NON-ADIABATIC NON-ABELIAN GEOMETRIC PHASE

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The non-integrable geometric phase factor is generalized to a non-abelian phase factor which in the adiabatic limit is the Wilczek–Zee generalization of the Berry phase. It is then extended to the evolution of mixed states. A theorem of Narasimhan and Ramanan is used to relate the gauge field connection to the generalized geometric connection.

It is well known that, in quantum mechanics, the physical state of a system is specified by the measurement of a complete set of commuting observables which determine a one-dimensional eigensubspace, called a ray of the Hilbert space $\mathscr{H}$. The set $\mathscr{P}$ of the rays of $\mathscr{H}$, which I shall call the projective Hilbert space of $\mathscr{H}$, represents, therefore, the set of all possible physical states of the system. The evolution of the system can therefore be described completely by a curve in $\mathscr{P}$. If $\mathscr{H}$ has finite dimension n then $\mathscr{P}$ is the usual complex projective space of dimension $n-1$. However, the phenomena of interference suggest that the state vectors that belong to $\mathscr{H}$ undergo a linear evolution and that the probability amplitude of transition during a measurement can be obtained from a linear inner product defined on $\mathscr{H}$. Therefore, the motion of any state vector in $\mathscr{H}$ can be obtained from a knowledge of the motions of a complete set of state vectors.

A given evolution of the system is then given by a curve C in $\mathscr{H}$ which projects to a curve $\hat{C}$ in $\mathscr{P}$ under the natural projection map Π: $\mathscr{H}\to\mathscr{P}$, that maps any state in $\mathscr{H}$ into the ray that contains it. If $\hat{C}$ is a closed curve then the evolution will be called cyclic and the state which undergoes this evolution will be called a cyclic state. Therefore, during a cyclic evolution, the state vector merely acquires a phase factor $e^{i\phi}$. Recently, a geometric part of this phase was defined by [1]

$$\beta\equiv\phi+\frac{1}{\hbar}\int\langle\psi(t)|H|\psi(t)\rangle\,dt\,, \tag{1}$$

where H is the hamiltonian that generates the evolution of the normalized state vector $|\psi(t)\rangle$ according to the Schrödinger equation. This implies [1]

$$\beta=\int\langle\tilde{\psi}|i d/dt|\tilde{\psi}\rangle\,dt$$
$$=\oint_{\hat{C}}\langle\tilde{\psi}|i\partial/\partial\lambda^{\mu}|\tilde{\psi}\rangle\,d\lambda^{\mu}\,, \tag{2}$$

where λ^{μ} are coordinates in $\mathscr{P}$ and $|\tilde{\psi}\rangle$ is any normalized, locally differentiable state vector field on $\mathscr{P}$ such that its value at any $p\in\mathscr{P}$ is contained in P. For a different choice $|\tilde{\psi}'(\lambda)\rangle=e^{i\Lambda(\lambda)}|\tilde{\psi}(\lambda)\rangle$, $A_{\mu}\equiv\langle\tilde{\psi}|i\partial/\partial\lambda^{\mu}|\tilde{\psi}\rangle$ transforms according to $A'_{\mu}=A_{\mu}-\partial\Lambda/\partial\lambda^{\mu}$. Therefore, (2) is independent of the choice of $|\tilde{\psi}\rangle$ and the coordinates λ^{μ} on $\mathscr{P}$, and is a property of only the unparametrized curve $\hat{C}$. Indeed, $e^{i\beta}$ is the holonomy transformation due to parallel transport around $\hat{C}$ with respect to a connection [1,2] on $\mathscr{P}$. The one-form $A=\langle\tilde{\psi}|i d|\tilde{\psi}\rangle$ is the connection coefficient of this connection with respect to the cross section defined by $|\tilde{\psi}\rangle$.

An example of a cyclic evolution could occur when the hamiltonian H depends on a set of parameters $\boldsymbol{R}$ which vary adiabatically along a closed curve Γ in the parameter space S. If the spectrum of energy eigenvalues is such that there is a finite number of them

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below or above a given eigenvalue [#1] then an eigenstate of $H(\boldsymbol{R})$ belonging to eigenvalue $E(\boldsymbol{R})$, that is simple on Γ, returns to its original state after $H(\boldsymbol{R})$ evolves around Γ. The motion of this eigenstate, therefore, maps Γ into a closed curve $\hat{\mathrm{C}}$ on projective Hilbert space. In this special case, the geometric phase β associated with $\hat{\mathrm{C}}$ is the same as Berry's phase [3] that was associated with Γ, which can be obtained from the holonomy of a connection [4,5] defined on S. However, if the eigenspace is constant along a part of Γ, then this part corresponds to a single point on $\hat{\mathrm{C}}$. Hence, even in this special case, it is better to associate $e^{i\beta}$ with the curve $\hat{\mathrm{C}}$ in the projective Hilbert space P, which does not have the redundancy in the earlier description [3,4] that uses instead the parameter space.

