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PARALLEL TRANSPORT AND "QUANTUM HOLONOMY" ALONG DENSITY OPERATORS

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"Quantum holonomy" as defined by Berry and Simon, and based on the parallel transport of Bott and Chern, can be considerably extended. There is a natural "parallelity" $W^* dW = (dW)^* W$ within the Hilbert–Schmidt operators W. This defines parallelity and holonomy along curves of density operators $\varrho = WW^*$. There is an intrinsic nonlinearity in the parallel transport which dissolves for curves of projection operators. In the latter case one comes back to the Bott–Chern parallel transport.

0. Introduction

"Quantum holonomy" arises by considering in Hilbert space a path of vectors with linearly dependent initial and final vectors. Then one transports the phase along the path according to the parallel transport of Bott and Chern [1], or according to Berry [2], by an adiabatic change in the sense of Ehrenfest [3] and Kato [4]. The equivalence of both procedures has been shown by Simon [5]. This method completely covers the case of pure states in which there are enough observables to distinguish every two linearly independent vectors by there expectation values.

Generally, however, a path in a Hilbert space may have linearly independent initial and final vectors, and, nevertheless has to be considered as "closed" by physical reasons. This situation appears when one assumes there are not enough observables at hand to discriminate between all pairs of linearly independent vectors. It is the intention of this note to show the existence of a rich formalism in this more general case extending and including the Bott, Chern, Berry, Simon procedure.

It is convenient and usual to describe mixed states by density operators. To become not to technical we shall stick to this description though a more satisfactory one is that in terms of states of operator algebras. From the point of differential geometry we are working in the bundle of Hilbert–Schmidt operators

based on the manifold (with boundary) of density operators. There is some nonlinearity in the parallel transport we are considering which seems unavoidable, and which dissolves by restricting to the projective manifold of the pure states (or to the Grassmann manifold of projections of a given rank). In the latter case the parallel transport is determined by the Kähler metric of these manifolds.

At the time being we do not touch the problem of adiabatic changes. We hope to come back to this question.

1. Parallelity

In the following we consider positive trace class operators, ϱ, which we shall interprete as (unnormalized) density operators:

Every such operator uniquely defines a state

$$A \to \langle A \rangle_\varrho = \mathrm{Tr}(A\varrho)/\mathrm{Tr}\,\varrho, \tag{1}$$

which is, in general, a mixture of pure states.

One calls (1) "faithful", iff all the eigenvalues of ϱ are non-zero. At first, until removing this restriction explicitly, we shall consider faithful states and their (eventually unnormalized) density operators only.

We shall introduce some simple terminology. An operator W is called an "amplitude of ϱ", and a unitary U is called a "phase factor of ϱ" iff

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

is valid. Thus the phase factor comes from a polar decomposition of the amplitude. Let us next consider an ordered pair $/\varrho_1, \varrho_2/$ of density operators and corresponding pairs $/W_1, W_2/$ and $/U_1, U_2/$ of amplitudes and phase factors. These pairs of amplitudes and phase factors are called *parallel* if and only if

$$W_1^* W_2 = W_2^* W_1 > 0. \tag{3}$$

The requirement (3) is a known and quite natural one in the theory of "transition probabilities" for pairs of mixed states [6, 7]: The square of the trace of (3) is the "transition probability" of the pair $/\varrho_1, \varrho_2/$. One simply deduces that the spectrum of the operator (3) is an invariant of the pair $/\varrho_1, \varrho_2/$.

Let $/W_1, W_2/$ be a pair of parallel amplitudes and $/U_1, U_2/$ of phase factors of $/\varrho_1, \varrho_2/$. Then

(a) $/W_2, W_1/$ and $/U_2, U_1/$ are parallel pairs for $/\varrho_2, \varrho_1/$.

(b) If r_1 and r_2 are positive numbers then $/(r_1)^{1/2} W_1, (r_2)^{1/2} W_2/$ and $/U_1, U_2/$ are parallel for $/r_1 \varrho_1, r_2 \varrho_2/$.

(c) $/VW_1, VW_2/$ and $/VU_1, VU_2/$ are parallel for $/V\varrho_1 V^*, V\varrho_2 V^*/$ for all unitaries V.

