Geometric Phase for Adiabatic Evolutions of General Quantum States

Biao Wu,[1,2] Jie Liu,[3] and Qian Niu[4]

[1]*Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China*
[2]*Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[3]*Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, Beijing 100088, China*
[4]*Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA*

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The concept of a geometric phase (Berry's phase) is generalized to the case of noneigenstates, which is applicable to both linear and nonlinear quantum systems. This is particularly important to nonlinear quantum systems, where, due to the lack of the superposition principle, the adiabatic evolution of a general state cannot be described in terms of eigenstates. For linear quantum systems, our new geometric phase reduces to a statistical average of Berry's phases. Our results are demonstrated with a nonlinear two-level model.

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A complete theory for the adiabatic evolution of quantum systems rests on three pillars. First, the adiabatic theorem dictates that the probability on each instantaneous eigenstate (nondegenerate) remains constant when the external condition, described by a set of control parameters, changes slowly in time [1]. Second, besides the usual dynamical phase, given by the time integral of the eigenenergy, the phase of an evolving eigenstate has a geometric part, called Berry's phase, which depends only on the geometric path in the parameter space [2]. Third, the linearity of the Schrödinger equation allows one to write the evolution of an arbitrary state as a linear superposition of the eigenstates with amplitudes whose magnitudes and phases are as prescribed above [3].

For a nonlinear quantum system, such as that described by the nonlinear Schrödinger equation, the third pillar is missing. The superposition principle no longer applies. While it is still possible to define eigenstates and describe their adiabatic evolution, one is clueless on the evolution of a general state when the control parameters are changed slowly. Nonlinear quantum systems have become increasingly important in physics. They often arise in the mean field treatment of many-body quantum systems, such as Bose-Einstein condensates (BECs) of dilute atomic gases [4,5], and as a possible fundamental nonlinear modification of quantum mechanics [6].

In this Letter we introduce the concept of a geometric phase for the adiabatic evolution of general quantum states including noneigenstates. It applies to both linear and nonlinear quantum systems. In the linear case, our geometric phase reduces to a statistical average of Berry's phases for the eigenstates, weighted by the probabilities that the system finds itself in the eigenstates.

Our effort to define a geometric phase for general quantum states is aided by the fact that quantum systems (linear or nonlinear) have an exact canonical structure of Hamiltonian dynamics, which has been known since long ago but not as widely as it deserves [6,7]. We can thus introduce classical concepts such as actions and angles to describe the motion of the quantum states without any approximation. The actions remain invariant during an adiabatic process, and the change in the angles has a geometric part called Hannay's angles [8]. Our new geometric phase is found to be related to these Hannay's angles in a derivative form. In defining the new phase, an average is taken over all possible initial states of the same actions. Therefore, our geometric phase can be viewed as a phase for a manifold of fixed actions, which is an invariant subspace of states in the adiabatic process (see Fig. 1).

The physical meaning of our phase is discussed in the context of a heavy particle interacting with a nonlinear quantum system. Our phase appears in the effective Lagrangian for the heavy particle. Similar to the original Berry's phase [2], we show that our phase for a general quantum state can be regarded as a geometric part of a generalized total phase. In the end, a nonlinear two-level model is used to illustrate our phase.

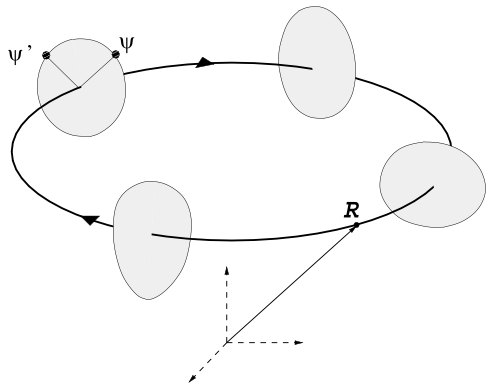

FIG. 1. Evolution of quantum states as the control parameters $\boldsymbol{R}$ traverse slowly along a closed path $\mathcal{O}$. At the end of the loop, an individual state (dot) may not come back to itself, but a collection of states (disk) does. This collection is characterized by a set of adiabatically invariant actions (illustrated by the disk area). Different disk shapes represent symbolically distinct dynamics at different values of $\boldsymbol{R}$.