The above geometric connection, which gives β for any closed curve $\hat{\mathrm{C}}$ in $\mathscr{P}$, can be used to parallel transport a state vector $|\psi^{\mathrm{P}}\rangle$ along *any* curve in $\mathscr{P}$ according to the condition [4,1]

$$\langle\psi^{\mathrm{P}}|\mathrm{d}/\mathrm{d}t|\psi^{\mathrm{P}}\rangle = 0\,. \tag{3}$$

It is then easy to show that the covariant derivative $\nabla|\psi\rangle = \langle\psi|\mathrm{d}|\psi\rangle|\psi\rangle$ where $|\psi\rangle$ is a normalized state vector field on P. Also, on defining the component Φ of $|\psi\rangle$ with respect to $|\tilde{\psi}\rangle$ by $|\psi\rangle = \Phi|\tilde{\psi}\rangle$, the component of $\nabla|\psi\rangle$ is then $\mathrm{d}\Phi - \mathrm{i}A\Phi$. If $|\tilde{\psi}\rangle$ is not necessarily normalized, then A must be defined more generally as

$$A = \mathrm{i}\,\frac{\langle\tilde{\psi}|\mathrm{d}|\tilde{\psi}\rangle - \mathrm{d}(\langle\tilde{\psi}|)|\tilde{\psi}\rangle}{2\langle\tilde{\psi}|\tilde{\psi}\rangle}\,.$$

Also, given an arbitrary hamiltonian $H(t)$ and an arbitrary time interval (t_1, t_2), the unitary time evolution operator $\mathrm{P}\exp(-\mathrm{i}\int_{t_1}^{t_2} H\,\mathrm{d}t)$, where P denotes Dyson time ordering, has a complete set of eigenstates, which, therefore, undergo cyclic evolutions during this time interval [#2]. Hence, the evolution of *any* state, which can of course be expressed as a superposition of the cyclic states, can be determined from the knowledge of the phase changes of the cyclic states. Thus, the study of cyclic evolutions is the study of all evolutions.

[#1] If this condition is not satisfied, then it may be possible for a given eigenstate to return to a different eigenstate after $\mathrm{H}(\boldsymbol{R})$ returns to its original value after the evolution along Γ. I thank D.R. Brill for pointing out this possibility.

[#2] I thank J. Garrison for pointing this out to me.

In a non-adiabatic cyclic evolution, it would be possible to measure β, experimentally, in the following situations: (A) The second term in (1) is zero or negligible, e.g. if H fluctuates rapidly during the cyclic evolution. Then β is the same as ϕ, which may be observed by interfering this cyclic state with another state. (B) The second term in (1) is the same for two cyclic states, e.g., this would be the case if H is invariant under a transformation that transforms one cyclic state into the other. Then the difference $\phi_1 - \phi_2$ of the total phases acquired by the cyclic states is the same as the difference $\beta_1 - \beta_2$ of their geometric phases. Therefore, $\beta_1 - \beta_2$ can be measured by observing the evolution of a superposition of the two cyclic states. (C) The second term in (1) is known from the experimental set up. The β can be measured using the techniques mentioned in (A) or (B). In the latter case, the superposition of the cyclic states would undergo an extra "precession" due to the geometric phase difference $\beta_1 - \beta_2$.

Sometimes, only a partial knowledge of the state of a system may be known through the measurement of a set of commuting observables that do *not* form a complete set. Then the state vector is known to be in an n-dimensional subspace V_n of $\mathscr{H}$ corresponding to the observed values of these observables. For example, if the system is known to have energy E for which H has a degenerate eigenspace V_n, then we can only say that its state vector belongs to V_n. In such cases, it may be of interest to follow the Schrödinger time evolution of a subspace $\mathrm{V}_n(t)$ with $\mathrm{V}_n(0) = \mathrm{V}_n$. Here, $\mathrm{V}_n(t)$ is defined to be the n-dimensional subspace of vectors obtained from the vectors in V_n by the linear Schrödinger evolution in the time interval $[0, t]$. If, furthermore, $\mathrm{V}_n(\tau) = \mathrm{V}_n(0)$ for some τ then we shall call the evolution of $\mathrm{V}_n(t)$ cyclic. When $n = 1$, this is the same as the cyclic evolution of a state [1]. Also, in the adiabatic limit and for a degenerate hamiltonian, this corresponds to the case considered by Wilczek and Zee [6].

