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In an open system, the geometric phase should be described by a distribution. We show that a geometric phase distribution for open system dynamics is in general ambiguous, but the imposition of reasonable physical constraints on the environment and its coupling with the system yields a unique geometric phase distribution that applies even for mixed states, nonunitary dynamics, and noncyclic evolutions.

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Introduction.—The geometric phase (GP) [1] identifies the portion of an overall (Abelian or non-Abelian [2]) phase shift of a quantum state that is due to the path of the state through projective Hilbert space; the GP and the dynamic phase combine to give the aggregate phase shift of the state that may be inferred by interferometric or other phase-sensitive methods. GP theory has been rigorously formulated for the general case of nonadiabatic [3], noncyclic [4], and nonunitary evolution (without quantum jumps) [5] of a pure state, but the importance of GP in realistic systems, for example, in the context of adiabatic quantum computation [6], has motivated recent important research into GP in open systems [7–14]. Quantum jump (or trajectory) analyses have been applied to certain physical systems, which show how the GP for a closed-system can be modified under open system dynamics [15,16], and a rigorous Kraus operator approach has been applied to define GP for general open system evolution [17]. These studies note the importance of GP beyond closed-system, unitary evolution of pure states.

In this Letter we argue that a complete description of Abelian GP in open systems has to identify the appropriate measure of phase distribution. We develop a theory of GP distributions for mixed states, nonunitary dynamics, and noncyclic evolutions. We show that, without further constraints, the GP distribution is ambiguous: an operational definition of GP that would resolve this ambiguity is not attainable because the GP is a nonlinear functional of the state. The ambiguity is rather subtle: we show that previous definitions of GP distributions and its spread implicitly assume a particular form of phase distribution. The imposition of reasonable physical constraints on the environment and its coupling with the system yields a unique GP distribution by taking the decomposition of the density matrix [17] into account.

Definition of geometric phase distributions for an open system.—Interferometric or other phase-sensitive measurements allow inference of the phase shift of a state, but separating geometric and dynamic components of the phase is not straightforward. For a pure state $|\psi(t)\rangle = V(t)|\psi(0)\rangle \in \mathcal{H}$ which is propagated by an arbitrary time-dependent evolution operator $V(t)$ (not necessarily cyclic or unitary), the mathematical definition of the geometric phase functional $\beta[\psi]$ is given by [4]

$$e^{i\beta[\psi]} \equiv \frac{Z[\psi]}{|Z[\psi]|}, \qquad Z[\psi] \equiv D[\psi]\langle\psi(0)|\psi(t)\rangle, \tag{1}$$

which is meaningful only for $Z[\psi] \neq 0$. The functional

$$D[\psi] \equiv \exp\left(-i\int_0^t dt' \mathrm{Im}\frac{\langle\psi(t')|\dot{\psi}(t')\rangle}{\langle\psi(t')|\psi(t')\rangle}\right) \tag{2}$$

removes the dynamic phase from the total phase shift. In some cases, the dynamic phase can be eliminated via interferometry of a state that follows a superposition of two paths, with the dynamic phase along each path being the additive inverse of the other [18,19], but this cancellation is not always achievable.

Nonunitary evolution of the type $V(t)$ may not satisfy the axioms of completely positive (CP) maps, which guarantee that a positive-definite operator on Hilbert space such as the density operator ρ is mapped to a positive-definite operator with identical trace, and linearity is preserved. Thus the GP should be established for general CP maps, not just for nonunitary evolution [11,20,21]. A physical picture for the CP emerges by considering a system S with Hilbert space $\mathcal{H}_S$ and a reservoir R (or set of ancillae) with Hilbert space $\mathcal{H}_R$, and joint Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$. At time $t = 0$ the density matrix factorizes, $\rho_{SR}(0) = \rho_S(0) \otimes \rho_R(0)$, and the unitary operator $U_{SR}(t)$ of the system + reservoir ($S + R$) is generated by a Hamiltonian $H_{SR}(t)$ such that $\rho_{SR}(t) = U_{SR}(t)\rho_{SR}(0)U_{SR}^\dagger(t)$. Dynamics for S alone is obtained by tracing over R; i.e., $\rho_S(t) = \mathrm{Tr}_R[U_{SR}\rho_{SR}(0)U_{SR}^\dagger]$ is a CP mapping, which can be decomposed into a sum of mappings corresponding to various measurement records obtained by readouts of the environments. For $\rho_S(0) = \sum_s q_s|\psi_s\rangle\langle\psi_s|$ and $\rho_R(0) = \sum_r p_r|r\rangle\langle r|$ this Kraus decomposition results in

