PRAMANA — journal of physics © Indian Academy of Sciences Vol. 56, Nos 2 & 3 Feb. & Mar. 2001 pp. 305–319

Density operator description of geometric phenomena in the ray space

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Abstract. A general gauge-invariant formalism for parallel transport, geodesics and geometric phase based on the pure state density operator is propounded. A single-query quantum search algorithm is proposed.

Keywords. Density operator; quantum search; parallel transport; geometric phase; geodesics.

PACS No. 03.65.Bz

1. Introduction

Geometric phase has been studied extensively since Berry [1] discovered it in adiabatic and cyclic evolutions of a general quantal system. Geometric phase has since been identified with the phase anholonomy of a parallel transported quantal system and shown to arise in completely general evolutions [2–7]. Determined solely by the geometry of the curve traced in the ray space, geometric phase encompasses a broad range [8–10] of scientific fields.

In this paper, we present a density operator-based, hence gauge-invariant, formalism for geometric phase and associated features of quantal evolutions, from a physicist's viewpoint. We delineate the properties of the finite difference $\Delta\rho$ between a pair of pure state density operators of a general quantal system. Using ρ and $\Delta\rho$, we construct a complete set of generators for the related 2-sphere ray subspace (§2), highlighting the physical operations performable with each generator. In the limit of an infinitesimal separation between the pair of rays, we characterise the differential density operator $\mathrm{d}\rho$ (§3). We derive an expression for the general curve length S in the ray space (§4) and examine its relationship with a time-energy uncertainty principle enunciated previously [11]. Using the 2-subspace generators, we propose a *single*-query quantum search algorithm to extract a desired ray *exactly* from a given array of n rays (§5). Showing that each infinitesimal step of a general evolution is confined to the local 2-subspace, we express the most general Hamiltonian $\mathcal{H}_s$ generating a given ray space evolution in terms of Pauli operators in local 2-subspaces constructed from ρ and $\mathrm{d}\rho$ (§6). This leads to a natural physical delineation of dynamical and geometric phase components, the latter originating from the parallel transport (§7) effected by the commutator between ρ and dρ, in $\mathcal{H}_s$. In §8, we obtain a density operator equation for geodesics. Section 9 expresses the general geometric phase as the integral of the projected solid angles in 2-subspaces, evaluated with an appropriately selected reference ray.

2. The difference density operator

A general wavefunction Ψ in the Hilbert space is shown of its norm and phase information, by multiplying it with a nonzero complex number, to be represented in the ray space by a normalized ray ψ. An n-state wavefunction therefore has a $\mathcal{C}P^{n-1}$ complex , i.e. $(2n-2)$ dimensional real, ray space. The pure state density operator $\rho = \Psi\Psi^{\dagger}/\Psi^{\dagger}\Psi = \psi\psi^{\dagger}$ is thus a ray space quantity with the properties : $\rho^{\dagger} = \rho, \rho^2 = \rho$ and $\mathrm{Tr}\rho = 1$. Furthermore, the density operator is gauge invariant, unlike the ray. Curves, surfaces and evolutions in the ray space can therefore be described in terms of the density operator in a gauge-independent manner.

For two distinct density operators $\rho_1 = \rho$ and $\rho_2 = \rho + \Delta\rho$, say, in the ray space, the difference operator $\Delta\rho$ is Hermitian and traceless. Using the equalities $(\rho+\Delta\rho)^2 = \rho+\Delta\rho$ and $\rho^2 = \rho$, we obtain

$$\Delta\rho = \rho\Delta\rho + (\Delta\rho)\rho + (\Delta\rho)^2 \ . \tag{1}$$

On post- and pre-multiplying eq. (1) with ρ, we get

$$(\Delta\rho)^2\rho = \rho(\Delta\rho)^2 = -\rho(\Delta\rho)\rho = \rho(\Delta\rho)^2\rho = \rho\mathrm{Tr}\rho(\Delta\rho)^2 = \rho(\Delta l)^2 \ . \tag{2}$$

Here $\Delta l = \Delta S/2$ denotes the semi-distance between the two rays, defined by the relation

$$(\Delta l)^2 = 1 - \mid \psi_1^{\dagger}\psi_2 \mid^2 = 1 - \mathrm{Tr}\rho(\rho + \Delta\rho) = -\mathrm{Tr}\rho\Delta\rho = \mathrm{Tr}\rho(\Delta\rho)^2 \ . \tag{3}$$

Equation (2) shows that the operator $(\Delta\rho)^2$ commutes with ρ. Similarly,

$$(\Delta\rho)^2(\rho + \Delta\rho) = (\rho + \Delta\rho)(\Delta\rho)^2 = (\rho + \Delta\rho)(\Delta l)^2 \ , \tag{4}$$

i.e. $(\Delta\rho)^2$ also commutes with $\rho + \Delta\rho$. It therefore commutes with every density operator representing an arbitrary linear combination of ψ_1 and ψ_2, i.e. belonging to the ray subspace shared by ρ_1 and ρ_2. This implies that

$$\left(\frac{\Delta\rho}{\Delta l}\right)^2 = \mathcal{I} \ , \tag{5}$$

$\mathcal{I}$ being the 2-dimensional projector, the unity operator for this 2-subspace $(\mathrm{Tr}\,\mathcal{I} = 2)$ and a null operator for all rays orthogonal to this subspace. Pre- or post-multiplying eq. (1) with $\Delta\rho$, dividing by $(\Delta l)^2$ and using eq. (5), we obtain

$$\left(\frac{\Delta\rho}{\Delta l}\right)^2 = \rho + \frac{\Delta\rho}{\Delta l}\rho\frac{\Delta\rho}{\Delta l} + \Delta\rho = \rho + \overline{\rho} = \mathcal{I} \ . \tag{6}$$

Thus the density operator $\overline{\rho} = (\Delta\rho/\Delta l)\rho(\Delta\rho/\Delta l) + \Delta\rho$ corresponds to the ray $\overline{\psi}_1$ orthogonal to ψ_1 and co-habiting the 2-subspace (cf. eq. (10)).

Any density operator belonging to this 2-subspace may be expressed as $\rho_a = (\mathcal{I} + \boldsymbol{\sigma} \cdot \mathbf{s}_a)/2$. The corresponding ray ψ_a then gets represented by the direction $\mathbf{s}_a = \mathrm{Tr}\rho_a\boldsymbol{\sigma}$ on the $\mathcal{C}P^1$ complex, i.e. 2-sphere real, ray subspace. Here $\boldsymbol{\sigma}$ is the vector of the Pauli spin operators in this 2-subspace and a null operator for rays orthogonal to the subspace. Hence the finite difference ratio

$$\frac{\Delta\rho}{\Delta l} = \boldsymbol{\sigma} \cdot \frac{\Delta\mathbf{s}}{\Delta S} = \sigma_{\mathrm{dif}} \ , \tag{7}$$

becomes the component of $\boldsymbol{\sigma}$ along the direction of the difference $\Delta\mathbf{s} = \mathbf{s_2} - \mathbf{s_1}$ between the respective directions in the 2-subspace associated with the rays ψ_2 and ψ_1. Since $\sigma_{\mathrm{dif}}^2 = \mathcal{I}$, the unitary operation

$$\exp\left(-i\sigma_{\mathrm{dif}}\alpha/2\right) = 1 - \mathcal{I} + \mathcal{I}\cos\frac{\alpha}{2} - i\frac{\Delta\rho}{\Delta l}\sin\frac{\alpha}{2} \ , \tag{8}$$

effects a rotation α about the direction $\Delta\mathbf{s}/\Delta S$ in this 2-subspace and leaves the remaining $n-2$ substates of the wavefunction, orthogonal to this subspace, unaltered. Here 1 is the full unity operator ($\mathrm{Tr}1 = n$).

