PARALLEL TRANSPORT OF PHASES.

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1. Introduction

Parallel transport of phases is a natural structure in the fundamentals of Quantum Theory. It is my aim to describe some essentials of that structure according to Berry [1] and Simon [2], which is defined via transport conditions for vectors and phases along curves of pure states. A further purpose is to introduce to the extension of these constructions to curves of more general states (i.e. mixtures) [3]. To do so is a problem of internal consistency: In Quantum Theory - and in contrast to Classical Statistical Mechanics - the question wether a state is a pure or a mixed one is decided by the set of observables and can, consequently, be changed by adding or neglecting observables (operators). The criteria for parallelity should be compatible with this feature. On the other hand, the case of pure states is basic and most important, and serves as a guide. See also [4].

The vectors of a Hilbert space $\mathcal{H}$ represent *pure* states if two of them can be distinguished by their expectation values provided they are linearly independent. To do so one needs enough *observables* acting as operators on $\mathcal{H}$. The simplest and also natural assumption for this is that potentially every selfadjoined operator is allowed to become an observable. It is however sufficient, and for technical reasons highly desirable, to use the bounded hermitian operators of $\mathcal{H}$, i.e. the hermitian elements of the algebra $\mathcal{B}(\mathcal{H})$ of all bounded operators acting on $\mathcal{H}$.

A vector ψ describes a state by the collection of its *expectation values*

$$A \mapsto \frac{< \psi, A\psi >}{< \psi, \psi >} \tag{1}$$

and for this reason two vectors describe the same state if and only if they are linearly dependent. Excluding the zero of $\mathcal{H}$ and identifying two linearly dependent vectors defines the *projective space*, $\mathbf{P}\mathcal{H}$, which labbels uniquely the pure states. It can hence be considered as the *space of pure states*. $\mathbf{P}\mathcal{H}$ can be realized either

a) as the space of 1-dimensional linear subspaces of $\mathcal{H}$ – the first Grassmann manifold of $\mathcal{H}$,
b) or as the space of rays of $\mathcal{H}$. A ray is 1-dimensional linear subspace with the exclusion of the zero of $\mathcal{H}$,
c) or as the space of the 1-dimensional projection operators, i.e. of the operators $P = P^2 = P^*$ which project $\mathcal{H}$ onto an 1-dimensional subspace.

Here always exclusively $\mathbf{P}\mathcal{H}$ is interpreted as the set of 1-dimensional projections. The merit in doing so is: The points of $\mathbf{P}\mathcal{H}$ appear as operators, and $\mathbf{P}\mathcal{H}$ is canonically imbedded into $\mathcal{B}(\mathcal{H})$ as a subset.

An unconvenience in using case c) above is in the double role the projections of rank one are playing: Such an operator represents as well a state as a genuine observable asking with which apriori probability this state is realized.

$\mathcal{H} - \{0\}$, the Hilbert space without its zero element, can be considered as a $\mathbf{C}^\times$-fibre bundle over $\mathbf{P}\mathcal{H}$. Because the norming of vectors is a topological trivial operation it is further useful to introduce the unit sphere

$$\mathbf{S}(\mathcal{H}) = \{\psi \in \mathcal{H} : <\psi, \psi>= \mathbf{1}\} \tag{2}$$

of $\mathcal{H}$ which is a S^1-bundle over $\mathbf{P}\mathcal{H}$.

Every Schrödinger equation

$$H(t)\psi = \mathrm{i}\dot{\psi} \tag{3}$$

determines (not canonical) lifts from $\mathbf{P}\mathcal{H}$ of the integral curves of

$$[H(t), P] = \mathrm{i}\dot{P} \tag{4}$$

Indeed, if $t \mapsto P_t$ is a solution of (4) and $P_0 = |\psi_0 >< \psi_0|$ then their is just one solution $t \mapsto \psi(t)$ of (3) with $\psi(0) = \psi_0$. Now $t \mapsto \psi(t)$ is clearly a lift of $t \mapsto P_t$ into $\mathcal{H} - \{0\}$. This lift sits in the subbundle (2) because of the conservation of the norm.

Replacing within (3)

$$H(t) \mapsto H_{\mathrm{new}}(t) = H(t) - a(t)\mathbf{1} \tag{5}$$

the new curve

$$H_{\mathrm{new}}(t)\psi_{\mathrm{new}} = \mathrm{i}\dot{\psi}_{\mathrm{new}}, \qquad \psi_{\mathrm{new}}(0) = \psi_0 \tag{6}$$

in $\mathcal{H} - \{0\}$ is again a lift of $t \mapsto P_t$ with

$$\psi_{\mathrm{new}}(t) = \exp \mathrm{i} \int_0^t a(t)\mathrm{d}t \cdot \psi(t) \tag{7}$$

This shows that the lifting may produce rather arbitrary phases. Furthermore, (3) produce lifts only for solutions of (4), which is a rather restricted class of curves in the space of pure states. This explains, why the procedure above is *not* a canonical lifting procedure. A *canonical* or *natural* lifting procedure should be valid for all (sufficiently smooth) curves of $\mathbf{P}\mathcal{H}$, and the lifts should be uniquely determined by their basic curves up to its initial value.

The arbitrariness mentioned above can be avoided in going to the *adiabatic limit* [5] – provided this is possible. To do this one considers together with (3) the family of Schrödinger equations

$$H(t/T)\psi_T(t) = \mathrm{i}\dot{\psi}_T(t), \qquad \psi_T(0) = \psi_0 \tag{8}$$

with $T > 0$ and the corresponding family of equations (4) on $\mathbf{P}\mathcal{H}$ with solutions

$$t \mapsto P_{T,t} = |\psi_T(t) >< \psi_T(t)| \tag{9}$$

One refers to *adiabatic convergence* if

$$\lim_{T\to\infty} P_{T,tT} = P_t^{\mathrm{adi}} \tag{10}$$

is converging towards a new curve $t \to P_t^{\rm adi}$ in $\mathbf{P}\mathcal{H}$.

