IISER Mohali Lectures on Geometric Phases

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1 Overview: Scope of Lectures

Berry's discovery of 1983-1984, a new phase in the context of the adiabatic theorem in QM, initiated activity worldwide. Several independent assumptions were made. Initially it was called the Berry phase, later the Geometric Phase or GP. It is relevant also in classical wave optics context.

Many efforts were devoted to relaxing assumptions made by Berry, to define GP under more general conditions - Aharonov Anandan 1987, Samuel Bhandari 1988, NM RS 1993, all successive steps in generalization.

Simultaneously a search for earlier ideas pointing in this direction was taken up. Two important ones are: S. Pancharatnam's work in classical polarization optics in 1956, pointed out by Ramaseshan and Nityananda in 1986; V. Bargmann in 1964 in discussing Wigner's theorem of 1931 on symmetry operations in QM, pointed out by NM RS in 1993. In addition there is work in quantum chemistry too, referred to in Berry's original paper.

These lectures will describe all these and more in a more or less chronological order. Many features of QM will be reexamined and refined as well as some useful mathematical ideas will be described. Some applications of 'our' kinematic approach will be given.

2 Berry's discovery of "new" phase (in simplified form)

We have some QM system in mind, pure states being vectors in a Hilbert space \mathcal{H} . Given a time dependent hermitian Hamiltonian operator H(t), state vector $\psi(t)$ obeys the Schroedinger equation

$$i\hbar \frac{d}{dt}\psi(t) = H(t)\psi(t)$$
 (2.1)

If H is time independent, formally the general solution is easy to get. Use complete orthonormal set of eigenfunctions and real eigenvalues of H, assume for simplicity they are discrete and non-degenerate :use flexible notation :

$$H\psi_{n} = E_{n}\psi_{n} \qquad n = 1, 2, \dots; \qquad E_{n} \text{ real};$$

$$(\psi_{n'}, \psi_{n}) \equiv \langle \psi_{n'} | \psi_{n} \rangle = \delta_{n',n} \qquad \sum_{n} |\psi_{n}\rangle \langle \psi_{n}| = \mathbb{I} \text{ on } \mathcal{H};$$

$$\psi(0) = \sum_{n} c_{n}\psi_{n} \rightarrow \qquad \psi(t) = \sum_{n} c_{n}e^{-iE_{n}t/\hbar}\psi_{n} \qquad (2.2)$$

Each ψ_n is fixed upto a phase. The c_n are constants, the ψ_n are stationary states, this is the general solution to equation (2.1).

Now take up the case H(t). Its instantaneous eigenfunctions and eigenvalues will in general vary with time:

$$H(t)\psi_n(t) = E_n(t)\psi_n(t) \qquad n = 1, 2, \dots; \qquad E_n(t) \text{ real;}$$
$$(\psi_{n'}(t), \psi_n(t)) = \delta_{n',n} \qquad \sum_{n} |\psi_n(t)\rangle\langle\psi_n(t)| = \mathbb{I} \text{ on } \mathcal{H}$$
(2.3)

Each $\psi_n(t)$ is fixed upto a time dependent phase. To try and solve (2.1) we begin by expanding $\psi(t)$ in terms of the instantaneous eigenfunctions with phase factors generalizing those in (2.2):

$$\psi(t) = \sum_{n} c_n(t) e^{\frac{-i}{\hbar} \int_0^t dt' E_n(t')} \psi_n(t)$$
 (2.4)

This reduces to (2.2) in the time independent case with $c_n(t) \to c_n$, $E_n(t) \to E_n$. Use (2.4) in the Schroedinger equation (2.1):

$$i\hbar \sum_{n} \left(\dot{c}_n(t)\psi_n(t) - \frac{i}{\hbar} c_n(t) E_n(t)\psi_n(t) + c_n(t)\dot{\psi}_n(t) \right) e^{\frac{-i}{\hbar} \int_0^t dt' E_n(t')}$$
$$= \sum_{n} c_n(t) E_n(t)\psi_n(t) e^{\frac{-i}{\hbar} \int_0^t dt' E_n(t')},$$

i.e.
$$\sum_{n} \left(\dot{c}_n(t) \psi_n(t) + c_n(t) \dot{\psi}_n(t) \right) e^{\frac{-i}{\hbar} \int_0^t dt' E_n(t')} = 0$$
 (2.5)

This is exact. Taking the inner product with $\psi_n(t)$ for general n gives:

$$\dot{c}_n(t) = -\sum_m c_m(t) e^{\frac{i}{\hbar} \int_0^t dt' (E_n(t') - E_m(t'))} (\psi_n(t), \dot{\psi}_m(t)), \quad \forall n$$
 (2.6)

which is still exact. Now analyse the last factor on the rhs:

$$H(t)\psi_{m}(t) = E_{m}(t)\psi_{m}(t) \Longrightarrow$$

$$\dot{H}(t)\psi_{m}(t) + H(t)\dot{\psi}_{m}(t) = \dot{E}_{m}(t)\psi_{m}(t) + E_{m}(t)\dot{\psi}_{m}(t) \Longrightarrow$$

$$\left(\psi_{n}(t), \dot{H}(t)\psi_{m}(t)\right) + E_{n}(t)\left(\psi_{n}(t), \dot{\psi}_{m}(t)\right)$$

$$= \dot{E}_{m}(t)\delta_{n,m} + E_{m}(t)\left(\psi_{n}(t), \dot{\psi}_{m}(t)\right) \ \forall n, m$$

i.e.

$$(E_m(t) - E_n(t)) \left(\psi_n(t), \dot{\psi}_m(t) \right) = -\dot{E}_m(t) \delta_{n,m} + \left(\psi_n(t), \dot{H}(t) \psi_m(t) \right) \forall n, m$$
 (2.7)

For m = n this gives:

$$\dot{E}_m(t) = \left(\psi_m(t), \dot{H}(t)\psi_m(t)\right) \tag{2.8}$$

Assuming nondegeneracy again, for $m \neq n$ we get:

$$\left(\psi_n(t), \dot{\psi}_m(t)\right) = \frac{\left(\psi_n(t), \dot{H}(t)\psi_m(t)\right)}{\left(E_m(t) - E_n(t)\right)} \tag{2.9}$$

Each $\psi_n(t)$ is free upto a time dependent phase. Limit this freedom by requiring

$$\left(\psi_n(t), \dot{\psi}_n(t)\right) = 0 \ \forall n \tag{2.10}$$

Then equation (2.6) becomes

$$\dot{c}_n(t) = -\sum_{m \neq n} c_m(t) e^{i \int_0^t dt' \omega_{nm}(t')} \left(\psi_n(t), \dot{\psi}_m(t) \right)
= \sum_{m \neq n} \frac{c_m(t)}{\hbar \omega_{nm}(t)} e^{i \int_0^t dt' \omega_{nm}(t')} \left(\psi_n(t), \dot{H}(t) \psi_m(t) \right) \, \forall n, \text{ exact,}
\hbar \omega_{nm}(t) = E_n(t) - E_m(t)$$
(2.11)

Again this is exact. Now in the adiabatic case, H(t) is "slowly varying", so $\dot{H}(t)$ is "small", so also $\psi_n(t)$, $E_n(t)$, $c_n(t)$ are all expected to vary slowly. Suppose at t=0 we have $\psi(0)=n_0^{th}$ instantaneous eigenvector of H(0):

$$\psi(0) = \psi_{n_0}(0), \qquad c_n(0) = \delta_{nn_0}, \text{ some given } n_0$$
 (2.12)

We use this on the rhs in (2.11), and to get an estimate, as $\dot{H}(t)$ appears explicitly and is "small", we treat the other factors $c_m(t)$, $\omega_{km}(t)$ as constants; then we get the approximate results

$$\dot{c}_{n_0}(t) \approx 0, \quad c_{n_0}(t) \approx 1;$$

$$n \neq n_0 : \dot{c}_n(t) \approx \frac{1}{\hbar \omega_{nn_0}} e^{i\omega_{nn_0}t} \left(\psi_n(t), \dot{H}(t)\psi_{n_0}(t) \right),$$

$$c_n(t) \approx \frac{i}{\hbar \omega_{nn_0}^2} (1 - e^{i\omega_{nn_0}t}) \left(\psi_n(t), \dot{H}(t)\psi_{n_0}(t) \right).$$
(2.13)

So while $c_{n_0}(t)$ remains close to unity, the other $c_n(t)$ keep oscillating with no steady build up. So provided

$$\frac{1}{\omega_{nn_0}} \left| \langle \psi_n(t) | \dot{H}(t) | \psi_{n_0}(t) \rangle \right| << \hbar \omega_{nn_0}, \ \forall n \neq n_0$$
 (2.14)

an approximate solution to the Schroedinger equation (2.1) is:

$$\psi(t) \approx e^{-\frac{i}{\hbar} \int_0^t dt' E_{n_0}(t')} \psi_{n_0}(t), \text{ each } n_0; \text{ now set } n_0 \to n$$
(2.15)

Now comes the step taken by Berry. Suppose H(t) is cyclic as an operator, i.e. for some time T>0 we have

$$H(T) = H(0) \tag{2.16}$$

What about (each of) the approximate solutions (2.15) to the Schroedinger equation? Assume that in addition to nondegeneracy, for $0 \le t \le T$ there are no level crossings. Clearly then $E_n(T) = E_n(0)$ and

$$\psi(0) = \psi_n(0) \implies \psi(T) \approx e^{-\frac{i}{\hbar} \int_0^T dt' E_n(t')} \psi_n(T) \tag{2.17}$$

Is this also cyclic? Yes, because of the nondegeneracy and no crossings of levels, but only upto a phase. H(t) being cyclic, and the condition (2.10), give only

$$\psi_n(T) = (n - \text{dependent phase}) \psi_n(0)$$
 (2.18)

This is the geometric phase, one for each n. So we have the full set of relations

$$\psi_{n}(T) = e^{i\varphi_{\text{geom}}^{n}} \psi_{n}(0) :
\psi(T) = e^{i\varphi_{\text{tot}}^{n}} \psi(0) \quad \text{i.e. } \varphi_{\text{tot}}^{n} = \arg (\psi(0), \psi(T));
\varphi_{\text{tot}}^{n} = \varphi_{\text{geom}}^{n} + \varphi_{\text{dyn}}^{n} \quad \text{i.e.} \varphi_{\text{geom}}^{n} = \varphi_{\text{tot}}^{n} - \varphi_{\text{dyn}}^{n},
\varphi_{\text{dyn}}^{n} = \frac{-1}{\hbar} \int_{0}^{T} dt \ E_{n}(t)$$
(2.19)

Berry's original derivation using parameter space:

In this, the Hamiltonian $H(\mathbf{R})$ was supposed to depend on some real (external) parameters \mathbf{R} ; and by letting \mathbf{R} vary slowly with time, the Hamiltonian became time dependent. This treatment is useful from a practical point of view:

 $\mathbf{R} \in \text{multidimensional parameter space}$

$$\mathbf{R} \to \mathbf{R}(t) \implies H(\mathbf{R}) \to H(\mathbf{R}(t))$$
 becomes explicitly time dependent (2.20)

Assume this is adiabatic. Let $\mathbf{R}(t)$ run over a closed loop as $0 \le t \le T$:

$$C = \{ \mathbf{R}(t) \mid 0 \le t \le T \} = \text{closed loop in parameter space}, \tag{2.21a}$$

$$\mathbf{R}(T) = \mathbf{R}(0). \tag{2.21b}$$

For each fixed **R** (in the domain of interest), we have eigenvectors and eigenvalues for $H(\mathbf{R})$:

$$H(\mathbf{R}) | n; \mathbf{R} \rangle = E_n(\mathbf{R}) | n; \mathbf{R} \rangle, \quad E_n(\mathbf{R}) \text{ real};$$
 (2.22a)

$$\langle n'; \mathbf{R} | n; \mathbf{R} \rangle = \delta_{n'n}, \quad \sum_{n} |n; \mathbf{R} \rangle \langle n; \mathbf{R} | = \mathbb{I} \text{ on } \mathcal{H}.$$
 (2.22b)

We assume nondegeneracy and no level crossings in the domain of interest in \mathbf{R} - space. Also, in contrast to (2.10), we assume $|n; \mathbf{R}\rangle$ is continuous and single valued in \mathbf{R} over the domain of interest.

