Annalen der Physik. 7. Folge, Band 46, Heft 1, 1989, S. 63–69 VEB J. A. Barth, Leipzig

On Berry Phases Along Mixtures of States

By A. Uhlmann

Karl-Marx-University Leipzig, Dep. of Physics, GDR

Dedicated to Günter Vojta at the Occasion of his 60th Birthday

Abstract. Concepts connected with Berry's phase can be extended to curves and loops in state spaces defined by von Neumann algebras. This includes the important space of density operators.

Berry-Phasen längs gemischter Zustände

Inhaltsübersicht. Mit der Berry-Phase verbundene Begriffe können auf Wege in Zustandsräumen von Neumannscher Algebren ausgedehnt werden. Der wichtige Raum der Dichteoperatoren wird dabei mit berücksichtigt.

1. The Problem

Let $\mathscr{H}$ be an Hilbert space and $\mathscr{A}$ a von Neumann algebra acting on it unitally. We think of $\mathscr{A}$ as of an "algebra of observables", the elements of which serve to distinguish different states. In other words two normalized vectors of $\mathscr{H}$ define the same state if their expectation values are the same for all elements of $\mathscr{A}$.

We therefore define states (with respect to the algebra of observables $\mathscr{A}$) by the functionals

$$\omega_\psi \colon A \to \omega_\psi(A) = \langle \psi, A\psi \rangle / \langle \psi, \psi \rangle \text{ with } A \in \mathscr{A}, \tag{1}$$

and we define the state space Ω to be the set of all functionals on $\mathscr{A}$ of the form (1). Now we may consider $\mathscr{H} - \{0\}$ as a space with a foliation. The foliation is induced by $\mathscr{A}$, with base space Ω, and with leaves given as following: Two vectors, ψ and φ, belong to the same leaf iff $\omega_\psi = \omega_\varphi$ is valid.

Given a curve

$$\boldsymbol{c} \colon s \to \omega_s \in \Omega, \quad 0 \leq s \leq 1, \tag{2}$$

living in the state space and hence in the base space of our foliation. We then ask for lifts C of $\boldsymbol{c}$ into $\mathscr{H} - \{0\}$, i.e. for

$$C \colon s \to \psi_s \in \mathscr{H} \text{ with } \omega_s = \omega_{\psi_s}. \tag{3}$$

The question is whether there is a "natural" transport mechanism, a sort of "parallel transport" with the properties

a) it depends only on the pair, $\mathscr{H}$, $\mathscr{A}$, and
b) for a given curve $\boldsymbol{c}$ and an initial vector ψ_0 sitting in the leaf given by ω_0 it determines exactly one lift C.

Up to certain regularity assumptions we shall confirm the existence of such a "universal" transport mechanism which generalizes the well known parallel transport behind Berry's phase factor [1, 2, 3]. The important particular case of a type I factor $\mathscr{A}$, and with the set of density operators as state space Ω has been considered in [4] and [5].

At first we recall shortly some properties of the Berry phase as defined for pure states, thereby preparing the treatment of state mixtures. The treatment of the latter can be based on the requirement that the adiabatic (i.e. Berry's) transport condition is not destroyed by operators commuting with all the observables. In other words, the transport condition should be stable against the application of operators out of $\mathscr{A}'$, the commutant of $\mathscr{A}$, to the lifted path of states. If one arranges Ω to be (isomorphic to) the set of density matrices and $\mathscr{A}$ the Hilbert space of Hilbert Schmidt operators, the transport mechanisms can be explicitly described.

2. On Berry's Phase Factor

The original and presently most important case is that of pure states. Here $\mathscr{A} = \mathscr{B}(\mathscr{H})$ is the algebra of all bounded operators, and two state vectors belong to the same leaf if they are linearly dependent, i.e. the states ω are given by the one-dimensional subspaces of $\mathscr{H}$ or, equivalently, by the projection operators of rank one. Thus Ω is the projective space given naturally by $\mathscr{H}$. We realize it by

$$\Omega = \mathrm{P}(\mathscr{H})\text{: space of all rank one projections.} \tag{4}$$

This gives an additional structure to Ω by viewing their elements as trace class (or simply as bounded) operators.