If it is possible – after a suitable substitution (5) – to reach convergence of ψ_T towards a curve $\psi^{\rm adi}$ in the sense of

$$\text{w}-\lim_{T\to\infty} T\left(\psi_T(tT)-\psi^{\rm adi}(t)\right)=0 \tag{11}$$

then one may heuristically (i.e. up to the interchange of two limiting procedures) argue as following:

$$\begin{aligned} <\psi^{\rm adi},\dot\psi^{\rm adi}> &= \lim_{T\to\infty}\ <\psi^{\rm adi},\frac{\rm d}{{\rm d}t}\psi_T(tT)> \\ &= -\lim {\rm i}T\ <\psi^{\rm adi},H(t)\psi_T(tT)> \\ &= -\lim {\rm i}T\ <H(t)\psi^{\rm adi},\psi_T(tT)>\,. \end{aligned} \tag{12}$$

Because of (11) this can become reasonable only with $<H(t)\psi^{\rm adi},\psi^{\rm adi}>=0$ and vanishing right hand side.

The question wether convergence (10) and (11) takes place is difficult and only solved [6] using rather strong assumptions. However, in the cases one can prove adiabatic convergence it results in

$$<\psi^{\rm adi},\frac{\rm d}{{\rm d}t}\psi^{\rm adi}>=0 \quad\text{with}\quad <\psi^{\rm adi},\psi^{\rm adi}>=1 \tag{13}$$

It is perhaps better to consider (13) as a necessary condition for the convergence of (11). It forces the vanishing of the *dynamical phase* by requiring a suitable shift (5) before performing (11). It is thus a kind of renorming the hamiltonian in order that adiabatic convergence (10) in the state space can imply (11).

At this point we arrived at a *natural* or *canonical* lifting procedure which induces indeed a well known *parallel transport* in the bundle $\mathbf{S}(\mathcal{H})$ respectively $\mathcal{H}-\{0\}$. It is reasonable to 'forget' the adiabatic origin of (13) and to treat this transport condition as a concept in its own right. Let

$$s\mapsto P_s,\qquad 0\le s\le 1, \tag{14}$$

be an arbitrary (but sufficiently regular) curve in $\mathbf{P}\mathcal{H}$. A lift

$$s\mapsto\psi(s)\quad\text{with}\quad P_s=|\psi(s)><\psi(s)| \tag{15}$$

is called *parallel* iff it fulfills

$$<\psi,\frac{\rm d}{{\rm d}s}\psi>=<\frac{\rm d}{{\rm d}s}\psi,\psi> \tag{16}$$

However, $<\psi,\dot\psi>$ is purely imarinary for a curve (15) of constant norm, and (16) reduces to

$$<\psi,\frac{\rm d}{{\rm d}s}\psi>=0. \tag{16a}$$

Parallel lifts are integral curves of connection 1-forms. A good choice for them is

$$< \psi, \mathrm{d}\psi > \tag{17}$$

for the fibre bundle $\mathbf{S}(\mathcal{H})$ and

$$\frac{1}{2} \frac{< \psi, \mathrm{d}\psi > - < \mathrm{d}\psi, \psi >}{< \psi, \psi >} \tag{18}$$

for the larger bundle $\mathcal{H} - \{0\}$.

At this place I like to give a first account for an extension to curves of not necessarily pure states. Let the algbra of observables be a unital *-subalgebra $\mathcal{A}$, i.e. a subalgebra containing the identity map and with every operator its hermitian conjugate. Then two linearly independent vectors may not be distinguishable by the elements of $\mathcal{A}$, and the *vector states* of $\mathcal{A}$

$$\omega = \omega_\psi : \; A \mapsto \omega(A) := \frac{< \psi, A\psi >}{< \psi, \psi >}, \qquad A \in \mathcal{A}, \tag{19}$$

generate a foliation of $\mathcal{H} - \{0\}$. Two vectors belong to the same leaf of this foliation iff their vector states (19) coincide. On every leaf act the unitaries (and, in a certain way, the partial isometries) of the commutant $\mathcal{A}'$ of $\mathcal{A}$.

Given a curve

$$s \mapsto \omega_s, \qquad 0 \leq s \leq 1, \tag{20}$$

of vector states of $\mathcal{A}$ there are i.g. many essentially different lifts

$$s \mapsto \psi(s) \quad \text{with} \quad \omega_s = \omega_{\psi(s)} \tag{21}$$

into $\mathcal{H} - \{0\}$. It is an obviously meaningful question wether there is a natural criterium distinguishing certain of these lifts, a *transport condition* selecting - up to the choice of the initial vector - just one lift (21) of a given curve (20). Let me call such a transport condition a *natural parallel transport* where the word *natural* means that the transport depends on $\mathcal{H}$ and $\mathcal{A}$ only.

Such a natural parallel transport gives rise to an *holonomy problem*: A closed curve of vector states will generally not induce a closed parallel lift. If things work well, and (21) is a parallel lift of (20) then the linear functional

$$A \mapsto \nu(A) =< \psi(0), A\psi(1) >, \qquad A \in \mathcal{A}, \tag{22}$$

should depend *only* on the original curve (20). In particular, $\nu(\mathbf{1})$ then would generalize what is called Berry's phase factor (see next section).

An ansatz which will be sufficient for an important class of curves (20) is the following preliminary definition [7]: A lift (21) of (20) is parallel if it is of constant norm and fulfills

$$(\dot{\psi}, B\psi) = (\psi, B\dot{\psi}) \quad \text{for all} \quad B \in \mathcal{A}'. \tag{23}$$

This is, as will be shown later on, a reasonable set of conditions which are similar to the Berry - Simon one.

If the algebra of observables is $\mathcal{B}(\mathcal{H})$, as it was assumed at the beginning, its commutant consists of the multiples of the identity map only, and (23) means that the lift (21) in this case satisfies (16) resp. (16a), i.e. the condition of Berry and Simon.

