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The Metric of Bures and the Geometric Phase.

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After the appearance of the papers of Berry [1], Simon [2], and of Wilczek and Zee [3], I tried to understand [4], whether there is a reasonable extension of the *geometric phase* - or, more accurately, of the accompanying phase factor - for general (mixed) states. A known recipe for such exercises is to use *purifications*: One looks for larger, possibly fictitious, quantum systems from which the original mixed states are seen as reductions of pure states. For density operators there is a standard way to do so by the use of Hilbert Schmidt operators (or by Hilbert Schmidt maps from an auxiliary Hilbert space into the original one).
Thus let

$$\mathbf{c}: \quad t \mapsto \varrho_t, \qquad 0 \le t \le 1 \tag{1}$$

be a path of density operators. A *standard purification* of (1) is a path

$$t \mapsto W_t, \qquad \varrho_t = W_t W_t^* \tag{2}$$

sitting in the Hilbert space of Hilbert Schmidt operators with scalar product

$$< W_1, W_2 >:= \operatorname{tr} W_1^* W_2 \tag{3}$$

The construction of standard purifications is by no means unique. Indeed, not only (2) but every *gauged* path

$$W_t \to W_t U_t, \qquad U_t \quad \text{unitary}, \tag{4}$$

is a purification of the same path of density operators.

The problem is, therefore, to distinguish within all purifications of the curve (1) of mixed states exceptional ones. In [4] this has been achieved as following. Let $W_1, ..., W_m$ be a *subdivision* of (2), i.e. a time-ordered subset of operators (2). These operators are of norm one since the density operators have trace one. Now the expression

$$\xi =< W_m, W_{m-1} > ... < W_3, W_2 >< W_2, W_1 > \tag{5}$$

will be considered according to (4) for all gauges

$$\xi \mapsto \tilde{\xi} \quad \text{by} \quad W_j \mapsto W_j U_j, \qquad U_j \quad \text{unitary}, \tag{6}$$

and it will be looked within the set of gauged $\tilde{\xi}$ for choices with

$$|\tilde{\xi}| = \text{maximum!} \tag{7}$$

The necessary and sufficient condition for (7) reads [5], [6]:

$$| < \tilde{W}_{j+1}, \tilde{W}_j > | = \mathrm{tr}\,(\varrho_j^{1/2} \varrho_{j+1} \varrho_j^{1/2})^{1/2} \quad \text{for} \quad j = 1, \ldots, m-1 \tag{8}$$

It should be remarked that

$$p(\varrho_1, \varrho_2) := (\mathrm{tr}\,(\varrho_1^{1/2} \varrho_2 \varrho_1^{1/2})^{1/2}) \tag{9}$$

is called *transition probability* of the pair ϱ_1, ϱ_2.
If (8) and hence (7) is fulfilled, the remaining arbitrariness is in a regauging $\tilde{W}_j \to \epsilon_j U \tilde{W}_j$ of the subdivision by numbers of modulus one and by an independent of j unitary U - provided the rank of the density operators (1) remains constant. This, however, means the gauge invariance of the quantity

$$X \mapsto \nu_{\mathbf{c}}^{subdivision}(X) = \xi \; < \tilde{W}_1, X \tilde{W}_m > \tag{10}$$

and it depends therefore only on the ordered set of the density operators $\varrho_k = W_k W_k^*$. In the limit of finer and finer subdivisions,

$$X \mapsto \nu_{\mathbf{c}}(X) := \lim \nu_{\mathbf{c}}^{subdivision}(X), \tag{11}$$

one obtains a gauge invariant linear form depending only on the original path (1). For closed loops of pure states the number $\nu_{\mathbf{c}}(\mathbf{1})$ is exactly Berry's phase factor.
(11) defines a certain noncommutative product integral. For curves of faithful density operators it can be conveniently expressed by the help of the geometric (quadratic) mean

$$a\#b := a^{\frac{1}{2}} \, (a^{-\frac{1}{2}} b a^{-\frac{1}{2}})^{\frac{1}{2}} \, a^{\frac{1}{2}} \tag{12}$$

of two positive operators [8], [9]. To this end one introduces the *holonomy* $V(\mathbf{c})$ of $\mathbf{c}$ by

$$\nu_{\mathbf{c}}(X) = \mathrm{tr} V(\mathbf{c}) \varrho_0 X \tag{13}$$

to find [20] (- in [20] the exponents are not correctly assigned -)

$$V(\mathbf{c}) = \lim_{subdivisions} (\varrho_m \# \varrho_{m-1}^{-1})(\varrho_{m-1} \# \varrho_{m-2}^{-1}) \cdots (\varrho_2 \# \varrho_1^{-1}) \tag{14}$$

