Uniquely defined geometric phase of an open system

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Various types of unravelings of Lindblad master equation have been used to define the geometric phase for an open quantum system. Approaches of this type were criticized for lacking in unitary symmetry of the Lindblad equation [A. Bassi and E. Ippoliti, Phys. Rev. A **73**, 062104 (2006)]. We utilize quantum state diffusion (QSD) approach to demonstrate that a geometric phase invariant on the symmetries of the Lindblad equation can be defined. It is then shown that such a definition of the geometric phase could be either invariant on the decomposition of the initial mixed state or gauge invariant, but not both. This alternative is inherent to the definitions based on quantum trajectories. The QSD geometric phase is computed for a qubit in different types of environments.

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State vectors $|\psi\rangle$ of a quantum system are normalized and the overall phase α in $e^{i\alpha}|\psi\rangle$ has no physical relevance. Nevertheless, two vectors on an orbit of the evolution governed by the Schrödinger equation can have nonzero relative phase $\alpha_{tot}=\arg\langle\psi(0)|\psi(t)\rangle$, which is measurable. It was Berry [1] who first realized that the total relative phase α_{tot} can be represented as a sum of the dynamical part that depends explicitly on the Hamiltonian and the part that is of a geometric origin. Berry considered evolution with Hamiltonian $\hat{H}(\mathbf{R}(t))$ depending on adiabatically and periodically changing parameters $\mathbf{R}$ and was able to show that a part of the total phase acquired by the systems state vector during one period of $\mathbf{R}(t)$ depends only on the geometric properties of the curve $\mathbf{R}(t)$ in the parameter space [1,2]. It was soon realized that there is a whole class of such geometric phases that appear responsible for important physical effects [3]. In particular, the geometric phase was defined for curves in the space of pure states that did not relay on the adiabatic [4] nor cyclic evolution [5,6]. It became clear that these geometric phases are always related to the geometry of the system's evolution in the state space $\mathbf{P}\mathcal{H}$, which has a nonzero curvature in the natural connection determined by the Hilbert space scalar product [2,7,5]. It is no surprise that the quantum information processing revolution brought the idea that the geometric phase can be used for quantum computing, which has been termed geometric or, more generally, holonomic computing (see, for example, [8]).

However, realistic quantum systems must be treated as open systems, i.e., together with their environment. The state of an open system is in general not pure and is described by a density matrix. Evolution of open quantum systems is necessarily described in terms of transformations of the density matrices even if the initial state is pure. There have been several attempts to define the geometric phase for mixed states of an open system (see, for example, [9–15]). Most of them explore the representation of the mixed state of the open system in terms of a collection of pure states of the open system or in terms of reduction in a pure state of a larger isolated system. For example, the quantum jumps unraveling of the Lindblad master equation for the evolution of the mixed state $\hat{\rho}(t)$ was used in [13] to define the geometric phase using the quantum trajectories that appear in the unraveling. Approaches based on pure states quantum trajectories were criticized in [16] because they imply a phase that is not invariant under the symmetry of the mixed state master equation.

However, there is a stochastic unraveling of the master equation in terms of pure state stochastic evolution, given by the quantum state diffusion (QSD) theory [17], which has the same symmetry as the master equation. We shall show that QSD unraveling can be used to define the geometric phase that retains the symmetry of the Lindblad equation. Thus, the objections raised in [16] are not the problem of all definitions of the geometric phase based on quantum trajectories. In addition, we study the problem of invariance with respect to equivalent pure state decompositions of the initial mixed state and we demonstrate that there is the following alternative: the QSD geometric phase can be defined such that it is either invariant with respect to the initial pure state decompositions or it is gauge invariant, but cannot satisfy both. Thus, the real issue with all geometric phase definitions based on pure state quantum trajectories is the nonuniqueness on decomposition of initial mixed state and not the unitary noninvariance.

