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Geometric phase for mixed states: a differential geometric approach

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Abstract. A new definition and interpretation of the geometric phase for mixed state cyclic unitary evolution in quantum mechanics are presented. The pure state case is formulated in a framework involving three selected principal fiber bundles, and the well-known Kostant–Kirillov–Souriau symplectic structure on (co-) adjoint orbits associated with Lie groups. It is shown that this framework generalizes in a natural and simple manner to the mixed state case. For simplicity, only the case of rank two mixed state density matrices is considered in detail. The extensions of the ideas of null phase curves and Pancharatnam lifts from pure to mixed states are also presented.

1 Introduction

The theory of the geometric phase (GP) for pure state unitary quantum evolution [1] attained a definitive status in all essential respects quite some time ago. On the one hand the original conditions of adiabatic cyclic unitary evolution were relaxed quite early [2,3] and a purely kinematic approach was also elaborated [4]. On the other hand the differential geometric framework in which the GP is best viewed has been fully delineated [3–5] – this will be recalled in a specific format below.

As against this situation, the generalization of the GP concept from pure states to generic mixed states of quantum systems has turned out to be non-unique, and several different approaches have been suggested. This is only to be expected, as one is making a transition from the particular to the general. The approaches include exploiting the process of purification of a mixed state of a given quantum system by tensoring it with another suitably chosen quantum system and so attaining a pure state [6]; setting up interferometric schemes in which phase shifts experienced by a system in a mixed state can be experimentally isolated [7]; using a real metric on the space of Hilbert–Schmidt operators leading to a natural connection via the Kaluza–Klein mechanism [8], and so on.

The purpose of the present work is to approach this problem from a differential geometric and, in a sense, a minimalist point of view, including also an essentially unique interpretation based on the general principles of quantum measurement theory. The main ingredients are the unitary matrix groups $U(n)$ for general (unspecified) n, some of their coset spaces, and associated structures. We will first show that the pure state GP problem can be treated in a systematic way using a set-up involving three principal fiber bundles (PFB): the first two are specific $U(n)$ coset spaces, the third is an associated bundle (AB) based on the second. In the second and the third PFB's, the base space consisting of unitarily related pure state quantum density matrices is a (co-) adjoint orbit in (the dual to) the Lie algebra $\underline{U}(n)$ of $U(n)$. As is well known, such orbits carry a unique symplectic structure – the Kostant–Kirillov–Souriau (KKS) symplectic structure [9–12] – and this is directly related to GP's for cyclic evolutions. Each of the three PFB's plays a specific role in the overall picture, with GP's being realized only in the third one as elements of the $U(1)$ holonomy group. Certain connections arising naturally in these PFB's will be made use of, and we will find that the familiar results are immediately obtained.

The advantage of this set-up, which may appear somewhat elaborate for the pure state case, is that it immediately, easily and unambiguously generalizes to the mixed state situation depending only upon general quantum principles. One of the important points we will emphasize is that, for cyclic unitary evolutions of such states, there is no such thing as *the* associated GP, but rather there is a collection of several such phases. However, the natural KKS symplectic structure singles out a specific combina-

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tion of them as having a preferred significance, and it is this that can be directly interpreted along the lines of quantum measurement theory.

The "minimalist" aspect of the treatment to be given here consists in the fact that we use only the structures that are already present in the quantum mechanical description of mixed states. We merely display them in a particular manner and then exploit them to the fullest possible extent. Any other approach, it would thus appear, must involve ideas and elements in addition to what is presented here; but in a sense these additions are not really necessary.

For the pure state GP problem, the case of non-cyclic evolutions [3], the relation to the Bargmann invariants (BI) [4], uses of geodesics [4], and the more recently discovered null phase curves (NPC) [13,14] have all been intensively studied. In the present work, as we wish to bring out as sharply as possible the most important features of mixed state GP's in exclusion to everything else, we shall limit ourselves to cyclic evolutions alone. While we will freely use geometric and group theoretic ideas intrinsic to the problem, we will also introduce local coordinate calculations so as to be able to carry out explicit calculations and make the entire treatment very tangible.

The contents of this paper are organized as follows. In Sect. 2 we reformulate the GP associated with pure state unitary cyclic evolution in the framework of three PFB's, pointing out the role played by each PFB in the overall argument. Section 3 then shows how this framework can be generalized in a natural way to evolution of mixed states in the rank two case, leading to a physically well-defined meaning of the GP to be associated with such cyclic evolution. The important role of the KKS symplectic structure in helping us identify the mixed state GP is clearly brought out. Section 4 provides the physical interpretation of the results of Sect. 3, bringing in the familiar meaning of mixed state density matrices in the context of quantum measurement theory. In Sect. 5 we discuss the role that the recently introduced NPC's [13,14] play in the mixed state situation; this involves generalizing these and the associated ideas of Pancharatnam lifts and null phase manifolds from pure states to mixed states. The concluding section, Sect. 6, outlines some general features of the extension of our approach from rank two mixed states to higher rank mixed states; contrasts our approach and interpretation with some other treatments, and mentions some open problems.

2 Reformulation of pure state GP

In this section we reformulate the pure state GP using the framework of coset space PFB's and AB [15–18]. As explained in the Introduction we consider only the case of cyclic evolution, as our main purpose is to extend the treatment to mixed states in later sections.

We denote by $\mathcal{H}$ the Hilbert space of pure states of some quantum system. We will suppose that $\mathcal{H}$ is of (complex) dimension n; however, in the final GP formulae the parameter n will in fact drop out. The group $U(n)$ of unitary transformations on $\mathcal{H}$ will hereafter be denoted by G; for the most part we deal with the defining representation of this group. In the latter case, its Lie algebra $\underline{U}(n)$ can be described as follows. The generators consist of all $n \times n$ hermitian matrices. These may be separated into pure imaginary antisymmetric matrices $J_{jk} = -J_{kj}$, generating the $SO(n)$ subgroup of $U(n)$: $(J_{jk})_{\ell m} = \mathrm{i}(\delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell})/\sqrt{2}$; and real symmetric "quadrupole" matrices $Q_{jk} = Q_{kj}$: $(Q_{jk})_{\ell m} = (\delta_{j\ell}\delta_{km} + \delta_{jm}\delta_{k\ell})/\sqrt{2}$. Here the indices j, k run over the range $1, 2, \ldots, n$. The basis made up of $J_{jk} = -J_{kj}$, $Q_{jk} = Q_{kj}$, $j \neq k$, $Q_j = \sqrt{2}Q_{jj}$ (no sum on j) is trace orthonormal. Thus we can write a general element of $\underline{U}(n)$ as a real linear combination of the form $X = x_j Q_j + \frac{1}{2}x_{jk}J_{jk} + \frac{1}{2}x'_{jk}Q_{jk}$ with $x_{jk} = -x_{kj}$ $x'_{jk} = x'_{kj}$ for $j \neq k$, and we have the trace formula $\mathrm{Tr}(XY) = x_j y_j + \frac{1}{2}x_{jk}y_{jk} + \frac{1}{2}x'_{jk}y'_{jk}$. Notice that the Q_j are the generators of the Abelian torus subgroup $U(1) \times U(1) \times \ldots \times U(1)$ of $U(n)$, consisting of all diagonal matrices U.

The unit sphere in $\mathcal{H}$ is denoted by $\mathcal{B}$:

$$\mathcal{B} = \{\psi \in \mathcal{H} | \ ||\psi|| = 1\} \subset \mathcal{H}, \tag{2.1}$$

and the space of unit rays by $\mathcal{R}$:

$$\mathcal{R} = \mathcal{B}/U(1) = \{\rho_\psi = \psi\psi^\dagger | \ \psi \in \mathcal{B}\}. \tag{2.2}$$

The projection π maps $\mathcal{B}$ onto $\mathcal{R}$. The preferred or natural connection one-form on $\mathcal{B}$, whose importance for pure state GP theory is well known, is

$$A = -\mathrm{i}\psi^\dagger \mathrm{d}\psi. \tag{2.3}$$

The two-form $\mathrm{d}A$ on $\mathcal{B}$,

$$\mathrm{d}A = -\mathrm{i}\mathrm{d}\psi^\dagger \wedge \mathrm{d}\psi, \tag{2.4}$$

is the pull-back of a symplectic two-form Ω on $\mathcal{R}$:

$$\mathrm{d}A = \pi^* \Omega. \tag{2.5}$$

The intrinsic definition of Ω is as follows [19]. At each point $\rho \in \mathcal{R}$, vectors in the tangent space $T_\rho\mathcal{R}$ arise by evaluating the commutators of hermitian operators K on $\mathcal{H}$ (generators of G) with ρ:

$$\rho \in \mathcal{R}, \ \ X \in \ T_\rho\mathcal{R} \ \ : \ \ X = -\mathrm{i}[K, \rho], \ \ K^\dagger = K. \tag{2.6}$$

Here K is determined by X up to an operator commuting with ρ, but this ambiguity does not matter in the definition of Ω below. If $\rho = \psi\psi^\dagger$, then a general X and a K can be expressed in terms of a vector χ orthogonal to ψ [4]:

$$K = \mathrm{i}(\chi\psi^\dagger - \psi\chi^\dagger), \ \ X = \chi\psi^\dagger + \psi\chi^\dagger \ \ , \ \ (\psi, \chi) = \psi^\dagger\chi = 0. \tag{2.7}$$

Now Ω is defined at each ρ by giving its evaluation on two tangent vectors there:

$$X, \ X' \in T_\rho\mathcal{R} \ \ : \Omega_\rho(X, X') = -\mathrm{i}\mathrm{Tr}(\rho[K, K']) = 2 \ \mathrm{Im}(\chi, \chi'). \tag{2.8}$$

This Ω is in fact the Kostant–Kirillov–Souriau (KKS) symplectic two-form on $\mathcal{R}$ viewed as a non-generic (co-) adjoint orbit in the Lie algebra $\underline{G}$ of G.