My next aim is to obtain expressions of the above procedure which are more manageable. One idea is to use an infinitesimal variant of (8). Indeed one may sharpen (8) by adding the requirement

$$\tilde{W}_{j+1}^* \, \tilde{W}_j \; \geq \; 0 \tag{15}$$

which in turn implies (8) for faithful density operators. Going to finer and finer subdivisions - and removing the tilde - (15) results in ($\dot{W}$ denotes the t-derivation of W)

$$W^* \, \dot{W} = \dot{W}^* \, W, \tag{16}$$

the so-called *parallelity condition* [4] : A lift (2) of (1) fulfilling (16) is called a (standard) *parallel purification* or a *parallel lift*. Thus choosing a parallel purification of (1), it is

$$\nu_{\mathbf{c}}(X) \; = < W_0, X W_1 > \tag{17}$$

where W_0 and W_1 are the starting and the end point of a parallel lift.
Though the word *parallel* points to a parallel transport governed by a connection form (described later on), a more elementary explanation is possible. The scaler products of the subdivision attain their maximal possible value if (8) is true. The vectors W_j have norm one and hence the scalar product is the cosine between neighbouring vectors. Therefore (8) indicates that the angles between neighbouring vectors is as small as possible. Hence for infinitesimal neighbouring they are parallelly directed.
Note that from (16) it follows for parallel lifts

$$W^* \ddot{W} = \ddot{W}^* W, \tag{18}$$

Another idea is already indicated in a paper of Fock [7], who tried to minimize the arbitrariness in the transport of phases of degenerate eigenstates of Hamiltonians. The observation [10] is as following: After choosing appropriate phases in (5) the scalar products $< W_{j+1}, W_j >$ can be made real and positive. But then ξ in (7) attains its maximum if and only if

$$\parallel W_m - W_{m-1} \parallel + ... + \parallel W_3 - W_2 \parallel + \parallel W_2 - W_1 \parallel \tag{19}$$

attains its minimum. On the other hand, in going to finer and finer subdivisions, (19) tends to the length of the curve (2) in the metric given by (3). Therefore a purification (2) is a parallel one iff it solves the variational problem

$$\int \sqrt{< \dot{W}, \dot{W} >} \mathrm{d}t = \mathrm{Min} \; ! \tag{20}$$

However, the Euler equations of this variational problem are nothing else than the parallelity condition (16) !

One can calculate the minimal length (20), which, indeed, is the *Bures length* [9] of the path (1) of density operators. To do so one has to solve the parallelity condition. According to Dabrowski and Jadczyk [12], and to [13], this is done by an ansatz

$$\dot{W} = \; G W, \qquad G^* = G \tag{21}$$

which gives easily the equation

$$\dot{\varrho} = G\varrho + \varrho G \tag{22}$$

for the unknown G. G is gauge invariant, and depends only on the pair $\{\varrho, \dot{\varrho}\}$. This reflects the fact that the Bures length of the path (1) can be expressed without using lifts (2) : Inserting (21) into (20) one gets

$$L^{\mathrm{Bures}}(\mathbf{c}) \; = \; \int \sqrt{< GW, GW >} \mathrm{d}t \tag{23}$$

and a straightforward calculation shows

$$dt^2_{\text{Bures}} =< GW, GW >= \text{ tr } \varrho G^2 = \frac{1}{2}\text{tr } G\dot{\varrho} \tag{24}$$

There is a formal solution of (22) which reads for faithful density operators

$$G = \int_0^\infty (\exp -s\varrho)\dot{\varrho}(\exp -s\varrho)\, ds \tag{25}$$

and which implies for the metric form (24) the expression

$$\frac{1}{2}\text{tr} \int_0^\infty (\exp -s\varrho)\dot{\varrho}(\exp -s\varrho)\, \dot{\varrho}\, ds \tag{26}$$