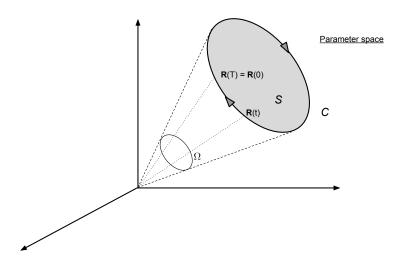


Figure 1:

Each $|n; \mathbf{R}\rangle$ is free upto a phase dependent on n and \mathbf{R} but is otherwise assumed to be well-defined (single-valued) in the relevant domain of \mathbf{R} -space.

The Schróedinger equation is

$$i\hbar\dot{\psi}(t) = H(\mathbf{R}(t))\psi(t).$$
 (2.23)

By the adiabatic theorem:

$$\psi(0) = |n; \mathbf{R}(0)\rangle \Rightarrow \psi(t) \approx \exp\left(-\frac{i}{\hbar} \int_0^t dt' E_n(\mathbf{R}(t')) + i\gamma_n(t)\right) |n; \mathbf{R}(t)\rangle, \qquad (2.24a)$$

$$\gamma_n(0) = 0. \qquad (2.24b)$$

We will find that $\gamma_n(t)$ is non-integrable, it is not a function of $\mathbf{R}(t)$ alone. So $\gamma_n(t)$ cannot be absorbed into the defintion of $|n; \mathbf{R}(t)\rangle$. Put (2.24) into (2.23) to get :

$$i\hbar \left[\frac{-i}{\hbar} E_n(\mathbf{R}(t)) |n; \mathbf{R}(t)\rangle + i\dot{\gamma}_n(t) |n; \mathbf{R}(t)\rangle + \frac{d}{dt} |n; \mathbf{R}(t)\rangle \right] \approx E_n(\mathbf{R}(t)) |n; \mathbf{R}(t)\rangle$$

i.e.
$$\dot{\gamma}_n(t)|n; \mathbf{R}(t)\rangle \approx i \frac{d}{dt}|n; \mathbf{R}(t)\rangle,$$

i.e. $\dot{\gamma}_n(t) \approx i \langle n; \mathbf{R}(t)| \frac{d}{dt}|n; \mathbf{R}(t)\rangle$

$$= i \langle n; \mathbf{R}(t)|\nabla|n; \mathbf{R}(t)\rangle \cdot \dot{\mathbf{R}}(t), \qquad \nabla \equiv \nabla_{\mathbf{R}}$$
(2.25)

(This is just $\frac{d}{dt} \left(e^{i\gamma_n(t)} | n; \mathbf{R}(\mathbf{t}) \right) \approx 0$, as is clear from (2.23) & (2.24). The \approx sign is essential, it means $\langle m; \mathbf{R}(t) | \frac{d}{dt} | n; \mathbf{R}(t) \rangle$ can be neglected for $m \neq n$, a consequence of the adiabatic theorem). So at the end of the cycle, when $\mathbf{R}(T)$ returns to $\mathbf{R}(0)$, we have:

$$\psi(T) \approx e^{-\frac{i}{\hbar} \int_0^T dt E_n(\mathbf{R}(t)) + i\gamma_n(T)} \psi(0),$$

$$\gamma_n(T) \equiv \gamma_n(C) = i \oint_C \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle \cdot d\mathbf{R}$$
(2.26)

A simple argument shows that the integrand here is pure imaginary:

$$\nabla \langle n; \mathbf{R} | n; \mathbf{R} \rangle = 0 = \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle + (\nabla \langle n; \mathbf{R} |) | n; \mathbf{R} \rangle$$
$$= 2 \operatorname{Re} \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle,$$

i.e.
$$\langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle = i \text{ Im } \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle$$
 (2.27)

Then (2.26) becomes:

$$\gamma_n(C) = -\operatorname{Im} \oint_C \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle \cdot d\mathbf{R}$$
 (2.28)

Now, in order to use Stokes theorem in its simplest form, Berry assumes parameter space is three dimensional. Then, with S being any two dimensional surface (within the domain of interest) with boundary C, i.e. $\partial S = C$, we get;

$$\gamma_{n}(C) = -\operatorname{Im} \int \int_{S} d\mathbf{S} \cdot \nabla_{\wedge} \langle n; \mathbf{R} | \nabla | n; \mathbf{R} \rangle$$

$$= -\operatorname{Im} \int \int_{S} d\mathbf{S} \cdot (\nabla \langle n; \mathbf{R} |)_{\wedge} (\nabla | n; \mathbf{R} \rangle)$$

$$= -\operatorname{Im} \int \int_{S} d\mathbf{S} \cdot \sum_{m \neq n} (\nabla \langle n; \mathbf{R} |) | m; \mathbf{R} \rangle_{\wedge} \langle m; \mathbf{R} | \nabla | n; \mathbf{R} \rangle$$
(2.29)

The term m = n doesn't contribute as, by (2.27), each factor in the integrand is purely imaginary. For $m \neq n$:

$$H(\mathbf{R})|n;\mathbf{R}\rangle = E_n(\mathbf{R})|n;\mathbf{R}\rangle$$

$$\implies \langle m;\mathbf{R}| [(\nabla H(\mathbf{R}))|n;\mathbf{R}\rangle + H(\mathbf{R})(\nabla |n,\mathbf{R}\rangle)] = E_n(\mathbf{R})\langle m;\mathbf{R}|\nabla |n;\mathbf{R}\rangle$$

i.e.

$$\langle m; \mathbf{R} | \nabla | n; \mathbf{R} \rangle = \frac{\langle m; \mathbf{R} | \nabla H(\mathbf{R}) | n; \mathbf{R} \rangle}{E_n(\mathbf{R}) - E_m(\mathbf{R})}$$
 (2.30)

Using this in (2.29) gives

$$\gamma_{n}(C) = -\operatorname{Im} \int \int_{S} d\mathbf{S} \cdot \sum_{m \neq n} \frac{\langle n; \mathbf{R} | \nabla H(\mathbf{R}) | m; \mathbf{R} \rangle_{\wedge} \langle m; \mathbf{R} | \nabla H(\mathbf{R}) | n; \mathbf{R} \rangle}{(E_{n}(\mathbf{R}) - E_{m}(\mathbf{R}))^{2}}$$

$$= -\int \int_{S} d\mathbf{S} \cdot \mathbf{V}_{n}(\mathbf{R}),$$

$$\mathbf{V}_{n}(\mathbf{R}) = \operatorname{Im} \left(\nabla \langle n; \mathbf{R} | \rangle \wedge \nabla | n; \mathbf{R} \rangle \right)$$

$$= \operatorname{Im} \sum_{m \neq n} \frac{\langle n; \mathbf{R} | \nabla H(\mathbf{R}) | m; \mathbf{R} \rangle_{\wedge} \langle m; \mathbf{R} | \nabla H(\mathbf{R}) | n; \mathbf{R} \rangle}{(E_{n}(\mathbf{R}) - E_{m}(\mathbf{R}))^{2}}$$
(2.31)

As stated by Berry, in this form we see that $\mathbf{V}_n(\mathbf{R})$ and so $\gamma_n(C)$ are independent of the choice of phases in $|n; \mathbf{R}\rangle$.

Near a two-fold degeneracy: With parameter space 3-dimensional, we can assume the degeneracy is at $\mathbf{R} = \mathbf{0}$. For $\mathbf{R} \neq \mathbf{0}$ we have two eigenstates of $H(\mathbf{R})$ close in energy but nondegenerate. Ignoring all other eigenstates, we reduce to a two dimensional problem. So for \mathbf{R} near $\mathbf{0}$ we set:

$$H(\mathbf{R}) = H(\mathbf{0}) + \mathbf{R} \cdot (\nabla H(\mathbf{R}))_{\mathbf{0}}; \quad H(\mathbf{0}) = 0;$$

$$H(\mathbf{R})|\pm; \mathbf{R}\rangle = E_{\pm}(\mathbf{R})|\pm; \mathbf{R}\rangle;$$

$$E_{+}(\mathbf{0}) = E_{-}(\mathbf{0}) = 0; \quad E_{+}(\mathbf{R}) > E_{-}(\mathbf{R}) \quad \text{for } \mathbf{R} \neq \mathbf{0}$$
(2.32)

Using Pauli matrices we have with no loss of generality in suitable basis and by suitable choice or identification of \mathbf{R} :

$$\nabla H(\mathbf{0}) = \frac{1}{2}\sigma; \quad H(\mathbf{R}) = \frac{1}{2}\mathbf{R} \cdot \sigma; \quad E_{\pm}(\mathbf{R}) = \pm \frac{1}{2}R, \quad R = |\mathbf{R}|;$$

$$|+;\mathbf{R}\rangle\langle+;\mathbf{R}| = \frac{1}{2}(1+\hat{R}\cdot\sigma), \quad |-;\mathbf{R}\rangle\langle-;\mathbf{R}| = \frac{1}{2}(1-\hat{R}\cdot\sigma).$$
 (2.33)

Using all these in Eq. 2.31 we get for , say, $V_{+}(\mathbf{R})$ the expression:

$$\mathbf{V}_{+}(\mathbf{R}) = \operatorname{Im} \left\{ \langle +; \mathbf{R} | \frac{1}{2} \sigma | -; \mathbf{R} \rangle_{\wedge} \langle -; \mathbf{R} | \frac{1}{2} \sigma | +; \mathbf{R} \rangle / R^{2} \right\}$$

$$= \frac{1}{16R^{2}} \operatorname{Im} \operatorname{Tr} \left\{ (1 + \hat{R} \cdot \sigma) \sigma_{\wedge} (1 - \hat{R} \cdot \sigma) \sigma \right\}$$
(2.34)

 $\mathbf{V}_{+}(\mathbf{R})$ has three components in parameter space, like \mathbf{R} . The j^{th} component is

$$V_{+,j}(\mathbf{R}) = \frac{1}{16R^2} \epsilon_{jkl} \text{ Im Tr } \{ (1 + \hat{R} \cdot \sigma)\sigma_k (1 - \hat{R} \cdot \sigma)\sigma_l \}$$

$$= \frac{1}{16R^2} \epsilon_{jkl} \text{ Im Tr } \left[\{ (1 + \hat{R} \cdot \sigma), \sigma_k \}_+ (1 - \hat{R} \cdot \sigma)\sigma_l \} \right] \text{ as } (\hat{R} \cdot \sigma)^2 = 1$$

$$= \frac{1}{16R^2} \epsilon_{jkl} \text{ Im Tr } \left[(2\sigma_k + 2\hat{R}_k)(1 - \hat{R} \cdot \sigma)\sigma_l \} \right]$$

$$= \frac{1}{8R^2} \epsilon_{jkl} \text{ Im Tr } \left[(1 - \hat{R} \cdot \sigma)\sigma_l\sigma_k + \hat{R}_k(1 - \hat{R} \cdot \sigma)\sigma_l \right]$$

$$= -\frac{1}{8R^2} \epsilon_{jkl} \text{ Im Tr } \left(\hat{R} \cdot \sigma \ i \ \epsilon_{lkm}\sigma_m \right) = \frac{1}{4R^2} \text{ Im Tr } (i\hat{R} \cdot \sigma\sigma_j)$$

$$= \hat{R}_j/2R^2,$$
i.e. $\mathbf{V}_+(\mathbf{R}) = \frac{1}{2} \frac{\mathbf{R}}{R^3}$ (2.35)

Berry calls this the "magnetic field" of a "magnetic monopole" of strength -1/2 at the origin in the parameter space; but equally well we can say it is the "Coulomb field" of a point "electric charge" of strength 1/2 at $\mathbf{R} = \mathbf{0}$ in parameter space. In any case the Berry phase for the state $|+; \mathbf{R}\rangle$ for a closed circuit C near $\mathbf{0}$ is from Eq. (2.31):

$$\gamma_{+}(C) = \frac{-1}{2} \iint_{S} d\mathbf{S} \cdot \mathbf{R} / R^{3} = \frac{-1}{2} \Omega[C],$$

$$\Omega[C] = \text{solid angle subtended at } \mathbf{R} = \mathbf{0} \text{ by loop } C.$$
(2.36)

Comment: There seems to be no simple physical way to combine Berry's 'parameter space' approach with the 'direct' method presented first. Because with only time as parameter and no multidimensional \mathbf{R} , there is no room for Stokes' theorem. In the direct method we do not get an expression for φ_{geom}^n with squares of energy differences in the denominator. In more detail, in place of Eq. 2.10, in the spirit of the 'parameter' approach we would have:

$$H(t)|n;t\rangle = E_n(t)|n;t\rangle; \quad \langle n';t|n;t\rangle = \delta_{n'n}$$

 $H(T) = H(0), \quad |n;T\rangle = |n;0\rangle, \quad \text{phase of } |n;t\rangle \text{ free in between.}$ (2.37)

Then by the adiabatic theorem:

$$\psi(0) = |n; 0\rangle \to \psi(t) \simeq e^{\frac{-i}{\hbar} \int_0^t dt' E_n(t') + i\gamma_n(t)} |n; t\rangle, \quad \gamma_n(0) = 0$$
 (2.38)

and the Schrodinger equation (2.1) leads to

$$\dot{\gamma_n}(t)|n;t\rangle \simeq i\frac{d}{dt}|n;t\rangle,$$

$$\dot{\gamma_n}(t) \simeq i\langle n;t|\frac{d}{dt}|n;t\rangle = -\text{Im }\langle n;t|\frac{d}{dt}|n;t\rangle,$$

$$\gamma_n(T) \simeq -\text{Im }\int_0^T dt\langle n;t|\frac{d}{dt}|n;t\rangle$$
(2.39)

in place of Eq (2.28). So this is an adaptation of Berry's **R**-space method, with $|n; \mathbf{R}\rangle$ single valued in the domain of interest, to the earlier direct derivation of φ_{qeom} .

