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Geometric phases for mixed states during cyclic evolutions

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Abstract
The geometric phases of cyclic evolutions for mixed states are discussed in the framework of unitary evolution. A canonical 1-form is defined whose line integral gives the geometric phase, which is gauge invariant. It reduces to the Aharonov and Anandan phase in the pure state case. Our definition is consistent with the phase shift in the proposed experiment (Sjöqvist *et al* 2000 *Phys. Rev. Lett.* **85** 2845) for a cyclic evolution if the unitary transformation satisfies the parallel transport condition. A comprehensive geometric interpretation is also given. It shows that the geometric phases for mixed states share the same geometric sense with the pure states.

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1. Introduction

When a pure quantal state undergoes a cyclic evolution the system returns to its original state but may acquire a nontrivial phase factor of purely geometric origin. This was first discovered by Berry [1] in the adiabatic context, and generalized to non-Abelian by Wilczek and Zee [2]. A nice interpretation was given by Simon [3] in terms of a natural Hermitian connection, as the parallel transport holonomy in a Hermitian line bundle. An extension to the nonadiabatic cyclic case was given by Aharonov and Anandan [4]. Based on Pancharatnam's earlier work on interference of light [5], this concept was generalized to noncyclic evolutions and nonunitary evolutions [6, 7]. The geometric phases for entangled states have also been discussed [8]. Applications of the geometric phase have been found in molecular dynamics [9], response function of the many-body system [10] and geometric quantum computation [11]. In all these developments the geometric phases have been discussed only for pure states. However, in some applications we are interested in mixed state cases [11, 12].

Uhlmann was probably the first to address the issue of mixed state in the context of purification, but as a purely mathematical problem [13]. Recently, Sjöqvist *et al* [12] gave a new formalism of the geometric phase for mixed state in the experimental context of quantum interferometry under parallel transport condition. It has been pointed out [14] that the latter geometric phase can be undefined at nodal points in the parameter space where the interference visibility vanishes. Anyway, the geometric phases for mixed states proposed in [12, 13] are generically different in the unitary case and match only under very special conditions such as in terms of pure states [15].

In this paper, we give a definition of the geometric phase for a cyclic evolution of mixed quantal state in the dynamical context of a quantum system. The reasons for employing the cyclic evolution are two: (i) the cyclic evolution of a physical system is of most interest in physics both experimentally and theoretically, (ii) the phase shift in a cyclic evolution should be definite. Firstly, we give a straightforward generalization of the Aharonov and Anandan (AA) phase for the global cyclic evolution where the total phase is explicit. Though this case seems a trivial extension of the AA phase, it contains the essence of geometric phase of mixed state. Then, we give the discussion of the general case based on a definition of the total phase. This geometric phase reduces to the AA phase [4], the standard geometric phase for pure state undergoing a cyclic evolution. We find that if the evolution satisfies the parallel transport condition the geometric phase is consistent with the result in [12]. Moreover, we give the geometric meaning of the geometric phases of mixed states which share the same sense with the pure states for the first time.

2. Geometric phases for mixed states

Supposing a quantum system with the Hamiltonian $H(t)$, the density operator $\rho(t)$ of this system undergoes the following evolution:

$$\rho(t) = U(t)\rho(0)U^{+}(t) \tag{1}$$

where $U(t) = \mathbf{T}\,\mathrm{e}^{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'/\hbar}$ is a unitary transformation, here $\mathbf{T}$ is the chronological operator. If $U(\tau)$ and $\rho(0)$ are commutative: $[U(\tau), \rho(0)] = 0$, i.e., $\rho(\tau) = \rho(0)$, we say this state undergoes a cyclic evolution with period τ. Furthermore, if $U(\tau) = \mathrm{e}^{\mathrm{i}\phi} I$, this evolution can be called the global cyclic evolution since for any $\rho(0)$ we have $\rho(\tau) = \rho(0)$.