The vector $\Delta\mathbf{s}$ bisects the directions $\mathbf{s_1}$ and $-\mathbf{s_2}$. A π rotation about $\Delta\mathbf{s}$ therefore takes $\mathbf{s_1}$ to $-\mathbf{s_2}$. Hence the operation (8) with $\alpha = \pi$ brings the ray ψ_1 to the ray $\overline{\psi}_2$ orthogonal to ψ_2 in the 2-subspace and represented by the density operator $\overline{\rho}_2$, i.e.

$$-i\frac{\Delta\rho}{\Delta l}\psi_1 = \overline{\psi}_2 \quad \Rightarrow \quad \overline{\rho}_2 = \overline{\rho + \Delta\rho} = \frac{\Delta\rho}{\Delta l}\rho\frac{\Delta\rho}{\Delta l} = \mathcal{I} - \rho_2 \ . \tag{9}$$

The same π rotation operation takes the unit vector $\mathbf{s_2}$ to $-\mathbf{s_1}$ and hence the ray ψ_2 to the ray $\overline{\psi}_1$ corresponding to the density operator $\overline{\rho}$ orthogonal to ρ in the 2-subspace. Thus

$$\overline{\rho}_1 = \overline{\rho} = \frac{\Delta\rho}{\Delta l}(\rho + \Delta\rho)\frac{\Delta\rho}{\Delta l} = \frac{\Delta\rho}{\Delta l}\rho\frac{\Delta\rho}{\Delta l} + \Delta\rho = \mathcal{I} - \rho \ . \tag{10}$$

For a non-orthogonal pair ρ_1, ρ_2, we can define a generator

$$\sigma_{\mathrm{sum}} = \frac{\rho_1 - \overline{\rho}_2}{\sqrt{\mathrm{Tr}\rho_1\rho_2}} = \frac{\rho - \frac{\Delta\rho}{\Delta l}\rho\frac{\Delta\rho}{\Delta l}}{\sqrt{1 - (\Delta l)^2}} = \boldsymbol{\sigma} \cdot \frac{\mathbf{s}_1 + \mathbf{s}_2}{\mid \mathbf{s}_1 + \mathbf{s}_2 \mid} \ , \tag{11}$$

viz. the component of $\boldsymbol{\sigma}$ along the vector sum of $\mathbf{s}_1$ and $\mathbf{s}_2$. The generator (11) operated on by σ_{dif} (7) leads to the generator

$$\begin{aligned} \sigma_{\perp} = i\sigma_{\mathrm{dif}}\sigma_{\mathrm{sum}} &= \frac{i[\rho_2, \rho_1]}{\sqrt{(1 - \mathrm{Tr}\rho_1\rho_2)\mathrm{Tr}\rho_1\rho_2}} \\ &= \frac{i[\frac{\Delta\rho}{\Delta l}, \rho]}{\sqrt{1 - (\Delta l)^2}} = \boldsymbol{\sigma} \cdot \frac{\mathbf{s}_1 \times \mathbf{s}_2}{\mid \mathbf{s}_1 \times \mathbf{s}_2 \mid} \ . \end{aligned} \tag{12}$$

Thus σ_{sum}, σ_{dif} and $\sigma_{\perp}$ form a trinity of $\boldsymbol{\sigma}$ components along the triad of orthogonal unit vectors parallel to $\mathbf{s}_1 + \mathbf{s}_2$, $\mathbf{s}_2 - \mathbf{s}_1$ and $\mathbf{s}_1 \times \mathbf{s}_2$, satisfying the familiar Pauli commutation and anticommutation relations. For the 2-subspace defined by ρ_1 and ρ_2 therefore, σ_{sum}, σ_{dif}, $\sigma_{\perp}$ and $\mathcal{I}$ constitute a complete set of generators. The ray 2-subspace is thus a unit 2-sphere of 'spin' directions $\mathbf{s}_a$ and the distance $2\Delta l$ between rays ψ_1 and ψ_2 is the length of the chord joining the tips of unit vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ on this 2-sphere. During the discussion of geodesics (§8), we will return to the generator $\sigma_{\perp}$.

3. Density operator and its differential

Applying the limit $\Delta l \to 0$ to eqs (1), (2), (3) and (5), we arrive at the following relations for the Hermitian and traceless differential $\mathrm{d}\rho$:

$$\mathrm{d}\rho = \rho \mathrm{d}\rho + (\mathrm{d}\rho)\rho \ , \tag{13}$$

$$\rho(\mathrm{d}\rho)\rho = \mathsf{O} \ , \quad \mathrm{Tr}\rho\mathrm{d}\rho = 0 \tag{14}$$

and

$$\left(\frac{\mathrm{d}\rho}{\mathrm{d}l}\right)^2 = \mathcal{I} = \rho + \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l} \ . \tag{15}$$

Equation (14) implies that $\mathrm{d}\rho\psi$ is orthogonal to ψ. Up to the irrelevant factor $-i$ in eq. (9), the unitary operation $\mathrm{d}\rho/\mathrm{d}l$ takes the ray ψ to its orthogonal ray $\overline{\psi}$ in the 2-subspace, i.e.

$$\frac{\mathrm{d}\rho}{\mathrm{d}l}\psi = \overline{\psi} \ , \tag{16}$$

corresponding to the density operator

$$\overline{\rho} = \overline{\psi\psi}^{\dagger} = \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l} \ , \tag{17}$$

orthogonal to ρ (cf. eq. (15)). One more operation $\mathrm{d}\rho/\mathrm{d}l$ brings the ray back to ψ, due to the identity (15). Each successive operation $\mathrm{d}\rho/\mathrm{d}l$ hence flips the ray between ψ and its orthogonal ray $\overline{\psi}$.

