Topological aspects of the non-adiabatic Berry phase

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Abstract. The topology of the non-adiabatic parameter space bundle is discussed for evolution of exact cyclic state vectors in Berry's original example of split angular momentum eigenstates. It turns out that the change in topology occurs at a critical frequency. The first Chern number that classifies these bundles is proportional to angular momentum. The non-adiabatic principal bundle over the parameter space is not well defined at the critical frequency.

1. Introduction

In a previous paper [1] the relation between the parameter space and the projective space approach to the problem of geometric (Berry) phase is discussed. The key idea is to use the classification theorem for principal bundles or alternatively for vector bundles. This method suggests a way of constructing fibre bundles over parameter space, even for the non-adiabatic evolution of state vectors (at least for a particular class of quantum systems).

Let M denote the smooth, compact§ manifold of parameters x, and $H = H(x)$ be a Hamiltonian which depends smoothly on $x \in M$. As described in [1], the cyclic state vectors are not energy eigenvectors. The adiabaticity assumption, therefore, does not describe the actual situation, rather it provides just an approximation. One has to distinguish two regions: the adiabatically related region for which the adiabatcity assumption yields a limiting case, and the non-adiabatic region. In the non-adiabatic region, one cannot use the adiabatic theorem and the cyclic state vectors cannot be approximated by the eigenvectors of the Hamiltonian.

The relation between Berry–Simon (BS) [2] parameter space bundle interpretation of the geometric phase, and the Aharonov–Anandan (AA) [3] approach of using the projective space bundle, is the following: the former principal bundle

$$\lambda_N : G \longrightarrow \cdots \longrightarrow M \tag{1}$$

is obtained as a pullback bundle from the latter

$$\eta_N : G \longrightarrow V_N \longrightarrow Gr_N . \tag{2}$$

In (1) and (2), $G = U(\mathcal{N})$ or $O(\mathcal{N})$ depending on whether the Hilbert space is real or complex, $\mathcal{N} < \infty$ is the dimension of the degeneracy subspace where the cyclic state vector belongs, V_N, and Gr_N are infinite-dimensional (real or complex) Stiefel and Grassmann

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§ In most physical examples M is compact. However, compactness is not a necessary condition in a large part of our analysis. As far as the mathematical results are concerned, M must at least be para-compact.

manifolds, respectively [1]. In other words, there is a continuous map $f : M \rightarrow Gr_N$ such that the following diagram commutes:

$$
\begin{array}{ccc}
\lambda_N & \xleftarrow{f^*} & \eta_N \\
\downarrow & \circ & \downarrow \\
M & \xrightarrow{f} & Gr_N
\end{array}
\tag{3}
$$

and f^* is a bundle isomorphism, i.e. $\lambda_N \cong f^*(\eta_N)$.

For the adiabatic case f is given by the Hamiltonian, namely

$$
\forall x \in M \qquad f(x) \equiv |\psi_x\rangle\langle\psi_x|
\tag{4}
$$

where $|\psi_x\rangle\langle\psi_x|$ is the eigenstate of $H(x)$ which evolves in time as x traverses a closed loop

$$
C : [0, T] \ni t \longrightarrow x(t) \in M \qquad x(0) = x(T) .
\tag{5}
$$

To repeat the same construction for the non-adiabatic case, one needs to consider a class of quantum systems, for which

(i) The cyclic state vectors exist and are eigenvectors of an operator $\tilde{H} = \tilde{H}(x)$.

(ii) $\tilde{H}(x) = H(F(x))$, for some continuous (smooth) function $F : M \rightarrow M$.

For this class of quantum systems, one can still use the classification theorem. This is realized by replacing f by a map $\tilde{f}$ defined by

$$
\tilde{f} \equiv f \circ F : M \longrightarrow Gr_N.
$$

Then the exact (non-adiabatic) bundle $\tilde{\lambda}_N$ over the parameter space is obtained as the pullback bundle $\tilde{\lambda}_N = \tilde{f}^*(\eta_N)$.

f and $\tilde{f}$ pullback the canonical connection of the universal bundles η_N onto λ_N and $\tilde{\lambda}_N$, and yield the adiabatic and non-adiabatic Berry connections, respectively. The geometric (Berry) phase is identified with the holonomy of these connections, in each case.

