Geometry and Topology in Quantum Mechanics –
Mathematical Properties of Geometric Phases

N. Mukunda

Bengaluru

1 States of quantum systems

Quantum system $\mathcal{S}$ — Pure states

Quantum system $\mathcal{S}$ — Mixed states

Pure states $\sim$ vectors ψ in some Hilbert space $\mathcal{H}$.

$$\mathcal{B} = \{\psi \in \mathcal{H} | (\psi, \psi) = 1\} \subset \mathcal{H} \tag{11}$$

$$\psi \in \mathcal{B} \to \text{corresponding pure state of } \mathcal{S}. \tag{12}$$

Many-to-one map: ψ and $\mathrm{e}^{\mathrm{i}\alpha}\psi \to$ same pure state.

$$\mathcal{R} = \mathcal{B}/U(1) = \{\rho(\psi) = |\psi\rangle\langle\psi| \mid \psi \in \mathcal{B}\} \tag{13}$$

Projection $\pi : \mathcal{B} \to \mathcal{R}$:

$$\psi \in \mathcal{B} \to \pi(\psi) = \rho(\psi) \in \mathcal{R} \tag{14}$$

$\mathcal{B} = U(1)$ principal fibre bundle over base $\mathcal{R}$.

$$\psi_1, \psi_2 \in \mathcal{B} \to |(\psi_2, \psi_1)|^2 = \mathrm{Tr}(\rho(\psi_2)\rho(\psi_1)) = \text{transition probability} \tag{15}$$

2 Wigner 1931 Theorem, Bargmann Invariants

Symmetry of $\mathcal{S}$: one-to-one onto map $\mathcal{T} : \mathcal{R} \to \mathcal{R}$ preserving $\mathrm{Tr}(\rho_1\rho_2)$.

$$\mathcal{R} \to \mathcal{R} : \rho_1 \to \mathcal{T}(\rho_1) = \rho_1', \quad \rho_2 \to \mathcal{T}(\rho_2) = \rho_2' :$$

$$\mathrm{Tr}(\rho_2'\rho_1') = \mathrm{Tr}(\rho_2\rho_1). \tag{21}$$

At vector level:

$$\mathcal{T}(\rho(\psi)) = \rho(\psi') : \psi' \text{ determined upto phase} \tag{22}$$

i.e.

$$\psi \in \mathcal{B} \xrightarrow{\pi} \rho(\psi) \in \mathcal{R} \xrightarrow{\mathcal{T}} \mathcal{T}(\rho(\psi)) = \rho(\psi') \in \mathcal{R} : \psi' \text{ fixed upto phase} \tag{23}$$

Theorem

$$\mathcal{T}(\rho(\psi)) = \rho(U\psi) \begin{array}{l} \nearrow \quad U \text{ linear unitary}, (U\psi_2, U\psi_1) = (\psi_2, \psi_1) \\ \qquad\qquad\qquad \text{or} \\ \searrow \quad U \text{ antilinear antiunitary}, (U\psi_2, U\psi_1) = (\psi_1, \psi_2) \end{array} \tag{24}$$

Bargmann 1964 method to determine option instantly

$$\text{BI} \quad \Delta_3(\psi_1, \psi_2, \psi_3) = (\psi_1, \psi_2)(\psi_2, \psi_3)(\psi_3, \psi_1) = \mathrm{Tr}(\rho_1\rho_2\rho_3). \tag{25}$$

$$\mathcal{T} : \Delta_3(\psi_1, \psi_2, \psi_3) \begin{array}{l} \nearrow \quad \Delta_3(\psi_1, \psi_2, \psi_3) : U \text{ linear unitary} \\ \qquad\qquad\qquad \text{or} \\ \searrow \quad \Delta_3(\psi_1, \psi_2, \psi_3)^* : U \text{ antilinear antiunitary} \end{array} \tag{26}$$

3 Pancharatnam 1956

Pure polarization states of plane EM waves, fixed $\mathbf{k}, \omega$

$$\mathbf{k} = (0, 0, |\mathbf{k}|) : \ \mathbf{k} \cdot \mathbf{E} = 0, \mathbf{E} = \begin{pmatrix} E_x \\ E_y \end{pmatrix} . \tag{31}$$

$$\dim \mathcal{H} = 2, \mathcal{B} \sim S^3, \mathcal{R} = \text{Poincaré sphere } \mathcal{P} = S^2 \tag{32}$$

