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Non-Abelian geometric phase, Floquet theory and periodic dynamical invariants

Ali Mostafazadeh†

Department of Mathematics, Koç University, Istinye 80860, Istanbul, Turkey

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Abstract. For a periodic Hamiltonian, periodic dynamical invariants may be used to obtain non-degenerate cyclic states. This observation is generalized to the degenerate cyclic states, and the relation between the periodic dynamical invariants and the Floquet decompositions of the time-evolution operator is elucidated. In particular, a necessary condition for the occurrence of cyclic non-adiabatic non-Abelian geometrical phase is derived. Degenerate cyclic states are obtained for a magnetic dipole interacting with a precessing magnetic field.

1. Introduction

Since Berry's article [1] on adiabatic geometric phase, there have been a growing number of publications on the subject. The most notable developments have been the characterization of Berry's adiabatic phase as the holonomy of a spectral bundle [2], the discovery of the non-Abelian [3] and classical [4] analogues of Berry's adiabatic phase, and its generalization to non-adiabatic cyclic [5] and even non-cyclic evolutions [6]. The main reason for the enormous excitement generated by Berry's finding [1] has been the wide range of its application in different areas of physics [7] and its rich mathematical structure [8].

Indeed, it is quite surprising that geometric phases were not discovered much earlier. There are a few older papers [9] in the literature where the authors come very close to discovering the geometric phase. Perhaps one of the most important of these is the classic 1969 paper of Lewis and Riesenfeld [10] on dynamical invariants. The correspondence of Berry's phase and Lewis's phase has been pointed out by Morales [11]. More recently, Monteoliva *et al* [12] showed that if a periodic-invariant operator $I(t)$ with non-degenerate spectrum was known, then one could obtain all the pure cyclic states as the eigenstates of $I(0)$ and compute the corresponding geometric phases directly in terms of $I(t)$. These authors also pointed out that for a periodic Hamiltonian $H(t)$ their method was more convenient than performing a Floquet decomposition $Z(t) e^{iMt}$ of the time-evolution operator $U(t)$ and obtaining the pure cyclic states as the eigenstates of the operator M , as originally suggested by Moore and Stedman [13, 14] (see also the paper by Furman [15]).

In the present paper, we shall generalize the results of Monteoliva *et al* [12] to degenerate cyclic evolutions. This generalization involves the analysis of the relationship between the periodic dynamical invariants $I(t)$ and the Floquet operators $Z(t)$ and M . In particular, we obtain a necessary condition for the occurrence of non-adiabatic non-Abelian geometrical phases factors, and show that a non-degenerate Hamiltonian may support degenerate cyclic

† E-mail address: amostafazadeh@ku.edu.tr

evolutions. A simple example is provided by the quantum dynamics of a magnetic dipole interacting with a precessing magnetic field.

The organization of the paper is as follows. In section 2, we recall the basic results of the Floquet theory for periodic Hamiltonians. In section 3, we discuss the relevance of the Lewis–Riesenfeld theory of dynamical invariants to the geometric phase. In particular, we derive the expression for the non-Abelian Lewis phase and demonstrate its coincidence with the non-adiabatic non-Abelian geometric phase [16]. In section 4, we offer a generalization of the results of Monteoliva *et al* [12] to degenerate cyclic evolutions and discuss a characterization of degenerate cyclic states. In section 5, we apply these results to obtain a degenerate cyclic state of a magnetic dipole (of spin $j = 1$) interacting with a precessing magnetic field. In section 6, we present a summary of our results and conclude the paper with some final remarks.

In the following we shall set $\hbar = 1$, represent quantum states with projection operators and assume that

- (i) the Hamiltonian $H(t)$ is a T -periodic Hermitian operator with a discrete spectrum, and
- (ii) during the evolution of the system there are no level crossings. In particular, the degree of degeneracy of the eigenvalues of the relevant operators will not depend on time.