Any general differential variation $\mathrm{d}\rho$ in ρ therefore takes place in the 2-subspace of the orthogonal density operators ρ and $(\mathrm{d}\rho/\mathrm{d}l)\rho(\mathrm{d}\rho/\mathrm{d}l)$. As Δl approaches zero, the generator (11)

$$\sigma_{\mathrm{sum}} \to \sigma_s = \rho - \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l} = 2\rho - \mathcal{I} \ , \tag{18}$$

becomes the component of $\boldsymbol{\sigma}$ along the 'spin' direction $\mathbf{s} = \mathrm{Tr}\rho\boldsymbol{\sigma}$ of the equivalent spin-1/2 particle for the 2-subspace. In the limit $\Delta l \to 0$, the generators (7) and (12) likewise tend to

$$\sigma_{\mathrm{dif}} \to \frac{\mathrm{d}\sigma_s}{\mathrm{d}S} = \boldsymbol{\sigma}\cdot\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S} = \frac{\mathrm{d}\rho}{\mathrm{d}l} \tag{19}$$

and

$$\sigma_{\perp} \to \boldsymbol{\sigma}\cdot\mathbf{s}\times\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S} = i\left[\frac{\mathrm{d}\rho}{\mathrm{d}l}, \rho\right] \ , \tag{20}$$

respectively. For the local 2-subspace of the orthogonal density operators ρ and $(\mathrm{d}\rho/\mathrm{d}l)\rho(\mathrm{d}\rho/\mathrm{d}l)$, the three generators (18), (19), (20) form the components of $\boldsymbol{\sigma}$ along the orthogonal directions $\mathbf{s}$, $\mathrm{d}\mathbf{s}/\mathrm{d}S$ and $\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S$.

4. Curve length and energy uncertainty

Adjacent rays represented by density operators ρ and $\rho + \mathrm{d}\rho$ are separated by the infinitesimal length segment (cf. (3))

$$\mathrm{d}S = 2\mathrm{d}l = 2\sqrt{\mathrm{Tr}\rho(\mathrm{d}\rho)^2}\ . \tag{21}$$

Hence the length of any curve $\mathcal{C}$ traversed in the ray space is given by

$$S = 2\int_{\mathcal{C}} \sqrt{\mathrm{Tr}\rho(\mathrm{d}\rho)^2}\ . \tag{22}$$

Since

$$\mathrm{Tr}\rho(\mathrm{d}\rho)^2 = \psi^\dagger(\mathrm{d}\rho)^2\psi = \psi^\dagger(\mathrm{d}\rho)(\mathrm{d}\rho)\psi = [(\mathrm{d}\rho)\psi]^\dagger[(\mathrm{d}\rho)\psi] = ||(\mathrm{d}\rho)\psi||^2 \tag{23}$$

and

$$(\mathrm{d}\rho)\psi = \overline{\rho}\mathrm{d}\psi = (\mathcal{I} - \rho)\mathrm{d}\psi = \mathrm{d}\psi - \psi(\psi^\dagger\mathrm{d}\psi)\ , \tag{24}$$

it follows that

$$\mathrm{d}S = 2||(\mathrm{d}\rho)\psi||\ , \tag{25}$$

i.e. the elementary curve length $\mathrm{d}S$ identifies with twice the norm of the resolved part of $\mathrm{d}\psi$ orthogonal to ψ. The semi-curve length $\mathrm{d}l$ may be expressed as

$$(\mathrm{d}l)^2 = (\mathrm{d}\psi^\perp)^\dagger\mathrm{d}\psi^\perp\ , \tag{26}$$

where

$$\mathrm{d}\psi^\perp = \mathrm{d}\psi - (\psi^\dagger\mathrm{d}\psi)\psi\ , \tag{27}$$

symbolises the part of $\mathrm{d}\psi$ orthogonal to ψ. Comparing eqs (24) and (27), we note that

$$\mathrm{d}\psi^\perp = (\mathrm{d}\rho)\psi\ , \tag{28}$$

thus establishing the equivalence between the expressions (26) and (21) for the elementary curve length. The result (21) however expresses the gauge-invariant length element $\mathrm{d}S$ directly in terms of the gauge-invariant operators ρ and $\mathrm{d}\rho$.

So far we have taken the quantum kinematic approach, characterising the ray space purely in terms of a gauge-independent ray space quantity, viz. the density operator. We have taken recourse neither to a Hamiltonian driving a quantal system nor indeed to any equation governing the evolution of the system. Anandan and Aharonov [11] derived the curve length in the projective Hilbert (i.e. ray) space for a quantal system from its Schrödinger evolution in a Hermitian Hamiltonian $\mathcal{H}$. The corresponding density operator variation

$$i\hbar\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right) = [\mathcal{H}, \rho]\ , \tag{29}$$

operated on the wavefunction Ψ yields

$$i\hbar\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)\Psi=(\mathcal{H}\rho-\rho\mathcal{H})\Psi=\mathcal{H}\Psi-\langle\mathcal{H}\rangle\Psi=(\mathcal{H}-\langle\mathcal{H}\rangle\sigma_s)\Psi\ . \tag{30}$$

Hence the change $(\mathrm{d}\rho)\Psi$, orthogonal to Ψ, is produced in Ψ by the parallel transport Hamiltonian $\mathcal{H}-\langle\mathcal{H}\rangle\sigma_s$, viz. that part of the Hamiltonian $\mathcal{H}$ which effects a change in the *ray* ψ (cf. §7 and eqs (43) and (49)). The Hermitian conjugate of eq. (30), viz.

$$-i\hbar\Psi^\dagger\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)=\Psi^\dagger(\mathcal{H}-\langle\mathcal{H}\rangle\sigma_s)\ , \tag{31}$$

operated on eq. (30) yields

$$\hbar^2\Psi^\dagger\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)^2\Psi=\Psi^\dagger(\mathcal{H}-\langle\mathcal{H}\rangle\sigma_s)^2\Psi\ , \tag{32}$$

i.e.

$$\hbar^2\mathrm{Tr}\rho\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\right)^2=\langle\mathcal{H}^2\rangle-\langle\mathcal{H}\rangle^2=(\Delta E)^2\ . \tag{33}$$

Here ΔE signifies the energy uncertainty. The elementary curve length (21) therefore becomes

$$\mathrm{d}S=\frac{2\Delta E\mathrm{d}t}{\hbar} \tag{34}$$

and the finite curve length

$$S=\frac{2}{\hbar}\int_0^{\Delta t}\Delta E\mathrm{d}t=\frac{2}{\hbar}\langle\Delta E\rangle\Delta t\ , \tag{35}$$

$\langle\Delta E\rangle=\int_0^{\Delta t}\Delta E\mathrm{d}t/\Delta t$ denoting the time-averaged uncertainty in energy during the time interval Δt. For the curve length between two orthogonal rays which must at least equal π, viz. the geodesic (cf. §8) length, Anandan and Aharonov arrived at the relation [11]

$$\langle\Delta E\rangle\Delta t\geq\frac{h}{4} \tag{36}$$

and termed it a new and more stringent time-energy uncertainty principle. It is true that smaller the averaged uncertainty in energy, the longer a ray takes to traverse a given curve length S (eq. (35)). An eigenstate for instance has a null uncertainty in energy and the ray therefore remains stationary ($S=0$). However Δt here is the time taken to traverse a curve between a pair of orthogonal rays and does not quite represent the time uncertainty in the spirit of Heisenberg's principle. It would be more appropriate therefore to regard eq. (36) as just a restatement of the geometric fact that no curve joining a pair of orthogonal rays can ever be shorter than π in length.