The connection A is now used to define horizontal lifts of smooth curves in $\mathcal{R}$. If

$$C = \{\rho(s) \in \mathcal{R} | s_1 \leq s \leq s_2,\ \rho(s_1) = \rho(s_2)\} \subset \mathcal{R} \quad (2.9)$$

is a parametrized closed curve in $\mathcal{R}$, and

$$\mathcal{C}_h = \{\psi(s) \in \mathcal{B} | s_1 \leq s \leq s_2\} \subset \mathcal{B} \quad (2.10)$$

is a horizontal lift of C to $\mathcal{B}$, then at each point of $\mathcal{C}_h$ we have

$$A_{\psi(s)}(\dot{\psi}(s)) = -\mathrm{i}(\psi(s), \dot{\psi}(s)) = \mathrm{Im}(\psi(s), \dot{\psi}(s)) = 0.$$

This lift $\mathcal{C}_h$ of C is in general not closed, as $\psi(s_1)$ and $\psi(s_2)$ may differ by a phase. This is the $U(1)$ holonomy group element and gives the GP associated with C:

$$\varphi_{\mathrm{geom}}[C] = \arg(\psi(s_1), \psi(s_2)) = -\int\int_S \Omega\,,\ \partial S = C, \quad (2.12)$$

where $S \in \mathcal{R}$ is any smooth two-dimensional surface with boundary C.

Now we explain the way in which this pure state GP emerges in a systematic and generalizable manner from a set-up involving three PFB's, each being used for a particular purpose.

The group G acts transitively on $\mathcal{B}$. Choose as a "reference point" or "origin" in $\mathcal{B}$ the first canonical basis vector in $\mathcal{H}$,

$$\psi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix}. \quad (2.13)$$

The stability group of $\psi_1^{(0)}$, namely the subgroup of G leaving $\psi_1^{(0)}$ invariant, is $H_0 = U(n-1)$ acting on dimensions $2, 3, \ldots, n$ in $\mathcal{H}$. Therefore $\mathcal{B}$ is the coset space $G/H_0 = U(n)/U(n-1)$. The first coset space PFB we introduce is $(G, \mathcal{B}, \ldots, H_0)$, where for simplicity here and later we omit the symbol for the relevant projection map. The purpose of this PFB is to help us compute the Maurer–Cartan one-forms on G in a practically useful form. For a general $\psi \in \mathcal{B}$, let $\ell(\psi)$ be some (local) choice of coset representative, namely an element of G carrying $\psi_1^{(0)}$ to ψ. Therefore $\ell(\psi)$ has the form

$$\ell(\psi) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ & \cdot & & \\ \psi & \cdot & \cdot & \cdot \\ & \cdot & & \\ & \cdot & \cdot & \cdot \end{pmatrix}, \quad (2.14)$$

with the first column being ψ and the rest determined up to an element of H_0 on the right. A general matrix $U \in G$ is then parametrized in the following way:

$$U = U(\psi, h_0) = \ell(\psi) h_0, \quad h_0 \in H_0, \quad (2.15)$$

with $\psi \in \mathcal{B}$ and $h_0 \in H_0$ being (local) coordinates on G. If we write the generators of H_0 as J_a and the remaining generators of G as J_μ, the full set of Maurer–Cartan one-forms on G ($\hat{\theta}^{(0)a}, \hat{\theta}^{(0)\mu}$) are given by [11, 12]

$$\begin{aligned} & U(\psi, h_0)^{-1} \mathrm{d}U(\psi, h_0) \quad (2.16) \\ & = -\mathrm{i}\hat{\theta}^{(0)a} J_a - \mathrm{i}\hat{\theta}^{(0)\mu} J_\mu \\ & = \psi^\dagger \mathrm{d}\psi\ Q_1\ + \underline{H}_0 \text{ terms } + \text{cross terms}, \end{aligned}$$

$$Q_1 = \begin{pmatrix} 1\ 0 & \cdot & \cdot & 0 \\ 0 & & & \\ \cdot & & & \\ \cdot & & 0 & \\ 0 & & & \end{pmatrix}.$$

To make contact with previous notation, the generators J_a of H_0 are $Q_j,\ J_{jk},\ Q_{jk}$ for $j, k = 2, 3, \ldots, n$; the ψ-dependent term is the unambiguous contribution involving the first diagonal generator Q_1, and the cross terms involve $J_{1k},\ Q_{1k}$ for $k = 2, 3, \ldots, n$, all outside $\underline{H}_0$. The coefficient of Q_1 is independent of the freedom in the choice of $\ell(\psi)$, and is essentially the one-form A in (2.3).

Next we turn to the second coset space PFB. The origin $\psi_1^{(0)} \in \mathcal{B}$ determines a corresponding point $\rho^{(0)} = \psi_1^{(0)} \psi_1^{(0)\dagger} \in \mathcal{R}$. The stability group of $\rho^{(0)}$ is the subgroup $H = U(1) \times H_0 = U(1) \times U(n-1) \subset G$, $U(1)$ being generated by Q_1, and $\mathcal{R}$ is the coset space G/H. The second coset space PFB is taken to be $(G, \mathcal{R}, \ldots, H)$. Here the base is a particular (co-) adjoint orbit in the Lie algebra $\underline{G}$. On this PFB, we have a preferred connection by retaining the terms in (2.16) involving generators of H alone, and dropping the cross terms:

$$\begin{aligned} \omega^{(2)} &= -\mathrm{i}\left(U(\psi, h_0)^{-1} \mathrm{d}U(\psi, h_0)\right)_H \\ &= -\mathrm{i}\psi^\dagger \mathrm{d}\psi\ Q_1 + \underline{H}_0 \text{ terms}. \end{aligned} \quad (2.17)$$

Finally we bring in a PFB associated to $(G, \mathcal{R}, \ldots, H)$: the base remains the same, while G and H are replaced by suitably chosen E and F. These are the $F = U(1)$ subgroup of the $H = U(1) \times H_0$ subgroup of G generated by Q_1 and $E = \mathcal{B}$. So this AB is $(\mathcal{B}, \mathcal{R}, \ldots, U(1))$. The action of H on F which is needed is defined by making H_0 in H act trivially, while $U(1)$ in H acts on $F = U(1)$ by the (Abelian) $U(1)$ group composition law. Thus the connection $\omega^{(2)}$ of (2.17) goes over in this third PFB to the connection

$$\omega^{(3)} = -\mathrm{i}\psi^\dagger \mathrm{d}\psi = A. \quad (2.18)$$

Thus we have arrived at (2.3). The $\underline{H}_0$-terms in $\omega^{(2)}$ have been dropped since H_0 is defined to act trivially on $F = U(1)$, and we have also set $Q_1 = 1$. In this final result, the dependence on n and the freedom in the choice of $\ell(\psi)$ have both disappeared. What we have seen already is the connection (2.5) between $\mathrm{d}A$ on $\mathcal{B}$ and the KKS symplectic two-form Ω on $\mathcal{R}$.

3 Mixed state GP's

A pure state density matrix is a rank one operator, with one non-zero eigenvalue unity and the remaining eigenvalues equal to zero. A mixed state density matrix has in general a spectrum of positive eigenvalues each with some multiplicity, followed by a remainder (in general) of zero eigenvalues. Whereas pure state density matrices are acted upon transitively by G, this is not true for the mixed state case since both the rank of the density matrix and its spectrum of eigenvalues are preserved under unitary transformations. For each rank k the generic case is when the spectrum of non-zero eigenvalues κ_a is non-degenerate, i.e., they obey

$$0 < \kappa_k < \kappa_{k-1} < \ldots < \kappa_2 < \kappa_1 < 1, \ \sum_{a=1}^{k} \kappa_a = 1. \tag{3.1}$$

The corresponding set of density matrices may be denoted by $\mathcal{R}_{\underline{\kappa}}$. Keeping k and $\underline{\kappa}$ fixed, each of these sets is acted upon transitively by G, and is homeomorphic in a $\underline{\kappa}$-dependent manner to the coset space $G/(U(1)^k \times U(n-k))$. Cases of degeneracy among the κ_a correspond to non-generic lower dimensional situations described by other coset spaces.

