

Geometric phase from a combined evolution-operator-invariant technique

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The quantum phase problem is investigated by a synthesis of the evolution operator technique and method of invariants. This approach has been found to be quite effective to disclose interrelationship between geometric phases differing in the nature of evolution and to obtain results for them without invoking the concept of parallel transport in the projective Hilbert space. The usefulness of the method developed is ascertained by studying the geometric phases associated with spinor evolutions in rotating magnetic field.

1. Introduction

Followed by early implications in optics [27] and chemical physics [12,13,20–22], the quantum phase problem has been studied in great detail in the context of nonrelativistic quantum mechanics. For example, when a quantal system in a given eigenstate is transported *adiabatically* around a closed circuit in the parameter space of the Hamiltonian, it acquires, in addition to the usual dynamical phase, a geometrical phase often called the Berry's phase [4]. In a followup to the original work, Aharonov and Anandan (AA) [1] removed the constraint implied by the adiabatic assumption and derived an approach to the phase problem in which the phase was shown to arise from the dynamical evolution of the quantal system in the projective Hilbert space rather than in the parameter space of the Hamiltonian. Later, Berry's phase has been found to appear in a still more general context. Neither adiabaticity [1], nor unitarity [30], nor even cyclicity [33] is a prerequisite for the evolution of a state to produce the geometrical phase. Also there exists a description [24] of the phase problem purely in terms of the geometry of the (open) curve in the ray space without invoking a Hamiltonian or a Schrödinger-like governing equation.

Besides all approaches noted above, the method of invariants (MI) [19] has been judiciously used [8,9,17,23] for a conceptually simple and elementary way of defining the geometric phase. In the MI, the exact solutions of a time-dependent (TD) Schrödinger equation are related to those of a Hermitian invariant of the Hamiltonian by a phase factor often called the LR phase according to the names of the originator (Lewis and Riesenfeld [19]) of the method. In studying the phase problem within the

framework of this approach one is led to a projective Hilbert space which is spanned by the instantaneous eigenstates of the LR invariant, and the geometric phase is due to holonomy in a line bundle over the generalized parameter space associated with the invariant. Although the adiabatic hypothesis is apparently removed [8,9,17,19,23] in the MI, the relation of the phase obtained to that of Berry or of AA is not immediately clear. One of our objectives in the present work is to reveal the interrelationship between the geometric phases. We propose to accomplish this by dealing with a variant of the evolution-operator technique (EOT) derived by Cheng and Fung [10]. The other point of our interest is to seek a realization of the geometric phase without making recourse to the use of so called parallel transport which has always played a central role [1,32] in such studies. Interestingly, we shall demonstrate that the initial conditions on the invariant determine the nature of evolution of the quantal system.

In section 2, we quote some of the results from the theory of time-dependent invariants [19] for a general quantum system whose Hamiltonian operator $H(t)$ is explicitly time dependent. We derive in section 3 an evolution-operator technique with particular emphasis on those points which in conjunction with the results of MI could achieve the objectives of the present work. In section 4, we seek a realization for the geometric phases in terms of variations in the initial condition of the invariant. Here we also clarify how the nature of evolution of the quantal system depends crucially on the choice for initial condition. In order to demonstrate the usefulness of the method developed we calculate in section 5 the result for Berry's and AA phases for a spin-1/2 particle in a rotating magnetic field. Finally, in section 6 we make some concluding remarks.

2. Time-dependent invariants

Consider a quantal system whose Hamiltonian operator $H(t)$ is an explicit function of time. The non-trivial Hermitian operator $I(t)$ is an invariant of the problem if

$$\frac{dI(t)}{dt} = \frac{\partial I(t)}{\partial t} + \frac{1}{i\hbar}[I, H] \equiv \left[-i\frac{\partial}{\partial t} + \frac{H}{\hbar}, I(t) \right] = 0. \quad (1)$$