Projection map

$$\mathbf{E} \in \mathcal{H} \to \frac{\mathbf{E}}{|\mathbf{E}|} \in \mathcal{B} \xrightarrow{\pi} \hat{n} = \frac{\mathbf{E}^\dagger \boldsymbol{\sigma} \mathbf{E}}{|\mathbf{E}|^2} \in S^2, |\mathbf{E}|^2 = \mathbf{E}^\dagger \mathbf{E}. \tag{33}$$

'In phase' concept:

$$\mathbf{E}_1, \mathbf{E}_2 \text{ `in phase'} \ \Leftrightarrow \mathbf{E}_1^\dagger \mathbf{E}_2 \text{ real} > 0 \tag{34}$$

Non transitive!

$$\mathbf{E}_1^\dagger \mathbf{E}_2 \text{ real} > 0, \mathbf{E}_2^\dagger \mathbf{E}_3 \text{ real} > 0 \nRightarrow \mathbf{E}_3^\dagger \mathbf{E}_1 \text{ real} > 0. \tag{35}$$

Measure of non transitivity:

$$\begin{aligned}
\hat{n}_{1,2,3} &= \pi(\mathbf{E}_{1,2,3}) \in \mathcal{P} : \\
\arg \mathbf{E}_3^{\dagger}\mathbf{E}_1 &= -\frac{1}{2}\Omega(\hat{n}_1, \hat{n}_2, \hat{n}_3), \\
\Omega(\hat{n}_1, \hat{n}_2, \hat{n}_3) &= \text{Solid angle of spherical triangle on } \mathcal{P}, \text{vertices} \\
&\quad \hat{n}_1, \hat{n}_2, \hat{n}_3, \text{sides geodesics.}
\end{aligned} \tag{36}$$

4 Berry (1983) adiabatic geometric phase and generalisations

Schrodinger equation in adiabatic approximation and condition of cyclic evolution $\rightarrow$ new phase of geometric nature in solution to Schrodinger equation.

$$\left.\begin{array}{ll}\text{Aharonov–Anandan: no need for adiabaticity} \\ \text{Samuel–Bhandari: no need for cyclic condition}\end{array}\right\} \begin{array}{l}\text{geometric phase} \\ \text{always exists}\end{array} \tag{41}$$

System $\mathcal{S}$ of dimension N: $\mathcal{H}$ has complex dimension N;

$\mathcal{B}$ has real dimension $(2N-1), \mathcal{R} = CP^{N-1}$ has real dimension $2(N-1)$.

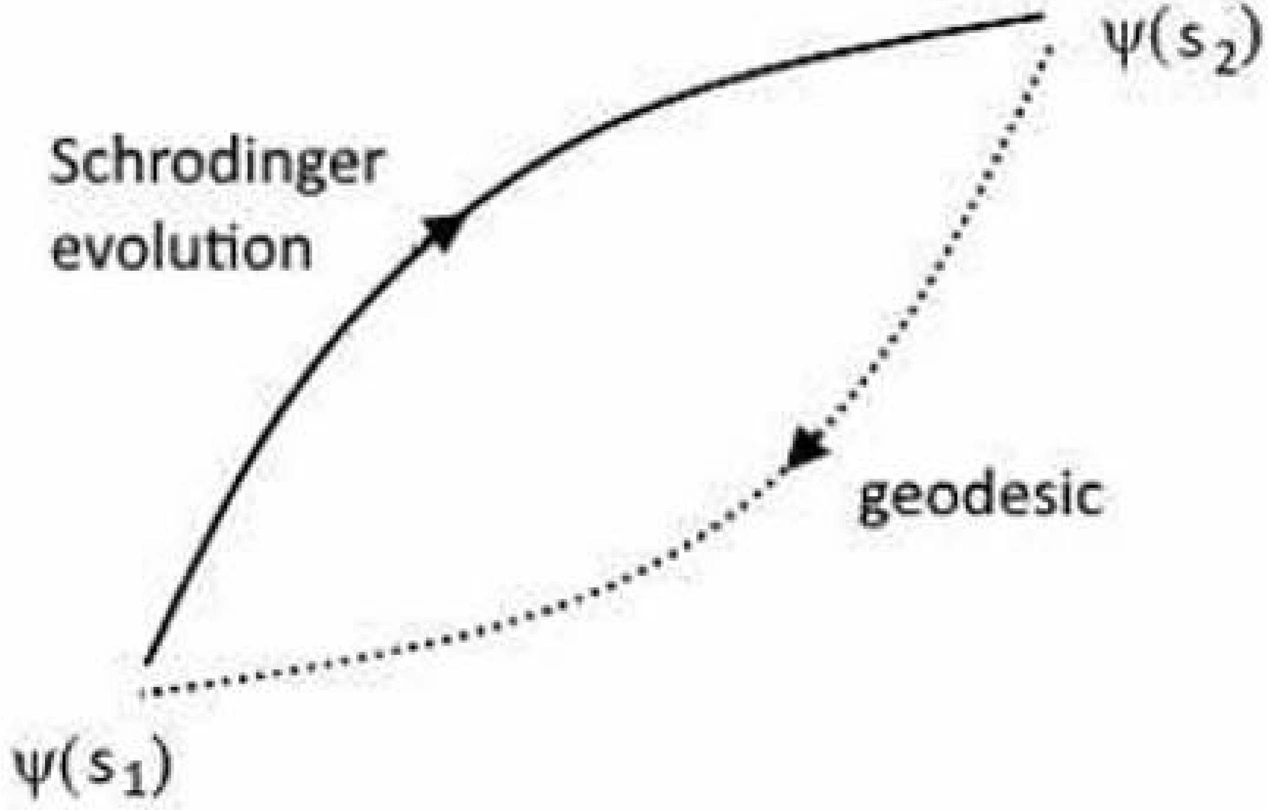
Ray space $\mathcal{R}$ = Riemannian manifold, also symplectic manifold.