Most important, however, is the following. Let $/\tilde{W}_1, \tilde{W}_2/$ be another pair of

parallel amplitudes belonging to the same pair $/\varrho_1, \varrho_2/$ of density matrices. Then there are unitaries, V_1, V_2 such that $\tilde{W}_j = W_j V_j$.

Parallelity requires

$$\tilde{W}_1^* \tilde{W}_2 = V_1^* W_1^* W_2 V_2 > 0$$

together with (3). By the uniqueness of the polar decomposition one now concludes $V_1 = V_2$.

STATEMENT 1. *Let $/W_1, W_2/$ and $/U_1, U_2/$ be pairs of parallel amplitudes and phase factors of $/\varrho_1, \varrho_2/$ respectively. Then all other parallel pairs are gained by the simultaneous replacement*

$$W_j \to W_j V \quad \text{and} \quad U_j \to U_j V, \tag{4}$$

where V runs through all the unitary operators.

One sees that

$$W_1 W_2^* \quad \text{and} \quad U_1 U_2^*$$

only depend on the ordered pair of density matrices and not on the particular choice of the pairs of parallel amplitudes and phase factors.

Thus we may *uniquely* define relative amplitudes and phase factors

$$AMP(\varrho_1, \varrho_2) = W_1 W_2^* \quad \text{and} \quad RPF(\varrho_1, \varrho_2) = U_1 U_2^*. \tag{5}$$

Before giving explicit expressions we draw some conclusions from (2) and (3).

$$AMP(\varrho_1, \varrho_2) = \varrho_1^{1/2} RPF(\varrho_1, \varrho_2) \varrho_2^{1/2}, \quad (AMP)^2 = \varrho_1 \varrho_2. \tag{6}$$

It is easily seen that

$$\text{iff } \varrho_1 \varrho_2 = \varrho_2 \varrho_1 \text{ then } AMP = \varrho_1^{1/2} \varrho_2^{1/2} \quad \text{and} \quad RPF = \mathbf{1}, \tag{7}$$

i.e. a commuting pair of density matrices gives raise to trivial RPF. The following relations can be expressed also through AMP by using (6):

$$RPF(\varrho_1, \varrho_2) = RPF(\varrho_2, \varrho_1)^* \tag{8}$$

$$RPF(V\varrho_1 V^*, V\varrho_2 V^*) = VRPF(\varrho_1, \varrho_2) V^* \tag{9}$$

for all unitaries, V. For all positive real numbers r_1, r_2 the equality

$$RPF(r_1 \varrho_1, r_2 \varrho_2) = RPF(\varrho_1, \varrho_2) \tag{10}$$

holds. Hence RPF depends only on the states (1) induced by the density operators involved.

There are several ways of constructing parallel pairs of amplitudes and phase factors for a given ordered pair $/\varrho_1, \varrho_2/$ of density matrices. An example is

$$W_1 = \varrho_1^{1/2}, \quad W_2 = \varrho_1^{-1/2} (\varrho_1^{1/2} \varrho_2 \varrho_1^{1/2})^{1/2}. \tag{11}$$

It provides us with

$$AMP(\varrho_1, \varrho_2) = \varrho_1^{1/2}(\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{1/2}\varrho_1^{-1/2}, \tag{12}$$

$$RPF(\varrho_1, \varrho_2) = (\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{1/2}\varrho_1^{-1/2}\varrho_2^{-1/2} = (\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{-1/2}\varrho_1^{1/2}\varrho_2^{1/2}. \tag{13}$$

To get the last expression in (13) the unitarity of RPF has been used. Let us adapt the notation of absolute value $|A| = (AA^*)^{1/2}$ for operators. Then

$$|\varrho_1^{1/2}\varrho_2^{1/2}| = (\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{1/2} \tag{14}$$

and we see from the last expression in (13) that

$$\varrho_1^{1/2}\varrho_2^{1/2} = |\varrho_1^{1/2}\varrho_2^{1/2}|\, RPF(\varrho_1, \varrho_2). \tag{15}$$

Remark 1. Equation (15) provides good grounds for extending our notations to all (not only faithful) density operators. To define RPF by this equation one considers it as a polar decomposition, i.e. one demands $RPF(\varrho_1, \varrho_2)$ to be a partial isometry the left (and right) support of which coincides with the right (and left) support of $\varrho_1^{1/2}\varrho_2^{1/2}$. We shall adapt this as a definition of RPF for all pairs of density operators. Then AMP will be defined through the first relation of (6). In (7), in the case of commuting density operators, RPF is equal to the support of AMP.

