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Connections and metrics respecting purification of quantum states

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Standard purification interlaces Hermitian and Riemannian metrics on the space of density operators with metrics and connections on the purifying Hilbert–Schmidt space. We discuss connections and metrics which are well adopted to purification, and present a selected set of relations between them. A connection, as well as a metric on state space, can be obtained from a metric on the purification space. We include a condition, with which this correspondence becomes one to one. Our methods are borrowed from elementary *-representation and fiber space theory. We lift, as an example, solutions of a von Neumann equation, write down holonomy invariants for cyclic ones, and ''add noise'' to a curve of pure states. © *1999 American Institute of Physics.* [S0022-2488(99)02107-6]

I. INTRODUCTION

In Ref. 1, see also Ref. 2, the monotone Hermitian and Riemannian metrics in the (finite dimensional) spaces of all density operators are classified. Based on the theory of operator means[3] they are indexed by a real function, *f*, operator monotone[4] on $(0,\infty)$. These metrics play an important role in domains like quantum information geometry, quantum versions of statistical estimation, and decision rules.[5–7]

D. Petz communicated his main results to us prior to publication, and about that time we started to ask for the effect of a purifying lift to these metrics. There are clear reasons for this. One of the present authors (A.U.) had defined 1986 in Ref. 8 an extension of the geometric phase,[9,10] see also Refs. 11 and 12, to curves of density operators by the help of a ''parallelity condition.'' The condition singles out, up to a global gauge (or a global partial isometry), a distinguished ''parallel lift'' within all purifying lifts of a curve of density operators. It turns out[13] that a connection form (a gauge potential), here called $\mathbf{a}^{\mathrm{geo}}$, is governing the transport of the purifying vectors, such that the parallelity condition results from the request for horizontality. In 1992 G. Rudolph and one of the authors (J.D.) considered a large class of gauge potentials, including $\mathbf{a}^{\mathrm{geo}}$, which rests on a purification scheme and which enables variants of the geometric phase along curves of density operators. It seems natural to ask for a link between these objects: (a) the connection forms just mentioned, (b) certain Hermitian (Riemannian) metrics on the purification space, and, if respecting the symmetry of the scheme, (c) metrics induced from (b) on the space of density operators.

Purification is essentially representation theory of observables and of the algebra in which they are contained. Principally one may use any unital *-representation of the ''algebra of observables'' over which the states can be defined. Its Hilbert representation space should only be large enough to allow for a representation of the states by vectors. If this condition is fulfilled, transport mechanism, its noncommutative phases, metrics, and other geometric objects can be constructed by relying on their form and appearance in the pure state case.

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In our paper we remain within an elementary setting: Our density operators live on a Hilbert space $\mathcal{H}$ of finite dimension n. In our convention, a density operator should not necessarily be normalized. We speak of ''density operators'' whether their trace is one or not. The algebra of observables is the algebra $\mathcal{B}(\mathcal{H})$ of all operators acting on $\mathcal{H}$. The representation or purification space, $\mathcal{W}$, is identified with the algebra of operators and equipped with the Hilbert–Schmidt scalar product. (In infinite dimensions $\mathcal{W}$ will be the space of Hilbert–Schmidt operators.) We try to emphasize the different meaning of operators by different notations: Operators acting on $\mathcal{H}$ are denoted by lower case letters, those acting on $\mathcal{W}$ often by capital letters. [Some authors call the operators of $\mathcal{B}(\mathcal{W})$ ''superoperators.''] Section II is devoted to explaining our notation in more details. In our paper purification takes place in the standard representation of $\mathcal{B}(\mathcal{H})$, i.e., in the GNS-representation based on the trace. For that reason we called it *standard purification*. In Sec. III the formalism is extended to velocity vectors, i.e., to tangents, at density operators and at their purifications. Purification defines vertical tangents in a canonical way. A tangent, orthogonal to the space of vertical tangents, is called horizontal, provided the tangent spaces carry a real Hilbert space structure, i.e., a Riemannian metric. Equivalently, within all purifying lifts of a given curve of density operators, those with the least length are horizontal.

Section IV exemplifies our task in defining horizontality by the real part of the Hilbert–Schmidt metric. As one knows, the Bures length of a curve of density operators and the Hilbert–Schmidt length of an horizontal lift are equal one to another. In deriving the parallelity condition we meet some peculiarities with tangents of purifying vectors if they belong to density operators with some vanishing eigenvalues. The reader will find a short account of the relation between the connection form $\mathbf{a}^{\mathrm{geo}}$ (Ref. 13) governing the geometric phase, and the Riemannian Bures metric.

Indeed, we devote some time to asking, and giving an affirmative answer to the following question: Is the topological metric of Bures Riemannian?[14–16] Essential differential geometric properties are in Ref. 17, see also Ref. 18 for $\dim \mathcal{H}=3$. Relations to quantum information theory can be seen in Refs. 19 and 20. However, a parameterization in terms of the operators' matrix elements remains cumbersome, except for $\dim \mathcal{H}=2$.

Concerning $\mathbf{a}^{\mathrm{geo}}$, which extends the geometric phase to (closed) curves of density operators, examples are shown in Sec. VIII. There is a further issue to be mentioned: The gauge potential for the two-dimensional density operators[21] living on a four-dimensional purification space, satisfies the Yang–Mills equations. With a certain cosmological constant, it even is a solution of the combined Yang–Mills–Einstein equations.[22] Meanwhile we know[23] $\mathbf{a}^{\mathrm{geo}}$ satisfies the Yang–Mills equations for every finite dimension of the supporting Hilbert space $\mathcal{H}$. These findings may be seen as extensions to mixed states of numerous examples relating the original Berry phase to Dirac monopoles, and the Wilczek and Zee phase[24] to instantons.

Section VI is devoted to the class of connections introduced in Ref. 25, which are, so to say, ''relatives'' of $\mathbf{a}^{\mathrm{geo}}$, compatible with the purification scheme. They are characterized by a function F, defined on $(0,\infty)$, and fulfilling $\overline{F}(1/t)=-F(t)$. Some equations become more appealing by using the function r, the arithmetic mean of $\overline{F}$ and 1. The connection forms $\mathbf{a}$ assign to every tangent x at the lift $w\in\mathcal{W}$ of $\varrho=ww^*$ a value in the Lie algebra of $U(n)$. The action of the gauge group induces the ''canonical'' connection $\mathbf{a}^{\mathrm{can}}$. The canonical connection is gained with the choice $F=0$. The connection $\mathbf{a}^{\mathrm{geo}}$ is constructed with $F(t)=(t-1)/(t+1)$. As we shall see, only connections with real F can be obtained from an appropriate Hermitian metric. We believe the complete class is a more natural object at the complexified tangents. They all decompose as $\theta-\theta^*$ with θ of type (1,0).

We specify the class of Hermitian metrics by another positive and real valued function, k, on the positive half-axis. The metrical form for the tangents at a purifying vector, w, will be given by the inverse of the (''super'')operator $k(\Delta_w)$, where Δ is the field of modular operators. There is an antilinear operator, a modification of Tomita–Takasaki's S_w operator, which admits just the horizontal tangents as fix points. The connection adjusted to the metric is characterized by various relations between the functions k, F, and r. Moreover, every one of the Hermitian metrics considered on the tangent space of $\mathcal{W}$ is a lift of exactly one Hermitian form on the space of density operators. The latter depends on a function f which is related to k. The Riemannian metric on the density operators is gained as the real part of the Hermitian one, and it corresponds to the harmonic mean of $f(t)$ and $tf(1/t)$. Further we discuss an additional condition, which enables us to assign a unique connection form to a given monotone Riemannian state space metric. These metrics are induced from the Hilbert–Schmidt metric by some constraints on the purifying vectors replacing the orthogonality condition of the Bures case.

The starting point has been a set of connections, compatible with the purification procedure, to define reasonable parallel transports along curves of density operators. We return to this issue in purifying horizontally solutions of von Neumann equations. Cyclic solutions give rise to some holonomy invariants. There are constraints on F for extending the parallelity conditions to the boundary, in particular to pure states. If they are fulfilled, the holonomy invariants reduce to the well-known geometric phase of Berry for pure states. At the end we ask what happened if ''noise'' is added to a closed path of pure states.

II. STANDARD PURIFICATION

We start by reviewing some basic ideas of the purification procedure. Let $\mathcal{H}$ be a complex Hilbert space of finite dimension n with scalar product $\langle .,. \rangle$ antilinear in its left argument. $\mathcal{B}(\mathcal{H})$ denotes the $*$-algebra of linear operators acting on $\mathcal{H}$. A *state* is a positive linear form over the algebra which takes the value 1 at the identity of $\mathcal{B}(\mathcal{H})$. Generally, a linear form l over our algebra is uniquely represented by

$$l(b) = \mathrm{Tr}\, b\omega, \quad \forall b \in \mathcal{B}(\mathcal{H}).$$

The linear form is positive if and only if ω is a positive element of $\mathcal{B}(\mathcal{H})$. We then call ω a *density operator* in accordance with its usage in physics. A density operator represents a state iff its trace is one.

A *purification* of a positive linear form over $\mathcal{B}(\mathcal{H})$ is a lift to a pure linear form of a larger algebra. A way to do so is as follows: With another auxiliary Hilbert space $\mathcal{H}^{\mathrm{aux}}$, with at least the same dimension, we consider

$$\mathcal{H} \otimes \mathcal{H}^{\mathrm{aux}}, \quad n = \dim \mathcal{H} \leqslant \mathcal{H}^{\mathrm{aux}}$$

and the inclusion (which, indeed, is a $*$-representation)

$$\mathcal{B}(\mathcal{H}) \hookrightarrow \mathcal{B}(\mathcal{H}) \otimes 1^{\mathrm{aux}} \subset \mathcal{B}(\mathcal{H} \otimes \mathcal{H}^{\mathrm{aux}}) \tag{1}$$

into the operator algebra of the extended Hilbert space. Let ϱ be the density operator of a positive linear form l over $\mathcal{B}(\mathcal{H})$. A vector ψ of $\mathcal{H} \otimes \mathcal{H}^{\mathrm{aux}}$ is said to *purify* l, and hence ϱ, iff

$$l(b) \equiv \mathrm{Tr}\, b\varrho = \langle \psi, b \otimes 1^{\mathrm{aux}} \psi \rangle \quad \forall b \in \mathcal{B}(\mathcal{H}). \tag{2}$$

A distinguished way to choose the auxiliary Hilbert space is to require

$$\mathcal{H}^{\mathrm{aux}} = \mathcal{H}^*, \quad \mathcal{W} := \mathcal{H} \otimes \mathcal{H}^*, \tag{3}$$

which results in the *standard purification,* based on the standard representation of $\mathcal{B}(\mathcal{H})$. In what follows this choice is assumed, and we have to fix some notations and conventions at the beginning.

