– –

Published in:
“Nonlinear, Dissipative, Irreversible Quantum Systems”,
Proceedings of the International Symposium on Mathematical Physics, Clausthal, August 1994, edited by H.-D. Doebner, V.K. Dobrev & P. Nattermann. World Scientific, 1995, 296 - 302
With an addendum from my Torun lecture December 1994

– –

On Cyclic Evolution of Mixed States in Two-Level Systems

Armin Uhlmann

Mathematical Institute
University of Leipzig
Augustusplatz
D-04109 Leipzig, Germany

Abstract

Cyclic evolutions of quantum states are accompanied by geometric phases. This should remain true not only for pure but also for mixed states, then resulting in non-commutative phases. After a short introduction expressions for the parallel transport of these phases along geodesic polygons are derived. They become rather explicit for two-level systems, predicting definite deviations from the pure state case which should be detectable experimentally.

1 Introduction

It is the aim of this paper to give manageable expressions for the geometric phase of certain cyclic evolutions of mixed states.

The phase of a single state is not an observable quantity. In particular, the phase commutes with the observables which define the system. Nevertheless the change of states is generally accompanied by a change of the phase that can be called *phase transport*. If a state ω is changed in two different ways to become another state ω', the transport of the phases may yield different phases. Then their "difference", the *relative phase*, may become observable by virtue of the superposition principle. A particular case is the cyclic change where ω comes back to itself and the change of the phase will be compared with that of a "trivial" process where ω remains stationary.

All this is obvious, both experimentally and theoretically, for pure states. But it should remain true, to a certain instant, for mixed states: At first, in deviating from the pure to the mixed states, i. e. in going from the extreme part into the inner parts of the state space, coherence and correlations will not be destroyed suddenly but gradually, continuously. Secondly, if embedded in a larger system, the mixed states may be seen as restrictions of pure states. Then some "parts" of the relative phase of a cyclic change in the larger system may become decodable already by observables of the smaller system in which the states appear as mixed ones.

The phase transport and the relative phase consist (at least) of two parts, a *dynamical* and a *geometrical* one. The geometric part depends only on the shape of the curve in state space which describes the changes of the system, and *not* on the time needed for that changes. It is this feature that allows to distinct the geometric phase and its transport from the total phase change.

This remarkable fact also opens an heuristic way to see why the geometric phase survives the adiabatic approximation in which the changes become "infinitely slow". Thus, seen from to-day, it seems quite natural that the geometric phase firstly appeared within applications of the Born Oppenheimer approximation, Herzberg and Longuet-Higgens 1958, [3], Mead and Truhlar 1979, [8]. Berry 1984, [10], has shown, beside others, the generality of the phenomenon for adiabatically guided Hamiltonians, remarking that the transport condition appears, in the language of Mechanics, as an anholonomic constraint. Simon 1983, [9] elegantly explained its geometric structure in showing that it is a morphism from the cyclic evolutions, which form a loop group in the state space, into the holonomy group of a natural parallel transport. Because he restricted himself to pure states, that holonomy group is $U(1)$. Then, 1987, Aharonow and Anandan [13] settled the existence of the geometric phase in *every* cyclic evolution of pure states, whether adiabatic or not.

F. Wilczek and A. Zee, 1984, [11] have been the first in considering the geometric phase of degenerate eigenstates of a parameter dependent Hamiltonian. Here the state ω can be described by the projection P onto the subspace of eigenvectors. Choose in the Hilbert space $\mathcal{H}$ any ortho-frame $\psi_1, \dots, \psi_m$ of length m of eigenvectors. It can be considered as a point of an orthogonal Stiefel manifold which is an $U(n)$-bundle over the Graßmann manifold of projections P of rank m. Changing the projections along a curve C, $t \to P(t)$, calls for a (parallel) transport of the ortho-frames, which constitute the fibers over the projections. For a cyclic evolution of the projections, one comes back to the same subspace, and hence to another ortho-frame. This latter one is related to the one chosen at the beginning of the evolution by a $U(m)$-transformation U. In [11] the transport condition reads