EXAMPLE 1. Let P_1 and P_2 be two projection operators of rank m. They can be represented by two orthonormal systems of m vectors as

$$P_j = |j, 1\rangle\langle 1, j| + |j, 2\rangle\langle 2, j| + \ldots + |j, m\rangle\langle m, j|. \tag{16}$$

Using the freedom in the choice of the orthonormal systems we can achieve

$$\langle k, 1|2, i\rangle = 0 \text{ if } k \neq i \quad \text{and} \quad \langle k, 1|2, k\rangle \geqslant 0. \tag{17}$$

If then $|1\rangle, |2\rangle, \ldots, |m\rangle$ denotes an arbitrary third orthonormal system of the same length the amplitudes

$$W_j = |j, 1\rangle\langle 1| + |j, 2\rangle\langle 2| + \ldots + |j, m\rangle\langle m| \tag{18}$$

of the projections satisfy (3). Using (15) to define AMP and RPF according to Remark 1 we get

$$RFP(P_1, P_2) = |1, 1\rangle\langle 1, 2| + |1, 2\rangle\langle 2, 2| + |1, m\rangle\langle m, 2| = AMP(P_1, P_2). \tag{19}$$

Remark 2. Using Remark 1 it is possible to define RPF and AMP for pairs of normal states in W^*-algebras in a representation independent manner.

2. Transport of phase factors: the discrete case

We shall now consider ordered sets of density operators, at first discrete ones and then curves, and try to transport phases "parallely" along them. As previously,

we suppose the density operators induce faithful states. Thus let

$$C = /\varrho_1, \varrho_2, \ldots, \varrho_{n+1}/ \tag{20}$$

be an ordered set of density matrices. For every ϱ_j we choose an amplitude W_j and a phase U_j according to (2) as follows. We choose W_1 (or U_1) arbitrary. But then we choose inductively W_{j+1} to be parallel to W_j for $j = 1$ to $j = n$. We obtain ordered sets

$$/W_1, W_2, \ldots, W_{n+1}/ \quad \text{and} \quad /U_1, U_2, \ldots, U_{n+1}/, \tag{21}$$

where nearest neighbours are parallel in the sense of (3).

Apart from C in (20) these sets depend on the choice of W_1 (or U_1) only, and changing W_1 into $W_1 V$ and U_1 into $U_1 V$ with a unitary V implements the change of W_j and U_j into $W_j V$ and $U_j V$ for all j.

Therefore the expressions

$$RFP(C) = U_1 U_{n+1}^* \quad \text{and} \quad AMP(C) = W_1 W_{n+1}^* = \varrho_1^{1/2} RFP(C) \varrho_2^{1/2} \tag{22}$$

are *uniquely* attached to the ordered set C of density matrices we started with.

One may glue together two ordered sets provided the last member of the first coincides with the first member of the last: If

$$C' = /\varrho_{n+1}, \ldots, \varrho_{n+m}/ \text{ then } CC' = /\varrho_1, \varrho_2, \ldots, \varrho_{n+1}, \ldots, \varrho_{n+m}/. \tag{23}$$

Now the following rule is obvious from the definition

$$RPF(CC') = RPF(C) RPF(C'). \tag{24}$$

Define further $C^* = /\varrho_{n+1}, \varrho_n, \ldots, \varrho_1/$ if C is given by (24). Then

$$RPF(C)^* = RPF(C^*). \tag{25}$$

The map $C \to RPF(C)$ is the "discrete" version of the "*parallel transport* of phase factors" in the case where all density operators give rise to faithful states.

We shall now skip the faithfulness assumption. Thus let C be given as above but we allow the ϱ_j to have zero eigenvalues too. We then try to write

$$RPF(C) = RPF(\varrho_1, \varrho_2) RPF(\varrho_2, \varrho_3) \ldots RPF(\varrho_n, \varrho_{n+1}) \tag{26}$$

and try to assure this to give an partial isometry.

Let us call C "admissable" iff for $j = 2$ to $j = n$ the right support of $RPF(\varrho_{j-1}, \varrho_j)$ equals the left support of $RPF(\varrho_j, \varrho_{j+1})$. This, indeed, guarantees $RPF(C)$ to be a partial isometry, and it gives no further condition in the "faithful case".