We consider an N-level quantum system governed by a general nonlinear Schrödinger equation ($\hbar = 1$),

$$i\frac{d}{dt}|\psi\rangle = H(\psi^*, \psi; \boldsymbol{R})|\psi\rangle. \quad (1)$$

Here $|\psi\rangle = (\psi_1, \psi_2, \ldots, \psi_N)$ with ψ_j being its jth component over an orthonormal basis; the vector $\boldsymbol{R}$ represents all the control parameters subject to adiabatic change. For all problems of physical interest, we can assume that the system is globally gauge invariant. Therefore, the norm of the wave function is conserved. When H is independent of ψ^* and ψ, Eq. (1) is the usual linear Schrödinger equation.

Eigenstates for Eq. (1) can be defined as usual,

$$H(\boldsymbol{R})|\varphi_n(\boldsymbol{R})\rangle = \mu_n(\boldsymbol{R})|\varphi_n(\boldsymbol{R})\rangle. \quad (2)$$

Then for fixed values of $\boldsymbol{R}$, $e^{-i\mu_n(\boldsymbol{R})t}|\varphi_n(\boldsymbol{R})\rangle$ is a solution of the nonlinear Schrödinger equation (1). In the context of BEC physics, μ_n plays the role of a chemical potential. When $\boldsymbol{R}$ varies slowly in time, such a state remains to be a solution of Eq. (1) with the phase replaced by $\int dt\mu_n(\boldsymbol{R})$ (dynamical phase), minus Berry's phase defined by

$$\gamma_n(\mathcal{O}) = \int_{\mathcal{O}} d\boldsymbol{R}\langle\varphi_n(\boldsymbol{R})|i\frac{\partial}{\partial\boldsymbol{R}}|\varphi_n(\boldsymbol{R})\rangle. \quad (3)$$

This phase depends on the path $\mathcal{O}$ in the parameter space, but does not depend on the rate of change in $\boldsymbol{R}$.

However, it is not clear how a similar geometric phase can be defined for noneigenstates, which is imperative for nonlinear quantum systems due to their lack of the superposition principle as mentioned in the introduction. One can check that various existing generalizations of Berry's phase do not help here [9]. To overcome this difficulty, we notice a long-known fact [6,7] that the quantum system Eq. (1) is mathematically equivalent to Hamilton's equations of motion with a Hamiltonian energy functional $\mathcal{H}(\psi^*, \psi; \boldsymbol{R})$ and Poisson brackets $\{\psi_j^*, \psi_k\} = i\delta_{jk}$. That is, Eq. (1) can be reformulated as

$$i\frac{d}{dt}\psi_j = \frac{\partial}{\partial\psi_j^*}\mathcal{H}(\psi^*, \psi; \boldsymbol{R}). \quad (4)$$

In this formulation, the eigenstate defined in Eq. (2) is variationally an extremum solution of the energy functional $\mathcal{H}$, with μ_n viewed as the value of the Lagrange multiplier enforcing the conserved norm of a wave function. We emphasize that this canonical Hamiltonian structure is exact and applies to both the linear and the nonlinear Schrödinger equations. It is not related to the usual classical-quantum correspondence in the limit of $\hbar \to 0$. Using the language of Hamiltonian dynamics, the system of Eq. (1) can be classified into integrable or nonintegrable as for any classical systems. In this sense, all linear quantum systems are integrable.

We focus on the case that Eq. (1) is locally integrable even in the presence of nonlinearity. As we point out later, generalization to chaotic systems is possible. For fixed control parameters $\boldsymbol{R}$, in the integrable regions, the system can be described by a set of action and angle variables, $\boldsymbol{I} = \{I_1, I_2, \ldots, I_N\}$, $\boldsymbol{\theta} = \{\theta_1, \theta_2, \ldots, \theta_N\}$; the actions are constant while the angles vary in time with frequencies $\omega_\ell = \partial\mathcal{H}/\partial I_\ell$. In other words, the wave function can be expressed in terms of these action-angle variables, $|\psi\rangle = |\psi(\boldsymbol{I}, \boldsymbol{\theta}; \boldsymbol{R})\rangle$, with a ($\boldsymbol{R}$-dependent) canonical transformation parametrizing the amplitudes ψ_j with these new variables. When $\boldsymbol{R}$ are time dependent, we can still use the same expression of the wave function, $|\psi\rangle = |\psi(\boldsymbol{I}, \boldsymbol{\theta}; \boldsymbol{R})\rangle$, although the action-angle variables will lose the above simple properties.