As the simplest case of a mixed state we consider rank two density matrices ρ for which the non-zero eigenvalues are non-degenerate:

$$\rho = \kappa_1 \psi_1 \psi_1^\dagger + \kappa_2 \psi_2 \psi_2^\dagger, \tag{3.2}$$

where $0 < \kappa_2 < \kappa_1 < 1$, $\kappa_1 + \kappa_2 = 1$ and the vectors $\psi_a, a = 1, 2$, each determined up to a phase factor, form an ordered pair of orthonormalized eigenvectors of ρ:

$$(\psi_a, \psi_b) = \psi_a^\dagger \psi_b = \delta_{ab}. \tag{3.3}$$

Hereafter we keep κ_a fixed. So each such ρ is in a unique one to one correspondence with an ordered pair of pure state density matrices defined as and obeying

$$\rho = \kappa_1 \rho_1 + \kappa_2 \rho_2; \ \ \rho_a = \psi_a \psi_a^\dagger \ , \ \rho_a \rho_b = \delta_{ab} \rho_a \ \ \text{(no sums!)}. \tag{3.4}$$

This set of ρ's forms a (co-) adjoint orbit under G. At the vector space level we have to deal with ordered orthonormal pairs $\psi_a, a = 1, 2$. We recognize here the generalizations of $\mathcal{B}$ and $\mathcal{R}$ of the pure state situation to mixed states of the form (3.2), in which for any $\underline{\kappa} = (\kappa_1, \kappa_2)$ with $0 < \kappa_2 < \kappa_1$ and $\kappa_1 + \kappa_2 = 1$, we have an orbit $\mathcal{R}^{(2)}_{\underline{\kappa}}$ replacing $\mathcal{R}$. We now define and describe these spaces in detail, stressing that we need something at the vector space level "on top of" density matrices.

The space $\mathcal{B}^{(2)}$

We define this space to consist of ordered pairs of orthonormal vectors in $\mathcal{H}$, with no explicit mention of κ_a. For later convenience we write the pair of vectors in a particular notation:

$$\mathcal{B}^{(2)} = \{\Psi = (\psi_1 \ \ \psi_2) | \psi_a \in \mathcal{B}, \psi_a^\dagger \psi_b = \delta_{ab}\}. \tag{3.5}$$

In an obvious manner, the group G acts transitively on $\mathcal{B}^{(2)}$. A convenient "origin" consists of the first two canonical basis vectors in $\mathcal{H}$:

$$\Psi^{(0)} = (\psi_1^{(0)} \ \ \psi_2^{(0)})$$

$$\psi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \ , \ \psi_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ \cdot \\ \cdot \\ 0 \end{pmatrix}. \tag{3.6}$$

The stability group of $\Psi^{(0)}$ is the subgroup $H_0 = U(n-2) \subset G$ acting on the dimensions $3, 4, \ldots, n$ in $\mathcal{H}$. (The use of the same letter H_0, and later H, as in the previous section, should cause no confusion.) Thus we recognize $\mathcal{B}^{(2)}$, the orbit of $\Psi^{(0)}$ under G action, as a coset space:

$$\mathcal{B}^{(2)} = G/H_0 = U(n)/U(n-2),$$
$$\dim \mathcal{B}^{(2)} = 4(n-1). \tag{3.7}$$

Elements of the tangent space to $\mathcal{B}^{(2)}$ at Ψ can be described as follows. Each $\Phi \in T_\Psi \mathcal{B}^{(2)}$ is a pair $\Phi = (\phi_1 \ \ \phi_2)$, $\phi_a \in \mathcal{H}$, obeying restrictions which follow from (3.3). After inserting $\psi_a' = \psi_a + \epsilon \phi_a$ $(a = 1, 2)$ into the latter equation and retaining only terms linear in ϵ, one finds

$$(\psi_1, \phi_1), (\psi_2, \phi_2) = \text{pure imaginary},$$
$$(\psi_1, \phi_2) + (\phi_1, \psi_2) = 0. \tag{3.8}$$

Taking out a factor of i we can write each such Φ uniquely as

$$\Phi = \mathrm{i}\Psi h + \overline{\underline{\chi}},$$
$$h^\dagger = h = 2 \times 2 \ \ \text{matrix},$$
$$\overline{\underline{\chi}} = (\chi_1 \ \ \chi_2), \tag{3.9}$$
$$\chi_a \in \mathcal{H}_\perp(\Psi) = \text{subspace of } \mathcal{H} \text{ orthogonal to } \psi_1 \text{ and } \psi_2.$$

Thus we have the one to one correspondence

$$\Phi \in T_\Psi \mathcal{B}^{(2)} \leftrightarrow h, \ \overline{\underline{\chi}}. \tag{3.10}$$

This is a generalization of the pure state case where any $\phi \in T_\psi \mathcal{B}$ has the unique form [4]

$$\phi = \mathrm{i}a\psi + \chi \, ; \ a^* = a, \ \chi \in \mathcal{H}_\perp(\psi). \tag{3.11}$$

The real number a gets generalized to a 2×2 hermitian matrix h, while $\chi \in \mathcal{H}_\perp(\psi)$ has been replaced by an ordered pair $\overline{\underline{\chi}} = (\chi_1 \ \ \chi_2)$ with each $\chi_a \in \mathcal{H}_\perp(\Psi)$.

The space $\mathcal{R}^{(2)}$

This is the space of mixed state density matrices we are interested in, and it can be described in several useful ways:

$$\mathcal{R}^{(2)} = \{\rho^\dagger = \rho \geq 0, \mathrm{Tr}\rho = 1 | \text{Spectrum of}$$
$$\rho = (\kappa_1, \kappa_2, 0, \ldots, 0)\}$$

$$= \{U\rho^{(0)}U^{-1} | U \in G, \rho^{(0)} = \kappa_1 \psi_1^{(0)} \psi_1^{(0)\dagger} + \kappa_2 \psi_2^{(0)} \psi_2^{(0)\dagger}\}$$
$$= \{(\rho_1 \ \ \rho_2) | \rho_a \in \mathcal{R}, \rho_1 \rho_2 = 0\}. \quad (3.12)$$

The last description of $\mathcal{R}^{(2)}$ (we omit $\underline{\kappa}$ in $\mathcal{R}^{(2)}_{\underline{\kappa}}$ since $\underline{\kappa}$ is kept fixed in the discussion), in which κ_a do not appear explicitly, is actually equivalent to the earlier description, via a $\underline{\kappa}$-dependent diffeomorphism. However, we do not mention this repeatedly.

Under the action of G, the stability group of $\rho^{(0)}$ is $H = U(1) \times U(1) \times H_0$, the $U(1)$ factors acting on the first and the second directions in $\mathcal{H}$. Thus we exhibit $\mathcal{R}^{(2)}$ as a coset space which is in fact a (co-) adjoint orbit in $\underline{G}$, as well as a quotient space starting from $\mathcal{B}^{(2)}$:

$$\mathcal{R}^{(2)} = \text{(co-) adjoint orbit of } \rho^{(0)} =$$
$$G/H = \mathcal{B}^{(2)}/U(1) \times U(1),$$
$$\dim \mathcal{R}^{(2)} = \dim \mathcal{B}^{(2)} - 2 = 2(2n-3). \quad (3.13)$$

The ($\underline{\kappa}$-dependent) projection $\pi : \mathcal{B}^{(2)} \to \mathcal{R}^{(2)}$ takes $\Psi \in \mathcal{B}^{(2)}$ to $\rho_\Psi \in \mathcal{R}^{(2)}$ according to

$$\rho_\Psi = \pi(\Psi) = \Psi \kappa \Psi^\dagger, \ \ \kappa = \begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix}. \quad (3.14)$$

The description of the tangent spaces $T_\rho \mathcal{R}^{(2)}$ involves a little effort. If we use the representation (3.14) for ρ_Ψ, and take some $\Phi \in T_\Psi \mathcal{B}^{(2)}$, a general $X \in T_{\rho_\Psi} \mathcal{R}^{(2)}$ is certainly expressible as

$$X = \Psi \kappa \Phi^\dagger + \Phi \kappa \Psi^\dagger \in \underline{G}. \quad (3.15)$$

Using (3.9) for Φ and writing out and grouping terms, we see that

$$X = \mathrm{i}\Psi[h, \kappa]\Psi^\dagger + \Psi \kappa \overline{\underline{\chi}}^\dagger + \overline{\underline{\chi}} \kappa \Psi^\dagger. \quad (3.16)$$

This is certainly determined by h and $\overline{\underline{\chi}}$, but h_{11} and h_{22} are not needed since

$$[h, \kappa] = (\kappa_1 - \kappa_2) \begin{pmatrix} 0 & -h_{12} \\ h_{21} & 0 \end{pmatrix}, \quad h_{21} = h_{12}^*. \quad (3.17)$$

Therefore, as is easily confirmed, each $X \in T_{\rho_\Psi} \mathcal{R}^{(2)}$ is determined by, and corresponds in a one-to-one fashion to, a complex number h_{12} and a pair $\overline{\underline{\chi}}$:

$$X(h_{12}, \overline{\underline{\chi}}) = -\mathrm{i}(\kappa_1 - \kappa_2)(h_{12} \psi_1 \psi_2^\dagger - h_{12}^* \psi_2 \psi_1^\dagger) \quad (3.18)$$
$$+ \kappa_1 (\psi_1 \chi_1^\dagger + \chi_1 \psi_1^\dagger) + \kappa_2 (\psi_2 \chi_2^\dagger + \chi_2 \psi_2^\dagger).$$

If we alter ψ_a by independent phases $\mathrm{e}^{\mathrm{i}\alpha_a}$ which leave ρ_Ψ invariant, to keep X unchanged we must replace $h_{12} \to \mathrm{e}^{\mathrm{i}(\alpha_2 - \alpha_1)} h_{12}, \chi_a \to \mathrm{e}^{\mathrm{i}\alpha_a} \chi_a$. Returning to $\Phi \in T_\Psi \mathcal{B}^{(2)}$ in (3.9), we can tentatively separate it into vertical and horizontal parts, the former being the h_{11}, h_{22} terms and the latter the rest:

$$\Phi = \mathrm{i}\Psi h + \overline{\underline{\chi}} = \mathrm{i}\, \Psi \begin{pmatrix} h_{11} & 0 \\ 0 & h_{22} \end{pmatrix} + \mathrm{i}\Psi \begin{pmatrix} 0 & h_{12} \\ h_{12}^* & 0 \end{pmatrix} + \overline{\underline{\chi}}. \quad (3.19)$$

The horizontal part is in unambiguous correspondence with X in (3.18).