Lewis and Riesenfeld [19] found that if $I(t)$ is one of the complete set of commuting observables having no time derivative with eigenstates $|\lambda, \kappa, t\rangle$ satisfying

$$I(t)|\lambda, \kappa, t\rangle = \lambda|\lambda, \kappa, t\rangle \quad (2a)$$

and

$$\langle \lambda', \kappa', t | \lambda, \kappa, t \rangle = \delta_{\lambda\lambda'} \delta_{\kappa\kappa'}, \quad (2b)$$

then the eigenvalues λ are time independent (TI) although the eigenstates are TD. The set of exact solution $|\psi(t)\rangle$ of the Schrödinger equation are related to $|\lambda, \kappa, t\rangle$ by

$$|\psi_{\lambda\kappa}(t)\rangle = e^{i\alpha_{\lambda\kappa}(t)}|\lambda, \kappa, t\rangle \quad (3)$$

with the phase factor

$$\alpha_{\lambda\kappa}(t) = \frac{1}{\hbar} \int_{t_0}^t \left\langle \lambda, \kappa, t' \left| i\hbar \frac{\partial}{\partial t'} - H(t') \right| \lambda, \kappa, t' \right\rangle dt'. \quad (4)$$

Clearly, the LR phase $\alpha_{\lambda\kappa}(t)$ is a part of the Schrödinger wave function and appears to be derivable without adiabatic hypothesis. The second term in (4) stands for the dynamical phase. It is of interest to identify the first term with any of the geometrical phases because for any situation the geometric phase is the difference of a total phase and a dynamical phase, and also because it was not obvious from the pioneering work of Mizrahi [23].

3. Evolution-operator technique

Let us assume for the sake of generalization that $H(t)$ is not necessarily cyclic in some parameters which induce the time evolution. Since in the Schrödinger picture, observables are regarded as constant in time, it will be tempting to consider the evolution equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (5)$$

in the interaction picture. Let $U(t)$ be a unitary operator that recovers $H(t)$ from a different Hamiltonian $\tilde{H}(t)$ through the similarity transformation

$$H(t) = U^\dagger(t) \tilde{H}(t) U(t) \quad (6)$$

and construct a new state

$$|\tilde{\psi}(t)\rangle = U(t) |\psi(t)\rangle \quad (7)$$

from the state $|\psi(t)\rangle$. Clearly,

$$\langle \psi(t) | H(t) | \psi(t) \rangle = \langle \tilde{\psi}(t) | \tilde{H}(t) | \tilde{\psi}(t) \rangle. \quad (8)$$

Equation (8) shows that dynamical phases of $H(t)$ and $\tilde{H}(t)$ are the same. Use of (7) in (5) gives the evolution equation for $|\tilde{\psi}(t)\rangle$ as

$$i\hbar \frac{\partial}{\partial t} |\tilde{\psi}(t)\rangle = \mathcal{H}(t) |\tilde{\psi}(t)\rangle, \quad (9)$$

where

$$\mathcal{H}(t) = \tilde{H}(t) - i\hbar U(t) \dot{U}^\dagger(t). \quad (10)$$

Interestingly, the evolution equations (5) and (9) for $|\psi(t)\rangle$ and $|\tilde{\psi}(t)\rangle$ have the same form. But an added advantage of the latter is that, it can be put into a *Schrödinger-like* picture by an appropriate choice for the operator $U(t)$ in (6) and (7) such that $\mathcal{H}(t)$ is Hermitian and

$$[\mathcal{H}(t), \mathcal{H}(t')] = 0 \quad \forall t, t'. \quad (11)$$

This implies that $\mathcal{H}(t)$ is diagonal for all time in some representation. More specifically, for a class of TD Hamiltonian that satisfies

$$H(t) = e^{-i\varepsilon At} H(0) e^{i\varepsilon At}, \quad (12)$$

the result in (9) describes the evolution equation in the Schrödinger picture with TI Hamiltonian

$$\mathcal{H} = H(0) - \varepsilon A. \quad (13)$$

Thus, equation (5) with $H(t)$ given in (12) can be regarded as an evolution equation in the interaction picture with εA playing the role of the unperturbed Hamiltonian H_0 in the transformation [29] between (12) and (13).

