by equation (22) which shows that the line element on S^4 is a combination of a line element on $\mathbf{B}^3$ of the form

$$4\mathrm{d}l_B^2 = \frac{\mathrm{d}\mathcal{C}^2}{1 - \mathcal{C}^2} + (1 - \mathcal{C}^2)\,\mathrm{d}\Omega \tag{62}$$

and the line element of a circle $S_{\mathcal{C}}^1$, $\mathrm{d}l_{S_{\mathcal{C}}^1}^2 = \mathcal{C}^2\,\mathrm{d}\chi^2$ with its radius parametrized by the value of the concurrence $\mathcal{C}$. The line element in (62) is that corresponding to the Bures metric [26] on the space of density matrices defined by

$$d_B(\rho, \omega) = \sqrt{2 - 2\mathrm{Tr}(\omega^{1/2}\rho\omega^{1/2})^{1/2}} \tag{63}$$

where ρ and ω are density matrices. Indeed, by restricting our attention to 2×2 density matrices, for the infinitesimal form of (63) we obtain the relation [27]

$$\mathrm{d}l_B^2 = \tfrac{1}{2}\mathrm{Tr}(\mathrm{d}\rho\,\mathrm{d}\rho) + \mathrm{d}(\det\rho)^{1/2}\,\mathrm{d}(\det\rho)^{1/2}. \tag{64}$$

Parametrizing ρ as in the first expressions preceding (35) and recalling that $\det\rho = \mathcal{C}^2/4$ we obtain (62). Hence the line element on S^4 is of the form $\mathrm{d}l^2 = 4\,\mathrm{d}l_B^2 + \mathcal{C}^2\,\mathrm{d}\chi^2$.

The space of 2×2 density matrices $\mathcal{D}_2$ is stratified into the submanifold of rank 1 density matrices $\mathcal{D}_2(1) \simeq \partial\mathbf{B}^3 \simeq S^2$, and the submanifold of rank 2 density matrices $\mathcal{D}_2(2) \simeq \mathrm{int}\,\mathbf{B}^3$. We realize that rank 1 density matrices correspond to separable states with $\mathcal{C} = 0$, and rank 2 density matrices correspond to the entangled states with $\mathcal{C} > 0$.

Having clarified the correspondence between reduced density matrices and the base space, we now turn to total space S^7 of the Hopf bundle. S^7 can be regarded as the space of purifications for the reduced density matrix ρ_1. The structure of these purifications was studied in [28]. Here we use these results to give some new insight into the geometry of two-qubit entanglement.

Let us denote by $\mathcal{M}_2$ the space of complex 2×2 matrices with elements $\Lambda \in \mathcal{M}_2$ satisfying the constraint $\mathrm{Tr}\,\Lambda\Lambda^\dagger = 1$. It is clear that in our case $\Lambda = \frac{1}{\sqrt{2}}C$ of equation (1), moreover due to normalization $\mathcal{M}_2 \simeq S^7$. Then the mapping $f : \Lambda \in \mathcal{M}_2 \mapsto \rho_1 = \Lambda\Lambda^\dagger \in \mathcal{D}_2$ defines a stratification (see also equation (2)). This stratification is the union of fibre bundles

$$\mathcal{M}_2 = \bigcup_k \mathcal{M}_2(k) \to \mathcal{D}_2 = \bigcup_k \mathcal{D}_2(k) \qquad k = 1, 2 \tag{65}$$

where $\mathcal{M}_2(k)$ denotes the manifold of rank k matrices in $\mathcal{M}_2$.

For the nonsingular case $\det\Lambda = \frac{1}{2}\det C = \frac{1}{2}w \neq 0$. Write $w = |w|\,\mathrm{e}^{\mathrm{i}\chi} = \mathcal{C}\,\mathrm{e}^{\mathrm{i}\chi}$. Since the quantity $\Lambda\Lambda^\dagger$ is invariant with respect to right multiplication by an element of $U(2)$ (the unitary V of equation (11)) the mapping $f_2 : \mathcal{M}_2(2) \to \mathcal{D}_2(2)$ is a principal bundle with $U(2)$ fibre. There is a subbundle $\mathcal{B}_2$ of this bundle defined by the constraint $\chi \equiv 0$, i.e. $\det\Lambda \in \mathbf{R}_+$. As one can check $\mathcal{B}_2$ is an $SU(2) \simeq Sp(1)$ bundle over $\mathrm{int}\,\mathbf{B}^3$. This bundle will turn out to be important in the following considerations.

