General Description of Mixed State Geometric Phase

Mingjun Shi\textsuperscript{1} and Jiangfeng Du\textsuperscript{1,2,3,4}

\textsuperscript{1}Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China
\textsuperscript{2}Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China
\textsuperscript{3}Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117542

We consider arbitrary mixed state in unitary evolution and provide a comprehensive description of corresponding geometric phase in which two different points of view prevailing currently can be unified. Introducing an ancillary system and considering the purification of given mixed state, we find that different results of mixed state geometric phase correspond to different choice of the representation of Hilbert space of the ancilla. Moreover we demonstrate that in order to obtain Uhlmann’s geometric phase it is not necessary to resort to the unitary evolution of ancilla.

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The notion of geometric phase was firstly demonstrated in Pancharatnam’s study of the interference of light in different states of polarization. Afterwards, Berry discovered a non-trivial phase factor in adiabatic, cyclic and parametric variations of quantal systems. This discovery has prompted more attention and more activities on search for the geometric structure involved in the evolution of quantum system. Aharanov and Anandan gave the formalism for geometric phase in the nonadiabatic case. Samuel and Bhandari made the extension to nonadiabatic and non-cyclic evolution. Further generalized case of nonadiabatic, non-cyclic and non-unitary evolution has also been carried out in recent investigation. It should be emphasized that the above-mentioned considerations refer to the pure quantal state. The definition of geometric phase in mixed state scenario is still an open question. Uhlmann firstly considered this issue within the mathematical context of purification. In contrast with the abstract formalism of Uhlmann’s definition, Sjöqvist et al presented a more concrete formalism of geometrical phase for mixed states in the experimental context of quantum interferometry. Such two definitions—that is, Uhlmann’s and Sjöqvist’s—would result in different geometric phase of mixed states. In other words, they are accordant with each other only in the case of pure states. It is unsatisfactory in theoretical point of view to have two different definitions and results for the same thing. On the other hand, geometric phase has important significance in quantum computation. Its potential application to fault-tolerant quantum computation has been the subject of recent investigations. There is no conflict in treating with the pure state geometric phase, but in actual and experimental situation the issue of mixed states is unpreventable. Unidentical explanation on the latter would be a trouble for experimentalist.

Recently in [12], Ericsson et al compared Uhlmann’s and Sjöqvist’s geometric phase for a mixed states undergoing unitary evolution and concluded that the former depends not only on the geometry of the path of system alone but also on a constrained bilocal unitary evolution of the purified entangled state, whereas the latter is essentially the property of system alone. Nevertheless there is not a consistent definition and interpretation of mixed state geometric phase so far.

In this paper, we propose a new definition of parallel transport for mixed state and give a general description of mixed state geometric phase in unitary evolution, from which Uhlmann’s phase and Sjöqvist’s phase can be deduced. In other words, such two definitions of geometric phase can be embodied in our statement. In our approach we deal with the mixed state not in view of spectrum decomposition (i.e., orthogonal decomposition), but by means of non-orthogonal decomposition. Of course for given mixed state there are infinite forms of non-orthogonal decomposition. We will seek the specific one among them and let each pure component undergo parallel transport. The geometric phase associated with each pure component is simply the total phase difference during an interval of unitary evolution. Then we think that the whole ensemble also undergoes parallel transport and the corresponding geometric phase factor is the sum of weighted geometric phase factor of pure component with related visibility. To this end, we adopt the usual method to deal with a mixed state of some quantum system, that is, introducing an ancilla and considering the purification of the mixed state in a larger Hilbert space. As a consequence we find that two different choice of the basis of ancilla Hilbert space will result in Sjöqvist’s and Uhlmann’s phase respectively. Our consideration need not ask for the help of unitary evolution of ancilla.

Consider a mixed state of some quantum system with \( n \) energy levels. In \( n \)-dimensional Hilbert space \( \mathcal{H}^S \) the initial state can be expressed as

\[
\rho(0) = \sum_{j=1}^{n} \lambda_j |e_j\rangle \langle e_j|,
\]

where \( \lambda_j \)'s and \( |e_j\rangle \)'s are respectively the eigenvalues and eigenstates of \( \rho(0) \). We choose \( \{ |e_j\rangle \}_{j=1, \ldots, n} \) as the basis of \( \mathcal{H}^S \). Some unitary operator \( U(t) \) determines the
evolution of the system, that is
\[
\rho(t) = U(t) \rho(0) U^\dagger(t).
\]
(2)