$$\rho_S(t) = \sum_{b_R,r,s} p_r q_s U_{r,b_R}(t)|\psi_s\rangle\langle\psi_s|U_{b_R,r}^\dagger(t), \tag{3}$$

with Kraus operators $U_{b_R,r} \equiv \langle b_R|U_{SR}(t)|r\rangle$, where $\{|b_R\rangle\}$ is a basis for the reservoir Hilbert space . This corresponds

to an incoherent mixture of nonunitarily evolving states $|\psi_{b_R,r,s}\rangle \equiv U_{b_R,r}(t)|\psi_s\rangle$, weighted with the initial probabilities $p_r q_s$. For each state the GP is given by Eq. (1) with $Z[\psi_{b_R,r,s}] \propto \langle\psi_{b_R,r,s}(0)|\psi_{b_R,r,s}(t)\rangle$. Because $|\psi_{b_R,r,s}(0)\rangle = \langle b_R|r\rangle|\psi_s\rangle$, it is obvious that $Z[\psi_{b_R,r,s}] = 0$ whenever the basis state $|b_R\rangle$ is orthogonal to the reservoir state $|r\rangle$, so that the associated GP is not well defined. To avoid this problem we start by choosing a different basis set $\{|b_R(r)\rangle\}$ for each term in the sum over r in Eq. (3), such that $\langle b_R(r)|r\rangle = \delta_{b_R,0}$. Consequently, when one introduces a distribution for complex numbers of the form

$$P(z) = \sum_{b_R,r,s} w(r, s, b_R)\delta(z - Z[\psi_{b_R,r,s}]), \qquad z \in \mathbb{C}, \quad (4)$$

with $w(r, s, b_R)$ denoting the weight functions, terms with $b_R \neq 0$ do not contribute to any moment $\langle z^n\rangle = \int z^n P(z) d^2z$ and can therefore be omitted. Hence, it is sufficient to keep only terms with $b_R = 0$ so that the complex number distribution induced by Eq. (3) becomes

$$P_Z(z) \equiv \sum_{r,s} p_r q_s \delta(z - Z[\psi_{r,s}]), \quad (5)$$

with $|\psi_{r,s}(t)\rangle = \langle r|U_{SR}(t)|r\rangle|\psi_s\rangle$. For a total system $S + R$ with a continuous spectrum the sums in this distribution would be replaced by integrals.

The definition for a corresponding GP distribution faces the same subtleties that arise for any phase distribution. Usually, a positive operator-valued measure (POVM) is introduced to describe a phase distribution for quantum systems. However, through the dynamic phase functional $D[\psi]$, the GP depends nonlinearly on the states of the system, so that it is generally not possible to provide a GP POVM based on linear operators. Instead, one has to construct a GP phase distribution differently. We investigate two natural definitions of GP distributions. The first possibility to introduce a GP distribution is to derive the GP directly from the complex number distribution P_Z of Eq. (5); for example, the mean GP is given by the first moment [22]

$$e^{i\langle\beta\rangle} \equiv \frac{\langle z\rangle_Z}{|\langle z\rangle_Z|} = \frac{\sum_{r,s} p_r q_s Z[\psi_{r,s}]}{|\sum_{r,s} p_r q_s Z[\psi_{r,s}]|}. \quad (6)$$

By definition, $D[\psi_{r,s}]$ becomes unity if each $|\psi_{r,s}\rangle$ is parallel transported. Equation (6) then coincides with the usual GP [9] for mixed states, $\langle\beta\rangle = \mathrm{Arg}[\mathrm{Tr}(U_{SR}(t)\rho_{SR}(0))]$.