The topologies of λ_N and $\tilde{\lambda}_N$ depend only on the homotopy classes of $[f]$ and $[\tilde{f}]$ in $[M, Gr_N]$. Hence, if F is a diffeomorphism† (homotopic to identity will suffice) $[f] = [\tilde{f}]$, and $\lambda_N \cong \tilde{\lambda}_N$.

For the non-degenerate (Abelian) case, $N = 1$ $(G = U(1))$ and

$$
Gr_1 = \mathbb{C}P(\infty) = K(2, \mathbb{Z})
$$

is an Eilenberg–McLane space. This allows one to have the following one-to-one correspondence:

$$
[M, \mathbb{C}P(\infty)] \cong H^2(M, \mathbb{Z}) .
$$

Hence, it is the first Chern class $c_1 \in H^2(M, \mathbb{Z})$ that determines the topology of $U(1)$ bundles, $\lambda \equiv \lambda_1$ and $\tilde{\lambda} \equiv \tilde{\lambda}_1$.

In this paper, we study a particular example for which the assumptions (i) and (ii) are valid‡. Thus, we explore the topology of the bundles λ and $\tilde{\lambda}$, and discuss the rather interesting implications of the topological information.

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† Note that in the adiabatic limit $\tilde{f}$ approaches f, hence, if F is a diffeomorphism it will be necessarily homotopic to identity. In other words, F as an element of Diff(M) belongs to the connected component to the identity.

‡ Except for one instance.

2. Non-adiabatic evolution in Berry's example

We consider a magnetic dipole μ in a magnetic field $B(x(t))$. The Hamiltonian of this system is given by [4]

$$H(x) = -\mu \cdot B(x) = bx \cdot J \qquad b = Bge/2mc. \tag{6}$$

The parameter space is S^2 and the closed loops considered are the following circular loops:

$$C : [0, T] \ni t \longrightarrow x(t) = (\theta = \text{constant}, \varphi = \omega t) \in S^2 \tag{7}$$

where $x \in S^2 \subset \mathbb{R}^3$ and (θ, φ) are spherical coordinates with respect to a standard Cartesian coordinate basis $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ or $(\hat{i}, \hat{j}, \hat{k})$ of $\mathbb{R}^3$.

The Schrödinger equation is exactly solvable in this case [5, 6]. The Hamiltonian H can be written in the following form:

$$H = U^\dagger H_0 U \tag{8}$$

where

$$U \equiv \exp((it\omega/\hbar) J_3)$$

$$H_0 \equiv bx_0 \cdot J = b(\cos\theta J_3 + \sin\theta J_1)$$

$$x_0 \equiv (\theta, \varphi = 0)$$

and J is the angular momentum operator. Note that due to (7), H_0 is time independent. Now, let $|\psi'\rangle \equiv U|\psi\rangle$ and substitute $|\psi\rangle = U^\dagger|\psi'\rangle$ in the Schrödinger equation

$$i\hbar\partial_t|\psi\rangle = H|\psi\rangle$$

$$i\hbar U \partial_t(U^\dagger|\psi'\rangle) = U H(U^\dagger|\psi'\rangle)$$

$$i\hbar\partial_t|\psi'\rangle = (UHU^\dagger - i\hbar U \partial_t U^\dagger)|\psi'\rangle$$

$$= H_0'|\psi'\rangle \tag{9}$$

where H_0' is defined by

$$H_0' \equiv UHU^\dagger - i\hbar U \partial_t U^\dagger$$

$$= H_0 - \omega J_3$$

$$= b[(\cos\theta - \omega/b)J_3 + \sin\theta J_1].$$

Again, because of (7), H_0' is time independent and hence (9) can be immediately integrated to give

$$|\psi'(t)\rangle = e^{-(it/\hbar)H_0'}|\psi'(0)\rangle. \tag{10}$$

Using the definition of $|\psi'\rangle$ one has

$$|\psi(t)\rangle = U^\dagger|\psi'(t)\rangle = e^{-(it\omega/\hbar)J_3}e^{-(it/\hbar)H_0'}|\psi(0)\rangle \tag{11}$$