For the singular case it was proved in [28] that we have $\mathcal{M}_2(1) \simeq S^3 \times_{U(1)} S^3$, hence we have an embedding of the complex Hopf bundle into $\mathcal{M}_2(1)$. This is the precise mathematical statement of the observation in [12] that in this case the quaternionic Hopf fibration can be 'iterated' to include the complex Hopf fibration. Moreover, in the light of this result it is not surprising that we have obtained in section 4 the magnetic monopole connection (the canonical connection on the complex Hopf bundle) on this stratum.

An interesting topic to discuss here is the relationship between Uhlmann's connection for parallel transport for mixed states [29] and our connection governing the entanglement properties of our qubits. Uhlmann introduced 'amplitudes' of density matrices. In our case these are the matrices Λ_1 and Λ_2 purifying two different nonsingular reduced density matrices ρ and ω. It is understood that ρ and ω correspond to the reduced density matrices of two different entangled states with coordinates $z_{1,2}, w_{1,2}$ and concurrences $\mathcal{C}_{1,2} \neq 0$. This means that we have $\rho = \Lambda_1 \Lambda_1^\dagger = \frac{1}{2} C_1 C_1^\dagger$ and $\omega = \Lambda_2 \Lambda_2^\dagger = \frac{1}{2} C_2 C_2^\dagger$. According to Uhlmann, two such amplitudes are parallel iff $C_1^\dagger C_2 = C_2^\dagger C_1 > 0$. It was also shown that on $\mathcal{M}_2(2)$ this parallel transport law is implemented by a connection form $\mathcal{A}$ satisfying $C^\dagger \, \mathrm{d}C - \mathrm{d}C^\dagger C = C^\dagger C \mathcal{A} + \mathcal{A} C^\dagger C$. Now we take the trace of this expression and then use the identity $MN + NM = \mathrm{Tr}(M)N + M\mathrm{Tr}(N) + (\mathrm{Tr}(MN) - \mathrm{Tr}(M)\mathrm{Tr}(N))$ valid for our 2×2 complex matrices to get

$$\mathcal{A} = \tfrac{1}{2}(C^\dagger \, \mathrm{d}C - \mathrm{d}C^\dagger C) - \tfrac{1}{4}\mathrm{Tr}(C^\dagger \, \mathrm{d}C - \mathrm{d}C^\dagger C). \tag{66}$$

Here we have taken into account $\mathrm{Tr}(C^\dagger C) = 2$ and the restriction $\mathrm{Tr}(\mathcal{A}) = 0$ which is valid on the subbundle $\mathcal{B}_2$ [28]. Now writing $A = \mathrm{Im}\langle u| \, \mathrm{d}u\rangle$ as a pure imaginary quaternion-valued 1-form in the quaternionic notation of (12) and $\mathcal{A}$ as an $su(2)$ valued 1-form in the complex notation for C as given by (5), one can see that the two connections coincide [28]. It is important to stress once again that $\mathcal{A} = A$ only for entangled states lying in the subbundle with $\chi = \arg w = 0$. For such states the line element of the metric on S^4 is the Bures line element, so the identification of the relevant connections is not surprising. Since the connections for this class of entangled states coincide, so does the anholonomy properties of entangled states parallel transported in the subbundle $\mathcal{B}_2$ of $\mathcal{M}_2(2)$. Using the results of the previous section we can generate curves in the space of reduced density matrices and calculate the anholonomy of the entangled states regarded now as purifications lying in $\mathcal{B}_2$. In this way in the context of two-qubit entanglement we managed to find a nice application for Uhlmann's parallel transport for density matrices.