In the setting above it is without further assumptions unclear, which states of the algebra $\mathcal{A}$ can be given by vector states, and how to handle the other states. To circumvent this a more satisfying way is in performing extensions instead of reductions of states. First of all this is nothing than inverting the point of view: One starts with $\mathcal{A}$ and asks for unital embeddings of $\mathcal{A}$ into $\mathcal{B}(\mathcal{H})$ such that all or a reasonable part of the states of $\mathcal{A}$ become reductions of pure vector states of $\mathcal{B}(\mathcal{H})$. One has to ensure, however, that the final results do *not* depend on the choice of the embedding.

2. Parallel Transport

The parallel transport can be realized in rather different bundle spaces and I describe one which is embedded in $\mathcal{B}(\mathcal{H})$. Again I start with problems for pure states before switching to a slightly larger class and to the general case.

An operator V is called a *partial isometry* iff VV^* and (consequently) V^*V are projection operators referred to as the *left* and the *right support* of V respectively.

Working with pure states one remains in the set of partial isometries of rank one. A partial isometry of rank one, V, can be written as

$$V = |\psi(1) >< \psi(0)|, \quad VV^* = P_1 \quad V^*V = P_0 \tag{1}$$

with two normed vectors, and it may be interpreted as annihilating the 'in state' $P_0 = |\psi(0) >< \psi(0)|$ and creating the 'out state' $P_1 = |\psi(1) >< \psi(1)|$. Given the in- and out-states this operation is fixed up to a phase factor because every $\mathbf{P}\mathcal{H}$-invariant for pairs of states depends 0nly on the transition probability

$$\mathrm{tprob}(P_0, P_1) = | < \psi(0), \psi(1) > |^2 = \mathrm{tr}(P_0 P_1) \tag{2}$$

This slight arbitrariness cannot be removed without introducing a new structural element.

This new structural element is a curve, $\mathbf{c}$, connecting smoothly P_0 and P_1:

$$\mathbf{c} \, : \, s \mapsto P_s, \quad 0 \le s \le 1, \tag{3}$$

With the aid of the following construction it is possible to fix the phase factor in dependence on $\mathbf{c}$. One takes subdivisions

$$1 > s_1 > s_2 > \, \ldots \, > s_m > 0 \tag{4}$$

of the parameter s of the curve and perform [8], [9],

$$V = V(\mathbf{c}) := \lim P_1 P_{s_1} P_{s_2} \ldots P_{s_m} P_0 \tag{5}$$

where the limiting procedure is taken over finer and finer subdivisions (4). To calculate V one uses a *lifted* path

$$\mathbf{c}^{\mathrm{lift}}: \quad s \mapsto \psi(s), \qquad \text{with} \quad P_s = |\psi(s)><\psi(s)| \tag{6}$$

of unit vectors with which (5) is converted into

$$V = |\psi(1)><\psi(0)| \lim <\psi(1), \psi(s_1)><\psi(s_1), \psi(s_2)> \ldots <\psi(s_m), \psi(0)> \tag{7}$$

If (6) is twice differentiable one estimates by Taylor's theorem

$$|1 + (t-s) <\dot{\psi}(s), \psi(s)> - <\psi(s), \psi(t)>| \leq (t-s)^2 \,\mathrm{const.}. \tag{8}$$

where the constant is independent of s and t. One knows that (7) converges absolutely if

$$\lim \sum |<\psi(s_{k+1}), \psi(s_k)> -1| \tag{9}$$

is absolutely converging. But (8) guaratees that (9) converges absolutely towards

$$\int |<\dot{\psi}(s), \psi(s)>| \,\mathrm{d}s. \tag{9a}$$

The existence of (5) is now established.

It is convenient to require

$$<\psi(s), \dot{\psi}(s)>= 0 \tag{10}$$

before performing (7). At this place the parallelity condition appears as a technical device, and the result of (5) or (7) does *not* depend on it. With (10) the estimate (8) results in

$$V(\mathbf{c}) = |\psi(1)><\psi(0)| \quad \text{if} \quad <\psi, \dot{\psi}>= 0. \tag{11}$$

For an *arbitrary* lift (5) it follows

$$V(\mathbf{c}) = |\psi(1)><\psi(0)| \,\exp \int <\mathrm{d}\psi, \psi> \tag{11a}$$

because its right hand side is compatible with (10) and invariant against gauge transformations

$$\psi(s) \mapsto \epsilon(s)\psi(s), \qquad |\epsilon(s)| = 1 \tag{12}$$

Only one eigenvalue of (11) can be different from zero, and its value is Berry's phase factor

$$\mathrm{Berry}(\mathbf{c}) = \exp \int <\mathrm{d}\psi, \psi>= \,\mathrm{tr}\, V(\mathbf{c}) \tag{13}$$

The modulus of (13) is at most one. It equals one iff $\mathbf{c}$ is closed, i.e. a loop.

Essential parts of what was and will be said in this section is true for projections and partial isometries of arbitrary finite rank. A first assertion is:

If (3) is a smooth curve of projection operators of rank k then (5) converges, and the result is a partial isometry $V(\mathbf{c})$ of rank k with left support P_1 and right support P_0.

It will further become evident that for these curves there is a completely invariant characterization of (1-22) by

$$\nu_{\mathbf{c}}(A) = \frac{1}{k}\mathrm{tr}\,\big(V(\mathbf{c})A\big) \tag{14}$$

such that Berry's phase factor is

$$\mathrm{Berry}(\mathbf{c}) = \frac{1}{k}\mathrm{tr}\,\big(V(\mathbf{c})\big) = \nu_{\mathbf{c}}(1) \tag{15}$$

To prove (3) for projections of rank k one writes

$$P_s = \sum |\psi_j(s) >< \psi_j(s)| \tag{16}$$

and requires for the curve of orthonormal k-frames $\psi_1, \cdots, \psi_k$ the auxiliary condition

$$< \psi_j, \dot{\psi}_i >= 0 \quad \text{for all} \quad i, j \tag{17}$$

To my knowledge (17) appeared first in an appendix of Fock's paper [10] as a condition that the phases of k-frames belonging to a degenerate eigenvalue of a time-dependent hamiltonian change as slowly as possible in the course of time. (17) is also known as defining a parallel transport in the fibre bundle of orthonormal k-frames (Stiefel manifolds). Extending Berry's anholonomy to curves of degenerate eigenstates and introducing the associated gauge theory is the idea of [11].