Let $\phi \in \mathcal{H}$. The element $\phi^* \in \mathcal{H}^*$, is defined by $\phi^*(\phi') = \langle \phi, \phi' \rangle$. In Dirac's notation:

$$\phi \leftrightarrow |\phi\rangle, \quad \phi^* \leftrightarrow \langle \phi|.$$

Being in finite dimensions, every operator is Hilbert–Schmidt, and $\mathcal{W}$ is canonically isomorphic to $\mathcal{B}(\mathcal{H})$. This can be made explicit with two arbitrarily chosen orthonormal bases $\phi_1, \phi_2, \ldots$ and $\phi'_1, \phi'_2, \ldots$ of $\mathcal{H}$ in writing

$$w=\sum |\phi_j\rangle\langle\phi_j, w\phi'_k\rangle\langle\phi'_k|, \quad w\in\mathcal{W}. \tag{4}$$

The Hilbert–Schmidt scalar product on $\mathcal{W}$ is

$$(w_2,w_1):=\mathrm{Tr}\, w_2^* w_1=\sum \langle w_2\phi'_k,\phi_j\rangle\langle\phi_j, w_1\phi'_k\rangle. \tag{5}$$

The star operation in $\mathcal{B}(\mathcal{H})$ is equivalent with a conjugation in $\mathcal{W}$,

$$w\mapsto w^* \quad \text{or} \quad (\phi\otimes\tilde{\phi}^*)^*=\tilde{\phi}\otimes\phi^*.$$

We need some operators acting on $\mathcal{W}$. The standard representation of $\mathcal{B}(\mathcal{H})$ is the inclusion (1), specified by (3), and acting as follows:

$$b\mapsto L_b, \quad L_b w:=bw, \quad b\in\mathcal{B}(\mathcal{H}).$$

We also need the right multiplication R_b, i.e., $R_b w=wb$. The right multiplication can be used to implement the standard representation of $\mathcal{B}(\mathcal{H}^*)$. Notice the different meaning of the *-operations on $\mathcal{W}=\mathcal{B}(\mathcal{H})$ and on $\mathcal{B}(\mathcal{W})$ seen in

$$(L_b)^*=L_{b^*}, \quad (L_b w)^*=(R_b)^* w^*$$

and in similar relations after exchanging L_b and R_b. Now, let $\hat{l}$ be a linear form on $\mathcal{B}(\mathcal{W})$ and l its *restriction* or reduction onto $\mathcal{B}(\mathcal{H})$. The relation

$$\hat{l}\mapsto l, \quad l(b):=\hat{l}(L_b), \quad b\in\mathcal{B}(\mathcal{H}) \tag{6}$$

encodes the partial trace over $\mathcal{H}^*$ on $\mathcal{W}$. Focusing our attention on the purification procedure, we shall apply this well-known mapping mainly to linear functionals of rank one. In that case the essence of the reduction mapping to the factors of $\mathcal{W}$ is contained in

$$(w_2, L_b R_c w_1)=\mathrm{Tr}\, w_2^* b w_1 c. \tag{7}$$

Its left-hand-side defines a linear form $B\mapsto(w_2,Bw_1)$ over $\mathcal{B}(\mathcal{W})$, and, varying w_1 and w_2 within $\mathcal{W}$, one can get every linear functional of rank one. Presently we need to consider (7) with $w_1=w_2=w$ and with either c or b the identity operator. Then, for $B\in\mathcal{B}(\mathcal{W})$ and $b,c\in\mathcal{B}(\mathcal{H})$, the left- and the right-hand sides of (7) may be rewritten

$$\hat{l}(B)=(w,Bw), \quad l(b)=\mathrm{Tr}\, ww^*b, \quad l'(c)=\mathrm{Tr}\, w^*wc.$$

$\varrho=\varrho_l:=ww^*$ is called the *density* or the *density operator* of l, while w is said to *purify* l. In the same spirit, a positive linear functional $\hat{l}$ of rank one, which reduces to l, is a *purification* of l.

From now on, instead of switching forth and back between linear forms and their densities, we remain mainly with the latter. Accordingly we define the mappings

$$\Pi w=ww^*, \quad \Pi' w=w^*w.$$

The mapping Π (and similarly the mapping Π'), is slightly more subtle than the reduction mapping (6). Its domain of definition is $\mathcal{W}$. Thus Π is composed of a Hopf bifurcation from w to the rank one density operator $|w)(w|$, representing the linear form $B\to(w,Bw)$, followed by the reduction (6):

$$w\mapsto|w)(w|\mapsto ww^*.$$

Here we used Dirac's notation relative to the scalar product (5) in $\mathcal{W}$. Π is a bundle projection, where the bundle space is $\mathcal{W}$ and the base space is the cone of (not necessarily normalized) density operators (i.e., positive trace class operators). Being in finite dimension, the base space is the positive cone of $\mathcal{B}(\mathcal{H})$. The bundle fibers are manifolds. However, the dimension of the fibers vary with the rank n_w of $w \in \mathcal{W}$. Therefore certain discontinuities occur if the rank is changing.

All this can be seen by the ''diagonal'' form of (4), which is the Gram–Schmidt decomposition of w. Let $\lambda_1, \lambda_2, \ldots$ be the n_w nonzero eigenvalues of ww^* and $\phi_1, \phi_2, \ldots$ their orthonormal eigenvectors,

$$ww^* = \sum \lambda_j |\phi_j\rangle\langle\phi_j|, \quad \lambda_k > 0.$$

There exists exactly one other orthonormal basis of vectors, $\phi'_1, \phi'_2, \ldots$ of the same length n_w, fulfilling

$$w = \sum \sqrt{\lambda_k} |\phi_k\rangle\langle\phi'_k|, \quad w^* w = \sum \lambda_j |\phi'_j\rangle\langle\phi'_j| \tag{8}$$

and the positive numbers λ_j sum up to (w,w). From (8) one can read off the polar decompositions

$$w = \sqrt{ww^*} v = v \sqrt{w^* w}, \quad v = \sum |\phi_k\rangle\langle\phi'_k|. \tag{9}$$

The index k runs from 1 to n_w. One may call v the *phase of w relative to* $\varrho = ww^*$. The projection operators $v^* v$ and vv^*, attached to the partial isometry v, map $\mathcal{H}$ onto the support spaces of $w^* w$ and ww^*, respectively. Later on we need the operator $J = J_w$,

$$J_w x = v x^* v = \sum |\phi_j\rangle\langle\phi'_j, x^* \phi_k\rangle\langle\phi'_k|, \tag{10}$$

which, for completely entangled w, is the well-known *modular conjugation*. One easily establishes

$$(J_w)^2 x = (vv^*) x (v^* v), \quad (Jx, y) = (Jy, x). \tag{11}$$

If $\varrho \geqslant 0$ is a density operator, the set $\Pi^{-1}\varrho$ consists of all w satisfying $\varrho = ww^*$. Along this fiber the orthoframe $\phi'_1, \phi'_2 \ldots$ in (8) and (9) varies arbitrarily. Thus the fiber at ϱ is isomorphic, though not canonically, to a complex Stiefel manifold.[26] These isomorphisms are parametrized by the different possibilities to choose an orthoframe for the nonzero eigenvalues of ϱ. The *structure* or *gauge group* of $\Pi^{-1}\varrho$ consists of all unitary $u \in \mathcal{B}(\mathcal{H})$ acting by R_u.

Iff ϱ is already pure, $\varrho = |\phi\rangle\langle\phi|$, its purifications reads $w = |\phi\rangle\langle\phi'|$. That is, the purifying vectors are necessarily product vectors (''unentangled'' vectors).

In case the rank of ϱ is larger than one, w is called *entangled* in the domain of quantum information theory. Accordingly, *complete entanglement* of w is reached if the density operator ϱ is of maximal rank $n_w = \dim \mathcal{H}$. In this case, in traditional $*$-representation theory, ϱ is called *faithful* and *w separating*. $\varrho = ww^*$ is faithful iff w is invertible.

The set of all faithful ϱ is the base space of a principal fiber bundle with free action of the unitaries R_u. The fiber space consists of all invertible w, the projection is Π.

III. PURIFICATION AND TANGENTS

A smooth, oriented curve in $\mathcal{W}$, passing through w, defines at w a *tangent* or *velocity vector* x. Hence the tangent space, $\mathcal{T}_w$ at w, may be identified with $\mathcal{W}$ if considered as a real linear space.

Assume that w and the unitaries u depend smoothly on a parameter, and let us use a dot to show parameter differentiation. The gauge transformation $w \mapsto w' := wu$ induces the relation

$$x \mapsto x' = xu + w\dot{u}, \quad x = \dot{w}, \quad x' = \dot{w}'. \tag{12}$$

Let us now consider Π, and assume $\Pi w = \varrho$. Π induces a mapping Π_* from the tangent space of $\mathcal{W}$ into the density operator's tangents.

Being a first-order problem, it is sufficient for the following to assume a curve as simple as possible, say $w(\lambda) = w + \lambda x$. The curve is projected by Π to a curve of density operators $\varrho_\lambda = w(\lambda)w^*(\lambda)$ of $\mathcal{B}(\mathcal{H})$. Differentiating at $\lambda = 0$ results in a tangent $\Pi_* x = \xi$ at ϱ,

$$\xi = \dot{\varrho}, \quad \xi = (ww^*)^{\cdot} = xw^* + wx^*. \tag{13}$$

A tangent vector x at w is called *vertical* iff $\Pi_* x = 0$. The real vector space of the vertical tangents at w is denoted by $\mathcal{T}_w^{\mathrm{ver}}$. It is a straightforward and well-known exercise to show: The gauge transformation $x \mapsto x'$ of (12) maps vertical tangents at w to vertical tangents at w'.

