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PARALLEL LIFTS AND HOLONOMY ALONG DENSITY OPERATORS: COMPUTABLE EXAMPLES USING O(3)-ORBITS.

Armin Uhlmann

University of Leipzig
Department of Physics
Leipzig, Germany

Introduction, Generalities.

The parallel transport governing Berry's phase [1], [2], and the Wilzcek and Zee [3] holonomy for degenerate states extends naturally to *density operators* [4] (and, up to the peculiarities of infinite dimensional analysis, at least partly to state spaces of certain *-algebras [5].) Our approach is consistent, for the pure states case, with the point of view of [6].

Let

$$t \mapsto \varrho_t \tag{1}$$

be a curve of density operators in the set

$$\Omega = \{\varrho \geq 0, \quad \operatorname{trace} \varrho = 1\} \tag{2}$$

of all density operators of an Hilbert space $\mathcal{H}$.
One considers now *extensions*

$$\mathcal{H}^{\text{ext}} = \mathcal{H} \otimes \mathcal{H}^{\text{aux}} \tag{3}$$

of $\mathcal{H}$ such that the original Hilbert space can be considered as a *subsystem* of the extended one. Every unit vector of the extension can be reduced to a density operator of $\mathcal{H}$. The inverse operation is called *purification*. Therefore, a curve of vectors sitting in $\mathcal{H}^{\text{ext}}$ is called a purification of (1) if its reduction onto $\mathcal{H}$ coincides with the curve (1).
The task of purification is of course not a unique one. However, in the set of all possible purifications of a given curve of density operators (1) there are exceptional ones. These exceptional ones are those purifications for which the usual Berry transport condition

remains stable after applying operators out of the commutant of $\mathcal{B}(\mathcal{H})$ in $\mathcal{B}(\mathcal{H}^{\text{ext}})$. (Remind that every imbedding (3) induces a well defined imbedding of the operators acting on $\mathcal{H}$ into those acting on $\mathcal{H}^{\text{ext}}$.) Purifications of this type are called *parallel*, and the condition just mentioned *(extended) parallel condition.*
Under certain continuity assumptions a parallel purification of a given curve of density operators is already determined by its initial value. Two parallel purifications of the same curve of density operators do not intersect or they are identical. Thus parallel purifications give rise to holonomy invariants if the curve which is to be lifted is closed.
For our present purposes it is sufficient to consider only standard purifications. This means to identify $\mathcal{H}^{\text{aux}}$ with the dual of $\mathcal{H}$ in (3). Then $\mathcal{H}^{\text{ext}}$ can be realized by the Hilbert space of the Hilbert - Schmidt operators defined on $\mathcal{H}$, i.e. by the linear space of operators W such that

$$\operatorname{trace} WW^* = \operatorname{trace} W^*W < \infty \tag{4}$$

Its scalar product is given by

$$(W_1, W_2) := \operatorname{trace} W_1^* W_2 \tag{5}$$

A *standard purification* of (1) is nothing but a curve

$$t \mapsto W_t, \qquad W_t \quad \text{Hilbert - Schmidt} \tag{6}$$

such that

$$\varrho_t = W_t W_t^* \quad \text{for all} \quad t \tag{7}$$

The (extended) parallelity condition can now be expressed [4] as

$$\dot{W}^* \, W \;=\; W^* \, \dot{W} \tag{8}$$

Indeed, this condition is equivalent with the more general recipe above, as seen as follows. If A is an operator acting on $\mathcal{H}$ then

$$A \mapsto AW := L_A \, W \tag{9}$$

is the canonical embedding of the operators of $\mathcal{H}$ into the operators acting on the Hilbert space $\mathcal{H}^{\text{ext}}$ of Hilbert Schmidt operators. The commutant of this embedding is given by the operations

$$A \mapsto WA := R_A \, W \tag{10}$$

Hence the stability of the Berry condition under the operators of the commutant is expressed by

$$(R_A \dot{W}, R_A W) = (R_A W, R_A \dot{W}) \quad \text{for all} \quad A \tag{11}$$

Now R_A can be moved from the left hand side to the right hand side in the scalar products, giving there an additional operator R_{A^*}. Every operator R_B can be represented by a linear combination of operators of the form $R_{A^*} R_A$. As a consequence equation (11) is equivalent with

$$(\dot{W}, R_A W) = (W, R_A \dot{W}) \quad \text{for all} \quad A \tag{12}$$

Using (5) one immediately derives (8) from (12) and vice versa.

