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Geometric phase as a simple closed-form integral

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Abstract. For a general evolution of a quantal system, the geometric phase measured with reference to a given initial state is derived as an integral of a function of the pure state density operator by invoking the Pancharatnam connection continuously.

Keywords. Geometric phase; density operator; Pancharatnam connection.

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1. Introduction

It was a decade ago that a general nonintegrable, Hamiltonian-independent part of the phase, viz. geometric phase, was delineated [1] in the context of adiabatic quantal evolutions. The prevalence of geometric phase in completely general evolutions and in a wide range of physical phenomena has since been recognised. The origin of geometric phase has been traced to the anholonomy in the ray space [2] of a parallel transported [3, 4] quantum state. The geometric phase is thus a property of the ray space alone.

In this communication, we bring out in a simple manner the exclusive dependence of the geometric phase on the geometry of the curve C traced in the ray space, without any reference to the Hilbert space. We present the general geometric phase as an explicit closed-form integral in the ray space.

When a quantal system evolves from an initial state $|\psi_0\rangle$ to a state $|\psi\rangle$, it acquires a phase Φ prescribed by the Pancharatnam connection [3, 4] as

$$\exp(i\Phi) = \langle\psi_0|\psi\rangle / |\langle\psi_0|\psi\rangle| = \langle\psi_0|\psi\rangle / (\langle\psi_0|\psi\rangle\langle\psi|\psi_0\rangle)^{1/2}. \tag{1}$$

Hence

$$i\mathrm{d}\Phi = \langle\psi_0|\mathrm{d}\psi\rangle/\langle\psi_0|\psi\rangle - \tfrac{1}{2}\langle\psi_0|\mathrm{d}(|\psi\rangle\langle\psi|)|\psi_0\rangle/(\langle\psi_0|\psi\rangle\langle\psi|\psi_0\rangle).$$

i.e.

$$\Phi = \tfrac{1}{2}i\int_{|\psi_0\rangle}^{|\psi\rangle}\{\langle\psi_0|(|\psi\rangle\langle\mathrm{d}\psi| - |\mathrm{d}\psi\rangle\langle\psi|)|\psi_0\rangle/(\langle\psi_0|\psi\rangle\langle\psi|\psi_0\rangle)\}. \tag{1a}$$

The integrable, Hamiltonian-dependent part of this phase Φ, viz. the dynamical phase Φ_D, can be expressed as [2, 5]

$$\Phi_D = \mathrm{Im}\int_{|\psi_0\rangle}^{|\psi\rangle}\{\langle\psi|\mathrm{d}\psi\rangle/\langle\psi|\psi\rangle\}$$

$$= -\tfrac{1}{2}i\int_{|\psi_0\rangle}^{|\psi\rangle}\{(\langle\psi|\mathrm{d}\psi\rangle - \langle\mathrm{d}\psi|\psi\rangle)/\langle\psi|\psi\rangle\}$$

$$= -\tfrac{1}{2}i\int_{|\psi_0\rangle}^{|\psi\rangle}\{\langle\psi_0|(\rho|\mathrm{d}\psi\rangle\langle\psi| - |\psi\rangle\langle\mathrm{d}\psi|\rho)|\psi_0\rangle/(\langle\psi_0|\psi\rangle\langle\psi|\psi_0\rangle)\}. \tag{2}$$

Here $\rho = |\psi\rangle\langle\psi|/\langle\psi|\psi\rangle$, represents the pure state density operator with the familiar properties: $\rho^\dagger = \rho, \rho^2 = \rho$ and $\mathrm{tr}(\rho) = 1$. The operator ρ remains unaltered if $|\psi\rangle$ is multiplied by a complex number. Thus the information about the variations in the phase and the norm of $|\psi\rangle$ is switched off in the ρ representation. Therefore ρ yields an image of $|\psi\rangle$ in the ray space.

The remaining part of Φ, viz. the geometric phase, therefore equals

$$\Phi_G = \Phi - \Phi_D = \tfrac{1}{2}i\int_{\rho_0}^{\rho}\left\{\langle\psi_0|[\rho,\mathrm{d}\rho]|\psi_0\rangle/\langle\psi_0|\rho|\psi_0\rangle\right\}$$
$$= \tfrac{1}{2}i\int_{\rho_0}^{\rho}\{\mathrm{tr}\,\rho_0[\rho,\mathrm{d}\rho]/\mathrm{tr}\,\rho_0\rho\}. \tag{3}$$

Geometric phase thus originates directly from the noncommutability between the density operator and its differential and from the consequent geometric anholonomy in the ray space.

If the final ray is orthogonal to the initial ray, i.e. $\langle\psi_0|\psi\rangle = 0$ and $\rho_0\rho = \mathbf{0}$, the total phase Φ and therefore the geometric phase Φ_G, becomes indeterminate (eqs (1) and (3)). However for a nonorthogonal final ray, (3) is valid even if the curve C passes through an orthogonal ray during its evolution. At the orthogonal ray, both the numerator and denominator of the integrand in (3) vanish, yet the integrand is determinate, given by its limit at the orthogonal ray along C.