In the following we would like to make some comments on the conformal structure of our metric on S^4. Let us consider first the line element $\mathrm{d}l_B^2$ associated with the Bures metric. Use the notation $R^2 = \xi_0^2 + \xi_1^2 + \xi_2^2 = 1 - \mathcal{C}^2$ and introduce the new coordinate $-\infty \leqslant \beta \leqslant \infty$ via the relation $R \equiv \tanh \beta$. Since $-1 \leqslant R \leqslant 1$ this is a good parametrization for R. Note that β behaves as the rapidity parameter in the special theory of relativity. For $\beta = 0$ we obtain maximally entangled states and for $\beta = \pm\infty$ we get the separable states. It is straightforward to check that using this new parametrization the Bures line element takes the following form: $4\mathrm{d}l_B^2 = \cosh^{-2}\beta(\mathrm{d}\beta^2 + \sinh^2\beta \, \mathrm{d}\Omega)$. Since the line element $\mathrm{d}l_{\mathbf{H}^3}^2 = \mathrm{d}\beta^2 + \sinh^2\beta \, \mathrm{d}\Omega$ is the line element on the upper sheet of the double sheeted hyperboloid $\mathbf{H}^3$, we can conclude that the Bures metric is conformally equivalent to the standard metric of hyperbolic geometry. The hyperboloid $\mathbf{H}^3$ can be stereographically projected to the Poincaré ball $\mathbf{B}^3$ with the standard Poincaré metric on it. Since the space of 2×2 density matrices is $\mathbf{B}^3$, the Bures metric is, up to a conformal factor, the Poincaré metric. Hence the space of density matrices can be given a hyperbolic structure. In this hyperbolic structure separable states are infinitely far away (i.e. on the boundary $\partial\mathbf{B}^3$) from the maximally entangled ones. This observation has already been made in a different context by Ungar in his study of gyrovector spaces and the geometry of 2×2 density matrices [30]. We can take one more step by realizing that the line element (22) for the 4-sphere can also be given a conformal form after noting that $(1 - R^2) \, \mathrm{d}\chi^2 = \mathrm{d}\chi^2 / \cosh \beta$ i.e. we have $\mathrm{d}l^2 = \cosh^{-2}\beta(\mathrm{d}\beta^2 + \sinh^2\beta \, \mathrm{d}\Omega + \mathrm{d}\chi^2)$. This means that conformally we have $S^4 \simeq \mathrm{int}\,\mathbf{B}^3 \times S^1$. Note that for this conformal equivalence we had to remove the boundary of $\mathbf{B}^3$ i.e. the separable states.

Concluding this section as an interesting application of these ideas, we calculate the geodesic distance between two entangled states $|\Psi\rangle$ and $|\Phi\rangle$ represented by the quaternionic spinors $|u\rangle$ and $|v\rangle$. These spinors map to points ξ_μ and η_ν $\mu, \nu = 0, 1, \ldots, 4$ of S^4 via the projection of the Hopf fibration. The first three components of the vectors ξ_μ and η_ν are denoted by the vectors $\mathbf{u}$ and $\mathbf{v}$. We relate as usual the remaining components to the concurrences as $\xi_3 + \mathbf{i}\xi_4 = \mathcal{C}_1 \, e^{i\chi_1}$ and $\eta_3 + \mathbf{i}\eta_4 = \mathcal{C}_2 \, e^{i\chi_2}$. We denote the reduced density matrices corresponding to $|u\rangle$ and $|v\rangle$ by ϱ and ω. Then the transition probability related to the geodesic distance (18) between our entangled states is given by the formula

$$|\langle u|v\rangle|^2 = \mathrm{Tr}_{\mathbf{H}}(P_u P_v) = \tfrac{1}{2}(1 + \xi_\mu \eta_\mu) = \tfrac{1}{2}(1 + \mathbf{uv} + \mathcal{C}_1\mathcal{C}_2 \cos(\chi_1 - \chi_2)). \quad (67)$$

For the subbundle $\mathcal{B}_2$ this is the Bures fidelity [28] $[\mathrm{Tr}(\omega^{1/2}\varrho\omega^{1/2})^{1/2}]^2$ occurring in the Bures distance (63). In terms of the rapidities $\beta_{\mathbf{u}}$ and $\beta_{\mathbf{v}}$ after introducing the Lorentz factors $\gamma_{\mathbf{u},\mathbf{v}} = \cosh\beta_{\mathbf{u},\mathbf{v}} = 1/\sqrt{1 - |\mathbf{u}, \mathbf{v}|^2}$, we can rewrite this as

$$\cos\frac{\Delta_{uv}}{2} = |\langle u|v\rangle|^2 = \frac{1}{2\gamma_{\mathbf{u}}\gamma_{\mathbf{v}}}(\gamma_{\mathbf{t}} + \cos(\chi_1 - \chi_2)) \qquad \gamma_{\mathbf{t}} \equiv \gamma_{\mathbf{u}}\gamma_{\mathbf{v}}(1 + \mathbf{uv}) \qquad (68)$$

where $\gamma_{\mathbf{t}}$ is obtained by the addition law of velocities for $\mathbf{u}$ and $\mathbf{v}$ in special relativity (the cosine theorem of hyperbolic geometry [30]). As a special case for the subbundle $\mathcal{B}_2$ and for states with $\chi_1 = \chi_2$, we obtain the formula of [32] for the Bures fidelity amenable for a nice interpretation in hyperbolic trigonometry.