As a consequence of (11), $|\tilde{\psi}(t)\rangle$ in (9) can be found from $|\tilde{\psi}(0)\rangle$ as [6]

$$|\tilde{\psi}_n(t)\rangle = e^{-\frac{i}{\hbar} \int^t \mathcal{H}(t') dt'} |\tilde{\psi}_n(0)\rangle, \quad (14)$$

where $|\tilde{\psi}(0)\rangle$ satisfies the eigenvalue equation

$$\mathcal{H}(0) |\tilde{\psi}_n(0)\rangle = \lambda_n |\tilde{\psi}_n(0)\rangle. \quad (15)$$

Using (14) in (7), one can obtain the solution of (5) as

$$|\psi_n(t)\rangle = e^{-\frac{i}{\hbar} \int^t \langle \mathcal{H}(t') \rangle_n dt'} U^\dagger(t) |\tilde{\psi}_n(0)\rangle \quad (16)$$

with the initial condition

$$|\psi(0)\rangle = U^\dagger(0) |\tilde{\psi}_n(0)\rangle. \quad (17)$$

Substituting (10) in (16) we have

$$|\psi_n(t)\rangle = e^{i\gamma_D(t) + i\gamma_G(t)} [U^\dagger(t) |\tilde{\psi}_n(0)\rangle]', \quad (18)$$

where $[U^\dagger(t) |\tilde{\psi}_n(0)\rangle]'$ does not involve any explicit TD phase factor. The dynamical and geometrical phases $\gamma_D(t)$ and $\gamma_G(t)$ are then given by

$$\gamma_D(t) = -\frac{1}{\hbar} \int^t \langle \tilde{\psi}_n(t') | \tilde{H}(t') | \tilde{\psi}_n(t') \rangle dt' \quad (19a)$$

and

$$\gamma_G(t) = -\frac{1}{\hbar} \int^t \langle \mathcal{H}(t') \rangle_n dt' - \gamma_D(t) + \theta(t), \quad (19b)$$

with $\theta(t)$, the phase of $U^\dagger(t) |\tilde{\psi}_n(0)\rangle$, which appears to introduce some kind of non-uniqueness for $\gamma_G(t)$. Since the actual geometric phase is a uniquely defined property of the closed path in the projective Hilbert space [20–22] our choice for $U(t)$ should be constrained to give $\theta(t) = 0$. This choice reduces $\gamma_G(t)$ into the form

$$\gamma_G(t) = i \int^t \langle \tilde{n}(u) | \dot{\tilde{n}}(u) \rangle du, \quad |\tilde{n}(t)\rangle = U^\dagger(t) |\tilde{\psi}_n(0)\rangle. \quad (20)$$

The geometrical phase has been expressed in the same way as that in Berry. In the treatment of Berry, $|\tilde{n}(t)\rangle$ refers to an instantaneous eigenstate of the Hamiltonian $H(t)$ because of the assumed adiabatic approximation. But in (20), $|\tilde{n}(t)\rangle$ need not necessarily be the instantaneous eigenstate. This waives the adiabatic assumption.

4. Method of invariant and geometric phase

We can now exploit some of the results obtained in sections 2 and 3 to examine the effectiveness of MI to obtain phases of Berry [4] and of Aharonov and Anandan [1]. In their work with the EOT, Cheng and Fung [10] obtained an equation similar to that in (9) by factoring out the evolution operator for (5) in the form

$$U(t, 0) = U(t)R(t) \quad (21)$$

and found

$$|\psi(t)\rangle = e^{i\bar{\gamma}_D(t)+i\bar{\gamma}_B(t)}|\bar{n}(t)\rangle. \quad (22)$$