For the later determination of the KKS two-form on $\mathcal{R}^{(2)}$, we need to express each $X \in T_{\rho_\Psi} \mathcal{R}^{(2)}$ as the commutator of some hermitian operator $K \in \underline{G}$ with ρ_Ψ. This is easily done:

$$X(h_{12}, \overline{\underline{\chi}}) = -\mathrm{i}[K(h_{12}, \overline{\underline{\chi}}), \rho_\Psi], \quad (3.20)$$
$$K(h_{12}, \overline{\underline{\chi}}) = \mathrm{i}(\overline{\underline{\chi}} \Psi^\dagger - \Psi \overline{\underline{\chi}}^\dagger) - \Psi \begin{pmatrix} 0 & h_{12} \\ h_{12}^* & 0 \end{pmatrix} \Psi^\dagger.$$

The presence of new terms compared to (2.7) in the pure state case should be noted.

We may add the following remark. Each (co-) adjoint orbit (fixed by $\underline{\kappa}$ as explained above) meets the subalgebra of diagonal matrices in as many points as the number of diagonal matrices we get by applying the permutation group (Weyl group) to the starting diagonal matrix $\rho^{(0)} = \kappa_1 \psi_1^{(0)} \psi_1^{(0)\dagger} + \kappa_2 \psi_2^{(0)} \psi_2^{(0)\dagger} + \ldots \kappa_k \psi_k^{(0)} \psi_k^{(0)\dagger}$, just intersecting each Weyl chamber exactly once. Fixing $\underline{\kappa}$ in such a way that $0 < \kappa_k < \kappa_{k-1} < \ldots < \kappa_2 < \kappa_1 < 1$ is then equivalent to choosing a particular Weyl chamber. Therefore, we have as many orbits as the points in the interior of a Weyl chamber, the boundary points corresponding to the case where the mixed state density matrix has degenerate eigenvalues. For example, in the rank two case, analyzed explicitly in this section, the Weyl chamber is a one-dimensional segment that we have chosen to parametrize by $\kappa_1 \in [1/2, 1)$.

Local coordinates on $\mathcal{B}^{(2)}$ and $\mathcal{R}^{(2)}$

In order to later connect Hilbert space notations with differential geometric ones, we now describe correlated local coordinate choices around general points in $\mathcal{B}^{(2)}$ and in $\mathcal{R}^{(2)}$. Take a point $\Psi_0 = (\psi_{01} \ \ \psi_{02}) \in \mathcal{B}^{(2)}$, not necessarily the "origin" $\Psi^{(0)}$ of (3.6). Its image in $\mathcal{R}^{(2)}$ is

$$\Psi_0 \in \mathcal{B}^{(2)} \to \rho_0 = \pi(\Psi_0) = \Psi_0 \kappa \Psi_0^\dagger \in \mathcal{R}^{(2)}. \quad (3.21)$$

Convenient neighborhoods of Ψ_0, ρ_0 will get determined as we describe them. The orthogonal complement to Ψ_0, a subspace of $\mathcal{H}$ of complex dimension $n-2$, is defined as

$$\mathcal{H}_\perp(\Psi_0) = \{\psi \in \mathcal{H} | (\psi_{0a}, \psi) = 0, \ a = 1, 2\} \subset \mathcal{H}. \quad (3.22)$$

Let $\Psi = (\psi_1 \ \ \psi_2) \in \mathcal{B}^{(2)}$ be "near" Ψ_0. Then each of ψ_1 and ψ_2 is expressible as a unique linear combination of ψ_{01}, ψ_{02} plus some vector in $\mathcal{H}_\perp(\Psi_0)$. Let us write

$$\psi_a = S_{ba} \psi_{0b} + \chi_{0a}, \ \chi_{0a} \in \mathcal{H}_\perp(\Psi_0) \ (a = 1, 2);$$

i.e.,

$$\Psi = \Psi_0 \, S + \overline{\underline{\chi}}_0, \quad (3.23)$$

with S a complex 2×2 matrix. The condition (3.3) becomes

$$S^\dagger S = 1_{2\times 2} - \overline{\underline{\chi}}_0^\dagger \overline{\underline{\chi}}_0. \quad (3.24)$$

Let us then limit $\underline{\overline{\chi}}_0$ so that the two eigenvalues of $\underline{\overline{\chi}}_0^\dagger \underline{\overline{\chi}}_0 = (\chi_{0a}^\dagger \chi_{0b})$ both lie in $[0,1)$. (This means that $\underline{\overline{\chi}}_0$ involves $4(n-2)$ real independent variables.) This makes S non-singular, the general solution being

$$S = \mathcal{U}(1 - \underline{\overline{\chi}}_0^\dagger \underline{\overline{\chi}}_0)^{1/2},\ \mathcal{U} \in U(2). \tag{3.25}$$

Here the square root is the unique hermitian positive definite one, so this is the polar decomposition of S.

If we allow $\mathcal{U}$ to be a general $U(2)$ element, that brings in four new independent variables, so $\mathcal{U}$ and $\underline{\overline{\chi}}_0$ together account for $4(n-1)$ real independent variables which would be right for $\mathcal{B}^{(2)}$. However, the action of $U(1)\times U(1)$ on Ψ amounting to a motion along the fibers is

$$\Psi \to \Psi \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha_1} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\alpha_2} \end{pmatrix}, \tag{3.26}$$

and it is convenient to have the charts on $\mathcal{B}^{(2)}$ and $\mathcal{R}^{(2)}$ related in this way. We therefore limit $\mathcal{U}$ in (3.25) to a two parameter family. We see easily that if $\mathcal{U} \in U(2)$ has real positive diagonal elements, then it is actually an element of $SU(2)$ and takes the form

$$\mathcal{U}(z) = \begin{pmatrix} \sqrt{1-|z|^2} & z \\ -z^* & \sqrt{1-|z|^2} \end{pmatrix},\ |z|<1. \tag{3.27}$$

We thus have a local coordinate description of a neighborhood of ρ_0 in $\mathcal{R}^{(2)}$ as follows: a point $\rho \in \mathcal{R}^{(2)}$ near ρ_0 is

$$\begin{aligned} \rho &= \Psi \kappa \Psi^\dagger, \\ \Psi &= \Psi_0 \mathcal{U}(z)(1 - \underline{\overline{\chi}}_0^\dagger \underline{\overline{\chi}}_0)^{1/2} + \underline{\overline{\chi}}_0. \end{aligned} \tag{3.28}$$

In all, z and $\underline{\overline{\chi}}_0$ amount to $2(2n-3)$ real independent parameters, the dimension of $\mathcal{R}^{(2)}$. The neighborhood of ρ_0 is defined by the conditions on $\underline{\overline{\chi}}_0$ and z in (3.25) and (3.27). For each ρ in this neighborhood, we have a unique lift $\Psi \in \mathcal{B}^{(2)}$ given in (3.28). A general $\Psi' \in \pi^{-1}(\rho)$ differs from Ψ by a diagonal phase matrix:

$$\Psi' = \Psi \begin{pmatrix} \mathrm{e}^{\mathrm{i}\alpha_1} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\alpha_2} \end{pmatrix},\ 0 \le \alpha_1, \alpha_2 < 2\pi. \tag{3.29}$$

Both ρ and Ψ in (3.28) are functions of z and $\underline{\overline{\chi}}_0$. In addition Ψ' involves α_1 and α_2. At ρ_0 and Ψ_0 both z and $\underline{\overline{\chi}}_0$ vanish. At Ψ_0, $\alpha_1 = \alpha_2 = 0$ as well. For a comparison of (3.28) and (3.29) with the pure state case, see [14].