Now the setting (2), (3), reads

$$\boldsymbol{c}\colon\ s \to P_s,\ 0 \leq s \leq 1,\ P_s \in \mathrm{P}(\mathscr{H}), \tag{5}$$

$$C\colon\ s \to \psi_s,\ P_s = |\psi_s\rangle\langle\psi_s|,\ \langle\psi_s, \psi_s\rangle = 1. \tag{6}$$

The condition for the natural parallel transport of the lift (6) of (5) simply reads

$$\left\langle \psi_s, \frac{d}{ds}\psi_s \right\rangle = 0. \tag{7}$$

Up to an overall phase, (7) defines a unique lift (6) of (5). If in addition $P_0 = P_1$ then $\psi_1 = \varepsilon\psi_0$, and $\varepsilon = \mathit{Berry}(\boldsymbol{c})$ is Berry's phase factor. The more, even with a general, not necessarily closed curve $\boldsymbol{c}$ in our state space, the expression

$$\mathit{Berry}(\boldsymbol{c}) = \langle\psi_0, \psi_1\rangle \tag{8}$$

depends only on $\boldsymbol{c}$ provided (6) and (7) is valid. The same is true for the rank one operator

$$I(\boldsymbol{c}) = |\psi_1\rangle\langle\psi_0|. \tag{9}$$

The map

$$\boldsymbol{c} \to I(\boldsymbol{c}) \tag{10}$$

is a morphism of the groupoid of curves contained in $\mathrm{P}(\mathscr{H})$ into the groupoid of rank one partial isometries, namely

$$I(\boldsymbol{c}^{-1}) = I(\boldsymbol{c})^*, \quad I(\boldsymbol{c}_1\boldsymbol{c}_2) = I(\boldsymbol{c}_1)\, I(\boldsymbol{c}_2). \tag{11}$$

In this setting two curves can be composed if the final point of the first one coincides with the initial point of the second. The multiplication, IJ, of operators, I, J, within the groupoid of partial isometries is allowed if $(I^*)\, I = J(J^*)$.

For a smooth enough path (5) one verifies

$$I(\boldsymbol{c}) = \lim P_{s_n} P_{s_{n-1}} \dots P_{s_1}, \tag{12}$$

with

$$0 \leq s_1 \leq s_2 \leq \dots \leq s_n,$$

and the limes goes through the filter of finer and finer subdivisions of the unit interval. Denoting by d total differentiation the connection form belonging to (7) reads

$$\operatorname{Im} \langle \psi, d\psi \rangle / \langle \psi, \psi \rangle \tag{13}$$

within $\mathscr{H} - \{0\}$. The trace of the operator valued 2-form $dP \wedge P \wedge dP$, divided by $2\pi i$, is the Chern class associated with (13) [6]. Let $\boldsymbol{f}$ be a 2-manifold bounded by $\boldsymbol{c}$, i.e. $\partial \boldsymbol{f} = \boldsymbol{c}$. Define

$$\boldsymbol{f}_{0p} = \int_{\boldsymbol{f}} dP \wedge P \wedge dP. \tag{14}$$

For smooth enough $\boldsymbol{f}$ this defines a trace class operator and

$$Berry(\boldsymbol{c}) = \exp \operatorname{tr} \boldsymbol{f}_{0p} = \det(\exp \boldsymbol{f}_{0p}). \tag{15}$$

The content of what has been said on $Berry(\boldsymbol{c})$ applies with appropriate modifications as well to the case discussed in [3].

3. A General Setting

We now return to an arbitrary von Neumann algebra $\mathscr{A}$ acting unitally on our Hilbert space $\mathscr{H}$. Again Ω denotes the set of all states given by (1), and we consider a curve (2), $\boldsymbol{c}$, and one of its lifts (3), C.

A lift C is called parallel, or better $\mathscr{A}$-parallel, if

$$\operatorname{Im}\langle \varphi_s, \mathring{\varphi}_s \rangle = 0 \text{ for all } \varphi_s = B\Psi_s \text{ with } B \in \mathscr{A}'. \tag{16}$$

We abbreviate the derivative by the dot notation: $dx/ds = \dot{x}$, and we denote the algebra of all operators commuting with $\mathscr{A}$ by $\mathscr{A}'$. The condition (16) is trivially equivalent to

$$\langle \psi_s, B\mathring{\psi}_s \rangle = \langle \mathring{\psi}_s, B\psi_s \rangle \text{ for all } B \in \mathscr{A}'. \tag{17}$$

If $s \to \psi_s$ is parallel, and if $r = r_s$ is a positive real and smooth function, then $s \to r_s\psi_s$ is parallel.

