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A generalization of Berry's connection

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Abstract. A generalization of Berry's connection is proposed for quantum mechanical models whose wavefunctions are sections of a vector bundle over a bundle space with fibre the configuration space of the model and base space a space of parameters. The transformation properties of the generalized Berry's connection under diffeomorphisms of the parameter space are also studied.

1. Introduction

The study of geometric phases in quantum mechanics started in the pioneer work of Aharonov and Bohm [1], and continued in the work of Berry [2] and Simons [3] on the phases of classical systems dependent on parameters.

Let $h(x, p; r)$ be the Hamiltonian of a classical system with parameters. r is a coordinate of a manifold R of parameters and $x(p)$ is the position (momentum) of the classical system. We denote the configuration space of this system as M . After the quantization of the theory, the Hamiltonian operator \hat{h} depends on the parameter r . Let \hat{h} be a self-adjoint (elliptic) operator with respect to a measure μ on M (for example the measure of a metric on M) with eigenvalues $\lambda = \lambda(r)$,

$$\hat{h}\psi_\lambda = \lambda(r)\psi_\lambda \quad (1.1)$$

where ψ_λ are the eigenstates of \hat{h} with eigenvalue λ .

If the wavefunctions of the theory are C^∞ complex functions $C^\infty(M \times R)$ on $M \times R$, Berry's connection [2] is given by

$$A_a^\lambda = i\langle \psi_\lambda, \partial_a \psi_\lambda \rangle = i \int_M (\psi_\lambda, \partial_a \psi_\lambda)(x, r) d\mu(x) \quad (1.2)$$

where (\cdot, \cdot) is a pointwise inner product on the space of wavefunctions (for example $(\psi_1, \psi_2) = \bar{\psi}_1 \psi_2$), $a = 1, \dots, \dim R$, and

$$\langle \psi_1, \psi_2 \rangle = \int_M (\psi_1, \psi_2)(x, r) d\mu(x). \quad (1.3)$$

If the eigenvalue λ is n -fold degenerate then A^λ is an $n \times n$ matrix. Since ψ_λ transforms as a function under reparametrizations of $M \times R$, A^λ in (1.2) transforms as a one-form on the parameter space R . Moreover A^λ transforms as a connection under rotations that mix the eigenstates ψ_λ with the same eigenvalue, preserve the inner product (\cdot, \cdot) and depend only on the parameters r , i.e. A^λ is a (non-Abelian) unitary connection over R [4].

An alternative way to define Berry's connection [3] is to consider the space of functions $C^\infty(M \times R)$ as an infinite dimensional vector bundle over R with fibre $C^\infty(M)$. This bundle admits a flat covariant derivative $\nabla_a = \partial_a$. The covariant derivative ∇^λ of the connection A^λ , (1.2), is defined by projecting ∇ on the subbundle $C^\infty_\lambda(M \times R)$ of $C^\infty(M \times R)$ of wavefunctions with eigenvalue λ , i.e.

$$\nabla^\lambda = P_\lambda \nabla P_\lambda \quad (1.4)$$

where P_λ is the projection from $C^\infty(M \times R)$ onto $C^\infty_\lambda(M \times R)$.

Amongst other applications, Berry's connection is useful in the study of the quantum mechanics of systems with slow and fast variables in the Born-Oppenheimer approximation. In most examples the Born-Oppenheimer Hamiltonian of the slow variables resembles the Hamiltonian of a charged particle minimally coupled to a magnetic field, which in this case is Berry's connection.

Next consider an infinitesimal transformation

$$\delta r^a = \varepsilon^A \xi_A^a(r) \quad (1.5)$$

generated by a group action of a group G , where ξ_A , $A = 1, \dots, \dim G$ are the vector fields generated by the group action and ε_A , $A = 1, \dots, \dim G$ are constant parameters. Then it was suggested in references [5, 6] that if this transformation induces a rotation on the space of eigenfunctions $C^\infty_\lambda(M \times R)$ that preserves the inner product $\langle \cdot, \cdot \rangle$ then the connection A^λ changes up to a gauge transformation. This implies that there is an infinitesimal gauge transformation η_A which depends on the parameter r such that

$$L_A A^\lambda = \nabla^\lambda \eta_A \quad (1.6)$$

where L_A is the Lie derivative of the vector field ξ_A . This was applied in the study of the diatom in the Born-Oppenheimer approximation [5]. In particular, it was shown that Berry's connection is invariant under rotations of the nuclear coordinates (slow variables) and consequently the Born-Oppenheimer Hamiltonian is invariant under the same transformations [5].