We look at vertical tangents as labels for the physical phase. The phase of a single state or of its density operator is not an observable. Which purifying vector w we choose is physically irrelevant. What can be observed are relative phases, for example in interference experiments. The relative phases should depend on the way a density operator is changed to become another one. There should be a protocol according to which the tangents, and hence the phases, are transported along a curve within the space of density operators. This can be achieved by the help of a parallel transport.

The standard procedure is to split the tangent space at every w into a direct sum of the vertical and of an horizontal part. Respecting the complex linear structures, we restrict ourselves to decompositions defined by the real part of an Hermitian metric: We assume at every w a distinguished positive Hermitian sesquilinear form

$$w \mapsto (x_2, x_1)_w, \quad x_1, x_2 \in \mathcal{T}_w. \tag{14}$$

For completely entangled w it should be positive definite. Now $\mathrm{Re}\,(.,.)_w$, the real part of (14), converts the tangent space at w into a *real* Hilbert space. The *velocity* with which a curve goes through w is the square root of $(x,x)_w$ with x the tangent at that point. In this setting, parallel transport is asking for a minimal velocity lift of a given tangent at the base space. This, in turn, induces a metrical structure at the base space: One calls the *velocity of a base space tangent* the minimum of the velocities of all possible lifts.

Thus, the *horizontal part*, x^{hor}, of a tangent x at w is the unique element of the set $x + \mathcal{T}_w^{\mathrm{ver}}$ with the smallest velocity. This is in accordance with the definition of $\mathcal{T}_w^{\mathrm{hor}}$ as the orthogonal complement of $\mathcal{T}_w^{\mathrm{ver}}$ in the real Hilbert space $\mathcal{T}_w$, the latter equipped with the scalar product $\mathrm{Re}\,(.,.)_w$.

There is a distinguished real subspace, $\mathcal{T}_w^{\mathrm{Ver}} \subset \mathcal{T}_w^{\mathrm{ver}}$, containing all tangents

$$x = wa, \quad a = -a^* \in \mathcal{W},$$

which are obviously vertical. If w is invertible (completely entangled), every vertical tangent can be uniquely expressed in that way. But generally, $\mathcal{T}_w^{\mathrm{Ver}}$ is a proper subspace of $\mathcal{T}_w^{\mathrm{ver}}$. We call a vertical tangent *neutral* iff it is orthogonal to $\mathcal{T}_w^{\mathrm{Ver}}$ with respect to $\mathrm{Re}\,(.,.)_w$. Hence, every tangent x allows for an orthogonal decomposition

$$x = x^{\mathrm{hor}} + x^{\mathrm{ver}}, \quad x^{\mathrm{ver}} = x^{\mathrm{neutral}} + x^{\mathrm{Ver}}. \tag{15}$$

IV. PHASE TRANSPORT AND BURES METRIC

The most natural and simple choice for the Hermitian metric $(x_2, x_1)_w$ of (14) is certainly the Hilbert–Schmidt scalar product (5). This choice is particularly interesting for several reasons.

At first it gives a straightforward generalization of the geometric phase by the parallel transport evolving from this choice. Indeed, one obtains a natural extension of the Fock,[27], Berry,[9] Simon,[10] Wilczek and Zee[24] parallel transport to density operators.

Transport of state vectors along closed curves generates a holonomy problem. In the period between V. Fock and M. Berry this has become clear. B. Simons explained how to calculate the holonomy by the second Chern class of the Hilbert space if considered as a line bundle. There is an extensive literature on the transport of phases along curves and loops of pure states, see Ref. 28 for a selection of important results, applications, and references. Particular examples in using and calculating the geometric phase can already be found in papers of decades past.

Second, one gets a Riemannian metric[14] on the (not necessarily normalized) density operators of $\mathcal{B}(\mathcal{H})$. Its distance function is the distance introduced by Bures[29] in following a similar construction of Kakutani[30] in probability spaces. Being the infinitesimal version of *Bures' distance*, we call this Riemannian metric *Bures' metric*.

And, finally, already the choice

$$(x_2,x_1)_w=(x_2,x_1), \quad \forall w,$$

shows essential problems in deviating from a genuine fiber bundle.

We start by enumerating the tangents y orthogonal to $\mathcal{T}_w^{\mathrm{Ver}}$

$$(y,wa)+(wa,y)=0, \quad \forall a+a^*=0.$$

That condition straightforwardly comes down to

$$y^*w=w^*y \tag{16}$$

and y is orthogonal to all Ver-tangents iff w^*y is Hermitian. (16) is the *parallelity condition*,[8] which extends the transport condition for the geometric phase from pure to mixed states.

To decompose y in its neutral and horizontal part, we start by completing the two orthonormal systems of the Schmidt decomposition (8) arbitrarily and set $\lambda_j=0$ if $j>n_w$. By sandwiching (16) between the orthobase $\{\phi_i'\}$ we get

$$\sqrt{\lambda_k}\langle\phi_j',y^*\phi_k\rangle=\sqrt{\lambda_j}\langle\phi_j,y\phi_k'\rangle.$$

There evolve two conditions on the matrix elements:

$$j\leqslant n_w, \quad k>n_w \Rightarrow \langle\phi_j',y\phi_k\rangle=0.$$

$$k,j\leqslant n_w \Rightarrow \frac{\langle\phi_j',y^*\phi_k\rangle}{\sqrt{\lambda_j}}=\frac{\langle\phi_j,y\phi_k'\rangle}{\sqrt{\lambda_k}}.$$

No restriction occurs for $j>n_w$, $k\leqslant n_w$. There is an Hermitian g such that

$$\langle\phi_j,g\phi_k\rangle=\frac{\langle\phi_j,y\phi_k'\rangle}{\sqrt{\lambda_k}}, \quad k\leqslant n_w.$$

One may choose the matrix elements of g with indices both larger than n_w arbitrarily but consistent with $g=g^*$.

The tangent $y_1=gw$ *is horizontal*[31,32] because it is orthogonal to all ver-tangents x. Indeed, $xw^*+wx^*=0$ implies $(gw,x)+(x,gw)=(g,xw^*+wx^*)=0$. What remains to check is the case of a tangent y_0, real orthogonal to all gw, $g=g^*$, and to all Ver-tangents. From the first condition it follows $wy_0^*+y_0w^*=0$, hence verticality, and from the second we obtain $w^*y_0=y_0^*w$. This is equivalent with

$$\langle\phi_j,y_0\phi_k'\rangle=0, \quad \forall j,k\leqslant n_w$$

or

$$y \quad \text{neutral} \quad \Leftrightarrow w^* y = y w^* = 0. \tag{17}$$

We conclude that every tangent x allows for a unique decomposition

$$x = gw + x_0 + wa \tag{18}$$

in a horizontal, a neutral, and a vertical part where g is Hermitian, a anti-Hermitian, and x_0 satisfies (17). With the extra conditions

$$\langle \phi_j, g\phi'_k \rangle = \langle \phi_j, a\phi'_k \rangle = 0, \quad k,j \geqslant n_w,$$

both g and a are unique. The last conditions are equivalent to the choice of maximal null-spaces, i.e., *minimal supports* for g and a. They allow one to define g and a uniquely.

The transformation property (12) implies

$$w \mapsto w' = wu \Rightarrow a \mapsto a' = u^* a u + u^* \dot{u}, \tag{19}$$

so that $x \mapsto a$ is a connection form (gauge potential) **a** for the gauge group $u \mapsto R_u$. However, support properties may not change continuously. For parameter values at which the rank of w is changing, one has to understand g or a as equivalence class with respect to the kernel of $g \mapsto gw$ or $a \mapsto wa$, respectively. Then (19) remains meaningful even in those cases.

In our next step we look at g and a. g, which describes the horizontal part of a tangent vector x, can be expressed by $\xi := \Pi_* x$ and $\varrho := ww^* = \Pi w$. We need the pair x and $\tilde{\varrho} := w^* w$ to gain a. We get

$$\varrho g + g \varrho = \xi, \quad \tilde{\varrho} a + a \tilde{\varrho} = w^* x - x^* w. \tag{20}$$

The first equation[32,31] is obtained from (13). To see the second one,[13] insert (18) into its right-hand side.

Apart from an obvious restriction on ξ, (20) can be solved to get g or a, and several ways to do so are well known. A review is in Ref. 33. The restriction in question reads $\langle \phi, \xi \phi \rangle = 0$ whenever ϕ is in the null space of ϱ for the first equation, and $\langle \phi', \xi \phi' \rangle = 0$ whenever ϕ' is in the null space of $\tilde{\varrho}$. Below we assume they are satisfied.

With the solvability conditions in mind we rewrite (20) as equations between operators in $\mathcal{B}(\mathcal{W})$. In order not to overload notations we abbreviate

$$\mathrm{L} \equiv L_\varrho, \quad \mathrm{R} \equiv R_\varrho, \quad \tilde{\mathrm{L}} \equiv L_{\tilde{\varrho}}, \quad \tilde{\mathrm{R}} \equiv R_{\tilde{\varrho}}.$$

These are families of operators indexed by ϱ or $\tilde{\varrho}$.