2. Floquet theory

A classic result of the Floquet theory [17] is that for a periodic Hamiltonian $H(t)$ with period T , the time-evolution operator $U(t)$ can be expressed as

$$U(t) = Z(t) e^{iMt} \quad (1)$$

where $Z(t)$ is a unitary T -periodic operator, i.e. $Z(T) = Z(0) = 1$, and M is a Hermitian operator. Clearly, $U(T) = e^{iMT}$ and the cyclic states of the system with period T are the eigenstates of M^\dagger .

We shall assume that

- (i) M has a discrete spectrum,
- (ii) the eigenvalues μ_n of M are m_n -fold degenerate, and the corresponding eigenvectors $|\mu_n, a\rangle$ with $a \in \{1, 2, \dots, m_n\}$ form a complete orthonormal set of basis vectors of the Hilbert space \mathcal{H} .

In view of equation (1), if $|\psi(t)\rangle$ is the solution of the Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (2)$$

with the initial condition

$$|\psi(0)\rangle = |\mu_n, a\rangle \quad (3)$$

then

$$|\psi(T)\rangle = U(T) |\mu_n, a\rangle = e^{i\mu_n T} |\mu_n, a\rangle. \quad (4)$$

Therefore the total phase angle associated with the cyclic state vector $|\mu_n, a\rangle$ is given by

$$\alpha_n = \mu_n T. \quad (5)$$

† In some cases, there are special values of T for which an eigenvector of e^{iMT} is not an eigenvector of M . For example let $T = 4\pi$ and $M = J_3$, where J_3 is the z -component of the angular momentum operator. Then $e^{iMT} = e^{4\pi i J_3}$ is the identity operator, and any vector $|\psi\rangle$ is an eigenvector of e^{iMT} . Taking $|\psi\rangle$ to be the sum of two eigenvector of J_3 , we have an example of a vector which is an eigenvector of e^{iMT} but not an eigenvector of M . In this paper we shall not consider these special cases.

This phase angle consists of a dynamical part δ_n and a geometric part γ_n (i.e. $\alpha_n = \delta_n + \gamma_n$) which are expressed in the form [5, 13, 18]

$$\delta_n = - \int_0^T \langle \psi(t) | H(t) | \psi(t) \rangle dt \tag{6}$$

$$\gamma_n = i \int_0^T \langle \phi(t) | \frac{d}{dt} | \phi(t) \rangle dt \tag{7}$$

where $|\phi(t)\rangle$ is a single-valued state vector defining the same pure state as $|\psi(t)\rangle$ [5, 19]. A particular choice for $|\phi(t)\rangle$ is $Z(t)|\mu_n, a\rangle$ [13]. Hence,

$$\gamma_n = i \int_0^T \langle \mu_n, a | Z^\dagger(t) \frac{d}{dt} Z(t) | \mu_n, a \rangle dt. \tag{8}$$

Note that in general $m_n > 1$, i.e. μ_n is degenerate. Nevertheless, the associated eigenvectors $|\mu_n, a\rangle$ undergo cyclic evolutions, and the corresponding geometric phase factors are Abelian.

3. Periodic dynamical invariants and degenerate cyclic evolutions

By definition a dynamical invariant $I(t)$ is a solution of

$$\frac{dI(t)}{dt} = i[I(t), H(t)]. \tag{9}$$

In the following we shall assume that

- (i) $I(t)$ is a Hermitian operator with a discrete spectrum,
- (ii) the eigenvalues λ_n of $I(t)$ are l_n -fold degenerate, and the corresponding eigenvectors $|\lambda_n, a; t\rangle$ with $a \in \{1, 2, \dots, l_n\}$ form a complete orthonormal set of basis vectors of the Hilbert space \mathcal{H} .

Note that the eigenvalue equation

$$I(t)|\lambda_n, a; t\rangle = \lambda_n|\lambda_n, a; t\rangle \tag{10}$$

determines the eigenvectors $|\lambda_n, a; t\rangle$ uniquely up to possibly time-dependent unitary transformations u which act on the degeneracy subspace

$$\mathcal{H}_{\lambda_n}(t) := \text{Span} \{ |\lambda_n, 1; t\rangle, |\lambda_n, 2; t\rangle, \dots, |\lambda_n, l_n; t\rangle \} \tag{11}$$

associated with the eigenvalue λ_n . In other words, one may choose another set of complete orthonormal eigenvectors $|\lambda_n, a; t'\rangle$ of $I(t)$ which are related to $|\lambda_n, a; t\rangle$ according to

$$|\lambda_n, b; t'\rangle = \sum_{a=1}^{l_n} |\lambda_n, a; t\rangle u_{ab}(t) \tag{12}$$

where $u_{ab}(t)$ are entries of an $l_n \times l_n$ unitary matrix u .