With (17) the right hand side of (5) decomposes into a sum of k independent product integrals (7). But their convergence to rank one projections is already established. Hence the assertion is proved.

For k fixed the mapping

$$\mathbf{c} \mapsto V(\mathbf{c}) \tag{18}$$

can be interpreted as morphism from the groupoid of curves onto the groupoid of rank k partial isometries. The term *groupoid* indicates that two curves can be multiplicated if and only if the end of the first coincides with the beginning of the second. In the same spirit the multiplication of two partial isometries is allowed iff the right support of the first equals the left support of the second. It is now plain to see from (5)

$$V(\mathbf{c}_1\mathbf{c}_2) = V(\mathbf{c}_1)V(\mathbf{c}_2), \tag{19}$$

$$V(\mathbf{c}^{-1}) = V(\mathbf{c})^*. \tag{20}$$

Let me comment on (20) as follows. (5) implies that $V(\mathbf{c})$ does not depend on the way $\mathbf{c}$ is parametrized. But it depends on its orientation. Reversing the orientation gives $\mathbf{c}^{-1}$.

By the help of (5) one can get a differential equation for the morphism (18) of a curve (3) with varying endpoint. To this end one considers the curve

$$\mathbf{c}_s \,:\, t \mapsto P_t, \quad 0 \leq t \leq s \tag{21}$$

and the corresponding

$$V_s \,:=\, V(\mathbf{c}_s) \tag{22}$$

to arrive at

$$\dot{V}_s = \dot{P}_s V_s \tag{23}$$

(22) as defined by (21) and (5) is the unique solution of the differential equation (23) with initial value $V_0 = P_0$.

One can give to the solutions of (23) a special format. At first an arbitrary (sufficiently regular) curve $s \mapsto V_s$ may be represented in the following way. One chooses orthonormal k-frames

$$s \mapsto \{\psi_1(s), \ldots \psi_k(s)\} \in V_s\mathcal{H} \quad \text{with} \quad < \psi_j, \dot{\psi}_i >= 0 \tag{24}$$

fulfilling the transport condition (17). Then, reminding $P = VV^*$, there is a *unique* second orthoframe

$$s \mapsto \{\tilde{\psi}_1(s), \ldots \tilde{\psi}_k(s)\} \in P_s\mathcal{H} = V_s^*\mathcal{H} \tag{25}$$

such that

$$V_s = \sum |\psi_j >< \tilde{\psi}_j|. \tag{26}$$

(26) is a solution of (23) if and only if the orthoframe (25) does *not* depend on s, provided (24) is valid.

The proof is a simple matter of calculation after inserting (26) into (23). In the same straightforward manner one proves:

The following three condition on a curve $s \mapsto V_s$ are mutually equivalent:

$$\dot{V} = \dot{P}V, \qquad V^*\dot{V} = 0, \qquad V^*\dot{V} = \dot{V}^*V. \tag{27}$$

If one - and hence all - of these conditions are fulfilled the curve $s \mapsto V_s$ is called a *parallel* lift of $s \mapsto P_s$ into the space of partial isometries of rank k. Equivalently one may characterize such parallel lifts as being *integral curves* of the differential 1-forms

$$\mathrm{d}V - (\mathrm{d}P)V, \qquad V^*\mathrm{d}V, \qquad \frac{1}{2}\big(V^*\mathrm{d}V - \mathrm{d}V^*V\big). \tag{28}$$

The last one is an antihermitian connection form. This requires a comment and I denote for that purpose by $\mathcal{I}_k$ the space of partial isometries of rank k. For any k-dimensional projection operator, P, the fibre $\mathcal{I}_k^P$ is the set of all V with $VV^* = P$. Let

$$V \mapsto VU, \quad V^*V \leq UU^* \tag{29}$$

be a map with partial isometries U depending on V. Then one gets from (29)

$$V^*\mathrm{d}V - \mathrm{d}V^*V \mapsto U\big(V^*\mathrm{d}V - \mathrm{d}V^*V\big)U^* + U^*\mathrm{d}U - \mathrm{d}U^*U \tag{30}$$

However, the partial isometries do not constitute a group. To get a *gauge group* one has to use in (29) the *unitary* transformations. But then $-\mathrm{d}U^* U = U^* \mathrm{d}U$. Hence the third expression of (28) is a connection form of the unitary group of $\mathcal{H}$.

It remains to say how all this could fit to the last part of section 1. Of course $\mathcal{I}_k$ is not a Hilbert space but it is elegantly embedded in the Hilbert space of Hilbert Schmidt operators

$$\mathcal{H}^{HS} = \{W \in \mathcal{B}(\mathcal{H}) : \mathrm{tr}\, W W^* < \infty\}, \quad < W_1, W_2 >= \mathrm{tr}\, W_1^* W_2 \tag{32}$$

To that space one applies what has been said at the end of section 1 where the *-subalgebra $\mathcal{A}$ of $\mathcal{B}(\mathcal{H}^{HS})$ is identified with the set of mappings

$$\mathcal{A} = \{W \mapsto AW,\ A \in \mathcal{B}(\mathcal{H})\} \tag{33}$$

A curve of projections of rank k can be understood as coming from a curve of density operators on $\mathcal{H}$ of the form

$$s \mapsto \varrho_s := \frac{1}{k} P_s \tag{34}$$

This curve will now be interpreted as the *reduction* of any curve

$$s \mapsto \frac{1}{\sqrt{k}} V_s \in \mathcal{H}^{HS}, \quad V_s V_s^* = P_s \tag{35}$$

