Geometric phase for mixed states: a differential geometric approach

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A new definition and interpretation of 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 Fibre Bundles, and the well known Kostant-Kirillov-Souriau symplectic structure on (co) adjoint orbits associated with Lie groups. It is shown that this framework generalises 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 aspects 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 generalisation 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 fibre 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

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(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 realised 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 generalises 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 combination 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 noncyclic 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 organised as follows. In Section 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 generalised 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 Section 3, bringing in the familiar meaning of mixed state density matrices in the context of quantum measurement theory. In Section 5 we discuss the role the recently introduced NPC's [13],[14] play in the mixed state situation.; this involves generalising them and the associated ideas of Pancharatnam lifts and Null Phase Manifolds from pure states to mixed states. The Concluding Section 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. 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. Its Lie algebra is described in Appendix A.

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

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

The two form dA on $\mathcal{B}$,

$$dA = -id\psi^\dagger \wedge d\psi, \tag{2.4}$$

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

$$dA = \pi^* \Omega. \tag{2.5}$$

The intrinsic definition of Ω is as follows [15]. 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:

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

Here K is determined by X upto 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 producing it can be expressed in terms of a vector χ orthogonal to ψ [4]:

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

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

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

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

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

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

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

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

$$\begin{aligned} A_{\psi(s)}(\dot{\psi}(s)) &= -i(\psi(s), \dot{\psi}(s)) \\ &= \mathrm{Im}(\psi(s), \dot{\psi}(s)) = 0. \end{aligned} \tag{2.11}$$

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 GP associated with C, and is the $U(1)$ holonomy group element in the sense of (B.20) in this case:

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

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 generalisable 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 $\mathcal{H}$,

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

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 $2, 3, \cdots, n$ 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 $(G, \mathcal{B}, \cdot\cdot, H_0)$, 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

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

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

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

with $\psi \in \mathcal{B}$ and $h_0 \in H_0$ being (local) coordinates on G. The full set of Maurer-Cartan one-forms on G can now be computed using eq. (B.10). In the general notation of Appendix B, if we write the generators of H_0 as J_a and the remaining generators of G as J_μ, eq.(B.10) gives [11],[12]:

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

To make contact with the notation of appendix A, the generators J_a of H_0 are $Q_j, \; J_{jk}, \; Q_{jk}$ for $j, k = 2, 3, \cdots, n$; 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 $k = 2, 3, \cdots, n$, 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 eq.(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 $(G, \mathcal{R}, \cdot\cdot, H)$. Here the base is a particular (co)adjoint orbit in the Lie algebra $\underline{G}$. On this PFB, by the definition (B.33), we have a preferred connection by retaining the terms in eq.(2.16) involving generators of H alone, and dropping the cross terms:

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

Lastly we bring in a PFB associated to $(G, \mathcal{R}, \cdot\cdot, H)$: the base remains the same, while G and H are replaced by suitably chosen E and F. These are: $F = U(1)$ subgroup of $H = U(1)$ subgroup of G generated by Q_1; and $E = \mathcal{B}$. So this AB is $(\mathcal{B}, \mathcal{R}, \cdot\cdot, U(1))$. 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 eq. (2.17) goes over in this third PFB to the connection

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

Thus we have arrived at eq. (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 dA on $\mathcal{B}$ and the KKS symplectic two-form Ω on $\mathcal{R}$.

To recapitulate, the first coset space PFB $(G, \mathcal{B}, \cdot\cdot, H_0)$ is used along with a choice of coset representative $\ell(\psi)$ to calculate the Maurer-Cartan one-forms on G (at least the terms of interest to us) in a convenient manner. This result is used to define a preferred connection $\omega^{(2)}$ in the second coset space PFB $(G, \mathcal{R}, \cdot\cdot, H)$, at the same time bringing in $\mathcal{R}$ as the base space. This connection is then 'transferred' to the AB $(\mathcal{B}, \mathcal{R}, \cdot\cdot, U(1))$ and gives back the connection A needed for pure state GP's. In both the second and third PFB's the base $\mathcal{R}$ is a (co)adjoint orbit in $\underline{G}$, carrying the KKS symplectic two-form Ω. In the third PFB, we recognise that dA on $\mathcal{B}$ is related to Ω by pull-back, and the sequence of operations is complete.

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 non zero 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 nonzero eigenvalues κ_a is non degenerate i.e., they obey

$$\begin{aligned} 0 \ < \ \kappa_k \ < \ \kappa_{k-1} < \cdots \quad < \kappa_2 \ < \kappa_1 \ < \ 1, \\ \sum_{a=1}^{k} \kappa_a = 1. \end{aligned} \tag{3.1}$$

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. Let us write $\kappa_a, a = 1, 2$, for these eigenvalues and agree that

$$0 < \kappa_2 < \kappa_1 < 1 \ , \quad \kappa_1 + \kappa_2 = 1. \tag{3.2}$$

Then ρ has the form

$$\rho = \kappa_1 \psi_1 \psi_1^\dagger + \kappa_2 \psi_2 \psi_2^\dagger, \tag{3.3}$$

where the vectors $\psi_a, a = 1, 2$, each determined upto a phase factor, form an ordered orthonormal pair:

$$(\psi_a, \psi_b) = \psi_a^\dagger \psi_b = \delta_{ab}. \tag{3.4}$$

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

$$\begin{aligned} \rho_a &= \psi_a \psi_a^\dagger \ , \ \rho_a \rho_b = \delta_{ab} \rho_a \ \ \text{(no sums!)}, \\ \rho &= \kappa_1 \rho_1 + \kappa_2 \rho_2. \end{aligned} \tag{3.5}$$

This set of ρ's forms a (co)adjoint orbit under G. At the vector space level we have to deal with ordered pairs $\psi_a, a = 1, 2$, as in eqs.(3.3, 3.4). We recognise here the generalisations of $\mathcal{B}$ and $\mathcal{R}$ of the pure state situation to mixed states of the form (3.3), in which for any $\underline{\kappa} = (\kappa_1, \kappa_2)$ with $\kappa_2 \ < \ \kappa_1$ 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:

$$\mathcal{B}^{(2)} = \{\Psi = (\psi_1 \ \ \psi_2) | \psi_a \in \mathcal{B}, \psi_a^\dagger \psi_b = \delta_{ab}\}. \tag{3.6}$$

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 $\mathcal{H}$:

$$\begin{aligned} \Psi^{(0)} &= (\psi_1^{(0)} \ \ \psi_2^{(0)}) \\ \psi_1^{(0)} = \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \quad &, \quad \psi_2^{(0)} = \begin{pmatrix} 0 \\ 1 \\ \cdot \\ \cdot \\ 0 \end{pmatrix}. \end{aligned} \tag{3.7}$$

