Derivation of the geometrical phase

Arno Bohm, Luis J. Boya,* and Brian Kendrick

Center for Particle Theory, Department of Physics, The University of Texas at Austin, Austin, Texas 78712

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The geometric (Berry) phase is shown to have its origin in the nontrivial geometry of the fiber bundle: Hilbert space→space of states. The nontrivial geometry comes simply from the scalar product in Hilbert space. A comprehensive treatment of the geometrical phase is presented, bringing together the various ideas in the literature.

I. INTRODUCTION

The mathematical language of fiber bundles[1,2] provides a powerful tool for the study of geometric phases. We want to discuss the geometric phase using these tools. The following points will be stressed.

(a) The splitting of the total phase into geometrical and dynamical parts is determined by a choice of connection.

(b) A natural connection is provided by the scalar product. This connection produces the standard geometrical (Berry) phase.

(c) The geometrical phase is independent of the choice of gauge. For cyclic evolution, gauge transformations are given by $|\phi(t)\rangle \rightarrow e^{i\theta(t)}|\phi(t)\rangle$, where $\theta(T)=\theta(0)+2\pi n$.

We want to consider unitary time evolution of a quantum system undergoing cyclic evolution. A state vector will be denoted by $|\psi(t)\rangle$ which is an element of an $(N+1)$-dimensional or infinite-dimensional complex vector space denoted by $C^{N+1}-\{0\}$ or $\mathcal{H}-\{0\}$ (we have subtracted out the null vector). We can denote this vector by $|\psi(t)\rangle=(Z_0(t),Z_1(t),\ldots,Z_N(t))$ where $Z_i(t)\in C^1$. This vector space is endowed with the usual scalar product or Hermitian metric. We also want to consider normalized state vectors, namely all $|\psi\rangle \in C^{N+1}-\{0\}$ or $\mathcal{H}-\{0\}$ such that $\langle\psi(t)|\psi(t)\rangle=1$ for all time. Written in terms of components this is

$$\sum_{i=0}^{N(\infty)} \bar{Z}^{i}(t) Z_i(t)=1 \ .$$

This equation defines the sphere S^{2N+1} or S^{∞} as a submanifold of $C^{N+1}-\{0\}$ or $\mathcal{H}-\{0\}$. Unitary evolution preserves the scalar product, therefore normalized state vectors remain normalized and motion is restricted to the sphere S^{2N+1} or S^{∞}.

In quantum mechanics a physical state is not represented by a normalized state vector $|\psi(t)\rangle\in\mathcal{H}-\{0\}$ but by a ray. A ray is the one-dimensional subspace to which this vector belongs. Two normalized vectors are equivalent $|\psi\rangle' \sim |\psi\rangle$ if they belong to the same ray, i.e., if $|\psi\rangle'=e^{i\theta}|\psi\rangle$ where $e^{i\theta}\in U(1)$. This equivalence relation forms equivalence classes on S^{2N+1} or S^{∞}. The set of all equivalence classes $S^{\infty}/\mathrm{U}(1)$ forms the space of physical states (rays) which we denote by

$$P(\mathcal{H})=S^{\infty}/\mathrm{U}(1)=\frac{\mathcal{H}-\{0\}}{C-\{0\}}$$

or by CP^N (N-dimensional projective space) when N is finite. $P(\mathcal{H})$ or CP^N can be interpreted as the space of one-dimensional complex subspaces of $\mathcal{H}$ with the zero vectors removed. It can also be understood as the space of the one-dimensional projection operators $|\psi\rangle\langle\psi|$ which project onto these one-dimensional subspaces. $P(\mathcal{H})$ is not only a linear space but also a complex analytic manifold.

We can express the above ideas in terms of fiber bundles. A fiber bundle consists of a topological space E called the total space, a topological space M called the base space, a fiber space F, a group G acting on the fibers (called the structure group) and a projection map π which projects the fibers above M to points in M. In our case the fiber bundle consists of a total space E which is the normalized state vectors in $C^{N+1}-\{0\}$ or $\mathcal{H}-\{0\}$, the base space M is the complex projective space CP^N or $P(\mathcal{H})$ whose elements are the rays (one-dimensional subspaces of $\mathcal{H}-\{0\}$), a fiber consists of all unit vectors from the same ray, the group G is U(1), and the association of the unit vector $|\psi(t)\rangle$ to the operator $|\psi(t)\rangle\langle\psi(t)|$ is the projection map π. This fiber bundle is a particular type of fiber bundle called a principal fiber bundle over CP^N or $P(\mathcal{H})$ with group U(1).[2]