\(U(t)\) can be represented as \(U(t) = \exp(-iHt)\), where \(H\) is the Hamiltonian of the system and assumed to be independent of time for simplicity (here \(\hbar = 1\)). Introduce an ancillary system. The Hilbert space describing the ancilla, named as \(\mathcal{H}^A\), has the same dimension as \(\mathcal{H}^S\). The basis of \(\mathcal{H}^A\) is labeled by \(\{|f_j\}\) \(j = 1, \ldots, n\). Then the purification of \(\rho(0)\) is
\[
|\Psi(0)\rangle = \sum_{j=1}^{n} c_j |e_j\rangle \otimes |f_j\rangle,
\]
where \(c_j\)'s can be regarded as real and positive numbers and in fact \(c_j = \sqrt{\lambda_j}\). Under bilocal unitary transformation \(U(t) \otimes V(t)\), the time evolution of \(|\Psi(0)\rangle\) is
\[
|\Psi(t)\rangle = \sum_{j=1}^{n} c_j U(t) |e_j\rangle \otimes V(t) |f_j\rangle.
\]
(4)

Obviously after tracing out ancilla, we always have \(\rho(t) = Tr_A|\Psi(t)\rangle \langle \Psi(t)|\) for arbitrary \(V(t)\). Also we express \(V(t)\) as \(V(t) = \exp(-iKt)\) where \(K\) is the time-independent Hamiltonian of ancilla.

Eq. (4) can be rewritten as
\[
|\Psi(t)\rangle = \sum_{j=1}^{n} U(t) CV^T(t) |e_j\rangle \otimes |g_j\rangle,
\]
where \(V^T(t)\) is the transpose of \(V(t)\) and \(C\) is a diagonal matrix, i.e., \(C = \text{diag}[c_1, c_2, \cdots, c_n]\). Define
\[
|\tilde{\psi}_j(t)\rangle = U(t) CV^T(t) |e_j\rangle,
\]
where the symbol ”\(\sim\)” means that \(|\tilde{\psi}_j(t)\rangle\)'s are not necessarily orthogonal with one another and are definitely non-normalized. We have
\[
|\Psi(t)\rangle = \sum_{j=1}^{n} |\tilde{\psi}_j(t)\rangle \otimes |f_j\rangle.
\]
(7)

As for the system, \(\rho(t)\) is expressed as
\[
\rho(t) = \sum_{j=0}^{n} |\tilde{\psi}_j(t)\rangle \langle\tilde{\psi}_j(t)|.
\]
(8)

Generally it is a non-orthogonal decomposition. Denote the normalized form of \(|\tilde{\psi}_j(t)\rangle\) as \(|\psi_j(t)\rangle = \frac{|\tilde{\psi}_j(t)\rangle}{\langle\tilde{\psi}_j(t)|\tilde{\psi}_j(t)\rangle}^{1/2}\). Then \(|\psi_j(t)\rangle\), as the pure component of \(\rho(t)\), appears in the ensemble with the probability \(p_j(t) = \langle\tilde{\psi}_j(t)|\tilde{\psi}_j(t)\rangle\). Now we ask such a question: Under what condition each \(|\psi_j(t)\rangle\) undergoes parallel transport, i.e., \(\langle\psi_j(t)|\frac{d}{dt}\psi_j(t)\rangle = 0\) for \(j = 1, 2, \cdots, n\)?

Note that the form of \(V(t)\) is unknown. Usually \(p_j(t)\) is not invariant. So we are above all faced with such a trouble that the pure components of \(\rho(t)\) come forth with time-dependent weights (or probabilities). To avoid this trouble we would ”see” the system state from the ancilla in another viewpoint. Formally speaking, we would choose another basis of \(\mathcal{H}^S\), say \(|\{g_j\}\rangle\), and suppose the relationship between \(|\{f_j\}\rangle\) and \(|\{g_j\}\rangle\) is a time-independent unitary transformation \(Z\) which will be determined later, that is, \(|f_j\rangle = Z|g_j\rangle\). Rewrite (4).