An important conclusion is: Let $t \mapsto W_t$ be a parallel lift of $t \mapsto \varrho$ for $0 \leq t \leq \tau$. Then

$$t \mapsto W_t W_0^*, \qquad 0 \leq t \leq \tau \tag{13}$$

depends only on ϱ_s, $\quad 0 \leq s \leq t$. If the curve of density operators closes for $t = \tau$ then $W_\tau W_0^*$ is an *holonomy invariant.* (It should be remarked that (13) defines trace class operators, and hence a path of normal linear functionals $A \mapsto \text{trace}(A W_t W^*)$ on the bounded operators of $\mathcal{H}$.)

The parallelity condition (8), (12) allows for links to a peculiar Riemannian metric on Ω, i.e. on the set of density operators, and to a connection (a gauge field) on the unit sphere of $\mathcal{H}^{\text{ext}}$. One gets the first link by the observation, that the parallelity condition (8) can be considered as the Euler equations of the variational problem

$$\text{length}(\, t \mapsto \varrho_t \,) = \inf \int \sqrt{(\dot{W}, \dot{W})}\, dt \tag{14}$$

if the infimum is running over all purifications of the curve of density operator in question [7]. This extends nicely an idea of Fock (see appendix of [8]) to fix the arbitrary phases of moving orthogonal m-frames by requiring their minimal change during their movement. Further aspects of this observations are discussed more recently in [9].

The length obtained by (14) is measured equally well by Riemannian metric on Ω. This metric has been at first considered in the context of W^*-algebra representations by Bures [10], who defined it as a distance function for positive functionals of W*-algebras. On Ω the line element of the metric equals

$$ds^2 := \frac{1}{2} \, \text{trace}\, \mathbf{G} \, d\varrho \tag{15}$$

where d denotes the total differential. $\mathbf{G}$ is determined by the Bloch-like equation [11], [12]

$$d\varrho = \varrho \mathbf{G} + \mathbf{G} \varrho \tag{16}$$

The metric (15) extends the Study Fubini metric from the pure states to the mixed states.

To obtain the second link one is looking for a connection form $\mathbf{A}$ for the gauge transformations

$$W \mapsto WU, \quad U \quad \text{unitary} \tag{17}$$

acting in the fibre of all W purifying a given ϱ. Again, within the many possibilities to satisfy this demand there is a canonical one. It can be defined by [13]

$$W^* \text{d}W - (\text{d}W^*) W = W^* W \cdot \mathbf{A} + \mathbf{A} \cdot W^* W \tag{18}$$

Denoting by D the covariant differential that goes with the connection form $\mathbf{A}$ one computes

$$\text{D}W := \text{d}W - W\mathbf{A} = \mathbf{G} W \tag{19}$$

and this is one way to see how strongly $\mathbf{A}$ and the gauge invariant $\mathbf{G}$ are bound together. And further:
Because of (18) $\mathbf{A} = 0$ is a gauge fixing along a lift. In a gauge with this property the parallelity condition is satisfied. The gauge fixing is up to a global gauge transformation, i.e. it is a local one.
According to (19) this gauge fixing is equivalent with solving the system of partial differential equations $\mathrm{d}W - \mathbf{G}W = 0$ [11].

Lifts of Hamiltonian motion.

If the eigenvalues of the density operators of a sufficiently regular curve (1) remain unchanged, this curve is a solution of a von Neumann - Liouville equations with a time-dependent Hamiltonian.