In this paper, we will define a generalization of Berry's connection for quantum systems whose wavefunctions are sections of a vector bundle \mathcal{E} over a manifold Z . Z^\dagger is a bundle whose fibre M is the configuration space of the system and whose base space R is the parameter space of the system.

There are many quantum mechanical models whose wavefunctions are sections of a vector bundle instead of functions. For example the wavefunctions of a charged particle coupled to a magnetic field, the wavefunctions of supersymmetric quantum mechanical models and the wavefunctions of all quantum systems whose phase spaces are compact manifolds.

This paper is organized as follows. In section 2, a generalization of Berry's connection is defined using the theory of families of operators. In section 3, models with parameter space R that admits a group action of a group G is considered. The obstructions to the transformations on R to induce gauge transformations on the generalized Berry's connection are examined. Finally in section 4, we give our conclusions.

† The transition functions of the bundle Z are diffeomorphisms of M that depend smoothly on the coordinates of R .

2. The generalized Berry's connection

Let $\hat{h}(r)$ be the Hamiltonian operator of a quantum system that depends on the coordinates r of the manifold R of parameters, i.e. there is a family of operators that depends smoothly on the parameters r . We will now use the definition of family of operators[†] to construct a generalization of Berry's connection.

We start with the bundle

$$M \rightarrow Z \rightarrow R \tag{2.1}$$

where M , the configuration space of the system, is a compact connected manifold without boundary and R is the space of parameters. The space of wavefunctions of the theory are sections of a hermitian vector bundle \mathcal{E} over Z with a compatible connection D . The space $\Gamma^\infty(\mathcal{E})$ of C^∞ sections of \mathcal{E} can be thought as an infinite dimensional vector bundle over R with fibre $\Gamma^\infty(E)$ [‡] where E is the restriction of \mathcal{E} to the fibre M of Z . We can define a fibrewise inner product on $\Gamma^\infty(\mathcal{E})$ by

$$\langle \psi_1, \psi_2 \rangle(r) = \int_{M_r} (\psi_1, \psi_2)(x, r) \, d\mu_r(x) \tag{2.2}$$

where (\cdot, \cdot) is a fibrewise inner product on \mathcal{E} , $\psi_1, \psi_2 \in \Gamma^\infty(\mathcal{E})$ and μ_r is a measure that depends on the coordinates of R (for example the measure of a metric on M that depends on the coordinates of R). In the following, we assume that $\hat{h}(r)$ is a self-adjoint operator in the completion of $\Gamma^\infty(\mathcal{E})|_r$ with respect to the inner product (2.2) for every $r \in R$.

Now, given a connection B on the bundle Z , the tangent bundle TZ of Z splits to horizontal $T^H Z$ and vertical $T^V Z$ subspaces

$$TZ = T^H Z \oplus T^V Z \tag{2.3}$$

where $T^H Z$ is isomorphic to $\pi^* TR$ (π is the projection of Z onto R) and $T^V Z = TM$. A horizontal frame in TZ is given by

$$e_a = \partial_a + B_a^i(x, r) \partial_i \tag{2.4}$$

and a vertical frame is given by

$$e_i = \partial_i \tag{2.5}$$

where $i = 1, \dots, \dim M$.

Next we define a connection ∇ on $\Gamma^\infty(\mathcal{E})$. Indeed

$$\nabla_X \psi = D_X \psi \tag{2.6}$$

where X is a vector field on R and $X^H = X^a(r) e_a$ is the horizontal lifting of X . ψ is a section of $\Gamma^\infty(\mathcal{E})$. Locally on R the connection ∇_X is given by

$$\nabla_a \psi = D_a \psi + B_a^i D_i \psi. \tag{2.7}$$

[†] See [7].

[‡] We restrict ourselves to the space of C^∞ sections $\Gamma^\infty(\mathcal{E})$ because its completion is not always a smooth vector bundle over R .