$$\langle \psi_j, \frac{d}{dt}\psi_k \rangle = 0, \quad 1 \leq j \leq m, \quad 1 \leq k \leq m \tag{1}$$

and U becomes the geometric phase. In that scheme the fiber bundle depends on the length of the ortho-frames. A reformulation without that defect is as follows: With an auxiliary ortho-frame $\varphi_1, \dots, \varphi_m$ define the partial isometry $W := \sum |\psi_j\rangle\langle\varphi_j|$. Then (1) can be expressed by

$$W^* \frac{d}{dt} W = 0, \quad W W^* = P, \quad \mathrm{rank}\, P = m \tag{2}$$

Indeed, let $C : t \to P = P(t)$ be a curve of projections of rank m and C' a path of ortho-frames $\psi_1, \dots, \psi_m$ of $P\mathcal{H}$. The path $\tilde{C} : t \to W = W(t)$ respects (2) if and only if it is of the form $W := \sum |\psi_j\rangle\langle\varphi_j|$ where the path C' fulfils (1) and the auxiliary ortho-frame remains unchanged along the path, $W^*W = \mathrm{const.}$

If W with $WW^* = P$ runs through all lifts of a given curve, C, of fixed rank projections, parallelity is characterized by

$$\int (\frac{dW}{dt}, \frac{dW}{dt}) dt = \mathrm{Min!} \quad \text{or} \quad \int \sqrt{(\frac{dW}{dt}, \frac{dW}{dt})} dt = \mathrm{Min!},$$

$$\text{with} \quad (W_1, W_2) := \mathrm{Tr}\, W_1^* W_2 \tag{3}$$

As a device to transport ortho-frames of degenerate eigenvectors Fock (1928), [1] appendix, minimizes an "energy integral", similar to (3), to obtain (1).

But a finite rank projection is nothing than a rather special density operator, and the present author could extend (1986) [12] the scheme to *all* density operators: Assume a curve of states is given by a curve of density operators (normalized or not):

$$t \to \omega_t, \qquad \omega_t(A) = \mathrm{Tr} D(t) A \,/\, \mathrm{Tr} D(t), \quad \mathrm{rank}\, D(t) = \mathrm{const.} \tag{4}$$

a lift

$$t \to W(t), \qquad D(t) = W(t)\, W(t)^* \tag{5}$$

is called *parallel* iff

$$W^* \frac{dW}{dt} = \frac{dW^*}{dt} W \tag{6}$$

See also Dabrowski and Jadcyk (1989) [17]. One may regard every W with $WW^* = D$ as an *amplitude* of the state given by D, so that two amplitudes of the same state differ by an unobservable unitary (or partial isometric) phase U, $W \to WU$.

In 1987, [15], I observed that the parallel condition (6) follows from the variational principle (3).

2 Parallelity and Geodesics

Let us shortly return to the pure states. Pancharatnam (1956), [2], asked for the relative phase of two photon beams such that their superposition is of maximal intensity. For two states $P_j = |\psi_j\rangle\langle\psi_j|$ one has to adjust phases so that the norm of $\psi_2 + \psi_1$ is maximal. The requirement is satisfied if $\langle\psi_1, \psi_2\rangle$ is real and positive. The norm in question is maximal if the distance of ψ_1 and ψ_2 is minimal. There is a geodesic arc connecting these vectors that satisfies the Berry transport condition, and the phase transported from ψ_1 to ψ_2 fulfils Pancharatnam's rule.

Let now W_1, W_2 be amplitudes of faithful density operators D_1, D_2. Let us assume that their Hilbert space distance with respect to $(.,.)$ of (3) is as small as possible. This minimal distance equals the Bures distance (1969) [4] from D_1 to D_2 and

$$W_2^* W_1 = W_1^* W_2 > 0, \quad (W_2, W_1) = p(D_1, D_2) := \sqrt{(D_1^{1/2} D_2 D_1^{1/2})^{1/2}} \tag{7}$$

where the last expression was first obtained by Araki (1972) [5]. (For various definitions and properties of the transition probability $p(.,.)$ see [7].) In the state space, D_1 is connected by a geodesic arc (see [22]) with D_2. After choosing an amplitude W_1 of D_1 the transport along a parallel lift of a short geodesic arc results in the unique amplitude W_2 of D_2 determined by (7).