In the sequel we consider open quantum systems that satisfy Markov property. The most general continuous evolution of such a system is given by the Gorini-Kossakowski-Lindblad master equation (LME) [18] for the density matrix $\hat{\rho}(t)$,

$$\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H},\hat{\rho}] + \sum_m (2\hat{L}_m\hat{\rho}\hat{L}_m^\dagger - \hat{L}_m^\dagger\hat{L}_m\hat{\rho} - \hat{\rho}\hat{L}_m^\dagger\hat{L}_m), \quad (1)$$

where $\hat{H}$ generates unitary evolution and the Lindblad operators $\hat{L}_m$ describe the nonunitary influences of the environment. The LME (1) is invariant on the unitary transformations of the Lindblad operators:

$$\hat{L}_m \to \sum_k u_{mk}\hat{L}_k, \quad \sum_m u_{mk}u^*_{mk'} = \delta_{kk'}, \quad (2)$$

where $*$ denotes complex conjugation of the complex numbers u_{mk}. Consequently, an observable quantity related to an

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orbit $\hat{\rho}(t), t\in(t_0,t_1)$ of Eq. (1), like the would be geometric phase, must not depend on u_{mk}. However, it was pointed out in Ref. [16] that the definitions of the geometric phase based on stochastic unraveling of Eq. (1) using a particular stochastic Schrödinger equation with real Wiener noise or the quantum jumps approach are not invariant on the transformations of the type $\hat{L}_m \to e^{i\alpha}\hat{L}_m$, which are the symmetries of Eq. (1) in form (2).

The idea to analyze the deterministic mixed state evolution (1) by an equivalent random evolution of pure states is known as the quantum trajectory approach to open system dynamics and is also called unraveling of master equation (1) [18]. The advantages of the description in terms of random pure states over the description by density matrix $\hat{\rho}$ are twofold. The computations are much more practical, as soon as the size of the Hilbert space is moderate or large [18]. On the theoretical side, the stochastic evolution of pure states provides valuable insights that cannot be inferred from the density-matrix approach [17–21]. Nonuniqueness of the representation of the mixed state in terms of pure states implies that there are several different types of unraveling that provide different insights into the dynamics of the open system.

We shall exploit the fact that the QSD equation is the unique unraveling of Eq. (1), which has the same invariance as Eq. (1) under the unitary transformations of environment operators (2) [17]. The linear form of QSD equation is given by the following formula:

$$|d\phi\rangle = \left[-i\hat{H}dt - \sum_m \hat{L}_m^\dagger \hat{L}_m dt + \sum_m \hat{L}_m dw_m\right]|\phi(t)\rangle, \quad (3)$$

where w_m are complex Wiener processes with respect to the probability measure $\mathbb{Q}$ satisfying

$$\mathbb{E}_{\mathbb{Q}}[dw_m] = \mathbb{E}_{\mathbb{Q}}[dw_m dw_{m'}] = 0, \quad \mathbb{E}_{\mathbb{Q}}[dw_m dw^*_{m'}] = 2\delta_{m,m'}dt. \quad (4)$$

$\mathbb{E}_{\mathbb{Q}}[\cdot]$ denotes the expectation with respect to the stochastic process. The stochastic process with increment $|d\phi\rangle$ given by Eq. (3) satisfies the unraveling property,

$$\mathrm{Tr}[\hat{\rho}(t)\hat{A}] = \mathbb{E}_{\mathbb{Q}}[\langle\phi(t)|\hat{A}|\phi(t)\rangle], \quad (5)$$

for any operator $\hat{A}$ and for all times t. Equation (3) is linear and does not preserve the norm of wave function. There exists a nonlinear norm preserving form of QSD equation that is more convenient for efficient simulations of an open system dynamics. However, we shall use, in a crucial way, the linear form of the QSD theory.

It can be easily seen that stochastic process (3) is invariant under transformation (2). In fact, the substitution of Eq. (2) leads to the same Eq. (3) with $dw'_m = \Sigma_k u_{km} dw_k$ and $dw^{*\prime}_m = \Sigma_k u^*_{km} dw^*_k$ instead of dw_m and dw^*_m, but these have the same stochastic properties [Eq. (4)].