3 The Aharonov Anandan and Samuel Bhandari generalisations, first mathematical interlude

3.1 Aharonov-Anandan generalization

We can list the independent assumptions in the Berry treatment: unitary quantum evolution governed by the Schrodinger equation, adiabatic hypothesis, cyclic condition on the Hamiltonian operator. The first important step in relaxing these assumptions was taken in 1987 by Aharonov and Anandan- the adiabatic condition on H(t) is not necessary to define the geometric phase. For any time dependent Hamiltonian H(t), given any (exact) cyclic solution to Eq (2.1) in the sense

$$i\hbar \frac{d}{dt}\psi(t) = H(t)\psi(t), \quad \psi(T) = e^{i\varphi_{\text{tot}}}\psi(0)$$
 (3.1)

a geometric phase can be reconstructed:

$$\varphi_{\text{geom}} = \varphi_{\text{tot}} - \varphi_{\text{dyn}}, \quad \varphi_{\text{dyn}} = \frac{-1}{\hbar} \int_0^T dt \ (\psi(t), H(t)\psi(t)).$$
(3.2)

Of course, in the adiabatic cyclic case, this reduces to Berry's result Eq. (2.19). Moreover they showed that this phase depends only on the ray space projection or image of the curve traced by $\psi(t)$ in the Hilbert space. Thus, the focus on the role of ray space was achieved. The parameter space used by Berry was also seen to be inessential. Of course Berry too had pointed out that his final formula Eq. (2.31) for geometric phases is unaffected by phase changes in the eigen vectors $|n; \mathbf{R}\rangle$ of $H(\mathbf{R})$. Here are the details. We are given $\psi(t)$ obeying

$$i\hbar \frac{d\psi(t)}{dt} = H(t)\psi(t), \quad \psi(T) = e^{i\Phi}\psi(0)$$
 (3.3)

If we make a phase transformation we get a new $\psi'(t)$ and a new H'(t) and Φ' :

$$\psi'(t) = e^{i\alpha(t)}\psi(t), \text{ any } \alpha \Rightarrow$$

$$H'(t) = H(t) - \hbar \dot{\alpha}(t), \quad \Phi' = \Phi + \alpha(T) - \alpha(0)$$
(3.4)

Taking expectation values, we have:

$$\hbar \dot{\alpha}(t) = (\psi(t), H(t)\psi(t)) - (\psi'(t), H'(t)\psi'(t)),$$

$$\alpha(T) - \alpha(0) = \frac{1}{\hbar} \int_0^T dt \{(\psi(t), H(t)\psi(t)) - (\psi'(t), H'(t)\psi'(t))\},$$
ie.
$$\Phi' + \frac{1}{\hbar} \int_0^T dt (\psi'(t), H'(t)\psi'(t)) = \Phi + \frac{1}{\hbar} \int_0^T dt (\psi(t), H(t)\psi(t))$$

$$= \text{ray space quantity} = \varphi_{\text{geom}},$$
(3.5)

so

$$\psi(T) = \exp\left\{i(\varphi_{\text{geom}} - \frac{1}{\hbar} \int_0^T dt(\psi(t), H(t)\psi(t))\right\} \psi(0)$$
(3.6)

We can identify the dynamical phase:

$$\Phi = \varphi_{tot} = \varphi_{geom} + \varphi_{dyn}, \varphi_{dyn} = -\frac{1}{\hbar} \int_0^T dt(\psi(t), H(t)\psi(t)). \tag{3.7}$$

Two interesting choices of $\alpha(t)$ can be exhibited:

$$\begin{array}{lll} \operatorname{General} \psi(t) & \operatorname{Choice} \ (1) & \operatorname{Choice} \ (2) \\ \psi(T) = e^{i\Phi} \psi(0), & \alpha(T) - \alpha(0) = \varphi_{\mathrm{tot}}, & \dot{\alpha}(t) = \frac{1}{\hbar} (\psi(t), H(t) \psi(t)), \\ \varphi_{\mathrm{dyn}} = -\frac{1}{\hbar} \int_0^T dt (\psi(t), H(t) \psi(t)), & \varphi'_{\mathrm{tot}} = 0, & \varphi'_{\mathrm{dyn}} = 0, \\ \varphi_{\mathrm{geom}} = \varphi_{\mathrm{tot}} - \varphi_{\mathrm{dyn}}, & \varphi_{\mathrm{geom}} = -\varphi'_{\mathrm{dyn}} & \varphi_{\mathrm{geom}} = \varphi'_{\mathrm{tot}}. \end{array}$$

3.2 First mathematical interlude

Before going on to the second important generalisation, we assemble some notations and definitions relating to QM for later use. For some given QM system, let \mathcal{H} be the Hilbert space to describe pure states, with complex dimension N which could be infinite. Vectors in \mathcal{H} are ψ, ϕ, \ldots and inner product (.,.) or $\langle .|. \rangle$. The unit sphere \mathcal{B} is

$$\mathcal{B} = \{ \psi \in \mathcal{H} | (\psi, \psi) = 1 \} \subset \mathcal{H}$$
(3.8)

This has real dimension 2N-1, it is a subset and not a subspace of \mathcal{H} . The group U(1) acts on \mathcal{B} (and also on \mathcal{H}):

$$\psi \in \mathcal{B} \implies \psi' = e^{i\alpha}\psi \in \mathcal{B}, \quad 0 < \alpha < 2\pi$$
 (3.9)

Ray space \mathcal{R} is the quotient of \mathcal{B} with respect to this action, obtained by regarding two vectors ψ , ψ' as related above as "equivalent"; in terms of density matrices or projection operators we have

$$\mathcal{R} = \{ \rho(\psi) = |\psi\rangle\langle\psi| \quad or \quad \psi\psi^{\dagger} \quad | \quad \psi \in \mathcal{B} \}$$
 (3.10)

 \mathcal{R} is also not a linear vector space, it is of real dimension 2(N-1) as a manifold, it is CP^{N-1} so it has complex dimension N-1; it is not a subset of \mathcal{H} or \mathcal{B} . What we have is a projection map $\pi: \mathcal{B} \to \mathcal{R}$:

$$\pi: \mathcal{B} \to \mathcal{R}: \quad \psi \in \mathcal{B} \to \ \rho(\psi) = \psi \psi^{\dagger} \in \mathcal{R}$$
 (3.11)

Pictorially this is represented in Fig:(2)

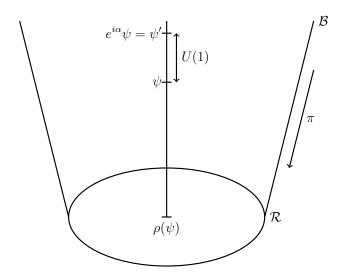


Figure 2:

The one dimensional U(1) 'fibre' sitting "on top of" $\rho(\psi) \in \mathcal{R}$ is an entire equivalence class of vectors related by phases to one another, all projecting down to one point in \mathcal{R} :

$$\rho(\psi) \in \mathcal{R} \to \pi^{-1}(\rho(\psi)) = \{ \psi' = e^{i\alpha} \psi \in \mathcal{B} \mid \psi \text{ fixed, } 0 \le \alpha < 2\pi \} \subset \mathcal{B}$$
 (3.12)

Let us denote by \mathcal{C} a 'sufficiently smooth' curve of unit vectors in \mathcal{B} :

$$C = \{ \psi(s) \in \mathcal{B} \mid s_1 \le s \le s_2 \} \subset \mathcal{B}$$
(3.13)

parametrized by a real variable s. Applying π to the points of \mathcal{C} we get its "image", a curve $C \subset \mathcal{R}$:

$$C = \pi[\mathcal{C}] = \{ \rho(\psi(s)) = \psi(s)\psi^{\dagger}(s) \in \mathcal{R} \mid s_1 \le s \le s_2 \} \subset \mathcal{R}$$
(3.14)

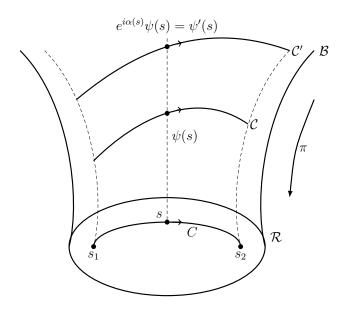


Figure 3:

Every parametrised $\mathcal{C} \subset \mathcal{B}$ projecting onto the same $C \subset \mathcal{R}$ is called a 'lift' of C from \mathcal{R} to \mathcal{B} . Any other lift \mathcal{C}' is related to \mathcal{C} by a smooth pointwise phase change, a 'gauge transformation':

$$\mathcal{C}' = \{ \psi'(s) = e^{i\alpha(s)}\psi(s) \mid \psi(s) \in \mathcal{C}, s_1 \le s \le s_2 \} \subset \mathcal{B}, \quad \pi[\mathcal{C}'] = \pi[\mathcal{C}] = C$$

$$(3.15)$$

Given $\mathcal{C} = {\psi(s)} \subset \mathcal{B}$, the tangent vector to \mathcal{C} at each point is

$$u(s) = \frac{d\psi(s)}{ds} = \dot{\psi}(s) \tag{3.16}$$

From $\psi(s)$ being normalised we get

$$(\psi(s), \psi(s)) = 1 \implies Re(\psi(s), u(s)) = 0, \quad i.e. \quad (\psi(s), u(s)) = i \text{ Im } (\psi(s), u(s))$$

$$(3.17)$$

Under the phase or gauge transformation Eq. (3.15) we find:

$$u'(s) = e^{i\alpha(s)}(u(s) + i\dot{\alpha}(s)\psi(s))$$
(3.18)

which is a linear inhomogeneous transformation law. Then the projection of u(s) orthogonal to $\psi(s)$ has a simpler behaviour:

$$u_{\perp}(s) = u(s) - \psi(s)(\psi(s), u(s)) :$$

$$u'_{\perp}(s) = u'(s) - \psi'(s)(\psi'(s), u'(s)) = e^{i\alpha(s)}u_{\perp}(s)$$
(3.19)

which is linear homogeneous. We then define the length of C gauge invariantly as

$$L[C] = \int_{s_1}^{s_2} ds \ (u_{\perp}(s), u_{\perp}(s))^{1/2}$$

$$= \int_{s_1}^{s_2} ds \ \{(\dot{\psi}(s), \dot{\psi}(s)) - (\psi(s), \dot{\psi}(s))(\dot{\psi}(s), \psi(s))\}^{1/2}$$
(3.20)

This is a ray space quantity, to compute it we can use any lift C, C'... of C from R to B. It is both reparametrisation invariant- therefore geometrical- and gauge invariant- therefore belongs to ray space.