Let us start now from (20). The equations can be solved by

$$g = (\mathrm{L} + \mathrm{R})^{-1} \xi, \quad a = (\tilde{\mathrm{L}} + \tilde{\mathrm{R}})^{-1} (w^* x - x^* w). \tag{21}$$

The operationally defined inverse exists by the solvability condition above. With two tangents ξ_j at ϱ and their horizontal lifts x_j^{hor} we get the Riemannian metric[16,14] belonging to the Bures distance

$$(\xi_2, \xi_1)^{\text{Bures}} := \operatorname{Re}(x_1^{\text{hor}}, x_2^{\text{hor}}) = \tfrac{1}{2} \operatorname{Tr} \varrho (g_1 g_2 + g_2 g_1) \tag{22a}$$

or, equivalently,

$$(\xi_2, \xi_1)^{\text{Bures}} = \tfrac{1}{2} \operatorname{Tr} \xi_2 g_1 = \tfrac{1}{2} \operatorname{Tr} \xi_2 (\mathrm{L} + \mathrm{R})^{-1} \xi_1. \tag{22b}$$

There is a similar procedure with the second equation of (21) resulting in the connection $\mathbf{a}^{\text{geo}}$ with $\mathbf{a}^{\text{geo}}(x) := wa$. The superscript "geo," if used, is a reminder for the physical important geometric phase. From (21) we get

$$\mathbf{a}^{\text{geo}} = \frac{\tilde{\mathrm{L}}}{\tilde{\mathrm{L}}+\tilde{\mathrm{R}}}(w^{-1}dw) - \frac{\tilde{\mathrm{R}}}{\tilde{\mathrm{L}}+\tilde{\mathrm{R}}}(w^{-1}dw)^*, \tag{23a}$$

where $w^{-1}\,dw$ is the left canonical 1-form with values in the Lie algebra of $\mathrm{GL}(\mathcal{H})$. $\mathbf{a}^{\text{geo}}$ takes values in the Lie algebra of the gauge group $U(\mathcal{H})$ acting from the right via $u \mapsto R_u$.

Formula (23a) represents $\mathbf{a}^{\text{geo}}$ as the difference of two Hermitian conjugated parts of type (1,0) and (0,1), respectively:

$$\mathbf{a}^{\text{geo}} = \mathbf{a}_{1,0} - \mathbf{a}_{0,1}, \quad \mathbf{a}_{0,1} = \mathbf{a}_{1,0}^*.$$

Another interesting equation expresses $\mathbf{a}^{\text{geo}}$ as sum of the canonical 1-form $\mathbf{a}^{\text{can}}$ of the bundle $\mathrm{GL}(\mathcal{H})/U(\mathcal{H})$ and a horizontal Ad-1-form[25]

$$\mathbf{a}^{\text{geo}} = \frac{w^{-1}\,dw - (w^{-1}\,dw)^*}{2} + \frac{\tilde{\mathrm{L}}-\tilde{\mathrm{R}}}{\tilde{\mathrm{L}}+\tilde{\mathrm{R}}}\,\frac{w^{-1}dw + (w^{-1}dw)^*}{2}. \tag{23b}$$

Since the second form is horizontal, it can be rewritten in terms of $d\varrho$ and we get

$$\mathbf{a}^{\text{geo}} = \mathbf{a}^{\text{can}} + w^{-1}\left(\frac{\mathrm{L}-\mathrm{R}}{2(\mathrm{L}+\mathrm{R})}\,d\varrho\right)(w^{-1})^* \tag{23b$'$}$$

$$= w^{-1}dw - w^{-1}\left(\frac{\mathrm{R}}{\mathrm{L}+\mathrm{R}}d\varrho\right)(w^{-1})^*. \tag{23c}$$

It becomes immediately clear that $\mathbf{a}^{\text{geo}}(x) = \mathbf{a}^{\text{can}}(x)$ iff $\mathrm{L}\xi = \mathrm{R}\xi$, where $\xi := wx^* + xw^*$, i.e., iff ϱ commutes with $\dot{\varrho}$.

This observation motivates the decomposition

$$\mathcal{T}_\varrho = \mathcal{T}_\varrho^{\parallel} + \mathcal{T}_\varrho^{\perp} \tag{24}$$

of the tangent space $\mathcal{T}_\varrho$ into a direct sum, where $\xi \in \mathcal{T}_\varrho^{\parallel}$ iff ξ commutes with $\varrho = ww^*$ or, equivalently, iff $\langle \phi_j, \xi\phi_k \rangle = 0$ for any two eigenvectors ϕ_j, ϕ_k, of ϱ with different eigenvalues. On the other hand, $\xi \in \mathcal{T}_\varrho^{\perp}$ iff it can be written as a commutator $i[b,\varrho]$ with a suitable Hermitian b. (24) is a well-known matrix decomposition: Assume ϱ represented as block diagonal matrix, every block belongs to just one eigenvalue. This induces a block representation of any matrix ξ. One gets $\xi^{\parallel}$ by setting zero every off-diagonal block of ξ. If the entries in the diagonal blocks are set to zero, one obtains $\xi^{\perp}$. In our present field of interest Hübner[18] obtained a decomposition (24) of the Bures Riemannian metric. For larger classes of metrics this has been done by Hasegawa and Petz (Refs. 34 and 35).

This brings us back to the metric (22). There is a solution g_1 commuting with ϱ iff ξ_1 does so: The support ϱ cannot be smaller than the support of ξ. Hence $2g_1 = \varrho^{-1}\xi_1 = \xi_1\varrho^{-1}$ is operational well defined. Inserting in (22b) results in

$$(\xi_2,\xi_1)^{\text{Bures}} = \tfrac{1}{4}\mathrm{Tr}\,\xi_2\xi_1\varrho^{-1}, \quad \xi_1 \in \mathcal{T}_\varrho^{\parallel}. \tag{25}$$

Comparing this with the Riemannian metric

$$(\xi_2,\xi_1)^{\text{can}} := \tfrac{1}{8}\mathrm{Tr}\,(\xi_2\xi_1 + \xi_1\xi_2)\varrho^{-1} = \mathrm{Tr}\,\xi_2(\mathrm{L}^{-1}+\mathrm{R}^{-1})\xi_1,$$

the inequality $4/(\mathrm{L}+\mathrm{R}) \leq (1/\mathrm{L}) + (1/\mathrm{R})$ gives[36]

$$(\xi,\xi)^{\text{Bures}} \leqslant (\xi,\xi)^{\text{can}}$$

and equality holds if and only if $\xi \in \mathcal{T}_\varrho^{\parallel}$, or, what is the same, if ξ commutes with ϱ.

Let $\phi_1, \ldots$ be a complete orthonormal eigenvector basis of $\varrho = ww^*$ and ξ with eigenvalues λ_j and $\dot{\lambda}_j$, respectively. Then we get from (25) the following quadratic form:

$$\frac{1}{4} \sum d\lambda_j^2 \lambda_j^{-1} = \sum d\mu_j^2, \quad \mu_j := \sqrt{\lambda_j}.$$

This is an Euclidean metric. However, restricted to the state space, where $\lambda_1, \ldots$ becomes a probability vector, we get Fisher's metric (''Fisher–Rao metric'').[37]

If the Bures metric is restricted to a submanifold of mutual commuting states, the Fisher metric is obtained. Moreover, *on any submanifold of commuting density operators*, whether normalized or not, *the phase transport is holonomically trivial.*

Indeed, we can form the lift $\varrho \rightarrow w = \sqrt{\varrho}$. The assumed commutativity provides us with Hermitian and commutative w and $x = \dot{w}$, and with $\varrho = ww^* = w^*w = \tilde{\varrho}$. Hence (21) comes down to $\mathbf{a}(x) = 0$, and the lift is horizontal. There is no room for a nontrivial phase.

We see a nontrivial geometric phase is definitely an effect of noncommutativity. We need for them curves with mutually not commuting density operators.

V. AUXILIARY TOOLS

In order to extend our previous considerations to a larger class of connections[25] we need some auxiliary tools.

Looking at Eqs. (23) one can identify functions of L/R and $\tilde{\mathrm{L}}/\tilde{\mathrm{R}}$. These operators are relatives of $\mathrm{L}/\tilde{\mathrm{R}} = \Delta_w$, the Tomita–Takesaki modular operator of the representation $b \mapsto L_b$ with GNS-vector w. The operators are defined if w^{-1} exists, that is for completely entangled w. But, as (23) shows, certain functions of these operators can be defined for every w.

Let $t \mapsto f(t)$ be a function defined for $0 < t < \infty$. We assume the existence of

$$f(0) := \lim_{t \to 0} f(t), \quad f(\infty) := \lim_{t \to \infty} f(t). \tag{26}$$

The assumption is necessary if we like to extend the formalism to density operators which are not invertible. Without it, we have to restrict ourselves to completely entangled w, i.e., to faithful density operators.

To treat an example with the assumption (26), we define $f(\mathrm{L}/\tilde{\mathrm{R}}) =: f(\Delta)$. The positive operators L and $\tilde{\mathrm{R}}$ commute. Let λ_j be the eigenvalue of ww^* and of w^*w with the eigenvectors ϕ_j and ϕ'_j. The eigenvectors, suitably chosen, collect in a complete orthonormal basis satisfying the Gram–Schmidt decomposition (8). λ_j is zero if $j > n_w$ and positive otherwise. Now

$$\mathrm{L} v_{jk} = \lambda_j v_{jk}, \quad \tilde{\mathrm{R}} v_{jk} = \lambda_k v_{jk}, \quad v_{jk} := |\phi_j\rangle\langle\phi'_k|.$$

The elements v_{jk} constitute a complete orthonormal basis of the Hilbert–Schmidt space $\mathcal{W}$. We like $f(\Delta)$ to be diagonalizable with eigenvectors v_{jk}. Remembering $\Delta = \mathrm{L}/\tilde{\mathrm{R}}$ we start with

$$f(\Delta) v_{jk} = f(\lambda_j/\lambda_k) v_{jk}, \quad \text{if } \lambda_k > 0.$$

The remaining possibility is done ''by hand'' in requiring

$$f(\Delta) v_{jk} = f(\infty) v_{jk}, \quad \text{if } \lambda_j > 0, \quad \lambda_k = 0,$$

$$f(\Delta) v_{jk} = f(1) v_{jk}, \quad \text{if } \lambda_j = \lambda_k = 0.$$

With this convention v_{jj} is an eigenvector of $f(\Delta)$ with eigenvalue $f(1)$ for all j.