The time evolution of a state vector is determined by the Hamiltonian via the Schrödinger equation. This evolution produces a path in the total space E. The corresponding path in the space of physical states [$M=P(\mathcal{H})$ or CP^N] is found by projecting the path in E down onto a path in M. We will consider cyclic evolution, i.e., evolution in which the physical state returns to the original state. Cyclic evolutions are thus represented by closed paths in M. Closed paths in M do not only correspond to closed paths in E but also to paths which are open in E. This means that a state vector for a cyclic evolution returns to the same fiber, but in general to another state vector which differs from the original state vector by an overall phase.

As we will show below, part of this phase depends only on the geometry of the fiber bundle. The geometry is given once a connection is chosen. Intuitively a connection provides a way to compare fibers at different points on the space M. Mathematically a connection is specified by defining a horizontal subspace H of the tangent space TE to E. Complementary to the horizontal subspace is a vertical subspace V such that $TE = H \oplus V$. Consider a point u in E; the vertical subspace at u is defined to consist of those tangent vectors in TE which are tangent to the fiber passing through u, i.e., whose projections to the tangent space on M are zero. While the vertical subspace is defined by the fibers, the horizontal subspace (connection) is a matter of choice. Once a connection is specified, the notion of a horizontal lift can be introduced. A horizontal lift is defined by lifting the tangent vectors of a curve in M to tangent vectors of a curve in E such that they are horizontal. The horizontal lift of a closed curve is in general open. Starting at a given point in the fiber, the horizontal lift will return to a different point on the same fiber. This difference is called holonomy, and in our case it is a phase. In this way, the horizontal lift will respect to a given connection defines the geometrical phase. The total phase of a state vector can then be decomposed into a geometrical part and a remaining part called dynamical.

II. THE CONNECTION, HORIZONTAL LIFT, AND HOLONOMY

Before choosing a horizontal subspace (connection) we will identify the vertical subspace (or vertical direction). The action of the group U(1) on S^{2N+1} or S^{∞} generates the fibers. Each element of a fiber points in the same direction (they just differ by a phase). This direction generated by the U(1) action is called the vertical direction.

The scalar product provides a natural choice for the horizontal subspace. To see this consider $|\dot{\phi}(t)\rangle$, the tangent vectors to the curve $|\phi(t)\rangle$ in E. These tangent vectors are in TE and can be decomposed into vertical and horizontal parts via the scalar product,

$$|\dot{\phi}(t)\rangle = \langle \phi(t)|\dot{\phi}(t)\rangle |\phi(t)\rangle + |h_{\phi}(t)\rangle \ . \tag{1}$$

From the above discussion we know that $|\phi(t)\rangle$ points in the vertical direction [so does $|\phi'(t)\rangle = e^{i\theta}|\phi(t)\rangle$]. Thus $\langle \phi(t)|\dot{\phi}(t)\rangle$ is the vertical part of $|\dot{\phi}(t)\rangle$. We note that the above decomposition is independent of the particular fiber element we choose to represent the vertical direction.

The horizontal component satisfies

$$\langle \phi(t)|h_{\phi}(t)\rangle = 0 \ . \tag{2}$$

This equation defines the horizontal subspace as being orthogonal to the vertical subspace providing a natural connection on the fiber bundle. Vertical tangent vectors are proportional to $|\phi(t)\rangle$, and horizontal tangent vectors are proportional to $|h_{\phi}(t)\rangle$.

In order to evaluate the connection explicitly, we will consider a local patch U on M and the region of E over U. Tangent vectors in TE are produced by the operator d/dt. In the usual way this operator is expressed in terms of vertical and horizontal operators as

$$\frac{d}{dt} = \alpha \frac{\partial}{\partial \theta} + B^{\mu} D_{\mu} \tag{3}$$

where the operator $\partial/\partial\theta$ is called the vertical basis and D_{μ} the horizontal basis. The coefficients α and B^{μ} represent the components in each direction. The horizontal basis D_{μ} is called the covariant derivative and is given by

$$D_{\mu} = \frac{\partial}{\partial X^{\mu}} + A_{\mu}\frac{\partial}{\partial \theta}$$

where $\tilde{A} = A_{\mu} dX^{\mu}$ and $X \in CP^N$ or $P(\mathcal{H})$. The one-form $\tilde{A}$ is the connection form.