Now following Lewis and Riesenfeld [10], let us differentiate both sides of equation (10), take the inner product of both sides of the resulting equation with $|\lambda_m, b; t\rangle$, for some m and $b \in \{1, \dots, l_m\}$, and use equations (9) and (10) to simplify the result. This leads to

$$(\lambda_n - \lambda_m) \left[\langle \lambda_m, b; t | H | \lambda_n, a; t \rangle - i \langle \lambda_m, b; t | \frac{d}{dt} | \lambda_n, a; t \rangle \right] = i \delta_{mn} \delta_{ab} \frac{d}{dt} \lambda_n \tag{13}$$

where δ 's are the Kronecker delta functions. Equation (13) implies:

- (i) Eigenvalues λ_n do not depend on time.

(ii) Eigenvectors $|\lambda_n, a; t\rangle$ satisfy

$$\langle \lambda_m, b; t | H | \lambda_n, a; t \rangle - i \langle \lambda_m, b; t | \frac{d}{dt} | \lambda_n, a; t \rangle = 0 \quad \text{for } m \neq n. \tag{14}$$

Clearly if equation (14) is also satisfied for $m = n$, then

$$\langle \lambda_m, b; t | \left(H - i \frac{d}{dt} \right) | \lambda_n, a; t \rangle = 0 \quad \text{for all } m \text{ and } b \tag{15}$$

and $|\lambda_n, a; t\rangle$ is a solution of the Schrödinger equation (2).

A central result of Lewis and Riesenfeld [10] is that although equation (15) may not be satisfied, there are unitary transformations of the form (12) which map $|\lambda_n, a; t\rangle$ to a new set of eigenvectors $|\lambda_n, a; t\rangle'$ of $I(t)$ which do satisfy equation (15) and provide solutions of the Schrödinger equation. Lewis and Riesenfeld do not, in fact, derive the defining equation for the matrix u . They suffice to say that this matrix may be diagonalized and obtain the equation satisfied by its eigenvalues, the Lewis phases.

In order to obtain the appropriate unitary transformation u for a given eigenvalue λ_n , we demand that equation (15) be fulfilled for the primed eigenvectors. Setting $m = n$, using equations (12) and (14), and simplifying the resulting expression, we obtain

$$i \frac{d}{dt} u(t) = \Delta(t) u(t) \tag{16}$$

where $\Delta(t)$ is an $l_n \times l_n$ matrix with entries

$$\Delta_{ab}(t) := \mathcal{E}_{ab}(t) - \mathcal{A}_{ab}(t) \tag{17}$$

$$\mathcal{E}_{ab}(t) := \langle \lambda_n, a; t | H | \lambda_n, b; t \rangle \tag{18}$$

$$\mathcal{A}_{ab}(t) := i \langle \lambda_n, a; t | \frac{d}{dt} | \lambda_n, b; t \rangle. \tag{19}$$

Since equation (16) has the form of a matrix Schrödinger equation, its solution can be written implicitly as

$$u(t) = \mathcal{T} e^{-i \int_0^t \Delta(t') dt'} u(0) = \mathcal{T} e^{i \int_0^t [-\mathcal{E}(t') + \mathcal{A}(t')] dt'} u(0) \tag{20}$$

where \mathcal{T} is the time-ordering operator. If the matrices $\mathcal{E}(t) = (\mathcal{E}_{ab})$ and $\mathcal{A} = (\mathcal{A}_{ab})$ commute, then equation (20) can be expressed as

$$u(t) = \mathcal{T} e^{-i \int_0^t \mathcal{E}(t') dt'} \mathcal{T} e^{i \int_0^t \mathcal{A}(t') dt'} u(0). \tag{21}$$