An ordered finite set of faithful density operators determines a *geodesic polygon*

$$D_1 \Rightarrow D_2 \Rightarrow \ldots \Rightarrow D_n \Rightarrow D_{n+1} = D_1 \tag{8}$$

in the state space. (There is just one short geodesic between two faithful density operators.) Now one fixes an amplitude W_1 of D_1 and chooses successively the unique amplitude W_{j+1} of D_{j+1} by $W_{j+1}^* W_j > 0$ for $j = 1, \ldots, n$. The *geometric phase*, U of the geodesic polygon is now implicitly given by $W_{n+1} = W_1 U$.

Expressions in terms of the density operator follow from squaring (7)

$$W_2^* W_1 = \sqrt{W_2^* W_1 W_1^* W_2} = \sqrt{W_2^* D_1 W_2} \tag{9}$$

by the help of polar decompositions. Abbreviating the Pucz and Woronowicz geometric mean [6] by (S, R positive)

$$S \# R := R^{1/2} (R^{-1/2}\, S\, R^{-1/2})^{1/2} R^{1/2} \tag{10}$$

one gets

$$W_{j+1} = (D_{j+1} \# D_j^{-1})\, W_j \tag{11}$$

$$W_1 U := W_{n+1} = (D_1 \# D_n^{-1})(D_n \# D_{n-1}^{-1}) \ldots (D_2 \# D_1^{-1})\, W_1 \tag{12}$$

U can be decomposed into relative phases $U_{j+1,j}$ defined by

$$W_j = D_j^{1/2} V_j, \quad W_{j+1} = D_{j+1}^{1/2} V_{j+1} = D_{j+1}^{1/2} U_{j+1,j} V_j \tag{13}$$

which implies by virtue of (11)

$$U_{j+1,j} = D_{j+1}^{-1/2} D_j^{-1/2} (D_j^{1/2} D_{j+1} D_j^{1/2})^{1/2} \tag{14}$$

Let us now stick to finite dimensions. Then the unitaries (14) are expressed through products of positive operators. Therefore, their determinants have to be one:

$$\det U_{j+1,j} = \det U = 1, \quad U \in \mathrm{SU}(n) \tag{15}$$

The reduction to $SU(n)$ in the interior of the state space is due to Dittmann and Rudolph [20], and Alberti [19]. If one or both the density operators involved in (14) tend to the boundary by prolonging the geometric arc, the uniqueness of the limits is guaranteed. Hence, with some caution, the equation

$$W_1 U = W_{n+1} = D_1^{1/2} U_{n+1,n} U_{n,n-1} \dots U_{2,1} V_1 \tag{16}$$

can be used if one or more of the polygons edges touch the boundary. Problems can arise with geodesics contained in the boundary ("level crossings", pairs of focal points). See Alberti (1992) [19].

3 Two-level Systems

To the first experiments [14] establishing Berry's phase belong configurations with mirrors or mirror-like devices which can be described by geodesic polygons in the space of pure states equipped with the Study Fubini metric. (The metric of Bures is restricting to the Study Fubini on the extreme boundary of the state space.) If one respects helicity reversals by an extra $i\pi$ phase, the polygon can be thought as consisting of short geodesic arcs. These and similar situations (use of filters) with "quantum jumps" are clearly examined in [16].