Geodesics in \mathcal{R} are curves C for which L[C] is stationary. Here are the results of detailed analysis:

- 1. Given any two "non orthogonal" points $\rho_1 = \rho(\psi_1)$, $\rho_2 = \rho(\psi_2)$ in \mathcal{R} , $\text{Tr}(\rho_1\rho_2) = |(\psi_1, \psi_2)|^2 \neq 0$, there is a unique shortest geodesic C_0 connecting them.
- 2. Without loss of generality, choose $\psi_1 \in \pi^{-1}(\rho_1), \psi_2 \in \pi^{-1}(\rho_2)$, so that

$$(\psi_1, \psi_2) = \cos \theta, \quad 0 < \theta < \pi/2 \tag{a}$$

3. Then, with s chosen to be arc length (affine choice of parameter), a lift of this geodesic C_0 is C_0 defined by and characterised by:

$$C_{0} = \{\psi_{0}(s) = \psi_{1}\cos s + (\psi_{2} - \psi_{1}\cos\theta)\frac{\sin s}{\sin\theta} | 0 \leq s \leq \theta\} \subset \mathcal{B},$$

$$\dot{\psi}_{0}(s) = u_{0}(s) = -\psi_{1}\sin s + (\psi_{2} - \psi_{1}\cos\theta)\frac{\cos s}{\sin\theta},$$

$$(u_{0}(s), u_{0}(s)) = 1, \quad (\psi_{0}(s), u_{0}(s)) = 0, \quad u_{\perp}(s) = u_{0}(s), \quad \pi[C_{0}] = C_{0};$$

$$L[\pi[C_{0}]] = \theta \qquad (b)$$

4. The most general lift of C_0 is any $\mathcal{C} \subset B$ obtained from \mathcal{C}_0 by a smooth phase transformation:

$$C = \{ \psi(s) = e^{i\alpha(s)} \psi_0(s) \mid 0 \le s \le \theta \}$$
 (c) (3.21)

All such lifts of geodesics in \mathcal{R} will be called geodesics in \mathcal{B} .

A last item in this interlude: we define the one-form on $\mathcal B$ important for calculation of geometric phases:

$$A = -i\psi^{\dagger}d\psi = \text{one-form on } \mathcal{B}$$
 (3.22)

Then along any smooth $\mathcal{C} \subset \mathcal{B}$, recalling Eq (3.17):

$$-i \int_{s_1}^{s_2} ds \ (\psi(s), \frac{d\psi(s)}{ds}) = \text{Im} \ \int_{s_1}^{s_2} ds (\psi(s), u(s)) \equiv \int_{\mathcal{C}} A$$
 (3.23)

The $\mathcal{H} - \mathcal{B} - \mathcal{R}$ framework, and the concept of geodesics in \mathcal{R} (and \mathcal{B}) are both important. The latter will lead us later to a Riemannian metric, the Fubini- Study metric or F-S metric on \mathcal{R} . The simplest examples are:

- 1. dim $\mathcal{H}=2$; $\mathcal{B}\simeq S^3$; $\mathcal{R}\simeq S^2=$ Poincaré sphere, geodesics are great circle arcs of length $<\pi$. $\mathcal{R}=CP^1$ here.
- 2. dim $\mathcal{H}=3$; $\mathcal{B}\simeq S^5$; $\mathcal{R}\simeq CP^2$; more difficult to picture. \mathcal{R} is of real dimension 4, has been studied by Simon et. al. and initially by some of us.

3.3 Samuel-Bhandari generalisation

In this step it was shown that the geometric phase can be defined even without the cyclic condition on the state vector, (and of course without the adiabatic condition either). The key result involved is a property of (lifts of) geodesics in \mathcal{R} . As we have just seen, given non orthogonal points ρ_1, ρ_2 in \mathcal{R} , a "preferred" lift of the geodesic C_0 from ρ_1 to ρ_2 is C_0 given in Eq. (3.16b), while a general lift is \mathcal{C} in Eq. (3.16c). Then using Eq. (3.16 b,c), (3.23) and also (3.18) we find \mathcal{C} = general lift of geodesic in \mathcal{R} :

$$\int_{\mathcal{C}} A = \operatorname{Im} \int_{0}^{\theta} ds \ (\psi(s), u(s)) = \operatorname{Im} \int_{0}^{\theta} ds \ (\psi_{0}, u_{0}(s) + i\dot{\alpha}(s)\psi_{0}(s)) = \alpha(\theta) - \alpha(0),$$
i.e. $\operatorname{arg} \ (\psi(0), \psi(\theta)) = \int_{\mathcal{C}} A$
(3.24)

So this is a property of geodesics in \mathcal{B} , derived by them. Using it, the geometric phase of any noncyclic evolution is defined as follows. Let $\psi(t)$, $0 \le t \le T$ be any solution of the Schrodinger equation Eq. (2.1), for any stretch of time. Then we adjoin any geodesic (in the generic case) in \mathcal{B} to take us back from $\psi(T)$ to $\psi(0)$, and combining the two curves we obtain a closed loop \mathcal{C}' , say:

$$\mathcal{C}' = (\text{Schrodinger evolution from } \psi(0) \text{ to } \psi(T)) \cup (\text{any geodesic from } \psi(T) \text{ to } \psi(0))$$
 (3.25)

and define

$$\varphi_{\text{geom}}[\text{noncyclic Schrodinger evolution}] = \oint_{\mathcal{C}'} A$$
 (3.26)

To understand the details of the argument it is good to see their paper, and appreciate the role of the property Eq. (3.24) of geodesics. (Incidentally, Samuel and Bhandari do not use the unit sphere $\mathcal{B} \subset \mathcal{H}$ as done here, but work with generally unnormalized but nonzero vectors in \mathcal{H}). In this treatment then, geodesics play the role of converting a generic noncyclic evolution into a related cyclic one.

4 The kinematic approach and the Bargmann Invariants

The third step in the continuing generalisation of the Berry framework is due to RS and me in 1993. The key point was to construct invariant expressions with respect to two groups of continuous transformations on parametrised curves in Hilbert space - local phase changes and reparametrisations. The Bargmann invariants (BI) were then brought into the discussion in an important manner, and their connection to GP's was systematically explored. This latter connection was mentioned by Samuel and Bhandari in a preliminary way.

We have set up the $\mathcal{H} - \mathcal{B} - \mathcal{R}$ framework in Section 3. Parametrised curves $\mathcal{C} \subset \mathcal{B}$, the action of local phase changes on them, and their images $C = \pi[\mathcal{C}] \subset \mathcal{R}$, have been introduced in (3.8, 3.9, 3.10). In addition to the phase change $\mathcal{C} \to \mathcal{C}'$ in (3.10), we now introduce reparametrisation transformations.

A smooth monotonic reparametrisation of C in (3.13) acts in this way:

$$C \to C' = \{ \psi'(s') = \psi(s) \mid s' = f(s), \frac{df(s)}{ds} \ge 0 \}$$

$$(4.1)$$

This then leads to a reparametrisation of the image $C = \pi[\mathcal{C}]$, giving $C' = \pi[\mathcal{C}']$. Therefore the traces of \mathcal{C} and \mathcal{C} , as sets of points in \mathcal{B} and \mathcal{R} , are maintained.

An elementary calculation now shows that the simplest functional of C invariant under both groups of transformations is essentially the geometric phase defined as

$$\varphi_{\text{geom}}[C] = \varphi_{\text{tot}}[C] - \varphi_{\text{dyn}}[C] ,$$

$$\varphi_{\text{tot}}[C] = \arg(\psi(s_1), \psi(s_2)) ,$$

$$\varphi_{\text{dyn}}[C] = \operatorname{Im} \int_{s_1}^{s_2} ds \left(\psi(s), \frac{d\psi(s)}{ds}\right)$$

$$= -i \int_{s_1}^{s_2} ds \left(\psi(s), \frac{d\psi(s)}{ds}\right) = \int_{\mathcal{C}} A$$
(4.2)

(It is assumed that $\psi(s_1)$ and $\psi(s_2)$ are not orthogonal). The points to note are: this phase is immediately defined for any open curve $C \subset \mathcal{R}$ as the difference of two terms, any lift \mathcal{C} of C being used to compute them; the construction is purely kinematic, not using any Hamiltonian or Schrodinger equation. The invariances under phase changes and under reparametrisations lead respectively to $\varphi_{\text{geom}}[C]$ being a ray space quantity, and a geometric object. From this definition, the earlier results are all recovered as special cases.

Using eq. (3.16) it is an immediate consequence that

$$\varphi_{\text{geom}}[\text{any geodesic in } \mathcal{R}] = 0$$
 (4.3)

Based on equations (3.21a,b,c):

$$\mathcal{C} = \left\{ \psi(s) = e^{i\alpha(s)} \psi_0(s) | 0 \le s \le \theta \right\};
\varphi_{\text{tot}}[\mathcal{C}] = \arg(\psi(0), \psi(\theta)) = \alpha(\theta) - \alpha(0) :
\varphi_{\text{dyn}}[\mathcal{C}] = \operatorname{Im} \int_0^\theta ds \left(e^{i\alpha(s)} \psi_0(s), \frac{d}{ds} e^{i\alpha(s)} \psi_0(s) \right) = \alpha(\theta) - \alpha(0),
\therefore \varphi_{\text{geom}}[\pi[\mathcal{C}]] = 0.$$
(4.4)

The content of this is essentially the same as in (3.24) but the status is very different. In the work of Samuel and Bhandari, (3.24) was used to set up the definition of the GP for a non-cyclic evolution. Here that is done kinematically in (4.2), and the property (4.3) of geodesics is derived as a consequence.

4.1 The Bargmann Invariants

These were introduced by V. Bargmann in 1964 while giving a new proof of Wigner's 1931 theorem on representation of symmetry operations in QM. The theorem is this: A symmetry operation is a one-to-one onto map of the set of pure physical states onto itself, preserving transition probabilities. Any such operation results from a unitary or an antiunitary transformation acting on the Hilbert space vectors. The simplest non-trivial BI is of order three. For any three mutually non-orthogonal vectors $\psi_j \in \mathcal{B}, j = 1, 2, 3$, it is defined as

$$\Delta_3(\psi_1, \psi_2, \psi_3) = (\psi_1, \psi_2)(\psi_2, \psi_3)(\psi_3, \psi_1) = Tr(\rho(\psi_1)\rho(\psi_2)\rho(\psi_3)) \tag{4.5}$$

Clearly this is a ray space quantity, and for dim $\mathcal{H} \geq 2$, it is in general complex. Now connect $\rho(\psi_1)$ to $\rho(\psi_2)$, $\rho(\psi_2)$ to $\rho(\psi_3)$ and $\rho(\psi_3)$ to $\rho(\psi_1)$ by geodesics C_{12} , C_{23} , C_{31} ; let C_{12} , C_{23} , C_{31} be any lifts of them connecting ψ_1 to ψ_2 , ψ_2 to ψ_3 , ψ_3 to ψ_1 . Then $C_{12} \cup C_{23} \cup C_{31}$ and $C_{12} \cup C_{23} \cup C_{31}$ are closed loops in \mathcal{B} and \mathcal{R} respectively. Repeated use of the property (4.3) of geodesics then shows:

$$\arg \Delta_{3}(\psi_{1}, \psi_{2}, \psi_{3}) = \arg(\psi_{1}, \psi_{2}) + \arg(\psi_{2}, \psi_{3}) + \arg(\psi_{3}, \psi_{1})$$

$$= \varphi_{\text{dyn}}[\mathcal{C}_{12}] + \varphi_{\text{dyn}}[\mathcal{C}_{23}] + \varphi_{\text{dyn}}[\mathcal{C}_{31}]$$

$$= \varphi_{\text{dyn}}[\mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31}] = -\varphi_{\text{geom}}[\mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31}]$$
(4.6)

Thus the phase of a third order BI is the negative of the geometric phase of a triangle in \mathcal{R} with geodesic sides. Generalisation to order n is immediate: $\psi_i \in \mathcal{B}, j = 1, 2, \ldots, n, (\psi_i, \psi_{i+1}) \neq 0$:

$$\Delta_n(\psi_1, \psi_2, \dots, \psi_n) = (\psi_1, \psi_2)(\psi_2, \psi_3) \dots (\psi_{n-1}, \psi_n)(\psi_n, \psi_1),$$
arg $\Delta_n(\psi_1, \psi_2, \dots, \psi_n) = -\varphi_{\text{geom}}[C = n\text{-sided polygon with vertices}$

$$\rho(\psi_1), \rho(\psi_2), \dots, \rho(\psi_n) \text{ connected by successive geodesics}]$$
(4.7)

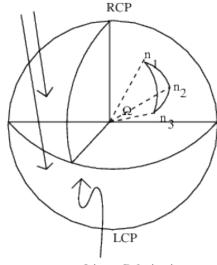
4.2 Some examples

a) We begin with examples in 2-dimensional Hilbert space. We have already seen Berry's analysis of GP's for adiabatic evolutions near a two-fold degeneracy, leading to a 'magnetic monopole' structure in a 3-dimensional parameter space. A much older example in the non-adiabatic case is the work of Pancharatnam in classical polarization optics in 1956. It is in a sense purely a kinematic analysis.