5. Quantum search algorithm

In a classical computer, a search for a desired number from an array of n numbers involves, on an average, $(n+1)/2$ comparisons or 'queries'. On the other hand, the quantum computer search for a desired ray ψ_d from a given array of n rays stored in the form of a normalized n-state ray ψ_g, is implemented [12] with an algorithm making successive identical 'queries', Q in number, to reach as close as possible to the desired ray. Each query comprises the unitary operation $(2\rho_g - 1)(1 - 2\rho_d)$. As seen in §2, these operations are confined to the 2-subspace of ψ_g and ψ_d. In this 2-subspace, let the two rays be represented by 'spin' directions $\mathbf{s}_g$ and $\mathbf{s}_d$ respectively enclosing an angle ($\pi - \delta$), with an inner product $\psi_g^\dagger \psi_d = \sqrt{\mathrm{Tr}\rho_g \rho_d} = \sin(\delta/2) = 1/\sqrt{n}$. Applied to any ray in this 2-subspace, each of the quantum queries performs the operation (cf. eq. (18))

$$(2\rho_g - 1)(1 - 2\rho_d)\mathcal{I} = -\sigma_g \sigma_d = \mathcal{I}\cos\delta - i\sigma_\perp \sin\delta \ , \tag{37}$$

i.e. successive π rotations $-i\sigma_d$ and $-i\sigma_g$ about $\mathbf{s}_d$ and $\mathbf{s}_g$ respectively, yield a net rotation 2δ about the direction of the vector $\mathbf{s}_g \times \mathbf{s}_d$ in this 2-subspace. The net rotation $2Q\delta$ along the geodesic (cf. §8) between ψ_g and ψ_d, achieved in Q queries should equal the desired rotation $\pi - \delta$ to within $\pm\delta/2$, i.e. Q should be the integer closest to $(\pi/\delta - 1)/2 = [\pi/2 \arcsin(1/\sqrt{n}) - 1]/2$. For large arrays therefore, Q equals the integer closest to $(\pi\sqrt{n} - 2)/4$. In contrast to the linear rise with n of the number of classical queries, this rise with $\sqrt{n}$ of Q renders the quantum search a far more efficient and economic process.

We now explore the possibility of effecting the quantum search with a *single* query. For any two directions $\mathbf{s}_1$ and $\mathbf{s}_2$ in the $\mathbf{s}_g - \mathbf{s}_d$ plane and enclosing an angle $(\pi + \delta)/2$, the operation

$$-\sigma_1\sigma_2 = \mathcal{I}\cos\frac{\pi - \delta}{2} - i\sigma_\perp \sin\frac{\pi - \delta}{2} \ , \tag{38}$$

would produce the required rotation $(\pi - \delta)$ about $\mathbf{s}_\perp$ to take ψ_g to the desired ray ψ_d. In the special case $\mathbf{s}_2 = \mathbf{s}_g$, the direction $\mathbf{s}_1$ is given by $-\mathbf{s}_b$, where

$$\mathbf{s}_b = \frac{\mathbf{s}_g + \mathbf{s}_d}{2\sin(\delta/2)} = \frac{\sqrt{n}(\mathbf{s}_g + \mathbf{s}_d)}{2} \ , \tag{39}$$

denotes the bisector of $\mathbf{s}_d$ and $\mathbf{s}_g$. The corresponding component of the Pauli operator is expressible as σ_{sum} (cf. eq. (11)) for σ_d and σ_g, viz.

$$\sigma_b = \frac{\sqrt{n}(\sigma_g + \sigma_d)}{2} = \frac{\sqrt{n}(2\rho_g - \mathcal{I} + 2\rho_d - \mathcal{I})}{2} = \sqrt{n}(\rho_g + \rho_d - \mathcal{I}) \ . \tag{40}$$

Since the operation σ_g leaves the given ray ψ_g unaltered, the required query $-\sigma_{-b}\sigma_g$ can be replaced with just

$$-\sigma_{-b} = \sigma_b = 2\rho_b - \mathcal{I} \ \to \ 2\rho_b - 1 \ , \tag{41}$$

viz. a π rotation about the bisector $\mathbf{s}_b$. This quantum search therefore extracts the desired ray *exactly* in a *single* query. The proposed query (38), (41), when realized, will constitute a powerful search algorithm.

6. Ray space evolution

We will now extend results derived previously [13–19] for a 2-state system, epitomised by a spin-1/2 particle, to a general quantal system undergoing an arbitrary evolution $\rho(t)$ in the ray space. With each density operator ρ, we may associate a 'full' Pauli-like operator $\boldsymbol{\Sigma} \cdot \boldsymbol{\mathcal{S}} = 2\rho - 1$ and a corresponding 'full spin' $\boldsymbol{\mathcal{S}}$, defined over the entire $(2n-2)$ dimensional real ray space, having a one-to-one correspondence with ρ. As shown in §3, each infinitesimal step $\mathrm{d}\rho(t)$ in the evolution is confined to the 2-subspace of the two orthogonal density operators $\rho(t)$ and $\dot{\rho}\rho\dot{\rho}/\dot{l}^2$ and their sum $\mathcal{I}(t)$, the overdots signifying differentiation w.r.t. time t. During this infinitesimal evolution, the projection $\sigma_s = \mathcal{I}(t)\boldsymbol{\Sigma}\cdot\boldsymbol{\mathcal{S}}\mathcal{I}(t) = 2\rho - \mathcal{I}(t)$ of this operator in the instantaneous 2-subspace (cf. eq. (18)) alone becomes operational. The corresponding Pauli operator $\boldsymbol{\sigma}\cdot\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S$ (cf. eq. (20)) evolves the ray in the 2-subspace, thus changing only the projection $\mathbf{s}$ in this 2-subspace of the full spin $\boldsymbol{\mathcal{S}}$. The projection of $\boldsymbol{\mathcal{S}}$ in the remaining $(2n-4)$ dimensional ray-subspace orthogonal to this 2-subspace remains unaltered during this time interval $\mathrm{d}t$ at t. This infinitesimal evolution yields the density operator $\rho(t+\mathrm{d}t)$ with the associated full spin $\boldsymbol{\mathcal{S}}(t+\mathrm{d}t)$. The next step $\mathrm{d}\rho(t+\mathrm{d}t)$ may in general occur in another 2-subspace characterized by $\rho(t+\mathrm{d}t)$ and a corresponding $\mathcal{I}(t+\mathrm{d}t)$. As ρ evolves, a triad of mutually orthogonal directions in the ray space attached to $\mathbf{s}(t)$, gets transported through the instantaneous 2-subspaces, along the curve traversed in the ray space. A Hermitian Hamiltonian $\mathcal{H}$ effects a unitary evolution of the wavefunction. The corresponding ray space evolution $\rho(t)$ then satisfies the relation $[\mathcal{H}, \rho] = i\hbar\dot{\rho}$. Since each infinitesimal step $\mathrm{d}\rho(t)$ of this general evolution takes place in a 2-subspace, we can express the Hamiltonian at each instant t in terms of the generators (18), (19), (20) appropriate for the 2-subspace visited during the time interval $\mathrm{d}t$ at t. A given evolution $\rho(t)$ can thus be implemented by any member of the infinite set of Hermitian Hamiltonians

$$\mathcal{H}_s = \hbar\left\{i[\dot{\rho}, \rho] + \frac{\omega_s(t)}{2}\left(\rho - \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l}\right)\right\}\ , \tag{42}$$