The stability group of $\Psi^{(0)}$ is the subgroup $H_0 = U(n-2) \subset G$ acting on the dimensions $3, 4, \cdots, n$ 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 recognise $\mathcal{B}^{(2)}$, the orbit of $\Psi^{(0)}$ under G action, as a coset space:

$$\begin{aligned} \mathcal{B}^{(2)} &= G/H_0 = U(n)/U(n-2), \\ \dim\mathcal{B}^{(2)} &= 4(n-1). \end{aligned} \tag{3.8}$$

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 eq.(3.4):

$$\begin{aligned} (\psi_1, \phi_1), (\psi_2, \phi_2) &= \text{pure imaginary}, \\ (\psi_1, \phi_2) + (\phi_1, \psi_2) &= 0. \end{aligned} \tag{3.9}$$

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

$$\begin{aligned} \Phi &= i\Psi h + \underline{\chi}, \\ h^\dagger &= h = 2 \times 2 \ \text{ matrix}, \\ \underline{\chi} &= (\chi_1 \;\; \chi_2), \\ \chi_a &\in \mathcal{H}_\perp(\Psi) = \text{subspace of } \mathcal{H} \text{ orthogonal to } \psi_1 \text{ and } \psi_2. \end{aligned} \tag{3.10}$$

Thus we have a one to one correspondence

$$\Phi \in T_\Psi\mathcal{B}^{(2)} \leftrightarrow h, \ \underline{\chi}. \tag{3.11}$$

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

$$\begin{aligned} \phi &= ia\psi + \chi, \\ a^* &= a, \\ \chi &\in \mathcal{H}_\perp(\psi). \end{aligned} \tag{3.12}$$

The real number a gets generalised to a 2×2 hermitian matrix h, while $\chi \in \mathcal{H}_\perp(\psi)$ has been replaced by an ordered pair $\underline{\chi} = (\chi_1 \;\; \chi_2)$ 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:

$$\begin{aligned} \mathcal{R}^{(2)} &= \{\rho^\dagger = \rho \geq 0, \mathrm{Tr}\rho = 1 | \text{Spectrum of } \rho = (\kappa_1, \kappa_2, 0, \cdots, 0)\} \\ &= \{U\rho^{(0)}U^{-1} | U \in G, \rho^{(0)} = \kappa_1\psi_1^{(0)}\psi_1^{(0)\dagger} + \kappa_2\psi_2^{(0)}\psi_2^{(0)\dagger}\} \\ &= \{(\rho_1 \;\; \rho_2) | \rho_a \in \mathcal{R}, \rho_1\rho_2 = 0\}. \end{aligned} \tag{3.13}$$

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 G action, 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 $\mathcal{B}^{(2)}$:

$$\begin{aligned} \mathcal{R}^{(2)} &= \text{(co) adjoint orbit of } \rho^{(0)} \\ &= G/H \\ &= \mathcal{B}^{(2)}/U(1) \times U(1), \\ \dim\mathcal{R}^{(2)} &= \dim\mathcal{B}^{(2)} - 2 = 2(2n-3). \end{aligned} \tag{3.14}$$

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

$$\begin{aligned} \rho_\Psi &= \pi(\Psi) = \Psi\kappa\Psi^\dagger, \\ \kappa &= \begin{pmatrix} \kappa_1 & 0 \\ 0 & \kappa_2 \end{pmatrix}. \end{aligned} \tag{3.15}$$

The description of the tangent spaces $T_\rho\mathcal{R}^{(2)}$ involves a little effort. If we use the representation (3.15) 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

$$X = \Psi\kappa\Phi^\dagger + \Phi\kappa\Psi^\dagger \in \underline{G}. \tag{3.16}$$

Using eq.(3.10) for Φ and writing out and grouping terms, we see that

$$X = i\Psi[h,\kappa]\Psi^\dagger + \Psi\kappa\underline{\chi}^\dagger + \underline{\chi}\kappa\Psi^\dagger. \tag{3.17}$$

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

$$\begin{aligned} [h,\kappa] &= (\kappa_1-\kappa_2)\begin{pmatrix} 0 & -h_{12} \\ h_{21} & 0 \end{pmatrix}, \\ h_{21} &= h_{12}^*. \end{aligned} \tag{3.18}$$

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 $\underline{\chi}$:

$$X(h_{12},\underline{\chi}) = -i(\kappa_1-\kappa_2)(h_{12}\psi_1\psi_2^\dagger - h_{12}^*\psi_2\psi_1^\dagger) + \kappa_1(\psi_1\chi_1^\dagger + \chi_1\psi_1^\dagger) + \kappa_2(\psi_2\chi_2^\dagger + \chi_2\psi_2^\dagger). \tag{3.19}$$

If we alter ψ_a by independent phases $e^{i\alpha_a}$ which leave ρ_Ψ invariant, to keep X unchanged we must replace $h_{12} \to e^{i(\alpha_2-\alpha_1)}h_{12}, \chi_a \to e^{i\alpha_a}\chi_a$. Returning to $\Phi \in T_\Psi\mathcal{B}^{(2)}$ in (3.10), we can tentatively separate it into vertical and horizontal parts, the former being the h_{11}, h_{22} terms and the latter the rest:

$$\begin{aligned} \Phi &= i\Psi h + \underline{\chi} \\ &= i\Psi\begin{pmatrix} h_{11} & 0 \\ 0 & h_{22} \end{pmatrix} + i\Psi\begin{pmatrix} 0 & h_{12} \\ h_{12}^* & 0 \end{pmatrix} + \underline{\chi}. \end{aligned} \tag{3.20}$$

The horizontal part is in unambiguous correspondence with X in eq. (3.19).

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:

$$\begin{aligned} X(h_{12},\underline{\chi}) &= -i[K(h_{12},\underline{\chi}),\rho_\Psi], \\ K(h_{12},\underline{\chi}) &= i(\underline{\chi}\Psi^\dagger - \Psi\underline{\chi}^\dagger) - \Psi\begin{pmatrix} 0 & h_{12} \\ h_{12}^* & 0 \end{pmatrix}\Psi^\dagger. \end{aligned} \tag{3.21}$$

The presence of new terms compared to eq.(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 $\rho^{(0)} = \kappa_1\psi_1^{(0)}\psi_1^{(0)\dagger} + \kappa_2\psi_2^{(0)}\psi_2^{(0)\dagger} + \cdots \kappa_k\psi_k^{(0)}\psi_k^{(0)\dagger}$, just intersecting each Weyl chamber exactly once. Fixing $\underline{\kappa}$ in such a way that $0 < \kappa_k < \kappa_{k-1} < \cdots < \kappa_2 < \kappa_1 < 1$ 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, analysed 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 $\mathcal{R}^{(2)}$

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 eq (3.7). Its image in $\mathcal{R}^{(2)}$ is

$$\Psi_0 \in \mathcal{B}^{(2)} \to \rho_0 = \pi(\Psi_0) = \Psi_0\kappa\Psi_0^\dagger \in \mathcal{R}^{(2)}. \tag{3.22}$$