However, if $\boldsymbol{R}$ vary slowly in time, the actions continue to be conserved [10]. In this case, $|\psi\rangle$ changes with time only through the rotating $\boldsymbol{\theta}$ and the slowly varying $\boldsymbol{R}$. This allows us to do the following expansion:

$$\langle\psi|d|\psi\rangle = \sum_{\ell=1}^{N}\langle\psi|\frac{\partial}{\partial\theta_\ell}|\psi\rangle d\theta_\ell + \langle\psi|\frac{\partial}{\partial\boldsymbol{R}}|\psi\rangle\cdot d\boldsymbol{R}. \quad (5)$$

The second term is clearly related to the geometry of the parameter space $\boldsymbol{R}$. It motivates us to define our geometric phase as

$$\gamma(\mathcal{O}) = \int_{\mathcal{O}} d\boldsymbol{R}\overline{\langle\psi(\boldsymbol{I}, \boldsymbol{\theta}; \boldsymbol{R})|i\frac{\partial}{\partial\boldsymbol{R}}|\psi(\boldsymbol{I}, \boldsymbol{\theta}; \boldsymbol{R})\rangle}, \quad (6)$$

where the overbar indicates an average after the integration along $\mathcal{O}$ over all initial angles with the same actions. This averaging wipes out the dependence of our phase γ on the dynamical angles $\boldsymbol{\theta}$ and makes it geometric. Such an averaging technique has been used in defining Hannay's angles [8].

The phase γ in Eq. (6) is the geometric phase that we have sought for general quantum states. Two remarks are in order: (i) One can check that our phase γ reduces to γ_n for an eigenstate $|\varphi_n\rangle$. (ii) Because of the averaging, the phase γ is a geometric characterization of the manifold of all states with a given set of actions. Such a manifold is an invariant subspace in an adiabatic process.

The physical meaning of our phase γ can be seen by considering a coupled system described by the following Lagrangian:

$$\mathcal{L} = \langle\psi|i\frac{d}{dt}|\psi\rangle - \mathcal{H}(\psi^*, \psi; \boldsymbol{R}) + \mathcal{L}'(\boldsymbol{R}, \dot{\boldsymbol{R}}), \quad (7)$$

where the first two terms are the Lagrangian for the nonlinear Schrödinger Eq. (1) and $\mathcal{L}'$ is a Lagrangian for a heavy particle moving slowly. In terms of action and angle variables, the Lagrangian becomes

$$\mathcal{L} = \boldsymbol{I}\cdot\dot{\boldsymbol{\theta}} + \langle\psi|i\frac{\partial}{\partial\boldsymbol{R}}|\psi\rangle\cdot\dot{\boldsymbol{R}} - \mathcal{H}(\boldsymbol{I}; \boldsymbol{R}) + \mathcal{L}'(\boldsymbol{R}, \dot{\boldsymbol{R}}). \quad (8)$$

Since the angles $\boldsymbol{\theta}$ change much faster than the particle's coordinates $\boldsymbol{R}$, we can take an average over the angles and obtain an effective Lagrangian for the dynamics of the heavy particle,

$$\mathcal{L}_{\text{eff}} = \overline{\langle\psi|i\frac{\partial}{\partial \boldsymbol{R}}|\psi\rangle} \cdot \dot{\boldsymbol{R}} - \mathcal{H}(\boldsymbol{I};\boldsymbol{R}) + \mathcal{L}'(\boldsymbol{R},\dot{\boldsymbol{R}}). \quad (9)$$

Our phase γ shows how the fast dynamics of a nonlinear quantum system influences the heavy particle.

Let us go back to Eq. (5) and examine the other two terms. After integration, the term on the left becomes

$$\beta = i\int_{\mathcal{O}}\langle\psi|d|\psi\rangle = \int_{\mathcal{O}}\langle\psi|H|\psi\rangle dt, \quad (10)$$

which is apparently a dynamical phase. For the first term on the right of Eq. (5), we have

$$\mathcal{T} = \int_{\mathcal{O}}\sum_{\ell=1}^{N} d\theta_\ell\langle\psi(\boldsymbol{I},\boldsymbol{\theta};\boldsymbol{R})|i\frac{\partial}{\partial\theta_\ell}|\psi(\boldsymbol{I},\boldsymbol{\theta};\boldsymbol{R})\rangle. \quad (11)$$