$\omega_s(t)$ denoting an arbitrary real function of time. We have omitted here physically uninteresting terms in $\mathcal{I}$ and 1 which would just add $U(1)$ phases to the wavefunction. The set of interaction Hamiltonians may be expressed in terms of the local 2-subspace Pauli operators as

$$\mathcal{H}_s = \frac{\hbar}{2}\boldsymbol{\sigma}\cdot\{\mathbf{s}\times\dot{\mathbf{s}} + \omega_s(t)\mathbf{s}\}\ . \tag{43}$$

The ray space evolution corresponds to successive 'precessions' [13] of instantaneous 'spins' $\mathbf{s}(t)$ about 'magnetic fields' [14,15] $\boldsymbol{\omega}_B(t) = \mathbf{s}\times\dot{\mathbf{s}} + \omega_s(t)\mathbf{s}$, expressed in appropriate angular velocity units. Only the first term in $\mathcal{H}_s$ (42), (43) brings about the ρ variation, since the second term commutes with ρ. In a frame of reference r say, rotating with a time-dependent angular velocity $\mathbf{s}\times\dot{\mathbf{s}}$, the instantaneous changes in the full spin $\boldsymbol{\mathcal{S}}$ due to these rotations get continuously nullified. In this frame r, therefore the ray ψ and the full spin $\boldsymbol{\mathcal{S}}$ remain fixed at their initial values ψ_i and $\boldsymbol{\mathcal{S}}_i$, say, respectively. The inverse of the ordered product $U^{-1}(t)$ of successive unitary transformations given by

$$U^{-1}(t) = \mathcal{P}\exp\left(-i\int_0^t \boldsymbol{\sigma}\cdot\mathbf{s}\times\dot{\mathbf{s}}\mathrm{d}t/2\right), \tag{44}$$

yields the wavefunction $\Psi_r = U(t)\Psi$ in the rotating frame r. The wavefunction Ψ_r evolves satisfying the Schrödinger equation under the effective Hamiltonian [16]

$$\mathcal{H}_r = U\mathcal{H}_s U^{-1} + i\hbar\dot{U}U^{-1} = \frac{\hbar}{2}\omega_s(t)\boldsymbol{\sigma}\cdot\mathbf{S}_i\ , \tag{45}$$

for the rotating frame r, corresponding to a 'magnetic field' [16,17] of magnitude ω_s directed along the now stationary spin $\boldsymbol{\mathcal{S}}_i$. This Hamiltonian effects a rotation $\int\omega_s(t)\mathrm{d}t$ of $\boldsymbol{\mathcal{S}}_i$ about its own direction, implementing the evolution $\Psi_r(t) = \exp\{-\int i\omega_s(t)\mathrm{d}t/2\}\Psi_i$. The wavefunction in the lab frame is then derived by making the inverse transformation at time t, viz.

$$\Psi(t) = U^{-1}(t)\Psi_r(t) = \exp\left(-\int i\omega_s(t)\mathrm{d}t/2\right)\mathcal{P} \times \exp\left(-i\int_0^t \boldsymbol{\sigma}\cdot\mathbf{s}\times\dot{\mathbf{s}}\mathrm{d}t/2\right)\Psi_i\ . \tag{46}$$

The operations of the two terms in (42), (43) thus stand separated. The first term causes a variation of the ray while the second yields a pure dynamical phase [4,18]

$$\Phi_D = -\int\langle\mathcal{H}_r\rangle_r\mathrm{d}t/\hbar = -\frac{1}{2}\int\omega_s(t)\mathrm{d}t = -\int\langle\mathcal{H}_s\rangle\mathrm{d}t/\hbar\ . \tag{47}$$

The second term in the Hamiltonian (42), (43) is thus the exclusive source of the dynamical phase (47) acquired by the wavefunction during the evolution. The first term parallel transports the wavefunction and transports the full spin $\boldsymbol{\mathcal{S}}$ parallel to itself, generating a pure geometric phase as shown in the next section. An evolution wherein the final ray coincides with the initial ray ($\rho_f = \rho_i, \boldsymbol{\mathcal{S}}_f = \boldsymbol{\mathcal{S}}_i$), is said to be cyclic. The angle anholonomy associated with the parallel transport part of a cyclic evolution equals the sum Ω of solid angles spanned in the 2-subspaces traversed. The parallel transport operation is hence equivalent to a local spin rotation equal to the angle anholonomy Ω about $\boldsymbol{\mathcal{S}}_i$ $(= \boldsymbol{\mathcal{S}}_f)$ for the equivalent spin-1/2 particle, yielding $\exp(-i\boldsymbol{\Sigma}\cdot\boldsymbol{\mathcal{S}}_i\Omega/2)\Psi_i = \exp(-i\Omega/2)\Psi_i$. The geometric phase, viz. the parallel transport phase anholonomy, therefore is given by $-\Omega/2$. Geometric phase acquired in a noncyclic evolution ($\boldsymbol{\mathcal{S}}_f \neq \boldsymbol{\mathcal{S}}_i$) can similarly be obtained by suitably closing (cf. §9) the open curve between ψ_i and ψ_f traced in the ray space.

Experimentally, the first clear separation of geometric and dynamical phases was achieved neutron interferometrically [19]. For spin-polarized neutrons used in this experiment, geometric and dynamical phases arose from a relative rotation and translation respectively between π spin flippers in the two arms of the interferometer. In the neutron polarimetric version [20] of this experiment performed subsequently, agreement of the observed geometric and dynamical phases with theory was improved to about 1%.

Since in a noncyclic evolution, the final ray is distinct from the initial ray, the interference amplitude [2,3,21] is less than unity and varies with the noncyclicity. The interferogram for a noncyclic evolution is hence governed by both the phase and the amplitude. The first observation [22] of noncyclic amplitudes and phases was made in a neutron interference experiment. For neutrons polarized at an angle θ to $\hat{\mathbf{z}}$, the noncyclic evolution comprised a fractional revolution of the spin about a magnetic field $B\hat{\mathbf{z}}$ applied in one arm of the interferometer. The phase and amplitude for the noncyclic evolution were determined from the shift and attenuation respectively of the interference pattern relative to a pattern recorded simultaneously for a cyclic evolution.