Our proposed generalization of Berry's connection is the restriction ∇^λ of ∇ (2.7) to the space $\Gamma_\lambda^\infty(\mathcal{E})$ of eigenfunctions of \hat{h} with eigenvalue λ , i.e.

$$\nabla^\lambda = P_\lambda \nabla P_\lambda \tag{2.8}$$

where P_λ is the projection of $\Gamma^\infty(\mathcal{E})$ onto $\Gamma_\lambda^\infty(\mathcal{E})$. To define ∇^λ we have assumed that the operators $\hat{h}(r)$ are elliptic so that all their eigenfunctions are C^∞ sections of \mathcal{E} , and $\Gamma_\lambda^\infty(\mathcal{E})$ is a well defined vector bundle over R .

The covariant derivative ∇ and consequently the covariant derivative ∇^λ encode the non-triviality of the topology of the bundle Z as well as the fact that the wavefunctions of the system are sections of a topologically non-trivial vector bundle \mathcal{E} over Z . Both covariant derivatives are dependent on the choice of connection B on Z and covariant derivative D on \mathcal{E} . Additional data must be supplied in a model to specify these connections. The fibre metric (2.2) is not always covariantly constant with respect to $\bar{\nabla}^\lambda$. However, we can always define another connection $\hat{\nabla}^\lambda$ which is compatible with (2.2)†.

If $Z = M \times R$ and \mathcal{E} is a trivial complex line bundle over Z , $\Gamma^\infty(\mathcal{E}) = C^\infty(M \times R)$. Then we can set $B = 0$ and $D = (\partial_a, \partial_i)$ and (2.8) reduces to Berry's connection (1.4).

Even if $Z = M \times R$, \mathcal{E} may not be a trivial vector bundle over Z . Indeed let $\hat{h} = \kappa r^a T_a$ be the interaction part of the Hamiltonian operator of a particle with spin coupled to a magnetic field r . T_a is an orthonormal basis in $\text{Lie}(\text{SU}(2))$, the magnetic field is chosen such that $r^a r^a = 1$, and κ is the gyromagnetic ratio. The space of parameters of the theory is the space of magnetic fields and is diffeomorphic to a two-sphere S^2 . If the wavefunctions of this system are taken to be functions of the parameter space S^2 , then Berry's connection (1.4) is the familiar magnetic monopole connection of reference [2]. However there is another possibility to consider. Indeed we can take the wavefunctions of the system to be sections of a non-trivial complex line bundle L over S^2 . In the latter case, the connection ∇ (2.7) is not flat and a modification of the Berry's connection is necessary to take into account the non-triviality of L .

Another example that requires the introduction of the connection (2.8) is given by supersymmetric quantum mechanics and in particular the quantization of $N = 1$ supersymmetric sigma models with parameters. The wavefunctions of an $N = 1$ sigma model without parameters are Dirac spinors (vector bundle valued spinors) over the target space M of the sigma model. The supersymmetric charge after quantization becomes a (twisted) Dirac operator \mathcal{D} and the Hamiltonian operator of the theory \hat{h} is given by $\hat{h} = \mathcal{D}^2$. Now given any space R of parameters, we can construct a family of (twisted) Dirac operators that are parametrized by R for any bundle Z with fibre M and base space R . Moreover there is a vector bundle \mathcal{E} over Z whose sections are the wavefunctions of the theory; when \mathcal{E} is restricted to M it becomes the bundle of Dirac spinors over M (multiplied with a vector bundle). Given a connection on \mathcal{E} and a connection on Z , we can define a connection ∇ (equation (2.7)) and from this we can construct the generalized Berry's connection.

A similar construction can be made for a charged particle coupled to a magnetic field. In this case, we take the bundle \mathcal{E} to be a complex line bundle over Z with connection D . Z is any bundle with fibre M and parameter space R . Let g_M be a metric on the configuration space M and g_R be a metric on the parameter space or the theory. Then we define a metric g_Z on Z : $g_Z = g^V + g^H$ where $(g^V)^{-1} = g_M^i e_i \otimes e_j$,

† Given a connection A of a vector bundle with fibre metric U such that $\nabla U \neq 0$, we can construct another connection $\hat{A} = A + \frac{1}{2}U^{-1}\nabla U$ such that $\hat{\nabla}U = 0$.

and $(g^H)^{-1} = g_R^{ab} e_a \otimes e_b$. The operator $\hat{h} = -\frac{1}{2}(g^\nu)^{\mu\nu} \mathcal{D}_\mu \mathcal{D}_\nu$ is the Hamiltonian operator of a charged particle with parameters coupled to a magnetic field where \mathcal{D} is the connection D of \mathcal{E} twisted with the Levi-Civita connection of g_Z and projected appropriately on the vertical directions of TZ . Using the covariant derivative D of \mathcal{E} and the connection B of Z , we can construct a generalized Berry's connection for the charged particle.