Two-by-two density operators may described by

$$D = \frac{1}{2}\underline{1} + x_1\sigma_1 + x_2\sigma_2 + x_3\sigma_3 = \frac{1-s}{2}\underline{1} + s\,P \tag{17}$$

where s is the degree of polarization, and

$$s^2 = 4(x_1^2 + x_2^2 + x_3^2), \quad 4x^2 := \det D = 1 - s^2 \tag{18}$$

The transition probability in (7) can be computed to [21]

$$p(D, D') = \frac{1}{2} + 2(x_1 x_1' + x_2 x_2' + x_3 x_3' + x x') \tag{19}$$

One may establish

$$D' \# D^{-1} == \frac{D' + x' x\, D^{-1}}{\sqrt{p(D', D)}} \tag{20}$$

and for the relative phases (14) one gets

$$U(D' \leftarrow D) = \frac{(D)^{1/2}\,(D')^{1/2} + x\,x'\,(D)^{-1/2}\,(D')^{-1/2}}{\sqrt{p(D', D)}} \tag{21}$$

This is valid for all short geodesics of length smaller than $\pi/2$, i. e. if $p(D', D) \neq 0$.

A particular simple case appears if the degree of polarization does not change, $s = s', x = x'$. Then

$$\sqrt{p(D', D)}\, D' \# D = \underline{1} + D' - D = \underline{1} + s(P' - P) \tag{22}$$

As an application let us compute the geometric phase U of geodesic triangles and quadrangles consisting of short geodesic arcs. Let us denote the common degree of polarization by s, and the projections of the involved density operators D_j by $P_j = |j\rangle\langle j|$, see (17). We abbreviate

$$a_{12} := \langle 1|2\rangle\,\langle 2|1\rangle, \quad a_{321} := \langle 3|2\rangle\,\langle 2|1\rangle\,\langle 1|3\rangle \text{ and so on} \tag{23}$$

geodesic triangles
The expression relevant for the intensities is

$$\sqrt{a_{12}a_{23}a_{31}}\,\mathrm{Tr}D_1U = s^4 a_{321} + s^3(1-s)\frac{a_{12}+a_{23}+a_{31}+2a_{321}-3}{2} +$$

$$+s^2(1-s)^2\frac{a_{12}+a_{23}+a_{31}+6}{2} + 4s(1-s)^3 + (1-s)^4 \qquad (24)$$

For $s = 1$ on gets $\epsilon = a_{321}/|a_{321}|$ as it should be for pure states.
geodesic quadrangles

$$\sqrt{a_{12}a_{23}a_{34}a_{41}}\,\mathrm{Tr}D_1U = s^5\, a_{4321} + \frac{s^4(1-s)}{2}$$

$$(6a_{4321} - a_{432} - a_{421} + 3a_{431} + 3a_{321} + a_{43} + a_{21} + a_{41} + a_{23} + a_{42} - 3a_{13} + 2) + \dots \qquad (25)$$

Acknowledgment

For valuable discussions and remarks I am grateful to P. M. Alberti, B. Crell, J. Dittmann, G. Rudolph, L. Stodolsky, H. Urbantke. I like to thank Deutsche Forschungsgemeinschaft for support under contract Al 374/1-3.

References

[1] V. Fock, *Z. Phys.* **49** (1928) 323

[2] S. Pancharatnam, *Proc. Indian Acad. Sci.* **A 44** (1956) 247

[3] G. Herzberg and H. C. Longuet-Higgens, *Discuss. Faraday Soc.* **35** (1963) 77

[4] D. J. C. Bures, *Trans. Amer. Math. Soc.* **135** (1969) 199

[5] H. Araki, *Publ. RIMS*, Kyoto Univ. **8** (1972) 335-362

[6] W. Pusz and L. Woronowicz, *Rep. Math. Phys.* **8** (1975) 159

[7] V. Cantoni, *Comm. Math. Phys.* **44** (1975) 125; A. Uhlmann, *Rep. Math. Phys.* **9** (1976) 273; H. Araki and G. A. Raggio, *Lett. Math. Phys.* **6** (1982) 237; P. M. Alberti, *Lett. Math. Phys.* **7** (1983) 25; P. M. Alberti and A. Uhlmann, *Lett. Math. Phys.* **7** (1983) 107