Convenient neighbourhoods 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

$$\mathcal{H}_\perp(\Psi_0) = \{\psi \in \mathcal{H} | (\psi_{0a},\psi) = 0,\ a = 1,2\} \subset \mathcal{H}. \tag{3.23}$$

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

$$\begin{aligned} \psi_a &= S_{ba}\psi_{0b} + \chi_{0a}, a = 1, 2, \\ \chi_{0a} & \in \mathcal{H}_\perp(\Psi_0), \\ \text{i.e.}\Psi &= \Psi_0\, S + \underline{\chi}_0, \end{aligned} \tag{3.24}$$

with S a complex 2×2 matrix. The condition (3.4) becomes:

$$S^\dagger S = 1_{2\times 2} - \underline{\chi}_0^\dagger \underline{\chi}_0. \tag{3.25}$$

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

$$S = \mathcal{U}(1 - \underline{\chi}_0^\dagger \underline{\chi}_0)^{1/2},\ \mathcal{U} \in U(2). \tag{3.26}$$

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 $\underline{\chi}_0$ 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 fibres is

$$\Psi \to \Psi \begin{pmatrix} e^{i\alpha_1} & 0 \\ 0 & e^{i\alpha_2} \end{pmatrix}, \tag{3.27}$$

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 eq.(3.26) 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

$$\mathcal{U}(z) = \begin{pmatrix} \sqrt{1 - |z|^2} & z \\ -z^* & \sqrt{1 - |z|^2} \end{pmatrix}\ , |z| < 1. \tag{3.28}$$

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

$$\begin{aligned} \rho &= \Psi \kappa \Psi^\dagger, \\ \Psi &= \Psi_0 \mathcal{U}(z)(1 - \underline{\chi}_0^\dagger \underline{\chi}_0)^{1/2} + \underline{\chi}_0. \end{aligned} \tag{3.29}$$

In all, z and $\underline{\chi}_0$ amount to $2(2n - 3)$ real independent parameters, the dimension of $\mathcal{R}^{(2)}$. The neighbourhood of ρ_0 is defined by the conditions on $\underline{\chi}_0$ and z in eqs. (3.26, 3.28). For each ρ in this neighbourhood, we have a unique lift $\Psi \in \mathcal{B}^{(2)}$ given in (3.29). A general $\Psi' \in \pi^{-1}(\rho)$ differs from Ψ by a diagonal phase matrix :

$$\Psi' = \Psi \begin{pmatrix} e^{i\alpha_1} & 0 \\ 0 & e^{i\alpha_2} \end{pmatrix},\ \ 0 \le \alpha_1, \alpha_2 < 2\pi. \tag{3.30}$$

Both ρ and Ψ in eq (3.29) are functions of z and $\underline{\chi}_0$. In addition Ψ' involves α_1 and α_2. At ρ_0 and Ψ_0 both z and $\underline{\chi}_0$ vanish. At Ψ_0, $\alpha_1 = \alpha_2 = 0$ as well. To compare eqs.(3.29), (3.30) with the pure state case, see [14].

Vectors and forms at Ψ_0

Since the matrix $(1 - \underline{\chi}_0^\dagger \underline{\chi}_0)^{1/2}$ 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 eq.(3.10). We will actually need expressions for $X_{\Phi'}$, $A^{(a)}$ and $dA^{(a)}$ (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 $\underline{\chi}_0$. From eqs. (3.29, 3.30) we have:

$$\begin{aligned} \psi_1' &= \psi_{01}(1 + i\alpha_1) - z^*\psi_{02} + \chi_{01}, \\ \psi_2' &= \psi_{02}(1 + i\alpha_2) + z\psi_{01} + \chi_{02}. \end{aligned} \tag{3.31}$$

Next we let $\Phi' \in T_{\Psi_0}\mathcal{B}^{(2)}$ correspond to the pair $h', \underline{\chi}'$ in the sense of (3.10). 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 eq. (3.31):

$$\begin{aligned}\Psi' &= \Psi_0 + \epsilon\Phi' : \\ &\quad \delta\alpha_1 = \epsilon h'_{11}, \;\; \delta\alpha_2 = \epsilon h'_{22}, \\ &\quad \delta z = i\epsilon h'_{12}, \;\; \delta z^* = -i\epsilon h'_{21}, \\ &\quad \delta\chi_{01} = \epsilon\chi'_1, \;\; \delta\chi_{02} = \epsilon\chi'_2. \end{aligned} \tag{3.32}$$

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

$$\begin{aligned} X_{\Phi'} &= h'_{11}\frac{\partial}{\partial\alpha_1} + h'_{22}\frac{\partial}{\partial\alpha_2} + ih'_{12}\frac{\partial}{\partial z} - ih'_{21}\frac{\partial}{\partial z^*} \\ &+ \frac{\partial}{\partial\chi_{01}}\chi'_1 + \frac{\partial}{\partial\chi_{02}}\chi'_2 + \chi_1'^{\dagger}\frac{\partial}{\partial\chi_{01}^{\dagger}} + \chi_2'^{\dagger}\frac{\partial}{\partial\chi_{02}^{\dagger}}. \end{aligned} \tag{3.33}$$

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

$$A^{(a)} = -i\psi_a'^{\dagger}d\psi'_a = d\alpha_a, \tag{3.34}$$

which implies

$$i_{X_{\Phi'}}A^{(a)} = h'_{aa}, \;\; a = 1, 2. \tag{3.35}$$

Thus as anticipated in eq.(3.20)

$$\Phi' \text{ horizontal} \Leftrightarrow i_{X_{\Phi'}}A^{(a)} = 0 \Leftrightarrow h'_{11} = h'_{22} = 0. \tag{3.36}$$

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

$$\begin{aligned} dA^{(1)} &= -idz \wedge dz^* - id\chi_{01}^{\dagger} \wedge d\chi_{01}, \\ dA^{(2)} &= +idz \wedge dz^* - id\chi_{02}^{\dagger} \wedge d\chi_{02}. \end{aligned} \tag{3.37}$$

We can contract these with tangent vectors Φ', Φ'' using eq.(3.33) and we then get

$$\begin{aligned} dA^{(1)}(X_{\Phi'}, X_{\Phi''}) &= i_{X_{\Phi''}}i_{X_{\Phi'}}\, dA^{(1)} \\ &= -i(h'_{12}h''_{21} - h'_{21}h''_{12}) + i(\chi_1''^{\dagger}\chi'_1 - \chi_1'^{\dagger}\chi''_1), \\ dA^{(2)}(X_{\Phi'}, X_{\Phi''}) &= i_{X_{\Phi''}}i_{X_{\Phi'}}\, dA^{(2)} \\ &= +i(h'_{12}h''_{21} - h'_{21}h''_{12}) + i(\chi_2''^{\dagger}\chi'_2 - \chi_2'^{\dagger}\chi''_2). \end{aligned} \tag{3.38}$$

