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Geometric phase within the complex quantum Hamilton-Jacobi formalism

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ABSTRACT

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1. Introduction

The concept of *quantum geometric phase* has attracted considerable attention in a wide range of areas of physics. Berry pointed out that a quantum system can obtain a geometric phase when it evolves adiabatically along a closed path in the parameter space of the Hamiltonian [1,2]. After Berry's publication, several studies were devoted to the removal of the restrictions on the evolution of a quantum system. The geometric phase was generalized to nonadiabatic cyclic evolutions in the projective Hilbert space [3]. Moreover, the evolution of the quantum system need be neither unitary nor cyclic [4]. In addition, Mukunda and Simon developed the theory of the geometric phase from the quantum kinematic approach, and showed that the geometric phase is a natural consequence of quantum kinematics [5].

As a variant of Bohmian mechanics [6–11], the *complex quantum trajectory method* based on the quantum Hamilton–Jacobi formalism [12,13] has been developed not only to provide insightful understanding of quantum phenomena but also to provide a useful approach in computational applications. As an analytical approach, complex quantum trajectories determined from the analytical form of the wave function have been analyzed for several stationary and nonstationary problems [14–19]. In addition, quantum interference demonstrated by the head-on collision of two Gaussian wave packets leads to the formation of quantum caves, and this method

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We derive a geometric phase using the quantum kinematic approach within the complex quantum Hamilton–Jacobi formalism. The single valuedness of the wave function implies that the geometric phase along an arbitrary path in the complex plane must be equal to an integer multiple of 2π . The nonzero geometric phase indicates that we travel along the path through the branch cut of the phase function from one Riemann sheet to another.

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provides a unified description of interference as well as an elegant method to define the lifetime for interference features [20–22]. As a synthetic approach, the derivative propagation method [23] has also been used to obtain approximate complex quantum trajectories and the wave function for wave-packet scattering problems [24–29].

The geometric phase in Bohmian mechanics has been explored in several studies [30-38], but the geometric phase has not been investigated within the complex quantum Hamilton-Jacobi formalism. Therefore, the purpose of the current study is to analyze the geometric phase in the complex quantum trajectory method using the quantum kinematic approach of Mukunda and Simon, and we transfer the concept of geometric phase to an individual complex quantum trajectory. Focusing on one-dimensional problems extended to the complex plane, we derive a reparametrization and gauge invariant geometric phase associated with an arbitrary open or closed path, which is not necessarily a quantum trajectory. The geometric phase consists of the total phase measuring the phase change at the endpoints of the path and the dynamical phase arising from the phase change locally accumulated along the path. In addition, we derive the rate equations describing the rate of change in the phase and amplitude of the wave function along a path in the complex plane. The single valuedness of the complexextended wave function implies that the geometric phase along a path must be equal to an integer multiple of 2π . The nonzero geometric phase indicates that we travel through the branch cut of the phase function from one Riemann sheet to another along the path. For stationary states, quantum vortices exhibiting the quantized circulation integral can be regarded as a manifestation of the geometric phase.

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This Letter is organized as follows. We begin by reviewing the complex quantum trajectory method in Section 2. In Section 3, we derive a reparametrization and gauge invariant geometric phase using the quantum kinematic approach and the rate equations for the phase and amplitude of the wave function. In Section 4, relevant properties for this geometric phase are discussed. In Section 5, a nonstationary state is used as an example to demonstrate those concepts developed in the previous sections. Finally, we make some comments and conclude with a discussion about future research.

2. Complex quantum trajectory method

In the complex quantum Hamilton–Jacobi formalism [12,13,18], the wave function analytically extended to complex space is expressed by

$$\Psi(z,t) = \exp\left[\frac{i}{\hbar}S(z,t)\right],\tag{1}$$

where S(z, t) is the complex action and time remains real valued. Substituting this expression into the complex-extended time-dependent Schrödinger equation, we obtain the complex-valued quantum Hamilton–Jacobi equation (QHJE) in complex space

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} \left(\frac{\partial S}{\partial z}\right)^2 + V(z) + \frac{\hbar}{2mi} \frac{\partial^2 S}{\partial z^2}.$$
 (2)

Complex quantum trajectories are defined by the guidance equation

$$m\frac{dz}{dt} = p(z,t) = \frac{\partial S(z,t)}{\partial z},$$
(3)

where p(z, t) is the quantum momentum function (QMF). The terms on the right side of Eq. (2) correspond to the kinetic energy, the classical potential, and the complex quantum potential given by

$$Q(z,t) = \frac{\hbar}{2mi} \frac{\partial^2 S}{\partial z^2}.$$
 (4)

Through Eq. (1), we can express the QMF in terms of the wave function by

$$p(z,t) = \frac{\hbar}{i} \frac{1}{\Psi(z,t)} \frac{\partial \Psi(z,t)}{\partial z}.$$
(5)

From Eq. (3), the wave function determines the dynamics of complex quantum trajectories through the QMF. It has been pointed out that the trajectory dynamics is influenced by stagnation points and poles of the QMF corresponding to those points where $\partial \Psi(z, t)/\partial z = 0$ and nodes of $\Psi(z, t)$, respectively [18–21,39,40].

