Parallel Transport and Holonomy along Density Operators

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Abstract: We describe a parallel transport and "quantum" holonomy along curves of density operators. We present arguments to show the naturality of our notation.

There is a rich geometric structure, though somewhat hidden, already in the very fundamentals of Quantum Physics.
It is my intention to point at a certain corner of recent interest of those structures. This interest has been triggered by a paper [1] of M. BERRY and a commenting one [2] to that by B. SIMON concerning phase transport accompanying adiabatic ("slow") changes of exterior parameters, for instance within an Hamiltonian.
If one finds adiabatic invariants they can be typically expressed by the help of certain path integrals, and identified with elements of an holonomy group.
In their considerations, BERRY and SIMON arrived at a well known parallel transport within the vector or U(1) bundle which comes naturally with the HILBERT space and its projective structure. In [3] WILCZEK and ZEE extended it to the natural parallel transport in the STIEFEL manifold of m-frames which is based on the GRASSMANN manifold of projectors of rank m . A path within the latter may be given by the degenerated ground states of a slowly varying family of Hamiltonians.
A curve of projection operators (of finite rank) can already be considered as a path of density operators (up to normalization) .
It has been pointed out [4] a rather natural generalization to curves of (not necessarily normalized) density operators. Meanwhile there is even more evidence that this is a "canonical" concept.

Let us denote by $\mathbf{H}$ an HILBERT space, by $\mathbf{S}$ the set of positive semidefinite trace class operators which are considered as density operators up to normalization. (We exclude the zero operator.) Every density operator S gives rise to a state

$$A \rightarrow \langle A \rangle_S = \mathrm{tr}.AS \,/\, \mathrm{tr}.S \tag{1}$$

Thus let us consider a smooth path

$$C : \quad S = S(t) \quad , \quad t \in [0,1] \tag{2}$$

The first step is to lift the path (2) by adding new observables to a curve consisting of pure vector states only. After this procedure our original system is a subsystem of a larger system, and every state (1) is seen as the reduction of a pure state. There is indeed a minimal extension that purifies all possible states (1). It can be described by the HILBERT space $\mathcal{HS}$ of all HILBERT SCHMIDT operators.
Let us call "amplitude of S " every element W of $\mathcal{HS}$ and "phase of S " every partial isometry U satisfying

$$S = W W^* \quad \text{and} \quad W = S^{1/2} U \tag{3}$$

where the support of S and the left support of U coincides. Now at every element of $\mathcal{S}$ (3) defines a fibre within $\mathcal{HS}$ and within the set of partial isometries. Note that the fibre of the phases is indepedent of the normalization of S , and hence it can be considdred as a fibre over the state (1). Therefore, starting with a path of states (2), the problem is in lifting this path into the space $\mathcal{HS}$ and then, by a polar decomposition, into the space of isometries.
Thus let us consider all smooth pathes

$$W = W(t) \quad \text{and} \quad U = U(t) \tag{4}$$

where S , W , U , fulfil (3) for every t . Of course this lifting procedure is up to now highly non-unique. Hence we need a parallel transport mechanism. In the following we shall suppress the subsript t usually, and write $dW = (dW/dt)dt$ for short as well as to handle the case of an arbitrary parameter space.
In [4] the parallel transport condition was argued to be

$$(dW/dt)^* W = W^* (dW/dt) \tag{5a}$$

or, more generally,

$$dW^* W = W^* dW \tag{5b}$$

This requirement is the infinitesimal version of

$$W_1^* W_2 > 0 \tag{6}$$

a condition coming from the theory of transition probabilities for pairs of states [5], see also [6], [7]. If (6) is valid the amplitudes of two faithful states are called "parallel". In this case their scaler product is not only real and positive but attains its maximally possible value for any simultaneous purification of the two states started with. We shall give some further characterizing properties of (5) later on, and let us now list some general consequences of the lifting procedure connected with (5). We introduce for any lifting (4) the forms