The same game is to play with $f(\mathrm{L}/\mathrm{R})$ and $f(\tilde{\mathrm{L}}/\tilde{\mathrm{R}})$. While the spectra of $f(\mathrm{L}/\mathrm{R})$ and $f(\tilde{\mathrm{L}}/\tilde{\mathrm{R}})$ coincide with that of $f(\Delta)$, their eigenvectors are, respectively,

$$|\phi_j\rangle\langle\phi_k| = v_{ji}v_{ik}^*, \quad |\phi_j'\rangle\langle\phi_k'| = v_{ji}^*v_{ik}.$$

VI. A CLASS OF CONNECTIONS

Our aim is to describe a class of connections, essentially that of Dittmann and Rudolph[25]. These objects, as will be seen, are particularly well adapted to the purification of the $\mathcal{H}$-system by that of $\mathcal{W} = \mathcal{H}\otimes\mathcal{H}^*$. We assume w to be completely entangled, so that $\varrho = \Pi w$ is faithful (invertible). Whether it is possible to skip this assumption, either by calculating modulo neutral tangents or by continuity arguments, depends on the asymptotic behavior of certain functions to be introduced below.

Let $[0,\infty] \ni s \mapsto r(s) \in \mathbb{C}$ be a smooth function and $r(1) = 1/2$. Then

$$(r(\tilde{\mathrm{L}}/\tilde{\mathrm{R}})y)^* = \overline{r}(\tilde{\mathrm{R}}/\tilde{\mathrm{L}})y^*.$$

Mimicking Eq. (23a) we define the form

$$\mathbf{a} := \overline{r}(\tilde{\mathrm{L}}/\tilde{\mathrm{R}})(w^{-1}\,dw) - r(\tilde{\mathrm{R}}/\tilde{\mathrm{L}})(w^{-1}\,dw)^*. \tag{27a}$$

It transforms like a connection and takes anti-Hermitian values. To be a connection it must take the correct values at vertical vectors, i.e., $\mathbf{a}(wa) = a$, for all anti-Hermitian a. Thus we need to have

$$\overline{r}(t) + r(1/t) = 1, \quad F(t) := \overline{r}(t) - r(1/t) = -\overline{F}(1/t), \tag{28}$$

to get a genuine connection with respect to the gauge group $\mathrm{U}(\mathcal{H})$ acting by $u \mapsto R_u$. Furthermore, as a consequence of $r(1) = 1/2$, one observes rescaling invariance of this connection form. Indeed, $\mathbf{a}$ is invariant under $w \mapsto \lambda(w)w$, where $\lambda : \mathcal{W} \to \mathbb{R}$:

$$\mathbf{a}_w(x) = \mathbf{a}_{\lambda w}(d\lambda(x)w + \lambda x),$$

so that there is no need to normalize w in calculating $\mathbf{a}$. The second equation in (28) introduces the function F used in Ref. 25 to label their gauge potentials, and we are allowed now to rewrite (27a) in a manner known already from (23):

$$\mathbf{a} = \mathbf{a}^{\mathrm{can}} + F(\tilde{\mathrm{L}}/\tilde{\mathrm{R}})\frac{(w^{-1}\,dw) + (w^{-1}\,dw)^*}{2} \tag{27b$'$}$$

$$= \mathbf{a}^{\mathrm{can}} + w^{-1}(F(\mathrm{L}/\mathrm{R})\,d\varrho)(w^{-1})^* \tag{27b}$$

$$= w^{-1}\,dw - w^{-1}(r(\mathrm{R}/\mathrm{L})\,d\varrho)(w^{-1})^*. \tag{27c}$$

One returns to the Bures case by

$$\mathbf{a} = \mathbf{a}^{\mathrm{geo}} \Leftrightarrow r(t) = \frac{t}{1+t} \Leftrightarrow F(t) = (t-1)/(t+1).$$

Before deriving expressions for the vertical and horizontal part of a given tangent x, we draw an important conclusion:

The value of a connection at the lift of a $\|$-tangent is independent of F, respectively, r. Indeed, $F(1) = 0$ and $\mathrm{L}x = \mathrm{R}x$ for these tangents, and we get from (27b') immediately

$$\Pi_*(x) \in \mathcal{T}^{\parallel} \Rightarrow \mathbf{a}(x) = \mathbf{a}^{\mathrm{can}}(x), \quad \forall F$$

allowing to extend a conclusion of Sec. IV:

On submanifolds with mutually commuting density operators the holonomy of every loop is trivial for the whole class of connections considered here.

Indeed, the lift $\varrho \to \sqrt{\varrho}$ is horizontal along every curve of commuting densities.

To obtain the vertical and horizontal part of a tangent x let us apply Eq. (27c) to x multiplied by w from the left. We assumed w to be separating so that there are no nonvanishing neutral tangents. Therefore

$$x^{\mathrm{ver}} = x^{\mathrm{Ver}} = w\mathbf{a}(x) = x - (r(\mathrm{R}/\mathrm{L})\xi)(w^*)^{-1} \tag{29a}$$

$$= x - r(\Delta^{-1})(x + wx^* w^{*-1}) \tag{29b}$$

$$= x - r(\Delta^{-1})[x + \Delta^{1/2} J x], \tag{29c}$$

reminding $wx^*(w^*)^{-1} = \Delta^{1/2} J x = J \Delta^{-1/2} x$. (29) reflects the decomposition of a general tangent into a vertical and a horizontal part, see (15). We conclude

$$x^{\mathrm{hor}} = (r(\mathrm{R}/\mathrm{L})\xi)(w^*)^{-1} = r(\Delta^{-1})[x + \Delta^{1/2} J x]. \tag{30}$$

A connection form $\mathbf{a}$ regulates the change of the phase v along a horizontal lift, $w_t = \sqrt{\varrho_t} v_t$, of a curve ϱ_t. We express $\mathbf{a}$ by

$$\begin{aligned}
\mathbf{a}(\dot{w}) = \mathbf{a}(\sqrt{\varrho}\dot{v} + (\sqrt{\varrho})^{\cdot} v) &= \mathbf{a}(\sqrt{\varrho} v v^* \dot{v} + (\sqrt{\varrho})^{\cdot} v) \\
&= v^* \dot{v} + v^* \mathbf{a}(\sqrt{\varrho}^{\cdot}) v \\
&= v^* \dot{v} + v^* \mathbf{a}\left(\frac{1}{\sqrt{\mathrm{L}} + \sqrt{\mathrm{R}}} \dot{\varrho} \right) v \\
&= v^* \dot{v} + v^* \frac{1}{2} \frac{1}{\sqrt{\mathrm{LR}}} \left(F(\mathrm{L}/\mathrm{R}) + \frac{\sqrt{\mathrm{R}} - \sqrt{\mathrm{L}}}{\sqrt{\mathrm{R}} + \sqrt{\mathrm{L}}} \right) (\dot{\varrho}) v.
\end{aligned}$$

and see that the horizontality of w_t is equivalent with

$$0 = \dot{v} v^* + \frac{1}{2} \frac{1}{\sqrt{\mathrm{LR}}} \left(F(\mathrm{L}/\mathrm{R}) + \frac{\sqrt{\mathrm{R}} - \sqrt{\mathrm{L}}}{\sqrt{\mathrm{R}} + \sqrt{\mathrm{L}}} \right) (\dot{\varrho}). \tag{31}$$

One observes, that there is one and only one connection in our setting with a global horizontal section, $\varrho \mapsto \sqrt{\varrho}$. That connection is given by

$$F(t) = -\frac{1 - \sqrt{t}}{1 + \sqrt{t}}, \quad r(t) = \frac{\sqrt{t}}{1 + \sqrt{t}}.$$

VII. CONNECTION AND METRIC

In this section we specify a class of Hermitian metrics (14) on $\mathcal{W}$, which respects the purification scheme. Our first task is to ask for Hermitian metrics on the complex manifold $\mathcal{W}$, the real part of which is compatible with a given connection form of Sec. VI. We demand: At every completely entangled $w \in \mathcal{W}$, the vertical tangents are real orthogonal to the horizontal ones. In the case where there exists a Hermitian metric doing this task, the functions F and r characterizing the connection have to be real. In the next step we describe the Hermitian and Riemannian metric one obtains by reduction from the purification space to that of (unnormalized) density operators.

Starting with a connection (27a), (28), there is some freedom in the choice of the Hermitian metric. It is an interesting question in its own right, whether, by a reasonable condition, the Hermitian metric becomes unique. We explain in the last part of this section how this can be done. If we start from a Riemannian metric on the density operators, the uniqueness problem is more involved. Nevertheless, our additional condition solves it also, at least for the monotone Riemannian metrics.

To start our little program we construct Hermitian metrics (14) by modifying the Hilbert Schmidt scalar product on $\mathcal{W}$ by a function $k(\Delta)$ of the modular operator. Like R and L the modular operator Δ depends on w. Our ansatz for the Hermitian product in $T_w\mathcal{W}$ reads

$$(x_2,x_1)_w := (x_2, k(\Delta_w)^{-1}x_1), \tag{32}$$

where k is a real positive smooth function defined either only on $0<t<\infty$ or on the closed interval $0\leqslant t\leqslant\infty$. We use the rules explained in Sec. V. There are two main merits with such a choice of the modified Hermitian metric: The symmetry group of the metric contains the unitary group $\mathrm{U}(\mathcal{H})\times\mathrm{U}(\mathcal{H}^*)$. The second is the rescaling invariance of Δ under $w\mapsto\lambda(w)w$, where $\lambda(w)$ denotes (a sufficiently smooth) real function on $\mathcal{W}$. Rescaling invariance is a further reason not to insist on normalized density operators.

In determining the connection form compatible with (32), we follow the recipe of Sec. III. We need the real-orthogonal complement of the vertical directions. They are to gain by the metrical independence of verticality. Namely, if a tangent x is real orthogonal to all vertical ones, $k(\Delta)^{-1}x$ is horizontal with respect to the Hilbert–Schmidt metric. Therefore, as shown in Sec. IV, we are allowed to write $x=gw$ with a Hermitian g. Conclusion:

A tangent x is horizontal with respect to (32), if it can be represented as

$$x=k(\Delta)(gw)=k(\mathrm{L}/\mathrm{R})(g)w, \quad g=g^*. \tag{33}$$

The real space of horizontal tangents is the fix point set of an antilinear operator, S_w^k, acting on $\mathcal{W}$. Our notation is borrowed from that of the Tomita–Takesaki operator $S_w=J\sqrt{\Delta}$, which will be returned if $k\equiv 1$. Our definition is

$$S_w^k := Jk(\Delta^{-1})k(\Delta)^{-1}\sqrt{\Delta}=k(\Delta)k(\Delta^{-1})^{-1}S_w. \tag{34a}$$

If this operator acts on $x=k(\Delta)(gw)$ the result is $k(\Delta)(g^*w)$. Comparison with (33) establishes: x is a fix point of S_w^k if and only if x is horizontal.