A second method to introduce a GP distribution is motivated by Holevo's approach to moments of a phase distribution [23]. While the definition (6) depends on the modulus of $Z[\psi]$, too, this is not necessarily desirable. Instead, one can introduce a phase distribution

$$P_H(s) = \sum_{r,s} p_r q_s \delta\left(e^{is} - \frac{Z[\psi_{r,s}]}{|Z[\psi_{r,s}]|}\right). \quad (7)$$

The corresponding first moment is given by

$$\langle e^{i\beta}\rangle \equiv \langle e^{is}\rangle_H = \sum_{r,s} p_r q_s e^{i\beta[\psi_{r,s}]}. \quad (8)$$

The phase of this expression can be considered as a mean GP, while its modulus is related to a measure

$$W = |\langle e^{i\beta}\rangle|^{-2} - 1 \quad (9)$$

for the spread of the GP. Equations (6) and (8) yield different results for the mean GP, which reflects the choice available in obtaining an average for the GP from the same distribution. Ideally, in each run one of the states $|\psi_{r,s}\rangle$ is realized and leads to a well-defined complex value for $Z[\psi_{r,s}]$. It is then only a matter of definition how the average of the complex values over all runs is performed.

Initially pure systems and density matrix decomposition.—To concentrate on the effects of the reservoir we consider the case $\rho_S(0) = |\psi_S\rangle\langle\psi_S|$, so that

$$P_Z(z) = \sum_r p_r \delta(z - Z[\psi_r]), \quad (10)$$

with $|\psi_r(t)\rangle = \langle r|U_{SR}(t)|r\rangle|\psi_S\rangle$. A consequence for a reservoir in a pure state (e.g., its ground state) is that the GP distribution is sharp, i.e., a δ distribution.

For the reservoir in a mixed state, however, the nonlinear dependence of $D[\psi]$ on $|\psi\rangle$ leads to an ambiguity in Eqs. (7) and (10) if the density matrix can be decomposed into mixtures of two different sets of states [17]. The GP then not only depends on the choice of distribution but also on the density matrix decomposition. We argue here that, with respect to the mean GP, the introduction of physical constraints can resolve both ambiguities. Naturally occurring reservoirs do not exhibit coherence between different energy levels, so we assume the density is block diagonal in the energy basis (with block sizes determined by degeneracies); a thermal reservoir with $\rho_R \propto \exp(-\beta H_R)$ is a typical example. It is then physically reasonable to only admit decompositions of the density matrix which differ with respect to the decomposition in degenerate subspaces. As the dynamic phase functional $D(E)$ is identical for all states sharing the same energy eigenvalue E, the contribution of the respective subspace $\mathcal{H}_E$ takes the form

$$\sum_{r\in\mathcal{H}_E} p_r \delta[z - D(E)\langle\psi_S|\langle r|U_{SR}|r\rangle|\psi_S\rangle]. \quad (11)$$

Hence, the corresponding contribution to $\langle z\rangle_Z$ can be written as $\mathrm{Tr}_{S,\mathcal{H}_E}[U_{SR}\rho(0)]$, which is independent of the decomposition. This is not the case for the mean GP in the Holevo measure, so that the resolution of the decomposition problem favors the choice of the measure $P_Z(z)$ for a

GP distribution. We note that for higher moments the decomposition ambiguity remains for both choices of GP distribution. However, we will see below that for a weakly coupled reservoir the GP distributions coincide and are independent of the decomposition.