Applying the operator of Eq. (3) to $|\phi(t)\rangle = |\phi(\theta, X)\rangle \in E$ we find

$$|\dot{\phi}(t)\rangle = \alpha \frac{\partial}{\partial \theta}|\phi\rangle + B^{\mu} D_{\mu}|\phi\rangle \ . \tag{4}$$

By comparing the vertical and horizontal parts of Eq. (1) with those of Eq. (4), we see

$$\langle \phi|\dot{\phi}\rangle|\phi\rangle = \alpha \frac{\partial}{\partial\theta}|\phi\rangle \ , \tag{5}$$

$$|h_{\phi}\rangle = B^{\mu} D_{\mu}|\phi\rangle \ . \tag{6}$$

From Eq. (6) we write

$$\langle \phi|h_{\phi}\rangle = \langle \phi|B^{\mu} D_{\mu}|\phi\rangle$$

and from Eq. (2) we see

$$\langle \phi|B^{\mu} D_{\mu}|\phi\rangle = 0 \ .$$

Since B^{μ} is arbitrary we have

$$\langle \phi|D_{\mu}|\phi\rangle = 0 \ ,$$

$$\left\langle \phi \left| \left[\frac{\partial}{\partial X^{\mu}} + A_{\mu}\frac{\partial}{\partial\theta} \right] \right| \phi \right\rangle = 0 \ ,$$

$$A_{\mu}\left\langle \phi \left| \frac{\partial}{\partial\theta} \right| \phi \right\rangle = -\left\langle \phi \left| \frac{\partial}{\partial X^{\mu}} \right| \phi \right\rangle \ .$$

By considering an infinitesimal U(1) action

$$|\phi\rangle_{\theta_0+\delta\theta} = |\phi\rangle_{\theta_0} + i\delta\theta|\phi\rangle_{\theta_0}$$

and a Taylor-series expansion

$$|\phi\rangle_{\theta_0+\delta\theta} = |\phi\rangle_{\theta_0} + \delta\theta \left.\frac{\partial|\phi\rangle}{\partial\theta}\right|_{\theta_0}$$

we find (θ_0 arbitrary)

$$\left.\frac{\partial|\phi\rangle}{\partial\theta}\right|_{\theta_0} = i|\phi\rangle_{\theta_0} \ . \tag{7}$$

Therefore the above expression for A_{μ} becomes

$$A_{\mu} = i\left\langle \phi \left| \frac{\partial}{\partial X^{\mu}} \right| \phi \right\rangle \tag{8}$$

where we have used $\langle \phi|\phi\rangle = 1$. We have seen explicitly how the scalar product on Hilbert space defines the connection form $\tilde{A}$.

In mathematical terminology, $|\phi\rangle$ is a local section of the fiber bundle. A local section is a continuous mapping of a patch U in M into the fibers above U. A change to a different patch U' on M corresponds to a change in the section $|\phi\rangle \rightarrow |\phi'\rangle$. The change in section is given by the structure group and, in our case,

$$|\phi(x)\rangle' = e^{i\theta(x)}|\phi(x)\rangle$$

where $\theta(x)$ is a real function of the coordinates X^μ on M. This transformation is called a gauge transformation. The connection form transforms in the usual way:

$$A'_\mu(x) = -\frac{\partial\theta(x)}{\partial X^\mu} + A_\mu(x) . \quad (9)$$

A local section maps a closed path in M [$X^\mu(T)=X^\mu(0)$, $0\le t\le T$] into a closed path in E. We will denote the closed path in E as $|\phi(t)\rangle$ [$|\phi(T)\rangle = |\phi(0)\rangle$]. A gauge transformation gives a different closed path in E,

$$|\phi'(t)\rangle = e^{i\theta(t)}|\phi(t)\rangle . \quad (10)$$

In order for $|\phi'(t)\rangle$ to be closed, the function $\theta(t)$ must satisfy

$$\theta(T) = \theta(0) + 2\pi n \quad (11)$$

where n is an integer.