$$i\,\dot{\varrho} = [H(t), \varrho] \tag{20}$$

If (1) is a solution of (20), and if $W = W_t$ is an arbitrary lift then one may write with a suitable $\tilde{H}(t)$

$$i\dot{W} = H(t)W - W\tilde{H}(t) \tag{21}$$

This relation can be considered as a Schrödinger equation

$$i\dot{W} = H^{\text{ext}}(t)W \quad \text{with} \quad H^{\text{ext}}(t) := (L_H - R_{\tilde{H}}) \tag{22}$$

in $\mathcal{H}^{\text{ext}}$. In [13] it is shown how to choose $\tilde{H}(t)$ for parallel purifications.
In the following the Hamiltonian in (20) is always assumed to be independent of time. The formal solution of this equation reads

$$t \mapsto \varrho_t := U(t)\varrho_0 U(-t), \quad U(t) = e^{-itH} \tag{23}$$

The corresponding solution for (21) with $\tilde{H}$ independent of time too is given by

$$W(t) = U(t)\varrho_0^{1/2}V(t), \qquad V(t) = e^{it\tilde{H}} \tag{24}$$

where the initial value for $t = 0$ is the positive square root of ϱ_0. Assuming that this is already a parallel lift, the gauge invariant (13) can be written as

$$U(t)\varrho_0^{1/2}V(t)\varrho_0^{1/2}$$

If now (1) is a loop, and the curve of density operator closes for $t = \tau$, then $U(\tau)$ commutes with ϱ_0. Thus the associated holonomy invariant reads

$$\varrho_0^{1/2}\,U(\tau)\,V(\tau)\,\varrho_0^{1/2} \quad \text{with} \quad \varrho_\tau = \varrho_0 \tag{25}$$

The parallelity condition demands the hermiticity of

$$W^*\,\frac{dW}{dt} = V^*\varrho_0^{1/2}[-iH]\varrho_0^{1/2}V + V^*\varrho_0[i\tilde{H}]V \tag{26}$$

resulting in

$$2\varrho_0^{1/2} H \varrho_0^{1/2} = \varrho_0 \tilde{H} + \tilde{H} \varrho_0 \tag{27}$$

If ϱ is faithful this equation defines $\tilde{H}$. Otherwise, in order to determine $\tilde{H}$ uniquely, one may require

$$< \psi, \tilde{H}\psi >= 0 \quad \text{if} \quad \varrho_0 |\psi >= 0$$

However, in calculating the gauge invariants (13), the holonomy invariant (25), or the line element of the Bures metric the ambiguity coming from (27) is cancelled automatically.

Let us assume for simplicity the faithfulness of ϱ_0. Then (27) defines a linear map

$$H \mapsto \tilde{H} \tag{28}$$

in the linear space of Hamiltonians. This map satisfies the following
a) If $H\varrho = \varrho H$ then $H = \tilde{H}$.
b) If $H\varrho = \varrho H$ then $[H, H'] = [H, \tilde{H}']$ for all $\tilde{H}'$.
c) The map (28) is trace preserving for $\dim \mathcal{H} < \infty$.
d) It is $\mathrm{trace}\varrho H = \mathrm{trace}\varrho \tilde{H}$

Denoting the eigenvalues and eigenvectors of ϱ by λ_m and ψ_m respectively, one writes

$$\varrho_0 = \sum \lambda_m \, |\psi_m >< \psi_m| \tag{29}$$

Inserting this into (27) results in

$$\tilde{H} = \sum \frac{2\sqrt{\lambda_m \lambda_n}}{\lambda_m + \lambda_n} \, |\psi_m >< \psi_m, H\psi_n >< \psi_n| \tag{30}$$

The coefficient in (30) is the quotient of the geometric mean by the arithmetic mean, and hence a number between 0 and 1. (30) can be rewritten as

$$\tilde{H} = H - \sum \frac{(\lambda_n^{\frac{1}{2}} - \lambda_m^{\frac{1}{2}})^2}{\lambda_m + \lambda_n} \, |\psi_m >< \psi_m, H\psi_n >< \psi_n| \tag{31}$$

Another useful relation is

$$\begin{aligned} (\dot{W}, \dot{W}) &= \mathrm{trace}\varrho_0^2 \{H^2 - \tilde{H}^2\} \\ &= \frac{1}{2} \sum \frac{(\lambda_m - \lambda_n)^2}{\lambda_m + \lambda_n} | < \psi_m, H\psi_n > |^2 \end{aligned} \tag{32}$$

The following section is devoted to Hamiltonians H which are generators of the rotation group. There eigenvalues are integers or half integers, and (23) closes after a time period of 2π. Thus

$$W_{2\pi} = (-1)^{2j} \, \varrho_0^{1/2} \exp 2\pi i \, \tilde{H}, \qquad j \text{ denotes spin} \tag{33}$$

and the holonomy invariant (25) of a loop will be

$$W_{2\pi}W_0^* = (-1)^{2j}\, \varrho_0^{1/2}\, e^{2\pi i\, \tilde{H}}\, \varrho_0^{1/2} \tag{34}$$

Rotationally symmetric 2-spheres of states.