Before using the definition of parallelity we need a simple property of lifts. Consider two arbitrary lifts,

$$s \to \psi_s \text{ and } s \to \varphi_s \text{ with } \langle \psi_s, \psi_s \rangle = \langle \varphi_s, \varphi_s \rangle, \tag{18}$$

of $\boldsymbol{c}$ as given by (2). There is a curve of partial isometries $s \to U_s \in \mathscr{A}'$ satisfying for every s

$$U_s\psi_s = \varphi_s, \tag{19}$$

and these partial isometries become unique by the requirement

$$U_s^* U_s \mathscr{H} = \mathscr{A} - \operatorname{supp} \psi_s := \text{closure}\,[A\psi_s,\, A \in \mathscr{A}]. \tag{20}$$

While the curves (18) may be smooth in the Hilbert space topology, this is not automatically granted for their $\mathscr{A}$-supports. But in the following we need the smoothness of the $\mathscr{A}$-supports. Let us hence call a curve $s \to \psi_s$ "good" if this curve and the curve of its $\mathscr{A}$-supports is smooth (say strongly continuous and, up to some discrete points, two times differentiable). The smoothness of the $\mathscr{A}$-support excludes accidental degeneracies as level crossings, which have to be considered as singularities within this context.

Theorem. For all parameter values s the infimum

$$\inf \langle \mathring{\varphi}, \mathring{\varphi} \rangle / \langle \varphi, \varphi \rangle \tag{21}$$

running over all good lifts $s \to \varphi = \varphi_s$ of $\boldsymbol{c}$ will be reached exactly for the parallel lifts with constant (in s) norm.

Proof: We consider an arbitrary good lift $s \to \varphi = \varphi_s$ and a further one, $s \to \psi = \psi_s$, which is parallel. We may assume both, ψ and φ, to be curves of norm one vectors, because it is easily seen that a curve of vectors with varying norms cannot minimize (21). Now there is $U = U_s \in \mathscr{A}'$ satisfying (19) and (20). Hence we have

$$\langle \mathring{\varphi}, \mathring{\varphi} \rangle = \langle \mathring{U}\psi, \mathring{U}\psi \rangle + \langle U\mathring{\psi}, U\mathring{\psi} \rangle + \langle \mathring{U}\psi, U\mathring{\psi} \rangle + \langle U\mathring{\psi}, \mathring{U}\psi \rangle . \tag{22}$$

The last two terms of (22) will be rewritten by the aid of the relation $\mathring{P} = (\mathring{U}^*)\, U + (U^*)\, \mathring{U}$, where $P = (U^*)\, U$ is the $\mathscr{A}$-support of ψ:

$$\langle \mathring{U}\psi, U\mathring{\psi} \rangle + \langle U\mathring{\psi}, \mathring{U}\psi \rangle = \langle \psi, \mathring{P}\mathring{\psi} \rangle - \langle \psi, (U^*)\, \mathring{U}\mathring{\psi} \rangle + \langle \mathring{\psi}, (U^*)\, \mathring{U}\mathring{\psi} \rangle .$$

But U is commuting with $\mathscr{A}$, and by parallelity of ψ the last two terms vanish. We get

$$\langle \mathring{\varphi}, \mathring{\varphi} \rangle = \langle \mathring{U}\psi, \mathring{U}\psi \rangle + \langle U\mathring{\varphi}, U\mathring{\psi} \rangle + \langle \psi, \mathring{P}\mathring{\psi} \rangle . \tag{22a}$$