$$X = W^* dW - W^* dW \quad , \quad Y = U\, dU^* \tag{7}$$

and look at their transformation properties if W , U , and W' , U' denote two liftings (4) belonging to the same path (2). Then there is

$$W' = W V \quad , \quad U' = U V \tag{8}$$

where the left support of the partial isometry V coincides with the right supports of W and U . One gets

$$Y' = Y + U (V dV^*) U^* \tag{9}$$

$$X' = V^* X V + V^* W^* W dV + dV^* W^* W V \tag{10}$$

Of course V generally depends on the parameter t introduced in (2). One has to have this in mind too for the various projection operators defined as the right (or initial) and left (or final) supports of the isometries involved. These supports are defined as

$$L = U U^* \quad , \quad R = U^* U \tag{11}$$

and in the same way L' and R' using the isometries U' instead. By its very definition we have

$$V\,V^* = R \quad \text{and} \quad V^*\,V = R' \tag{12}$$

Let us call "proper" a lifted path (4) if and only if $X = 0$.
The following statements can shown to be true [4] where the proof at least in the case all partial isometries involved are unitaries is straightforward.
There is, however, one further restriction: Not only the path of density operators has to be sufficiently regular but also the path of their supports. (This excludes certain level crossings and similar things.)
Let us call "proper" a lifted path (4) if and only if $X = 0$.

$$\text{If} \quad X = 0 \quad \text{then} \quad dR = 0 \tag{13}$$

This means: While the left support L equals the support of S and will hence vary according to the structure of the path (2), the right support R of W will not depend on the parameter t . This is a strong restriction for a lifted path to be a proper one. Furthermore,

$$\text{If} \quad X = X' = 0 \quad \text{then} \quad Y = Y' \tag{14}$$

One concludes from this: Two proper liftings connected by (8) are isometrically isomorphic one to another, i. e. V does not vary along the path.

This allows for the following constructions:
Let C be a given path (2) of density operators, and let us select a <u>proper</u> lift (4) . Then

$$\text{AMP}(C) = W(0)\,W(1)^* \quad \text{and} \quad \text{PHASE}(C) = U(0)\,U(1)^* \tag{15}$$

is independent of the choice of the proper lifting of the given path C of density operators. The more PHASE is <u>uniquely</u> defined by the path of states as defined by (1) with $S = S(t)$. (In [4] the functor PHASE has been called RPF i.e. "relative phase factor".)
Let us consider the group of <u>closed</u> curves (2) starting and terminating at $S°$. Then $C \rightarrow \text{PHASE}(C)$ is a group homomorphism into the group of partial isometries the left and right support of which are equal to the support of $S°$. Thus PHASE(C) is an <u>holonomy</u>

invariant attached to the group of curves (2) starting and terminating at the given S° . Of course, AMP(C) is an holonomy invariant too - it does not, however, respect the group structure of the group of pathes. As a matter of fact one gets by PHASE the same invariants as discussed in [1], [2], and [3], provided the curve is a path of finite rank projection operators. In particular, if C consists of 1-dimensional projections, i.e. of pure states, PHASE(C) is a multiple of S° and the multiplier is nothing than (the complex conjugate of) BERRY's phase factor.

For general closed curves of states PHASE(C) depends not only on C but also on the choice of the starting point. If C and C' denote two curves differing only in the choice of their starting points then PHASE(C) and PHASE(C') are isometrically isomorph. This includes identical spectral properties up to the zero-eigenvalues. (The latter can vary by selecting different proper liftings.) This means:
The spectral properties of the restriction of the operator PHASE(C) to its support is an holonomy invariant not depending on the choice of the starting point of the closed curve C .
If it exists

$$\mu(C)^* \qquad \text{where} \qquad \mu(C) = \mathrm{tr.\ PHASE}(C) \tag{16}$$

is the correct generalization of BERRY's phase factor.