Consider an orbit $\hat{\rho}(t), t\in(t_0,t_1)$ of Eq. (1). The initial mixed state is a convex combination of pure state projectors $\hat{\rho}(t_0) = \Sigma_k p_k|\phi_0^k\rangle\langle\phi_0^k|$. Starting from initial condition $\phi_w^k(t_0) = \phi_0^k$ each of the pure states is evolved stochastically through the space of pure states using Eq. (3) resulting in $|\phi_w^k(t)\rangle$, where subindex w corresponds to the sample paths of Eq. (3). Deterministic evolution through mixed states by Eq. (1) from the initial pure state $|\phi_0^k\rangle\langle\phi_0^k|$ gives the curve $\hat{\rho}^k(t)$, which is equal to $\mathbb{E}_{\mathbb{Q}}[|\phi_w^k(t)\rangle\langle\phi_w^k(t)|]$, $t\in(t_0,t_1)$. Physical motivation based on the interferometric approach, elaborated in [16], requires the total phase to be defined using the linear QSD equation as follows:

$$\alpha^k_{tot}(t) = \arg \mathbb{E}_{\mathbb{Q}}[\langle\phi_w^k(t_0)|\phi_w^k(t)\rangle]. \quad (6)$$

The dynamical phase related with the curve $\hat{\rho}^k(t)$ can be defined as

$$\alpha^k_{dyn}(t) = \mathrm{Im}\int_{t_0}^{t} \mathbb{E}_{\mathbb{Q}}[\langle\phi_w^k(s)|d\phi_w^k(s)\rangle]. \quad (7)$$

Phases (6) and (7) are well defined and uniquely associated with the curve of mixed states $\hat{\rho}^k(t)$, as will be presently demonstrated and illustrated with examples. Finally, the geometric phase of the curve $\hat{\rho}^k(t)$ is uniquely defined as the difference of the total and the dynamical phases

$$\alpha^k_g(t) = \alpha^k_{tot}(t) - \alpha^k_{dyn}(t). \quad (8)$$

This completes the definition of the phases in the case of pure initial states.

Let us briefly demonstrate that phases (6) and (7) are invariant under transformation (2). The expression $\langle\phi|d\phi\rangle$ after substitution of Eq. (2) into Eq. (3) and using the properties of u_{mk} becomes

$$\langle\phi|d\phi\rangle = -i\langle\hat{H}\rangle_\phi dt - \sum_k \langle\hat{L}_k^\dagger\hat{L}_k\rangle_\phi dt + \sum_k \langle\hat{L}_k\rangle_\phi dw'_k, \quad (9)$$

where $\langle\cdot\rangle_\phi$ denotes the quantum expectation in the state $|\phi(t)\rangle$. Notice that due to the unitarity of u_{mk} the stochastic increments dw'_k in Eq. (9) satisfy the same properties (4) as dw_k and thus generate the same stochastic process $|\phi_w^k(t)\rangle$. From the invariance of $\langle\phi|d\phi\rangle$ follows the invariance of dynamical phase (7) along an orbit $\hat{\rho}^k(t)$ of Eq. (1). In a similar manner, it is obvious that total phase (6) is also invariant because the same stochastic process $|\phi_w^k(t)\rangle$ is generated. Furthermore, the imaginary part of Eq. (9) is always equal to $-\langle\hat{H}\rangle_\phi dt$. Using the unraveling property (5) we get the simple expression of dynamical phase

$$\alpha^k_{dyn}(t) = -\int_{t_0}^{t} \mathrm{Tr}[\hat{\rho}^k(s)\hat{H}]ds. \quad (10)$$

Note that the dynamical phase depends on the environment only through the evolution of the state. Thus, the geometric phase is well defined and uniquely associated with the orbit $\hat{\rho}^k(t)$ of LME (1).

Let us now focus on the phases for mixed initial states. Dynamical phase is naturally generalized as

$$\alpha_{dyn}(t) = \sum_k p_k \alpha^k_{dyn}(t) = -\int_{t_0}^{t} \mathrm{Tr}[\hat{\rho}(s)\hat{H}]ds, \quad (11)$$

which is clearly the quantity related to the evolution of $\hat{\rho}(t)$. One possible way to choose the total phase is