At first, we study the case of the global cyclic evolution. Now define $\widetilde{U}(t) = \mathrm{e}^{-\mathrm{i}\phi(t)} U(t)$ such that $\widetilde{U}(\tau) = I$. We define the geometric phase for such a state during the global cyclic evolution as

$$\phi_g = \mathrm{i}\int_0^{\tau} \mathrm{Tr}\left[\rho(0)\widetilde{U}^{+}(t)\frac{\mathrm{d}\widetilde{U}(t)}{\mathrm{d}t}\right]\mathrm{d}t. \tag{2}$$

Using the transformation between $\widetilde{U}(t)$ and $U(t)$, one can have

$$\phi_g = \phi - \phi_d \tag{3}$$

and

$$\begin{aligned}\phi_d &= -\mathrm{i}\int_0^{\tau}\mathrm{d}t\,\mathrm{Tr}\left[\rho(0)U^{+}(t)\frac{\mathrm{d}U(t)}{\mathrm{d}t}\right] \\ &= -\frac{1}{\hbar}\int_0^{\tau}\mathrm{d}t\,\mathrm{Tr}[\rho(t)H(t)].\end{aligned} \tag{4}$$

Obviously ϕ_d is just the dynamical phase during the cyclic evolution.

We can prove that if $\rho(t)$ is the density operator of a pure state the geometric phase defined by equation (2) is just the Aharonov and Anandan phase [4]. Assuming

$\rho(0) = |\psi(0)\rangle\langle\psi(0)|$, $|\psi(t)\rangle = U(t)|\psi(0)\rangle$. Let $|\varphi(t)\rangle = \mathrm{e}^{-\mathrm{i}\phi(t)}|\psi(t)\rangle$, then we have $|\varphi(t)\rangle = \widetilde{U}(t)|\varphi(0)\rangle$. So, equation (2) can be written as $\phi_g = \mathrm{i}\int_0^\tau \langle\varphi(t)|\dot{\varphi}(t)\rangle\,\mathrm{d}t$ which is just the result of [4].

An initial state can always be diagonalized, namely,

$$\rho(0) = \sum_k w_k |k\rangle\langle k| \tag{5}$$

where $|k\rangle$ are bases for the system and w_k are classical probability of finding a member of the ensemble in the corresponding state. For the global cyclic evolution we have $U(\tau)|k\rangle = \mathrm{e}^{\mathrm{i}\phi}|k\rangle$, then the AA phase of $|k\rangle$ is $\phi_g^k = \phi - \phi_d^k$, where $\phi_d^k = -\frac{1}{\hbar}\int_0^\tau \mathrm{d}t\,\mathrm{Tr}[|k\rangle\langle k|U^+(t)\dot{U}(t)]$. Substituting (5) into (4), and from (3) we obtain

$$\phi_g = \phi - \sum_k w_k\phi_d^k = \sum_k w_k\phi_g^k. \tag{6}$$

So, for the global cyclic evolution the geometric phases of mixed states have explicit meanings: the geometric phases of a mixed state are the weighted average of the geometric phases of the constituent pure states.

Example I. Suppose that a qubit (a spin-$\frac{1}{2}$ particle) with a magnetic moment is in a homogenous magnetic field $\mathbf{B}$ along the z-axis. Then the Hamiltonian in the rest frame is $H = -\mu B\sigma_z$. Suppose the initial state is

$$\rho(0) = \tfrac{1}{2}[I + r(\sin\theta\sigma_x + \cos\theta\sigma_z)] \tag{7}$$

where r is a constant and $0 \leqslant r \leqslant 1$. So we have $\rho(t) = U(t)\rho(0)U^+(t)$ with

$$U(t) = \exp(\mathrm{i}\mu Bt\sigma_z/\hbar). \tag{8}$$

This unitary evolution is periodic with period $\tau = \pi\hbar/\mu B$, i.e., $\rho(\tau) = \rho(0)$. It is easy to see that $U(\tau) = \exp(\mathrm{i}\pi)I$. Let $\widetilde{U}(t) = \mathrm{e}^{-\mathrm{i}\mu Bt/\hbar}U(t)$, then $\widetilde{U}(\tau) = U(0)$. From equation (2), and after some elaboration we can obtain the geometric phase

$$\phi_g = \pi(1 - r\cos\theta). \tag{9}$$

Obviously, if $r = 1$, we get $\phi_g = \pi(1 - \cos\theta)$ which is just the AA phase [4].