3. Symmetries and topological obstructions

Let f_g be the action of a group G on the parameter space R . It can be shown that the group action f_g leaves the covariant derivative ∇^λ (equation (2.8)) of the vector bundle $\Gamma_\lambda = \Gamma_\lambda^\infty(\mathcal{E})$ over R invariant, if there is a lifting f_g^\uparrow on Γ_λ^\uparrow . The lifting f_g^\uparrow of the group action f_g of the group G on R is a group action of G on Γ_λ such that $\pi f_g^\uparrow = f_g \pi$ where π is the projection of Γ_λ onto R . The connection corresponding to the covariant derivative ∇^λ transforms up to gauge transformations under the action of G on R . In general there are obstructions to the existence of a lifting f_g^\uparrow for the group action f_g . If this is the case, ∇^λ will not be invariant under f_g .

In the case where Γ_λ is a complex line bundle over R and G is a compact group the necessary and sufficient conditions for the existence of a lifting of the group action f_g are given by the Hattori-Yoshida theorem [10]. Indeed, the group action f_g accepts a lifting if and only if the line bundle Γ_λ is the pullback of a line bundle over $EG \times_G R$ with the inclusion i of R in $EG \times_G R$. EG is the classifying bundle of the group G . Using the spectral sequence of the fibration

$$R \rightarrow EG \times_G R \rightarrow BG \quad BG = EG/G \tag{3.1}$$

we can show that the obstructions to a line bundle Γ_λ over R being the pullback of a line bundle over $EG \times_G R$ are represented by $d_2 c_1(\Gamma_\lambda) \in H^2(BG, H^1(R, \mathbb{Z}))$ and $d_3 c_1(\Gamma_\lambda) \in H^3(BG, \mathbb{Z})$ where d_2, d_3 are the differentials of the spectral sequence and $c_1(\Gamma_\lambda)$ is the first Chern class of the line bundle Γ_λ .

If we assume in addition that the group G is connected, then the obstructions can be represented as follows [11]: Let $f: R \times G \rightarrow R$ be the group action. From the Kunneth formulae we get

$$f^* c_1(\Gamma_\lambda) = c_1(\Gamma_\lambda) + O_1 + O_2 \tag{3.2}$$

where $O_1 \in H^1(G, H^1(R, \mathbb{Z}))$ and $O_2 \in H^2(G, \mathbb{Z})$. The obstructions to lifting f_g are represented by the classes O_1 and O_2 . If O_1 and O_2 are zero the obstructions vanish. For example, the classes O_1 and O_2 always vanish provided that G is a semisimple, simply connected and compact group, i.e. any action of the group G always lifts to any complex line bundle. To give an example of an obstruction‡, we set $G = SO(3)$ and $M = S^2$ with the standard action of $SO(3)$ on S^2 . This action does not lift to the Hopf line bundle over S^2 or to any other complex line bundle over S^2 with odd Chern number. The obstruction is represented by the non-trivial element of the cohomology group $H^2(SO(3), \mathbb{Z}) = \mathbb{Z}_2$. This can be applied to Berry's connection of a particle with spin coupled to a magnetic field. The magnetic monopole connection with odd first Chern number§ is not invariant (up to a gauge transformation) under the action of $SO(3)$ on S^2 .

† The proof of this theorem was given in [8]; see also [9].

‡ For more examples see [11] and [13].

§ For the definition of this number see [3].

In the case where Γ_λ is a vector bundle and cannot be reduced to a sum of line bundles, the Hattori-Yoshida theorem gives the necessary conditions for the existence of a lifting of the group action f_g on Γ_λ . These conditions can be considered as topological obstructions to extended the classifying map of Γ_λ from R to $EG \times_G R$ [12, 13].

4. Conclusions

In conclusion we generalized Berry's connection for quantum mechanical systems with wavefunctions whose are sections of a vector bundle over a manifold Z . Z is a bundle with fibre the configuration space M of the system and base space the space R of parameters of the theory. Several examples of such quantum mechanical systems were given including supersymmetric quantum mechanical models and the charged particle in a magnetic field. Finally, we discussed the topological obstructions for a group of transformations of the parameter space R to transform the generalized Berry's connection up to a gauge transformation.

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