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 $(G, \mathcal{B}^{(2)}, \cdot\cdot, H_0)$ with $H_0 = U(n-2)$. A choice of coset representative at $\Psi \in \mathcal{B}^{(2)}$ is of the form

$$\begin{aligned} \ell(\Psi) &= \begin{pmatrix} & \cdot & \cdots \\ & \cdot & \\ \Psi & \cdot & \cdots \\ & \cdot & \\ & \cdot & \cdots \end{pmatrix} \in G, \\ \ell(\Psi)\Psi^{(0)} &= \Psi. \end{aligned} \tag{3.39}$$

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

$$U(\Psi, h_0) = \ell(\Psi)h_0, \;\; h_0 \in H_0 \tag{3.40}$$

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

$$U(\Psi, h_0)^{-1} dU(\Psi, h_0) = \psi_1^\dagger d\psi_1 \, Q_1 \; + \psi_2^\dagger d\psi_2 \, Q_2 \; + \underline{H}_0 \text{ terms } + \text{cross terms}. \tag{3.41}$$

The second coset space PFB is $(G, \mathcal{R}^{(2)}, \cdot\cdot, H)$ with $H = U(1) \times U(1) \times H_0$. The preferred connection on this PFB is obtained from eq.(3.41) by dropping the cross terms and retaining only the H-terms:

$$\begin{aligned} \omega^{(2)} &= -i \left(U(\Psi, h_0)^{-1} dU(\Psi, h_0) \right)_H \\ &= -i\psi_1^\dagger d\psi_1 \, Q_1 - i\psi_2^\dagger d\psi_2 \, Q_2 + \underline{H}_0 - \text{terms}. \end{aligned} \tag{3.42}$$

which replaces eq.(2.17).

The third PFB is an AB to the previous one in which we replace G and H by 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

$$\omega^{(3)} = -i\psi_1^\dagger d\psi_1 \, Q_1 - i\psi_2^\dagger d\psi_2 \, Q_2, \tag{3.43}$$

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 $\mathcal{B}^{(2)}$:

$$A^{(a)} = -i\psi_a^\dagger d\psi_a \;\; (\text{no sum}). \tag{3.44}$$

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

$$\omega^{(3)} = A^{(1)} \, Q_1 + A^{(2)} \, Q_2. \tag{3.45}$$

The evaluations of $A^{(a)}$ and $dA^{(a)}$ on tangent vectors at general points on $\mathcal{B}^{(2)}$ are contained in eq. (3.35, 3.38).

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:

$$\begin{aligned} A^{(a)}_{\Psi(s)}(\dot{\Psi}(s)) &= 0, \\ \text{i.e., } (\psi_a(s), \dot{\psi}_a(s)) &= 0, \;\; a = 1, 2. \end{aligned} \tag{3.46}$$

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 $dA^{(a)}$ 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 $dA^{(a)}$ is related to Ω via pullback. We now find this combination.

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

In eq.(3.21) 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 [15]:

$$\Omega_\rho(X', X'') = -i \text{Tr}_{\mathcal{H}}(\rho \, [K', K'']). \tag{3.47}$$

For clarity we have indicated that the trace has to be computed on the Hilbert space $\mathcal{H}$. Using eq.(3.21) we find after some algebra:

$$\begin{aligned} \Omega_\rho(X', X'') &= -i(\kappa_1 - \kappa_2)(h'_{12} h''_{21} - h'_{21} h''_{12}) \\ &- i\kappa_1 (\chi_1'^\dagger \chi_1'' - \chi_1''^\dagger \chi_1') - i\kappa_2 (\chi_2'^\dagger \chi_2'' - \chi_2''^\dagger \chi_2'). \end{aligned} \tag{3.48}$$

Comparing this with the expressions for $dA^{(a)}(X_{\Phi'}, X_{\Phi''})$ in eq.(3.38) we see that we have the relation

$$\sum_a \kappa_a dA^{(a)} = \pi^* \Omega. \tag{3.49}$$

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 2 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 $\mathcal{R}^{(2)}$:

$$\begin{aligned} \varphi^{(a)}_{\text{geom}}[C] &= \arg(\psi_a(s_1), \psi_a(s_2)) \ , \ a = 1, 2 \ ; \\ \sum_a \kappa_a \varphi^{(a)}_{\text{geom}}[C] &= -\int\int_S \Omega \quad , \partial S = C. \end{aligned} \tag{3.50}$$

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 eqs. (3.47, 3.48). The symplectic area integral of Ω is a weighted average of the two GP's, as in eq. (3.50). 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 [16]:

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

(Of course there must be at least two terms present). Here the p_r are any set of classical probabilities. 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, characterised as a whole by ρ, can be synthesised. 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

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

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 realisations 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 realisations (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 eq.(4.1) cannot exceed dim $\mathcal{H} = n$). Our result (3.50) for mixed state GP's suggests that we use this canonical ensemble realisation of ρ.

We now go back to the rank two case and use the canonical decomposition (3.3). 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 are pure state evolutions. We assume 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 eq.(3.50) 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 realisation of ρ, and involves an average of phases, not of unimodular phase factors $\exp(i\varphi^{(a)}_{\text{geom}}[C])$. This implies that the experimental measurements of the $\varphi^{(a)}_{\text{geom}}[C]$ must not be just modulo 2π, but must keep careful 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 noncyclic 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.

Let us start by recalling some of the geometrical structures we have studied in the preceding sections. We have seen that, for each $\underline{\kappa} = (\kappa_1, \kappa_2),\ \kappa_1 + \kappa_2 = 1$, the space $\mathcal{R}^{(2)}_{\underline{\kappa}}$ can be identified with the adjoint orbit under the $U(n)$ action of a given rank-two density matrix $\rho^{(0)} = \kappa_1 \rho_1^{(0)} + \kappa_2 \rho_2^{(0)}$. This orbit is, in turn, isomorphic to the coset space $U(n)/U(1) \times U(1) \times U(n-2)$, via a $\underline{\kappa}$-dependent map which fixes the two $U(1)$'s as being generated by $\rho_j^{(0)}$, $j = 1, 2$. On each orbit $\{\rho = U\rho^{(0)}U^{-1} = \kappa_1 U\rho_1^{(0)}U^{-1} + \kappa_2 U\rho_2^{(0)}U^{-1} \,|\, U \in U(n)\}$, the KKS symplectic form is given by $\Omega_\rho = \mathrm{Tr}(\rho\, dU^\dagger \wedge dU)$ and its pull-back to the full $U(n)$ as well as to the bundle space $\mathcal{B}^{(2)}$ is exact, with $\pi^\star_{\underline{\kappa}}\Omega_\rho = dA_\rho,\ A_\rho = \kappa_1 A_1 + \kappa_2 A_2 = \mathrm{Tr}(\rho\, U^\dagger dU)$. We notice that both Ω_ρ and A_ρ depend explicitly on $\underline{\kappa}$ i.e. they are specific to the chosen orbit, on which we confine the evolution to define geometric phases. For this reason, in the following we drop the subscript $\underline{\kappa}$.