Now, switching to density operators of finite dimension n, one may choose a base E_k , where $k = 1, \dots, n^2 - 1$, of traceless hermitian matrices, and write

$$\varrho = \frac{1}{n}\mathbf{1} + \sum x^k E_k \tag{27}$$

to get from (26)

$$\frac{1}{2}\text{tr } \dot{\varrho}G = \sum g_{jk}\dot{x}^j\dot{x}^k \quad \text{with} \quad g_{jk} = \frac{1}{2}\text{tr} \int_0^\infty (\exp -s\varrho)E_j(\exp -s\varrho)E_k\, ds \tag{28}$$

Therefore one has for the "moments conjugate to the coordinates", x_k,

$$p_k = 2\sum g_{kj}\dot{x}^j = \text{tr } GE_k \tag{29}$$

Example 1.
Here I show the simplest possible case, the Bures metric for $n = 2$. That this case can be solved is due to the following: Let δ be a derivation, $X > 0, Y$, 2-by-2 matrices, then

$$\delta X = YX + XY \tag{30}$$

is solved by

$$Y\, \text{tr}X = \delta X + \frac{1}{2}X^{-1}\delta \det X - \mathbf{1}\,\frac{1}{2}\text{tr}X \tag{31}$$

which is easily derived by δ-differentiating the characteristic equation of X. Describing now the density operators by

$$\varrho = \frac{1}{2}(\mathbf{1} + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3) \tag{32}$$

which is a variant of (27), the metric space

$$\{\varrho > 0, \quad \text{tr}\varrho = 1, \quad dt^2_{\text{Bures}}\} \tag{33}$$

can be isometrically imbedded into a sphere $\mathcal{S}^3$ given by

$$1 = x_1^2 + x_2^2 + x_3^2 + x_4^2 \tag{34}$$

where x_4 is defined by

$$x_4 \geq 0, \qquad x_4^2 = 4 \det \varrho \tag{35}$$

and which is equipped with the metric

$$\frac{1}{4}(\mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2 + \mathrm{d}x_4^2) \tag{36}$$

This example shows that the Bures metric turns the set of all 2-by-2 density matrices into a piece of a symmetric space, i.e. into half of a 3-sphere, see also [14], showing a hidden O(4)-symmetry. Further, let

$$\omega = \frac{1}{2}(\mathbf{1} + y_1\sigma_1 + y_2\sigma_2 + y_3\sigma_3) \tag{c}$$

be another 2-by-2 density operator. Then one calculates

$$p(\varrho, \omega) = \frac{1}{2}(x_1y_1 + x_2y_2 + x_3y_3 + x_4y_4 + 1) \tag{d}$$

showing that for $n = 2$ the transition probability characterize the relative position of ϱ and ω up to an O(4)-rotation.

Example 2.

Here the restriction of the Bures metric to maximal commutative sub-manifolds will be described. In a suitable base such a sub-manifold can be given by diagonal density matrices.

$$\varrho = (\, \lambda_j \, \delta_{jk} \,), \qquad G = (\, g_j \, \delta_{jk} \,) \tag{39}$$

Now (22) yields

$$g_j = \frac{\dot{\lambda}_j}{2\lambda_j} \tag{40}$$

Introducing the new variables

$$\lambda_j = y_j^2 \tag{41}$$

the metric of Bures reads

$$dt^2_{\mathrm{Bures}} = \sum \dot{y}_j^2 \tag{42}$$

Hence the restriction on a maximal commutative subset of the Bures metric is isometrically isomorph to a piece of a sphere, i.e. of a symmetric space.

The set of density operators, equipped with the Bures metric, is metrically incomplete. One may ask whether there is a completion in which all geodesics close for dim > 2. To support this question let us consider

Example 3.

The geodesic connecting two faithful density operators, ϱ_j, $j = 1, 2$, within the space of density operators can be described as follows. Let $\varrho_j = W_j W_j^*$. Then the geodesic in the W-space connecting W_1 with W_2 is part of a large circle of the unit sphere. Its equation is

$$W = \lambda_1 W_1 + \lambda_2 W_2, \qquad < W, W >= 1 \tag{43}$$

where

$$a := \text{Real } < W_1, W_2 > \tag{44}$$

$$\lambda_1 = \cos\vartheta - \frac{a}{\sqrt{1-a^2}} \sin\vartheta \tag{45}$$

$$\lambda_2 = \frac{\sin\vartheta}{\sqrt{1-a^2}} \tag{46}$$

The (oriented) length is hence the arc ϑ_0 given by

$$\cos\vartheta_0 = \text{Real} < W_1, W_2 > \quad \text{with} \quad -\frac{\pi}{2} < \vartheta_0 < \frac{\pi}{2} \tag{47}$$