Explicit GP expression for a weakly coupled reservoir.—We consider a total Hamiltonian of the form $H(t) = H_S(t) + H_R + H_I$ with constant weak coupling H_I and time-dependent system Hamiltonian $H_S(t)$, which generates a unitary evolution $U_{SR}(t) = T\exp[-i\int_0^t dt' H(t')]$ of the total system. The reservoir is initially in a mixture of eigenstates $|r\rangle$ of the time-independent Hamiltonian H_R. In the interaction picture, $U_{SR}(t) = U_S(t)U_R(t)\tilde{U}(t)$, with $U_R(t) = \exp(-itH_R)$ and $U_S(t) = T\exp[-i\int_0^t dt' H_S(t')]$. Standard second-order perturbation theory then leads to $\tilde{U}(t) = 1 + A + B + O(H_I^2)$ with $A \equiv -i\int_0^t dt' \tilde{H}_I(t')$ as well as $B \equiv -\int_0^t dt' \int_0^{t'} dt'' \tilde{H}_I(t')\tilde{H}_I(t'')$ and the interaction-picture Hamiltonian $\tilde{H}_I = U_R^\dagger U_S^\dagger H_I U_S U_R$.

Instead of explicitly deriving closed expressions for the operators A and B, we relate them to a corresponding CP mapping of the reduced density matrix ρ_S, which is assumed to be of Lindblad type [24],

$$\dot{\rho}_S = -i[H_S + \eta, \rho_S] - Q\rho_S - \rho_S Q + 2\sum_\alpha L_\alpha \rho_S L_\alpha^\dagger, \tag{12}$$

where $Q \equiv \sum_\alpha L_\alpha^\dagger L_\alpha$ and L_α are the jump operators. The Hermitian operator η describes any energy shifts (such as the Lamb shift for atom-light interaction) associated with $S + R$ interaction. On the other hand, we can also directly calculate $\dot{\rho}_S$ to second order in H_I by use of Eq. (3). A simple calculation yields

$$\dot{\rho}_S = -i[H_S, \rho_S] + \{U_S\langle\dot{B}\rangle_R U_S^\dagger \rho_S + U_S \sum_{r,r'} p_r \langle r|\dot{A}|r'\rangle U_S^\dagger \rho_S U_S \langle r'|A^\dagger|r\rangle U_S^\dagger + \text{H.c.}\}. \tag{13}$$

Expectation values are denoted by $\langle\cdots\rangle_q$ for a state $|\psi_q\rangle$; in particular, $\langle\cdots\rangle_S$ refers to $\langle\psi_S|\cdots|\psi_S\rangle$ and $\langle\cdots\rangle_R$ to $\mathrm{Tr}_R[\rho_R(0)\cdots]$. Comparing Eq. (13) with the Lindblad form (12) allows us to identify $U_S\langle\dot{B}\rangle_R U_S^\dagger = -i\eta - Q$, while the operator A is related to the jump terms.

To keep the presentation concise we now focus on a coupling of the form $H_I = -\sum_\mu R_\mu S_\mu$, where R_μ and S_μ are operators which act only on $\mathcal{H}_R$ and $\mathcal{H}_S$, respectively. Furthermore, we assume that $\langle r|R_\mu|r\rangle = 0\ \forall r$, which is the case for energy-transferring $S + R$ interactions, for instance. An immediate consequence is that $\langle A\rangle_r = 0$. It follows that $Z[\psi_r] = Z[\psi_S](1 + \langle\Delta Z\rangle_{r,S})$ with

$$\Delta Z \equiv \frac{U_S B}{\langle U_S\rangle_S} - \frac{B - B^\dagger}{2} + i\int_0^t dt'(B^\dagger \Delta\tilde{H}_S + \Delta\tilde{H}_S B), \tag{14}$$

with $\tilde{H}_S \equiv U_S^\dagger H_S U_S$ and $\Delta\tilde{H}_S \equiv \tilde{H}_S - \langle\tilde{H}_S\rangle_S$. Using Eq. (14) one easily finds the following expression for the moments associated with each of the two different GP distributions introduced above,

$$\langle e^{ins}\rangle_H = \frac{\langle z^n\rangle_Z}{|\langle z\rangle_Z|^n} = e^{in\beta[\psi_S]}(1 + in\mathrm{Im}\langle\Delta Z\rangle_{\rho_{SR}(0)}). \tag{15}$$