We have plane electromagnetic waves with fixed propagation direction along the positive zaxis, in various pure polarization states. Each wave is determined by its transverse two-component
complex electric vector in the x-y plane:

$$\mathbf{E} = \begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \in \mathbb{C}^2, \quad \text{Intensity } I \simeq \mathbf{E}^{\dagger} \mathbf{E} \; ;$$
 Polarization state $\sim \hat{n} = \frac{1}{I} \mathbf{E}^{\dagger} \tau \mathbf{E} \in \mathbb{S}^2$, the Poincarè sphere (4.8)

Elliptic Polarizations



Linear Polarizations

Figure 4: S^2 for Pancharatnam phase

We are here in the $\mathcal{H} - \mathcal{B} - \mathcal{R}$ framework with dim $\mathcal{H} = 2$, $\mathcal{B} \sim \mathbb{S}^3$, $\mathcal{R} \sim \mathbb{S}^2$. The Pauli matrices $\boldsymbol{\tau}$ used in classical polarization optics follow a different convention than in QM:

$$\tau_1 = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tau_2 = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_3 = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$(4.9)$$

To display an example of Eq (4.6) we choose three electric field vectors $\mathbf{E}^{(1)}, \mathbf{E}^{(2)}, \mathbf{E}^{(3)}$ and consider the corresponding BI

$$\Delta_3(\mathbf{E}^{(1)}, \mathbf{E}^{(2)}, \mathbf{E}^{(3)}) = \frac{1}{I_1 I_2 I_3} \mathbf{E}^{(1)\dagger} \mathbf{E}^{(2)} \mathbf{E}^{(2)\dagger} \mathbf{E}^{(3)\dagger} \mathbf{E}^{(3)\dagger} \mathbf{E}^{(1)}$$
(4.10)

Keeping $\mathbf{E}^{(1)}$ fixed, suppose we adjust the 'overall phase' of $\mathbf{E}^{(2)}$ to make the first factor real positive. Then by the Pancharatnam convention or definition, $\mathbf{E}^{(1)}$ and $\mathbf{E}^{(2)}$ are 'in phase': superposing them leads to maximum constructive interference. Next we can similarly adjust the overall phase of $\mathbf{E}^{(3)}$ to make the second factor also real positive, so $\mathbf{E}^{(2)}$ and $\mathbf{E}^{(3)}$ are 'in phase'. But then we have no more phase freedoms left, the third factor is in general complex and $\mathbf{E}^{(3)}$ and $\mathbf{E}^{(1)}$ are 'out of phase'. Their 'relative phase', a measure of the non-transitivity of the 'in phase' concept, is given by Eq. (4.6) to be:

$$\arg \mathbf{E}^{(3)\dagger} \mathbf{E}^{(1)} = \arg \Delta_3(\mathbf{E}^{(1)}, \mathbf{E}^{(2)}, \mathbf{E}^{(3)}) = -\varphi_{\text{geom}}[C = C_{12} \cup C_{23} \cup C_{31}],$$

$$C_{12} = \text{great circle on } \mathbb{S}^2 \text{ from } \hat{n_1} \text{ to } \hat{n_2} \text{ etc.} ,$$

$$= -\frac{1}{2}\Omega[C]$$

$$(4.11)$$

with $\Omega[C]$ being the solid angle subtended at the centre of \mathbb{S}^2 by the geodesic triangle C. Establishing this is an easy exercise in spherical trigonometry.

b) Next we consider three-level systems in QM. The passage from a two-dimensional Hilbert space and the Poincarè sphere \mathbb{S}^2 to a three-dimensional Hilbert space and its ray space involves interesting algebraic as well as geometric features, and new group theoretical aspects as well. We summarise the main facts, the derivations being quite straightforward.

Let $\mathcal{H}^{(3)}$ be a three-dimensional Hilbert space with vectors ψ, ϕ, \ldots written as three-component complex column vectors. The unitary group acting on $\mathcal{H}^{(3)}$ is the nine-dimensional U(3); removing

an overall phase we have the eight parameter unitary unimodular group SU(3):

$$SU(3) = \{ A = 3 \times 3 \text{ complex matrix } | A^{\dagger} A = \mathbb{I}_{3 \times 3}, \det A = 1 \}$$

$$\tag{4.12}$$

This replaces SU(2) familiar from the study of spin- $\frac{1}{2}$ systems in QM. For the Hermitian generators in the defining representation (4.11), we go from the Pauli σ_j 's to the Gell-Mann λ_r 's:

$$\lambda_{1} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{2} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{4} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$\lambda_{5} = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \lambda_{6} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_{7} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \lambda_{8} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \tag{4.13}$$

These are eight independent Hermitian traceless matrices. Their commutators, anti-commutators and products bring in two different three-index symbols or invariant tensors:

$$\begin{split} [\lambda_r, \lambda_s] &= 2i \, f_{rst} \, \lambda_t, \\ f_{123} &= 1 \,, \, f_{458} = f_{678} = \frac{\sqrt{3}}{2} \,, \, f_{147} = f_{246} = f_{257} = f_{345} = f_{516} = f_{637} = \frac{1}{2}; \\ \{\lambda_r, \lambda_s\} &= \frac{4}{3} \, \delta_{rs} \, + \, 2 \, d_{rst} \, \lambda_t, \\ d_{118} &= d_{228} = d_{338} = -d_{888} = \frac{1}{\sqrt{3}} \,, \, d_{448} = d_{558} = d_{668} = d_{778} = -\frac{1}{2\sqrt{3}}, \\ d_{146} &= d_{157} = -d_{247} = d_{256} = d_{344} = d_{355} = -d_{366} = -d_{377} = \frac{1}{2}; \\ \lambda_r \lambda_s &= \frac{2}{3} \, \delta_{rs} \, + \, i \, f_{rst} \, \lambda_t \, + \, d_{rst} \, \lambda_t, \, Tr \lambda_r \lambda_s = 2 \, \delta_{rs} \end{split} \tag{4.14}$$

Only the independent components of the completely anti-symmetric f's and the completely symmetric d's have been listed.

The two-to-one homomorphism $SU(2) \to SO(3)$ is well-known. With SU(3) the situation is more intricate. We have a particular real eight-dimensional adjoint or octet representation of SU(3) given by certain 8×8 real orthogonal unimodular matrices, which is irreducible. All real orthogonal unimodular 8×8 matrices taken together form the 28 dimensional group SO(8); the matrices of the octet representation of SU(3) are a 'very small' eight-dimensional subset of SO(8), in fact a subgroup:

$$A \in SU(3) \to D_{rs}(A) = \frac{1}{2} Tr(\lambda_r A \lambda_s A^{\dagger}), D(A) \in SO(8);$$

$$D(A')D(A) = D(A'A)$$
(4.15)

Given any two (real) 'octet vectors' $\mathbf{a}, \mathbf{b} \in \mathbb{R}^8$, we can form one scalar and two octet vectors from them:

$$\mathbf{a} \cdot \mathbf{b} = a_r b_r;$$

$$(\mathbf{a} \wedge \mathbf{b})_r = -(\mathbf{b} \wedge \mathbf{a})_r = f_{rst} \, a_s \, b_t;$$

$$(\mathbf{a} * \mathbf{b})_r = (\mathbf{b} * \mathbf{a})_r = \sqrt{3} \, d_{rst} \, a_s \, b_t;$$

$$D(A)\mathbf{a} \wedge D(A)\mathbf{b} = D(A)(\mathbf{a} \wedge \mathbf{b}),$$

$$D(A)\mathbf{a} * D(A)\mathbf{b} = D(A)(\mathbf{a} * \mathbf{b})$$

$$(4.16)$$

Now to the generalisation of the Poincarè sphere \mathbb{S}^2 . For any unit vector $\psi \in \mathcal{H}^{(3)}$, we expand the density matrix in terms of the λ 's as:

$$\rho = \psi \psi^{\dagger} = \frac{1}{3} \left(\mathbb{I} + \sqrt{3} \, \mathbf{n} \cdot \lambda \right), \ n_r = n_r^* = \frac{\sqrt{3}}{2} \, Tr(\rho \lambda_r);$$

$$\mathbf{n} \cdot \mathbf{n} = 1, \qquad \mathbf{n} * \mathbf{n} = \mathbf{n}$$
(4.17)

Thus $\mathbf{n} \in \mathbb{S}^7$, a real unit vector in \mathbb{R}^8 , obeying further conditions so that only 4 of the n_r are algebraically independent. The ray space for pure states of a three-level system is then:

$$\mathcal{R} = CP^2 = \{ \mathbf{n} \in \mathbb{S}^7 | \mathbf{n} * \mathbf{n} = \mathbf{n} \} = \mathcal{O} \subset \mathbb{S}^7 \subset \mathbb{R}^8$$
(4.18)

The geometric object \mathcal{O} , which replaces the Poincarè sphere \mathbb{S}^2 , is a connected simply connected 4-dimensional region embedded within \mathbb{S}^7 ; in fact it is the coset space SU(3)/U(2), just as $\mathbb{S}^2 = SU(2)/U(1)$. It is somewhat difficult to picture the 'shape' of \mathcal{O} , one must get used to its unusual features. For instance,

$$\mathbf{n} \in \mathcal{O} \implies -\mathbf{n} \notin \mathcal{O},$$
 (4.19)

so the idea of antipodal points fails here. Actually if $\psi, \psi' \in \mathcal{H}$ are mutually orthogonal, their representative points $\mathbf{n}, \mathbf{n}' \in \mathcal{O}$ make an angle of $\frac{2\pi}{3}$ radians:

$$1 \ge Tr(\rho \rho') = \frac{1}{3} (1 + 2\mathbf{n} \cdot \mathbf{n}') \ge 0 \iff -\frac{1}{2} \le \mathbf{n} \cdot \mathbf{n}' \le 1;$$
$$\psi'^{\dagger} \psi = 0 \iff \cos^{-1}(\mathbf{n} \cdot \mathbf{n}') = \frac{2\pi}{3}$$
(4.20)

Ray space geodesics for a general QM system are described in (3.21). It turns out that for two-level systems with $\mathcal{R} = \mathbb{S}^2$, these geodesics are great circle arcs on \mathbb{S}^2 , which are geodesics in the sense of three-dimensional Euclidean geometric notions inherited by \mathbb{S}^2 . However, for the three-level case, ray space geodesics are quite different from 'Euclidean' geodesics in $\mathbb{S}^7 \subset \mathbb{R}^8$.

Using SU(3) 'covariance', with no loss of generality we can choose the two non-orthogonal points $\rho_1, \rho_2 \in \mathcal{O}$ to be the images of $\psi_1, \psi_2 \in \mathcal{B}^5$, the unit sphere in $\mathcal{H}^{(3)}$, given by

$$\psi_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \psi_2 = \begin{pmatrix} 0 \\ \sin \theta \\ \cos \theta \end{pmatrix}, \ 0 < \theta < \pi/2. \tag{4.21}$$

Then $\mathbf{n}^{(1)}, \mathbf{n}^{(2)} \in \mathcal{O}$ are

$$\mathbf{n}^{(1)} = (0, 0, 0, 0, 0, 0, 0, 0, -1),$$

$$\mathbf{n}^{(2)} = \frac{\sqrt{3}}{2} (0, 0, -\sin^2 \theta, 0, 0, 2 \sin \theta \cos \theta, 0, \frac{1}{\sqrt{3}} (1 - 3\cos^2 \theta))$$
(4.22)

By (3.21), the ray space geodesic C_0 from ρ_1 to ρ_2 is the image of the following curve in $\mathcal{B}^{(5)}$:

$$\psi(s) = \begin{pmatrix} 0 \\ \sin s \\ \cos s \end{pmatrix}, \ 0 \le s \le \theta;
C_0 : \mathbf{n}(s) = \frac{\sqrt{3}}{2} \psi^{\dagger}(s) \lambda \psi(s)
= \frac{\sqrt{3}}{2} (0, 0, -\sin^2 s, 0, 0, 2 \sin s \cos s, 0, \frac{1}{\sqrt{3}} (1 - 3\cos^2 s)) \qquad 0 \le s \le \theta$$
(4.23)

As only $n_3(s), n_6(s), n_8(s)$ are non-zero, this curve $C_0 \in \mathcal{O}$ lies within a three-dimensional subspace of \mathbb{R}^8 . In fact it lies within the intersection of \mathcal{O} with the 3-6-8 subspace of \mathbb{R}^8 . It is also a plane curve since

$$n_8(s) + \sqrt{3}n_3(s) = -1 \tag{4.24}$$

which defines a two-dimensional plane in the 3-6-8 subspace. However this is 'off-centre',i.e., the origin of \mathbb{R}^8 is not in this plane. Therefore the geodesic C_0 is not part of the intersection of \mathbb{S}^7 with any two-dimensional plane in \mathbb{R}^8 containing the origin.