Since ρ and $\mathrm{d}\rho$ are both Hermitian operators, (3) can be rewritten as

$$\Phi_G = -\,\mathrm{Im}\int_{\rho_0}^{\rho}\{\mathrm{tr}\,\rho_0\rho\mathrm{d}\rho/\mathrm{tr}\,\rho_0\rho\}$$
$$= i\int_{\rho_0 \atop \mathrm{C}}^{\rho}\{\mathrm{tr}\,\rho_0(\rho - \tfrac{1}{2}\mathbf{1})\mathrm{d}\rho/\mathrm{tr}\,\rho_0\rho\}. \tag{4}$$

as the Hermitian part of $\rho\mathrm{d}\rho$ equals $[\rho\mathrm{d}\rho + (\mathrm{d}\rho)\rho]/2 = \mathrm{d}(\rho^2)/2 = \mathrm{d}\rho/2$. The symbol $\mathbf{1}$ denotes the unity operator. Equation (4) expresses the geometric phase as a simple closed-form integral purely over the parameters in the ray space, thus bringing out the sole dependence of Φ_G on the the geometry of the curve C traced out in the ray space. This relation holds for a general evolution; it does not require the evolution to be adiabatic, cyclic or even unitary. The relation (4) is identical to the equation

$$\Phi_G = i\int_C\langle\tilde{\psi}|\mathrm{d}\tilde{\psi}\rangle, \tag{5}$$

with $|\tilde{\psi}\rangle = |\psi\rangle\exp(-i\Phi)/\langle\psi|\psi\rangle^{1/2}$ symbolising the normalized form of $|\psi\rangle\exp(-i\Phi)$, Φ being specified by the Pancharatnam connection (1). In the special case of a unitary cyclic evolution, the curve C gets closed and (5) for Φ_G reduces to the nonadiabatic geometric phase [2] derived previously.

We illustrate the result (4) by applying it to the case of a 2-state system as a spin 1/2 particle. Here

$$\rho = (1 + \mathbf{s}\cdot\boldsymbol{\sigma})/2, \tag{6}$$

where $\mathbf{s} = \langle\psi|\boldsymbol{\sigma}|\psi\rangle$ denotes a unit vector in the direction of the 'spin', $\boldsymbol{\sigma}$ signifying the vector of the Pauli spin operators. Then

$$\begin{aligned}(\rho - \tfrac{1}{2}1)\mathrm{d}\rho &= \tfrac{1}{4}(\mathbf{s}\cdot\boldsymbol{\sigma})(\mathrm{d}\mathbf{s}\cdot\boldsymbol{\sigma}) = \tfrac{1}{4}i(\mathbf{s}\times \mathrm{d}\mathbf{s})\cdot\boldsymbol{\sigma})\\ &= \tfrac{1}{4}i(-\sin\theta \mathrm{d}\phi\,\hat{\theta} + \mathrm{d}\theta\,\hat{\phi})\cdot\boldsymbol{\sigma}.\end{aligned} \tag{7}$$

Here (θ, ϕ) stand for the polar coordinates of s on the unit sphere of spin directions. The mutually orthogonal unit vectors

$$\begin{aligned}\mathbf{s} &= (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)\\ \hat{\theta} &= (\cos\theta\cos\phi,\ \cos\theta\sin\phi,\ -\sin\theta)\ \text{and}\\ \hat{\phi} &= (-\sin\phi,\ \cos\phi,\ 0)\end{aligned} \tag{7a}$$

directed respectively along the local surface normal, longitude and latitude on the spin sphere form a right-handed triad [6]. The geometric phase (4) then becomes

$$\Phi_G = -\tfrac{1}{2}\int_{C} (\mathbf{s}_0\cdot\mathbf{s}\times \mathrm{d}\mathbf{s})/(1 + \mathbf{s}\cdot\mathbf{s}_0), \tag{8}$$

$\mathbf{s}_0 = \langle\psi_0|\boldsymbol{\sigma}|\psi_0\rangle$ representing the initial spin direction. A substitution from (7) and (7a) in (8) leads to the result [6]

$$\begin{aligned}\Phi_G &= \tfrac{1}{2}\left\{\int_{C\,(\theta_0,\phi_0)}^{(\theta,\phi)} \cos\theta\,\mathrm{d}\phi - \arctan\{\cos\tfrac{1}{2}(\theta_0 + \theta)\tan\tfrac{1}{2}(\phi - \phi_0)/\cos\tfrac{1}{2}(\theta_0 - \theta)\right\}\\ &= -\tfrac{1}{2}\Omega(C),\ \text{mod}\ 2\pi,\end{aligned} \tag{9}$$

derived previously. Here Ω (C) denotes the solid angle subtended at the centre of the spin sphere by the closed circuit obtained by joining [3, 4] the ends (θ, ϕ) and (θ_0, ϕ_0) of C with the shorter arc of the great circle passing through them.

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