In turn, every curve (35) *purifies* the curve of mixted states (34). Because one has in the present setting

$$\mathcal{A}' = \{W \mapsto WA,\ A \in \mathcal{B}(\mathcal{H})\} \tag{36}$$

it can be verified straightforwardly that (1-23) is equivalent to the last equation of (27). Indeed this calculation can be done in more general terms using the fact that *every* density operator ϱ of $\mathcal{H}$ can be purified by decompostions

$$\varrho = WW^*, \qquad W \in \mathcal{H}^{HS}. \tag{37}$$

Thus *every* curve of density operators of H

$$\mathbf{c} : s \mapsto \varrho_s \tag{38}$$

can be purified, i.e. lifted into a curve of pure vector states of the Hilbert space of Hilbert Schmidt operators, or, what is the same, can be gained by reductions of pure states

$$\mathbf{c}^{\text{lift}} : s \mapsto W_s \in \mathcal{H}^{HS}, \quad \varrho_s = W_s W_s^* \tag{39}$$

Because of (36) rewriting (1-19) results in

$$\mathrm{tr}\, \dot{W}^* (WA) = \mathrm{tr}\, W^* (\dot{W} A)$$

for all bounded operators A on $\mathcal{H}$. This can be valid only if

$$\dot{W}^* W = W^* \dot{W}, \tag{40}$$

and in this form (1-23) has been derived in [3]. It is therefore reasonable to call (39) a *parallel lift* or a *parallel purification* of (38) if (40) is valid.

To look at the set of unit vectors of $\mathcal{H}^{HS}$ as to a fibre bundle with the unitary group of $\mathcal{H}$ and with the (not singular) density operators as its base space has been stressed in [12]. See also [13] for problems of interpretation.

An ansatz

$$\dot{W}_s = G_s W_s \quad \text{with} \quad G_s = G_s^* \tag{41}$$

obviously solves (40). Differentiating (37) and replacing $\dot{W}$ by (41) immediatly shows

$$\dot{\varrho} = G\varrho + \varrho G. \tag{42}$$

That methode appeared in [12], [9]. It fits very well with (23) for curves of parallel isometries where $G = \dot{P}$.

3. The Minimal Length Property

The inequaltiy

$$\frac{<\dot{\psi}, \dot{\psi}>}{<\psi, \psi>} \geq \frac{<\dot{\psi}, \dot{\psi}>}{<\psi, \psi>} - \frac{<\psi, \dot{\psi}><\dot{\psi}, \psi>}{<\psi, \psi>^2} \tag{1}$$

where the right hand side is the lifted projective metric of $\mathbf{P}\mathcal{H}$, shows that Berry's parallelity condition results from minimizing $<\dot{\psi}, \dot{\psi}>$. Hence parallel lifts can be considered as those of shortest length.

Before combining this with the previously discussed scheme a historical remark is in order. If a k-dimensional subspace (or its projection) moves smoothly through its Hilbert space, there are numerous comoving orthonormal bases. How can one avoid 'unnecessary' rotations of these k-frames? The answer given in [10] was to require

$$\int \mathrm{d}t \sum <\dot{\psi}_j, \dot{\psi}_j> = \text{Min !} \tag{2a}$$

This simple variational problem implies as its necessary condition (its 'Euler equations')

$$<\psi_j, \dot{\psi}_k> = 0. \tag{2b}$$

These ideas can easily be used to produce the parallelity conditions (1-23), (2-40), and similar ones. To prepare this let $\mathcal{H}^{\text{ext}}$ be the Hilbert space of an extended system and $\mathcal{A}$ a unital *-subalgebra of $\mathcal{B}(\mathcal{H}^{\text{ext}})$.

Remark. Up to the notation 'ext' things are as in the last part of section 1. In section 2 the role of $\mathcal{H}^{\text{ext}}$ is played by $\mathcal{H}^{\text{HS}}$.

A curve

$$\mathbf{c} : s \mapsto \omega_s \qquad \text{with} \quad 0 \leq s \leq 1 \tag{3}$$

of states of $\mathcal{A}$ can be *purified* by embedding $\mathcal{A}$ into $\mathcal{B}(\mathcal{H}^{\rm ext})$ with large enough $\mathcal{H}^{\rm ext}$ so that there exists a curve

$$\mathbf{c}^{\rm lift} : s \mapsto \psi(s) \in \mathcal{H}^{\rm ext} \tag{4}$$

with

$$\omega_s(A) = < \psi(s), A\psi(s) > \quad \text{for all} \quad A \in \mathcal{A}. \tag{5}$$

(4) is clearly not fixed by (3) and the arbitrariness is the larger the bigger is $\mathcal{A}'$, the commutant of $\mathcal{A}$ in $\mathcal{B}(\mathcal{H}^{\rm ext})$. Indeed, every curve of paritial isometries

$$s \mapsto U_s \in \mathcal{A}' \quad \text{with} \quad \| \psi(s) \| = \| U_s\psi(s) \| \tag{6}$$

gives a new purifying curve

$$s \mapsto \psi'(s) = U_s\psi(s) \tag{7}$$

The purification ambiguity can be diminished by the requirement

$$\int \sqrt{< \dot\psi, \dot\psi >} \mathrm{d}s = \text{Min !} \quad \text{or} \quad \int < \dot\psi, \dot\psi > \mathrm{d}s = \text{Min !} \tag{8}$$

where the extrema are taken on the set of all lifts (4) satisfying (5). For sufficiently regular curves this is locally equivalent to

$$< \dot\psi, \dot\psi > = \text{Min !} \tag{9}$$

If (4) is an admissable curve and $B \in \mathcal{A}'$ then (6) with $U_s = \exp \mathrm{i}sB$ gives rise to another such curve. The assumption that (4) is already solving (9) or (8) will result in

$$0 \leq < B\psi, B\psi > + i[< \dot\psi, B\psi > - < \psi, B\dot\psi >] \tag{10}$$

This set of inequalties can valid for all B iff

$$< \dot\psi, B\psi > = < \psi, B\dot\psi > \quad \text{for all} \quad B \in \mathcal{A}' \tag{11}$$

(11) is proved above for hermitian B. But these operators span $\mathcal{A}'$ linearly.

Because of (5) one is working with unit vectors by definition. For curves within $\mathcal{H}^{\rm ext} - \{0\}$ one either requires the constancy of the vector norms explicitely, or, with the same effect, demands

$$\frac{< \dot\psi, \dot\psi >}{< \psi, \psi >} = \text{Min !} \tag{12}$$

for parallelity of the lifts (4). However, the conditions (11) remain valid under arbitrary rescaling of the vector norms.