Vectors and forms at Ψ_0

Since the matrix $(1 - \underline{\overline{\chi}}_0^\dagger \underline{\overline{\chi}}_0)^{1/2}$ is not easy to differentiate, we limit ourselves to small regions in $\mathcal{R}^{(2)}$ and $\mathcal{B}^{(2)}$ around ρ_0 and Ψ_0, respectively. By Φ' we denote a general tangent vector in $T_{\Psi'}\mathcal{B}^{(2)}$ in the manner of (3.9). We will actually need expressions for $X_{\Phi'}$, $A^{(a)}$ and $\mathrm{d}A^{(a)}$ (defined later) at Ψ_0, which means we ultimately take $\Phi' \in T_{\Psi_0}\mathcal{B}^{(2)}$. For these purposes we find that it is adequate to retain only terms linear in α_a, z and $\underline{\overline{\chi}}_0$. From (3.28) and (3.29) we have

$$\begin{aligned} \psi_1' &= \psi_{01}(1+\mathrm{i}\alpha_1) - z^*\psi_{02} + \chi_{01}, \\ \psi_2' &= \psi_{02}(1+\mathrm{i}\alpha_2) + z\psi_{01} + \chi_{02}. \end{aligned} \tag{3.30}$$

Next we let $\Phi' \in T_{\Psi_0}\mathcal{B}^{(2)}$ correspond to the pair $h', \underline{\overline{\chi}}'$ in the sense of (3.9). Then the nearby point $\Psi' = \Psi_0 + \epsilon\Phi'$, for small ϵ, involves small changes $\delta\alpha_1, \delta\alpha_2, \delta z, \delta\chi_{0a}$ around zero, obtained by comparison with (3.30):

$$\begin{aligned} \Psi' = \Psi_0 + \epsilon\Phi' :\ \ \delta\alpha_1 = \epsilon h_{11}',\ \ \delta\alpha_2 = \epsilon h_{22}',\ \ \delta z = \mathrm{i}\epsilon h_{12}', \\ \delta z^* = -\mathrm{i}\epsilon h_{21}',\ \ \delta\chi_{01} = \epsilon\chi_1',\ \ \delta\chi_{02} = \epsilon\chi_2'. \end{aligned} \tag{3.31}$$

Dropping ϵ, the standard differential geometric way of representing Φ' at Ψ_0 is as follows:

$$\begin{aligned} X_{\Phi'} = {} & h_{11}'\frac{\partial}{\partial\alpha_1} + h_{22}'\frac{\partial}{\partial\alpha_2} + \mathrm{i}h_{12}'\frac{\partial}{\partial z} - \mathrm{i}h_{21}'\frac{\partial}{\partial z^*} + \frac{\partial}{\partial\chi_{01}}\chi_1' \\ & + \frac{\partial}{\partial\chi_{02}}\chi_2' + \chi_1'^\dagger\frac{\partial}{\partial\chi_{01}^\dagger} + \chi_2'^\dagger\frac{\partial}{\partial\chi_{02}^\dagger}. \end{aligned} \tag{3.32}$$

In a similar spirit we compute $A^{(a)}$ and $\mathrm{d}A^{(a)}$ at Ψ_0. For the former we find

$$A^{(a)} = -\mathrm{i}\psi_a'^\dagger \mathrm{d}\psi_a' = \mathrm{d}\alpha_a, \tag{3.33}$$

which implies

$$i_{X_{\Phi'}} A^{(a)} = h_{aa}',\ \ a = 1,2. \tag{3.34}$$

Thus, as anticipated in (3.19),

$$\Phi' \text{ horizontal} \Leftrightarrow i_{X_{\Phi'}} A^{(a)} = 0 \Leftrightarrow h_{11}' = h_{22}' = 0. \tag{3.35}$$

Now we look at the two-forms $\mathrm{d}A^{(a)}$ again at Ψ_0. Simple calculations give the results

$$\begin{aligned} \mathrm{d}A^{(1)} &= -\mathrm{i}\mathrm{d}z \wedge \mathrm{d}z^* - \mathrm{i}\mathrm{d}\chi_{01}^\dagger \wedge \mathrm{d}\chi_{01}, \\ \mathrm{d}A^{(2)} &= +\mathrm{i}\mathrm{d}z \wedge \mathrm{d}z^* - \mathrm{i}\mathrm{d}\chi_{02}^\dagger \wedge \mathrm{d}\chi_{02}. \end{aligned} \tag{3.36}$$

We can contract these with the tangent vectors Φ', Φ'' using (3.32) and we then get

$$\begin{aligned} & \mathrm{d}A^{(1)}(X_{\Phi'}, X_{\Phi''}) \\ & = i_{X_{\Phi''}} i_{X_{\Phi'}}\, \mathrm{d}A^{(1)} \\ & = -\mathrm{i}(h_{12}'h_{21}'' - h_{21}'h_{12}'') + \mathrm{i}(\chi_1''^\dagger\chi_1' - \chi_1'^\dagger\chi_1''), \\ & \mathrm{d}A^{(2)}(X_{\Phi'}, X_{\Phi''}) \\ & = i_{X_{\Phi''}} i_{X_{\Phi'}}\, \mathrm{d}A^{(2)} \\ & = +\mathrm{i}(h_{12}'h_{21}'' - h_{21}'h_{12}'') + \mathrm{i}(\chi_2''^\dagger\chi_2' - \chi_2'^\dagger\chi_2''). \end{aligned} \tag{3.37}$$

With these preparations we can go on to GP considerations.

The PFB framework and GP's

We now follow the same pattern of arguments as in the previous section for pure states. The first coset space PFB is now $(G, \mathcal{B}^{(2)}, \ldots, H_0)$ with $H_0 = U(n-2)$. A choice of coset representative at $\Psi \in \mathcal{B}^{(2)}$ is of the form

$$\ell(\Psi) = \begin{pmatrix} & \cdots & \\ & \cdot & \\ \Psi & \cdots & \\ & \cdot & \\ & \cdots & \end{pmatrix} \in G,$$

$$\ell(\Psi)\Psi^{(0)} = \Psi. \tag{3.38}$$

This replaces (2.14), and $\ell(\Psi)$ is arbitrary up to an element of H_0 on the right. A general matrix $U \in G$ is parametrized as

$$U(\Psi, h_0) = \ell(\Psi)h_0, \;\; h_0 \in H_0 \tag{3.39}$$

in place of (2.15). The replacement for (2.16) involving all the Maurer–Cartan forms on G is

$$U(\Psi, h_0)^{-1}\mathrm{d}U(\Psi, h_0) \tag{3.40}$$
$$= \psi_1^\dagger \mathrm{d}\psi_1 \; Q_1 \; + \psi_2^\dagger \mathrm{d}\psi_2 \; Q_2 \; + \underline{H}_0 \text{ terms } + \text{cross terms}.$$

The second coset space PFB is $(G, \mathcal{R}^{(2)}, \ldots, H)$ with $H = U(1) \times U(1) \times H_0$. The preferred connection on this PFB is obtained from (3.40) by dropping the cross terms and retaining only the H-terms:

$$\omega^{(2)} = -\mathrm{i}\left(U(\Psi, h_0)^{-1}\mathrm{d}U(\Psi, h_0)\right)_H$$
$$= -\mathrm{i}\psi_1^\dagger \mathrm{d}\psi_1 \; Q_1 - \mathrm{i}\psi_2^\dagger \mathrm{d}\psi_2 \; Q_2 + \underline{H}_0 \text{ terms}, \tag{3.41}$$

which replaces (2.17).

The third PFB is an AB to the previous one in which we replace G and H by a suitable E and F: $E = \mathcal{B}^{(2)}$, $F = U(1) \times U(1)$ part of H. The action of H on F is defined again by making H_0 act trivially, while $U(1) \times U(1)$ acts on F following the abelian composition law. Thus from $\omega^{(2)}$ we arrive at the connection

$$\omega^{(3)} = -\mathrm{i}\psi_1^\dagger \mathrm{d}\psi_1 \; Q_1 - \mathrm{i}\psi_2^\dagger \mathrm{d}\psi_2 \; Q_2 \tag{3.42}$$

on this third PFB. Now we cannot delete Q_1 and Q_2 here as they are the two independent generators of the two $U(1)$ factors in $U(1) \times U(1)$. Alternatively we can say we have two independent one-forms $A^{(a)}$ on $\mathcal{B}^{(2)}$:

$$A^{(a)} = -\mathrm{i}\psi_a^\dagger \mathrm{d}\psi_a \;\; (\text{no sum}), \tag{3.43}$$

while the $\underline{U(1)} \times \underline{U(1)}$ valued connection $\omega^{(3)}$ is

$$\omega^{(3)} = A^{(1)} \; Q_1 + A^{(2)} \; Q_2. \tag{3.44}$$

The evaluations of $A^{(a)}$ and $\mathrm{d}A^{(a)}$ on tangent vectors at general points on $\mathcal{B}^{(2)}$ are contained in (3.34) and (3.37).

If we consider a closed curve $C \subset \mathcal{R}^{(2)}$ (cyclic mixed state evolution), a horizontal lift $\mathcal{C}_h \subset \mathcal{B}^{(2)}$ must obey two conditions at each point:

$$A^{(a)}_{\Psi(s)}(\dot{\Psi}(s)) = 0, \;\; \text{i.e. } (\psi_a(s), \dot{\psi}_a(s)) = 0, \;\; a = 1, 2. \tag{3.45}$$

In general now the end points of $\mathcal{C}_h$ differ by a pair of phases, an element of $U(1) \times U(1)$, not just by a single phase. Each of them is a GP and should be counted independently. This leads us to consider the two independent two-forms $\mathrm{d}A^{(a)}$ on $\mathcal{B}^{(2)}$. On the other hand, the KKS construction leads to a single symplectic two-form Ω on $\mathcal{R}^{(2)}$, so the question is to find out which linear combination of $\mathrm{d}A^{(a)}$ is related to Ω via a pull-back. We now find this combination.