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* iff $\psi_j(s), \rho_j(s)$ 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* iff $\psi_j(s), \rho_j(s)$ 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) iff

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

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:

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

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

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

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

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

There are additional properties of GP's that are worth mentioning and that can be recovered from 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

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

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:

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

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 with $\iota_M : M \hookrightarrow \mathcal{R}^{(2)}$ the corresponding inclusion map. By using eq. (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:

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

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

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 eq. (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 with $\mathcal{C}_{12}, \mathcal{C}_{12}'$ 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:

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

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

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

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 $(k+1), (k+2), \cdots, n$ of $\mathcal{H}$; $H = U(1) \times U(1) \times \cdots \times U(1) \times H_0$, with k $U(1)$ factors. Correspondingly at the vector and operator levels we have to deal with the spaces

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

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 $(G, \mathcal{B}^{(k)}, \cdot\cdot, H_0)$, $(G, \mathcal{R}^{(k)}, \cdot\cdot, H)$ and $(\mathcal{B}^{(k)}, \mathcal{R}^{(k)}, \cdot\cdot, U(1) \times U(1) \times \cdots \times U(1))$. On the last we obtain, following the set up given earlier, the connection one-form

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

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

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

The general interpretation follows lines similar to what is described in Sections 4 and 5 . As the holonomy group is $U(1) \times U(1) \times \cdots \times U(1)$ (k factors), a cyclic evolution of such mixed states naturally involves k separate $U(1)$ phases or k separate pure state GP's $\varphi^{(a)}_{\mathrm{geom}}[C]$. 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 $\kappa_1, \; \kappa_2, \cdots, \; \kappa_n$. Such a ρ determines an orthonormal basis or frame in Hilbert space upto n phases, namely upto an element of $U(1) \times \cdots \times U(1)$ (n factors). Given a closed trajectory (cyclic unitary evolution) of the density martrix 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$U(1) \times \cdots \times U(1)$ phases. The $U(1) \times \cdots \times U(1)$ 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 ($\mathcal{B}^{(k)}, \; \mathcal{R}^{(k)}, \cdots, U(1) \times \cdots \times U(1)$) and the connection $\omega^{(3)}$ of eq.(6.4) thereon. However, while our framework of three PFB's seems to play no explicit role in ref [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 [17], [18]. 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 [19], 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.

APPENDIX A: THE LIE ALGEBRA OF $U(n)$

The family of compact unitary groups $U(n)$ plays an important role in our analysis. Mainly for notational convenience we list the generators and commutation relations in the defining representation.

The definition of $U(n)$ is

$$U(n) = \{U = n \times n \text{complex matrix} | U^\dagger U = 1_{n\times n}\}. \tag{A.1}$$

Regarding this as a group of complex rotations in an n-dimensional complex space, subgroups $U(n-1), U(n-2), \cdots, U(1)$ can easily be identified in various ways.

The generators of this defining representation of $U(n)$ 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 $U(n)$, and real symmetric 'quadrupole' matrices $Q_{jk} = Q_{kj}$; here the indices j, k go over the range $1, 2, \cdots, n$. The definitions are

$$\begin{aligned} (J_{jk})_{\ell m} &= \frac{i}{\sqrt{2}}(\delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{k\ell}), \\ (Q_{jk})_{\ell m} &= \frac{1}{\sqrt{2}}(\delta_{j\ell}\delta_{km} + \delta_{jm}\delta_{k\ell}). \end{aligned} \tag{A.2}$$

Their commutation relations separate into three sets:

$$\begin{aligned} -i[J_{jk}, J_{\ell m}] &= \frac{1}{\sqrt{2}}(\delta_{k\ell}J_{jm} - \delta_{j\ell}J_{km} + \delta_{km}J_{\ell j} - \delta_{jm}J_{\ell k}), \\ -i[J_{jk}, Q_{\ell m}] &= \frac{1}{\sqrt{2}}(\delta_{k\ell}Q_{jm} - \delta_{j\ell}Q_{km} + \delta_{km}Q_{j\ell} - \delta_{jm}Q_{k\ell}), \\ -i[Q_{jk}, Q_{\ell m}] &= \frac{1}{\sqrt{2}}(\delta_{k\ell}J_{mj} + \delta_{j\ell}J_{mk} + \delta_{km}J_{\ell j} + \delta_{jm}J_{\ell k}). \end{aligned} \tag{A.3}$$

The numerical coefficients in eq.(A.2) have been chosen so that as far as possible these matrices are trace orthonormal. We have:

$$\begin{aligned} \mathrm{Tr}(J_{jk}J_{\ell m}) &= \delta_{j\ell}\delta_{km} - \delta_{jm}\delta_{kl}, \\ \mathrm{Tr}(J_{jk}Q_{\ell m}) &= 0, \\ \mathrm{Tr}(Q_{jk}Q_{\ell m}) &= \delta_{j\ell}\delta_{km} + \delta_{jm}\delta_{kl}. \end{aligned} \tag{A.4}$$

Thus while distinct generators are definitely 'trace orthogonal', each individual J_{jk} and each individual Q_{jk} for $j \neq k$ have normalised traces in the above sense. The exceptional cases are the generators $Q_{11}, Q_{22}, \cdots, Q_{nn}$ since for $j = k = \ell = m$ we have a factor of 2 on the right hand side in the last of eqs.(A.4). To have a strictly trace orthonormal basis for the Lie algebra $\underline{U}(n)$ of $U(n)$ in the defining representation we therefore may take the basis to be made up of

$$\begin{aligned} J_{jk} &= -J_{kj}, \\ Q_{jk} &= Q_{kj}, \quad j \neq k, \\ Q_j &= \sqrt{2}Q_{jj} \quad \text{no sum on } j. \end{aligned} \tag{A.5}$$

Each of the matrices J_{jk} and Q_{jk} for $j \neq k$ has no non vanishing diagonal matrix elements. On the other hand, each Q_j has a matrix element of unity at the j^{th} place in the diagonal, while all other matrix elements vanish. Using the basis (A.5) we can write a general element of $\underline{U}(n)$ as a real linear combination of the form:

$$\begin{aligned} X &= x_j Q_j + \frac{1}{2}x_{jk}J_{jk} + \frac{1}{2}x'_{jk}Q_{jk}, \\ & \quad x_{jk} = -x_{kj} \quad x'_{jk} = x'_{kj} \quad \text{for } j \neq k. \end{aligned} \tag{A.6}$$

Then we have the trace formula

$$\mathrm{Tr}(XY) = x_j y_j + \frac{1}{2}x_{jk}y_{jk} + \frac{1}{2}x'_{jk}y'_{jk}, \tag{A.7}$$

so each independent term appears with a coefficient of unity.