Next consider the spectral resolution of $I(t)$, namely

$$I(t) = \sum_n \lambda_n \Lambda_n(t) \tag{22}$$

where

$$\Lambda_n(t) := \sum_{a=1}^{l_n} |\lambda_n, a; t\rangle \langle \lambda_n, a; t| = \sum_{a=1}^{l_n} |\lambda_n, a; t\rangle' \langle \lambda_n, a; t|' \tag{23}$$

is the degenerate eigenprojector (state) associated with the eigenvalue λ_n or alternatively the degeneracy subspace $\mathcal{H}_{\lambda_n}(t)$. Now, if $I(t)$ is a periodic dynamical invariant with period T , i.e. $I(T) = I(0)$, then the degenerate eigenprojectors $\Lambda_n(t)$ will also be periodic, i.e. $\Lambda_n(T) = \Lambda_n(0)$. In other words, $\Lambda_n(0)$ undergo *degenerate cyclic evolutions*.

Let us choose a set of instantaneous eigenvectors $|\lambda_n, a; t\rangle$ of $I(t)$. Then $|\lambda_n, a; t\rangle$ are single-valued and periodic, $|\lambda_n, a; T\rangle = |\lambda_n, a; 0\rangle$. Now consider the evolution of a frame

$$\Psi(0) = \{ |\psi_1(0)\rangle, \dots, |\psi_n(0)\rangle \} \tag{24}$$

of $\mathcal{H}_{\lambda_n}(0)$. We can choose the initial condition in such a way that $|\psi_a(0)\rangle = |\lambda_n, a; 0\rangle = |\lambda_n, a; 0\rangle'$. Then the vectors constituting the frame evolve according to $|\psi_a(t)\rangle = |\lambda_n, a; t\rangle'$. After a complete cycle, therefore, one obtains a new frame $\Psi(T)$ of the degeneracy subspace $\mathcal{H}_{\lambda_n}(T) = \mathcal{H}_{\lambda_n}(0)$ which is related to $\Psi(0)$ by the unitary transformation (20), with $u(0) = 1$, or alternatively by (21) if the matrices $\mathcal{E}(t)$ and $\mathcal{A}(t)$ commute. For $t = T$, the second time-ordered exponential in (21) is precisely the non-adiabatic non-Abelian geometric phase factor of Anandan [16].

Note that under the single-valued unitary (gauge) transformations of the basis vectors $|\lambda_n, a; R(t)\rangle$, the non-Abelian geometric phase factor (20) transforms covariantly—not invariantly. This means that the physically observable quantities depend only on its invariants, namely, its eigenvalues. As discussed in [16], one can in general find an eigenbasis $\{|\lambda_n, a; R(t)\rangle\}$ in which the total non-Abelian phase factor (20) is diagonal. In this basis, the invariant diagonal elements which are of physical importance can be written as the product of a dynamical part and a geometrical part.

4. Periodic invariants and Floquet decompositions

As discussed in the preceding section, given a dynamical invariant $I(t)$ one can obtain solutions of the corresponding Schrödinger equation as eigenvectors of $I(t)$, provided that one performs the necessary unitary transformations. The converse of this procedure is also valid. In order to see this, let $\mathcal{C} := \{|\psi_n(0)\rangle\}$ be a complete set of state vectors, $c_n \in \mathbb{R}$, and $|\psi_n(t)\rangle := U(t)|\psi_n(0)\rangle$ be the solutions of the Schrödinger equation (2) corresponding to the initial conditions $|\psi_n(t=0)\rangle = |\psi_n(0)\rangle$. Then

$$I(t) := \sum_n c_n |\psi_n(t)\rangle \langle \psi_n(t)| = U(t) \left[\sum_n c_n |\psi_n(0)\rangle \langle \psi_n(0)| \right] U^\dagger(t) = U(t) I(0) U^\dagger(t) \quad (25)$$

is a dynamical invariant[†]. In fact, every dynamical invariant $I(t)$ can be viewed as associated with a complete set \mathcal{C} of initial state vectors, and expressed as