On the other hand, we can have two pure states $\rho_1(0) = \frac{1}{2}[I + (\sin\theta\sigma_x + \cos\theta\sigma_z)]$ and $\rho_2(0) = \frac{1}{2}[I + (\sin(\pi+\theta)\sigma_x + \cos(\pi+\theta)\sigma_z)]$, which can construct a set of orthonormal bases. From (7), we have $\rho(0) = \frac{1+r}{2}\rho_1(0) + \frac{1-r}{2}\rho_2(0)$. Obviously, this is a diagonal representation of the initial state $\rho(0)$. Then from equation (6), we can obtain $\phi_g = \frac{1+r}{2}\pi(1-\cos\theta) + \frac{1-r}{2}\pi(1-\cos(\pi+\theta)) = \pi(1 - r\cos\theta)$.

The above discussion of the general cyclic evolution seems a trivial extension of the AA phase, but it contains the essence of geometric phase of the mixed state.

For the general case of a cyclic evolution, the density matrix and transformation satisfy $[U(\tau), \rho(0)] = 0$. We cannot find the total phase explicitly from this condition. To factor out the total phase, we use the Pancharatnam's brilliant idea, i.e., the Pancharatnam connection [5]. We define the total phase of the mixed state during a cyclic evolution with the initial state $\rho(0)$ and the unitary transformation $U(t)$ as

$$\phi = \arg\mathrm{Tr}[\rho(0)U(\tau)]. \tag{10}$$

Let $\widetilde{U}(t) = \mathrm{e}^{-\mathrm{i}\phi(t)}U(t)$ such that $\phi(\tau) = \phi$. Based on this definition, the geometric phase of the cyclic evolution can also be defined by equation (2). Obviously, the geometric phase for a cyclic evolution takes the same form as in equation (3). Indeed equation (2) defines a canonical 1-form in the parameter space

$$\beta = \mathrm{i}\,\mathrm{Tr}[\rho(0)\widetilde{U}^+(t)\,\mathrm{d}\widetilde{U}(t)]. \tag{11}$$

It is not difficult to prove that β is a real number. The geometric phase can be obtained by its line integral, i.e.,

$$\phi_g = \oint \beta. \tag{12}$$

The equivalent of the above formula for the pure states case is well known [7, 16].

The geometric phase defined above is manifestly gauge invariant: it does not depend on the dynamics, but depends only on the geometry of the close unitary path given by the unitary transformation $U(t)$. Assuming α is a dynamic parameter of this system, the nature of the cyclic evolution requires $\alpha(0) = \alpha(\tau)$ [1]. Under the transformation $\widetilde{U}(t)' = \mathrm{e}^{\mathrm{i}\delta(\alpha)}\widetilde{U}(t)$, we can have $\beta' = \beta - \mathrm{d}\delta$. It is easy to prove that $\oint \beta' = \oint \beta$ since $\delta(a(\tau)) = \delta(a(0))$. Indeed the quantity $\beta = \mathrm{i}\,\mathrm{Tr}[\rho(0)\widetilde{U}^{+}(t)\,\mathrm{d}\widetilde{U}(t)]$ can be regarded as a gauge potential on the space of density operators pertaining to the system.

Example II. Consider a spin-$\frac{1}{2}$particle is initially in the state

$$\rho(0) = \tfrac{1}{2}(I + r\sigma_z) \tag{13}$$

where $r \leqslant 1$ is a constant. Suppose this particle is in a magnetic field $\mathbf{B}(t)$ with

$$\mathbf{B}(t) = \begin{cases} -(\omega\hbar/\mu)\widehat{e}_y & 0 \leqslant t \leqslant t_1 \\ -(\omega\hbar/\mu)\widehat{e}_z & t_1 \leqslant t \leqslant t_2 \\ -(\omega\hbar/\mu)(\sin\varphi\widehat{e}_x - \cos\varphi\widehat{e}_y) & t_2 \leqslant t \leqslant \tau \end{cases} \tag{14}$$

in which ω is a constant and $t_1 = \frac{\theta}{2\omega}$, $t_2 = \frac{\theta+\varphi}{2\omega}$ and $\tau = \frac{2\theta+\varphi}{2\omega}$. So, the unitary transformation is

$$U(t) = \begin{cases} \mathrm{e}^{-\mathrm{i}\omega t\sigma_y} & 0 \leqslant t \leqslant t_1 \\ \mathrm{e}^{-\mathrm{i}\omega(t-t_1)\sigma_z}\,\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}\sigma_y} & t_1 \leqslant t \leqslant t_2 \\ \mathrm{e}^{-\mathrm{i}\omega(t-t_2)(\sin\varphi\sigma_x - \cos\varphi\sigma_y)}\mathrm{e}^{-\mathrm{i}\frac{\varphi}{2}\sigma_z}\,\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}\sigma_y} & t_2 \leqslant t \leqslant \tau. \end{cases} \tag{15}$$

