J. Phys. A: Math. Gen. 22 (1989) 3167-3170. Printed in the UK

COMMENT

Quantum statistical holonomy

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Received 16 January 1989

Abstract. A (faithful) density matrix can be represented by a Hilbert–Schmidt operator up to composition with a unitary operator. This ambiguity can be described in terms of a principal fibre bundle which is a modification of a construction by Uhlmann. The HS norm provides a real metric which determines a natural connection via the Kaluza–Klein mechanism. We compute the curvature and show that at the boundary its holonomy reproduces the Berry phase for (pure) non-degenerate states and the non-Abelian holonomy of Wilczek and Zee for k-fold degenerate states.

The Berry phase [1], by now confirmed by several experiments [2], has a beautiful geometric interpretation. It is best described as a holonomy of a natural connection on the 'tautological' line bundle over the projective Hilbert space $P(H)$ (for non-degenerate states) or on the Stieffel bundle of k-frames over the Grassmannian of k-planes in H (for k-fold degeneracy) [3–5]. Recently Uhlmann [6] proposed to unify them and also include the density matrices $S=\{\rho|\mathrm{Tr}\,\rho<\infty,\ \rho\geqslant 0\}$, i.e. mixed states on the algebra of bounded operators in H. An important geometric ingredient there is the space of Hilbert–Schmidt operators J_2, together with the map $\pi: A\rightarrow AA^+$ onto S. As it stands, this is not a bundle (the fibres are not isomorphic) but there is some geometry behind it and the aim of this comment is to exhibit this geometry. We shall do this by cutting down π and obtaining a principal fibre bundle B with the structure group $\mathrm{U}(H)$ (unitary operators) over a subspace $\underline{S}\subset S$, which is dense in S. It turns out that B has a natural metric which provides a principal connection on B via the Kaluza–Klein mechanism. The related parallel transport coincides with Uhlmann's 'parallel amplitudes'.

The group $\mathrm{U}(H)$ acts on J_2 by right multiplication in a fibre-preserving way since $\mathrm{AU(AU)^+ = AA^+}$. However, this action is neither free nor transitive. To overcome this difficulty, we define B as the subset of J_2 consisting of operators with a trivial kernel. The image $\pi(B)=\underline{S}$ consists then of strictly positive density matrices, i.e. those which have no zero eigenvalues. Thus, among other things, we delete one-dimensional projectors (pure states on the boundary of S) as well as finite-dimensional projectors. But $\underline{S}$ is dense in S since we can always make $\rho=\Sigma\,\rho_n P_n$ invertible by adding a suitable perturbation, for instance $\rho_\varepsilon=\rho+\Sigma\,\varepsilon^n P'_n$, where $0<\varepsilon\ll 1$ and P'_n are projectors onto a basis of the kernel of ρ. Practically, for sufficiently small ε, ρ_ε and ρ describe the same physical state since no measurement can tell the difference between them.

The action of $\mathrm{U}(H)$ is now free and transitive on fibres of π. Thus $\mathrm{U}(H)\rightarrow B\rightarrow \underline{S}$ is a principal fibre bundle. (Strictly speaking, we should work with normalised states

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0305-4470/89/153167+04$02.50

and operators, $\operatorname{tr}\rho = 1$ and $\|A\|_{\mathrm{HS}} = 1$, but leaving them unnormalised provides no additional topology and simplifies the discussion). There is a global section of B over $\underline{S}$ (and of J_2 over S) which assigns to ρ its unique positive square root, therefore the bundle is topologically trivial but still has an interesting geometry.

The Hilbert–Schmidt norm provides a metric (non-degenerate real bilinear form)

$$(X, Y) = \tfrac{1}{2}\operatorname{tr}(X^\dagger Y + Y^\dagger X) \tag{1}$$

on J_2, thought of as a real vector space. Here, we use the linear structure to identify the tangent space to B at any A with J_2, so that the derivative of the projection π maps X into

$$Z = AX^\dagger + XA^\dagger. \tag{2}$$

The metric (1) is invariant under the action of $\mathrm{U}(H)$ and defines a principal connection on B as follows. A tangent vector X at A is called horizontal iff it is orthogonal to all vertical vectors. Now, using the infinitesimal action of $\mathrm{U}(H)$, we see that the vertical vectors at A are of the form AS, where $S \in \operatorname{Lie}(\mathrm{U}(H))$. Hence X is horizontal iff $(AS, X) = 0$ for all $S^\dagger = -S$, i.e.