We will now evaluate the holonomy produced by the horizontal lift of a closed curve in M with respect to the connection given above. We will denote the horizontal lift by $|\tilde{\psi}(t)\rangle$. By definition, the tangent vectors to the curve $|\tilde{\psi}(t)\rangle$ must be horizontal. From Eq. (1) this means

$$\langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle = 0 \quad (12)$$

(i.e., their vertical component is zero). We can express the open path $|\tilde{\psi}(t)\rangle$ in E terms of a closed path $|\phi(t)\rangle$ in E,

$$|\tilde{\psi}(t)\rangle = e^{if(t)}|\phi(t)\rangle \quad (13)$$

where $|\tilde{\psi}(T)\rangle = e^{i(f(T)-f(0))}|\tilde{\psi}(0)\rangle$ and $|\phi(T)\rangle = |\phi(0)\rangle$. Defining $\beta = f(T) - f(0)$, substituting Eq. (13) into (12), and integrating yields

$$\beta = i\int_0^T \langle\phi(t)|\dot{\phi}(t)\rangle dt .$$

The tangent vector $|\dot{\phi}\rangle$ is given by

$$\frac{d}{dt}|\phi(t)\rangle = \dot{\theta}\frac{\partial}{\partial\theta}|\phi\rangle + \dot{X}^\mu\frac{\partial}{\partial X^\mu}|\phi\rangle .$$

Contracting this equation with $i\langle\phi|$ from the left and integrating yields

$$\beta = i\int_0^T \dot{\theta}\left\langle\phi\left|\frac{\partial}{\partial\theta}\right|\phi\right\rangle dt + i\int_0^T \dot{X}^\mu\left\langle\phi\left|\frac{\partial}{\partial X^\mu}\right|\phi\right\rangle dt .$$

We now use Eq. (7) and $\langle\phi|\phi\rangle = 1$ to find

$$\beta = -\int_0^T \dot{\theta}\,dt + i\int_0^T \left\langle\phi\left|\frac{\partial}{\partial X^\mu}\right|\phi\right\rangle \dot{X}^\mu dt . \quad (14)$$

From Eq. (8), we can express the second integral in Eq. (14) as

$$i\int_0^T \left\langle\phi\left|\frac{\partial}{\partial X^\mu}\right|\phi\right\rangle \dot{X}^\mu dt = \oint_c \tilde{A} . \quad (15)$$

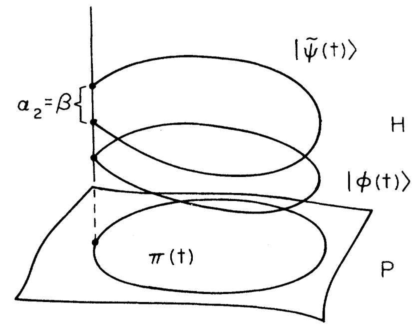

FIG. 1. Horizontal lift of the path $c = \pi(t)$.

The first integral in Eq. (14) yields

$$\int_0^T \dot{\theta}dt = \theta(T) - \theta(0) = 2\pi n .$$

This contribution to the phase represents the gauge freedom as discussed above [see Eqs. (9), (10), and (11)]. From Eqs. (9) and (15) we see that Eq. (14) is simply

$$\beta = \oint_c A'_\mu dX^\mu .$$

The holonomy (or geometric phase) $e^{i\beta}$ is independent of the choice of gauge:

$$e^{i\beta} = \exp\left[i\oint_c \tilde{A}'\right] ,$$

$$e^{i\beta} = \exp\left[i\oint_c \tilde{A}\right] e^{-i2\pi n} ,$$

$$e^{i\beta} = \exp\left[i\oint_c \tilde{A}\right] .$$

With this understanding we can effectively drop the prime (choose a gauge) and write

$$\beta = \oint_c \tilde{A} . \quad (16)$$

The phase angle β is the standard geometric phase angle. Equation (16) expresses β as a line integral of the connection form $\tilde{A}$ over a closed path C in M (see Fig. 1).

III. THE DYNAMICAL PHASE

The time evolution of a state vector is given by the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle . \quad (17)$$

The path in the space of physical states M is represented by the operator

$$\pi(t) = |\psi(t)\rangle\langle\psi(t)| .$$

For cyclic evolution the path in M is closed,

$$\pi(T) = \pi(0) .$$

Now consider a second system which is related to the above by a unitary transformation,

$$|\tilde{\psi}(t)\rangle = U(t)|\psi(t)\rangle \ ,$$
$$i\frac{\partial}{\partial t}|\tilde{\psi}(t)\rangle = \tilde{H}(t)|\tilde{\psi}(t)\rangle \ , \tag{18}$$

where

$$\tilde{H}(t) = U(t)H(t)U^{-1}(t) + i\left[\frac{\partial}{\partial t}U(t)\right]U^{-1}(t) \ , \tag{19}$$