Clearly, the length attains its minimum if we choose lifts such that a is of maximal value. This can be achieved if (15), and hence (8), is valid for $j = 1$.
Thus the Bures length ϑ_0 of the geodesic joining the two density operators is given by

$$\cos\vartheta_0 = \text{tr}\,(\varrho_1^{1/2}\varrho_2\varrho_1^{1/2})^{1/2}, \quad \text{with} \quad 0 < \vartheta_0 < \frac{\pi}{2} \tag{48}$$

One easily constructs pairs W_1, W_2 for which (43) is a parallel lift [4]. Expressing with them the holonomy (14) and the linear form (13) results in

$$V(\text{geodesic}) = \varrho_2 \# \varrho_1^{-1}, \qquad \nu_{\text{geodesic}}(X) = \text{tr}X(\varrho_2 \# \varrho_1^{-1})\varrho_1 \tag{e}$$

Comparing (48) with (d) of example 1 yields in the $n = 2$ case

$$x_1y_1 + x_2y_2 + x_3y_3 + x_4y_4 = \cos 2\theta_0 \tag{f}$$

The metric on the unit sphere of the Hilbert Schmidt W-space can be decomposed into a horizontal and a vertical part by an ansatz

$$< \dot{W}, \dot{W} > = < GW, GW > + < WA, WA >, \qquad A^* = -A \tag{51}$$

Then A can be defined equally well by [15]

$$W^*\dot{W} - \dot{W}^*W = \; A\,W^*W + W^*W\,A \tag{52}$$

This can be seen as follows. Going into (22) with an ansatz [15]

$$\dot{W} - WA = GW \tag{53}$$

and with $\varrho = WW^*$, it follows that A is anti-hermitian. Knowing this and the hermiticity of G one easily recovers (51). On the other hand, substituting (53) into the left side of (52), one arrives at the right side of this equation.
A is the restriction on the given lift of a connection 1-form, $\mathbf{A}$, for the gauge transformations (4), and one has

$$W^*\text{d}W - \text{d}W^*\,W = \; \mathbf{A}\,W^*W + W^*W\,\mathbf{A} \tag{54}$$

Introducing the $\mathbf{A}$-covariant derivation of an expression X transforming as W by

$$\mathrm{D}X = \mathrm{d}X - X\mathbf{A} \tag{55}$$

another form of (53) is

$$\mathrm{D}\,W \;=\; \mathbf{G}\,W \tag{56}$$

I now rewrite (54) in a form similar to (30). As a complex linear space defines a complex analytic structure, the total differential is decomposed naturally into $d = \partial + \bar{\partial}$. Using this one may rewrite (54) as

$$(\partial - \bar{\partial})\,(W^*W) = \;\mathbf{A}\,W^*W + W^*W\,\mathbf{A} \tag{57}$$

This may be contrasted to

$$\mathrm{d}(WW^*) = (\partial + \bar{\partial})(WW^*) = WW^*\mathbf{G} + \mathbf{G}WW^* \tag{58}$$

Thus we have

$$W^*\mathrm{d}W = \;\mathbf{A}^{1,0}\,W^*W + W^*W\,\mathbf{A}^{1,0} \tag{59}$$

$$\mathrm{d}W\,W^* = WW^*\mathbf{G}^{1,0} + \mathbf{G}^{1,0}WW^* \tag{60}$$

Remark: In the case of 2-by-2 density operators (51) can be solved effectively by (31) using $\delta = \partial - \bar{\partial}$, $X = W^*W$, and $Y = \mathbf{A}$. The first explicit expression for $\mathbf{A}$ was obtained in [16], see also [17].

For rank$(\varrho) = 1$ one falls back to the Berry case, and $\mathbf{A}$ describes the monopole structure. For rank$(\varrho) = 2$ one gets instanton structures [18]. It is unknown what is with rank$(\varrho) > 2$.

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Note added in proof: In a recent preprint [19] some of the constructions are generalized and examined for C*-algebras. It is further indicated how possibly to proceed if the states (or density operators) have mutually inequivalent supports.

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