Next, we show that the cyclic state vectors are eigenvectors of H_0'. Let $|\tilde{\psi}(0)\rangle$ be an exact cyclic state vector, i.e.

$$|\tilde{\psi}(T)\rangle = e^{i\alpha}|\tilde{\psi}(0)\rangle$$

where $T \equiv 2\pi/\omega$ is the period of a cycle and $\alpha \in \mathbb{R}$. Using (11) one then has

$$e^{-(2\pi i/\hbar)J_3} e^{-(iT/\hbar)H_0'} |\tilde{\psi}(0)\rangle = e^{i\alpha} |\tilde{\psi}(0)\rangle . \tag{12}$$

The last equation (12) says that $|\tilde{\psi}(0)\rangle$ is an eigenvector of the operator $\exp(-(2\pi i/\hbar)J_3)\exp(-(iT/\hbar)H_0')$. However, the two operators $\exp(-(2\pi i/\hbar)J_3)$ and $\exp(-(iT/\hbar)H_0')$ commute, hence $|\tilde{\psi}(0)\rangle$ must be a simultaneous eigenvector of these operators and so of H_0'. Furthermore, since H_0 and H_0' do not commute, $|\tilde{\psi}(0)\rangle$ is not an energy eigenvector. This justifies our first assumption, (i), namely that the cyclic state vectors are eigenvectors of an operator H_0'.

The second requirement, (ii), is also fulfilled. Let us define the map

$$F : M = S^2 \to S^2 = M$$

by†

$$\forall x = (\theta, \varphi) \in S^2 \qquad F(x) \equiv \tilde{x} = (\tilde{\theta}, \tilde{\varphi})$$

$$\cos\tilde{\theta} \equiv \frac{b}{\tilde{\omega}}\left(\cos\theta - \frac{\omega}{b}\right) \qquad \sin\tilde{\theta} \equiv \frac{b}{\tilde{\omega}}\sin\theta \qquad \tilde{\varphi} \equiv \varphi \tag{13}$$

$$\tilde{\omega} \equiv b\sqrt{\left(\frac{\omega}{b}\right)^2 - 2\left(\frac{\omega}{b}\right)\cos\theta + 1} .$$

Then, it is easy to see that F is a smooth function of $x \in S^2$‡, and

$$H_0'(x_0) = \frac{\tilde{\omega}}{b} H_0(\tilde{x}_0) = \frac{\tilde{\omega}}{b} H_0(F(x_0)) .$$

Let us now define the following Hermitian operator:

$$\tilde{H}_0(x_0) \equiv (H_0 \circ F)(x_0) .$$

Since $\tilde{H}_0$ is a scalar multiple of H_0', the cyclic state vectors are also eigenvectors of $\tilde{H}_0$. Thus condition (i) is satisfied for $\tilde{H}_0$ too. Next we realize that we have chosen a fixed coordinate frame in which the system is at $\varphi = 0$ at initial time: $t = 0$. Allowing for an arbitrary choice of coordinates we define

$$\tilde{H}(x) \equiv H(\tilde{x}) = H(F(x)) = (H \circ F)(x) \tag{14}$$

The cyclic state vectors $|\tilde{\psi}(x)\rangle$ are then eigenvectors of $\tilde{H}(x)$, $\forall x \in M = S^2$§. Hence, $\tilde{H}$ satisfies both (i) and (ii).

The adiabatic limit is $\omega \ll b$, in which F approaches to the identity map. The (adiabatic) Berry connection is given by [4, 6]

$$A = i\langle n, x|d|n, x\rangle$$

where $|n, x\rangle$ is a single-valued basis eigenvector of $H(x)$, and

$$|n, x(t = 0)\rangle = |\psi(0)\rangle \simeq |\tilde{\psi}(0)\rangle.$$

† These formulae are local expressions, valid only in the upper patch of S^2 (excluding the south pole), $\theta \neq \pi$. To get the expressions for the lower patch, one can simply take θ to $\theta - \pi$, in this case $\theta \neq 0$.
‡ Except for $\omega = b$ in which case F fails to be well defined at the north pole. We discuss this case in section 3.
§ Note that here the point $x = (\theta, \varphi)$ is the starting point ($t = 0$), hence $\tilde{H}(x)$ is still time independent and has all the properties of $\tilde{H}_0$.