The square of the operator (34a) is J^2; compare (11). J^2 is the identity of $\mathcal{W}$ iff w is invertible. Further, the adjoint of S_w^k with respect to (32) is $\sqrt{\Delta}J$ and, as it should be, independent of k. (Tomita–Takesaki theory calls it "F_w.") Finally we polar decompose (34a) to get the appropriate modifications of the modular operator, $\Delta=\Delta_w$, and of the modular conjugation, $J=J_w$,

$$S_w^k=J_w^k|S_w^k|, \quad \Delta_w^k := |S_w^k|^2, \tag{34b}$$

$$\Delta_w^k=k(\Delta^{-1})k(\Delta)^{-1}\Delta, \quad J_w^k=J\sqrt{k(\Delta^{-1})k(\Delta)^{-1}}. \tag{34c}$$

We now ask for the connection coming with the metric. The connection form belonging to (32) annihilates all the horizontal vectors (33). This reasoning, applied to (27a) or (27b), determines the function r or F. The calculation shows, in accordance with (28),

$$r(t)=\frac{tk(1/t)}{k(t)+tk(1/t)}, \quad \text{respectively}, \quad F(t)=\frac{tk(1/t)-k(t)}{tk(1/t)+k(t)}. \tag{35}$$

Obviously, *the functions r and F are real valued* if the connection is gained from a Hermitian metric (32). A cross check of (35) is in setting $k\equiv 1$. We get $r(t)=t/(1+t)$ and $F(t)=(t-1)/(t+1)$ as it should be for the Bures case.

On the other hand, given r or F, there is some freedom for k since the induced connection depends on $k(t)/k(1/t)$ only.

$$\frac{k(t)}{k(1/t)}=1\Leftrightarrow r(t)=\frac{t}{1+t},\quad F(t)=\frac{(t-1)}{(t+1)},\quad \mathbf{a}=\mathbf{a}^{\mathrm{geo}},$$

$$\frac{k(t)}{k(1/t)}=t\Leftrightarrow r(t)=\frac{1}{2},\quad F(t)=0,\quad \mathbf{a}=\mathbf{a}^{\mathrm{can}}.$$

In particular, there is no modification of the Tomita–Takesaki operators by (34) if the connection is $\mathbf{a}^{\mathrm{geo}}$. More generally, from (35) we get

$$\frac{k(t)}{k(1/t)}=t\frac{r(1/t)}{r(t)}=t\frac{1-F(t)}{1+F(t)} \tag{36}$$

and find, remarkably enough, the modified Tomita–Takesaki operators (34) depending on F only. Further, by (36), the positivity of k enforces the inequality

$$-1<F(t)<1 \tag{37}$$

for F to be obtained from a k. In order to invert (36), the inequality is also sufficient. According to (28) one needs only to check $F<1$ for real F. Then, given F, the general solution of the problem is

$$k(t):=\sqrt{t}(1-F(t))q(t),$$

q being an arbitrary positive function fulfilling $q(t)=q(1/t)$.

We started from a Hermitian metric on $\mathcal{W}$, derived conditions for horizontality, and determined the connection. Now we go back to $\mathcal{H}$ and to its density operators: We ask for the Hermitian and Riemannian metric induced on the space of density operators. That is, with two tangents ξ and η at $\Pi w=\varrho$, we are concerned with

$$(\eta,\xi)_\varrho:=(y^{\mathrm{hor}},x^{\mathrm{hor}})_w,\quad \mathrm{Re}\,(\eta,\xi)_\varrho=\frac{(\eta,\xi)_\varrho+(\xi,\eta)_\varrho}{2}.$$

x^{hor} and y^{hor} are the horizontal lifts of ξ and η. In the present paper the $\mathbb{C}$-valued $\mathbb{R}$-linear form $\xi,\eta\mapsto(\eta,\xi)_\varrho$ is defined on the real tangents. Nevertheless, for obvious reasons, we call it ''Hermitian.'' Relying on (30) we conclude

$$(y^{\mathrm{hor}},x^{\mathrm{hor}})_w=\mathrm{Tr}\,r(\mathrm{L/R})(\eta)\frac{r(\mathrm{R/L})}{\mathrm{R}k(\mathrm{L/R})}(\xi)=\mathrm{Tr}\,\eta\frac{r(\mathrm{R/L})^2}{\mathrm{R}k(\mathrm{L/R})}\xi,$$

so that

$$(\eta,\xi)_\varrho=\mathrm{Tr}\,\eta\frac{\mathrm{R}k(\mathrm{L/R})}{[\mathrm{R}k(\mathrm{L/R})+\mathrm{L}k(\mathrm{R/L})]^2}\xi, \tag{38a}$$

where r has been substituted by k by the aid of (35). The real part is a Riemannian metric. By standard rules we get

$$\mathrm{Re}\,(\eta,\xi)_\varrho = \frac{1}{2}\,\mathrm{Tr}\,\eta \frac{1}{\mathrm{R}k(\mathrm{L/R}) + \mathrm{L}k(\mathrm{R/L})}\,\xi. \tag{38b}$$

Petz[36,1,2] was able to classify all monotone Hermitian metrics on the state space, i.e., those for which $(\cdot,\cdot)_\varrho$ does not increase under the action of completely positive and unital mappings. At the heart of his result is the characterization of a monotone metric by an operator monotone function, *f*, defined on $0<t<\infty$, such that

$$(\eta,\xi)_\varrho = \frac{1}{4}\,\mathrm{Tr}\,\eta \frac{\mathrm{R}^{-1}}{f(\mathrm{L/R})}\,\xi. \tag{39}$$

(The factor 1/4 is a normalization convention.) Note that this Hermitian metric becomes symmetric, and hence a Riemannian one, if and only if the function *f* satisfies $f(t)=tf(1/t)$. A function with this algebraic property we call self-transposed, following the terminology for operator means introduced in Ref. 3. Presently, however, the monotonicity of the metric (39) or of its real part is *not* assumed. We need a more general frame. Having this in mind, we compare (39) with (38a) and obtain

$$f(t) = \frac{(k(t)+tk(1/t))^2}{4k(t)}. \tag{40}$$

This equation has a unique solution for *k* depending on *f*, therefore, every Hermitian metric (39) can be reached by exactly one Hermitian metric (32) on the purification space. Indeed, the harmonic mean of $f(t)$ and its transpose, $tf(1/t)$, yields

$$\frac{1}{f(t)} + \frac{1}{tf(1/t)} = \frac{4}{k(t)+tk(1/t)}$$

so that one can insert this into the right-hand side of (40) to express *k* by *f*:

$$k(t) = f(t)\frac{4t^2 f(1/t)^2}{[f(t)+tf(1/t)]^2}. \tag{41}$$

Moreover, using (35) we get

$$r(t) = \frac{f(t)}{f(t)+tf(1/t)}, \quad F(t) = \frac{f(t)-t(1/t)}{f(t)+tf(1/t)}. \tag{42}$$

These equations describe the relation between the connection on $\mathcal{W}$ and the Hermitian metric living on the density operators. It is Riemannian iff *f* is self-transposed. (41) yields $f=k$ in this case, and (42) degenerates to $r\equiv 1/2$. Hence, *if the induced Hermitian form is Riemannian, the induced connection is necessarily the canonical one.* This way we do not get an interesting mapping from the class of Riemannian metrics to the class of connections. Especially, the function $f(t)=(1+t)/2$ belonging to the Bures metric cannot be gained from $\mathbf{a}^{\mathrm{geo}}$ as one might expect.

Moreover, if we like to gain the connection form $\mathbf{a}^{\mathrm{geo}}$, $r(t)=t/(t+1)$, belonging to the geometric phase, we need, according to (42), $t^2 f(1/t) = f(t)$ or, equivalently, $k(t)=k(1/t)$. If *f* is operator monotone, so is $tf(1/t)$. Therefore, $t^2 f(1/t)$ is convex (lemma 5.2 of Ref. 3). Thus, *f* is convex and, as an operator monotone function, concave. Being convex and concave, *f* has to be affine. An affine function on the positive real axis, fulfilling $t^2 f(1/t)=f(t)$, is a multiple of *t*.

If $\mathbf{a}=\mathbf{a}^{\mathrm{geo}}$ *and f is operator monotone with* $f(1)=1$, *then* $f(t)=t$.

However, for $k(t)=1$ [respectively, $k(t)=2t/(t+1)$] we get $\mathbf{a}=\mathbf{a}^{\mathrm{geo}}$ (respectively, $\mathbf{a}=\mathbf{a}^{\mathrm{can}}$) and obtain from (38b) for the real part

$$\mathrm{Re}\,(\eta,\xi)_\varrho = \frac{1}{4}\,\mathrm{Tr}\,\eta\,\frac{R^{-1}}{f_s(L/R)}\,\xi \tag{43}$$

with $f_s(t)=(1+t)/2$ (respectively, $f_s(t)=2t/(t+1)$). These f_s are distinguished (self-transposed) operator monotone functions. Moreover, in these cases (38b) restricted to the horizontal vectors coincides with the real part of the Hilbert–Schmidt metric. This is the motivation to deal in the following with the real part of the Hermitian metric induced on the state space.

First of all, this Riemannian metric is of the form (43) with a certain self-transposed function f_s depending on k. From (38b) we get

$$f_s(t)=\frac{k(t)+tk(1/t)}{2}. \tag{44}$$

$f_s(t)$ is the harmonic mean of $f(t)$ and $tf(1/t)$, with f given by (40).