Geodesics in $\mathcal{R}$:

$$\rho_1 = \rho(\psi_1), \rho_2 = \rho(\psi_2) : \text{ choose } \psi_1, \psi_2 \text{ so that } (\psi_1, \psi_2) = \cos\theta, 0 < \theta < \pi/2. \tag{42}$$

Then

$$\begin{aligned} C_{\text{geo}} &= \pi[\mathcal{C}_{\text{geo}}] \subset \mathcal{R}, \\ \mathcal{C}_{\text{geo}} &= \{\psi(s) | 0 \le s \le \theta\} \subset \mathcal{B}, \\ \psi(s) &= \psi_1 \cos s + (\psi_2 - \psi_1 \cos\theta)\frac{\sin s}{\sin\theta}, \quad 0 \le s \le \theta; \\ \text{i.e.} \quad C_{\text{geo}} &= \{\rho(s) = |\psi(s)\rangle\langle\psi(s)| \mid 0 \le s \le \theta\}. \end{aligned} \tag{43}$$



Samuel–Bhandari treatment of noncyclic case.

5 Kinematic approach to Geometric Phase

Ingredients

$$\mathcal{C} = \{\psi(s) \in \mathcal{B} | s_1 \leq s \leq s_2\} \subset \mathcal{B},$$
$$C = \pi[\mathcal{C}] = \{\rho(s) = \rho(\psi(s)) \in \mathcal{R} | s_1 \leq s \leq s_2\} \subset \mathcal{R}. \qquad (51)$$

Two groups of transformations on curves $\mathcal{C}$:

Local phase changes $\mathcal{C} = \{\psi(s)\} \to \mathcal{C}' = \{\psi'(s)\}$,

$$\psi'(s) = \mathrm{e}^{\mathrm{i}\alpha(s)}\psi(s); \qquad \text{(a)}$$

Reparametrisations

$$s' = f(s), \quad \frac{\mathrm{d}f(s)}{\mathrm{d}s} > 0 :$$
$$\mathcal{C} = \{\psi(s)\} \to \mathcal{C}' = \{\psi'(s')\}, \psi'(s') = \psi(s). \qquad \text{(b)} \qquad (52)$$

Simplest invariant expression:

$$\varphi_g[C] = \varphi_{tot}[\mathcal{C}] - \varphi_{dyn}[\mathcal{C}],$$
$$\varphi_{tot}[\mathcal{C}] = \arg(\psi(s_1), \psi(s_2)), \quad \varphi_{dyn}[\mathcal{C}] = \mathrm{Im} \int_{s_1}^{s_2} \mathrm{d}s(\psi(s), \frac{\mathrm{d}\psi(s)}{\mathrm{d}s}). \qquad (53)$$

This is the geometric phase of AASB for general noncyclic situation.