$$X^\dagger A - A^\dagger X = 0. \tag{3}$$

(This agrees with equation (44) in [6]). Thus the horizontal lift of Z to A which obeys (2) and (3) is formally

$$X = \sum (\rho_m + \rho_n)^{-1} P_m Z P_n A. \tag{4}$$

The related connection form on B with values in skew-Hermitian operators is

$$\omega_A(X) = S_\alpha M_{\alpha\beta}(AS_\beta, X). \tag{5}$$

Here, and later on, we sum over repeated Greek indices, S_α is a basis of skew-Hermitian operators and $M_{\alpha\beta}$ is the inverse of the matrix of scalar products $(S_\alpha, A^\dagger A S_\beta)$.

The connection ω reproduces the known results on the boundary. Loosely speaking, one may slightly deform a loop in the boundary into the interior, compute its holonomy using ω and deform it back. The final result is independent on the details of the deformation. More rigorously, there is an injective homomorphism (over the identity) of the Stieffel bundle into the bundle $\pi : J_2 \to S$ given as follows. We think of a k-frame as an isometry $F : \mathbf{C}^n \to H$, $F^\dagger F = 1$ and of a k-plane as a k-dimensional projector. The bundle projection onto the Grassmannian is $F \to FF^\dagger$. Then, by choosing a fiducial frame F_0, we send F into the HS operator $FF_0^\dagger$ which projects onto $\rho = FF^\dagger$. To assure that the group actions commute, we map a unitary matrix U in $\mathbf{C}^n$ into the unitary operator $F_0 U F_0^\dagger$ in H. The pullback connection does not depend on F_0 and is equal to the canonical connection $\omega_F(X) = F^\dagger X$ on the Stieffel bundle (note that a vector X tangent to the Stieffel space at F obeys $F^\dagger X_\dagger + X^\dagger F = 0$).

The curvature (covariant derivative of (5)) is

$$\Omega_A(X, Y) = \Omega_A^\alpha(X, Y)S_\alpha = \mathrm{d}\omega_A(X, Y) + [\omega_A(X), \omega_A(Y)]$$

with

$$\Omega_A^\alpha(X, Y) = (S_\alpha S_\beta + S_\beta S_\alpha, A^\dagger X)(S_\beta, A^\dagger Y) - (S_\alpha S_\beta + S_\beta S_\alpha, A^\dagger Y)(S_\beta, A^\dagger X)$$
$$+ 2(S_\alpha, X^\dagger Y) + (S_\beta, A^\dagger X)(S_\gamma, A^\dagger Y)c^\alpha_{\beta\gamma}. \tag{6}$$

In this expression we have used an adapted A-dependent basis of the S_α such that $M_{\alpha\beta} = \delta_{\alpha\beta}$, for instance the following:

$$S_{m,n} = (e_m e_n^\dagger - e_n e_m^\dagger)(\rho_m + \rho_n)^{-1/2} \qquad m < n$$

$$S_{\underline{m,n}} = \mathrm{i}(e_m e_n^\dagger + e_n e_m^\dagger)(\rho_m + \rho_n)^{-1/2}(1 + \delta_{mn})^{-1/2} \qquad m \leqslant n$$

where the Greek indices become double Latin indices (no summation) and e_m are the orthonormal eigenvectors of $A^\dagger A$ with eigenvalues ρ_m. The only non-vanishing structure constants of this basis are:

$$c^{p,q}_{j,k;m,n} = (\rho_p + \rho_q)^{1/2}(\rho_j + \rho_k)^{-1/2}(\rho_m + \rho_n)^{-1/2}$$
$$\times (\delta_{km}\delta_{jp}\delta_{nq} - \delta_{km}\delta_{jq}\delta_{np} - \delta_{kn}\delta_{jp}\delta_{mq} + \delta_{kn}\delta_{jq}\delta_{mp}$$
$$- \delta_{jm}\delta_{kp}\delta_{nq} + \delta_{jm}\delta_{kq}\delta_{np} + \delta_{jn}\delta_{kp}\delta_{mq} - \delta_{jn}\delta_{kq}\delta_{mp})$$