Let us examine the last two terms of this equation. It is

$$\begin{aligned} \langle U\mathring{\psi}, U\mathring{\psi} \rangle + \langle \psi, \mathring{P}\mathring{\psi} \rangle &= \langle \mathring{\psi}, P\mathring{\psi} \rangle + \langle \psi, \mathring{P}\mathring{\psi} \rangle \\ &= \langle P\mathring{\psi}, \mathring{\psi} \rangle + \langle \mathring{P}\psi, \mathring{\psi} \rangle = \langle \mathring{\psi}, \mathring{\psi} \rangle , \end{aligned}$$

where the last equality sign comes from differentiating $P\psi = \psi$. Finally we arrived at

$$\langle \mathring{\varphi}, \mathring{\varphi} \rangle = \langle \mathring{U}\psi, \mathring{U}\psi \rangle + \langle \mathring{\psi}, \mathring{\psi} \rangle . \tag{23}$$

Hence parallel and constant in its norm lifts minimize (21) for all values of its parameter s. Let us now prove the second assertion assuming φ to be a minimizing lift too. Because of (23) this is true if and only if $\mathring{U}\psi = 0$. This is equivalent with $\mathring{U}P = 0$ for $\mathring{U}$ is commuting with $\mathscr{A}$. The last equation we write $\mathring{U}(U^*)\, U = 0$. But U maps $\mathscr{H}$ onto the $\mathscr{A}$-support of Φ. Thus $\mathring{U}(U^*) = 0$. Hence

$$\frac{d}{ds} U(U^*) = \mathring{U}(U^*) + (\mathring{U}(U^*))^* = 0$$

and we see the independence on the parameter s of $\mathscr{A}$-supp(φ). Changing the role of φ and ψ, which both we had assumed to reach the infimum of (21), we conclude $\mathring{P} = 0$. Remembering $\mathring{U}P = 0$ and differentiating $U = UP$ we get $\mathring{U} = \mathring{U}P + U\mathring{P} = 0$. Hence $U = U_s \in \mathscr{A}'$ as defined by (19) and (20) is independent of s. Using this knowledge on straightforwardly checks the validity of (17) for the lift φ. In addition we proved Corollary:

a) $\mathscr{A}$-supp(ψ_s) is independent of s for every good parallel lift $\psi = \psi_s$ of a given path $\boldsymbol{c}$.
b) Let be ψ_s and φ_s two good parallel lifts of $\boldsymbol{c}$ with $\langle \psi, \psi \rangle = \langle \varphi, \varphi \rangle$. If then $\varphi_s = U_s \psi_s$, $U \in \mathscr{A}'$, fulfills (21), U does not depend on s.

Corollary a) may be expressed as following: Every vector of a good parallel lift is a cyclic vector for one and the same GNS-representation of $\mathscr{A}$.

We now may draw several conclusions. First of all we can unambiguously define *Berry*($\boldsymbol{c}$) if there is a good parallel lift C of $\boldsymbol{c}$ for which we may require $\langle \psi_s, \psi_s \rangle = 1$ without loss of generality. By the use of the theorem. every other lift with the same properties is of the form $s \to U\psi_s$ with $U \in \mathcal{A}'$, $U^*U = \mathcal{A}\text{-supp}(\psi_s)$. But this change does not alter the expression

$$Berry(\boldsymbol{c}) = \langle \psi_0, \psi_1 \rangle, \tag{24}$$

which extends (8) to our general setting. We see even more: The linear functional on $\mathcal{A}$ defined by

$$A \to \boldsymbol{c}(A),\ \boldsymbol{c}(A) := \langle \psi_0, A\psi_1 \rangle \text{ with } A \in \mathcal{A}, \tag{25}$$

is uniquely attached to $\boldsymbol{c}$, provided $\boldsymbol{c}$ admits a good parallel lift. Clearly we get $Berry(\boldsymbol{c}) = \boldsymbol{c}(1)$.

For a path C of unit vectors of $\mathcal{H}$ it is convenient to introduce $I(C) = |\psi_1\rangle\langle\psi_0|$ if C starts at ψ_0 and terminates by ψ_1. Assuming C to be a good parallel lift of $\boldsymbol{c}$ consisting of unit vectors,

$$I(\boldsymbol{c}) = \{UI(C)\,U^* \text{ with } U \in \mathcal{A}',\ U^*U = \mathcal{A}\text{-supp}(\psi_s)\}, \tag{26}$$

as a set is uniquely associated to $\boldsymbol{c}$. If we allow for multiplication of partial isometries if and only if the result is partial isometric too, we can save the relations (11) relative to the definition (26).