Choosing $|n, x\rangle = |k, x\rangle$, k being an eigenvalue of $x(t) \cdot J$, one obtains [6]

$$A = -k(1 - \cos\theta)d\varphi. \tag{15}$$

The corresponding Berry's curvature two-form is then given by

$$\Omega = dA = -k \sin\theta d\theta \wedge d\varphi. \tag{16}$$

The non-adiabatic BS bundle $\tilde{\lambda}$ is the pullback of the AA bundle $\eta(\equiv \eta_{N=1})$ induced by

$$\tilde{f} = f \circ F. \tag{17}$$

Thus

$$\tilde{\lambda} = \tilde{f}^*(\eta) = (f \circ F)^*(\eta) = F^*(f^*(\eta)) = F^*(\lambda). \tag{18}$$

Similarly, since f and $\tilde{f}$ pullback the connections, one has

$$\tilde{A} = \tilde{f}^*(A) = F^*(f^*(A)) = F^*(A). \tag{19}$$

In (19) A and $\tilde{A}$ stand for the canonical (Stiefel) connection (on η), and the non-adiabatic (Berry) connection (on $\tilde{\lambda}$), respectively. To find the (local) expression for $\tilde{A}$, one can directly use (19). The result is

$$\tilde{A} = -k(1 - \cos\tilde{\theta})d\varphi. \tag{20}$$

An alternative method to calculate $\tilde{A}$ is to define the geometric phase to be the difference between the total phase and the dynamical phase. This is done in [6]. The result is identical with (20) but the derivation is much longer. The corresponding curvature two-form (to $\tilde{A}$) is given by

$$\tilde{\Omega} = d\tilde{A} = -k \sin\tilde{\theta}d\tilde{\theta} \wedge d\varphi$$

$$= -k\left(\frac{b}{\tilde{\omega}}\right)^3\left(1 - \frac{\omega}{b}\cos\theta\right)\sin\theta d\theta \wedge d\varphi. \tag{21}$$

The non-adiabatic Berry (geometric) phase angle is obtained as the holonomy element

$$\gamma = \oint_C \tilde{A} = \int_S \tilde{\Omega} \tag{22}$$

where $C = \partial S$ is defined in (7).

At this point we would like to emphasize that although conditions (i) and (ii) of section 1 seem to be quite restrictive, the system of (6) is certainly not the only case where they are satisfied. Indeed, equation (6) is a member of a class of quantum systems whose Hamiltonians belong to a semi-simple Lie algebra [9, 10]. The method presented in this paper applies to these systems. This is quite transparent in the analysis of [10].

3. Topology of λ and $\tilde{\lambda}$

First we introduce some notation. Let $\nu \equiv \omega/b$, $z \equiv \cos\theta$, $\tilde{z} \equiv \cos\tilde{\theta}$; we also define

$$F_0(z, \nu) \equiv \frac{z - \nu}{\sqrt{\nu^2 - 2z\nu + 1}} = \tilde{z}. \tag{23}$$

Note that the only difference between (13) and (23) is that in (23) we chose a different set of coordinates, namely (z, φ) and $(\tilde{z}, \varphi)$ instead of (θ, φ) and $(\tilde{\theta}, \varphi)$, respectively. In this notation equations (20) and (21) become

$$\tilde{A} = -k(1 - \tilde{z})\mathrm{d}\varphi \tag{24}$$

$$\tilde{\Omega} = k\mathrm{d}\tilde{z} \wedge \mathrm{d}\varphi = \frac{-kb^3 \sin\theta(1 - \nu\cos\theta)}{(\nu^2 - 2\nu\cos\theta + 1)^{3/2}}\mathrm{d}\theta \wedge \mathrm{d}\varphi . \tag{25}$$

The principal bundle $\tilde{\lambda} = \tilde{f}^*(\eta)$ is induced by

$$\tilde{f}(x) = (f \circ F)(x) = f(F(x)) = f(\tilde{x}) . \tag{26}$$

Thus using (4) one has

$$\tilde{f}(x) = |\psi_{\tilde{x}}\rangle\langle\psi_{\tilde{x}}| \tag{27}$$

where $|\psi_{\tilde{x}}\rangle$ is an eigenvector of $H(\tilde{x}) = \tilde{H}(x)$. As mentioned above the topologies of λ and $\tilde{\lambda}$ are determined by the homotopy classes of $[f]$ and $[\tilde{f}]$ in $[M = S^2, \mathbb{C}P(\infty)]$, respectively. Alternatively, one can use the fact that

$$[M, \mathbb{C}P(\infty)] \cong H^2(M, \mathbb{Z})$$

and look at the first Chern numbers c_1, which also classify all $U(1)$ bundles [1, 7].