Regarding $\underline{U}(n)$ as the abstract Lie algebra of $U(n)$ we may denote its basis elements corresponding to the above matrices as

$$Q_j \rightarrow e_j \ \ , J_{jk} \rightarrow e_{jk} = -e_{kj} \ \ , Q_{jk} \rightarrow e'_{jk} = e'_{kj} \ \text{ for } j \neq k. \tag{A.8}$$

The Q_j, or e_j in a general situation, are the generators of the Abelian torus subgroup $U(1) \times U(1) \times \cdots \times U(1)$ of $U(n)$, consisting of all diagonal matrices U.

APPENDIX B: PRINCIPAL FIBRE BUNDLES, ASSOCIATED BUNDLES, COSET SPACES AND CONNECTIONS

For setting notations and as a ready reference for the reader, we here collect briefly the basic definitions and properties of the structures named above [20]-[23].

Principal fibre bundles and connections

A principal fibre bundle (PFB) is a collection of four objects written as (P, M, π, H): P the total space; M the base space; π the projection map $P \rightarrow M$; and H a Lie group, the structure group and typical fibre. P, M and H are all differentiable manifolds, with dim P = dim M + dim H. Points in them will be denoted by $p, p', \cdots,\quad m, m', \cdots,\quad h, h', \cdots$, with $\pi(p) = m, \quad \pi(p') = m', \ \cdots$. For each element $h \in H$ there is a globally well defined fibre-preserving diffeomorphisn ψ_h of P onto itself, which is free and transitive on each fibre. In a local trivialization of the bundle, the portion $\pi^{-1}(M_\alpha) \subset P$ lying 'on top of' some open subset $M_\alpha \subset M$ 'looks like' the Cartesian product $M_\alpha \times H$. We express this with the compact notation

$$\pi(p) = m \in M_\alpha \ \ : \ \ p = (m, h)_\alpha, \ \ h \in H, \tag{B.1}$$

h being uniquely determined by p. As h varies over H with m kept fixed, we obtain all points $p \in \pi^{-1}(m)$. In the overlap of two such local trivializations we have a transition rule

$$\begin{aligned} \pi(p) = m \in M_\alpha \cap M_\beta : \quad & p = (m, h)_\alpha = (m, h')_\beta : \\ & h' = t_{\beta\alpha}(m) h, \ \ t_{\beta\alpha}(m) \in H, \end{aligned} \tag{B.2}$$

with the transition group element appearing by convention on the left hand side. In the relevant overlaps these transition functions obey

$$\begin{aligned} t_{\alpha\beta}(m)^{-1} &= t_{\beta\alpha}(m), \\ t_{\alpha\beta}(m) t_{\beta\gamma}(m) &= t_{\alpha\gamma}(m). \end{aligned} \tag{B.3}$$

The globally well defined map $\psi_{h'}$ representing $h' \in H$ appears locally (by convention, so as not to 'interfere' with the transition rule (B.2)) as a right translation along fibres:

$$\psi_{h'}(m, h)_\alpha = (m, h h'^{-1})_\alpha. \tag{B.4}$$

In this set up, we do not contemplate any action of H on M.

A connection on P is a one-form ω on P taking values in the Lie algebra $\underline{H}$ of H, and obeying two important conditions spelt out below. We denote by e_a the elements of a basis for $\underline{H}$, so $\underline{H} = \mathrm{Sp}\{e_a\}$. At each point $p \in P$, the tangent space $T_p P$ contains a vertical subspace V_p corresponding to motions within the fibre induced by the (right) actions ψ_h of elements $h \in H$. This leads to a natural isomorphism $\rho_p : V_p \rightarrow \underline{H}$ with $\rho_p^{-1} : H \rightarrow V_p$. The first condition on ω is that at each p, the contraction of vertical vectors with ω_p should agree with ρ_p:

$$v \in V_p : i_v \omega_p = \rho_p(v) \in \underline{H} \ , \tag{B.5}$$

the second is the 'equivariance' condition which controls the behaviour of ω_p as p runs over a fibre:

$$h \in H : \psi_h^* \omega = \mathcal{D}(h^{-1}) \circ \omega, \tag{B.6}$$

where $\mathcal{D}(h)$ is the adjoint representation of H on $\underline{H}$, with matrices $(\mathcal{D}^a{}_b(h))$. One can show that in a local trivialization of P over $M_\alpha \subset M$, ω necessarily has the form [23]:

$$m \in M_\alpha, p = (m,h)_\alpha : \omega_p = (\hat{\Theta}^{(0)a}(h) - \mathcal{D}^a{}_b(h^{-1})A^b(m))e_a, A^a \in \mathcal{X}^*(M_\alpha). \tag{B.7}$$

Here $\hat{\Theta}^{(0)a}$ are the left-invariant Maurer-Cartan one-forms on H, adapted to the basis $\{e_a\}$ for $\underline{H}$; and each A^a is a one-form defined locally over M_α. (We omit the extra label α on these one-forms). If m is in the overlap $M_\alpha \cap M_\beta$ of the domains of two local trivializations of P, then the two expressions for ω involving A^a over M_α and A'^a over M_β are related by the gauge transformation formula

$$A'^a(m) = \mathcal{D}^a{}_b(t_{\beta\alpha}(m))(A^b(m) + \hat{\Theta}^{(0)b}(t_{\beta\alpha}(m))). \tag{B.8}$$

Any $\underline{H}$-valued one-form ω on P obeying the two conditions (B.5, B.6), described locally as in (B.7) subject to the transition rule (B.8), is an acceptable connection on P, there being no preferred one.

Sometimes for practical calculations it is convenient to work within some (unspecified) matrix representation $\mathcal{U}(h)$ of H, with generators $e_a \to -iJ_a$. Then eqs.(B.7, B.8) have the convenient matrix forms

$$\begin{aligned} \omega_p &= \mathcal{U}(h)^{-1}(id - J_a A^a(m))\mathcal{U}(h), \\ J_a A'^a(m) &= \mathcal{U}(t_{\beta\alpha}(m))(J_a A^a(m) - id)\mathcal{U}(t_{\beta\alpha}(m))^{-1}, \end{aligned} \tag{B.9}$$

while the Maurer-Cartan one-forms appearing in eqs.(B.7, B.8) are obtainable from

$$\mathcal{U}(h)^{-1} d\mathcal{U}(h) = -i\hat{\Theta}^{(0)a} J_a. \tag{B.10}$$

Given a connection ω on P, at any $p \in P$ the horizontal subspace $H_p \subset T_pP$ is defined to be the null space of ω_p:

$$X \in T_pP : X \in H_p \Leftrightarrow i_X \omega_p = 0. \tag{B.11}$$

Then T_pP appears as the direct sum of vertical and horizontal subspaces:

$$T_pP = V_p \oplus H_p, \tag{B.12}$$

and the tangent map $(\pi_*)_p$, which annihilates V_p, gives an one-to-one onto map of H_p to T_mM in the base:

$$\pi(p) = m : (\pi_*)_p : V_p \to 0, H_p \to T_mM. \tag{B.13}$$

The last item in this brief recapitulation of PFB structure is the concept of parallel transport, or horizontal lift of a smooth curve in M upto P. Let $C = \{m(s)\} \subset M$ be a smooth parametrised curve in the base. Then a smooth parametrised curve $\mathcal{C} = \{p(s)\} \subset P$ is a horizontal lift of C (with respect to a given connection ω) if $\mathcal{C}$ projects onto C and at each point its tangent vector is horizontal:

$$\begin{aligned} \pi(p(s)) &= m(s), \\ X(s) &= \text{tangent to } \mathcal{C} \text{ at } p(s) \in H_{p(s)}. \end{aligned} \tag{B.14}$$