We similarly average $\mathcal{T}$ over all initial angles. Because of such an averaging, the integrand in Eq. (11) can be replaced with I_ℓ [11]. Letting $\Delta\theta_\ell$ be the total change in angle θ_ℓ for an adiabatic process along $\mathcal{O}$, we find

$$\overline{\mathcal{T}} = \sum_{\ell=1}^{N} I_\ell\Delta\theta_\ell, \quad (12)$$

which is the total action of the quantum state on average. Putting all these together, we arrive at

$$\sum_{\ell=1}^{N} I_\ell\Delta\theta_\ell = \overline{\beta} - \gamma(\mathcal{O}), \quad (13)$$

where the overbar stands for the averaging over all the initial angles as before. For an adiabatically evolving eigenstate $|\psi\rangle = e^{-i\lambda(t)}|\varphi_n(\boldsymbol{R})\rangle$, there is only one pair of nonzero action and angle, the norm $\langle\psi|\psi\rangle$ and the phase λ, respectively. In this special case, our total action $\overline{\mathcal{T}} = \mathcal{T}$ becomes the total phase $\Delta\lambda$, accumulated during the adiabatic evolution of the eigenstate. Therefore, the total action is also a generalization of the total phase, and relation (13) says that our phase γ is the geometric part of this generalized total phase. Finally, we note that this relation (13) can also be regarded as another expression for our phase γ, which is easier to be implemented numerically and is used to compute the results in Fig. 2.

According to Hannay [8], the rotating angles $\boldsymbol{\theta}$ pick up geometric angles $\boldsymbol{\alpha} = \{\alpha_1, \alpha_2, \ldots, \alpha_N\}$ in addition to the dynamical part as $\boldsymbol{R}$ traverse slowly round a loop $\mathcal{O}$. These angles $\boldsymbol{\alpha}$, known as Hannay's angles and regarded as a classical concept, have now shown up naturally in quantum systems. In light of this recognition, the geometric part of the total action $\mathcal{T}$ is apparently $\sum_\ell I_\ell\alpha_\ell$, which should equal our phase γ. Taking the derivative of Eq. (13) with respect to I_ℓ, we then obtain

$$\alpha_\ell(\mathcal{O}) = -\frac{\partial}{\partial I_\ell}\gamma(\mathcal{O}), \quad (14)$$

which relates our geometric phase and Hannay's angle in a derivative form. This relation can be viewed from another angle. The quantum system (linear or nonlinear) of Eq. (1) may be regarded as the classical limit of a second-quantized system $\hat{\mathcal{H}}$, where ψ_j becomes an operator $\hat{\psi}_j$. According to Ref. [12], our phase γ is the usual Berry's phase for this second-quantized system in the semiclassical limit. In other words, the relation (14) is also the semiclassical relation between Hannay's angles and Berry's phases, which has been known for a while [12–14].

So far, we have focused on completely integrable systems (or regions). Our phase γ can be generalized to other nonintegrable systems, including the class of chaotic systems studied in Ref. [15]. One can achieve this by expanding the averaging in Eq. (6). Namely, if the system has only $K(<N)$ adiabatic invariants, the averaging in Eq. (6) is then over all initial states with the same K invariants.

We now illustrate the new phase γ with two examples. First, we consider a general quantum state in linear systems, where the evolving quantum state can be expanded in terms of the normalized eigenstates,

$$|\psi(t)\rangle = \sum_{n=1}^{N} a_n(t)|\varphi_n(\boldsymbol{R})\rangle. \quad (15)$$

According to the quantum adiabatic theorem [1], the occupation probabilities of different eigenstates $|a_n|^2$ are adiabatic constants. In fact, they are actions $I_n = |a_n|^2$ when the system is regarded mathematically as a classical Hamiltonian system [16]; their corresponding angle variables θ_n's are the phases of a_n's. With these in mind, the computation of Eq. (6) with the state (15) is straightforward. We find that the off-diagonal terms become zero after the averaging, and the geometric phase γ is

$$\gamma(\mathcal{O}) = \sum_{n=1}^{N}|a_n|^2\gamma_n(\mathcal{O}). \quad (16)$$

Therefore, in linear quantum systems, the phase γ is just a weighted summation of Berry's phases of all the eigenstates involved. Interestingly, this kind of weighted summation of Berry's phases has already been applied in real physical systems [17,18]. Interestingly, if we apply Eq. (14) to Eq. (16), we find that these Hannay's angles differ from Berry's phases only by a sign, $\alpha_n = -\gamma_n$.