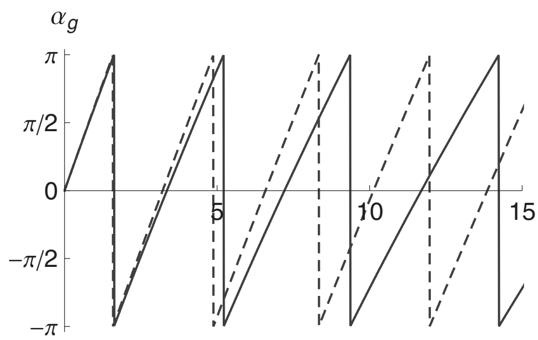

FIG. 1. Dependence on the dimensionless time $\tau=\mu Bt$ of the geometric phase α_g from initial state $|\uparrow\rangle$, for the thermal environment with $\bar{n}=0.2$ (dashed line) and $\bar{n}=1$ (solid line). $\mu B=1$, $\lambda=0.1$.

$$\alpha_{tot}(t) = \arg \mathbb{E}_{\mathrm{Q}}\left[\sum_k p_k\langle\phi_w^k(t_0)|\phi_w^k(t)\rangle\right], \qquad (12)$$

and it is invariant on decomposition of initial density matrix into convex combination of pure state projectors. Namely, let $\Sigma_k q_k|\chi_0^k\rangle\langle\chi_0^k|$ be some other decomposition of $\hat{\rho}(t_0)$. Then there exists a unitary matrix $\mathcal{U}=(\mathcal{U}_{km})$ such that [22]

$$\sqrt{p_k}|\phi_0^k\rangle = \sum_m \mathcal{U}_{km}\sqrt{q_m}|\chi_0^m\rangle. \qquad (13)$$

Taking $|\phi_0^k\rangle(|\chi_0^m\rangle)$ as initial state at t_0, evolution (3) gives a distribution of wave functions $|\phi_w^k(t)\rangle[|\chi_w^m(t)\rangle]$. Provided evolution (3) is *linear* the following relation must hold:

$$\sqrt{p_k}\mathbb{E}_{\mathrm{Q}}[|\phi_w^k(t)\rangle] = \sum_m \mathcal{U}_{km}\sqrt{q_m}\mathbb{E}_{\mathrm{Q}}[|\chi_w^m(t)\rangle]. \qquad (14)$$

Using relations (13) and (14) it is easy to show that

$$\mathbb{E}_{\mathrm{Q}}\left[\sum_k p_k\langle\phi_w^k(t_0)|\phi_w^k(t)\rangle\right] = \mathbb{E}_{\mathrm{Q}}\left[\sum_m q_m\langle\chi_w^m(t_0)|\chi_w^m(t)\rangle\right], \qquad (15)$$

which proves the invariance of the total phase on decomposition of initial density matrix. This conclusion assures that the definition of total phase (12) represents a quantity that does not depend on the convex decomposition of the initial mixed state.

However, the geometrical phase $\alpha_g(t)=\alpha_{tot}(t)-\alpha_{dyn}(t)$ for a mixed initial state obtained using definitions (11) and (12) for the dynamical and total phase, respectively, is not invariant on gauge transformations $|\phi_w^k(t)\rangle\to e^{i\alpha(t)}|\phi_w^k(t)\rangle$, $\hat{H}(t)\to\hat{H}(t)-d\alpha(t)/dt$, under which Eq. (3) and relation (5) remain unchanged. The reason can be traced back to choice (12) for the total phase which does not transform like a phase under gauge transformations. An alternative definition of the total phase could be

$$\alpha_{tot}(t) = \sum_k p_k \arg \mathbb{E}_{\mathrm{Q}}[\langle\phi_w^k(t_0)|\phi_w^k(t)\rangle], \qquad (16)$$

which has required transformation properties and yields a gauge invariant geometrical phase. In this case, however, the invariance on the convex decomposition of the initial mixed state is lost. Let us stress that these two alternatives arise for the case of mixed initial states and are inherent to definitions of a geometric phase that are based on quantum trajectories. In the case of a pure initial state the definition of the geometric phase for the open system using QSD unraveling is both unique and gauge invariant.