\[
|\Psi(t)\rangle = \sum_{j=1}^{n} U(t) CV^T(t) |e_j\rangle \otimes Z |g_j\rangle
\]
\[
= \sum_{j=1}^{n} U(t) CV^T(t) Z^T |e_j\rangle \otimes |g_j\rangle
\]
\[
= \sum_{j=1}^{n} |\tilde{\varphi}_j(t)\rangle \otimes |g_j\rangle,
\]
(9)

where \(|\tilde{\varphi}_j(t)\rangle\equiv U(t) CV^T(t) Z^T |e_j\rangle\) Then \(\rho(t) = \sum_{j=0}^{n} |\tilde{\varphi}_j(t)\rangle \langle\tilde{\varphi}_j(t)|\). Now we hope every \(\langle\tilde{\varphi}_j(t)|\tilde{\varphi}_j(t)\rangle\) is invariant. It is equivalent to say that all diagonal elements of matrix \(Z^* V^T C Z V^T Z^T\) are time-independent. Note that \(C\) is time-independent. If \(Z^*\) can diagonalize \(V^*\), i.e., \(Z^* V^* Z^T\) is diagonal (or equivalently \(K^T Z^\dagger\) is diagonal), then our hope is realized. Now suppose that we have the time-independent unitary \(Z\) such that
\[
\overline{K} \equiv Z^* K^T Z^T = Z K Z^\dagger
\]
\[
= \text{diag}[^{\kappa_1, \kappa_1, \cdots, \kappa_n}],
\]
where \(\kappa_j\)'s are all real numbers and in fact the eigenvalues of \(K\). Correspondingly \(V(t)\) is transformed to
\[
\overline{V}(t) = ZV(t)Z^\dagger
\]
\[
= \text{diag}[e^{-i\kappa_1 t}, e^{-i\kappa_2 t}, \cdots, e^{-i\kappa_n t}].
\]

Then we can say that given arbitrary non-diagonal \(V(t)\) (or Hamiltonian \(K\)) on the basis \(\{|f_j\}\) we can choose as new basis \(\{|g_j\}\) of \(\mathcal{H}^S\) the eigenstates of \(K\) so that in the view of \(\{|g_j\}\) the weight of each pure component of the system mixed ensemble is invariant. This invariant weight is presented as
\[
q_j = \langle\tilde{\varphi}_j(t)|\tilde{\varphi}_j(t)\rangle = \langle e_j|Z^* C^2 Z^T|e_j\rangle.
\]
(10)

Let \(|\varphi_j(t)\rangle = \overline{q}_j^{1/2}|\tilde{\varphi}_j(t)\rangle\). We have \(\rho(t) = \sum_{j=1}^{n} q_j |\varphi_j(t)\rangle \langle\varphi_j(t)|\). It is still a non-orthogonal decomposition of \(\rho(t)\).

Next, what about the exact form of Hamiltonian \(K\) such that guarantees \(\langle\varphi_j(t)|\frac{d}{dt}\varphi_j(t)\rangle = \langle\tilde{\varphi}_j(t)|\frac{d}{dt}\tilde{\varphi}_j(t)\rangle = 0\) for each \(j\)? That is, we further hope
\begin{align}
\langle e_j | [Z^*V^*(t)CU^\dagger(t)][\dot{U}(t)CV^T(t)Z^T + U(t)CV^T(t)Z^T] | e_j \rangle = 0, \\
\text{for } j = 1, 2, \cdots, n,
\end{align}

or equivalently
\begin{align}
\langle e_j | Z^*V^*(t)|CHC & \\
+C^2K^T| V^T(t)Z^T | e_j \rangle = 0,
\end{align}

for \( j = 1, 2, \cdots, n \). Remind ourselves that \( Z^* \) is time-independent and can diagonalize \( K^T \) and \( V^* \). Suppose \( K^T \) is determined by the following equation.
\begin{equation}
C^2K^T + K^TC^2 = -2CHC.
\end{equation}

That implies \( \langle \varphi_j(t) | \frac{d}{dt} | \varphi_j(t) \rangle = 0 \). Thus we have answered the above-mentioned question, that is, first the Hamiltonian of ancilla has to meet condition \( \text{13} \), and then the basis of Hilbert space of ancilla is such that the Hamiltonian has diagonal form. We regard this description as the parallel transport of mixed state in unitary evolution.

The geometric phase of \( |\varphi_j(t)\rangle \) is
\begin{align}
\gamma_j(t) &= \arg\langle \varphi_j(0) | \varphi_j(t) \rangle \\
&= \arg \langle e_j | Z^*CU(t)CV^T(t)Z^T | e_j \rangle \\
&= \arg \langle e_j | Z^*CU(t)CZ^T \dot{V}^T(t) | e_j \rangle \\
&= \arg \langle e_j | Z^*CU(t)CZ^T | e_j \rangle - \kappa_j.
\end{align}

The visibility is decided by \( \nu_j = |\langle \varphi_j(0) | \varphi_j(t) \rangle| \).