Then, $U(\tau) = \exp\left(-\mathrm{i}\frac{\theta}{2}(\sin\varphi\sigma_x - \cos\varphi\sigma_y)\,\mathrm{e}^{-\mathrm{i}\frac{\varphi}{2}\sigma_z}\,\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}\sigma_y}\right)$. We can prove that $U(\tau)\rho(0)$ $U^{+}(\tau) = \rho(0)$. Under this unitary transformation, the state undergoes a cyclic evolution with a closed path of the corresponding Bloch vector as shown in figure 1, where the vectors at points B and C are $\mathbf{r}_B = (r\sin\theta, 0, r\cos\theta)$ and $\mathbf{r}_C = (r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta)$, respectively. From equations (10) and (4), we have the total phase of this cyclic evolution $\phi = -\arctan\left[r\tan\frac{\varphi}{2}\right]$, and the dynamic phase $\phi_d = -\frac{\varphi}{2}r\cos\theta$. Then, the geometric phase of this cyclic evolution is

$$\phi_g = -\arctan\left[r\tan\frac{\varphi}{2}\right] + \frac{\varphi}{2}r\cos\theta. \tag{16}$$

We know that if $\theta = \frac{\pi}{2}$ the closed path on the Bloch sphere is geodesic [17], i.e., the dynamical phase is zero. At this time the geometric phase is $-\arctan\left[r\tan\frac{\varphi}{2}\right]$, which has also been pointed out in [12] and verified by the recent experimental observations [18].

If $\varphi = 2\pi$, i.e., the points B and C in figure 1 are the same. Obviously, the geometric phase for such a path should be equal to the case in example I except for the direction of magnetic field reversed. From (16), we have $\phi_g = \pi(1 + r\cos\theta)$ which is consistent with equation (9).

From our definition of the geometric phase, we can obtain a theorem for a composite quantum system.

Theorem. *Let ρ^{AB} be a density operator of a composite quantum system of A and B. If the system evolves under the unitary transformation $U(t) = I^A \otimes U^B$ with $U^B = \mathbf{T}\,\mathrm{e}^{-\mathrm{i}\int_0^t H(t')\,\mathrm{d}t'/\hbar}$*

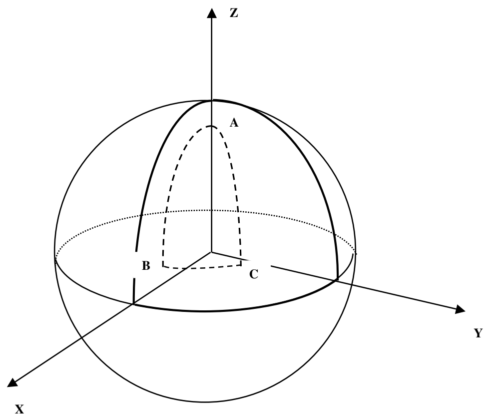

Figure 1. A path with cyclic evolution of the Bloch vector. The solid line represents a geodesic path of the unitary pure state case and defines a spherical triangle enclosing the solid angle $\pi/2$. The dashed line represents the closed path of the mixed state with the unitary evolution defined by (15), where the initial state is given in equation (13).

and $[\rho^{AB}, U(\tau)] = 0$*, then the geometric phase of such a composite system equals one of the subsystem B, i.e.,* $\phi_g^{AB} = \phi_g^B$.