We shall now apply the previous definitions (6)–(8) to two examples. In both the isolated system is a qubit in a constant magnetic field along the z axis: $\hat{H}=-\mu B\sigma_z$ and for the environments we use standard examples of the dephasing and the thermal environment. Consider first the dephasing environment represented here by $\hat{L}=\lambda\sigma_z$. This is almost a trivial example since the Hamiltonian and the only Lindblad operator commute, but it has been commonly used as the testing case for various definitions of the open system geometric phase [11,13]. The QSD equation assumes the following form:

$$|d\phi\rangle = [i\mu B\sigma_z dt - \lambda^2\sigma_z^2 dt + \lambda\sigma_z dw]|\phi\rangle, \qquad (17)$$

and we get $\langle\phi|d\phi\rangle=i\mu B\langle\sigma_z\rangle_t dt-\lambda^2 dt+\lambda\langle\sigma_z\rangle_t dw$. The dynamical phase associated with a pure initial state $|\phi_0\rangle=\cos(\theta/2)|+\rangle+\sin(\theta/2)|-\rangle$ is given by $-\int_0^t\mathbb{E}_{\mathrm{Q}}[\langle\hat{H}\rangle_s]ds$. Thus we have to compute the expectation of $\mu B\int_0^t\langle\sigma_z\rangle_s ds$ for which the time dependence of $\langle\sigma_z\rangle_t$ is needed. Using Itô calculus it can be easily seen that $d\langle\sigma_z\rangle_t=\lambda\langle\phi_t|\phi_t\rangle(dw+dw^*)$, which implies that $\mathbb{E}_{\mathrm{Q}}[\langle\sigma_z\rangle_t]=\mathrm{const}=\mathbb{E}_{\mathrm{Q}}[\langle\phi_0|\sigma_z|\phi_0\rangle]$. Thus the dynamical phase is $\alpha_{dyn}=\mu B\langle\sigma_z\rangle_0\int_0^t ds$. This is the same result as for the isolated system, which is to be expected since $\hat{L}$ and $\hat{H}$ commute. Integrating Eq. (17) we obtain

$$\begin{aligned}\arg \mathbb{E}_{\mathrm{Q}}[\langle\phi_0|\phi_t\rangle] &= \arg\langle e^{i\mu B\sigma_z t}\rangle_0\\ &= \arg[e^{i\mu B\sigma_z t}\cos^2(\theta/2) + e^{-i\mu B\sigma_z t}\sin^2(\theta/2)]\end{aligned}$$

for the total phase, the same as in [16].

Next we consider the same system $\hat{H}=-\mu B\sigma_z$ but with the thermal environment $\hat{L}=\lambda(\bar{n}+1)\sigma_-+\lambda\bar{n}\sigma_+$, where λ is a small coupling parameter and $\bar{n}$ is a parameter depending on the temperature. In this case the evolution is given by

$$\begin{aligned}|d\phi\rangle = \{&i\mu B\sigma_z dt + \lambda[(\bar{n}+1)\sigma_- + \bar{n}\sigma_+]dw - \lambda^2[(\bar{n}+1)^2\sigma_+\sigma_-\\ &+ \bar{n}^2\sigma_-\sigma_+ + \bar{n}(\bar{n}+1)(\sigma_+\sigma_+ + \sigma_-\sigma_-)]dt\}|\phi\rangle. \qquad (18)\end{aligned}$$

The dynamical and the geometric phases are computed using numerical solutions of Eq. (18) and are illustrated in Fig. 1. The initial state in Fig. 1 is pure and we present the geometrical phase for the open system evolution with two values of $\bar{n}$. Expectation values are computed using only 200 sample orbits. The curves for different u_{mk} coincide demonstrating the independence of the phases on the same transformations that characterize LME (1).

In summary, we have demonstrated that a geometric phase of an orbit $\hat{\rho}(t)$ of an open quantum system undergoing Markov evolution from a pure initial state can be well defined and uniquely related with the orbit using the QSD unraveling of the LME. The property of the QSD unraveling, not shared by other types of unravellings, that it is invariant under the same transformations as the LME is crucial for the unique association of the geometric phase with the orbit $\hat{\rho}(t)$. In the case of mixed initial state the geometric phase can be defined such that it is either invariant with respect to the initial pure state decompositions or it is gauge invariant, but cannot be both. This alternative is inherent to the definition of an open system geometric phase based on quantum trajectories and cannot be overcome within this type of approach.

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