We first claim the following:

Claim 1. The bundles λ and $\tilde{\lambda}$ have the same topology for $\omega < b$ $(\nu < 1)$.

We prove this result using two different methods:
 • by studying the homotopy classes;
 • by directly calculating the first Chern numbers.

We begin by using the first method. Let $\epsilon \in \mathbb{R}^+$, be arbitrarily small. Define the map $\mathcal{F} : [\epsilon, \nu] \times S^2 \to \mathbb{C}P(\infty)$ by

$$\mathcal{F}(\xi, x) \equiv f(F(x, \xi)) \qquad \forall x \in S^2 \qquad \forall \xi \in [\epsilon, \nu]$$

where $F(x, \xi) \equiv (F_0(z, \xi), \varphi)$ and F_0 is defined in (23). We claim that $\mathcal{F}$ is the desired homotopy map, i.e. it has the following properties:
  (a) $\mathcal{F}(\epsilon, x) \equiv f(F(x, \epsilon)) = f(x)$, since $\epsilon \ll 1$.
  (b) $\mathcal{F}(\nu, x) \equiv f(F(x, \nu)) = f(\tilde{x}) = \tilde{f}(x)$; this is obvious by (23) and (26).
  (c) $\mathcal{F}$ is continuous. To see this, note that $\mathcal{F} = f \circ F$. The continuity of f is assured by the continuity of $H = H(x)$, so $\mathcal{F}$ is continuous if and only if F is. As is seen from (23), F has a discontinuity at $(x = \text{north pole}, \xi = 1)$, i.e. $(z, \xi) = (1, 1)$. Hence, by requiring ν to be less than 1, i.e. $\omega < b$, we have $\xi < 1$ and F is continuous on its domain.

The alternative method is to explicitly calculate the first Chern numbers. Fortunately the integrals can be easily evaluated and the result is

$$\tilde{c}_1 = c_1 = -2k. \tag{28}$$

In (28), $\tilde{c}_1 = (1/2\pi) \int_{S^2} \tilde{\Omega}$ and $c_1 = (1/2\pi) \int_{S^2} \Omega$ stand for the first Chern numbers of $\tilde{\lambda}$ and λ respectively [8].

If we choose $\nu \geqslant 1$, the map F and hence $\mathcal{F}$ become discontinuous in the full domain of $\xi \in (0, \nu]$. This marks the possibility of a change in the topology of $\tilde{\lambda}$. Examining (23), we can prove that for $\nu > 1$, $\tilde{f}$ is homotopic to a constant map, hence

Claim 2. The bundle $\tilde{\lambda}$ undergoes a change of topology at $\nu = 1(\omega = b)$, and it is a trivial bundle for $\nu > 1(\omega > b)$.

To see this let us transform the domain $[\nu, \infty)$ to a closed one by considering the homotopy map $\mathcal{G} : [0, \frac{1}{\nu}] \times S^2 \to \mathbb{C} \, P(\infty)$, defined by

$$\mathcal{G}(\zeta, x) \equiv f(G(x, \zeta))$$

with

$$G(x, \zeta) = \begin{cases} F(x, \xi = 1/\zeta) & \text{for } 0 < \zeta \leqslant 1/\nu \\ \mathcal{S} : \text{south pole} & \text{for } \zeta = 0. \end{cases}$$

It is easy to see that, for $\xi \geqslant \nu > 1$(i.e. $\zeta \leqslant 1/\nu$), G and $\mathcal{G}$ are continuous. Furthermore

$$\mathcal{G}(1/\nu, x) = f(F(x, \nu)) = f(\tilde{x}) = \tilde{f}(x)$$

and

$$\mathcal{G}(0, x) \equiv f(\mathcal{S}) = \text{constant}.$$

Thus, $\tilde{f} \approx$ (a constant map).