The unit vectors $\vec{n}$ in 3-space characterize the points of a 2-sphere. By the help of the generators of an irreducible representation of $SU(2)$, J_x, J_y, J_z, one associate to it an 2-sphere of states with monopole-like structure. To this end one considers the vectors $|m, \vec{n}>$ of norm one satisfying

$$\vec{n}\, \vec{J}\, |m, \vec{n}> = m\, |m, \vec{n}> \tag{35}$$

If $\lambda_m > 0$ with $\sum \lambda_m = 1$ is given then

$$\varrho = \sum \lambda_m\, |\psi_m >< \psi_m| \quad \text{where} \quad \psi_m = |m, \vec{n}> \tag{36}$$

is a density operator.
Varying the direction of the unit vector $\vec{n}$ one gets a set of density operators which uniquely fill a 2-sphere $\mathbf{S} = \mathbf{S}_{j,\lambda}$. It is determined by the given eigenvalues λ_m, and the chosen irreducible representation labelled by j. It is an obviously rotational invariant sphere.
On this sphere we shall consider curves which are (parts of) circles. Their starting point ϱ_0 should be attached to the z-direction in the sense of (36), while $\vec{n} = \{0, \sin\theta, \cos\theta\}$ will be chosen as rotational axis. The resulting curve is given by

$$\phi \mapsto U(\phi)\varrho_0 U(-\phi), \qquad U(\phi) = e^{-i\phi\, (\sin\theta\, J_y + \cos\theta\, J_z)} \tag{37}$$

and the associated parallel lift of this curve with initial value $\varrho_0^{1/2}$ by

$$\phi \mapsto U(\phi)\varrho_0 V(\phi), \qquad V(\phi) = e^{i\phi\, (\sin\theta\, \tilde{J}_y + \cos\theta\, J_z)} \tag{38}$$

in accordance with (23) and (24). The holonomy invariant (34) can now be obtained by setting $\phi = 2\pi$. An obvious calculation shows for the linear map (28)

$$\begin{aligned} \tilde{J}_z &= J_z, \\ \tilde{J}^+ &= \sum a_{m+1,m} \sqrt{j(j+1) - m(m+1)}\, |\psi_{m+1} >< \psi_m|, \\ \tilde{J}^- &= \sum a_{m-1,m} \sqrt{j(j+1) - m(m-1)}\, |\psi_{m-1} >< \psi_m|, \end{aligned} \tag{39}$$

where

$$a_{m,m'} = \frac{2\sqrt{\lambda_m \lambda_{m'}}}{\lambda_m + \lambda_{m'}} \tag{40}$$

One remarks as a byproduct

$$[[\tilde{J}_x, \tilde{J}_y], J_z] = 0, \qquad [J_z, J^{\pm}] = \pm J^{\pm} \tag{41}$$

and further

$$(\dot{W}, \dot{W}) = \frac{1}{4} \sin^2\theta \sum_m \frac{(\lambda_{m+1} - \lambda_m)^2}{\lambda_{m+1} + \lambda_m} \{j(j+1) - m(m+1)\} \tag{42}$$

Things become simpler for suitable chosen eigenvalues of the ϱ.
At first, as a check, let $\mathbf{S}$ be a sphere of pure states, i.e. it consists of 1-dimensional projectors. Thus let ϱ_0 project onto a vector $|m>$ with J_z-eigenvalue m in a spin j representation. Then $\lambda_m = 1$, and all other eigenvalues are zero. Consequently the numbers (40) will be zero, and $\tilde{J}_y = 0$, therefore. Our holonomy invariant (34) reads

$$W_{2\pi} W_0^* = (-1)^{2j} \, \varrho_0^{1/2} \, e^{2\pi i \, \cos\theta \, J_z} \, \varrho_0^{1/2} = e^{-2\pi i m \, (1-\cos\theta)} \, |m><m| \tag{43}$$