[8] C. A. Mead and D. G. Truhlar, *J. Chem. Phys.* **70** (1979) 2284

[9] B. Simon, *Phys. Rev. Lett.* **51** (1983) 2167

[10] M. V. Berry, *Proc. Royal. Soc. Lond.* **A 392** (1984) 45

[11] F. Wilczek and A. Zee, *Phys. Rev. Lett.* **52** (1984) 2111

[12] A. Uhlmann, *Rep. Math. Phys.* **24** (1986) 229

[13] Y. Aharonow and J. Anandan, *Phys. Rev. Lett.* **58** (1987) 1593; J. Anandan and Y. Aharonow, *Phys. Rev.* **D 38** (1987) 1863

[14] R. Y. Chiao and Y. S. Wu, *Phys. Rev. Lett.* **57** (1986) 933; M. Kitano, T. Yabuzaki, and T. Ogawa *Phys. Rev. Lett.* **58** (1987) 523; D. Suter, G. Chingas, R. A. Harris, and A. Pines, *Mol. Phys.* **61** (1987, 1327); R. Y. Chiao, A. Antaramian, K. M. Ganga, H. Jiao, and S. R. Wilkinson, *Phys. Rev. Lett.* **60** (1988) 1214; J. Samuel and R. Bhandari, *Phys. Rev. Lett.* **60** (1988) 2339

[15] A. Uhlmann, in: Differential Geometric Methods in Theoretical Physics, *ed. H. D. Doebner, J. D. Hennig,* World Sci. Publ., 1987, 246

[16] J. Anandan and Y. Aharonow, *Phys. Rev.* **D 38** (1988) 1863; M. G. Benedict, L. Gy. Feher, *Phys. Rev.* **D 39** (1989) 3194

[17] L. Dabrowski, A. Jadcyk, *J. Phys. A: Math. Gen.* **22** (1989) 3167

[18] L. Dabrowski, H. Grosse, *Lett. Math. Phys.* **19** (1990) 205

[19] P. M. Alberti, *Z. Analysis Anw.* **11** (1992) 293 and **11** (1992) 455

[20] J. Dittmann and G. Rudolph, *J. Geom. and Phys.* **10** (1992) 93

[21] M. Hübner, *Phys. Lett.* **A 163** (1992) 239

[22] A. Uhlmann, *Rep. Math. Phys.* **33** (1993) 253

Addendum, March 1995

Another easy to calculate process makes use of

$$D'\#D^{-1} = D'^{1/2} D^{-1/2}, \quad U(D', D) = 1_{\mathrm{id}}, \quad \text{if} \quad D'D = D'D \tag{26}$$

for commuting density operators.

Let us consider the following cyclic process with photons travelling in z-direction. The in-state D_1 is linear polarized in, say, x-direction and with an polarization degree ξ. Then, conserving the polarization direction, its degree is changed to η. To do this we use (26) to get D_2. In the next step the degree of polarization remains constant but the linear polarization is changed by an angle α. We arrive at D_3. The third step consists of changing the degree of polarization back to ξ, leaving unchanged its direction. We obtain D_4. Finally the direction of the polarization is rotated back to the x-direction, so that the initial state D_1 is recovered.

To get from D_2 to D_3 we have to calculate the relative phase transporting the state along a piece of a SU(2)-orbit on the Poincaré sphere. This has been calculated in different settings in [12] and [18] yielding

$$U(D_3, D_2) = \exp(-i\,\alpha\,\eta\,\sigma_3) \tag{27}$$

Because of (26) the phase obtained in the cyclic process, its *holonomy*, is computed to

$$U = U(D_1, D_4)\, U(D_3, D_2) = \exp i\, \alpha(\xi - \eta)\sigma_3 \tag{28}$$

What can be observed from the relative phase U according to the formalism of quantum theory is basically encoded by the transition form

$$A \to \nu(A) = \mathrm{Tr}\, D_1^{1/2} A D_1^{1/2} U^* \tag{29}$$

Similar considerations can be done with spin 1/2 particles and other two-level systems.