Clearly, in starting with a self-transposed f_s there is some arbitrariness in choosing k respecting (44). Moreover, given a self-transposed f_s, the only restriction for F is $-F(1/t)=F(t)<1$. Indeed, Eqs. (35) and (44) then have the unique solution

$$k(t)=f_s(t)(1-F(t)). \tag{45}$$

In order to remove the arbitrariness in going from f_s to F and vice versa or from f_s to k, we impose an additional requirement on the class (32) of Hermitian metrics $(x,y)_w$. The aim is to ensure that, given f_s, there is only one k and one F fulfilling (35) and (44). We shall prove that we meet our goal for operator monotone f_s by the following natural demand:

Condition HS: For x and y belonging to the horizontal spaces defined by the Hermitian metric (32), the real part, Re $(x,y)_w$, *of* $(x,y)_w$ *coincides with the real part,* Re (x,y), *of the Hilbert–Schmidt product of x and y.*

At first, by the aid of (33), the condition HS becomes

$$\mathrm{Re}\,(k(\Delta)(gw),g'w)=\mathrm{Re}\,(k(\Delta)(gw),k(\Delta)(g'w))$$

with arbitrary Hermitian g and g'. It yields the constraint

$$k(t)+tk(1/t)=k(t)^2+tk(1/t)^2. \tag{46}$$

Next, we have the following crucial observation, which one verifies straightforwardly:

There is a one-to-one correspondence between positive functions k fulfilling the constraint (46) and functions F with $-F(1/t)=F(t)<1$. *The correspondence is given by (35) and*

$$k(t)=\frac{2t(1-F(t)}{(1+F(t))^2+t(1-F(t))^2}. \tag{47}$$

By (44) or, equally well, by (45) we get the relation between F and f_s,

$$f_s(t)=\frac{2t}{(1+F(t))^2+t(1-F(t))^2}. \tag{48}$$

Hence, under condition HS, a function f_s can be gained from a k iff f_s has a representation (48) with a suitable F, $F(t)<1$. To explain which functions f_s can be reached, we rewrite relation (48) into the equivalent form

$$\frac{1+t}{2}-f_s(t)=\frac{f_s(1/t)(1+t)^2}{4}\left(\frac{t-1}{t+1}-F(t)\right)^2.$$

Therefore, necessary conditions for f_s are $f_s(1)=1$, $f_s \leqslant (1+t)/2$ and, moreover, $t \mapsto (1+t)/2 - f_s(t)$ must be the square of a smooth function.

Now suppose we have such a pair f_s, F. We define an auxiliary smooth function

$$\delta(t) := \frac{\sqrt{f_s(1/t)}(1+t)}{2}\left(\frac{t-1}{t+1} - F(t)\right).$$

It fulfills

$$\delta(t)^2 = \frac{1+t}{2} - f_s(t), \quad \sqrt{t}\,\delta(1/t) + \delta(t) = 0. \tag{49}$$

The second equation is a consequence of $F(1/t) = -F(t)$ and $f_s(t) = t f_s(1/t)$. F can be expressed in terms of δ and f_s by

$$F(t) = \frac{t-1}{t+1} - \frac{2}{(1+t)\sqrt{f_s(1/t)}}\,\delta(t). \tag{50}$$

Conversely, for a given self-transposed f_s, $f_s(1)=1$, the possibilities in choosing δ with the properties (49) enumerate via (50) the solutions F of (48) and $-F(1/t) = F(t)$. But such an F may not fulfill $F(t) < 1$ if we did not choose appropriately the signs for δ in (49). The desired choice may be neither unique nor possible. But if so, the function k defined by

$$k(t) := \frac{2}{t+1}\left(f_s(t) + \sqrt{t f_s(t)\,\delta(t)}\right) \tag{51}$$

satisfies (44) and (35).

The question, which functions f_s, $f(1)=1$, bounded by $0 < f(t) \leqslant (1+t)/2$, can arise from F or, equivalently, from a Hermitian metric (32), depends also on regularity requirements on F and k. We do not discuss this in detail. Instead we have the following uniqueness result:

Lemma: For every self-transposed operator monotone function $f_s : (0,\infty) \to \mathbb{R}$ with $f(1)=1$ there exists exactly one positive real analytic function $k : (0,\infty) \to \mathbb{R}$ fulfilling (44) and (46). k and its corresponding function F are given by

$$k(t) = \frac{2 f_s(t)}{t+1}\left(1 + \frac{t-1}{|t-1|}\sqrt{t}\sqrt{\frac{1+t}{2 f_s(t)} - 1}\right), \tag{52}$$

$$F(t) = \frac{t-1}{t+1}\left(1 - \frac{2\sqrt{t}}{|t-1|}\sqrt{\frac{1+t}{2 f_s(t)} - 1}\right) \tag{53}$$

for $t \neq 1$ and $k(1)=1$, $F(1)=0$.

We prove this assertion in the Appendix. (It should be emphasized that k and F are real analytic although the last formulas involve $1/|t-1|$, see the Appendix.) From this lemma we get:

For every monotone Riemannian metric (43), $f_s(1)=1$, on the manifold of completely entangled states there exists exactly one Hermitian metric (32) satisfying the condition HS such that the real part of the induced Hermitian metric is just the given monotone metric. For a given f_s the Hermitian metric and the corresponding connection form are obtained from (52) and (53).

The obtained connection we call the connection associated to the monotone Riemannian metric. For the Bures metric we return to the Hilbert–Schmidt metric and the connection above called $\mathbf{a}^{\text{geo}}$.

Since we used only certain properties of operator monotone functions this assertion would be true for a larger class of metrics, but we will not deal with this problem.

Although the condition HS seems to be natural, perhaps a short comment would be worthwhile. The induced Riemannian metrics are obtained, essentially, by taking the real part of the Hermitian metric of horizontally lifted vectors. But, because of HS, this is the same as the real part of the Hilbert–Schmidt metric. Forgetting for a moment about the underlying Hermitian metric, which forced horizontality, we can take the following point of view: The monotone metrics are obtained from the originally given Hilbert–Schmidt metric similarly to the Bures metric (Sec. IV) whereas the deviation from the Bures metric is caused by some constraints on the purifying lifts.

VIII. EXAMPLES

At first we look at curves of density operators satisfying a von Neumann equation

$$i\dot{\varrho}=[h,\varrho],\quad h=h^*,\quad \dot{h}=0 \tag{54}$$

and their lifts. We may think of $h\in\mathcal{B}(\mathcal{H})$ as of a given Hamiltonian and of the curve parameter, t, as time. This interpretation is not obligatory: h may be the generator of any one-parameter group. (The parameter t should not be confused with the use of the same letter as a dummy variable in several functions like f, k, r, F.) To fix a solution of (54), we start at an initial time, $t_{\rm in}$, with an initial density operator $\varrho_{\rm in}$. The solution may be written

$$\varrho_t=u_t^*\varrho_{\rm in}u_t,\quad u_t:=\exp i(t-t_{\rm in})h. \tag{55}$$

Now a general lift w_t is polar decomposed, $w_t=\sqrt{\varrho_t}v_t$, according to (9).

Our aim is to prove the following: *Given a connection form and an initial $\varrho_{\rm in}$ at $t_{\rm in}$ there is a t-independent Hermitian $\tilde{h}$ such that*

$$u_tv_t=\exp i(t-t_{\rm in})\tilde{h} \tag{56}$$

implies horizontality of w_t. At first we see from (55) and (56) the validity of a Schrödinger equation in $\mathcal{W}$,

$$i\dot{w}=Hw,\quad Hw:=hw-w\tilde{h}. \tag{57}$$

By the help of our menagerie of equations it is not particularly difficult to prove the statement above and to obtain an expression for $\tilde{h}$. At first let us multiply (57) by w^* from the right. By (30) the condition for horizontality is in equating $i\dot{w}w^*$ with $r(R/L)i\dot{\varrho}$. Now (54) yields

$$r(\mathrm{R}/\mathrm{L})(h\varrho-\varrho h)=h\varrho-w\tilde{h}w^*.$$

This equation is sufficient to guarantee horizontality. Now $w\tilde{h}w^*$ can be computed by (56) to $u_t^*\sqrt{\varrho_{\rm in}}\tilde{h}\sqrt{\varrho_{\rm in}}u_t$. Therefore, our horizontality condition is the Ad-transform with u_t^* of the equation

$$r(\mathrm{R}_{\rm in}/\mathrm{L}_{\rm in})(h\varrho_{\rm in}-\varrho_{\rm in}h)=h\varrho_{\rm in}-\sqrt{\varrho_{\rm in}}\tilde{h}\sqrt{\varrho_{\rm in}},$$

where R and L at $t=t_{\rm in}$ is indexed by in. In other words, if we choose $\tilde{h}$ t-independent and v according to (56), we can satisfy the horizontality condition.

To get a unique $\tilde{h}$, we require the support of $\tilde{h}$ to be smaller than that of $\varrho_{\rm in}$. Finally, with the help of (28), we get the expression

$$\tilde{h}=(\sqrt{\mathrm{R}/\mathrm{L}}r(\mathrm{L}/\mathrm{R})+\sqrt{\mathrm{L}/\mathrm{R}}r(\mathrm{R}/\mathrm{L}))h,\quad t=t_{\rm in}. \tag{58}$$

Let us consider a solution (55) of (54) from $t_{\rm in}$ to $t_{\rm out}$. *Then $w_{\rm out}w_{\rm in}^*$ is a gauge invariant.* Its trace in $\mathcal{H}$,

$$(w_{\mathrm{in}}, w_{\mathrm{out}}) = (w_{\mathrm{in}}, [\exp i(t_{\mathrm{out}} - t_{\mathrm{in}})H] w_{\mathrm{in}}) = \mathrm{Tr}\, \sqrt{\varrho_{\mathrm{in}}} \sqrt{\varrho_{\mathrm{out}}} \exp(i(t_{\mathrm{in}} - t_{\mathrm{out}})h) \exp(i(t_{\mathrm{out}} - t_{\mathrm{in}})\tilde{h}), \tag{59}$$

may be called a *relative geometric phase*. For pure states that object has been introduced in Ref. 38. These authors called it the ''non-cyclic geometric phase.'' One may think of shortcutting the in- and the out-state to a closed curve by a Fubini Study geodesic arc. Whether one has a similar interpretation in our much more general case remains an open question.