In local coordinates, say q^μ for M and θ^a for H, along with an accompanying local trivialization of P, we get explicit formulae suitable for computations. The entire set (q^μ, θ^a) gives a local coordinate system for P. The Maurer-Cartan one forms $\hat{\Theta}^{(0)a}$ and the one-forms A^a determining ω may be written as

$$\begin{aligned} \hat{\Theta}^{(0)a}(h) &= \hat{\xi}^a_b(\theta)d\theta^b, \\ A^a(m) &= A^a_\mu(q)dq^\mu. \end{aligned} \tag{B.15}$$

Let us write the coordinates of points on C as $q^\mu(s)$; for a horizontal lift $\mathcal{C}$ we must determine the additional coordinates $\theta^a(s)$ such that condition (B.14) is obeyed. The tangents to C and $\mathcal{C}$ at corresponding points are

$$\begin{aligned} &\frac{dq^\mu(s)}{ds}\frac{\partial}{\partial q^\mu} \qquad\qquad\qquad\quad \in T_{m(s)}M, \\ X(s) = &\frac{dq^\mu(s)}{ds}\frac{\partial}{\partial q^\mu} + \frac{d\theta^a(s)}{ds}\frac{\partial}{\partial \theta^a} \in T_{p(s)}P. \end{aligned} \tag{B.16}$$

Then (B.14) becomes a system of first order ordinary differential equations for the coordinates $\theta^a(s)$ of a variable element $h(s) \in H$:

$$\hat{\xi}^a_b(\theta(s))\frac{d\theta^b(s)}{ds} = \mathcal{D}^a{}_b(h(s)^{-1})A^b_\mu(q(s))\frac{dq^\mu(s)}{ds}. \tag{B.17}$$

In a general matrix representation this takes the form

$$\frac{d}{ds}\mathcal{U}(h(s)) = -iJ_aA^a_\mu(q(s))\frac{dq^\mu(s)}{ds}\mathcal{U}(h(s)). \tag{B.18}$$

Thus each horizontal lift $\mathcal{C}$ of C is fully determined by the choice of an initial point $p(s_1) \in \pi^{-1}(m(s_1))$ at $s = s_1$, say,i.e., the choice of an element $h(s_1) \in H$. The solution to (B.18) is:

$$\mathcal{U}(h(s)) = \mathrm{P}\left(\exp(-i\int_{s_1}^{s_2} ds'\ A^a_\mu(q(s'))\frac{dq^\mu(s')}{ds'}\ J_a)\right)\mathcal{U}(h(s_1)), \tag{B.19}$$

where P is the path-ordering symbol keeping variables with later parameter values to the left. Keeping $C \subset M$ fixed and applying $\psi_{h_0},\ h_0 \in H$ to a horizontal lift $\mathcal{C}$ of C leads to another horizontal lift $\psi_{h_0}[\mathcal{C}]$ in which $h(s) \to h(s)h_0^{-1}$ pointwise. This just amounts to changing the initial point $h(s_1)$ to $h(s_1)h_0^{-1}$.

In case $C \subset M$ is a closed loop with $q^\mu(s_2) = q^\mu(s_1)$ for a final parameter value s_2, the lift is in general not closed: while the end points of $\mathcal{C}$ lie on the same fibre, they differ by a left translation by an element of H determined by the loop C,

$$\begin{aligned} h(s_2) &= h[C]h(s_1), \\ \mathcal{U}(h[C]) = & \quad \mathrm{P}\left(\exp(-i\oint_C ds\ A^a_\mu(q(s))\frac{dq^\mu(s)}{ds}\ J_a)\right). \end{aligned} \tag{B.20}$$

These elements of the structure group H form the holonomy group, in general a subgroup of H, associated with the connection ω.

Associated Bundles

To pass from the PFB (P, M, π, H) to an associated bundle (AB) we retain the base space M, replace the typical fibre H by a differentiable manifold F as the new typical fibre, and simultaneously change the total space from P to E. Thus the AB is written as a quartet (E, M, π_E, F), with π_E a new projection map $E \to M$. However it retains the memory of the structure group H since we require that there be an action of H on F by a family of diffeomorphisms $\{\varphi_h\}$ respecting the composition law in H. Locally, E looks like the Cartesian product $M \times F$, but this may not be so globally. We 'use up' the action of H on F in stating the transition rule connecting two overlapping local trivializations of E, in the spirit of eq.(B.2):

$$\begin{aligned} e \in E, \quad & \pi_E(e) = m \in M_\alpha \subset M : e = (m, f)_\alpha,\ f \in F; \\ & m \in M_\alpha \cap M_\beta : e = (m, f)_\alpha = (m, f')_\beta, \\ & f' = \varphi_{t_{\beta\alpha}(m)}(f). \end{aligned} \tag{B.21}$$

The transition group elements $t_{\beta\alpha}(m)$ are taken from the parent PFB (so implicitly the same open sets $M_\alpha, M_\beta, \cdots$ in M are used to locally trivialize the PFB and AB). There is now no 'other' global fibre preserving H action on E, in place of ψ_h in the PFB; and again no H action on M is contemplated.

Compared to a general fibre bundle (FB), which however we have not recalled here, an AB has more structure: there is the group H acting on the typical fibre F, and transition formulae connecting overlapping local trivializations.