7. Parallel transport

Kato [23] introduced the special Hamiltonian

$$\mathcal{H}_p = i\hbar[\dot{\rho}, \rho] \;, \tag{48}$$

as a generator of adiabatic evolutions. This Hamiltonian just equals the first term of the general Hamiltonian $\mathcal{H}_s$ (42), obtained by setting $\omega_s(t) = 0$. In terms of the local $\boldsymbol{\sigma}$ generators, it is expressible as

$$\mathcal{H}_p = \frac{\hbar}{2}\frac{\mathrm{d}S}{\mathrm{d}t}\boldsymbol{\sigma}\cdot\mathbf{s}\times\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S} \;, \tag{49}$$

Each infinitesimal step $\exp(-i\mathcal{H}_p\mathrm{d}t/\hbar)$ in the evolution under this Hamiltonian rotates $\mathbf{s}$ by $\mathrm{d}S$ about the direction $\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S$, transverse to $\mathbf{s}$. A triad in the ray space attached to $\mathbf{s}$ hence propagates without ever twisting about the local normals $\mathbf{s}$, i.e. gets transported parallel to itself. The infinitesimal evolution takes the wavefunction $\Psi(t)$ to

$$\begin{aligned}\Psi(t+\mathrm{d}t) &= \exp(-i\mathcal{H}_p\mathrm{d}t/\hbar)\Psi(t) = \exp(-i\boldsymbol{\sigma}\cdot\mathbf{s}\times\mathrm{d}\mathbf{s}/2)\Psi(t)\\ &= \left(\cos\left(\frac{\mathrm{d}S}{2}\right)\mathcal{I} + \sin\left(\frac{\mathrm{d}S}{2}\right)\boldsymbol{\sigma}\cdot\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S}\,\sigma_s\right)\Psi(t)\\ &= \cos(\mathrm{d}l)\Psi(t) + \sin(\mathrm{d}l)\overline{\Psi}(t) \;,\end{aligned} \tag{50}$$

which is in phase with $\Psi(t)$ in accordance with the Pancharatnam connection [2,3,5–7,21], since the inner product $\Psi^\dagger(t)\Psi(t+\mathrm{d}t) = \cos(\mathrm{d}l)$ is real positive [cf. (50)]. Here the normalized wavefunction $\overline{\Psi}(t) = (\mathrm{d}\rho/\mathrm{d}l)\Psi(t)$ is orthogonal to Ψ (cf. eqs (16), (19)). Such an evolution, wherein wavefunctions $\Psi(t)$ and $\Psi(t+\mathrm{d}t)$ before and after each infinitesimal duration $\mathrm{d}t$ are in phase, is said to parallel transport [6,24] the wavefunction. For any given ray space variation $\rho(t)$ therefore, the wavefunction Ψ can be parallel transported by choosing the Hermitian Hamiltonian $\mathcal{H}_p$ (48). When the direction $\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S$ is time dependent, the parallel transport is nontrivial. The triad $\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S - \mathbf{s} - \mathrm{d}\mathbf{s}/\mathrm{d}S$ attached to the 'field' $\mathbf{s}\times\dot{\mathbf{s}}$ then rotates with the instantaneous angular velocity [14,16],

$$\boldsymbol{\omega}_a(t) = \mathbf{s}\times\dot{\mathbf{s}} - \left|\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S)\right|\mathbf{s} \;, \tag{51}$$

viz. the difference between two mutually perpendicular vectors of magnitudes $|\mathbf{s}\times\dot{\mathbf{s}}| = |\dot{\mathbf{s}}|$ and $|\mathrm{d}(\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S)/\mathrm{d}t|$. The magnitude

$$\omega_a(t) = \sqrt{|\dot{\mathbf{s}}|^2 + \left|\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S)\right|^2} \;, \tag{52}$$

of this angular velocity can never be less than the magnitude $|\mathbf{s}\times\dot{\mathbf{s}}| = |\dot{\mathbf{s}}|$ of the precession rate for the spin $\mathbf{s}$. The direction $\mathbf{s}\times\mathrm{d}\mathbf{s}/\mathrm{d}S$ specifying the Hamiltonian $\mathcal{H}_p$ thus must change at least as fast as $\mathbf{s}$, which characterises the ray. A nontrivial parallel transport evolution is therefore *necessarily nonadiabatic* [16].

The dynamical phase $-\int\langle\mathcal{H}_p\rangle\mathrm{d}t/\hbar$ for the parallel transported wavefunction vanishes identically, since $\langle\mathcal{H}_p\rangle \equiv 0$. In the Hamiltonian $\mathcal{H}_p$, an initial wavefunction Ψ_i undergoes an ordered evolution $\mathcal{P}\exp\left(-i\int\mathcal{H}_p \mathrm{d}t/\hbar\right)$ to reach $\Psi_f = \mathcal{P}\exp\left(-i\int\boldsymbol{\sigma}\cdot\mathbf{s}\times\mathrm{d}\mathbf{s}/2\right)\Psi_i$, acquiring a phase [2,3,7]

$$\begin{aligned}\Phi_G &= \arg\ \Psi_i^\dagger\Psi_f = \arg\mathrm{Tr}\mathcal{P}\exp\left(-i\int\boldsymbol{\sigma}\cdot\mathbf{s}\times\mathrm{d}\mathbf{s}/2\right)\rho_i \\ &= \arg\mathrm{Tr}\mathcal{P}\exp\left(\int[\mathrm{d}\rho,\rho]\right)\rho_i\ ,\end{aligned} \tag{53}$$

which depends only on the geometry of the curve traced in the ray space. The phase anholonomy of a parallel transport evolution therefore is the geometric phase Φ_G. For a given ray space evolution $\rho(t)$, the geometric phase is independent of the actual Hamiltonian, i.e. of $\omega_s(t)$, selected from the infinite set $\mathcal{H}_s$ (42), (43), to implement the evolution.

In a general evolution effected by a Hamiltonian $\mathcal{H}_s$ (42), the parallel transport component $\mathcal{H}_p$ (48), viz. the first term in (42) corresponding to the component of the 'magnetic field' perpendicular to the instantaneous spin direction, alone evolves the spin and hence the ray, producing a concomitant pure geometric phase. The geometric phase is independent of the second term of $\mathcal{H}_s$ (42), (43), representing the component of the magnetic field along the spin $\mathbf{s}(t)$ which only makes the spin precess about its own direction, thus yielding the dynamical phase. The dynamical phase so generated by the non-parallel transport component of the evolution, is hence integrable and Hamiltonian-dependent, unlike the geometric phase.