Retrospecting \( \text{10} \), we can say that \( |\Psi(t)\rangle \) undergoes parallel transport, and hence give the geometric phase of \( |\Psi(t)\rangle \) as follows.
\begin{align}
\Gamma(t) &= \arg\langle \Psi(0) | \Psi(t) \rangle \\
&= \arg \sum_{j=1}^n \langle \tilde{\varphi}_j(0) | \tilde{\varphi}_j(t) \rangle \\
&= \arg \sum_{j=1}^n q_j \nu_j e^{i\gamma_j}.
\end{align}

Rewrite \( \text{15} \) as \( e^{i\Gamma(t)} = \sum_{j=1}^n q_j \nu_j e^{i\gamma_j} \) and consider the mixed ensemble of system. \( \text{15} \) is in actually the sum of weighted geometric phase factor of (non-orthogonal) pure component with the associated visibility. We regard \( \text{15} \) as the geometric phase of mixed state. Obviously it is gauge-invariant. We would rather review \( \text{15} \) from another point of view.

Note that \( \rho(0) = CC^\dagger \). \( |\Psi(t)\rangle \) being in bilocal unitary transformation \( U(t) \otimes V(t) \), we have \( \rho(t) = U(t)CV^T(t) \). It is evident that \( \rho(t) = C(t)C^\dagger(t) \). Then \( C(t) \) is the purification of \( \rho(t) \) in Uhlmann’s sense. Let \( W(t) = C(t)Z^T \). \( W(t) \) is another Uhlmann’s purification of \( \rho(t) \). Furthermore we have
\begin{align}
W^\dagger(t)W(t) &= \rho(t) \\
&= Z^*C^\dagger(t)C(t)Z^T \\
&= -iZ^*V^*(t)|CHC + C^2K^T|V^T(t)Z^T \\
&= iZ^*V^*(t)|CHC + K^TC^2|V^T(t)Z^T \\
&= W(t)W^\dagger(t),
\end{align}

where we have used \( \text{15} \). Thus \( W(t) \) satisfies Uhlmann’s parallel transport condition, and we obtain Uhlmann’s geometric phase of mixed state.
\begin{align}
\gamma^{Uhl}(t) &= \arg Tr \{ W^\dagger(0)W(t) \} \\
&= \arg Tr\{ Z^*CC(t)Z^T \} \\
&= \arg Tr[CC(t)].
\end{align}

It is straightforward to check \( \gamma^{Uhl}(t) = \Gamma(t) \). So our statement in fact results in Uhlmann’s geometric phase. In brief, after choosing the Hamiltonian of ancilla to meet \( \text{13} \), and selecting the specific basis of \( \mathcal{HH} \) to diagonalize such Hamiltonian, we indeed answer the question and meanwhile obtain Uhlmann’s phase.

Let’s consider a special case in which \( V(t) \) is already diagonal in the original basis \( \{|f_j\rangle\} \). Recall \( \text{8} \) and \( \text{9} \). It is easy to see that \( p_j(t) = \langle \tilde{\varphi}_j(t) | \tilde{\varphi}_j(t) \rangle \) is invariant and in fact is \( \lambda_j \). Define the Hamiltonian of ancilla as \( K_{kl} = -\delta_{kl}H_{kl} \), where \( H_{kl} \)’s are respectively the matrix elements of \( K \) and \( H \). The evolution of ancilla is given by \( V(t) = \text{diag}[e^{iH_{11}t}, e^{iH_{22}t}, \cdots, e^{iH_{nn}t}] \). We have
\( \langle \tilde{\varphi}_j(t), \frac{d}{dt} | \tilde{\varphi}_j(t) \rangle = 0 \). Similar to \( \text{15} \), the geometric phase of \( |\Psi(t)\rangle \) in this case is
\begin{align}
\Gamma'(t) &= \arg \langle \Psi(0) | \Psi(t) \rangle \\
&= \arg \sum_{j=1}^n \langle \tilde{\varphi}_j(0) | \tilde{\varphi}_j(t) \rangle \\
&= \arg \sum_{j=1}^n \lambda_j \langle e_j | U(t) | e_j \rangle e^{i\gamma_j},
\end{align}

where \( \lambda_j \) is the weighted geometric phase factor of (non-orthogonal) pure component with the associated visibility. We regard \( \text{15} \) as the geometric phase of mixed state. Obviously it is gauge-invariant. We would rather review \( \text{15} \) from another point of view.
where $\gamma_{j}(t) = \arg(\tilde{\psi}_{j}(0)|\tilde{\psi}_{j}(t))$. This is just the mixed state geometric phase based on Sjöqvist’s formalism\cite{8}.