Its trace is the well known [1] phase factor of Berry. Our loop is circle on a sphere. The radius of that circle in the Bures metric (which is for pure states that of the Study Fubini metric [6]) can be obtained from (42). On gets

$$\text{radius of the circle if } \varrho_0 = |m><m| \quad \text{equals} \quad \sin\theta \sqrt{\frac{j^2 + j - m^2}{2}} \tag{44}$$

Another interesting case constitute the Gibbsian states of the form

$$\varrho = \frac{e^{\alpha \, \vec{n}\vec{J}}}{\text{trace}\, e^{\alpha \, \vec{n}\vec{J}}} \tag{45}$$

which fill for a given value of α a 2-sphere called $\mathbf{S}_j^\alpha$ if $\vec{n}$ runs through all directions in 3-space. This problem has been partly considered in [4] and, for $j = \frac{1}{2}$, explicitly in [14], [15]. From the number (40) we only need

$$a := a_{m,m+1} = \frac{2\, e^{\frac{\alpha}{2}}}{1 + e^\alpha} = \frac{1}{\cosh \frac{\alpha}{2}} \tag{46}$$

It follows now (39) that $\tilde{J}^\pm = a J^\pm$, and hence

$$\tilde{H} = \cos\theta \, J_z + a \, \sin\theta \, J_y \tag{47}$$

It is now possible to look at $V(\phi)$ as a rotation with angle

$$\tilde{\phi} = \kappa\phi, \quad \kappa = \sqrt{\cos^2\theta + a^2 \sin^2\theta} \leq 1 \tag{48}$$

and rotation axis

$$\vec{\xi} = \{0, \frac{\sin\theta}{\kappa}, \frac{a\, \cos\theta}{\kappa}\} \tag{49}$$

The holonomy invariant can be written as

$$(-1^{2j})\varrho_0^{1/2}\, e^{2\pi i(\cos\theta\, J_z + a\, \sin\theta\, J_y)}\, \varrho_0^{1/2} = (-1^{2j})\varrho_0^{1/2}\, e^{2\pi i\kappa\vec{\xi}\vec{J}}\, \varrho_0^{1/2} \tag{50}$$

See also [14], [15], and [16] for $j = \frac{1}{2}$.
The Bures radius of the considered circle of density operators is easily computed from (32) because H and $\tilde{H}$ are known as linear combinations of J_y and J_z, and because ϱ_0 commutes with J_z. The result is

$$\text{radius of the circle:}\quad \sin\theta\,\sqrt{(1-a^2)\text{trace}\,\varrho_0 J_y^2} := \sin\theta\, r_j^\alpha \tag{51}$$

where r_j^α is the radius of the sphere $\mathbf{S}_j^\alpha$ as determined by the Bures metric.
As a cross check one may consider the limits

$$\alpha \mapsto \pm\infty, \quad \varrho_{,} \to |m >< m|, \quad m = \pm j$$

showing that (51) is consistent with (44).

The trace within (51) can be simplified.

$$\text{trace}\varrho_0 J_y^2 = \frac{1}{4}\text{trace}\varrho_0(J_+J_- + J_-J_+) = \frac{1}{2}\{j(j+1) - \text{trace}\varrho_0 J_z^2\} \tag{52}$$

The remaining trace can be explicitly computed, for example

$$\text{trace}\varrho_0 J_z^2 = \begin{cases} \frac{1}{4} & \text{if } j = \frac{1}{2} \\ \frac{e^\alpha + e^{-\alpha}}{1+e^\alpha+e^{-\alpha}} & \text{if } j = 1 \end{cases}$$

This yields according to (51) and (46)

$$r_j^\alpha = \begin{cases} \frac{1}{2}\sqrt{1-a^2} & \text{if } j = \frac{1}{2} \\ \sqrt{\frac{2(1-a^2)}{4-a^2}} & \text{if } j = 1 \end{cases}$$

In the most simple case of spin $\frac{1}{2}$ the spheres $\mathbf{S}_{\frac{1}{2}}^\alpha$ with varying α can be isometrically imbedded in a $\mathbf{S}^3$ - hemisphere [16], [17]. However, for larger spin and varying α the set of the 2-spheres $\mathbf{S}_j^\alpha$ form a more complicated piece of a Riemann 3-space.
See also [18].

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