This shows that ray space geodesics are not geodesic arcs in the sense of Euclidean geometry in eight dimensions as inherited by \mathbb{S}^7 . They are more like arcs of constant latitude on \mathbb{S}^2 .

Any ray space geodesic in \mathcal{O} is obtained from the above by the action of D(A) for some $A \in SU(3)$. Thus it lies within some three-dimensional subspace of \mathbb{R}^8 , is a plane curve, but is off-center.

Even though it has limitations, a local description of \mathcal{O} is useful for practical calculations. A vector $\psi \in \mathcal{B}^{(5)}$ has components ψ_1, ψ_2, ψ_3 . We introduce four independent local angle type coordinates for the portion of \mathcal{O} corresponding to $\psi_3 \neq 0$:

$$(\psi_1, \psi_2, \psi_3) = (\text{overall phase}) \left(e^{i\chi_1} \sin \theta \cos \phi, e^{i\chi_2} \sin \theta \sin \phi, \cos \theta \right), \tag{4.25}$$

where

$$0 \le \theta < \pi/2$$
 $0 \le \phi \le \pi/2$ $0 \le \chi_1, \chi_2 < 2\pi$.

The limits on θ and ϕ ensure $\psi_3 \neq 0$ as well as

$$(|\psi_1|, |\psi_2|, |\psi_3|) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{4.26}$$

which means that this is a point in the first octant of an \mathbb{S}^2 . Then $\theta, \phi, \chi_1, \chi_2$ are coordinates for this portion of \mathcal{O} .

Next we indicate the generalization of the Pancharatnam formula (4.10) for the geometric phase for a triangle in \mathcal{O} whose vertices are nonorthogonal and sides are (ray space) geodesics. (Incidentally, it can be shown that Schrodinger evolution along any geodesic in \mathcal{O} can be generated by a constant Hamiltonian with vanishing dynamical phase.) Using actions by successive SU(3) elements, it turns out that the vertices of such a triangle in \mathcal{O} can be taken to the following configurations:

$$\rho_{1} = \psi_{1}\psi_{1}^{\dagger}, \quad \psi_{1} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix};$$

$$\rho_{2} = \psi_{2}\psi_{2}^{\dagger}, \quad \psi_{2} = \begin{pmatrix} 0 \\ \sin \xi \\ \cos \xi \end{pmatrix}, 0 < \xi < \pi/2;$$

$$\rho_{3} = \psi_{3}\psi_{3}^{\dagger}, \quad \psi_{3} = \begin{pmatrix} \sin \eta \cos \zeta \\ e^{i\chi_{2}} \sin \eta \sin \zeta \\ \cos \eta \end{pmatrix}, 0 < \eta < \pi/2, \quad 0 \le \zeta \le \pi/2, \quad 0 \le \chi_{2} < 2\pi. \tag{4.27}$$

All three points ρ_1 , ρ_2 , ρ_3 lie in the portion of \mathcal{O} covered by the local coordinates (4.24). We see that up to an overall SU(3) transformation, the most general geodesic triangle in \mathcal{O} (with nonorthogonal vertices) involves four intrinsic angle parameters ξ , η , ζ , χ_2 determining its shape and size. This is consistent with the fact that SU(3) is eight dimensional, while the choice of three general vertices in \mathcal{O} requires specifying twelve independent coordinates. The geometric phase for the geodesic triangle with vertices ρ_1 , ρ_2 , ρ_3 in (4.26) is determined by the general GP-BI relation (4.5):

$$\varphi_{\text{geom}} \text{ [geodesic triangle with vertices } \rho_1, \rho_2, \rho_3]$$

$$= -\arg \Delta_3(\psi_1, \psi_2, \psi_3)$$

$$= \arg(\psi_3, \psi_2)$$

$$= \arg(\cos \xi \cos \eta + e^{-i\chi_2} \sin \xi \sin \eta \sin \zeta). \tag{4.28}$$

All four intrinsic angle parameters appear, and χ_2 must be nonzero for this GP to be nontrivial.

Lastly, in connection with three level systems we go back to the adiabatic situation. Possible three-fold degeneracies for a general system can be analyzed in the spirit of the Berry treatment of double degeneracies, and GP's for evolutions near them. This exploits the SU(3) machinery set up above. With three levels one has to work in an eight dimensional parameter space, some portion of \mathbb{R}^8 , and there are distinct kinds of degeneracies: double degeneracy of the two upper levels, double degeneracy of the two lower levels, and a genuine triple degeneracy. Each of the double degeneracies occurs over a corresponding five dimensional region in \mathbb{R}^8 , while the triple degeneracy

occurs at a point, say the origin in \mathbb{R}^8 . The general formula (2.31), in the form appropriate for an eight dimensional parameter space, has been analyzed to bring out these regions of degeneracies, a nontrivial extension of the Berry 'monopole' situation, and the delicate way in which the 'monopole' structure is recovered.

4.3 The Weyl Phase as a Geometric Phase

Now we consider $\mathcal{H} = L^2(\mathbb{R})$ which is infinite dimensional and describe a toy case of the GP. For a one dimensional Cartesian QM system the Heisenberg canonical commutation relation is

$$[\hat{q}, \hat{p}] = i\hbar. \tag{4.29}$$

In the exponentiated Weyl form this is

$$e^{ib\hat{q}}e^{ia\hat{p}}e^{-ib\hat{q}}e^{-ia\hat{p}} = e^{-iab\hbar}. (4.30)$$

The phase on the right is the Weyl phase, we now show it is a GP. Now set $\hbar = 1$.

Take any unit vector $\psi_1 \in \mathcal{H}$ as initial state, and 'evolve' it in four steps using as piecewise constant Hamiltonians either \hat{p} or \hat{q} alternately. Indicating also the parameter ranges we have:

$$0 \leq s \leq a : \psi(s) = e^{-is\hat{p}}\psi_{1}, \psi(a) = \psi_{2};$$

$$a \leq s \leq a+b : \psi(s) = e^{-i(s-a)\hat{q}}\psi_{2}, \psi(a+b) = \psi_{3};$$

$$a+b \leq s \leq 2a+b : \psi(s) = e^{i(s-a-b)\hat{p}}\psi_{3}, \psi(2a+b) = \psi_{4};$$

$$2a+b \leq s \leq 2a+2b : \psi(s) = e^{i(s-2a-b)\hat{q}}\psi_{4}, \psi(2a+2b) = \psi_{5} = e^{-iab}\psi_{1}.$$

$$(4.31)$$

Clearly $\psi(s)$ for $0 \le s \le 2(a+b)$ projects onto a closed loop in ray space. The total phase is immediate:

$$\varphi_{\text{tot}} = \arg(\psi_1, \psi_5) = -ab. \tag{4.32}$$

The dynamical phase is additive, there are four contributions:

$$\varphi_{\text{dyn}} = -\int_{0}^{a} ds \; (\psi(s), \hat{p}\psi(s)) - \int_{a}^{a+b} ds \; (\psi(s), \hat{q}\psi(s)) + \int_{a+b}^{2a+b} ds \; (\psi(s), \hat{p}\psi(s)) + \int_{2a+b}^{2a+2b} ds \; (\psi(s), \hat{q}\psi(s)) = -2ab \quad (4.33)$$

after some algebra. Taking the difference we see that for any choice of ψ_1 , we have the same geometric phase:

$$\varphi_{\text{geom}} = \varphi_{\text{tot}} - \varphi_{\text{dvn}} = ab \tag{4.34}$$

establishing the result.

5 Second Mathematical Interlude

In the first mathematical interlude in Section 3, we described the $\mathcal{H} - \mathcal{B} - \mathcal{R}$ framework in quantum mechanics; lengths of curves in \mathcal{R} , geodesics in \mathcal{R} and their lifts to \mathcal{B} ; and the one-form A on \mathcal{B} whose integrals along curves $\mathcal{C} \subset \mathcal{B}$ give dynamical phases. Now we explore some further aspects to get a better understanding of these spaces and of objects defined on them. Several useful facts will be described leaving proofs and derivations to the reader.

5.1 On \mathcal{B}

Given a Hilbert space \mathcal{H} of complex dimension N, the unit sphere $\mathcal{B} \subset \mathcal{H}$ was defined in (3.3). At a point $\psi \in \mathcal{B}$, the tangent space to \mathcal{B} is written as $T_{\psi}\mathcal{B}$, and consists of tangent vectors to smooth curves in \mathcal{B} passing through ψ . We then find:

$$\psi \in \mathcal{B}: \qquad T_{\psi}\mathcal{B} = \{\phi \in \mathcal{H} | \operatorname{Re}(\psi, \phi) = 0\}.$$
 (5.1)

This is a real linear space of dimension (2N-1). A one-dimensional vertical subspace of this is immediately recognized: it consists of tangent vectors to curves in \mathcal{B} passing through ψ and contained within the U(1) fibre containing ψ :

$$\psi \in \mathcal{B}: \qquad V_{\psi}\mathcal{B} = \{ia\psi | a \in \mathbb{R}\} \subset T_{\psi}\mathcal{B}.$$
 (5.2)

The one-form A on \mathcal{B} was defined in (3.17). By definition, any one-form on \mathcal{B} is defined at each $\psi \in \mathcal{B}$ as a real linear functional on $T_{\psi}\mathcal{B}$. In the case of A we have:

$$\psi \in \mathcal{B}, \phi \in T_{\psi}\mathcal{B}: \qquad A_{\psi}(\phi) = \operatorname{Im}(\psi, \phi) = -i(\psi, \phi).$$
 (5.3)

Then the horizontal subspace $H_{\psi}\mathcal{B}$ of $T_{\psi}\mathcal{B}$ is that subspace on which A_{ψ} vanishes:

$$\psi \in \mathcal{B}: \qquad H_{\psi}\mathcal{B} = \{\phi \in T_{\psi}\mathcal{B} | A_{\psi}(\phi) = 0 \text{ i.e. } (\psi, \phi) = 0\} \subset T_{\psi}\mathcal{B};$$

$$T_{\psi}\mathcal{B} = H_{\psi}\mathcal{B} \oplus V_{\psi}\mathcal{B}. \tag{5.4}$$

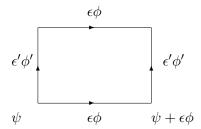
This $H_{\psi}\mathcal{B}$ is a complex linear space of complex dimension (N-1). It is the subspace of \mathcal{H} orthogonal to ψ :

$$H_{\psi}\mathcal{B} = \{\phi \in \mathcal{H} | (\psi, \phi) = 0\} \tag{5.5}$$

The exterior derivative dA of A is a two-form on \mathcal{B} . Any two-form on \mathcal{B} acts as an antisymmetric bilinear form on $T_{\psi}\mathcal{B}$, with real values. For dA, starting from (5.3) one can show that

$$\psi \in \mathcal{B}; \quad \phi, \phi' \in T_{\psi}\mathcal{B} : (dA)_{\psi} \ (\phi, \phi') = 2 \text{ Im } (\phi, \phi'). \tag{5.6}$$

We need to calculate the integral of A around a small quadrilateral pictured as:



to lowest order in ϵ and ϵ' :

$$A_{\psi}(\epsilon\phi) + A_{\psi+\epsilon\phi}(\epsilon'\phi') - A_{\psi}(\epsilon'\phi') - A_{\psi+\epsilon'\phi'}(\epsilon\phi)$$

$$= \operatorname{Im}\{\epsilon(\psi,\phi) + \epsilon'(\psi+\epsilon\phi,\phi') - \epsilon'(\psi,\phi') - \epsilon(\psi+\epsilon'\phi',\phi)\}$$

$$= 2\epsilon\epsilon' \operatorname{Im}(\phi,\phi') = (dA)_{\psi}(\epsilon\phi,\epsilon'\phi')$$
(5.7)