It is highly desirable to know for what curves (3) there exists a unique holonomy, i.e. a unique

$$\nu_{\mathbf{c}}(A) = < \psi(0), A\psi(1) >, \qquad A \in \mathcal{A} \tag{13}$$

depending on $\psi(0)$ and $\psi(1)$, the initial and finite vectors of an *arbirary* parallel lift. This amounts to the s-independence of U_s if (4) and (7) both produce the minima of (9) or fulfil (11). See also [9] for this problem.

Here I circumvent this problem by trying to establish the correctness of (13) directly for the particular but improtant case

$$\mathcal{A} = \mathcal{B}(\mathcal{H}) \quad \text{and} \quad \mathcal{H}^{\text{ext}} = \mathcal{H}^{\text{HS}}$$

already introduced in section 2. Let (3) be given as a curve of density operators on $\mathcal{H}$

$$\mathbf{c} : s \mapsto \varrho_s \qquad \text{with} \quad 0 \leq s \leq 1 \tag{14}$$

and a lift

$$\mathbf{c}^{\text{lift}} : s \mapsto W_s, \qquad \varrho_s = W_s W_s^* \tag{15}$$

of *minimal* length. The *Bures length* [14] of (14) is now the Hilbert space length of (15). Our next task is to use a polygon approximation to the curve (15), and to express this in terms of the curve (14).

With the aid of the polar decompoition

$$W_j = \varrho_j^{\frac{1}{2}} U_j \tag{16}$$

one gets

$$W_1 W_0^* = \varrho_1^{\frac{1}{2}} U_1 U_0^* \varrho_0^{\frac{1}{2}}. \tag{17}$$

For parallel lifts this gives rise to the definitions

$$V(\mathbf{c}) = U_1 U_0^*, \qquad \nu_{\mathbf{c}}(A) = \operatorname{tr} W_0^* A W_1 \quad \text{with} \quad A \in \mathcal{B}(\mathcal{H}) \tag{18}$$

and the aim is to show independence from the chosen parallel lift. This will be done for faithful (non-singular) density operators only. For every subdivision

$$1 > s_1 > s_2 > \ldots > s_m > 0$$

there is the identity

$$\begin{aligned} U_1 U_0^* &= U_1 (U_{s_1}^* U_{s_1})(U_{s_2}^* U_{s_2}) \cdots (U_{s_m}^* U_{s_m}) U_0 \\ &= (U_1 U_{s_1}^*)(U_{s_1} U_{s_2}^*) \cdots (U_{s_m} U_0^*) \end{aligned} \tag{19}$$

The next step is in approximating $U_s U_t^*$ for small $s - t$. Because the curve in question is of minimal length the approximation is done by replacing two neighboured W's by

$$\tilde{W}_s = \varrho_s^{\frac{1}{2}} V_s, \quad \tilde{W}_t = \varrho_t^{\frac{1}{2}} V_t \tag{20}$$

such that these two vectors are of minimal distance. This is settled by the requirement [3]

$$\tilde{W}_s \tilde{W}_t^* = \varrho_s^{\frac{1}{2}} V_s V_t^* \varrho_t^{\frac{1}{2}} \ > \ 0. \tag{21}$$

In this and only in this case $< \tilde{W}_t, \tilde{W}_s >$ is positive and attains its maximal value for all decompositions (20). That maximal value is the root of the transition probability [15] between the two density operators ϱ_s and ϱ_t

$$\text{tprob}(\varrho_s, \varrho_t) = \left(\text{tr}\,(\varrho_t^{\frac{1}{2}}\,\varrho_s \varrho_t^{\frac{1}{2}})^{\frac{1}{2}}\right)^2 \tag{22}$$

A solution of (21) is obviously

$$V_s V_t^* = \varrho_s^{-\frac{1}{2}}\,\varrho_t^{-\frac{1}{2}}\,(\varrho_t^{\frac{1}{2}}\,\varrho_s \varrho_t^{\frac{1}{2}})^{\frac{1}{2}} \tag{23}$$

and the solution is unique, for otherwise one comes into conflict with the uniqueness of the polar decomposition. Writing now

$$X_{s,t} = \varrho_t^{-\frac{1}{2}}\,(\varrho_t^{\frac{1}{2}}\,\varrho_s \varrho_t^{\frac{1}{2}})^{\frac{1}{2}}\,\varrho_t^{-\frac{1}{2}} \tag{24}$$

(19) can be approximated by

$$\varrho_1^{-\frac{1}{2}}\,X_{1,s_1} X_{s_1,s_2} \cdots X_{s_m,0}\,\varrho_0^{\frac{1}{2}}\,. \tag{25}$$

Hence

$$W_1 W_0^* = \lim X_{1,s_1} X_{s_1,s_2} \cdots X_{s_m,0}\,\varrho_0 \tag{26}$$

This indicates that the left hand side of the non-commutative product integral (26) is independent from the choice of the shortest lift of (14), and the same is true with (17) and (18). The aim, to show the correctness of the holonomy problem for parallel lifts for curves of non-singular density operators, has been reached.

It is worthwhile to rewrite (24) and (26) by the help of the non-commutative *geometric* (or *quadratic*) *mean* [16] which can be defined for two positive definite operators by [17]

$$A\#B := A^{\frac{1}{2}}\,(A^{-\frac{1}{2}} B A^{-\frac{1}{2}})^{\frac{1}{2}}\,A^{\frac{1}{2}} \tag{27}$$

Then

$$X_{s,t} = \varrho_s \,\#\, \varrho_t^{-1} \tag{28}$$

Inserting into (26) yields

$$W_1 W_0^* = \lim(\varrho_1 \# \varrho_{s_1}^{-1})(\varrho_{s_1} \# \varrho_{s_2}^{-1}) \cdots (\varrho_{s_m} \# \varrho_0^{-1})\,\varrho_0 \tag{29}$$

Therefore the parallel transport can be described by

$$W_1 = V(\mathbf{c}) W_0 \quad \text{with} \quad V(\mathbf{c}) = \lim(\varrho_1 \# \varrho_{s_1}^{-1})(\varrho_{s_1} \# \varrho_{s_2}^{-1}) \cdots (\varrho_{s_m} \# \varrho_0^{-1}) \tag{30}$$

A cross check ist now that

$$G := \lim_{\epsilon \to 0} \frac{X_{t+\epsilon,t} - \mathbf{1}}{\epsilon} \tag{31}$$

fulfils (2-42), i.e.

$$\dot{\varrho} = \varrho G + G \varrho \qquad (32).$$

The same arguments can be applied for curves of density operators of *constant support*. It should be possible to require only *constant rank* in order that the product integrals above and the ones discussed in section 2 should appear as special cases. Presently the correct format of that (hypothetical) product integral is not known to me.