The KKS two-form on $\mathcal{R}^{(2)}$

In (3.20) we have an expression for a general tangent vector $X \in T_\rho\mathcal{R}^{(2)}$, as well as a hermitian generator K leading to it upon commutation with ρ. The KKS symplectic two-form Ω on $\mathcal{R}^{(2)}$ is defined at each point by its evaluation on two tangent vectors [19]:

$$\Omega_\rho(X', X'') = -\mathrm{i}\mathrm{Tr}_{\mathcal{H}}(\rho\,[K', K'']). \tag{3.46}$$

For clarity we have indicated that the trace has to be computed on the Hilbert space $\mathcal{H}$. Using (3.20) we find after some algebra

$$\Omega_\rho(X', X'')$$
$$= -\mathrm{i}(\kappa_1 - \kappa_2)(h'_{12}h''_{21} - h'_{21}h''_{12}) - \mathrm{i}\kappa_1(\chi_1'^\dagger\chi_1'' - \chi_1''^\dagger\chi_1')$$
$$- \mathrm{i}\kappa_2(\chi_2'^\dagger\chi_2'' - \chi_2''^\dagger\chi_2'). \tag{3.47}$$

Comparing this with the expressions for $\mathrm{d}A^{(a)}(X_{\Phi'}, X_{\Phi''})$ in (3.37) we see that we have the relation

$$\sum_a \kappa_a \mathrm{d}A^{(a)} = \pi^*\Omega. \tag{3.48}$$

Here finally the non-zero eigenvalues κ_a of $\rho \in \mathcal{R}^{(2)}$ have reappeared, and at the same time dependences on n have disappeared.

This approach indicates that the unique GP we can associate with a cyclic evolution in the coadjoint orbit of a given rank two mixed state density operator is a linear combination of the two phases provided by the $U(1) \times U(1)$ holonomy group element, and this combination is expressible as the symplectic area of a surface in $\mathcal{R}^{(2)}$:

$$\varphi^{(a)}_{\mathrm{geom}}[C] = \arg(\psi_a(s_1), \psi_a(s_2)) \;, \; a = 1, 2 \;;$$
$$\sum_a \kappa_a \varphi^{(a)}_{\mathrm{geom}}[C] = -\int\int_S \Omega \;, \; \partial S = C. \tag{3.49}$$

Here $C = \{\rho(s)\}$ is a closed loop on $\mathcal{R}^{(2)}$ and $\mathcal{C}_h = \{\Psi(s)\}$ is a horizontal lift of it in $\mathcal{B}^{(2)}$.

We explore the physical interpretation of these results in the next section.

4 Physical interpretation of mixed state GP's

The present approach to mixed state unitary evolution based on the PFB framework has naturally emphasized the fact that (in the rank two case) the holonomy group is $U(1) \times U(1)$. So at the end of a cyclic evolution we have a pair of geometric phases $\varphi^{(a)}_{\text{geom}}[C]$, not simply one. On the other hand, the KKS definition of a canonical symplectic structure on the space of these density matrices, which form a (co-) adjoint orbit in $\underline{G}$, leads to a unique two-form Ω given in (3.46) and (3.47). The symplectic area integral of Ω is a weighted average of the two GP's, as in (3.49). We now construct an interpretation of this result, based on general quantum mechanical principles.

A mixed state density matrix ρ for a quantum system is a convex combination of any number of pure state density matrices [20]:

$$\rho = \sum_r p_r \rho_r, \quad \rho_r \in \mathcal{R}, \quad p_r > 0, \ \sum_r p_r = 1. \tag{4.1}$$

Here the p_r are any set of classical probabilities and the ρ_r do not have to be pairwise orthogonal. A mixed ρ can be expanded in this form in infinitely many ways, and each expansion represents a distinct physical way in which an ensemble of kinematically identical systems, characterized as a whole by ρ, can be synthesized. Given the particular expansion (4.1), we can imagine an ensemble of a very large number of systems, a fraction p_r of which form a sub-ensemble in the pure state ρ_r. The average of the results of measurements of any hermitian observable θ over the entire ensemble is given by

$$\langle \theta \rangle = \sum_r p_r \text{Tr}(\rho_r \theta) = \text{Tr}(\rho\theta). \tag{4.2}$$

In the final result only ρ appears, not the particular way in which the ensemble was physically prepared. This expresses the physical fact that the average of measurements over any one of these ensemble realizations of ρ is always the same. Of course, $\text{Tr}(\rho\theta)$ need not be any one of the eigenvalues of θ; even each individual $\text{Tr}(\rho_r\theta)$ need not be an eigenvalue of θ.

Among the infinitely many realizations (4.1) of ρ is of course a special or canonical one. This corresponds to the spectral resolution of ρ when the p_r are the non-zero eigenvalues κ_a of ρ (assumed non-degenerate for simplicity), and the ρ_a are the corresponding mutually orthogonal pure state projections. (In this case, the number of terms in (4.1) cannot exceed $\dim \mathcal{H} = n$.) Our result (3.49) for mixed state GP's suggests that we use this canonical ensemble realization of ρ.

We now go back to the rank two case and use the canonical decomposition (3.2). The measurement of GP's is not like the measurement of some hermitian operator observable belonging to the system under consideration. Let us nevertheless imagine that we have an ensemble of systems, a fraction κ_1 of which are in the pure state $\rho_1 = \psi_1^\dagger \psi_1$, and the remaining fraction κ_2 are in the orthogonal pure state $\rho_2 = \psi_2^\dagger \psi_2$. As ρ undergoes unitary cyclic evolution, so do each of ρ_1 and ρ_2, but these latter ones are pure state evolutions. We assume that an experimental arrangement has been set up which is capable of measuring these two pure state GP's. Then the ensemble average of the results of these measurements is exactly what appears in (3.49) on the left hand side, which need not be the same as either of the two individual GP's (or indeed any GP). However, this ensemble averaged GP is what is reproduced by the symplectic area calculation on $\mathcal{R}^{(2)}$, using the canonical KKS two-form Ω.

This "minimalist" interpretation works only with the canonical ensemble realization of ρ, and involves an average of phases, not of unimodular phase factors $\exp(\text{i}\varphi^{(a)}_{\text{geom}}[C])$. This implies that the experimental measurements of the $\varphi^{(a)}_{\text{geom}}[C]$ must not be just modulo 2π but must carefully keep track of the gradually accumulating value of each $\varphi^{(a)}_{\text{geom}}[C]$ as the cyclic evolution is experienced.

5 The relation of geometric phase to null phase curves for mixed states

In this section we would like to generalize some earlier results on Berry's phase for pure states [14]. In particular, we would like to show how geometric phase(s), for both cyclic and non-cyclic evolutions, can be directly obtained as a surface integral of the KKS symplectic two-form once a suitable class of curves, the null phase curves, has been defined. For definiteness, we will consider again the case of rank two density matrices, but the results can be easily generalized to the higher rank situation which will be briefly described in the last section. As before, to define geometric phases, we will confine ourselves to a unitary evolution on a specific adjoint orbit of a given density matrix ρ as given in (3.2).

We consider continuous parametrized curves $\mathcal{C} \in \mathcal{B}^{(2)}$ and their projections to $C = \pi(\mathcal{C}) \subset \mathcal{R}^{(2)}$:

$$\mathcal{C} = \{(\psi_1(s) \ \psi_2(s)) \in \mathcal{B}^{(2)} \,|\, s \in [s_1, s_2]\} \tag{5.1}$$

$$C = \{\rho(s) = \kappa_1 \rho_1(s) + \kappa_2 \rho_2(s) \in \mathcal{R}^{(2)} \,|\, s \in [s_1, s_2]\}, \tag{5.2}$$

with the following smoothness conditions.

The curves $\mathcal{C}$, C, are said to be *class I curves* if and only if $\psi_j(s), \rho_j(s)$ are continuous, piecewise differentiable and

$$(\psi_j(s_1), \psi_j(s_2)) \neq 0, \ j = 1, 2; \tag{5.3}$$

the curves $\mathcal{C}$, C, are said to be *class II curves* if and only if $\psi_j(s), \rho_j(s)$ are continuous, once differentiable and

$$(\psi_j(s), \psi_j(s')) \neq 0, \ j = 1, 2, \text{ for any } s, s' \in [s_1, s_2]. \tag{5.4}$$

In addition, a curve $\mathcal{C}$, C of class II is said to be a *null phase curve* (NPC) if and only if

$$\begin{aligned} &\text{Tr}(\rho_j(s)\rho_j(s')\rho_j(s'')) = \text{real positive} \\ &\quad \Leftrightarrow \ \text{Tr}(\rho_j(s)[\rho_j(s'), \rho_j(s'')]) = 0, \ j = 1, 2, \\ &\qquad \text{for any } s, s', s'' \in [s_1, s_2]. \end{aligned} \tag{5.5}$$

We can understand this definition also from a more geometrical point of view. Let us consider the subset of couples of vectors $(\psi_1\ \psi_2) \in \mathcal{B}^{(2)}$ such that ψ_j $(j = 1, 2)$ belongs to the real linear hull obtained by forming all real linear combinations of any number of vectors $\psi_j(s')$ (renormalized if necessary). This collection of couples is associated to a real subspace of $\mathcal{H}^{(2)} = \{(\psi_1\ \psi_2)\,|\,\psi_j \in \mathcal{H}\}$ which, because of (5.5), is $\pi^\star\Omega$ isotropic. We are thus led to characterize a NPC via such associated subspaces.