We shall abbreviate the notion "discrete ordered admissible set of density operators" by the three letters *AOS*.

Let us now consider two *AOS*, C and C', as in (20) and (23). We then allow to

form the "product" CC' iff the right support of $RPF(\varrho_n, \varrho_{n+1})$ equals the left support of $RPF(\varrho_{n+1}, \varrho_{n+2})$. With this condition CC' is an *AOS* for admissible C and C'.

The family of all *AOS* now forms a groupoid. *RPF* is a morphism into the groupoid of the partial isometries. In the latter multiplication of two partial isometries is allowed only if the right support of the first and the left support of the second factor coincides.

We have to add some technicalities.

1. It is worth considering an *AOS* consisting of one density operator only. We define

$$/\varrho//\varrho, \varrho', .../ = /\varrho, \varrho', .../ \quad \text{and} \quad /..., \varrho', \varrho//\varrho/ = /..., \varrho', \varrho/, \tag{27}$$

i.e. if the product exists $/\varrho/$ acts as a left (or right) unit. Furthermore, we set

$$RPF(/\varrho/) = \text{support}(\varrho). \tag{28}$$

2. We want to introduce an equivalence relation between admissible ordered sets of density operators. To this aim we consider certain subsequences of neighbouring density operators in such an *AOS* and replace them by "equivalent" ones.

Two *AOS*, C and $\hat{C}$, are called "equivalent" iff they can be transformed one into another by a sequence of the following steps:

a. A subsequence of the form ϱ, ϱ is replaced by ϱ.

b. A single element ϱ is replaced by ϱ, ϱ.

c. A subsequence $\varrho, \varrho', \varrho$ is replaced by ϱ.

d. A single element ϱ is replaces by $\varrho, \varrho', \varrho$, where $/\varrho, \varrho', \varrho/$ is admissible.

We shall write $C \sim \hat{C}$ iff C and $\hat{C}$ are equivalent.

STATEMENT 2. *If* $C \sim \hat{C}$ *then* $RPF(C) = RPF(\hat{C})$.

This simple consequence of the definition is satisfactory: Looking at an *AOS* it is tempting to interpret it as a discretized path. From this point of view equivalent sets should be modifications not touching the result of a "parallel transport".

The equivalence classes form a groupoid in a natural way: Assume $C \sim \hat{C}$ and $C' \sim \hat{C}'$. If CC' exists then there exists $\hat{C}\hat{C}'$ and it follows that $CC' \sim \hat{C}\hat{C}'$.

Let us now consider the *AOS*

$$C_1 = /\varrho_1, \varrho_2, ..., \varrho_n, \varrho_1/, ..., C_j = /\varrho_j, ..., \varrho_n, \varrho_1, ..., \varrho_j/, ... \tag{29}$$

They mimic a "closed path", the first starting and terminating at ϱ_1, the j-th doing the same at ϱ_j. We shall call an *AOS* "closed" iff it is of the form

$$/\varrho_1, \varrho_2, ..., \varrho_n, \varrho_1/ \text{ with } /\varrho_n, \varrho_1, \varrho_2/ \text{ admissible.} \tag{30}$$

There are some obvious facts. If one *AOS* is closed then all members of its

equivalence class are closed. If one of the *AOS* listed in (29) is closed then all *AOS* of (29) are closed.

Let us call *holomony invariant* each functor associating to every equivalence class of closed *AOS* an object which is constant on every family (29) of closed *AOS*.

Let now (29) and (30) be fulfiled. Then one finds, according to our rules,

$$C_2 \sim /\varrho_2, \varrho_1/\, C_1\, /\varrho_1, \varrho_2/ \tag{31}$$

and

$$RPF(C_2) = V^* RPF(C_1) V \quad \text{with} \quad V = RPF(\varrho_1, \varrho_2). \tag{32}$$

STATEMENT 3. *Up the zero eigenvalues the spectrum of $RFP(C)$ is an holonomy invariant for closed AOS.*