Thus for mixed states our proposal includes the origination of Sjöqvist’s phase and Uhlmann’s phase. We almost get a comprehensive interpretation on mixed state geometric phase. A remained discomfort in the above discussion is the time-evolution of the ancilla, i.e., $V(t)$. In the following we try to remove $V(t)$ and give a more concise expression.

Actually in the above discussion our purpose of applying $V(t)$ to the ancilla is to cancel out the dynamical phase of the system, or more strictly speaking, to cancel out the dynamical phase of each component of the mixed ensemble $\rho(t)$. Then we can re-explain our procedure in alternative viewpoint as follows. We firstly postulate that in some representation of $\mathcal{H}_A$, say $\{|j\rangle\}$, the ancilla is subjected to the Hamiltonian $K$ satisfying (13). Then choose another representation $\{|g\rangle\}$ of $\mathcal{H}_A$ in which $K$ is diagonal. As stated above, unitary $Z$ transforms $\{|g\rangle\}$ to $\{|j\rangle\}$. Afterwards we can disregard $K$ and the corresponding time evolution operator $V(t) = \exp(-iKt)$. So $|\Psi(t)\rangle$ is decided as the following.

$$
|\Psi(t)\rangle = \sum_{j=1}^{n} U(t) CZT |e_j\rangle \otimes |g_j\rangle.
$$

Let $|\tilde{\chi}_j(0)\rangle = CZT |e_j\rangle$ and $|\tilde{\chi}_j(t)\rangle = U(t)|\tilde{\chi}_j(0)\rangle$. Apparently $\langle \tilde{\chi}_j(t)|\tilde{\chi}_j(t)\rangle$ is invariant and is just $q_j$. Let $|\chi_j(t)\rangle = q_j^{-1/2} |\tilde{\chi}_j(t)\rangle$. We have

$$
\rho(t) = \sum_{j=0}^{n} |\chi_j(t)\rangle \langle \chi_j(t)|
= \sum_{j=0}^{n} q_j |\chi_j(t)\rangle \langle \chi_j(t)|. \tag{18}
$$

Also $|\chi_j(t)\rangle$’s are not orthogonal with one another and do not endure parallel transport. Let’s calculate the dynamical phase of $|\chi_j(t)\rangle$.

$$
\phi_{d}^{j}(t) = -i \int_{0}^{t} \langle \tilde{\chi}_j(t')|Z^*CHCZ^T|e_j\rangle dt'.
$$

If applying (13), we have $\phi_{d}^{j}(t) = \langle e_j|Z^*K^TZ|e_j\rangle t = \kappa_j t$. The total phase is

$$
\phi_{j}(t) = \arg(\chi_j(0)|\chi_j(t)) = \arg(e_j|Z^*CU(t)CZ^T|e_j).
$$

Then the geometric phase associated with each $|\chi_j(t)\rangle$ is $\gamma_{j}(t) = \phi_{j}(t) - \phi_{d}^{j}(t)$. Apparently $\phi_{d}^{j}(t) = \gamma_{j}(t)$ (see \cite{14}). Hence we have demonstrated that in order to obtain Uhlmann’s phase we may not resort to the evolution of ancillary system, and all we have to do is to find specific representation of $\mathcal{H}_A$ in which the hermitian matrix $K$ satisfying (13) is diagonal.

Conclusively, in the formalism proposed in this paper, the mixed state geometric phase is provided with unified interpretation. The key point is Eq. (13) which implies the representation transformation of the ancilla. As stated before, the unitary evolution of ancilla is not necessary, and it is the choice of representation of ancillary Hilbert space that results in particular geometric phase. For given mixed state and its purification, different choice of the representation of $\mathcal{H}_A$ can be considered as different kind of measurement. So the mixed state geometric phase behaves somewhat like the result of quantum measurement: Having nothing to do with $\mathcal{H}_A$, we would get Sjöqvist’s result; shifting to the other basis of $\mathcal{H}_A$, we would get Uhlmann’s result. The hidden significance of such basis transformation is not clear. We hope our discussion would be helpful to further research of geometric phase.

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1. Electronic address: shmj@ustc.edu.cn
2. Electronic address: djf@ustc.edu.cn

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