Let us now assume $\boldsymbol{c}$ closed, i.e. a loop in the state space Ω, and let $C\colon s \to \psi = \psi_s$ be a good parallel lift of unit vectors. Then the initial and the final vector of the curve C determine the same state in Ω, (and hence on $\mathcal{A}$). Then there is a unique partial isometry U with

$$\psi_1 = U\psi_0,\ U \in \mathcal{A}',\ (U^*)\,U = U(U^*) = \mathcal{A}\text{-supp}(\psi_s), \tag{27}$$

U is determined by $\boldsymbol{c}$ up to a similarity transformation $U \to VU(V^*)$ where V is any partial isometry out of $\mathcal{A}'$ such that the right carrier of V and the carrier of U coincide: $(V^*)\,V = U(U^*)$. The set of such similarity transforms constitute the conjugacy class of U in the groupoid of partial isometries of $\mathcal{A}'$. This conjugacy class is uniquely attached to the loop $\boldsymbol{c}$. It is a "pointed holonomy invariant" for it depends on the state at which the loop starts. On the other hand, U acts as a unitary operator on $U\mathcal{H}$. The spectrum of this unitary operator depends not on the starting point of $\boldsymbol{c}$. It is therefore an "absolute holonomy invariant" of the loop $\boldsymbol{c}$.

4. Density Operators

We now discuss shortly how this fits together with an state space

$$\Omega = \{\omega\colon \omega \geq 0,\ \text{tr.}\ \omega = 1\} \tag{28}$$

consisting of density operators defined as positive trace class operators on the Hilbert space $\mathcal{H}_{\text{pure}}$. We are then working in the Hilbert space of Hilbert Schmidt operators,

$$\mathcal{H} = \mathcal{S}_2(\mathcal{H}_{\text{pure}}) \subseteq \mathcal{B}(\mathcal{H}_{\text{pure}}), \tag{29}$$

with scalar product

$$\langle W_1, W_2 \rangle = \text{tr.}\ (W_1^*)\ W_2, \tag{30}$$

and $\mathcal{A}$ defined by the left multiplications $W \to AW$ with $A \in \mathcal{B}(\mathcal{H}_{\text{pure}})$ while $\mathcal{A}'$ is given by the multiplications $W \to WA$ from the right. Every element $W \in \mathcal{H} - \{0\}$ determines a definite element of Ω by

$$W \to \omega = \omega_W\colon \omega(A) = \text{tr.}\ W^*AW/\text{tr.}\ W^*W,\ A \in \mathcal{B}(\mathcal{H}_{\text{pure}}) \approx \mathcal{A}, \tag{31}$$

so that we consider it according to the context as linear functional or as a trace class operator. Within the latter notation one make use of the polar decomposition

$$W = (W^*W)^{1/2}U. \tag{32}$$

Then parallelity is a certain choice of $s \to U_s$ for curves $s \to \omega_s$. Let us now consider a smooth curve $\boldsymbol{c}$ in our state space (28), and a smooth lift C into $\mathscr{H}$. The lift is good if the curve of the projections onto the sets cl. $\{A W_s,\, A \in \mathscr{B}(\mathscr{H}_{\text{pure}})\}$ is smooth. For this it is necessary that

$$s \to \text{projection onto } \{\text{nullspace of } \omega_s\} \tag{33}$$

is smooth. In particular we have to assume for finite rank density operators that there rank does not change along the considered path $\boldsymbol{c}$.

The lift is parallel if

$$W_s^* \mathring{W}_s - \mathring{W}_s^* W_s = 0 . \tag{34}$$

Hence, using the interpretation of the vectors of $\mathscr{H}$ as operators of another Hilbert space, we may write the set of conditions (17) in a compact form. In the same spirit we introduce an operator valued "connection form"

$$\Theta = (W^*)\, dW - (dW^*)\, W / \operatorname{tr.}(W\, W^*) \tag{35}$$

vanishing just for parallel lift $s \to W_s$.