8. Geodesics

The equation of a curve in the ray space can be expressed as $\rho = \rho(S)$, by specifying the density operator as a function of the curve length S measured from a fixed point on the curve. We consider a curve along which

$$\left[\rho, \frac{\mathrm{d}^2\rho}{\mathrm{d}S^2}\right] = \mathsf{O}\ , \tag{54}$$

which on integration implies that the commutator

$$i\left[\frac{\mathrm{d}\rho}{\mathrm{d}l},\rho\right] = \mathcal{K}\ , \tag{55}$$

say, remains invariant. Such a curve is a geodesic. In the Pauli operator representation,

$$i\left(\boldsymbol{\sigma}\cdot\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S}\right)(\boldsymbol{\sigma}\cdot\mathbf{s}) = \boldsymbol{\sigma}\cdot\mathbf{s}\times\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S} = \sigma_c \quad\Rightarrow\quad \mathbf{s}\times\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S} = \mathbf{c}\ , \tag{56}$$

i.e. the unit vector $\mathbf{c}$ denoting the direction normal to both $\mathbf{s}$ and $\mathrm{d}\mathbf{s}/\mathrm{d}S$ remains a constant all along a geodesic. A parallel transport evolution along this geodesic implemented by the Hamiltonian $\mathcal{H}_p = \hbar\dot{l}\mathcal{K}$ (cf. eqs (48), (49)) takes an initial wavefunction Ψ_i to

$$\Psi_f = \cos\left(\frac{S}{2}\right)\ \Psi_i + \sin\left(\frac{S}{2}\right)\ \overline{\Psi}_i\ . \tag{57}$$

Here the ray $\overline{\psi}_i$ orthogonal to the initial ray is separated from it by $S = \pi$ along the geodesic. The final wavefunction Ψ_f is in phase [2,3,7] with Ψ_i for traversed curve lengths $S < \pi$. The final ray ψ_f also remains constrained to the 2-subspace of the pair of orthogonal rays ψ_i and $\overline{\psi}_i$. Since a parallel transport evolution produces a pure geometric phase (cf. §7), geometric phase vanishes identically [5,6] along a geodesic (55) less than π in length.

A differentiation of the operator $\sigma_s = \rho - (\mathrm{d}\rho/\mathrm{d}l)\rho(\mathrm{d}\rho/\mathrm{d}l)$ (cf. eqs (18), (19)) along a geodesic, viz.

$$\frac{\mathrm{d}\left[\rho - \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l}\right]}{\mathrm{d}S} = 2\frac{\mathrm{d}\rho}{\mathrm{d}S} = \frac{\mathrm{d}\rho}{\mathrm{d}l} = -i\mathcal{K}\left[\rho - \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l}\right] = i\left[\rho - \frac{\mathrm{d}\rho}{\mathrm{d}l}\rho\frac{\mathrm{d}\rho}{\mathrm{d}l}\right]\mathcal{K}\ , \tag{58}$$

i.e.

$$\frac{\mathrm{d}\sigma_s}{\mathrm{d}S} = -i\left(\boldsymbol{\sigma}\cdot\mathbf{s}\times\frac{\mathrm{d}\mathbf{s}}{\mathrm{d}S}\right)(\sigma_s) = -i\mathcal{K}\sigma_s = i\sigma_s\mathcal{K}\ , \tag{59}$$

is obtained by just pre-multiplying it with the invariant operator $-i\mathcal{K}$ or postmultiplying with its Hermitian conjugate. Applying this result repeatedly, we get

$$\frac{\mathrm{d}^N\sigma_s}{\mathrm{d}S^N} = (-i\mathcal{K})^N\sigma_s\ , \tag{60}$$

for any positive integer N. The special case $N = 2$ yields the second derivative

$$\frac{\mathrm{d}^2\sigma_s}{\mathrm{d}S^2} = -\sigma_s\ \Rightarrow\ \frac{\mathrm{d}^2\mathbf{s}}{\mathrm{d}S^2} = -\mathbf{s}\ , \tag{61}$$

which brings about a mere change of sign in σ_s (and $\mathbf{s}$). A geodesic therefore represents an arc of a great circle for the spin $\mathbf{s}$ on the 2-sphere subspace of orthogonal density operators ρ and $(\mathrm{d}\rho/\mathrm{d}l)\rho(\mathrm{d}\rho/\mathrm{d}l)$. A geodesic between two rays ψ_1 and ψ_2 is hence the shortest possible curve joining them and lies wholly in their 2-subspace, its invariant $\mathcal{K}$ being the operator $\sigma_\perp$ (cf. eq. (12)) defined in terms of the commutator between ρ_1 and ρ_2.

We have defined a geodesic here as the curve along which the density operator commutes identically with its second derivative. Conventionally, a geodesic is defined as the shortest curve between any two rays through which it passes. We observe that the two definitions of a geodesic are equivalent.

9. Geometric phase

Geometric phase is the phase acquired by a parallel transported wavefunction and depends only on the ray space geometry. The basic building block of geometric phase is the Pancharatnam 3-vertex phase [2,3,7] associated with the triangle formed by shorter geodesics between mutually nonorthogonal rays ψ_0, ψ_1 and ψ_2, say. The wavefunction Ψ_0 subjected to two successive phase-preserving projections, i.e. filtering measurements, along rays ψ_1 and ψ_2 picks the 3-vertex geometric phase

$$\Phi_G^\Delta = \arg \mathrm{Tr}\rho_0\rho_2\rho_1 = \arg \mathrm{Tr}\rho_0\mathcal{I}\rho_2\rho_1\mathcal{I}$$
$$= \arg \mathrm{Tr}\mathcal{I}\rho_0\mathcal{I}\rho_2\rho_1 = \arg \mathrm{Tr}\rho_{0p}\rho_2\rho_1 \ . \qquad (62)$$

Here $\mathcal{I}$ is the unity operator (5) for the 2-subspace of ρ_1 and ρ_2. The density operator $\rho_{0p} = \mathcal{I}\rho_0\mathcal{I}/\mathrm{Tr}\rho_0\mathcal{I}$ represents the normalized ray $\psi_{0p} = \mathcal{I}\psi_0/\sqrt{\mathrm{Tr}\rho_0\mathcal{I}}$ along the projection $\mathcal{I}\psi_0$ of ψ_0 in the 2-subspace of ψ_1 and ψ_2. Using eq. (18), we may express the triangle phase (62) as

$$\tan\Phi_G^\Delta = -\frac{\mathbf{s}_{0p}\cdot\mathbf{s}_1\times\mathbf{s}_2}{1+\mathbf{s}_{0p}\cdot\mathbf{s}_1+\mathbf{s}_1\cdot\mathbf{s}_2+\mathbf{s}_2\cdot\mathbf{s}_{0p}} \Rightarrow \Phi_G^\Delta = -\frac{\Omega_p^\Delta}{2} \ . \qquad (63)$$

The 3-vertex geometric phase thus equals minus half the solid angle subtended by the spherical triangle formed by the shorter geodesics between ψ_{0p}, ψ_1 and ψ_2, i.e. by the shorter great circle arcs joining the tips of the unit spin vectors $\mathbf{s}_{0p}$, $\mathbf{s}_1$ and $\mathbf{s}_2$, at the centre of the 2-sphere ray subspace. The Pancharatnam triangle phase Φ_G^Δ hence depends solely on the ray space geometry. It vanishes if and only if the triangle encloses null area, i.e. if the rays ψ_{0p}, ψ_1 and ψ_2 lie on a single geodesic of length S less than π.