Some differential geometric notation:

$$\varphi_{dyn}[\mathcal{C}] = \int_{\mathcal{C}} A, \quad A = -\mathrm{i}\psi^{+}\mathrm{d}\psi = \text{one form on } \mathcal{B}. \qquad (54)$$

This A does not 'descend' to $\mathcal{R}$, but $\mathrm{d}A$ does.

$$\mathrm{d}A = -\mathrm{i}\mathrm{d}\psi^+ \ \wedge \ \mathrm{d}\psi = \pi^*\omega,$$
$$\omega = \text{two-form on } \mathcal{R}, \text{nondegenerate, closed, i.e., } \mathrm{d}\omega = 0. \tag{55}$$

So

$$\varphi_g[C] = -\int_S \omega, \quad S \subset \mathcal{R}, \partial S = C \cup \pi(\text{geodesic from } \psi(s_2) \text{ to } \psi(s_1)). \tag{56}$$

Geometric phases are symplectic areas in ray spaces.

6 General connection between BI's and Geometric Phases

$$\text{Choose } \psi_1, \psi_2, \psi_3 \in \mathcal{B} \xrightarrow{\pi} \rho_1, \rho_2, \rho_3 \in \mathcal{R} \tag{61}$$

Then find:

$$\begin{aligned} &\arg \Delta_3(\psi_1, \psi_2, \psi_3) = -\varphi_g[C_{12} \cup C_{23} \cup C_{31}] = \int_S \omega, \\ &\partial S = C_{12} \cup C_{23} \cup C_{31}, C_{12} = \text{geodesic } \rho_1 \text{ to } \rho_2 \text{ etc.} \end{aligned} \tag{62}$$

Easily generalised to $\Delta_n(\psi_1, \psi_2, \ldots, \psi_n), n > 3$.

Simple fact:

$$\varphi_g \text{ [any geodesic in } \mathcal{R}] = 0. \tag{63}$$

7 Null Phase Curves (NPC)

These are the most general curves in $\mathcal{R}$ for which

$$\varphi_g \text{ [any NPC]} = 0. \tag{71}$$

Definition of NPC

$$\begin{aligned} &N = \{\rho(s) = \rho(\psi(s)) \in \mathcal{R} | s_1 \leq s \leq s_2\} \subset \mathcal{R}, \\ &\Delta_3(\psi(s), \psi(s'), \psi(s'')) = \text{real} > 0 \text{ for all } s, s', s'' \in [s_1, s_2]. \end{aligned} \tag{72}$$

Special 'Pancharatnam' lifts:

$N \subset \mathcal{R}$ is NPC $\Leftrightarrow$ there are lifts $\mathcal{N} = \{\psi(s)\} \subset \mathcal{B}$ such that