If now a connection ω is given on the parent PFB, it can be used to set up horizontal lifts in the AB. We limit ourselves to a local coordinate description. With coordinates q^μ for M and f^r for F, we have coordinates (q^μ, f^r) for E. Then, given the curve $C = \{q^\mu(s)\} \subset M$, a horizontal lift of it to E is a curve $\mathcal{C}_E = \{q^\mu(s), f^r(s)\} \subset E$ in which the coordinates $f^r(s)$ of points in the new fibre may be read off from eq.(B.19) (after taking $h(s_1)$ to be the identity in H):

$$\begin{aligned} f(s) &= \varphi_{h(s)}(f(s_1)), \\ \mathcal{U}(h(s)) &= \mathrm{P}\left(\exp(-i\int_{s_1}^{s} ds'\ A^a_\mu(q(s'))\frac{dq^\mu(s')}{ds'}\ J_a)\right)\ 1\!\!1. \end{aligned} \tag{B.22}$$

In case F in the AB is a linear vector space with vectors $\Psi, \Psi', \cdots$,and the diffeomorphisms φ_h are linear transformations on F with generators J_a, the AB is a vector bundle; and horizontal lifting is describable by a simple ordinary first order matrix differential equation:

$$\begin{aligned} (\frac{d}{ds} &+ iA^a_\mu(q(s))\frac{dq^\mu(s)}{ds}\ J_a)\Psi(s) = 0, \\ \Psi(s+\delta s) &= \exp\left(-iA^a_\mu(q(s))J_a\delta q^\mu\right)\Psi(s), \\ \delta q^\mu &= \frac{dq^\mu(s)}{ds}\delta s. \end{aligned} \tag{B.23}$$

We see that both the structure group H of a PFB and a connection ω given on it carry over to an AB set up as described above.

Lie group on coset space as PFB

Next we consider the coset space G/H of a Lie group G with respect to a Lie subgroup H. We take G/H to be the space of right cosets, and view G as a PFB over it as base. We wish to point out the particular new features that are present in this case. For the quartet (P, M, π, H) of a general PFB, we now make the identifications $P \to$ Lie group G, $M \to$ Coset space G/H, structure group and typical fibre $H \to$ subgroup H in G. The projection π maps any $g \in G$ to its right coset gH. So we denote such a PFB by $(G, G/H, \pi, H)$. Several new features are immediately recognized: the total space is a Lie group G, actions of G on itself by left and right translations, $L^{(0)}_g$ and $R^{(0)}_g$, are both available; the former translations $L^{(0)}_g$ descend to a transitive G action on the base G/H by maps L_g. For the globally well defined fibre preserving action of H on G by maps ψ_h we take $R^{(0)}_h$, a subset of $R^{(0)}_g$; so $R^{(0)}_g$ for $g \notin H$ play no immediate role.

Local trivilializations and transition formulae are connected now to choices of local coset representatives. Over some $M_\alpha \subset M$ a local coset representative is a map

$$m \in M_\alpha \to \ell_\alpha(m) \in G : \pi(\ell_\alpha(m)) = m. \tag{B.24}$$

This determines a local trivialization of G over $\pi^{-1}(M_\alpha)$:

$$\pi(g) = m \in M_\alpha \Rightarrow g = \ell_\alpha(m)h, h \in H, \tag{B.25}$$

so we can view g as the pair $(m, h)_\alpha$:

$$g = \ell_\alpha(m)h \Leftrightarrow g = (m, h)_\alpha. \tag{B.26}$$

In the overlap of two such choices of local coset representatives we necessarily have

$$m \in M_\alpha \cap M_\beta : \ell_\beta(m) = \ell_\alpha(m)t_{\alpha\beta}(m),\ \ t_{\alpha\beta}(m) \in H, \tag{B.27}$$

so that

$$g = (m, h)_\alpha = (m', h')_\beta \Leftrightarrow h' = t_{\beta\alpha}(m)h. \tag{B.28}$$

In this kind of PFB, there is a preferred connection. We have denoted a basis for $\underline{H}$ by $\{e_a\}$. They obey Lie bracket relations

$$[e_a, e_b] = C_{ab}{}^c e_c, \tag{B.29}$$

with $C_{ab}{}^c$ the structure constants of H. Now we add elements e_μ to get a basis for $\underline{G}$

$$G = \mathrm{Sp}\{e_a, e_\mu\}. \tag{B.30}$$

We assume that the Lie brackets $[e_a, e_\mu]$ have the simple form

$$[e_a, e_\mu] = C_{a\mu}{}^\nu e_\nu, \tag{B.31}$$

with no e_b terms on the right. The remaining Lie bracket relations for $\underline{G}$ are

$$[e_\mu, e_\nu] = C_{\mu\nu}{}^a e_a + C_{\mu\nu}{}^\lambda e_\lambda. \tag{B.32}$$

The full set of left-invariant Maurer-Cartan one-forms on G consists of $\hat{\Theta}^{(0)a}(g), \hat{\Theta}^{(0)\mu}(g)$. It now turns out that a preferred connection on $(G, G/H, \pi, H)$ is given by

$$\omega = \hat{\Theta}^{(0)a}(g)e_a, \tag{B.33}$$

which is indeed $\underline{H}$-valued. Here only a subset of the full set of Maurer-Cartan forms on G is used. This choice obeys both the conditions demanded of a general connection on a PFB. If now one brings in a local coset representative $\ell_\alpha(m)$ and the accompanying local trivialization (B.26) of G, one indeed finds

$$\begin{aligned} & g = \ell_\alpha(m)h = (m, h)_\alpha : \\ & \hat{\Theta}^{(0)a}(g) = \hat{\Theta}^{(0)a}_H(h) - \mathcal{D}_H{}^a{}_b(h^{-1})A^b(m), \end{aligned} \tag{B.34}$$

where A^a are specific one-forms over M_α arising out of the structure constants $C_{a\mu}{}^\nu, C_{\mu\nu}{}^a, C_{\mu\nu}{}^\lambda$. Here the Maurer-Cartan forms and adjoint representation matrices belonging to H have been denoted with a subscript H to distinguish them from objects belonging to G. Using (B.34) in (B.33) we see that the expected structure (B.7) for ω is indeed present, so this is a preferred connection determined by G in relation to G/H and H.

Associate bundle to a coset PFB

Lastly we point out the special features that accompany a bundle $(E, G/H, \pi_E, F)$ associated to a coset space PFB $(G, G/H, \pi, H)$. They share the same base G/H, while the total space and the typical fibre are E and F in place of G and H respectively. As with a general AB, we have H acting on F via diffeomorphisms φ_h. The transition functions $\{t_{\alpha\beta}(m)\}$ belonging to $(G, G/H, \pi, H)$ are used for $(E, G/H, \pi_E, F)$ as well. Compared to a general AB in which eq. (B.21) holds, we now have the feature that the transition functions arise from coset representatives via eq.(B.27), namely

$$t_{\alpha\beta}(m) = \ell_\alpha(m)^{-1}\ell_\beta(m), \tag{B.35}$$

though the $\ell_\alpha(m)$ themselves play no direct role in the AB. The left and right translations $L_g^{(0)}, R_g^{(0)}$ of G also have no role to play, though the present AB 'remembers' (if necessary) the transitive G action on the base G/H by maps L_g. Finally the preferred connection on $(G, G/H, \pi, H)$ given by eq.(B.33) leads to parallel transport and horizontal lifting operations in $(E, G/H, \pi_E, F)$ in a preferred manner, the details being of course given by eqs.(B.22, B.23).

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