EXAMPLE 2. Let $C = /P_1, P_2, \ldots, P_{n+1}/$ be an *AOS* of 1-dimensional projections. Then either $P_j P_{j+1} = 0$ always (trivial case) or never. In the non-trivial case we know from Example 1 that $RFP(P_j, P_{j+1}) = |j\rangle\langle j+1|$ iff $\langle j|\, j+1\rangle$ is a positive real number and the vectors are normalized. It follows that $RFP(C) = |1\rangle\langle n+1|$. If now $P_1 = P_{n+1}$, then C is a closed *AOS*. In this case there is a unimodular number ε with $|1\rangle = \varepsilon |n+1\rangle$. The essential spectrum of $RFP(C)$ consist of the eigenvalue ε only. It is clearly a discrete approximation to the Bott, Chern, Berry holonomy along a closed path of pure states.

3. Transport of phase factors

Let

$$C\colon\ s \to \varrho(s) \tag{33}$$

describe a *path* of density operators of sufficient regularity, in particular differentiability. We shall allow these operators to have a non-trivial null space.

The parameter, s, is supposed to run through a closed interval of the reals. We often write equations in a more general manner allowing s to vary in a higher dimensional manifold. If we wish to emphasise this we call (33) a *manifold* of density operators.

In particular, we sometimes prefer the use of the total differentiation, dW, instead of dW/ds even in the one-dimensional case.

Given (33) we consider smooth paths (or manifolds) of amplitudes and phases

$$s \to W(s) \quad \text{and} \quad s \to U(s) \tag{34}$$

satisfying (2).

In defining parallelity we need to translate the hermiticity statement of the requirement (3). Heuristically this is very easy: Applying (3) to two "infinitesimally near" amplitudes, W and $W+dW$, we arrive at

$$W^* dW = (dW)^* W \quad \text{or} \quad W^*(dW/ds) = (dW/ds)^* W. \tag{35}$$

We call a path or manifold (of amplitudes or phases) *parallel* iff (35) and (2) is fulfilled.

Let us consider two examples.

EXAMPLE 3. Let $s \to P(s)$ denote a smooth path of m-dimensional projection operators, and let us try the ansatz

$$W(s) = |s, 1\rangle\langle 1| + |s, 2\rangle\langle 2| + \ldots + |s, m\rangle\langle m| \tag{36}$$

similar to (18) of Example 1. Here $|s, k\rangle$, $k = 1, \ldots, m$, denotes an orthonormal set of eigenvectors of $P(s)$ with eigenvalue 1. $|1\rangle$, $|2\rangle$, ... denotes an auxiliary orthonormal system of length m. Inserting this into (35), one gets

$$\langle k, s|(d/ds)|s, i\rangle = 0 \quad \text{for } i, k = 1, 2, \ldots, m \tag{37}$$

using the fact that the matrix (37) is antihermitian by the orthonormality conditions. In the example at hand it even follows from (35) that $W^* dW = 0$. Furthermore, one sees how (35) induces the Bott, Chern parallel transport [1] in the bundle of orthonormal m-frames of a Hilbert space over the Grassmann manifold of its m-dimensional subspaces (assuming a finite-dimensional Hilbert space). Evidently, for 1-dimensional projections, i.e. for pure states, (37) reduces to the Berry–Simon transport [2, 5] giving the Berry phase factor for closed paths.

EXAMPLE 4. Let ϱ and ϱ' denote a pair of non-singular density operators and $/W, W'/$ a pair of parallel amplitudes. Then

$$s \to (1-s)W + sW', \quad 0 \leqslant s \leqslant 1, \tag{38}$$

is a parallel path of amplitudes belonging to

$$s \to (1-s)^2 \varrho + s^2 \varrho' + s(1-s)(W' W^* + W(W')^*). \tag{39}$$

In particular, every *AOS* gives rise to a piecewise smooth path of density operators and parallel amplitudes.

If (33) is a path starting at the parameter value s' and terminating at s'', one defines *AMP* and *RFP* by

$$AMP(C) = W(s')\, W(s'')^* \quad \text{and} \quad RPF(C) = U(s')\, U(s'')^* \tag{40}$$

provided W and U fulfil the parallelity condition.

There is, however, the problem of uniqueness of this definition. We shall discuss this and other problems below. We shall ignore the many technical questions arising in the analysis in infinite dimensions.