Suppose $\mathrm{H} = \mathrm{V}_n(t) \oplus \mathrm{V}_m(t)$ is a time dependent decomposition of the $(n+m)$-dimensional Hibert space into two subspaces of dimensions n and m, respectively, and $\mathrm{V}_n(t)$ undergoes cyclic evolution, so that $\mathrm{V}_n(\tau) = \mathrm{V}_n(0)$. Let $\{|\tilde{\psi}_a(t)\rangle, a = 1, ..., n\}$ be an orthonormal basis of $\mathrm{V}_n(t)$ with $|\tilde{\psi}_a(\tau)\rangle = |\tilde{\psi}_a(0)\rangle$ for every a. Let $\{|\psi_a(t)\rangle, a = 1, ..., n\}$ be another orthonormal basis which undergoes time evolution according to the Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi_a(t)=H|\psi_a(t)\rangle \tag{4}$$

with $|\psi_a(0)\rangle = |\tilde{\psi}_a(0)\rangle$. Then

$$|\psi_a(t)\rangle = \sum_{b=1}^{n} U_{ba}(t)|\tilde{\psi}_b(t)\rangle , \tag{5}$$

where U is a unitary matrix. Substituting (5) into (4), we obtain

$$U(t) = \mathrm{P}\exp\left(\int_0^t \mathrm{i}(A-K)\,\mathrm{d}t\right) \tag{6}$$

where $A_{ab} = \mathrm{i}\langle\tilde{\psi}_a|\mathrm{d}/\mathrm{d}t|\tilde{\psi}_b\rangle$ and $K_{ab} = (1/\hbar)\times\langle\tilde{\psi}_a|H|\tilde{\psi}_b\rangle$ are hermitian matrices and P denotes path ordering. This A_{ab} is geometrical in the sense that it is independent of the hamiltonian and depends only on the Hilbert space structure.

If we choose a different basis $|\tilde{\psi}'_a(t)\rangle = \sum_{b=1}^{n}\Omega_{ba}(t)|\tilde{\psi}_b(t)\rangle$, where Ω is a unitary operator, then the matrices A_{ab} and K_{ab} transform according to

$$A' = \mathrm{i}\Omega^+\dot{\Omega} + \Omega^+ A\Omega$$

and $K' = \Omega^+ K\Omega$. If $G_{n,m}$ is the set of all n-dimensional subspaces of $\mathscr{H}$ then it is possible to choose an open covering $\{U_\alpha\}$ of $G_{n,m}$ such that on each U_α, $|\tilde{\psi}_a\rangle$, $a=1,2,...,n$, are smooth fields, with their values at each $V_n \in U_\alpha$ forming an orthonormal basis of V_n. Then the matrix valued one-form $\mathrm{i}\langle\tilde{\psi}_a|\mathrm{d}|\tilde{\psi}_b\rangle$ may be regarded as the coefficients of a non-abelian connection or "gauge field" on the space $G_{n,m}$. Also, $|\psi\rangle \in V_n(t)$ is parallel transported with respect to this connection if

$$\langle\tilde{\psi}_a(t)|\mathrm{d}/\mathrm{d}t|\psi(t)\rangle = 0 , \quad a=1,2,...,n , \tag{7}$$

which generalizes (3).

In mathematical terms this connection is in a vector bundle $E_{n,m}$ over $G_{n,m}$ such that the fiber of $E_{n,m}$ over $V_n \in G_{n,m}$ is V_n itself. This $G_{n,m}$, which is called a Grassmann manifold [7], generalizes our projective Hilbert space that corresponds to the special case of $n=1$. Since the subgroup of the unitary group $U(n+m)$, that acts on $\mathscr{H}$, that leaves $V_n(t)$ invariant is $U(n)\times U(m)$, $G_{n,m}$ may also be taken to be $U(n,m)/U(n)\times U(m)$.