Here $|\bar{n}(0)\rangle$ is the eigenstate of $H(0)$ instead of $\mathcal{H}(0)$. In this approach one may make different choices of $U(t)$ and $R(t)$ to get a unique $|\psi(t)\rangle$ for (5). The value of the dynamical phase will not depend on the choice $U(t)$. But as one goes on changing the choice for $U(t)$, $|\bar{n}(t)\rangle$ in (20) will develop a phase. The change of phase is compensated by a change in the value $\bar{\gamma}_B(t)$ and makes $|\psi(t)\rangle$ choice independent. In particular, for cyclic evolution of period T , they recovered the Berry's phase by choosing $U_B(t)$ as

$$U_B(T)|n(0)\rangle = |n(0)\rangle. \quad (23)$$

Their second choice was the parallel transport

$$\langle n(0)|U_A(t)\dot{U}_A^\dagger(t)|n(0)\rangle = 0 \quad (24)$$

of the state vector along a closed circuit in the projective Hilbert space. In this case, $\bar{\gamma}_B(T)$ vanishes identically and one gets the geometric phase α from

$$U_A(T)|n(0)\rangle = e^{i\alpha}|n(0)\rangle, \quad (25)$$

which is precisely the result obtained by Anandan [2].

In the following we now examine how the form of the EOT derived by us gives the AA phase via equation (20) without going through any parallel transport. This will depend on the choice of the initial state as an eigenstate of $\mathcal{H}(0)$ and the relationship between MI and EOT. In the bargain, this will determine the conditions on the choice of the initial form of invariants to produce the phases of Berry and AA. To that end we start with (20) and impose the initial condition

$$I(0) = k\mathcal{H}(0) \quad (26)$$

on $I(0)$. From (15) and (26), it is clear that $|\tilde{\psi}_n(0)\rangle$ is also an eigenfunction of $I(0)$. The unitarity of $U(t)$ can be used to recast (15) into the form

$$I(t)|\tilde{n}(t)\rangle = \lambda|\tilde{n}(t)\rangle, \quad (27)$$

where

$$I(t) = U^\dagger(t)I(0)U(t). \quad (28)$$

With the help of equation (10), it can be shown that $I(t)$ satisfies the equation for a constant of the motion. This is explicitly demonstrated in appendix A. Similarly, exploiting the evolution equation for $U(t, 0)$ one can demonstrate in the notation of [10] that

$$I_B(t) = U(t, 0)I_B(0)U^\dagger(t, 0) \quad (29)$$

with

$$I_B(0) = kH(0) \quad (30)$$

also satisfies (1). This is proved in appendix B.

We like to emphasize that although $I_B(t)$ in (29) obeys the equation for the constant of the motion, initial condition (30) suggests $I_B(t)$ as a time-dependent action operator and $\dot{I}_B(t) = 0$ as the quantum analogue of the time average of the classical action variable I [18]. This identification can further be substantiated from the fact that in the zeroth order approximation, i.e., when the system is nearly closed, $U(t)\dot{U}^\dagger(t)$ is negligible. Consequently, in this limit the exact invariant in (28) is proportional to the action variable $I(\sim H)$ [3,11]. Thus the operator $I_B(t)$ in (29) may be regarded as the action operator close to the invariant for adiabatic evolution of the system. As a result the geometric phase obtained from (20) by using eigenstate of (30) refers to that of Berry while the one obtained by using $|\tilde{\psi}_n(0)\rangle$ gives precisely the AA phase. This shows that the conditions on $I(0)$ govern the evolution of the quantal system and thus supplement the usual interpretation based on parallel transport of the phase of the system according to some prescribed natural connection.