8. Conclusions

In this paper we related the basic quantities of two-qubit entanglement to the geometrical structure of the quaternionic Hopf fibration. The entangled state was represented by an element of the bundle space S^7. One of our qubits was associated with the base (S^4) and the other with the fibre (S^3) of this fibration. The nontriviality of the fibration i.e. the twisting of the bundle has been connected with the entanglement of the qubits via the use of the canonical connection and the natural metric on S^7. These quantities pull back via the use of sections to the base giving rise to the instanton gauge field with self-dual curvature, and the Mannoury–Fubini–Study metric.

The base space can be stratified to submanifolds of fixed entanglement. Separable states occupy a 2-sphere S^2, and maximally entangled states occupy a great circle S^1 of the equator of $\mathbf{HP}^1 \simeq S^4$. The complement of separable states in the base can be conformally represented as int $\mathbf{B}^3 \times S^1$. Here int $\mathbf{B}^3$ is the space of rank 2-reduced density matrices. The measure of entanglement was defined as the length of the shortest geodesic with respect to the Mannoury–Fubini–Study metric between the entangled state in question and the nearest separable state. This nearest separabe state expressed in the form of the standard section is one of the Schmidt states appearing in the Schmidt decomposition of the entangled state. The other Schmidt state is reproduced from the quaternionic phase between this separable state and the one obtained by parallel transport along the shortest geodesic from our initial entangled state. The other pair of Schmidt states is obtained by a similar procedure carried out by using the longer part of the geodesic, and the corresponding states.

We examined the anholonomy properties realized by quaternionic geometric phases for the two-qubit entangled states. We have shown that for quadrupole-like Hamiltonians we can generate closed curves using the standard Schrödinger type of evolutions (both adiabatic and nonadiabatic) in the stratification manifold of two qubits. These evolutions enable an implementation for anholonomic quantum computation. For a specific family of curves we explicitly constructed the anholonomy transformations corresponding to a special class of quantum gates.

By looking at the total space S^7 of our fibration as the space of purifications for our reduced density matrices, we have started working out a dictionary between the non-Abelian $SU(2)$ geometric phase governing the entanglement of our qubits and Uhlmann's law of parallel transport for purifications over the manifold of density matrices. The space of such purifications forms a stratification, i.e. a collection of fibre bundles. These bundles provide the natural geometrical setting for a deeper understanding of the results of [12]. We have shown how the Bures distance between reduced density matrices is related to the geodesic distance between entangled states. We have also reformulated the known relationship between the instanton connection and Uhlmann's connection from the viewpoint of two-qubit entanglement. Based on the results of Ungar *et al* we made connection with the geometric data of the Hopf fibration, entanglement and the hyperbolic geometry of the space of reduced density matrices.

It would be interesting to see whether the usefulness of quaternions is merely a specific property of two-qubit entanglement or it can be generalized for other entangled quantum systems. In the context of quaternionic quantum mechanics, or merely as a convenient representation we can consider the higher quaternionic Hopf fibrations $\pi : S^{4n+3} \to \mathbf{HP}^n$ with again an $Sp(1)$ fibre. The connection and metric used here can be generalized and have already been discussed elsewhere [18]. In this case one can use $n + 1$ component quaternionic vectors somehow representing entangled states. However, the structure of these bundles should be only capable of incorporating the twisting of merely one qubit (belonging to the fibre) with respect to another (possibly also entangled) state represented by the base degree of freedom. The other possibility to utilize the nontrivial fibre bundle structure as a geometric representation for quantum entanglement is to consider spin bundles, based on higher dimensional Clifford algebras. In particular the 2^n dimensional spin bundles over $2n$ dimensional spheres seem to be promising. For the $n = 2$ case we get essentially the Hopf fibration. For the general case the fibre is $SU(2^{n-1})$, and the tensor product structure of higher dimensional Γ matrices hints at a possible use for understanding a special subclass of entangled systems in the language of higher dimensional monopoles as connections on such bundles. Apart from the fact whether these expectations are realized or not, we hope that we have convinced the reader that the quaternionic Hopf fibration with its instanton connection is tailor-made to unveil the basic structure of two-qubit entanglement.

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