$$I(t) = U(t) I(0) U^\dagger(t). \quad (26)$$

For a periodic dynamical invariant $I(t)$ with period T , one has

$$I(0) = I(T) = U(T) I(0) U^\dagger(T) = e^{iMT} I(0) e^{-iMT}. \quad (27)$$

For a generic value of T , this implies[‡]

$$[I(0), M] = 0. \quad (28)$$

In particular, M and $I(0)$ have simultaneous eigenvectors, and

$$I(t) = Z(t) I(0) Z^\dagger(t). \quad (29)$$

Now let us recall that the eigenprojectors $\Lambda_n(0)$ of $I(0)$ represent the degenerate cyclic states. If $\Lambda_n(0)$ happens to also be an eigenprojector of M , then the corresponding total phase factor is Abelian. Therefore, a necessary condition for the occurrence of a non-Abelian geometric phase is the existence of a T -periodic dynamical invariant $I(t)$ such that $I(0)$ has a degenerate eigenprojector which is not an eigenprojector of the Floquet operator M , i.e. $I(0)$ and M have different degeneracy structures.

This observation suggests a way of obtaining degenerate cyclic states even for systems whose Hamiltonian and (or) evolution operator are non-degenerate.

[†] Note that the numbers c_n are not generally distinct.

[‡] There are special situations where $[e^{iMT}, I(0)] = 0$ will not imply $[M, I(0)] = 0$. See the footnote after equation (1) for an example. The results presented below can also be obtained using equation (27) directly.

5. Application to the spin system

Perhaps the best-known example of a model which leads to Abelian geometric phases is a magnetic dipole (a spin) interacting with a changing classical magnetic field [1, 18–20]. The Hamiltonian is given by

$$H(t) = b\vec{R}(t) \cdot \vec{J} \quad (30)$$

where b is (proportional to) the Larmor frequency, $\vec{R}(t) \in \mathbb{R}^3$ describes the magnetic field vector and \vec{J} is the angular momentum of the dipole. For $\vec{R}(t) \neq 0$, the eigenvalues of $H(t)$ are all non-degenerate and given by $b|\vec{R}|k$ where k is a half-integer. If the dipole has total angular momentum j , then $k \in \{-j, -j+1, \dots, j\}$.

In the following we shall restrict ourselves to the simplest possible dipole system which would allow for a degenerate cyclic evolution. Clearly, this is the $j = 1$ case, where the Hilbert space is three dimensional. The general problem of non-Abelian adiabatic geometrical phase for systems with a three-dimensional Hilbert space is discussed in [21]. Here we are interested in the non-adiabatic non-Abelian phases.

In view of the results of the Floquet theory, let us consider an evolution operator of the form (1) with

$$Z(t) = e^{i\Omega t J_1} \quad M = \omega J_3 \quad (31)$$

where $\Omega := 2\pi/T$ and ω is an arbitrary positive real constant. This corresponds to the T -periodic Hamiltonian,

$$H = -[\Omega J_1 + \omega \sin(\Omega t) J_2 + \omega \cos(\Omega t) J_3] \quad (32)$$

of a magnetic dipole interacting with a precessing magnetic field.

Clearly the pure cyclic states are eigenstates of $M = \omega J_3$. Since $j = 1$, J_3 has three non-degenerate eigenvalues, namely $-1, 0$ and 1 . We shall denote the corresponding eigenvectors by $|-\rangle, |0\rangle$ and $|+\rangle$, respectively. Therefore, we can write

$$M = \omega(|+\rangle\langle+| - |-\rangle\langle-|). \quad (33)$$

Now consider an invariant $I(t)$ of the form $Z(t)I(0)Z^\dagger(t)$ with

$$I(0) = \lambda_1(|+\rangle\langle+| + |0\rangle\langle 0|) + \lambda_2|-\rangle\langle-| \quad \lambda_1, \lambda_2 \in \mathbb{R} - \{0\}. \quad (34)$$

Obviously $I(0)$ commutes with M and $I(t)$ is T -periodic. Moreover, $\Lambda_1(0) := |+\rangle\langle+| + |0\rangle\langle 0|$ is a degenerate eigenprojector which undergoes a cyclic evolution.