Result (15) has some interesting consequences. First, P_Z and P_H generate exactly the same moments so that $\langle e^{i\beta}\rangle = e^{i\langle\beta\rangle}$ to second order in H_I. Hence for a weakly coupled reservoir P_Z and P_H are equivalent and, since $|\langle e^{i\beta}\rangle| \approx 1$, the GP distribution is sharp. Second, as a consequence of $\langle r|R_\mu|r\rangle = 0$, P_Z and P_H do not depend on the operator A and therefore not on the jump operators. Third, because of the "linearity" of expressions to lowest order in perturbation theory, the moments (15) are independent of the decomposition of $\rho_R(0)$.

Explicit calculations of Berry phase.—As illustration we consider the GP distribution defined above for some specific physical examples. First, we discuss a two-level atom with ground state $|g\rangle$ and excited state $|e\rangle$ interacting with a thermal radiation reservoir. The corresponding Hamiltonian is $H_S = -(h\omega/2)(|e\rangle\langle e| - |g\rangle\langle g|)$, and the jump operators of Eq. (12) are $L_1 = \sqrt{\gamma_0(n+1)}|g\rangle\langle e|$ and $L_2 = \sqrt{\gamma_0 n}|e\rangle\langle g|$. Here, γ_0 denotes the spontaneous emission rate and n the thermal mean number of resonant photons [25]. At temperature $T = 0$ we have $n = 0$ which describes spontaneous emission in vacuum. The operator B introduced above then reads $B = -\gamma_0(|e\rangle\langle e| + n\mathbf{1})$. For simplicity we have omitted the Lamb shift [26]. For an initial state $|\psi_S\rangle = \cos\frac{\theta}{2}|e\rangle + \sin\frac{\theta}{2}|g\rangle$ we find for the (sharp) GP at time $t = 2\pi/\omega$ the expression

$$\langle\beta\rangle = \beta[\psi_S] + \pi^2\frac{\gamma}{\omega}\sin^2\theta, \tag{16}$$

where the GP for a closed system is given by $\beta[\psi_S] = 2\pi\sin^2(\theta/2)$. An interesting feature of this result is that the mean GP does not depend on the temperature, even though for $T > 0$ the radiation reservoir is in a mixed state. This is a consequence of the n dependence of B being proportional to the identity: the effect of thermal fluctuations, which induce incoherent absorption and emission of thermal photons at equal rates, do exactly cancel each other. The asymmetric effect of spontaneous emission, however, changes the GP.

Alternatively, one can calculate the GP exactly by solving Eq. (12) in terms of Kraus operators K_i without explicit reference to the reservoir. This simply amounts to seeking for operators K_i and probability weights p_i for which $\sum_i p_i K_i \rho_S(0) K_i^\dagger$ is a solution of the master equation [27]. For the present case, the Kraus operators are

$$K_0 = e^{-i(\omega/2)t}|g\rangle\langle g| + e^{i(\omega/2)t - \gamma_n t}|e\rangle\langle e|, \tag{17}$$

$$K_1 = K_3^\dagger = \sqrt{1 - e^{-2\gamma_n t}}|g\rangle\langle e|, \tag{18}$$

and $K_2 = \sigma_x K_0^\dagger \sigma_x$, with $\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|$, $\gamma_n \equiv (2n+1)\gamma_0$, and weights $p_0 = p_1 = (n+1)/(2n+1)$ as well as $p_2 = p_3 = n/(2n+1)$. The operators K_1 and K_3 are related to the jump operators and, because of $K_1(0) = K_3(0) = 0$, do not contribute to the GP. Substituting K_0 and K_2 into Eqs. (6) and (8) we calculate the GP distribution at time $t = 2\pi/\omega$ to be