5.2 On \mathcal{R}

Now we move on to objects on the ray space $\mathcal{R} = \mathbb{C}P^{N-1}$, a manifold of complex dimension (N-1). The projection $\pi : \mathcal{B} \to \mathcal{R}$ is given in (3.6). At any $\rho \in \mathcal{R}$, the tangent space $T_{\rho}\mathcal{R}$ consists of a certain family of hermitian operators:

$$\rho = \psi \psi^{\dagger} \in \mathcal{R}: \quad T_{\rho}\mathcal{R} = \{B = \text{linear operator on } \mathcal{H}|B^{\dagger} = B, \text{Tr}B = 0, \{B, \rho\} = B\}$$
$$= \{\chi \psi^{\dagger} + \psi \chi^{\dagger} | \chi = B\psi \in H_{\psi}\mathcal{B}\} \quad (5.8)$$

In the second line we have made use of some (any) $\psi \in \pi^{-1}(\rho)$. Thus, for each such ψ , there is a one-to-one map $T_{\rho}\mathcal{R} \leftrightarrow H_{\psi}\mathcal{B}$. It is a nice exercise to show that elements of $T_{\rho}\mathcal{R}$ can be given another useful description:

$$T_{\rho}\mathcal{R} = \{B = i[\rho, K] | K = \text{hermitian linear operator on } \mathcal{H}\}.$$
 (5.9)

The connection to (5.8) is given by

$$K = i(\chi \psi^{\dagger} - \psi \chi^{\dagger}). \tag{5.10}$$

The two-form dA on \mathcal{B} is projectable onto \mathcal{R} , i.e. there is a two-form ω on \mathcal{R} of which dA is the pullback, $dA = \pi^*\omega$. In contrast, A on \mathcal{B} is not the pullback of any one-form on \mathcal{R} . As with dA, now ω too is defined at each $\rho \in \mathcal{R}$ as a real antisymmetric bilinear functional on $T_{\rho}\mathcal{R}$. Choosing some (any) $\psi \in \pi^{-1}(\rho)$:

$$\rho = \psi \psi^{\dagger} \in \mathcal{R}; B, B' \in T_{\rho} \mathcal{R} :$$

$$\omega_{\rho}(B, B') = -i \text{Tr} \left(\rho[B, B'] \right) = 2 \text{Im}(\chi, \chi')$$

$$\chi' = B' \psi, \chi = B \psi; \chi, \chi' \in H_{\psi} \mathcal{B}$$
(5.11)

This two-form ω on \mathcal{R} is nondegenerate, so it defines a symplectic structure on \mathcal{R} , or \mathcal{R} is a symplectic manifold.

Some of these relations can be understood more easily by using local coordinates over regions of \mathcal{R} , and their inverse images. They are useful also for practical calculations. For any chosen $\rho_0 = \psi_0 \psi_0^{\dagger} \in \mathcal{R}$, define a neighbourhood \mathcal{M} by

$$\mathcal{M} = \{ \rho \in \mathcal{R} | \text{Tr}(\rho_0 \rho) > 0 \} \subset \mathcal{R}. \tag{5.12}$$

For each $\rho \in \mathcal{M}$, choose a unique $\psi \in \pi^{-1}(\rho)$ such that (ψ_0, ψ) is real positive. This ψ has a unique decomposition into parts parallel and perpendicular to ψ_0 :

$$\psi = \psi_0 (1 - (\chi_0, \chi_0))^{1/2} + \chi_0, \chi_0 \in H_{\psi_0} \mathcal{B}, (\chi_0, \chi_0) < 1$$
(5.13)

A general $\psi' \in \pi^{-1}(\rho)$ is a phase times ψ : $\psi' = e^{i\alpha}\psi$, $0 \le \alpha < 2\pi$. Now choose an orthonormal basis $\{e_r\}$ for $H_{\psi_0}\mathcal{B}$, so $\{\psi_0, e_r\}$ is one for \mathcal{H} , here $r = 1, 2 \cdots N - 1$. Then χ_0 occurring in (5.11) can be expanded as

$$\chi_0 = \frac{1}{\sqrt{2}} \sum_r (q_r - ip_r)e_r, \qquad \sum_r (q_r^2 + p_r^2) < 2.$$
 (5.14)

Therefore $\{q_r, p_r\}$ are local coordinates over \mathcal{M} and $\{q_r, p_r, \alpha\}$ over $\pi^{-1}(\mathcal{M})$.

With these expressions we get local descriptions of A and dA on \mathcal{B} , ω on \mathcal{R} :

$$A_{\psi'} = -i\psi'^{\dagger}d\psi' = d\alpha - i\psi^{\dagger}d\psi$$

$$= d\alpha + \frac{1}{2}\sum_{r}(p_{r}dq_{r} - q_{r}dp_{r}),$$

$$(dA)_{\psi'} = \sum_{r}dp_{r} \wedge dq_{r}$$

$$\omega_{\rho} = \sum_{r}dp_{r} \wedge dq_{r}$$
(5.15)

It is the $d\alpha$ piece in A which makes it not related to any one-form on \mathcal{R} by pullback. The Fig:(5) explains these constructions.

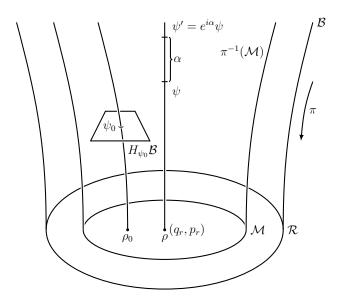


Figure 5: Domains of local coordinates on \mathcal{R} and \mathcal{B}

5.3 The geometric phase as a symplectic area

We know that any open curve $C \subset \mathcal{R}$ (with lift $\mathcal{C} \subset \mathcal{B}$) can be completed to a closed loop $C' \subset \mathcal{R}$ by connecting its endpoints by a geodesic. The geometric phase for C is then the same as that for C'. (This will be greatly generalized in the next Section.) Without loss of generality let us assume then that C is closed to begin with and let C be a closed lift of C to B. Then if S is any two dimensional surface in B with boundary C, and $S = \pi[S] \subset R$, we have:

$$C = \partial S; \quad \partial C = 0; \qquad C = \partial S; \quad \partial C = 0:$$

$$\varphi_{\text{geom}}[C] = -\varphi_{\text{dyn}}[C] = -\oint_{C} A$$

$$= -\int_{S} dA = -\int_{S} \omega \qquad (5.16)$$

This reveals the intrinsic nature of the geometric phase: it is a symplectic area. A nontrivial twodimensional surface S can have vanishing symplectic area. For example in a phase space of dimension ≥ 4 , if S lies in the $q^1 - q^2$ 'plane' or in the $q^1 - p^2$ or $p^1 - p^2$ 'planes', $\int_S \omega$ is zero.

5.4 The Fubini-Study Metric on \mathcal{R}

Given a parametrized curve $C = {\rho(s)} \subset \mathcal{R}$, its length is defined in (3.15) using any lift $C \to \mathcal{C} = {\psi(s)} \subset \mathcal{B}$. The element of length dl along C is determined by

$$(dl)^{2} = [(\dot{\psi}(s), \dot{\psi}(s)) - (\psi(s), \dot{\psi}(s))(\dot{\psi}(s), \psi(s))](ds)^{2}$$
(5.17)

and is reparametrization invariant. To extract the metric tensor on \mathcal{R} from this expression, we must express dl^2 at a general point $\rho \in \mathcal{R}$ in terms of a tangent vector there, i.e. an element of $T_{\rho}\mathcal{R}$. At $\rho(s) \in C$ the tangent space $T_{\rho(s)}\mathcal{R}$ is defined in (5.6) with $\rho(s)$ instead of ρ . Then a general $B \in T_{\rho(s)}\mathcal{R}$ is:

$$B \in T_{\rho(s)}\mathcal{R}: \qquad B = \psi(s)\chi^{\dagger} + \chi\psi(s)^{\dagger}, (\psi(s), \chi) = 0. \tag{5.18}$$

Therefore a nearby point $\rho(s + \delta s) \in C$ is of the form

$$\rho(s + \delta s) = \rho(s) + \delta s B \approx \psi(s + \delta s) \psi(s + \delta s)^{\dagger},$$

$$\psi(s + \delta s) = \psi(s) + \delta s \chi,$$
 (5.19)

for some $\chi \in \mathcal{H}$ orthogonal to $\psi(s)$. This gives $\dot{\psi}(s) = \chi$ and then (5.17) becomes

$$(dl)^{2} = (\chi, \chi) (ds)^{2} = \text{Tr} (\rho(s)B^{2}) (ds)^{2}.$$
(5.20)

The metric tensor is a symmetric nondegenerate covariant second rank tensor, defined pointwise on \mathcal{R} by :

$$\rho \in \mathcal{R}, \quad B \in T_{\rho}R \quad : \quad g_{\rho}(B,B) = 2\operatorname{Tr}\left(\rho B^{2}\right).$$
(5.21)

This leads by 'polarization' to the more general expression

$$\rho \in \mathcal{R}; \quad B, B' \in T_{\rho}R \quad : \quad g_{\rho}(B, B') = \operatorname{Tr}\left(\rho \left\{B, B'\right\}\right) = 2\operatorname{Re}\left(\chi, \chi'\right) \tag{5.22}$$

if we use (5.18) for B and similarly for B'. This is a particular way of expressing the metric on \mathcal{R} , there are other ways of expressing it.

This is the expression for the Fubini-Study metric on \mathcal{R} . On the other hand, the symplectic structure ω on \mathcal{R} is given pointwise by (5.11). Combining the two we have,

$$\operatorname{Tr}\left(\rho B B'\right) = \left(\chi, \chi'\right) = \frac{1}{2} g_{\rho}(B, B') + \frac{i}{2} \omega_{\rho}(B, B'). \tag{5.23}$$

The Riemannian metric on \mathcal{R} , and the symplectic structure on \mathcal{R} , are both determined by the inner product among Hilbert space vectors — they are the symmetric real part and the anti-symmetric imaginary part, respectively. From the GP perspective, as presented upto now, geodesics are determined by the former, and GP's by the latter (as symplectic areas, (5.16)); and geodesics provide the BI - GP link.

6 Null Phase Curves - The BI - GP link generalized

The general connection between BI's and GP's given in (4.6, 4.7) uses ray space geodesics to connect the vertices in a BI and build up a closed loop in ray space for which a GP can be computed. However there are some early results which look like 'counterexamples' to this connection based on geodesics. We describe one of them now. It involves the well-known harmonic oscillator coherent states.

6.1 The case of coherent states

This was studied by Chaturvedi, Sriram and Srinivasan in 1987. The Hilbert space involved is $\mathcal{H} = L^2(\mathbb{R})$ which is infinite dimensional, and so are \mathcal{B} and \mathcal{R} . But we actually use some finite dimensional submanifolds in them.

With standard notations for a single canonical pair of operators \hat{q} , \hat{p} obeying

$$[\widehat{q},\widehat{p}] = i\hbar \tag{6.1}$$

the coherent states are normalized eigenstates of the annihilation operator ($\hbar = 1$):

$$\widehat{a} = \frac{1}{\sqrt{2}} (\widehat{q} + i\widehat{p}). \qquad \widehat{a}^{\dagger} = \frac{1}{\sqrt{2}} (\widehat{q} - i\widehat{p}), \qquad \left[\widehat{a}, \widehat{a}^{\dagger}\right] = 1;$$

$$\widehat{a}|z\rangle = z|z\rangle, \qquad z \in \mathbb{C}$$
(6.2)

These states are related to the number states in the well known way, and have simple inner products:

$$|z\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle, \qquad \widehat{a}^{\dagger} \widehat{a} |n\rangle = n|n\rangle;$$

$$\langle z'|z\rangle = \exp\left(-\frac{1}{2}|z'|^2 - \frac{1}{2}|z|^2 + z'^*z\right),$$

$$\arg\left(\langle z'|z\rangle\right) = \operatorname{Im}\left(z'^*z\right). \tag{6.3}$$

Now take these coherent states as a collection and define submanifolds in \mathcal{B} and in \mathcal{R} as follows:

$$\Sigma_c = \{ |z\rangle \in \mathcal{B} | z \in \mathbb{C} \} \subset \mathcal{B} ;$$

$$\Omega_c = \pi \left(\Sigma_c \right) = \{ |z\rangle \langle z| \in \mathcal{R} | z \in \mathbb{C} \} \subset \mathcal{R}.$$
(6.4)

Clearly both Σ_c and Ω_c are of real dimension two, embedded in \mathcal{B} and \mathcal{R} respectively, and with an obvious one-to-one map between them.