One may use (10) to obtain an expression for Y if X = 0 . To do this one chooses for W' the positive square root of $S = S(t)$ which will imply $U' = L$. By (8) we have $V = U^*$. Thus

$$[\, S^{1/2} \,,\, d(S^{1/2}) \,] \quad = \quad S\,Y \; - \; Y^* S \tag{17}$$

$$\text{and} \qquad dL \; = \; Y \; + \; Y^* \tag{18}$$

There are several ways to handle these equations [4]. We shall restrict ourselves here to one simple particular case. If $S = S(t)$ is - up to normalization - a curve of projection operators of fixed finite rank then $L = S$ and the condition $X = 0$ reduces to $W^* dW = 0$. It follows

$$U(t) = |t,1\rangle\langle 1| + \ldots + |t,m\rangle\langle m| \qquad (19)$$

where $|1\rangle, \ldots, |m\rangle$ is an orthonormal system of the subspace the projection R is projecting on while $|t,1\rangle, \ldots, |t,m\rangle$ is an orthonormal base of $L\,\mathbf{H}$. The condition $X = 0$ may now be rewritten as

$$\langle i,t|\ (d/dt)\ |t,k\rangle = 0 \quad \text{for all } i,\ k\ . \qquad (20)$$

This is nothing else than the parallel transport condition in the STIEFEL manifold of orthoframes based an the GRASSMANN manifold of projection operators of rank m (of m-planes) given by $\mathbf{H}$.
It has been proposed in [3] to describe the adiabatic changing of degenerate ground states by the STIEFEL parallel transport shortly described above.
While this transport is well described by a connection (a gauge field structure, as remarked in [3]), there is quite another characterization. FOCK argued in an appendix to [8] that a slow variation of a degenerate ground state will show up in minimal phase changes: In fact, given (19) the relation (20) is the solution of the variation principle

$$\int \mathrm{tr.}\{\ dU^*/dt\ dU/dt\ \}^{1/2}\, dt = \mathrm{Min.!} \qquad (21)$$

(21) is FOCK's proposal and it indeed generalizes to the situation discussed in the present paper.
Let us consider a path C of density operators as given by (2). Then in the family of all liftings $W = W(t)$ of C we look for the minimal solutions of

$$\int \mathrm{tr.}\{\ dW^*\ dW\ \}^{1/2} = \mathrm{Min.!} \qquad (22)$$

It turns out the minimum is reached just for proper liftings and the solution of the variational problem (22) is nothing but $X = 0$.
The prove of this is elementary (assuming differentiability) for curves C consisting of faithful (i.e. non singular) density operators only. Otherwise one should take care of the support problems involved. It is indeed surprising how the additional property of the STIEFEL connection to satisfy an extremal principle with respect to the length of the lifted path remains true for proper liftings of curves (2).

There is a further consequence. The minimal value of (22) with respect to a given path C of density operators is uniquely assigned to C.

$$\mathrm{len}(C) = \int \mathrm{tr.}\{ dW^* dW \}^{\frac{1}{2}} \quad \text{with} \quad W^* dW = dW^* W \tag{23}$$

turns out to be the length of C measured by the metric discovered by BURES [9], i.e. $\mathrm{len}(C)$ is the BURES length of C.
This is derived from the expression of the BURES distance of two density operators S and S' given by

$$\mathrm{dist}(S,S') = \inf [\mathrm{tr.}(W - W')^* (W - W')]^{\frac{1}{2}} \tag{24}$$

where the infimum runs through all the pairs of amplitudes, W, W', of S, S'. For faithful density operators, as is easily seen, the inf is reached if $W^* W'$ is positive definite. It is always

$$\mathrm{dist}(S,S') = [\mathrm{tr.}\{S + S' - 2(S^{\frac{1}{2}} S' S^{\frac{1}{2}})^{\frac{1}{2}} \}]^{\frac{1}{2}} \tag{25}$$

To restate our assertion once more: $W = W(t)$ is a proper lifting of $S = S(t)$ iff the length of $W = W(t)$ measured in the HILBERT metric of $\mathbf{HL}$ equals the length of $S = S(t)$ measured in the BURES metric.