For a cyclic solution of (54), i.e., $\varrho_{\mathrm{in}} = \varrho_{\mathrm{out}}$, $t_{\mathrm{cycle}} = t_{\mathrm{out}} - t_{\mathrm{in}}$, the expression $w_{\mathrm{out}} w_{\mathrm{in}}^*$ is a (pointed) holonomy invariant, i.e., it depends on the choice of ϱ_{in}. To change the in-state of our cyclic curve one has to perform a u_t-transformation. Consequently, *all eigenvalues of* $w_{\mathrm{out}} w_{\mathrm{in}}^*$ *are (absolute) holonomy invariants*. of our cyclic curve. They are encoded in the traces

$$\mathrm{Tr}\,(w_{\mathrm{out}} w_{\mathrm{in}}^*)^m = \mathrm{Tr}\,[\varrho_{\mathrm{in}} \exp(-i t_{\mathrm{cycle}} h) \exp(i t_{\mathrm{cycle}} \tilde{h})]^m, \tag{60}$$

where $\exp(-i t_{\mathrm{cycle}} h)$ commutes with ϱ_{in}.

There are a few examples where one can become more explicit. One of them is in *adding noise to a curve of pure states* p_t. In this important example one can study the influence of ''noise'' on the geometric phase, and the behavior of gauge and holonomy invariants in coming from the interior to the extreme boundary of the cone of unnormalized density operators. For this purpose we fix two positive real numbers, α and β, and consider the curve of density operators ϱ,

$$\varrho = \alpha p + \beta \mathbf{1}, \quad p = |\psi\rangle\langle\psi|, \quad \langle\psi,\psi\rangle = 1. \tag{61}$$

$\alpha + \beta$ is a simple and β, if n denotes the dimension of $\mathcal{H}$, a $(n-1)$-fold eigenvalue of ϱ. ψ, p and ϱ depend on a parameter t, but we will not suppose a von Neumann equation.

Remark: The line element of this curve with respect to the metric induced from (32) is

$$ds^2 = \frac{2\alpha(1-\tau)}{\tau k(1/\tau) + k(\tau)} ds^2_{\mathrm{Bures}}, \quad \tau := \frac{\beta}{\alpha + \beta},$$

where ds^2_{Bures} denotes the Bures line element of the curve of pure states p_t. □

All t-derivations will be indicated by a dot, in particular

$$\dot{\varrho} = \alpha \dot{p}, \quad \dot{p} = \dot{p}p + p\dot{p}, \quad p\dot{p}p = 0.$$

$\dot{\varrho}$ belongs to $\mathcal{T}^{\perp}$. As an application one calculates

$$R_{\varrho}\dot{p} = \dot{p}(\alpha p + \beta \mathbf{1}) = (\alpha + \beta)\dot{p}p + \beta p\dot{p}.$$

In this manner one gets

$$R_{\varrho}(p\dot{p}) = \beta p\dot{p}, \quad R_{\varrho}(\dot{p}p) = (\alpha + \beta)\dot{p}p,$$

$$L_{\varrho}(p\dot{p}) = (\alpha + \beta)p\dot{p}, \quad L_{\varrho}(\dot{p}p) = \beta \dot{p}p$$

and, finally, skipping the index of L_{ϱ} and R_{ϱ},

$$(\mathrm{L/R})(p\dot{p}) = \left(\frac{\alpha + \beta}{\beta}\right) p\dot{p}, \quad (\mathrm{L/R})(\dot{p}p) = \left(\frac{\beta}{\alpha + \beta}\right) \dot{p}p.$$

For instance, $\dot{p}p$ and $\dot{p}p$ are eigenvectors of LR with the eigenvalue $(\alpha + \beta)\beta$. At this stage we do not suppose a von Neumann equation (54) but rely on (31). From the last equation and $F(t) = -F(1/t)$, we get

$$F(\mathrm{L/R})\dot{p}=F\left(\frac{\beta}{\alpha+\beta}\right)(\dot{p}p-p\dot{p}).$$

Hence, in solving (31) with (61) we are faced with an equation

$$\dot{v}v^*=\frac{1}{2}\frac{\alpha}{\sqrt{(\alpha+\beta)\beta}}\left[F\left(\frac{\beta}{\alpha+\beta}\right)+\frac{\sqrt{\alpha+\beta}-\sqrt{\beta}}{\sqrt{\alpha+\beta}+\sqrt{\beta}}\right](p\dot{p}-\dot{p}p), \tag{62}$$

which may be rewritten as

$$\dot{v}^*=v^*(1-\mu)(p\dot{p}-\dot{p}p), \quad \mu=\frac{1}{2}\frac{\alpha}{\sqrt{(\alpha+\beta)\beta}}\left[F\left(\frac{\beta}{\alpha+\beta}\right)+\frac{\alpha+2\beta}{\alpha}\right]. \tag{63}$$

Can we go by $\beta\to 0$ to the pure states? A necessary condition is

$$F(0)=-1$$

or, equivalently, $r(0)=0$. To be sufficient we additionally need the existence of

$$\kappa:=\lim_{\beta\to 0}\mu=\lim_{\lambda\to 0}\frac{1+F(\lambda)}{2\sqrt{\lambda}}=\lim_{\lambda\to 0}\lambda^{-1/2}r(\lambda). \tag{64}$$

Then the limit $\beta\to 0$ can be performed in (62):

$$(v\dot{v}^*)^{\mathrm{pure}}=(1-\kappa)(p\dot{p}-\dot{p}p). \tag{65}$$

With $\mathbf{a}^{\mathrm{geo}}$, or, more generally, with $s>1/2$ in $r(\lambda)=\lambda^s/(1+\lambda^s)$, we get $\kappa=0$. *With* $\kappa=0$ *we obtain the Berry phase for pure states.*

Indeed, imposing $\langle\psi,\dot{\psi}\rangle=0$ a la Berry[9] and Fock[27], we find $\dot{v}^*\psi+v^*\dot{\psi}=0$ from (63). Hence, with $\kappa=0$, the vector $v^*\psi$ is t-independent. This yields $w=|\psi\rangle\langle\varphi|$, $\dot{\varphi}=0$. It then follows

$$\mathrm{Tr}\,(w_{\mathrm{out}}w_{\mathrm{in}}^*)^m=\langle\psi_{\mathrm{in}},\psi_{\mathrm{out}}\rangle^m.$$

This is the mth power of the Berry phase, because we had supposed the validity of Berry's transport condition. Remark that this goes not through if $\kappa\neq 0$ or if, as for $\mathbf{a}^{\mathrm{can}}$, (64) does not exist.

Something more can be said if (61) satisfies a von Neumann equation (54). Computing $\tilde{h}$ with this assumption by the help of (58) ends up with

$$\tilde{h}=h+\mu[(\mathbf{1}-p_{\mathrm{in}})hp_{\mathrm{in}}+p_{\mathrm{in}}h(\mathbf{1}-p_{\mathrm{in}})]. \tag{66}$$

Looking at $\tilde{h}$ as a block matrix with respect to p_{in} and $\mathbf{1}-p_{\mathrm{in}}$, the deviation from h is in multiplying the off-diagonal blocks by μ. If (64) exists and $\kappa=0$ then the off-diagonal blocks become zero at the pure state limit.

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APPENDIX: PROOF OF THE LEMMA OF SECTION VII

Every self-transposed operator monotone function f_s with $f_s(1)=1$ has a unique integral representation

$$\begin{aligned} f_s(t) &= m(\{0\})\frac{1+t}{2} + \int_{(0,1]} \frac{1+x}{2}\left(\frac{t}{t+x}+\frac{t}{tx+1}\right) dm(x) \\ &= \frac{1+t}{2} + \int_{(0,1]}\left\{-\frac{1+t}{2}+\frac{1+x}{2}\left(\frac{t}{t+x}+\frac{t}{tx+1}\right)\right\} dm(x) \\ &= \frac{1+t}{2} - (1-t)^2 \int_{(0,1]} \frac{x(t+1)}{2(t+x)(tx+1)}\, dm(x), \end{aligned} \tag{A1}$$

where m is a normalized positive Radon measure on $[0,1]$, see Ref. 3. If the measure is not concentrated at 0, the last integral is strictly positive for all $t \in \mathbb{R}_+$. Its positive root, for the time being denoted by τ, is a real analytic function. Hence, every such function f_s can be represented as

$$f_s(t) = \frac{1+t}{2} - (t-1)^2 \tau(t)^2 \tag{A2}$$

with a certain τ, positive or trivial. Therefore, $(1+t)/2 - f_s(t)$ has exactly two real analytic roots,

$$\delta_+(t) = (t-1)\,\tau(t), \quad \delta_-(t) = -(t-1)\,\tau(t),$$

or is vanishing. The self-transposeness of f_s implies $\tau(1/t) = \sqrt{t}\,\tau(t)$ and both roots fulfill the condition (49). As explained in Sec. VII, a solution for k of our problem corresponds to such a root δ, which leads via (50) to $F(t)<1$. We infer: If selecting the root δ_+, the condition $F(t)<1$, $t>0$, is equivalent to $f_s(t)>1/2$ for all $t>1$. Because f_s is monotone increasing and $f_s(1)=1$ the latter inequality is true. On the other hand, F cannot fulfill $F(t)<1$ for all $t>1$ if the root δ_- is chosen, except $\delta_- = 0$. Otherwise we could conclude $f_s(t)>t/2$ for all $t>1$. But the self-transposeness effects $f_s'(1)=1/2$ and f_s must be concave. Therefore, $\delta := \delta_+$ is the only real analytic root leading to an appropriate F. Inserting

$$\delta(t) = (t-1)\,\tau(t) = \frac{t-1}{|t-1|}\sqrt{\frac{1+t}{2} - f_s(t)}, \quad \delta(1) = 0, \tag{A3}$$

into formulas (50), (51) yields (53) and (52).

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