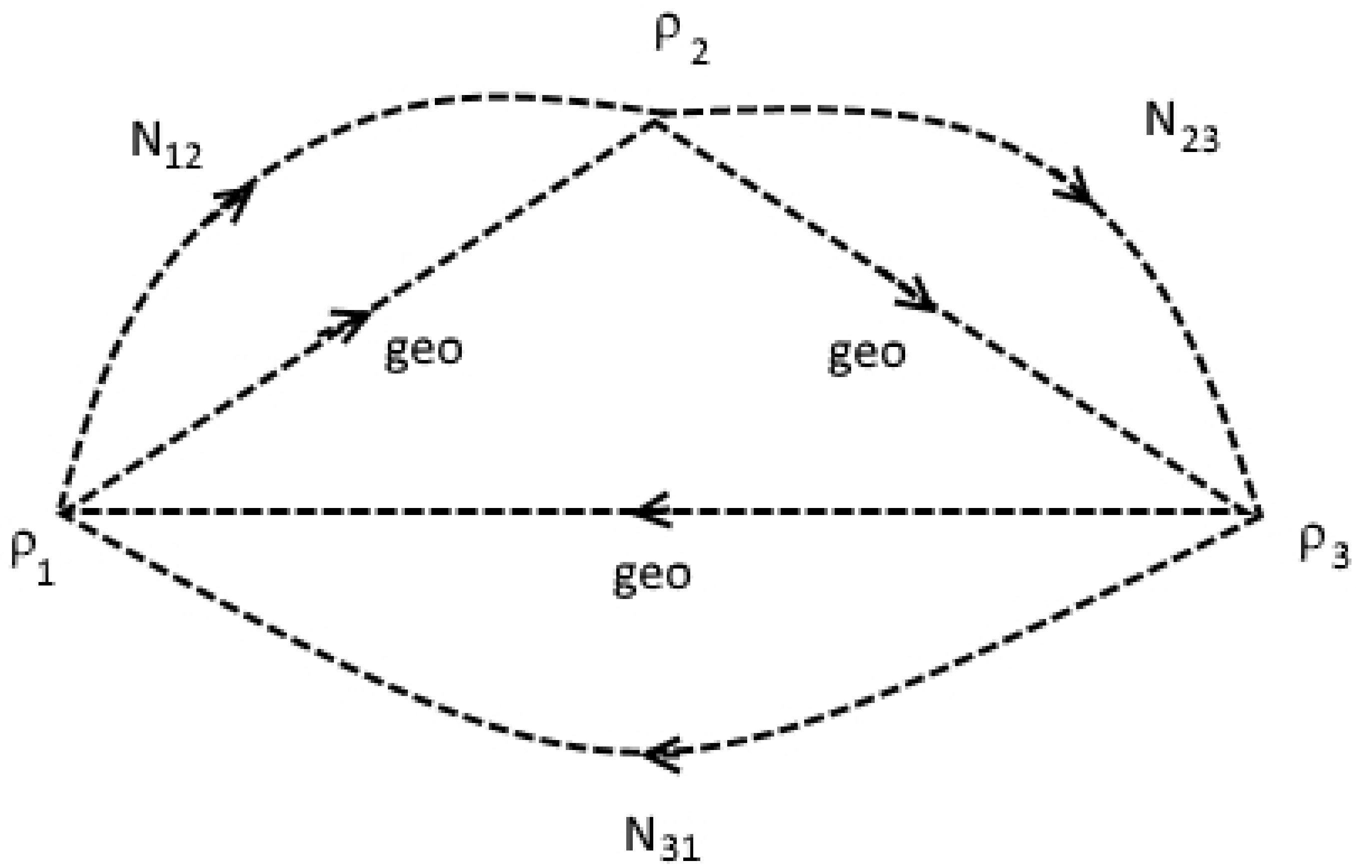
$$(\psi(s), \psi(s')) = \text{real} > 0 \text{ for all } s, s' \in [s_1, s_2]. \tag{73}$$

Dim $\mathcal{H} = 2, \mathcal{R} = S^2$: NPC $\equiv$ geodesic, great circle arc on S^2;

Dim $\mathcal{H} \geq 3$: geodesics are NPC's, but NPC's are far more numerous.

Most general BI-Geometric Phase connection:

$$\begin{aligned} \arg \Delta_3(\psi_1, \psi_2, \psi_3) &= -\varphi_g[N_{12} \cup N_{23} \cup N_{31}], \\ N_{12} &= \text{any NPC } \rho_1 \text{ to } \rho_2 \text{ etc.} \end{aligned} \quad (74)$$



ρ 2
N12
N23
geo
geo
ρ1
geo
ρ3
N31

8 Concluding remarks

Interesting class of geometric phases – associated with unitary representations of compact or noncompact simple Lie groups – detailed analysis possible.

In overall framework of quantum mechanics – ideas of Wigner, Pancharatnam, Bargmann deep and beautiful – their interconnections seen better thanks to Berry's profound discovery and the AASB generalisations.

Some References

[1] E. P. Wigner, Group Theory, Academic Press (NY) (1959), pp. 233–236.

[2] V. Bargmann, Jour. Math. Phys. **5**, 862 (1964).

[3] S. Pancharatnam, Proc. Indian Acad. Sci. **A44**, 247 (1956).

[4] M. V. Berry, Proc. Roy. Soc. **A392**, 45 (1984).

[5] Y. Aharonov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987).

[6] J. Samuel and R. Bhandari, Phys. Rev. Lett. **60**, 2339 (1988).

[7] N. Mukunda and R. Simon, Ann. Phys. (NY) **228**, 205, 269 (1993).

For the theory of NPC's see: N. Mukunda, Arvind, E. Ercolessi, G. Marmo, G. Morandi and R. Simon, Phys. Rev. **A67**, 042114 (2003); S. Chaturvedi, E. Ercolessi, G. Morandi, A. Ibort, G. Marmo, N. Mukunda and R. Simon, Jour. Math. Phys. **54**, 062106 (2013).