The density operator of such a system can be expressed by

$$\rho^{AB} = \frac{1}{N_A N_B}\big[I^A \otimes I^B + \mathbf{r}^A \cdot \vec{\lambda}^A \otimes I^B + I^A \otimes \mathbf{r}^B \cdot \vec{\lambda}^B + \beta_{ij}\lambda_i^A \otimes \lambda_j^B\big] \tag{17}$$

where N_A and N_B are the orders of density matrices for each subsystems, $\vec{\lambda}^A = \big(\lambda_i^A; i = 1, 2, \ldots, N_A^2 - 1\big)$ and $\vec{\lambda}^B = \big(\lambda_i^A; i = 1, 2, \ldots, N_B^2 - 1\big)$ are the generators of $SU(N_A)$ and $SU(N_B)$ respectively, $\mathbf{r}^A = \big(r_i^A; i = 1, 2, \ldots, N_A^2 - 1\big)$ and $\mathbf{r}^B = \big(r_i^B; i = 1, 2, \ldots, N_B^2 - 1\big)$ are two vectors, and β_{ij} are $\big(N_A^2 - 1\big)\big(N_B^2 - 1\big)$ real numbers. Because $\mathrm{Tr}\big(\lambda_i^{A,B}\big) = 0$, one can have $\phi^{AB} = \arg \mathrm{Tr}[\rho^{AB} U(\tau)] = \arg \mathrm{Tr}[\rho^B U^B(\tau)]$ where ρ^B is the reduced density operator for B, i.e., $\rho^B = \frac{1}{N_B}[I^B + \mathbf{r}^B \cdot \vec{\lambda}^B]$. From (4), we can also obtain $\phi_d^{AB} = -\mathrm{i}\int \mathrm{Tr}[\rho^{AB} U^+(t)\dot{U}(t)] = -\mathrm{i}\int \mathrm{Tr}[\rho^B U^{B^+}(t)\dot{U}^B(t)]$. So the geometric phase for ρ^{AB} is $\phi_g^{AB} = \phi^{AB} - \phi_d^{AB} = \phi^B - \phi_d^B$, where $\phi^B = \arg \mathrm{Tr}[\rho^B U^B(\tau)]$ and $\phi_d^B = -\mathrm{i}\int \mathrm{Tr}[\rho^B U^{B^+}(t)\dot{U}^B(t)]$. The geometric phase of the subsystem B is $\phi_g^B = \phi^B - \phi_d^B = \phi_g^{AB}$.

We know that for a pure state of an entangled composite quantum system ρ^{AB}, the reduced density operators $\rho^{A,B}$ are mixed states. So this theorem may have some important applications, at least to observe the geometric phase for mixed state, since the geometric phase for a pure state can be acquired by methods known before.

3. Geometric phase and parallel transport

Recently, Sjöqvist *et al* have also proposed geometric phases for mixed states under the parallel transport condition [12]. If the unitary transformation $U(t)$ satisfies a parallel condition we can prove that the geometric phase given by equation (2) is consistent with what was obtained in [12]. The parallel transport condition for a mixed state undergoing unitary evolution is

$$\mathrm{Tr}[\rho(t)U^+(t)\dot{U}(t)] = 0. \tag{18}$$

Under this condition, from the definition in [12] the geometric phase of the cyclic evolution can be expressed as $\overline{\phi}_g = \arg \mathrm{Tr}[\rho(0)U(\tau)]$.

Indeed, for the unitary operator $U(t)$ we can always obtain another unitary operator by a $U(1)$ transformation, $U'(t) = \mathrm{e}^{\mathrm{i}\xi(t)}U(t)$, so that $\mathrm{Tr}[\rho(t)U'^{+}(t)\dot{U}'(t)] = 0$. From this condition, it is easy to prove that

$$\dot{\xi}(t) = \mathrm{i}\,\mathrm{Tr}[\rho(0)U^{+}(t)\dot{U}(t)]. \tag{19}$$

So $\xi(\tau) = -\phi_d$. From (10) and (3), $\phi_g = \arg\mathrm{Tr}[\rho(0)U(\tau)] + \xi(\tau) = \arg\mathrm{Tr}[\rho(0)U'(\tau)]$. Obviously, such a parallel transport $U'(\tau)$ is unique for an initial state $\rho(0)$ and the unitary operator $U(t)$. So, if $U(t)$ satisfies the parallel transport condition, the dynamical phase in equation (3) vanishes identically, so $\overline{\phi}_g = \phi_g$, i.e., under the parallel transport condition our definition of the geometric phase is consistent with the definition in [12].