If we choose $\Psi(0) = \{|+\rangle, |0\rangle\}$ as the initial frame for the cyclic evolution the unitary operation relating $\Psi(0)$ to $\Psi(T)$ will be diagonal and the total phase factor will still be Abelian. However, if we choose an arbitrary initial frame,

$$\Psi(0) = \{|\psi_1(0)\rangle, |\psi_2(0)\rangle\} \quad |\psi_1(0)\rangle := \xi|+\rangle + \zeta|0\rangle \quad |\psi_2(0)\rangle := \zeta^*|+\rangle - \xi^*|0\rangle \quad (35)$$

with $\xi, \zeta \in \mathbb{C}$ and $|\xi|^2 + |\zeta|^2 = 1$, then we obtain a non-diagonal unitary operator and a non-Abelian phase. Using the basic properties of the angular momentum operators and the relation $|\lambda_1, a; t\rangle = Z(t)|\lambda_1, a; 0\rangle$, which follows from $I(t) = Z(t)I(0)Z^\dagger(t)$, we can easily obtain

$$\mathcal{E} = -\omega \begin{pmatrix} |\xi|^2 & \xi^*\zeta^* \\ \xi\zeta & |\zeta|^2 \end{pmatrix} - \frac{\Omega}{\sqrt{2}} \begin{pmatrix} \xi^*\zeta + \zeta^*\xi & -\xi^{*2} + \zeta^{*2} \\ -\xi^2 + \zeta^2 & -(\xi^*\zeta + \zeta^*\xi) \end{pmatrix} \quad (36)$$

$$\mathcal{A} = -\frac{\Omega}{\sqrt{2}} \begin{pmatrix} \xi^*\zeta + \zeta^*\xi & -\xi^{*2} + \zeta^{*2} \\ -\xi^2 + \zeta^2 & -(\xi^*\zeta + \zeta^*\xi) \end{pmatrix} \quad (37)$$

$$\Delta = -\omega \begin{pmatrix} |\xi|^2 & \xi^*\zeta^* \\ \xi\zeta & |\zeta|^2 \end{pmatrix}. \quad (38)$$

Since \mathcal{E} , \mathcal{A} and Δ do not depend on time, we have

$$\Psi(T) = e^{-iT\Delta}\Psi(0). \quad (39)$$

Note that \mathcal{E} and \mathcal{A} do not generally commute and equation (21) does not hold.

6. Conclusion

In this paper, we have explored the relationship between the Floquet decomposition of the evolution operator for a periodic Hamiltonian and the periodic dynamical invariants of Lewis and Riesenfeld. We showed that the degenerate cyclic states may be viewed as the eigenstates of a Hermitian operator $I(0)$ which serves as the initial value of a periodic dynamical invariant $I(t)$. We derived the expression for the corresponding non-Abelian non-adiabatic geometrical phase in terms of the eigenvectors of $I(t)$; thus generalizing the results of Monteoliva *et al* [12] to degenerate cyclic evolutions.

We used our results to show that the simple quantum system describing the dynamics of a magnetic dipole in a precessing magnetic field, which since Berry's paper [1] has served as the main example involving a non-trivial Abelian geometrical phase, also leads to degenerate cyclic evolutions.

We wish to conclude this paper with the following remarks:

- (i) The Moore–Stedman [13] method of generating the pure cyclic states as eigenstates of the Floquet operator M may be viewed as a special case of the method of invariants. This can be easily seen, by associating a T -periodic dynamical invariant, namely $I(t) := Z(t) M Z^\dagger(t)$, to a given Floquet decomposition $Z(t) e^{iMt}$ of the evolution operator.
- (ii) The method of invariants is superior to the method of Moore and Stedman [13], as it can also be used to generate degenerate cyclic states.
- (iii) For a general quantum system with a three-dimensional Hilbert space, one can easily apply the method developed in [21] to obtain the general form of a Hermitian invariant which leads to a degenerate cyclic evolution. In particular, one can show that the parameter space of such invariants has the manifold structure of $\mathbb{C}P^2$.

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