The triangle phase (62) can be expressed as

$$\sin\Phi_G^\Delta = -\sqrt{\frac{(1-\mathrm{Tr}\rho_{0p}\rho_1)(1-\mathrm{Tr}\rho_{0p}\rho_2)}{\mathrm{Tr}\rho_1\rho_2}}\sin\phi = -\frac{\Delta l_{p1}\Delta l_{p2}}{\sqrt{1-\Delta l_{12}^2}}\sin\phi \ , \qquad (64)$$

(cf. eq. (3)) in terms of the angle ϕ between the shorter geodesics joining ψ_{0p} to ψ_2 and ψ_1 and of the semidistances between the three pairs of these rays. In the limit ψ_1 tending to the ray $\overline{\psi}_{0p}$ orthogonal to ψ_{0p}, the triangle tends to an 'orange' slice between the two geodesics of length π each, joining ψ_{0p} and $\overline{\psi}_{0p}$. The phase Φ_G^Δ then tends to the angle ϕ. This is the phase jump encountered in a general evolution in passing a ray orthogonal to the reference ray ψ_0, discussed previously [6,7,14] and observed in interference [19,22] experiments.

If ψ_1 and ψ_2 are separated infinitesimally, $\rho_1 = \rho$ and $\rho_2 = \rho + \mathrm{d}\rho$, i.e. the spins $\mathbf{s}_1 = \mathbf{s}$ and $\mathbf{s}_2 = \mathbf{s} + \mathrm{d}\mathbf{s}$, the triangle phase becomes

$$\mathrm{d}\Phi_G^\Delta = -\frac{\mathrm{d}\Omega_p^\Delta}{2} = \frac{i\ \mathrm{Tr}\rho_{0p}[\rho,\mathrm{d}\rho]}{2\ \mathrm{Tr}\rho_{0p}\rho} = -(1-\mathrm{Tr}\rho_{0p}\rho)\mathrm{d}\phi = -\Delta l_p^2\mathrm{d}\phi \ , \qquad (65)$$

where Δl_p denotes the semidistance between ψ_{0p} and ψ, i.e. half the length of the chord joining the tips of unit spin vectors $\mathbf{s}_{0p}$ and $\mathbf{s}$.

The geometric phase $\Phi_G(\mathcal{C})$ acquired in any general evolution from ψ_i to ψ_f along a curve $\mathcal{C}$ can be obtained [6] by integrating the phases (65) associated with contiguous infinitesimal triangles having a common vertex ψ_0 and bases formed by infinitesimal segments of the curve $\mathcal{C}$. Such an integral

$$\Phi_G(\mathcal{C},\rho_0) = \int_{\rho_i}^{\rho_f}\mathrm{d}\Phi_G^\Delta = -\int_{\rho_i}^{\rho_f}\frac{\mathrm{d}\Omega_p^\Delta}{2}$$
$$= -\int_{\rho_i}^{\rho_f}(1-\mathrm{Tr}\rho_{0p}\rho)\mathrm{d}\phi = \Phi_G(\mathcal{C}) + \Phi_G^\Delta(\rho_0,\rho_i,\rho_f) \ , \qquad (66)$$

equals the sum [2,6] of the actual geometric phase acquired and the 3-vertex phase for the triangle $\psi_0 \to \psi_i \to \psi_f$. For a cyclic evolution, ($\mathcal{C}$ closed, i.e. $\rho_i = \rho_f$), the integral (66) yields the correct $\Phi_G(\mathcal{C})$ irrespective of the reference ρ_0 chosen, since the additional 3-vertex phase vanishes identically (cf. eq. (62)). A change of ρ_0 corresponds to a gauge transformation [6,14] of the ray ψ. The gauge freedom is therefore complete for a cyclic evolution. If $\mathcal{C}$ is open, however, the reference ray ψ_0 has to be selected so that the additional 3-vertex phase vanishes, i.e. ψ_{0p}, ψ_i and ψ_f lie on a single geodesic shorter than π. Here ψ_{0p} stands for the normalized projection of ψ_0 in the 2-subspace of ψ_i and ψ_f. The gauge freedom thus gets restricted for a noncyclic evolution.

Using a Stokes-like theorem, we may convert the line integral (66) into the integral [6,25]

$$\Phi_G(\mathcal{C}) = i\int_S \mathrm{Tr}\rho\mathrm{d}\rho \wedge \mathrm{d}\rho = -\int_S \frac{\mathrm{d}\Omega_p}{2}\ , \qquad (67)$$

of the curvature 2-form over the surface S enclosed by the curve $\mathcal{C}$, closed if necessary by joining its ends with the shorter geodesic. Since $\mathrm{d}\rho = \boldsymbol{\sigma}\cdot\mathrm{d}\mathbf{s}/2 = \boldsymbol{\sigma}\cdot(\mathrm{d}\theta\boldsymbol{\theta} + \sin\theta\mathrm{d}\phi\ \boldsymbol{\phi})/2$ (cf. eqs (18),(19)) in terms of the orthogonal triad $\mathbf{s}-\boldsymbol{\theta}-\boldsymbol{\phi}$ in the local 2-subspace [5], $\mathrm{Tr}\rho\mathrm{d}\rho\wedge\mathrm{d}\rho = i\sin\theta\mathrm{d}\theta\mathrm{d}\phi/2 = i\mathrm{d}\Omega_p/2$. The phase (67) is therefore just minus half the integral of the 2-subspace solid angles over the surface S in the ray space.

10. Conclusions

Two nonorthogonal density operators of a quantal system characterise a complete set of SU(2) generators (5), (7), (11), (12) for their 2-sphere ray-subspace. A quantum search algorithm harnessing these generators can retrieve a desired ray from an n-array with a *single* query (38), (41). Each infinitesimal displacement in the ray space takes place in the 2-subspace of orthogonal density operators ρ and $(\mathrm{d}\rho/\mathrm{d}l)\rho(\mathrm{d}\rho/\mathrm{d}l)$ (cf. eqs (15), (17)). It can therefore be treated as a 'spin' precession for the equivalent spin-1/2 particle in an effective magnetic field. Any general ray-space evolution comprises such successive 'spin' precessions in the local 2-subspaces. A Hamiltonian (48), (49) parallel transporting the 'spin' through successive 2-subspaces produces a pure geometric phase. Dynamical phase is the phase acquired in a rotating frame of reference r in which the 'spin' becomes stationary (cf. eqs (44), (45)), latched to the fixed direction of the effective magnetic field. A geodesic (cf. eqs (54), (55), (58), (61)) is an arc of a great circle on a 2-sphere ray subspace. An identically null geometric phase is obtained along a geodesic of length less than π. In any general ray-space evolution, the geometric phase (66), (67) equals minus half the integral of projected solid angles in the local 2-subspaces, evaluated with a proper choice of the reference ray.

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