$$c^{p,q}{}_{j,k;\underline{m,n}} = -c^{p,q}{}_{\underline{m,n};j,k} = (\rho_p + \rho_q)^{1/2}((\rho_j + \rho_q)^{1/2}((\rho_j + \rho_k)(\rho_m + \rho_n)(1 + \delta_{pq})(1 + \delta_{mn}))^{-1/2}$$
$$\times (\delta_{km}\delta_{jp}\delta_{nq} + \delta_{km}\delta_{jq}\delta_{np} + \delta_{kn}\delta_{jp}\delta_{mq} + \delta_{kn}\delta_{jq}\delta_{mp}$$
$$- \delta_{jm}\delta_{kp}\delta_{nq} - \delta_{jm}\delta_{kq}\delta_{np} - \delta_{jn}\delta_{kp}\delta_{mq} - \delta_{jn}\delta_{kq}\delta_{mp})$$

$$c^{p,q}{}_{\underline{j,k};\underline{m,n}} = (\rho_p + \rho_q)^{1/2}((\rho_j + \rho_k)(\rho_m + \rho_n)(1 + \delta_{jk})(1 + \delta_{mn}))^{-1/2}$$
$$\times (-\delta_{km}\delta_{jp}\delta_{nq} + \delta_{km}\delta_{jq}\delta_{np} - \delta_{kn}\delta_{jp}\delta_{mq} + \delta_{kn}\delta_{jq}\delta_{mp}$$
$$+ \delta_{jm}\delta_{kp}\delta_{nq} - \delta_{jm}\delta_{kq}\delta_{np} + \delta_{jn}\delta_{kp}\delta_{mq} - \delta_{jn}\delta_{kq}\delta_{mp})$$

where δ is the Kronecker symbol. We choose the basis of horizontal directions as $\mathrm{i}S_\alpha A$ and give the components of the curvature at $A = \rho^{1/2}$

$$\Omega_A^\alpha(\mathrm{i}S_\beta A, \mathrm{i}S_\gamma A) = -2(\rho_m\rho_n)^{1/2}(\rho_m + \rho_n)^{-1}c^\alpha_{\beta\gamma} \tag{7}$$

where $\alpha = m,n$ or $\alpha = \underline{m,n}$. We see that (formally) the holonomy is equal to $\mathrm{SU}(H)$ and the bundle with connection can be reduced to this group ($\mathrm{SU}(H)$ contains $\mathrm{U}(k)$ for arbitrary $k < \dim H$ at the boundary).

We close this comment with some remarks.

We left aside questions regarding differentiability of the manifolds and maps we consider if H is infinite dimensional. The problem is that then B is not an open subset of J_2 in the HS topology. We could consider as smooth those curves which are smooth as viewed from J_2, but this may ruin the linear structure of tangent spaces which in addition appear differently at different points. To be rigorous, one should work with the whole J_2, consider it as a stratified space and introduce a connection in the sense of [7]. Alternatively, since the fibres are homogeneous spaces for $\mathrm{U}(H)$, in the spirit of Kaluza–Klein (see e.g. [8]), one has a natural connection which agrees with the connections we have described.

We feel that we have shed more light on the geometry of the space S of quantum mechanical states. Because of the lack of space we just observe that the metric (1) is Kaehler and that more structure exists there. Namely, in addition to a connection, the metric (1) provides a metric on S which equals the standard invariant metrics on the Grassmannians, e.g. the Fubini–Study metric on the projective Hilbert Space. The parallel transport along the geodesics alows one to compare points in distinct fibres. How this relates to Uhlmann's notion of 'parallel amplitudes' (two points are parallel if the length in J_2 of their difference is minimal) and how Pancharatnam's ideas [9, 10] can be extended to mixed states, will be discussed elsewhere.

One may wonder why such a huge bundle and holonomy is employed. One reason is that J_2 and S are in a sense 'universal' since they embed all the Stieffel bundles on the boundary. Also, $\mathrm{U}(H)$ is roughly a limit of $\mathrm{U}(k)$ for $k \to \infty$ and we are dealing with all the Chern classes at the same time. Another reason is that in statistical physics it was often used to represent a mixed state in H by a vector in $H \otimes H$. In fact, this is equivalent [11] to the construction described above, which we regard as a natural generalisation to mixed states of the Berry phase.

Acknowledgments

One of us (LD) is grateful for the invitation and financial support from Istituto Nazionale di Fisica Nucleare, Padova, where part of this work was done.

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