In the special case when $[K, A]=0$, (6) may be written as

$$U(t) = \mathrm{P}\exp\left(-\mathrm{i}\int_0^t K\,\mathrm{d}t\right)B(t) ,$$

where $B(t) = \mathrm{P}\exp(\mathrm{i}\int_0^t A\,\mathrm{d}t)$ generalizes the geometric phase factor $\exp(\mathrm{i}\beta)$ for the special case $n=1$. An example, considered by Wilczek and Zee [8], is when $H(t)$ varies slowly so that the adiabatic approximation is valid and $V_n(t)$ is a degenerate eigensubspace of $\mathscr{H}$ corresponding to eigenvalue $E(t)$. Then $U(\tau) = \exp(-\mathrm{i}\int_0^\tau E\,\mathrm{d}t)B(\tau)$ with

$$B(\tau) = \mathrm{P}\exp\left(\mathrm{i}\oint_{\hat{C}} A_\mu(\lambda)\,\mathrm{d}\lambda^\mu\right) , \tag{8}$$

with $A_{\mu ab} = \mathrm{i}\langle\tilde{\psi}_a|\partial/\partial\lambda_\mu|\tilde{\psi}_b\rangle$, where (λ_μ) are coordinates on $G_{n,m}$, and $\hat{C}$ is the closed curve in $G_{n,m}$ corresponding to the cyclic evolution of $V_n(t)$. It is then possible to experimentally determine B [6]. From the holonomy transformations B, the connection A can be determined [8] on $G_{n,m}$ and it is then unique up to gauge transformations [9].

Returning now to the more general case in which $U(t)$ is given by (6), since $U(\tau)$ is a unitary operator, it has a set of eigenvectors $\{|\psi_a(0)\rangle\}$ which form an orthornormal basis of $V_n(0)$. Then $|\tilde{\psi}_a(t)\rangle$ can be chosen to be proportional to $|\psi_a(t)\rangle$ and $A-K$ is then diagonal, because of (4). Then $U(\tau)$ is also diagonal with its diagonal elements being

$$\exp\left(-\oint_{\hat{C}} \langle\tilde{\psi}_a|\mathrm{d}/\mathrm{d}t|\tilde{\psi}_a\rangle - \frac{\mathrm{i}}{\hbar}\langle\tilde{\psi}_a|H|\tilde{\psi}_a\rangle)\,\mathrm{d}t\right) .$$

Hence, each $|\psi_a\rangle$, which undergoes a cyclic evolution acquires the abelian geometric phase β, given by (1) or (2). The adiabatic cyclic evolution of a degenerate eigenspace considered by Wilczek and Zee [6] corresponds to the special case of $\langle\tilde{\psi}_a|H|\tilde{\psi}_a\rangle = E$ for $a=1, 2 ..., n$. The experiment of Tomita and Chiao [10], in which a degenerate eigenspace $V_2(t)$ consisting of the spin states of the photon undergoes a cyclic evolution, belongs to this category and not the more restrictive category considered by Berry [3] in which an eigenspace $V_1(t)$ belonging to a simple eigenvalue undergoes an adiabatic evolution. However, it is not possible to define $\{|\tilde{\psi}_a\rangle\}$ on $G_{n,m}$ so that, for *every* closed curve

$\hat{C}$ on $G_{n,m}$, $A-K$ or A is diagonal. Hence A does represent a non-abelian connection.

As an application, consider a density operator $\hat{\rho}(t)$ that represents a quantum statistical ensemble at time t. The set $\{|\psi_a(t)\rangle\}$ of orthonormal eigenvectors of $\hat{\rho}(t)$ belonging to non-zero eigenvalues span an n-dimensional subspace $V_n(t)$ of $\mathscr{H}$. Then the density matrix ρ with respect to the basis $\{|\tilde{\psi}_a(t)\rangle\}$ evolves as $\rho(t)=U(t)\rho(0)U^+(t)$, where $U(t)$ is given by (6). If $V_n(\tau)=V_n(0)$ and $V_n(t)$ is a degenerate subspace of $H(t)$, then $\rho(\tau)=B(\tau)\rho(0)B^+(\tau)$, with $B(\tau)$ defined by (8). In this case, the evolution of $\rho(t)$ is purely geometrical. When $n>1$, ρ describes a mixed state, and the non-abelian aspect of A plays an essential role because a basis cannot be chosen, in general, so that both A and ρ are diagonal. The set of pure state density operators for which $n=1$ may be regarded as the same as $\mathscr{P}$.