4. The Connection Form

To get parallel lifts of a curve of states one needs at first a suitable extension in order to represent the original curve as the reduction of a curve of pure states, or, what is the same, to allow for a puification. The arbitrariness of the lifting involved gives rise to a gauge group (or gauge groupoid). It is the aim of the following to show the existence of a natural *connection form* (respectively *gauge potential*) for the parallel transport already discussed. This can and will be done for the normal states of $\mathcal{B}(\mathcal{H})$. Such a state is given by a density operator ϱ of an Hilbert space $\mathcal{H}$ and described by their expectation values

$$\varrho : \quad A \mapsto \varrho(A) := \mathrm{tr}\, \mathrm{A} \varrho \qquad (1)$$

To achieve purification it is sufficient to consider factor extensions, the most important one, the space of Hilbert Schmidt operators, has already be considered. It is convenient to represent these extensions as spaces of Hilbert Schmidt mappings of an Hilbert space $\mathcal{H}'$ into the given Hilbert space $\mathcal{H}$:

$$\mathcal{H}^{\mathrm{ext}} = \mathcal{L}^2(\mathcal{H}', \mathcal{H}) \qquad (2)$$

consisting of all mappings

$$W : \quad \mathcal{H}' \to \mathcal{H} \qquad \text{with} \quad \mathrm{tr}_{\mathcal{H}'} W^* W = \mathrm{tr}_{\mathcal{H}} W W^* < \infty \qquad (3)$$

Here, as usual, W^* is a map from $\mathcal{H}$ into $\mathcal{H}'$ defined by

$$< \psi, W\psi' > = < W^*\psi, \psi' > \qquad \text{for all} \quad \psi \in \mathcal{H}, \quad \psi' \in \mathcal{H}' \qquad (4)$$

so that

$$W^* \in \mathcal{L}^2(\mathcal{H}, \mathcal{H}') \qquad \text{iff} \qquad W \in \mathcal{L}^2(\mathcal{H}', \mathcal{H}) \qquad (5)$$

The scalar product of $\mathcal{B}(\mathcal{H}^{\mathrm{ext}})$ reads

$$(W_1, W_2) := \mathrm{tr}_{\mathcal{H}'} W_1^* W_2 = \mathrm{tr}_{\mathcal{H}} W_2 W_1^* \qquad (6)$$

where $W_2 W_1^*$ respectively $W_1^* W_2$ is in $\mathcal{B}(\mathcal{H})$ respectively $\mathcal{B}(\mathcal{H}')$. One observes that (2) is nothing than $\mathcal{H}^{\mathrm{HS}}$ if $\mathcal{H}' = \mathcal{H}$. Contact with previous notations is reached with

$$\mathcal{A} = \{W \to AW,\, A \in \mathcal{B}(\mathcal{H})\} \qquad \mathcal{A}' = \{W \to WB,\, B \in \mathcal{B}(\mathcal{H}')\} \qquad (7)$$

With this setting a state ϱ can be purified if and only if

$$\operatorname{rank} \varrho \leq \dim \mathcal{H}' \tag{8}$$

The set of all states (densitiy operastors) which satisfy (7) can now be regarded as the base space of the bundle $\mathcal{H}^{\text{ext}} - \{0\}$ with the bundle projection

$$\pi \; : \qquad W \mapsto \varrho := WW^* \, / \, (W, W) \tag{9}$$

The bundle group is the group of unitaries of $\mathcal{B}(\mathcal{H}')$ acting as

$$W \mapsto \tilde{U} = WU \quad \text{whith} \quad U \in \mathcal{B}(\mathcal{H}') \tag{10}$$

The parallelity condition can now be written

$$(\dot{W}, WB) = (W, \dot{W}B) \quad \text{for all} \quad B \in \mathcal{B}(\mathcal{H}')$$

which results in (2-40) with vectors W of the form (3) out of (2). This can be reexpressed in the following way. For a curve of density operators

$$s \mapsto \varrho_s \qquad \text{with} \quad 0 \leq s \leq 1 \tag{11}$$

one looks for purifying curves

$$s \mapsto W_s \in \mathcal{H}^{\text{ext}} = \mathcal{L}^2(\mathcal{H}', \mathcal{H}) \tag{12}$$

annihilating the differential 1-form

$$W^* \mathrm{d}W - (\mathrm{d}W^*)W. \tag{13}$$

This is a form with values in $\mathcal{B}(\mathcal{H}')$ sitting on the space (2). However, it is *not* a connection form for the gauge transformations (10). To remedy that defect I introduce another differential 1-form $\mathbf{A}$ of a similar structure by [18]

$$W^* \mathrm{d}W - (\mathrm{d}W^*)W = W^*W \cdot \mathbf{A} + \mathbf{A} \cdot W^*W \tag{14}$$

It vanishs exactly along parallel lifts, and it is a connection form for the transformations (10). If the support of W equals $\mathcal{H}'$ then (14) determines $\mathbf{A}$ uniquely. Otherwise one has to require additionally

$$< \psi', \mathbf{A}\psi' >= 0 \quad \text{for all} \quad \psi' \in \mathcal{H}' \quad \text{with} \quad W\psi' = 0 \tag{15}$$

With (14) and (15) the differential form $\mathbf{A}$ is completely defined up to those tangential directions $\dot{W}$ for which there does not exist a solution of (14). These directions correspond to tangential directions at the boundary of the base space along which the rank of the density operator is changing.