However, for an initial state $\rho(0)$ and the unitary operator $U(t)$, one can construct alternative parallel transport by a unitary transformation, except for a $U(1)$ transformation, i.e., the parallel transport corresponding to the initial state and the unitary operator $U(t)$ is not unique [12, 19]. We must emphasize that only for the parallel transport obtained by the $U(1)$ transformation (which is unique), $U'(\tau) = \mathrm{e}^{\mathrm{i}\xi(t)}U(t)$ determined by equation (19), the geometric phase can be expressed as $\phi_g = \arg\mathrm{Tr}[\rho(0)U'(\tau)]$. For example, we consider the case of example I. For the state $\rho(0)$ given in (7), one can have two pure states $\rho_{\pm} = \frac{1}{2}[I \pm (\sin\theta\sigma_x + \cos\theta\sigma_z)]$ such that $\rho(0) = \frac{1+r}{2}\rho_{+} + \frac{1-r}{2}\rho_{-}$. For the unitary operator $U(t) = \exp(\mathrm{i}\mu Bt\sigma_z/\hbar)$, by unitary transformation $\exp(-\mathrm{i}[\mu Bt(\cos\theta)(\sin\theta\sigma_x + \cos\theta\sigma_z)/\hbar])$, we can construct $U'' = \exp(\mathrm{i}(\mu Bt\sigma_z/\hbar))\exp(-\mathrm{i}[\mu Bt(\cos\theta)(\sin\theta\sigma_x + \cos\theta\sigma_z)/\hbar])$ which satisfies $\mathrm{Tr}[\rho_{\pm}(U'')^{+}\dot{U}''(t)] = 0$. Obviously, this is a parallel transport of $\rho(t) = U''(t)\rho(0)U''^{+}(t) = U(t)\rho(0)U^{+}(t)$. It is easy to obtain $\arg\mathrm{Tr}[\rho(0)U''(\tau)] = \pi - \arctan[r\tan(\pi\cos\theta)]$ which does not equal the geometric phase given by equation (9).

In fact, the set of density operators constructs a base space $\mathcal{M}$ (the subspace corresponding to pure states is isomorphic to the projective Hilbert space). The unitary transformations U just define a line bundle $\mathcal{F}$ on the base space with the projection map Π as $\Pi^{-1}(\rho) = \{\rho : \rho \to c = \mathrm{Tr}(U\rho)/|\mathrm{Tr}(U\rho)|, c \in U(1)\}$. Then the cyclic evolution discussed in this paper just defines a closed curve $C : [0, \tau] \to \mathcal{M}$ on the base space, but on the bundle space the path is not closed with the final point lifted by a $U(1)$ factor $c(\tau)$. On the other hand, using $U(1)$ transformations, we can always obtain a unitary transformation $U'(t)$ determined by equation (19) which satisfies the parallel transport condition for a given closed path C. Then, the geometric phase defined in equation (3) can be expressed by the phase factor of the parallel lift: $\phi_g = \arg\mathrm{Tr}[\rho(\tau)U'(\tau)]$. Under this consideration the geometric phases of mixed states share the same geometric sense with the pure states for the cyclic evolution.

4. Conclusion

In summary, we give a definition of the geometric phase for a mixed state during a cyclic evolution. Our definition is consistent with the prescription proposed in [12] when the evolution satisfies parallel transport condition. We first give the geometric meaning of the geometric phases for mixed states which share the same sense with the pure states. Although our definition is only for cyclic evolution, the discussion can be straightforwardly generalized to noncyclic evolution except for a gauge condition[4] (for the pure states see [7]) which is automatically satisfied in cyclic evolution.

[4] Under a $U(1)$ transformation $\widetilde{U}(t)' = \mathrm{e}^{\mathrm{i}\delta(\alpha)}\widetilde{U}(t)$, we can have $\beta' = \mathrm{i}\,\mathrm{Tr}[\rho(0)\widetilde{U}'^{+}(t)\,\mathrm{d}\widetilde{U}'(t)] = \beta - \mathrm{d}\delta$. So the gauge function should satisfy: $\delta(\tau) = \delta(0) + 2n\pi$ where n is an integer number. The phase angle will be invariant mod 2π.

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