Associated with the vector bundle $E_{n,m}$ is a principal fiber bundle $F_{n,m}$ over $G_{n,m}$ with structure group $U(n)$ such that the fiber of $F_{n,m}$ over each $V_n\in G_{n,m}$ is the set of orthonormal frames in V_n. If $\mathscr{H}$ is infinite-dimensional then the corresponding $G_{n,\infty}$ is called a universal bundle and the connection A defined above in E_n has an associated universal connection B in $F_{n,m}$. Narasimhan and Ramanan [11] have shown that given any other principal fiber bundle P over a manifold M with structure group $U(n)$ and connection Γ, there exists a bundle homomorphism f: $P\to F_{n,\infty}$ such that Γ is the connection on P induced by the connection B. It follows that there exists a differentiable map

$$M\supset U\ni \boldsymbol{R}\xrightarrow{h}(|\tilde{\psi}_1^{\boldsymbol{R}}\rangle,|\tilde{\psi}_2^{\boldsymbol{R}}\rangle,\dots,|\tilde{\psi}_n^{\boldsymbol{R}}\rangle)\in F_{n,\infty}$$

such that

$$i\langle\tilde{\psi}_a^{\boldsymbol{R}}|\partial/\partial R^\mu|\tilde{\psi}_b^{\boldsymbol{R}}\rangle=-\Gamma_{\mu ab}(\boldsymbol{R}) \qquad (9)$$

where R^μ are the coordinates of $\boldsymbol{R}$ and $\Gamma_{\mu ab}(\boldsymbol{R})$ are the connection coefficients (gauge potential) with respect to a cross section (gauge) in P.

If M is space–time, then by suitably choosing f or h, which corresponds to the experiment being performed, the generalized Aharonov–Bohm effect due to an arbitrary gauge field [12,13] may be regarded as arising from the geometric connection. For the U(1) gauge field, an example of the map h was given by Berry [3] for the special case of a magnetic field confined to a line with flux Φ. In this case, M can be taken to be the three-dimensional space surrounding the flux line. Berry chose $\langle \boldsymbol{r}|\tilde{\psi}^{\boldsymbol{R}}\rangle$ to be a wave-function confined to a box centered at $\boldsymbol{R}\in$M. More generally, I consider a flux line of a $U(n)$ gauge field such that in some gauge, the gauge potential components $A_0^\alpha=0$ and A_i^α, $i=1, 2, 3$ are time independent. For every $\boldsymbol{R}\in$M, I choose a subspace $V_n(\boldsymbol{R})$ to be spanned by orthonormal states $|\tilde{\psi}_a^{\boldsymbol{R}}\rangle$, $a=1, 2, \dots, n$ which are eigenstates of the hamiltonian. These states may be regarded as confined to a box centered at $\boldsymbol{R}$ so that

$$\langle \boldsymbol{r}|\tilde{\psi}_a^{\boldsymbol{R}}\rangle=\mathrm{P}\exp\left(-ig\int_{\boldsymbol{R}}^{\boldsymbol{r}} A_j^\alpha T^\alpha\, dx^j\right)\psi_a^{\boldsymbol{R}}(\boldsymbol{r}),$$

where $\psi_a^{\boldsymbol{R}}(\boldsymbol{r})=\psi_a(\boldsymbol{R})\chi(\boldsymbol{r}-\boldsymbol{R})$ satisfies $\langle\psi_a^{\boldsymbol{R}}|\nabla_{\boldsymbol{R}}|\psi_b^{\boldsymbol{R}}\rangle_{\boldsymbol{R}}=0$ for all a, b and χ is gauge invariant, normalized and vanishes outside the box and T^α generate the gauge group. The $\psi_a(\boldsymbol{R})$, $a=1, 2, \dots, n$ are assumed to be orthonormal in the internal symmetry vector space at $\boldsymbol{R}$. The $\langle\tilde{\psi}_a^{\boldsymbol{R}}|\tilde{\psi}_b^{\boldsymbol{R}}\rangle=\delta_{ab}$. Also, (9) is satisfied with $\Gamma_{\mu ab}(\boldsymbol{R})=gA_\mu^\alpha(\boldsymbol{R})\times\langle\tilde{\psi}_a^{\boldsymbol{R}}|T^\alpha|\tilde{\psi}_b^{\boldsymbol{R}}\rangle$. Suppose the box containing a given $|\psi_a\rangle\in V_n(R)$ is taken adiabatically around a circuit surrounding the flux line in a time interval $[0,\tau]$. Then according to (5) and (6)

$$|\psi_a(\tau)\rangle=\exp\left(-\frac{i}{\hbar}\int_0^\tau E\,dt\right)\times\sum_{b=1}^{n}\left[\mathrm{P}\exp\left(i\oint\boldsymbol{\Gamma}(\boldsymbol{R})\cdot d\boldsymbol{R}\right)\right]_{ba}|\psi_b(0)\rangle .$$

If this state is interfered with a state that is coherent with it in a box which was not transported then the shift in the interference pattern would be similar to the generalized Aharonov–Bohm effect [12,13], due to a non-abelian gauge field.

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