5. Spin-1/2 particle in a rotating magnetic field

It is felt [34] that cyclic and/or noncyclic spinor evolutions resulting in a pure geometric phase may be realizable in neutron polarimetric experiments [5,28]. Therefore, it will be of some interest to study the geometric spinor phase in a rotating magnetic field through use of our results in (26) and (30), which we believe to be the most significant findings of the present work. The appropriate Hamiltonian for the two-state problem under consideration is given by

$$H(t) = \frac{b}{2}\vec{B}(t) \cdot \vec{\sigma} \quad (31)$$

with

$$\vec{B}(t) = B(\sin \theta \cos \omega t, \sin \theta \sin \omega t, \cos \theta). \quad (32)$$

In (31) and (32), B, θ, ω are constants and

$$b = -\frac{e}{2mc}gB$$

is related to the Larmor frequency. Obviously, $\vec{\sigma}$ stands for the Pauli spin matrices. Clearly, $H(t)$ can be written in the form of (12) with

$$U(t) = e^{\frac{i}{2}\omega\sigma_3 t} \quad (33)$$

and thus,

$$\mathcal{H} = \frac{b}{2} \begin{pmatrix} \cos \theta - \omega/b & \sin \theta \\ \sin \theta & -(\cos \theta - \omega/b) \end{pmatrix}. \quad (34)$$

Using the eigenvalues and eigenfunctions of (34), the eigenstates of $I(t)$ given in (28) can be written in the form

$$|\tilde{n}(t)\rangle = \frac{1}{\sqrt{\Omega}} \begin{pmatrix} \sqrt{\frac{\Omega}{2} + \frac{nb}{2} \left(\cos \theta - \frac{\omega}{b} \right)} e^{-\frac{i}{2}\omega t} \\ \frac{n \frac{b}{2} \sin \theta}{\sqrt{\frac{\Omega}{2} + \frac{nb}{2} \left(\cos \theta - \frac{\omega}{b} \right)}} e^{\frac{i}{2}\omega t} \end{pmatrix} \quad (35)$$

with

$$\Omega = b \sqrt{1 - \frac{2\omega}{b} \cos \theta + \frac{\omega^2}{b^2}} \quad \text{and} \quad n = \pm 1. \quad (36)$$

From (20) and (35)

$$\gamma_G = -n \left[\pi \frac{b}{\Omega} \left(\cos \theta - \frac{\omega}{b} \right) \right]. \quad (37)$$

Using the properties of spinor under a rotation of 2π , the geometric phase of the state $|\tilde{n}(0)\rangle$ can be found from (37) as

$$\gamma_G = -n\pi \left[1 - \frac{b}{\Omega} \left(\cos \theta - \frac{\omega}{b} \right) \right]. \quad (38)$$

Interestingly, (38) represents the phase factor of AA [2,6,26]. On the other hand, using the eigenstate of $H(0)$ rather than that of $\mathcal{H}(0)$, we could obtain the Berry's phase [6,26]

$$\gamma_B = -n\pi[1 - \cos \theta]. \quad (39)$$

6. Conclusion

The evolution operator technique represents a powerful method to study the geometric phase problem. Very recently, a family of unitary operators that characterizes the EOT has been used to provide an interesting description for the TD harmonic

oscillator problem [31]. We have chosen to work with a variant of the EOT which is essentially a quantum analogue of the time-dependent canonical transformation in classical mechanics. The form of the EOT used by us when tied in with the method of invariants imposes conditions on $I(0)$ for the time-dependent invariant $I(t)$ to be an action operator or a constant of the motion. This provides a basis to examine the relationship between the LR phase and that of Berry or AA and to obtain results for geometrical phases from a unified viewpoint.

The geometric phase was encountered in molecular systems [12,13,20–22] long before the work of Berry, and currently there has been a growing interest to study the effect of geometric phase on chemical reactions [7,14,16,25,35]. A similar problem was also envisaged and beautifully expounded by Kozumi and Sugano [15] for the two electronic level systems. In view of this we believe that the simple minded realization of the geometric phase sought in this paper will be of some interest for researchers working in this field of investigation.