Second, we study a nonlinear two-level model given by

$$i\frac{d\psi_1}{dt} = \left[c|\psi_2|^2 + \frac{Z}{2}\right]\psi_1 + \frac{X - iY}{2}\psi_2, \quad (17)$$

$$i\frac{d\psi_2}{dt} = \left[c|\psi_1|^2 - \frac{Z}{2}\right]\psi_2 + \frac{X + iY}{2}\psi_1. \quad (18)$$

This simple model can be used to describe the Josephson effect of Bose-Einstein condensates residing in a double-well potential [5,19]. The complex coupling constant, as denoted by X and Y, can be realized in experiment through phase imprinting on one of the two wells [20].

We first look at the geometric phase γ for eigenstates of this nonlinear quantum system. This is to find all the eigenstates $|\varphi_n(\boldsymbol{R})\rangle$, and then use them to calculate the

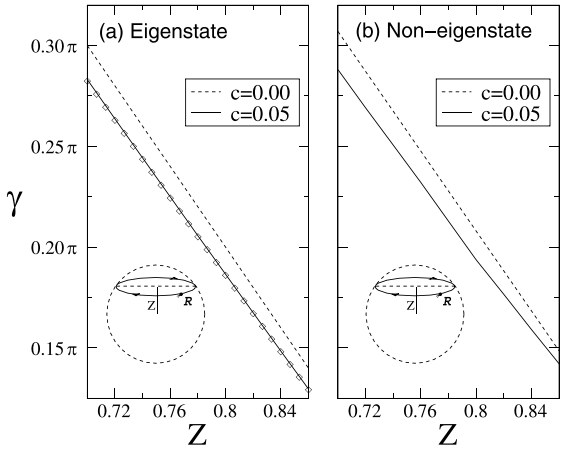

FIG. 2. Geometrical phases γ of the nonlinear two-level model (17) and (18): (a) the lower eigenstate and (b) the noneigenstate near the lower eigenstate. The noneigenstate has an action (or *AA* phase) of $I = 0.005$. The inset shows the closed path $\mathcal{O}$ used that is a circle on a unit sphere with Z fixed. The circle is traversed with a rate of 0.001. The results for eigenstates are compared to the analytical expression of Eq. (19) (denoted by diamonds): a very good match is found.

phase with Eq. (3). They could be done numerically; fortunately for this simple case, analytical results can be obtained. When the path is restricted on the unit sphere $X^2 + Y^2 + Z^2 = 1$, we find that the phases for these nonlinear eigenstates are

$$\gamma(\mathcal{O}) = \int_{\partial S=\mathcal{O}} \frac{\eta^3(\boldsymbol{R} + c\eta\hat{z}) \cdot d\boldsymbol{S}}{(c\eta + Z)^2(c\eta^3 + Z)}, \qquad (19)$$

where $\hat{z}$ is the unit vector along the z axis and η is one of the real roots of

$$c^2\eta^4 + 2cZ\eta^3 + (1 - c^2)\eta^2 - 2cZ\eta - Z^2 = 0. \qquad (20)$$

Different real roots η correspond to different eigenstates. Equation (20) can have more than two real roots, indicating that there can be more than two eigenstates [21]. Here we limit ourselves to the situations where Eq. (20) has only two real roots. For the path $\mathcal{O}$ that is a circle with a fixed Z, the geometric phase in Eq. (19) becomes $\gamma = (1 - \eta)\pi$. The diamonds in Fig. 2 show how γ for the lower eigenstate changes with Z.

For a general quantum state, we have to resort to numerical means. The path $\mathcal{O}$ is picked to be a circle with fixed Z. We then solve Eqs. (17) and (18) numerically after choosing a changing rate $\upsilon = 0.001$ for the parameters $\boldsymbol{R} = \{X, Y, Z\}$. The evolving states are recorded and used to compute the phase γ with Eq. (13), where the averaging is done for different initial states with the same action (or *AA* phase) I. Results for $c = 0.05$ are plotted in Fig. 2, showing how the phase changes with Z. Computation is done for both eigenstate and noneigenstate, and the results (solid lines) are compared to the phases for the linear case $c = 0.0$ (dashed lines). The changing rate of $\boldsymbol{R}$ ($\upsilon = 0.001$) is slow enough to be considered as adiabatic. This is witnessed by the good fit between the solid line and the diamonds in Fig. 2(a) as the diamonds are the analytical results of Eq. (19).

In conclusion, a geometric phase for the adiabatic evolution of general quantum states is introduced. It applies to noneigenstates as well as eigenstates in both linear and nonlinear quantum systems. Our geometric phase is related to Hannay's angles, which arise naturally in a canonical description of adiabatic dynamics of quantum states. Like the usual Berry's phase, it also affects the effective dynamics of slow variables. A nonlinear two-level system is used to demonstrate our results.

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