It should be emphasized that the triviality of $\tilde{\lambda}$ does not imply that the holonomy vanishes. As far as a non-flat connection exists on $\tilde{\lambda}$ the curvature $\tilde{\Omega}$ does not vanish, and the holonomy group is non-trivial. The only difference is that now one can smoothly deform the Hamiltonian in such a way that the phase vanishes.

Again, we could calculate the first Chern numbers directly. In general, the integrals may not be as readily calculable as they are in our case. The results are listed as (29), and confirm our homotopy analysis.

$$\tilde{c}_1 = \begin{cases} -2k & \text{for } \nu < 1 \\ 0 & \text{for } \nu > 1. \end{cases} \tag{29}$$

There are several remarkable consequences of (29). First of all, it shows a direct relation between a topological invariant of a $U(1)$ bundle and the eigenvalues of angular momentum. Secondly, for $\nu < 1$ the fact that $\tilde{c}_1$ is an integer, translates to k being a half-integer. One can also try to use (25) to calculate $(1/2\pi) \int_{S^2} \tilde{\Omega}$ even when $\nu = 1$, which corresponds to the *critical frequency*: $\omega = b$. However, one must realize that the function $F : S^2 \to S^2$ fails to be single valued at the north pole (N). Actually, F maps N to the equator. This is a consequence of the fact that $F(\theta, \varphi) = (\tilde{\theta}, \varphi)$, but at N, φ is not fixed. For $\nu < 1$ or $\nu > 1$, N is mapped to itself or to the south pole. In both of these cases, the indeterminacy in φ does not cause any problem. But for $\nu = 1$, the situation is different and F is not well defined over whole of S^2. Thus, one cannot use F and hence $\tilde{f}$ to pullback $\tilde{\lambda}$ from η, because the fibre over N would not be unique. However, one must note that this is not a counter-example to our method. For $\nu = 1$ there is no (well-defined) F that satisfy both conditions (i) and (ii) of section 1, and our construction does not apply†.

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† A rather trivial solution to this problem is to simply exclude N from the parameter space. In that case

$$F : M' \equiv S^2 - \{N\} \longrightarrow S^2$$

is well defined and can be used to pull back a bundle $\tilde{\lambda}'$ from λ. The bundle $\tilde{\lambda}' = F \mid^*_{M'} (\lambda)$ has obviously trivial topology. The geometric phase is again identified with the holonomy of $\tilde{\lambda}'$.

4. Conclusion

The study of the topology of fibre bundles encountered in the subject of Berry phase suggests many interesting relations between quantum mechanics and algebraic topology. Among these is the relation between spin and the topological invariants such as Chern numbers. For the example considered, there is a critical frequency at which a topological change of the bundle structure occurs.

Acknowledgments

References

[1] Bohm A, Boya L J, Mostafazadeh A and Rudolph G 1993 Classification theorem for principal fibre bundles, Berry's phase and exact cyclic evolution *J. Geom. Phys.* to appear
[2] Simon B 1983 *Phys. Rev. Lett.* **51** 2167
[3] Aharonov Y and Anandan J 1987 *Phys. Rev. Lett.* **58** 1593
   Anandan J and Aharonov Y 1988 *Phys. Rev.* D **38** 1863
[4] Berry M 1984 *Proc. R. Soc.* A **392** 45
[5] Rabi I I, Ramsey N F and Schwinger J 1954 *Rev. Mod. Phys.* **26** 167
[6] Bohm A 1993 *Quantum Mechanics: Foundations and applications* (Berlin: Springer) 3rd edn, in preparation
[7] Kostant B 1970 Quantization and unitary representation *Lectures in Modern Analysis and Applications (Lecture Notes in Mathematics 170)* (Berlin: Springer) p 87
[8] Nash C and Sen S 1983 *Topology and Geometry for Physicists* (New York: Academic)
[9] Anandan J and Stodolsky L 1987 *Phys. Rev.* D **35** 2597
[10] Wang S 1990 *Phys. Rev.* A **42** 5103