$$P_Z(z) = p_0\delta(z - f_-) + p_2\delta(z - f_+),$$
$$P_H(s) = p_0\delta\left(e^{is} - \frac{f_-}{|f_-|}\right) + p_2\delta\left(e^{is} - \frac{f_+}{|f_+|}\right),$$
$$f_\pm \equiv -e^{-\pi(\gamma_n/\omega)}\langle e^{\mp\pi(\gamma_n/\omega)\sigma_z}\rangle_S\langle e^{\mp 2\pi(\gamma_n/\omega)\sigma_z}\rangle_S^{\pm i(\omega/2\gamma_n)}. \tag{19}$$

For zero temperature we have $n = 0$ and therefore $p_2 = 0$. Both expressions then predict a sharp GP $\langle\beta\rangle = \pi + \frac{\omega}{2\gamma_0}\ln\langle\psi_S|e^{-2\pi\gamma_0\sigma_z/\omega}|\psi_S\rangle$. This result agrees with the expression found in Ref. [15] and, to first order in γ_0, also with the result (16) based on the weakly coupled reservoir. Any difference between $\exp i\langle\beta\rangle$ and $\langle\exp i\beta\rangle$ is of second order in γ_0. Also for finite temperatures, the two exact results still agree with the weak coupling result (16) to first order in γ_0. Hence, any dependence on the temperature through n is of higher order in γ_0.

Another illustrative case is phase damping which can be described by a jump operator of the form $L_1 = \sqrt{\alpha}(|e\rangle\langle e| - |g\rangle\langle g|)$ (and therefore $B \propto \mathbf{1}$), where α denotes the phase damping rate. This jump operator can be derived from a coupling to a nonresonant reservoir of harmonic oscillators with effective interaction Hamiltonian $H_I = S_0 R_0 = \sigma_z\sum_i g_i a_i^\dagger a_i$, where a_i is the annihilation operator of the ith oscillator and g_i the corresponding effective coupling parameter. In thermal equilibrium we have $\langle R_0\rangle = \sum_i g_i\langle a_i^\dagger a_i\rangle \neq 0$ so that $\langle r|R_\mu|r\rangle = 0$ is violated. Consequently, the (trivial) result predicted by Eq. (15) is spurious. We can again compare this to an exact calculation based on the Kraus operators

$$K_0 = \frac{1}{r}e^{-i(\omega/2)t - \alpha t}|g\rangle\langle g| + re^{i(\omega/2)t}|e\rangle\langle e|, \tag{20}$$

and $K_1 = \sigma_x K_0^\dagger \sigma_x$, with $r \equiv [1 + \sqrt{1 - \exp(-2\alpha t)}]^{1/2}$ and weights $p_0 = p_1 = 1/2$. For brevity we only discuss the first moments which are given by

$$e^{i\langle\beta\rangle} \approx e^{i\beta[\psi_S]}\left(1 + \frac{2i\pi^2\alpha}{3\omega}\cos\theta\sin^2\theta\right), \tag{21}$$

$$\langle e^{i\beta}\rangle \approx e^{i\beta[\psi_S]}\left[1 + \frac{2\pi^2\alpha}{\omega}\sin^2\theta\left(i\cos\theta - \frac{4}{9}\sin^2\theta\right)\right], \tag{22}$$

for $t = 2\pi/\omega$. Unlike Eq. (15), these moments include nontrivial corrections and differ from each other as well as from the result of Ref. [15]. By Eq. (9) they indicate a GP spread of $W \approx 16\pi^2\sin^4\theta\alpha/(9\omega)$ for phase damping.

In summary, we have established a theory for GP distributions based on operational considerations that employs a Kraus operator analysis. We resolve ambiguities concerning decomposition of the density matrix and GP by incorporating reasonable assumptions about the reservoir and solve specifically for spontaneous emission and phase damping of a two-level atom.

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