3. Geometric phase in complex space

3.1. Quantum kinematic approach to the geometric phase

Using the quantum kinematic approach of Mukunda and Simon [5], we derive a geometric phase within the complex quantum Hamilton–Jacobi formalism. For a wave function $\psi(z, t)$, we consider an arbitrary open or closed path z(t) in the complex plane starting at $t = t_1$ and ending at $t = t_2$, which is not necessarily a quantum trajectory. The time evolution of the wave function along this path arises from changes both in position and in time, $\psi(t) = \psi(z(t), t)$, where the parameter t labels the wave function. Thus, $\psi(t)$ forms a one-dimensional or one-parameter smooth curve in the *complex inner product space*, $C = \{\psi(t), t_1 \le t \le t_2\}$. The geometric phase is a property of a curve $\psi(t)$ in this space.

From the quantum kinematic approach [5], the geometric phase associated with this curve C is given by

 $\varphi_g = \varphi_{tot} - \varphi_{dyn}$

$$= \arg\left[\left(\psi(t_{1}), \psi(t_{2})\right)\right] - \int_{t_{1}}^{t_{2}} \operatorname{Im}\left[\frac{(\psi(t), d\psi(t)/dt)}{(\psi(t), \psi(t))}\right] dt, \qquad (6)$$

where φ_{tot} is the total phase, φ_{dyn} is the dynamical phase, and the brackets (.,.) denote the inner product of two complex numbers. The total phase measures the phase difference between the endpoints of this curve, and this endpoint relative phase is a *global* quantity. However, the dynamical phase measures the phase change *locally* accumulated along the curve in the complex inner product space.

Separating the complex action into its real and imaginary parts, S(z,t) = u(x, y, t) + iv(x, y, t) where u(x, y, t) and v(x, y, t) are real valued, we write the wave function in Eq. (1) as

$$\Psi(z,t) = \exp\left[\frac{i}{\hbar}S\right] = \exp\left[\frac{i}{\hbar}u - \frac{1}{\hbar}v\right].$$
(7)

Since the complex action is analytically extended into the complex plane, the phase function u(x, y, t) and the amplitude function v(x, y, t) are continuous and differentiable with respect to x and y and they can be regarded as differentiable multivariable functions of x, y, and t [41]. Substituting this expression into the first term in Eq. (6), we obtain the *real-valued* total phase along an arbitrary path z(t) = x(t) + iy(t),

$$\varphi_{tot} = \frac{1}{\hbar} \Big[u \big(x(t_2), y(t_2), t_2 \big) - u \big(x(t_1), y(t_1), t_1 \big) \Big]. \tag{8}$$

Specifically, the total phase is undefined if $\psi(t_1) = 0$ or $\psi(t_2) = 0$. On the other hand, to obtain the dynamical phase along a path z(t), we need to evaluate the time derivative of the wave function expressed in Eq. (7)

$$\frac{d\psi(t)}{dt} = e^{-\nu/\hbar} e^{iu/\hbar} \left(\frac{i}{\hbar} \frac{du}{dt} - \frac{1}{\hbar} \frac{d\nu}{dt} \right).$$
(9)

The *total* time derivative of the wave function gives the change of the wave function along a path originating from changes in both position and time. Thus, the *real-valued* dynamical phase in Eq. (6) becomes

$$\varphi_{dyn} = \frac{1}{\hbar} \int_{t_1}^{t_2} \frac{du}{dt} (x(t), y(t), t) dt.$$
 (10)

The expression clearly indicates that the dynamical phase describes the locally accumulated phase change along the path. Therefore, the geometric phase along the path in the complex plane is given by $\varphi_g = \varphi_{tot} - \varphi_{dyn}$.

3.2. Rate equations for the phase and amplitude of the wave function

It is noted from Eq. (10) that we need to derive a rate equation for the phase function describing the rate of change in u(x, y, t)along an *arbitrary* path z(t), which is not necessarily a quantum trajectory. Taking the total time derivative of the complex action, we obtain

$$\frac{dS}{dt} = \frac{\partial S}{\partial z}\frac{dz}{dt} + \frac{\partial S}{\partial t} = p\left(\frac{dz}{dt} - \frac{p}{m}\right) + L(z,t),$$
(11)

where $p = \partial S/\partial z$ and Eq. (2) have been used and the *complex quantum Lagrangian* is given by $L(z, t) = p^2/2m - (V + Q)$. Here, the grid point velocity (dz/dt) has not been assigned; thus, Eq. (11)

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