Given a class II curve $C = \{\rho(s) = \kappa_1\rho_1(s)+\kappa_2\rho_2(s)\} \in \mathcal{R}^{(2)}$, we can define its *Pancharatnam lift* to a curve $\mathcal{C}_0 = \{(\psi_1^0(s)\ \psi_2^0(s))\} \in \mathcal{B}^{(2)}$ such that, for each component,

$$(\psi_j^0(s), \psi_j^0(s')) = \text{real positive for any } s, s' \in [s_1, s_2], \tag{5.6}$$

in a way similar to the construction obtained in [14] for the pure state case. Choosing any reference point $(\psi_1^0(s_0)\ \psi_2^0(s_0)) \in \mathcal{B}^{(2)}$, this lift is explicitly determined by setting, for $j = 1, 2$,

$$\psi_j^0(s) = N_j(s)\rho_j(s)\psi_j^0(s_0), \tag{5.7}$$

$$N_j(s) = |(\psi_j^0(s_0), \psi_j(s))|^{-1} = [\mathrm{Tr}(\rho_j^0\rho_j)]^{-1/2}. \tag{5.8}$$

As a consequence of (5.6), any two points of $\mathcal{C}_0$ are in phase in the Pancharatnam sense and the curve $\mathcal{C}_0$ is horizontal:

$$\arg(\psi_j^0(s_1), \psi_j^0(s_2)) = 0,$$
$$\int_{\mathcal{C}_0} A_j = 0, \tag{5.9}$$

where $A_j = -\mathrm{i}\psi_j^\dagger \mathrm{d}\psi_j$. It is then not difficult to check that, for a general lift $\mathcal{C} = \{(\mathrm{e}^{\mathrm{i}\alpha_1(s)}\psi_1^0(s)\ \mathrm{e}^{\mathrm{i}\alpha_2(s)}\psi_2^0(s))\}$ of C obtained from $\mathcal{C}_0$ by a smooth local $U(1) \times U(1)$ phase transformation, one has

$$\begin{aligned}\int_{\mathcal{C}} A_j &= \int_{s_1}^{s_2} \mathrm{d}s \frac{\mathrm{d}\alpha_j(s)}{\mathrm{d}s} \\ &= \alpha_j(s_2) - \alpha_j(s_1) \\ &= \arg(\psi_j(s_1), \psi_j(s_2)).\end{aligned} \tag{5.10}$$

We are now ready to define the geometric phase (GP) associated to any class I curve $C = \{\rho(s)\}$ from $\rho(s_1)$ to $\rho(s_2)$. Let C' be any NPC from $\rho(s_2)$ to $\rho(s_1)$ so that $C \cup C'$ is a class I closed loop. Then, if S is a two-dimensional surface such that $\partial S = C \cup C'$, the GP associated to C is defined to be given by

$$\varphi_g[C] = -\int_S \Omega. \tag{5.11}$$

With some algebra, one can easily show that the integral (5.11) is indeed independent of the choice of the NPC C' and that the geometric phase associated to any NPC vanishes. Also the kinematic definition of the GP is recovered: if $\mathcal{C}$ is any lift of C, from $(\psi_1(s_1)\ \psi_2(s_1))$ to $(\psi_1(s_2)\ \psi_2(s_2))$, one has

$$\begin{aligned}\varphi_g[C] \equiv -\int_S \Omega = -\oint_{\mathcal{C}\cup\mathcal{C}'} A &= -\int_{\mathcal{C}} A - \int_{\mathcal{C}'} A \\ &= \arg(\psi_1(s_1), \psi_1(s_2)) + \arg(\psi_2(s_1), \psi_2(s_2)) \\ &\quad - \int_{\mathcal{C}} A.\end{aligned} \tag{5.12}$$

There are additional properties of GP's that are worth mentioning and that can be recovered from the definition (5.11) and from the property (5.10) of NPC's. Suppose first that C_{12}, C_{23}, C_{31} are projections of the NPC's $\mathcal{C}_{12}, \mathcal{C}_{23}, \mathcal{C}_{31}$ from $(\psi_1(s_1)\ \psi_2(s_1))$ to $(\psi_1(s_2)\ \psi_2(s_2))$, from $(\psi_1(s_2)\ \psi_2(s_2))$ to $(\psi_1(s_3)\ \psi_2(s_3))$ and from $(\psi_1(s_3)\ \psi_2(s_3))$ to $(\psi_1(s_1)\ \psi_2(s_1))$ respectively. Since both $C_{12} \cup C_{23} \cup C_{31}$ and $\mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31}$ are closed loops, we have

$$\begin{aligned}&\varphi_g[C_{12} \cup C_{23} \cup C_{31}] \\ &= -\oint_{\mathcal{C}_{12}\cup\mathcal{C}_{23}\cup\mathcal{C}_{31}} A = -\oint_{\mathcal{C}_{12}} A - \oint_{\mathcal{C}_{23}} A - \oint_{\mathcal{C}_{31}} A \\ &= -\kappa_1 \arg\mathrm{Tr}(\rho_1(s_1)\rho_1(s_2)\rho_1(s_3)) \\ &\qquad -\kappa_2 \arg\mathrm{Tr}(\rho_2(s_1)\rho_2(s_2)\rho_2(s_3)).\end{aligned} \tag{5.13}$$

More generally, for any class I curves C_{12}, C_{23}, C_{31} which are projections of $\mathcal{C}_{12}, \mathcal{C}_{23}, \mathcal{C}_{31}$ we can prove the relation

$$\begin{aligned}&\varphi_g[C_{12} \cup C_{23} \cup C_{31}] \\ &= \varphi_g[C_{12}] + \varphi_g[C_{23}] + \varphi_g[C_{31}] \\ &\qquad -\kappa_1 \arg\,\mathrm{Tr}(\rho_1(s_1)\rho_1(s_2)\rho_1(s_3)) \\ &\qquad -\kappa_2 \arg\,\mathrm{Tr}(\rho_2(s_1)\rho_2(s_2)\rho_2(s_3)),\end{aligned} \tag{5.14}$$

showing the lack of additivity of the GP.

Let us now consider a connected, simply connected smooth submanifold $M \in \mathcal{R}^{(2)}$ with dimension $m \geq 2$ in the real sense and let us denote by $\iota_M : M \hookrightarrow \mathcal{R}^{(2)}$ the corresponding inclusion map. By using (5.14) above, one can show that if M is a null phase manifold (NPM), i.e. a submanifold such that every once-differentiable curve $C \subset M$ is a NPC, then

$$M \text{ is isotropic: } \Omega_M \equiv \iota_M^\star\Omega = 0; \tag{5.15}$$

$$\begin{aligned}&\text{for any } \rho = \pi((\psi_1\ \psi_2)), \\ &\qquad \rho' = \pi((\psi_1'\ \psi_2')), \\ &\qquad \rho'' = \pi((\psi_1''\ \psi_2'')) \in M, \\ &\quad \mathrm{Tr}(\rho_1\rho_1'\rho_1''), \mathrm{Tr}(\rho_2\rho_2'\rho_2'') \text{ are real positive.}\end{aligned} \tag{5.16}$$

Let us first concentrate on (5.15), which shows that isotropy is a necessary condition for M to be a NPM. We will see now that it is not a sufficient one. To examine this point, let us suppose that M is such that $\mathrm{Tr}(\rho_1\rho_1') > 0$, $\mathrm{Tr}(\rho_2\rho_2') > 0$ for any $\rho = \kappa_1\rho_1 + \kappa_2\rho_2$, $\rho' = \kappa_1\rho_1' + \kappa_2\rho_2'$. In the spirit of the Pancharatnam lift defined in (5.6), we can construct a lift of M to a submanifold $M_0 \in \mathcal{B}^{(2)}$ as follows. Given a point $\rho \in M$, its lifted point $(\psi_1\ \psi_2) \in \mathcal{B}^{(2)}$ is given by the choice

$$\psi_1 = \frac{\rho_1\psi_1^0}{\sqrt{\mathrm{Tr}(\rho_1^0\rho^1)}}\ ,\ \psi_2 = \frac{\rho_2\psi_2^0}{\sqrt{\mathrm{Tr}(\rho_2^0\rho^2)}}. \tag{5.17}$$

where ρ^0, $(\psi_1^0\ \psi_2^0)$ are fiducial points in M, M_0 respectively, and $\pi((\psi_1^0\ \psi_2^0)) = \rho^0$. This lift is characterized by the fact that any point $(\psi_1\ \psi_2) \in M_0$ is in phase with $(\psi_1^0\ \psi_2^0)$ in the Pancharatnam sense:

$$(\psi_1^0, \psi_1), (\psi_2^0, \psi_2) > 0. \tag{5.18}$$

In general, however, two generic points $(\psi_1\ \psi_2), (\psi_1\prime\ \psi_2') \in M_0$ are not in phase, since

$$(\psi_j', \psi_j) = \mathrm{Tr}(\rho_j^0 \rho_j' \rho_j),\ j = 1, 2. \tag{5.19}$$