Let us consider a given path (33) and the paths (35) belonging to it. Let us

denote by

$$s \to Q(s) = U(s)\,U(s)^* \tag{41}$$

the path of supports of the density operators which is equally well the path of left supports of the amplitudes and phases (34). We further introduce

$$s \to R(s) = U(s)^*\,U(s). \tag{42}$$

To shorten notations we do not write explicitly the dependence on s.

One concludes from (41) and (42) in the usual manner that

$$WR = W, \quad QW = W, \quad UR = U, \quad QU = U. \tag{43}$$

Let us introduce the expressions

$$X = W^*\,dW - (dW)^*\,W \quad \text{and} \quad Y = U\,(dU)^*. \tag{44}$$

The knowledge of Y along a path (33) determines the curves (34) of amplitudes and phases completely up to the choice of initial data. Clearly, $X = 0$ is the parallelity condition.

STATEMENT 4. *One has*

$$\textit{If } X = 0 \textit{ then } dR = 0. \tag{45}$$

In particular, $U^*\,U = R$ is a constant projection operator on every sufficiently regular parallel manifold.

To see this one multiplies $X = 0$ from the right by R, and uses $WR = R$ to get the equality of $W^*\,dW$ and $W^*\,dWR$. Differentiating $WR = R$ and using this equality, we get $W^*\,WdR = 0$. The support of $W^*\,W$ is R, and hence $RdR = 0$. This implies $(dR)\,R = 0$. Because R is a projection operator one has $dR = (RdR + (dR)\,R)$ which implies the assertion.

We shall look at the transformation properties of X and Y in passing to different choices of the amplitudes for the same path (33). Hence we consider the change

$$W \to W' = WV \quad \text{and} \quad U \to U' = UV, \tag{46}$$

$$V = V(s), \quad VV^* = R, \quad V^*\,V = R'. \tag{47}$$

Using the substitution (46) we define Q', R', X', Y' by the help of the amplitudes W' and the phases U'.

Taking care of the support properties, a short calculation yields

$$Y' = Y + U\,(V(dV)^*)\,U^*, \tag{48}$$

$$X' = V^*\,XV + V^*\,W^*\,W\,dV - (dV)^*\,W^*\,WV. \tag{49}$$

As a first application let us solve the unicity problem. If $X = X' = 0$, we conclude

$$VV^* W^* WdVV^* = VdV^* W^* WVV^*. \tag{50}$$

One has

$$VV^* = R, \quad RW^* = W^*, \quad WR = W$$

which yields the equivalence of (50) with $W^* WdVV^* = VdV^* W^* W$. From (45) we know that VdV^* is antihermitian because $R = VV^*$. Hence

$$VdV^* W^* W + W^* WVdV^* = 0. \tag{51}$$

But W^*W is positive and of the trace class with R as its support. It follows that

$$VdV^* R + RVdV^* = 0. \tag{52}$$

From this and $RV = V$ we get $VdV^*(\mathbf{1}+R) = 0$. However, $1+R$ is invertible. We therefore get $VdV^* = 0$ and $Y = Y'$.

STATEMENT 5. *For sufficiently regular paths C of density operators $AMP(C)$ and $RFP(C)$ is uniquely defined by* (40).

We shall now calculate Y if $X = 0$. Note that $QY = Y$ because of (43). Differentiating (41) and multiplying from the right by $(\mathbf{1}-Q)$ provides us with

$$Y(\mathbf{1}-Q) = (dQ)(\mathbf{1}-Q) = Q\,dQ. \tag{53}$$

We apply (49) to the following situation:

We set $X = 0$ but $W' = \varrho^{1/2}$, and $U' = Q$.

Then (46) is fulfilled by $V = U^*$.

One gets

$$\begin{aligned} \varrho^{1/2} d(\varrho^{1/2}) - d(\varrho^{1/2})\varrho^{1/2} &= UW^* WdU^* - dUW^* WU^* \\ &= \varrho UdU^* - dUU^* \varrho, \end{aligned} \tag{54}$$

where we had used $Q = UU^*$ and $Q\varrho = \varrho$. Multiplying by Q from the left, and remembering that $Q(dQ)Q = 0$, one arrives at

$$Q[\varrho^{1/2}, d\varrho^{1/2}] = \varrho Y + Y\varrho. \tag{55}$$

To solve this equation one may use (for every s) a complete system of eigenvectors $k\rangle$ for the eigenvalues $e(k)$ of to get:

If $e(j) > 0$ then

$$\langle j|Y|k\rangle = \big(e(j)^{1/2} - e(k)^{1/2}\big)\big(e(j)+e(k)\big)\,\langle j|d(\varrho^{1/2})|k\rangle. \tag{56}$$

It is well known that such an expression may be converted into an integral relation. Denote by u a real auxiliary parameter. Then

$$Y = UdU^* = Q\int_0^\infty (\exp -u\varrho)\,[\varrho^{1/2}, d\varrho^{1/2}]\,(\exp -u\varrho)\,du. \tag{57}$$

Let us mention two important cases:

If C is a path of projection operators then (53) suffices to determine Y. On the contrary, if C is a path of non-singular density operators, for example Gibbs states, then $Q = \mathbf{1}$, and (53) is trivial. In any case, (54), (55), or (56) completely determine Y.

One can further see explicitly that Y only depends on the states (1) induced by the density operators, i.e. it is insensitive to the normalization of the density operators building up the path C.

There is a possibility of simplyfying the equations above. To this end let the path or manifold (33) of density operators be given by

$$\varrho = V\sigma V, \qquad F = V^* dV, \tag{58}$$

where $s \to V(s)$ is unitary, and $s \to \sigma(s)$ is a *commuting* manifold (path) of density operators. Then one can rearrange the left-hand side of (54) to the form

$$V\left[\sigma^{1/2}, \left[F, \sigma^{1/2}\right]\right] V^*. \tag{*}$$

Let us denote by P the support of σ such that $Q = VPV^*$, and let us try out the decomposition

$$U = VS, \tag{59}$$

which implies, because of $QU = U$, the relations

$$PS = S, \qquad SS^* = P. \tag{60}$$

It is now straightforward to express the right-hand side of (54) as

$$V\left[\sigma SdS^* - dSS^*\sigma\right] V^* - V\left[F\sigma + \sigma F\right] V^*. \tag{**}$$

Now the equation (54) means equality of the expressions (*) and (**). Computing the double commutator in (*), we get

$$2\sigma^{1/2} F\sigma^{1/2} = \sigma SdS^* - dSS^*\sigma. \tag{61}$$

If the supports $P = P(s)$ of the commuting set σ commute themselves, then P is constant along the manifold (path).

In this case $PdS = 0$, and

$$2\sigma^{1/2} F\sigma^{1/2} = \sigma SdS^* + SdS^*\sigma. \tag{62}$$

Of course one may now immediately write down resolutions for SdS^* as was done in (54) and (55) for Y. Explicit calculations of RPF remains difficult nevertheless.

EXAMPLE 5. We consider in an irreducible representation of the angular momentum (or spin) operators $\vec{J}$ an unormalized density operator of the form

$$\sigma = \exp(aJ_3). \tag{63}$$

We define a path of density operators (33) by (58), where V denotes a rotation around an axis that crosses the 3-axis by angle α. Hence we may choose

$$V = \exp is(\sin(\alpha) J_1 + \cos(\alpha) J_3). \tag{64}$$

It is then more or less straightforward to compute S by (62). Denoting by $\mathrm{ch}(a)$ the hyperbolic cosine of a one can express the result as

$$S = \exp is(b \sin(\alpha) J_1 + \cos(\alpha) J_3) \quad \text{with } b\,\mathrm{ch}(a/2) = 1. \tag{65}$$

A full turn around the rotation axis gives

$$RPF = U(0)\,U(2\pi)^* = \pm S(2\pi)^*, \tag{66}$$

where the even or odd sign comes from an integer or half integer representation of the rotation group under consideration.

The eigenvalues of (66) only depend on the closed path and not on the starting density operator (63), i.e. they do not depend on s in $U(s)\,U(s+2\pi)^*$. They are given by

$$\pm \exp\left[2i\,m(b^2 \sin(\alpha)^2 + \cos(\alpha)^2)^{1/2}\right], \tag{67}$$

where the number m runs through the eigenvalues of J_3 in the representation at hand.

In this example we had assumed not only constant eigenvalues of the density operators along the path but also a very simple path given by the action of a 1-parameter group of unitaries. If the latter is not the case, path integrals with Dyson ordering seem to be unavoidable in calculating relative phase factors.

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