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Appendix A

To show that $I(t)$ in (28) is a constant of the motion, we require to verify (1) for it. To that end we begin by recasting (10) in the form

$$U^\dagger \mathcal{H} - HU^\dagger = -i\hbar \dot{U}^\dagger(t), \quad (\text{A.1})$$

$$\mathcal{H}U - UH = i\hbar \dot{U}(t) \quad (\text{A.2})$$

and differentiating (28) partially with respect to 't'. The partial derivative is given by

$$\frac{\partial I}{\partial t} = \dot{U}^\dagger(t)I(0)U(t) + U^\dagger(t)I(0)\dot{U}(t). \quad (\text{A.3})$$

Using of (A.1) and (A.2) in (A.3) gives

$$\frac{\partial I}{\partial t} = \frac{1}{i\hbar} \{HU^\dagger I(0)U - U^\dagger \mathcal{H}(t)I(0)U + U^\dagger I(0)\mathcal{H}(t)U - U^\dagger I(0)UH\}. \quad (\text{A.4})$$

Equation (A.4) in conjunction with (26) and (28) leads to

$$\frac{\partial I}{\partial t} = \frac{1}{i\hbar} [H, I(t)] + \frac{k}{i\hbar} \{U^\dagger (\mathcal{H}(0)\mathcal{H}(t) - \mathcal{H}(t)\mathcal{H}(0))U\}. \quad (\text{A.5})$$

Now, by making use of (11), we recover our desired equation

$$\frac{dI(t)}{dt} = \frac{\partial I(t)}{\partial t} + \frac{1}{i\hbar} [I, H] = 0. \quad (\text{A.6})$$

We emphasize here that it is not possible to derive (A.6) from (A.5) in a straightforward manner unless one uses (26). Other choices of $I(0)$ as in (30) require to redefine the time evolution of $I(0)$. This is clarified in appendix B.

Appendix B

To derive equation (1) for $I_B(t)$ in (29) with the initial condition in (30) we follow the notations of Cheng and Fung [10]. Focusing our attention on (2.5) and (2.22) of [10] we write

$$H(0)|m(0)\rangle = \mu_m|m(0)\rangle \quad (\text{B.1})$$

and

$$U(t)|m(0)\rangle = |m(t)\rangle. \quad (\text{B.2})$$

Equation (B.1) implies that

$$I(0)|m(0)\rangle = \bar{\mu}_m|m(0)\rangle. \quad (\text{B.3})$$

Employing the unitarity properties of U and R , one can write equation (B.3) in the form

$$U(t)I(0)R(t)R^\dagger(t)U^\dagger(t)U(t)|m(0)\rangle = \bar{\mu}_m U(t)|m(0)\rangle. \quad (\text{B.4})$$

Since both R and $I(0)$ are diagonal in the basis $\{|m(0)\rangle\}$, equation (B.4) can further be rearranged to write

$$U(t)R(t)I(0)R^\dagger(t)U^\dagger(t)U(t)|m(0)\rangle = \bar{\mu}_m U(t)|m(0)\rangle. \quad (\text{B.5})$$

Using equations (21) and (29), one can reduce it as

$$I_B(t)|m(t)\rangle = \bar{\mu}_m|m(t)\rangle. \quad (\text{B.6})$$

It appears from equation (B.6) that although time evolution of $I_B(t)$ is guided by evolution operator $U(t, 0)$ its eigenfunction is evolved by one of its factor $U(t)$ in (21). Consequently, $|m(t)\rangle$ can be regarded as the part of the instantaneous eigenfunction of $H(t)$. Partial differentiation of equation (29) with respect to 't' gives

$$\frac{\partial I_B}{\partial t} = \dot{U}(t, 0)I_B(0)U^\dagger(t, 0) + U(t, 0)I_B(0)\dot{U}^\dagger(t, 0). \quad (\text{B.7})$$

To remove the time derivative of U and U^\dagger we use equation (2.4) of [10] and get

$$\frac{\partial I_B}{\partial t} = \frac{1}{i\hbar} [HU(t, 0)I_B(0)U^\dagger(t, 0) - U(t, 0)I_B(0)U^\dagger(t, 0)H]. \quad (\text{B.8})$$

Further use of equation (29) leads to

$$\frac{\partial I_B(t)}{\partial t} + \frac{1}{i\hbar} [I_B, H] = 0.$$

This completes the proof that $I_B(t)$ also satisfies equation (1) although it is not a constant of the motion.

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