Using uniqueness it is elementary to show

$$\mathbf{A} + \mathbf{A}^* = 0 \tag{16}$$

and it is a matter of straightforward calculation that a regauging (10) results in

$$\mathbf{A} \mapsto \tilde{\mathbf{A}} =: U^* \mathbf{A} U + U^* \mathrm{d} U \tag{17}$$

It is remarkable that (17) remains valid if one exchanges the auxiliary Hilbert space $\mathcal{H}'$ by another one, say $\mathcal{H}''$, and if U in (10) is an isometry from $\mathcal{H}''$ into $\mathcal{H}'$. Thus the connection forms living on different spaces (2) appear to be 'all the same up to gauge transformations'.

The introduced connection form respects further scale transformations which do not change (9): $\mathbf{A}$ remains *invariant* under scale transformations

$$W \ \mapsto \ \lambda W \tag{18}$$

where λ may arbitrarily vary with W. Hence $\mathbf{A}$ can be considered directly as a connection form defined on $\mathbf{P}\mathcal{H}^{\mathrm{ext}}$.
Remark. If $\mathcal{H}' = \mathcal{H}$ and finite dimensional, and if W^{-1} exists, then $\mathbf{A}$ remains unchanged if W is replaced by $(W^*)^{-1}$. In the base space that transformation becomes $\varrho \to (\varrho^{-1})/\mathrm{tr}(\varrho^{-1})$.

There is a further differential 1-form, $\mathbf{G}$, defined on $\mathcal{H}^{\mathrm{ext}}$ as given by (2) but with values in $\mathcal{B}(\mathcal{H})$ and invariant with respect to gauge transformations (10). It is implicetly defined by

$$\mathrm{d}(WW^*) = \mathbf{G}\, WW^* + WW^*\, \mathbf{G} \tag{19}$$

This is supplemented by

$$< \psi, \mathbf{A}\psi >= 0 \quad \text{for all} \quad \psi \in \mathcal{H} \quad \text{with} \quad W^*\psi = 0 \tag{20}$$

to take care of the null space of W. Again the definition (19) works up to certain directions in the tangent space along which the rank (or von Neumann dimension) of the density operator is diminishing. From the definition follows easily

$$\mathbf{G} = \mathbf{G}^* \tag{21}$$

The differential form $\mathbf{G}$ reflects the operator G introduced at the end of section 2, equation (2-42), and also in section 3, (3-31) and (3-32). Namely, $G\mathrm{d}s$ is the pull back of $\mathbf{G}$ into the base space of density operators along the curve (11).

¿From (2-41) it follows that $dW - \mathbf{G}W$ vanishes allong parallel lifts. Hence

$$\Theta := \mathrm{d}W - W\mathbf{A} - \mathbf{G}W$$

is vanishing along every parallel lift. On the other hand, the covariant $\mathbf{A}$-derivative $\mathrm{D}W$ transforms with (10) like

$$\mathrm{D}W := \mathrm{d}W - W\mathbf{A} \ \mapsto \ \mathrm{D}WU = (\mathrm{d}W - W\mathbf{A})U \tag{22}$$

This and because $\mathbf{G}$ is a gauge invariant, θ transforms covariantly with (10). Because every (smooth enough) lift can be gauged to become a parallel lift, Θ is vanishing for all lifts and has to be zero:

$$\mathrm{d}W - W\mathbf{A} = \mathbf{G}W \tag{23}$$

Having a connection form (a gauge potential) it is tempting to introduce its curvature 2-form

$$\mathbf{F} = \mathrm{d}\mathbf{A} + \mathbf{A} \wedge \mathbf{A} \tag{24}$$

Performing the exterior derivative of (23) one gets

$$W(\mathrm{d}\mathbf{A} + \mathbf{A} \wedge \mathbf{A}) + (\mathrm{d}\mathbf{G} - \mathbf{G} \wedge \mathbf{G})W = 0 \tag{25}$$

$$(\mathrm{d}\mathbf{A} + \mathbf{A} \wedge \mathbf{A})W^* = W^*(\mathrm{d}\mathbf{G} + \mathbf{G} \wedge \mathbf{G}) \tag{26}$$

An more explicite representation of $\mathbf{A}$ is possible by sandwiching (14) with eigenstates of W^*W. This, however, demands knowledge of the eigenvectors of an arbitrary hermitian trace class operator. With the exception of low dimensions, particulary two, this can scarcely be solved effectively. Another methode, using the integral representation (for positive definite X)

$$Y = \int_0^\infty (\exp -sX) Z (\exp -sX)\, ds \quad \text{if} \quad XY + YX = Z$$

is also not easy for calculating, say, $\mathbf{F}$. Therefore, with the exception of pure states, projections, and rank two density operators, up to now, a satisfactory geometrical interpretation of the gauge potential and the curvature remains to be given.

If $\dim \mathcal{H}' = 1$ then $\mathcal{H}^{\mathrm{ext}}$ coincides with $\mathcal{H}$ and it follows directly from (14), see also (1-18),

$$\mathbf{A} = \frac{1}{2} \frac{< \psi, \mathrm{d}\psi > - < \mathrm{d}\psi, \psi >}{< \psi, \psi >} \tag{27}$$

$$\mathbf{F} = \frac{< \mathrm{d}\psi, \mathrm{d}\psi >}{< \psi, \psi >} - \frac{< \psi, \mathrm{d}\psi > \wedge < \mathrm{d}\psi, \psi >}{< \psi, \psi >^2} \tag{28}$$

If W is proportional or equal to a partial isometry, V, see (2-30), then

$$\mathbf{A} = \frac{1}{2}\big(V^*\mathrm{d}V - \mathrm{d}V^*V\big) \tag{29}$$

An explicit expression for $\mathbf{A}$ in the case $\dim \mathcal{H} = 2$ has been given in [19]. While the rank one case shows up monopole structures [1], with rank two one arrives at instanton structures [20].

* * * * *

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