$$\tilde{\pi}(t) = U(t)\pi(t)U^{-1}(t) \ . \tag{20}$$

Equation (20) implies that the path in M can in general change under a unitary transformation. We wish to consider all systems which produce the same path in M. Namely, all transformations which satisfy

$$\tilde{\pi}(t) = \pi(t) \tag{21a}$$

or

$$[U(t), \pi(t)] = 0 \ . \tag{21b}$$

For cyclic evolution, the initial and final state vectors will differ by an overall phase which is defined as

$$|\psi(T)\rangle = e^{i\alpha_1}|\psi(0)\rangle$$

and for the second system as

$$|\tilde{\psi}(T)\rangle = e^{i\alpha_2}|\tilde{\psi}(0)\rangle \ .$$

We can express $|\psi(t)\rangle$ and $|\tilde{\psi}(t)\rangle$ in terms of a section $|\phi(t)\rangle$,

$$|\psi(t)\rangle = e^{if_1(t)}|\phi(t)\rangle \ , \tag{22a}$$

$$|\tilde{\psi}(t)\rangle = e^{if_2(t)}|\phi(t)\rangle \ , \tag{22b}$$

where $f_1(t)$ and $f_2(t)$ are real continuous functions of t which satisfy $f_1(T) - f_1(0) = \alpha_1$ and $f_2(T) - f_2(0) = \alpha_2$.

By substituting Eqs. (22a) and (22b) into Eqs. (17) and (18) we find[3]

$$\alpha_1 = i\int_0^T \langle\phi|\dot{\phi}\rangle dt - \int_0^T \langle\psi(t)|H(t)|\psi(t)\rangle dt \ , \tag{23a}$$

$$\alpha_2 = i\int_0^T \langle\phi|\dot{\phi}\rangle dt - \int_0^T \langle\tilde{\psi}(t)|\tilde{H}(t)|\tilde{\psi}(t)\rangle dt \ . \tag{23b}$$

The first term in Eq. (23a) is the same as the first term in Eq. (23b). We recognize this term as being β, the geometrical phase angle. Since the state vector $|\psi(t)\rangle$ was not horizontal, its total phase angle α_1 has an additional term which is called dynamical. The dynamical phase angle is the second term in Eq. (23a), and we see that it depends explicitly on the Hamiltonian. The second term in Eq. (23b) is the dynamical phase angle for system two. We see that the dynamical phase for system one is in general different from that of system two (see Fig. 2).

The transformation $U(t)$ represents a change in system [or effective Hamiltonian, Eq. (19)] which can alter the dynamical phase. The geometric phase does not change since the path in M does not change.

The transformation $U(t)$ can be used to eliminate the dynamical phase. This corresponds to transforming the state vectors $|\psi(t)\rangle$ into vectors $|\tilde{\psi}(t)\rangle$ which are horizontal [i.e., satisfy Eq. (12)]:

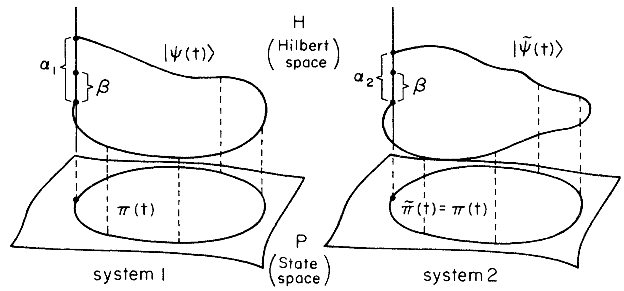

FIG. 2. System independence of the geometric phase β.

$$\langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle = -i\langle\tilde{\psi}(t)|\tilde{H}(t)|\tilde{\psi}(t)\rangle = 0 \ . \tag{24}$$

This equation means according to (19) that the transformation $U(t)$ must satisfy

$$\langle\psi(t)|H(t)|\psi(t)\rangle = i\left\langle\psi(t)\left|U^{-1}(t)\left[\frac{\partial U(t)}{\partial t}\right]\right|\psi(t)\right\rangle = 0 \ .$$

In addition, as the two systems are to produce the same path in M, $U(t)$ must satisfy Eq. (21b). It is straightforward to check that a solution to these two equations is

$$U(t) = \exp\left[i\int_0^t \langle\psi(t')|H(t')|\psi(t')\rangle dt'\right] \ .$$