Let us now take three points $z_1, z_2, z_3 \in \mathbb{C}$, equivalently three 'points' $|z_1\rangle, |z_2\rangle, |z_3\rangle \in \Sigma_c$. We can plot them in the complex plane: They define a BI and from (6.3) we can compute its phase:

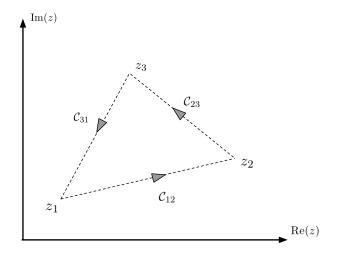


Figure 6:

$$\arg \Delta_3 (|z_1\rangle, |z_2\rangle, |z_3\rangle) = \arg \langle z_1|z_2\rangle \langle z_2|z_3\rangle \langle z_3|z_1\rangle$$

= Im $(z_1^*z_2 + z_2^*z_3 + z_3^*z_1)$. (6.5)

According to (4.6), this is the negative of a GP. We draw (lifts of) geodesics as follows:

$$\mathcal{C}_{12}^{\text{(geod)}}$$
 : $|z_1\rangle$ to $|z_2\rangle$; (6.6a)
 $\mathcal{C}_{23}^{\text{(geod)}}$: $|z_2\rangle$ to $|z_3\rangle$; (6.6b)
 $\mathcal{C}_{31}^{\text{(geod)}}$: $|z_3\rangle$ to $|z_1\rangle$. (6.6c)

$$C_{23}^{\text{(geod)}} : |z_2\rangle \text{ to } |z_3\rangle;$$
 (6.6b)

$$C_{31}^{\text{(geod)}} : |z_3\rangle \text{ to } |z_1\rangle.$$
 (6.6c)

Then (4.6) gives:

$$-\operatorname{Im}\left(z_{1}^{*}z_{2}+z_{2}^{*}z_{3}+z_{3}^{*}z_{1}\right)=-\varphi_{\operatorname{dyn}}\left[\mathcal{C}_{12}^{(\operatorname{geod})}\cup\mathcal{C}_{23}^{(\operatorname{geod})}\cup\mathcal{C}_{31}^{(\operatorname{geod})}\right]$$

$$=\varphi_{\operatorname{geom}}\left[\pi\left(\mathcal{C}_{12}^{(\operatorname{geod})}\cup\mathcal{C}_{23}^{(\operatorname{geod})}\cup\mathcal{C}_{31}^{(\operatorname{geod})}\right)\right]$$
(6.7)

We notice an important property of the curves (6.6): while each of them starts and ends on a coherent state which lies in Σ_c , at 'intermediate points' they are linear combinations of coherent states, as seen in (3.21) describing geodesics, which are not coherent states. Therefore the 'arguments' of φ_{dyn} and φ_{geom} appearing on the right hand side in (6.7) do not lie in Σ_c , Ω_c respectively but \mathbf{go} outside them.

However, Chaturvedi et al showed by direct calculation that the phase of the BI (6.5) is the GP (apart from a sign) of a 'triangle' within the manifold Σ_c , shown by dotted lines in Fig. (6). The sides are 'straight lines' in the complex plane, so we pass through coherent states throughout. These straight lines are denoted by C_{12}, C_{23}, C_{31} , so we have a triangle

$$\mathcal{C}(z_1, z_2, z_3) = \mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31} \subset \Sigma_c \tag{6.8a}$$

$$C(z_1, z_2, z_3) = \pi \left[C(z_1, z_2, z_3) \right] \subset \Omega_c.$$
 (6.8b)

Both are closed loops. So the former has zero total phase. Easy calculations give:

$$\varphi_{\text{geom}} [C(z_1, z_2, z_3)] = -\varphi_{\text{dyn}} [C_{12} \cup C_{23} \cup C_{31}]
= -\varphi_{\text{dyn}} [C_{12}] - \varphi_{\text{dyn}} [C_{23}] - \varphi_{\text{dyn}} [C_{31}]
= -\text{Im} (z_1^* z_2 + z_2^* z_3 + z_3^* z_1),$$
(6.9a)

that is,

$$\arg \Delta_3 (|z_1\rangle, |z_2\rangle, |z_3\rangle) = -\varphi_{\text{geom}} \left[\pi \left(\mathcal{C}_{12} \cup \mathcal{C}_{23} \cup \mathcal{C}_{31} \right) \right]$$
$$= -\varphi_{\text{geom}} \left[C \left(z_1, z_2, z_3 \right) \right]$$
(6.9b)

We can calculate $\varphi_{\text{dyn}}[\mathcal{C}_{12}]$ for instance a follows:

$$z(s) = (1-s)z_{1} + sz_{2}, \quad 0 \leq s \leq 1;$$

$$\varphi_{\text{dyn}}[C_{12}] = \text{Im} \int_{0}^{1} ds \langle z(s) | \frac{d}{ds} | z(s) \rangle$$

$$= \text{Im} \int_{0}^{1} ds \langle z(s) | \frac{d}{ds} \left(|e^{-\frac{1}{2}|z(s)|^{2} + z(s)\hat{a}^{\dagger}} | 0 \right) \right)$$

$$= \text{Im} \int_{0}^{1} ds \langle z(s) | \left(-\frac{1}{2} z^{*}(s) \dot{z}(s) - \frac{1}{2} \dot{z}^{*}(s) z(s) + \dot{z}(s)\hat{a}^{\dagger} \right) | z(s) \rangle$$

$$= \text{Im} \int_{0}^{1} ds \frac{1}{2} \left(z^{*}(s) \dot{z}(s) - \dot{z}^{*}(s) z(s) \right) = \text{Im} \int_{0}^{1} ds z^{*}(s) \dot{z}(s)$$

$$= \text{Im} \int_{0}^{1} ds \left((1-s)z_{1}^{*} + sz_{2}^{*} \right) (z_{2} - z_{1}) = \text{Im}(z_{1}^{*}z_{2}), \tag{6.10}$$

are similar for the other two terms.

In other words, in this example, the phase of the BI in (6.6) is the negative of a GP in two distinct ways - either as the GP of a geodesic triangle (in \mathcal{B} and in \mathcal{R}) involving linear combinations of coherent states, or as the GP of a triangle within Σ_c , Ω_c involving only coherent states at all stages.

A similar result was obtained by us (RS, NM) in 1993 in the context of centred Gaussian states obeying the paraxial wave equation in classical optics. We were studying the so-called Gouy phase and the BI involved was of order 4.

These two physically important examples - the existence of two ways of connecting BI's with GP's only one of which used ray space geodesics - led us to look for the most general way in which this connection could be established. The first analysis was made by Rabei , Arvind, Simon and me in 1999, in a preliminary way. Later the general idea of a Null Phase Curve was developed, and it turned out that using such curves we get the most general form of the BI-GP connection .

6.2 Definition and properties of Null Phase Curves (NPC)

Let us revert to the spaces $\mathcal{H}, \mathcal{B}, \mathcal{R}$ in (3.8 - 3.10) with any dimensions. When curves \mathcal{C} with a parameter s are considered in \mathcal{B} with parametrised images $C \subset \mathcal{R}$, the smoothness conditions vary depending on their use: to define geodesics, to be able to evaluate GP's or to be NPC's (to be defined now). These variations should be kept in mind though not spelt out here. A NPC is a smooth parametrised curve $C \subset \mathcal{R}$, along with any smooth lift $\mathcal{C} = \psi(s) \subset \mathcal{B}$, if

$$\Delta_3\left(\psi(s), \psi(s'), \psi(s'')\right) \equiv \text{Tr}(\rho(s)\rho(s')\rho(s'')) = \text{real positive, all } s, s', s''$$
(6.11)

From (3.21) we see that every geodesic in \mathcal{R} is a NPC. The key property of a NPC , captured by the definition (6.11) is this

$$\varphi_{\text{geom}}[\text{any connected portion of a NPC}] = 0,$$
 (6.12)

From (6.11) connected subsets of a NPC are themselves NPC's. The definition (6.11) is designed just so as to have the desired connection

$$\arg \Delta_3(\psi_1, \psi_2, \psi_3) = -\varphi_{\text{geom}}[C \subset R],$$
 $C = \text{any triangle with vertices } \rho(\psi_1), \rho(\psi_2), \rho(\psi_3) \text{ and any NPC's as sides.}$ (6.13)

The generalisation to $\Delta_n(\psi_1, \psi_2, \cdots, \psi_n)$ is immediate and obvious. The proof of (6.13) is left as a simple exercise based on (6.12) which itself is a consequence of the definition (6.11). Moreover, (6.13) is the most general way in which BI and GP can be connected. For a general open curve $C \subset R$, if N is any NPC connecting the end points of C such that $C \cup N$ is a closed loop, we get using (5.16)

$$\partial C \neq 0$$
: $\varphi_{\text{geom}}[C] = \varphi_{\text{geom}} [C \cup N] = -\iint_{S} \omega, \quad \partial S = C \cup N$ (6.14)

As said above, with the use of NPC's in place of geodesics, we get the maximum possible generalisation of the relation (4.7, 3.25, 3.26). Here are the important properties of NPC's:

- For dim $\mathcal{H} = 2$ with $\mathcal{R} = \mathcal{S}_P^2$, NPC's and geodesics coincide.
- For dim $\mathcal{H} \geq 3$, given any two non orthogonal points $\rho_1, \rho_2 \in \mathcal{R}$, there is only one (shorter) geodesic, but infinitely many NPC's connecting them. Thus while every geodesic is a NPC, the latter are far more numerous. So for given vertices the phases of BI's can be interpreted as GP's in infinitely many ways- varying each NPC does not change the GP.
- NPC 's have essentially non-local features, they cannot be described by any system of ordinary differential equations of any finite order. In contrast as we have seen , geodesics are solutions of second order ordinary differential equations.
- One can prove quite easily that Eq. (3.19) holds for any NPC, i.e.,

$$\arg(\psi(s_1), \psi(s_2)) = \int_{\mathcal{C}} A \tag{6.15}$$

as was the case with geodesics earlier.

• It can also be shown that any NPC possesses special lifts in \mathcal{B} along which any two vectors are in phase in the Pancharatnam sense, i.e., have an inner product which is real positive.

This should make it clear that it is NPC's that really belong to GP theory, the early use of geodesics is incidental as they are NPC's. For further properties of NPC's and so-called Null Phase Manifolds, the reader can look at a recent paper by some of us.

7 Concluding Remarks

We may mention some applications of the kinematic approach to GP's over the years, for completeness:

- 1. GP's which arise from unitary representations of Lie groups can be analyzed from both algebraic and differential geometric points of view. This leads to a general structure which is reminiscent of the well known Wigner-Eckart theorem. A complete list of possibilities in the SU(3) case has been obtained.
- 2. The Gouy phase in Gaussian wave optics has been studied using a 4^{th} order BI $\Delta_4(\psi_1, \psi_2, \psi_3, \psi_4)$.
- 3. The so-called 'off diagonal GP's' have been shown to be based essentially on BI's, and nothing else in principle is needed.

- 4. A definition and interpretation of GP's for mixed states has been given.
- 5. The case of three level degeneracy in the adiabatic limit has been analyzed in complete detail, in the spirit of Berry's two-level degeneracy analysis. Useful tools based on SU(3) tensors have been developed for this purpose.
- 6. The use of BI's in the study of higher order CKM matrices in particle physics has been explored.

This has been a brief review of developments in the theory of the GP beginning with Berry's work of 1983-84. His original arguments and important later generalizations, have been described. The role of BI's in this connection has been emphasized. Some instructive examples have been given, and the differential geometric structures relevant to the subject have been outlined.

The basic $\mathcal{H} - \mathcal{B} - \mathcal{R}$ framework is seen to be capable of handling GP's in both quantum mechanical and classical optical contexts. Ray spaces \mathcal{R} possess both a Riemannian metric and symplectic structure. GP's are closely connected to the latter, but initially geodesics determined by the former played an important role in GP considerations. The fact that actually NPC's are more natural in this context, and their definition in terms of BI's, have been brought out. As it is relatively new, the NPC concept deserves further study and use in interesting situations in imaginative ways. The mathematics of Kahler manifolds may help in this effort.

Equally importantly, it is desirable to find incisive uses of GP's to solve physical problems, going beyond recognizing past results as being instances of GP's. This attitude should lead to useful results, and the background provided in these notes should help.

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