With the assumption $\langle W, W \rangle = 1$ we can examine this condition for a good and parallel lift

$$C\colon s \to (\omega_s)^{1/2}\, U_s . \tag{36}$$

One finds the independence on s of $U_s^* U_s$, and the equation

$$[d(\omega^{1/2}), \omega^{1/2}] = \omega U\, dU^* - dU\, U^*\, \omega , \tag{37}$$

where the bracket denotes the commutator. Given a lift W_0 of the initial point of a curve $\boldsymbol{c}$ fulfilling (33), the equation (37) gives uniquely a good parallel lift (36). Then

$$\boldsymbol{c}(A) = \operatorname{tr.}(W_0^*\, A W_1),\ \mathit{Berry}(\boldsymbol{c}) = \operatorname{tr.}\,(W_0^*\, W_1) . \tag{38}$$

Further, in the case $\boldsymbol{c}$ is a loop, the left multiplication of the elements W of $\mathscr{H}$ by the $U_0^* U_1$ compares with the partial isometry of $\mathscr{A}'$ introduced by (27). The spectrum of the operator $U_0^* U_1$, with the exclusion of its zeros, is an absolute holonomy invariant.

Applying the condition (34) or (37) to a path of density operators which are (up to normalization) projection operators of rank k, as it happens for the ground state of degenerate Hamiltonians, reproduces the results of [3], see [4]. In this particular case an integral form of (21) has been proposed already in [7] (see its appendix).

Another particular case appears if the density operators of the path $\boldsymbol{c}$ does not possses zero eigenvectors, i.e. $\boldsymbol{c}$ is a curve of faithful states. Then we can use a lift (36) where the W_s are invertible and the "phases" U_s are unitaries. Then (34) may be rewritten as (we suppress the parameter index s)

$$G = G^* \text{ where } G = \mathring{W}\, W^{-1} , \tag{39}$$

and G is the unique hermitian solution of

$$\omega G + G \omega = \mathring{\omega} . \tag{40}$$

The simplest example possible is certainly a state space Ω consisting of density operators of rank 2. Using Pauli matrices we write (suppressing the s-dependence)

$$\omega = \frac{1}{2} \sigma_0 + \vec{x}\, \vec{\sigma},\ \mathring{\omega} = \vec{v}\, \vec{\sigma},\ G = y_0 \sigma_0 + \vec{y}\, \vec{\sigma} . \tag{41}$$

The solution of (40) reads

$$y_0 = \frac{1}{4} \frac{d}{ds} (\ln \Delta),\quad \vec{y} = \Delta^{1/2} \frac{d}{ds} (\vec{x}\, \Delta^{-1/2}),\ \Delta = \det \omega . \tag{42}$$

If the density operators constituting $\boldsymbol{c}$ are unitarily equivalent one to another, then Δ is constant. Substituting this into (39) results in the differential equation

$$\overset{\circ}{\vec{w}} = i\vec{v} \times \vec{w} + w_0\vec{v}, \; w_0 = \vec{v}\,\vec{w} \tag{43}$$

(the symbol $\times$ denotes the vector product). These equations allow for a general integral:

$$(w_0)^2 - \vec{w}\,\vec{w} = \det(\omega)^{1/2} = \text{const.} \tag{44}$$

The solution if Δ and v remain constant along $\boldsymbol{c}$ has been given in [4] by a direct use of (37).

References

[1] BERRY, M. V.: Proc. R. Soc. Lond. **A 392** (1984) 45.
[2] SIMON, B.: Phys. Rev. Let. **51** (1983) 2167.
[3] WILCZEK, F.; ZEE, A.: Phys. Rev. Lett. **52** (1984) 2111.
[4] UHLMANN, A.: Rep. Math. Phys. **24** (1986) 229.
[5] UHLMANN, A.: Parallel Transport and Holonomy along Density Operators. In: Differential Geometric Methods in Theoretical Physics, (Proc. of the XV DGM conference), H. D. DOEBNER and J. D. HENNIG (ed.), Singapore World Sci. Publ., 1987.
[6] AVRON, J. E.; SEILER, R.; YAFFE, L. G.: preprint 1986: Adiabatic Theorems and Applications to the Quantum Hall Effect.
[7] FOCK, V.: Z. Phys. **49** (1928) 323.

Bei der Redaktion eingegangen am 13. Juni 1988.

Anschr. d. Verf.: Prof. Dr. A. UHLMANN
Karl-Marx-Universität Leipzig
Department of Physics
Leipzig
DDR-7010