It is amusing to see a further aspect in the construction of proper liftings related to the "algebraic approach" which views observables and states through the eyes of *-algebras, in particular W*-algebras.
Let $\mathbf{M}$ be a W*-algebra, $f = f(t)$ a sufficiently regular path of its states, and ϕ a *-representation with HILBERT space $\mathbf{L}$ allowing for a smooth representation of f as a curve of vector states.
Thus in $\mathbf{L}$ there are normalized vectors $u = u(t)$ with

$$f(t)[a] = \langle u(t), \phi[a]\, u(t) \rangle \tag{26}$$

for all elements a from $\mathbf{M}$ and all t.
Let us denote by $\mathbf{N}$ the commutator algebra of $\phi[\mathbf{M}]$, i.e. the algebra of bounded operators acting on $\mathbf{L}$ and commuting with every $\phi[a]$. Let us now call $u(t)$ a "proper purification" of f if and only if the following two conditions are satisfied:

1) The closure of $\phi[\mathbf{M}]\,u(t)$ does not depend on t .

2) For every positive element b of $\mathbf{N}$

$$\mathrm{Im}\ \langle u(t),\ b\ du(t)/dt \rangle \ = \ 0 \quad \text{for all } t \qquad (27)$$

If $u = u(t)$ is a proper purification of $f(t)$ then the BURES length of f equals the HILBERT metric length of $u = u(t)$. (This can be deduced from [6].) As is seen in the general context of the algebraic approach, the notation of "proper purification" replace that of "proper lifting" the latter appears as a particular case.
Assume now the parameter t is going from 0 to 1 , and $f(0) = f(1)$ Then $u(0)$ and $u(1)$ represent the same vector state. For they are generating the same GNS - subrepresentation in $\mathbf{L}$ there is a unique partial isometry U in $\mathbf{N}$ the left and right support of which is the closure of $\phi[\mathbf{M}]\,u(t)$ and which satisfies $U\,u(0) = u(1)$.
It is possible to show representation independence of this definition provided the conditions 1) and 2) above are fulfilled. This unique U replaces the definition (15) of PHASE in the W^*-algebraic setting.
U is changing by changing in the closed curve f the starting point of the lifting or by multiplying the properly lifted curve by an isometry the right support of which coincides with the closure of $\phi(\mathbf{M})\,u(t)$. By these changes U varies within an equivalence class given by transformations $U \to V^*\,U\,V$ where the isometries V respect the support properties of U .(Remind that the left and right support of U coincide by the very construction of U . If the trace of U exists in $\mathbf{L}$ then it will not vary within the equivalence class just mentioned, and $\mathrm{tr}.U$ will be a good canditate for defining a phase factor a la BERRY in the context of W^*-algebra theory.

The connecting with our previous considerations are such: $\mathbf{M}$ plays the role of the algebra of all bounded operators of $\mathbf{H}$ while $\mathbf{HS}$ becomes the representation space $\mathbf{L}$. ϕ denotes multiplication of W by A from the left. The operators of $\mathbf{N}$ are given by the right multiplication of the elements W of $\mathbf{HS}$ by an operator A .

We have now seen several different possibilities to characterize or to define the same holonomy invariannts (including BERRY's phase factor) for closed curves of mixed ("thermal") states by an appropriate notation of "parallel transport". The latter one seems to be interesting for its own because it contains a certain "non - linearity". Only for curves consisting of multiples of projection operators this non-linearity dissolves and the result is an "ordinary" parallel transport determined by a well known connection.
It is possible to contact our differential geometric setting with different aspects of the adiabatic approximation (see [10], [11], [12]). This, however, will be reported elsewhere.

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