According to Eq. (24), Eq. (23b) now becomes

$$\alpha_2 = \beta = i\int_0^T \langle\phi(t)|\dot{\phi}(t)\rangle dt \ .$$

IV. SUMMARY

We have seen that the equivalence of state vectors which differ by a phase, along with the scalar product, define the geometry of Hilbert space (i.e., the fiber bundle and connection). The geometry is nontrivial. It induces a U(1) holonomy in a normalized state vector which undergoes cyclic evolution. This induced phase is called the geometric phase. It depends only on the path in the space of physical states, not on the Hamiltonian which generates this path. The total phase accumulated by a state vector undergoing cyclic evolution consists of a geometrical phase and a dynamical phase. The dynamical phase is system dependent, it depends explicitly on the Hamiltonian.

We have expressed the geometric phase in terms of a connection form $\tilde{A}$. We note that for unitary evolution [where $H(t)$ is Hermitian] Eq. (24) yields

$$\mathrm{Re}\langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle = 0 \tag{25}$$

which implies that Eq. (8) can be written as

$$\tilde{A} = -\mathrm{Im}\langle\phi|d|\phi\rangle \tag{26}$$

where d is the exterior derivative with respect to the coordinates X^μ on M. The curvature two-form of M is

$$\tilde{F} = d\tilde{A} \ ,$$
$$\tilde{F} = -\mathrm{Im}(d\langle\phi|) \wedge (d|\phi\rangle) \ , \tag{27}$$

and by using Stokes's theorem we can express β as

$$\beta=\int_S \tilde{F} \tag{28}$$

where S is the two-dimensional surface enclosed by the path C in M. It can be shown directly from Eqs. (26) and (27) that $\tilde{A}$ and $\tilde{F}$ are the standard connection one-form and curvature two-form for a complex projective space[4] (coming from the natural Fubini-Study metric on complex projective space).

We note that for nonunitary evolution the holonomy is C^* (a nonzero complex constant) not U(1).[5] The connection is still given by the scalar product, Eq. (2). However, Eq. (25) no longer holds and the connection form $\tilde{A}$ has both real and imaginary parts. The real part of $\tilde{A}$ gives the phase holonomy and the imaginary part of $\tilde{A}$ gives the magnitude holonomy. A straightforward calculation shows

$$\begin{aligned} \tilde{A} &= i\frac{\langle\phi|(d|\phi\rangle)}{\langle\phi|\phi\rangle} , \\ |\tilde{\psi}(T)\rangle &= \exp\left[i\oint_c \tilde{A}\right]|\tilde{\psi}(0)\rangle , \\ \exp\left[\oint_c \tilde{A}\right] &= \exp\left[-\oint_c \mathrm{Re}\frac{\langle\phi|(d|\phi\rangle)}{\langle\phi|\phi\rangle}\right] \\ &\quad \times\exp\left[-i\oint_c \mathrm{Im}\frac{\langle\phi|(d|\phi\rangle)}{\langle\phi|\phi\rangle}\right] . \end{aligned} \tag{29}$$

In the limit of unitary evolution, we see that Eq. (29) goes into $e^{i\beta}$ with β given by Eq. (16) and $\tilde{A}$ given by Eq. (26).

V. HISTORICAL REMARKS

The appearance of a phase factor in addition to the usual dynamical phase factor for Hamiltonians that depend upon time has been well known since the early days of the adiabatic approximations. This phase factor was always omitted because it was believed that it could be absorbed into the state vector by a phase transformation. The Born-Oppenheimer procedure of molecular physics was based on this belief. That something may be wrong with this procedure was first noticed in 1963 as sign ambiguities of electronic wave functions.[6] Mead and Truhlar[7] showed that these problems could be solved by the introduction of a vector potential and called this the "molecular Bohm-Aharanov effect." Berry[8] independently derived the same formula for the vector potential, now called the Berry connection, considering a general quantum system undergoing adiabatic evolution. Simon[9] presented the geometrical aspects in terms of a connection on a line bundle. The generalization to nonadiabatic evolution was developed by Aharonov and Anandan,[3] and its geometrical picture advanced by Page.[4] More geometrical ideas were presented by Samuel and Bhandari[10] for noncyclic evolution, and non-Abelian generalizations were discussed by Wilczek and Zee[11] and Anandan.[12] A multitude of applications are collected in the reprint book by Shapere and Wilczek.[13]

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*On leave of absence from Departamento de Fisica Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain.

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