If now we suppose M to be isotropic, one can easily prove that, for any two class I curves in M from $\rho(s_1)$ to $\rho(s_2)$, say C_{12} and C_{12}', one has

$$\varphi_g[C_{12}] = \varphi_g[C_{12}'], \tag{5.20}$$

i.e., denoting by $\mathcal{C}_{12}, \mathcal{C}_{12}'$ the corresponding lifts in M_0:

$$\int_{\mathcal{C}_{12}} A = \int_{\mathcal{C}_{12}'} A. \tag{5.21}$$

This means that the pull-back of A from $\mathcal{B}^{(2)}$ to M_0 is exact. Thus, setting $\iota_{M_0} : M_0 \hookrightarrow \mathcal{B}^{(2)}$, we have the result

$$\Omega_M = 0 \ \Leftrightarrow\ \iota_{M_0}^\star A = \mathrm{d}f. \tag{5.22}$$

If in addition M is a NPM we have the stronger result

$$\iota_{M_0}^\star A = 0, \tag{5.23}$$

which follows from the fact that now $(\psi_j', \psi_j) > 0, j = 1, 2$, for any two points in M_0. This result gives the extent to which the NPM property goes beyond isotropy.

To find a sufficient condition for M to be a NPM one has to consider (5.16). One can finally assert the following inverse result [14]: if M is such that for any three points $\rho = \pi((\psi_1\ \psi_2)), \rho' = \pi((\psi_1'\ \psi_2')), \rho'' = \pi((\psi_1''\ \psi_2''))$, the quantities $\mathrm{Tr}(\rho_1\rho_1'\rho_1''), \mathrm{Tr}(\rho_2\rho_2'\rho_2'')$ are real positive, then

$$\mathrm{Tr}(\rho_1\rho_1'),\ \mathrm{Tr}(\rho_2\rho_2') > 0; \tag{5.24}$$

$$M \text{ is an NPM;} \tag{5.25}$$

$$M \text{ is isotropic.} \tag{5.26}$$

Notice that these three statements are not independent, since the third is implied by the second.

6 Concluding remarks

We have set up what may be called a "minimalist" interpretation for the meaning to be given to the phrase "mixed state GP", limiting ourselves for clarity to the case of unitary cyclic evolutions. We have been guided by the structures of, and relationships among, certain PFB's which arise naturally in this context. They all flow out of the unitary group $G = U(n)$ acting on the n-dimensional Hilbert space of a quantum system. Our aim has been to bring into focus the role of the KKS symplectic structure existing on each (co-) adjoint orbit in $\underline{G}$. In the final results, as often stated, explicit dependences on n actually drop out. This is because in these results only the codimensions are relevant.

We considered the case of rank two density matrices ρ, with the two non-zero eigenvalues obeying $0 < \kappa_2 < \kappa_1 < 1$. It can be seen fairly easily that the framework set up in this paper, involving three PFB's in sequence and the use to which each is put, can be faithfully repeated for higher rank (but still non-degenerate for non-zero eigenvalues) density matrices. The main features for rank k, $0 < k < n$, would be that the non-zero eigenvalues of ρ would obey

$$0 < \kappa_k < \kappa_{k-1} < \ldots < \kappa_2 < \kappa_1 < 1,\ \sum_{a=1}^{k} \kappa_a = 1. \tag{6.1}$$

Then ρ has the decomposition

$$\rho = \sum_{a=1}^{k} \kappa_a \psi_a \psi_a^\dagger,\ \ (\psi_a, \psi_b) = \delta_{ab}. \tag{6.2}$$

The stability groups H_0 and H in this situation would be $H_0 = U(n-k)$ acting on dimensions $(k+1), (k+2), \ldots, n$ of $\mathcal{H}$; $H = U(1) \times U(1) \times \ldots \times U(1) \times H_0$, with k $U(1)$ factors. Correspondingly at the vector and operator levels we have to deal with the spaces

$$\begin{aligned}
\mathcal{B}^{(k)} &= \{\Psi = (\psi_1\ \ \psi_2\ \ \ldots \psi_k) | \psi_a \in \mathcal{B}, (\psi_a, \psi_b) = \delta_{ab}\} \\
&= G/H_0, \\
\mathcal{R}^{(k)} &= \left\{ \rho = \sum_{a=1}^{k} \kappa_a \rho_a | \rho_a = \psi_a \psi_a^\dagger \in \mathcal{R} \right\} \\
&= G/H \\
&= \mathcal{B}^{(k)}/U(1) \times U(1) \times \ldots \times U(1).
\end{aligned} \tag{6.3}$$

These spaces are of real dimensions $k(2n-k)$ and $k(2n-k-1)$ respectively, and the latter is always even, with $\mathcal{R}^{(k)}$ being a (co-) adjoint orbit in $\underline{G}$.

The sequence of three PFB's is now $(G, \mathcal{B}^{(k)}, \ldots, H_0)$, $(G, \mathcal{R}^{(k)}, \ldots, H)$ and $(\mathcal{B}^{(k)}, \mathcal{R}^{(k)}, \ldots, U(1) \times U(1) \times \ldots \times U(1))$. On the last we obtain, following the set-up given earlier, the connection one-form

$$\begin{aligned}
\omega^{(3)} &= \sum_{a=1}^{k} A^{(a)} Q_a, \\
A^{(a)} &= -\mathrm{i}\psi_a^\dagger \mathrm{d}\psi_a.
\end{aligned} \tag{6.4}$$

This serves to define the concept of horizontal lifts of a curve $C \subset \mathcal{R}^{(k)}$ to $\mathcal{C} \subset \mathcal{B}^{(k)}$. The KKS symplectic two-form Ω on $\mathcal{R}^{(k)}$ is, however, unique, and its relation to the above $A^{(a)}$ is

$$\sum_{a=1}^{k} \kappa_a \mathrm{d}A^{(a)} = \pi^* \Omega. \tag{6.5}$$

The general interpretation follows lines similar to what is described in Sects. 4 and 5. As the holonomy group is

$U(1) \times U(1) \times \ldots \times U(1)$ (k factors), a cyclic evolution of such mixed states naturally involves k separate $U(1)$ phases or k separate pure state GP's $\varphi^{(a)}_{\rm geom}[C]$. What the KKS structure does is to relate a particular linear combination of these to a two dimensional symplectic area integral in $\mathcal{R}^{(k)}$.

For emphasis, we may restate our results in the following intuitive manner. Consider the case of rank n (maximal rank) non-degenerate density matrices ρ, belonging to $\mathcal{R}^{(n)}$ and with eigenvalues arranged in decreasing order $\kappa_1,\ \kappa_2, \ldots,\ \kappa_n$. Such a ρ determines an orthonormal basis or frame in Hilbert space up to n phases, namely up to an element of $U(1) \times \ldots \times U(1)$ (n factors). Given a closed trajectory (cyclic unitary evolution) of the density matrix in $\mathcal{R}^{(n)}$, the different possible unitary evolutions which will carry the density matrix along the given trajectory will differ from one another at each point by independent $U(1) \times \ldots \times U(1)$ phases. The $U(1) \times \ldots \times U(1)$ relative phases at the level of $\mathcal{B}^{(n)}$ between the final and the initial frames have two parts: a dynamical part depending on the particular unitary evolution chosen, and one that depends only on the closed trajectory in $\mathcal{R}^{(n)}$. Then the available invariant or geometric quantities that remain are an n-tuple of $U(1)$ abelian phases. Any function of these is also a geometric invariant. Our analysis of the canonical KKS symplectic structure on $\mathcal{R}^{(n)}$ singles out a particular such function as having a preferred significance.

The considerations of [7] have certain points of similarity with the above. The concept of horizontal lift of an evolution in $\mathcal{R}^{(k)}$ to one in $\mathcal{B}^{(k)}$ is similar; in our treatment explicit use is made of the third PFB ($\mathcal{B}^{(k)}$, $\mathcal{R}^{(k)}, \ldots, U(1) \times \ldots \times U(1)$) and the connection $\omega^{(3)}$ of (6.4) thereon. However, while our framework of three PFB's seems to play no explicit role in [7], the use of the KKS symplectic structure on $\mathcal{R}^{(k)}$ above gives a satisfying underpinning to arrive at the weighted sum of geometric phases tied to the spectral decomposition of ρ.

The concept of off-diagonal GP's for multi- (n-) level quantum systems has been recently introduced and studied in the literature [21,22]. Here too for such systems we have n individual pure state GP's defined for generic unitary cyclic evolution, and in addition several algebraically independent Bargmann invariants (of order four) also enter the picture. The spirit of the present paper has some points of similarity with off-diagonal GP ideas.

In case we have degenerate mixed states, in the sense that some non-zero eigenvalues of ρ have non-trivial multiplicity, we have to deal with non-Abelian holonomy groups [23], rather than just products of $U(1)$ factors. This would naturally lead us to non-Abelian GP's, but the basic three-PFB scheme set up here would again be available.

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