DERIVATION OF THE GEOMETRICAL BERRY PHASE

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I. Introduction

The state vector of a quantum system which undergoes cyclic evolution develops not only the usual dynamical phase but also a geometrical phase [1],[2]. Cyclic evolution means that the physical state of a quantum system returns to the same physical state after some time period T. Since state vectors which differ by a phase represent the same physical state, the final state vector can differ from the initial state vector by a phase. The dynamical part of the phase depends explicitly on the Hamiltonian. The geometrical part of the phase is produced by the non-trivial geometry of the space of physical states. This geometry can be described using the mathematical theory of fiber bundles [3],[4]. We will begin by describing the geometry of Hilbert space in terms of a fiber bundle. We will then introduce the geometrical ideas of a connection and horizontal lift, and see that the scalar product defines the connection. The resulting geometric phase will be expressed in terms of the connection one-form.

II. The Geometry of Hilbert Space

A state vector will be denoted by $\mid \psi(t)\rangle$ which is an element of a $N+1$ dimensional or infinite dimensional complex vector space denoted by $C^{N+1} - \{0\}$ or $\mathcal{H} - \{0\}$. This vector space is endowed with the usual scalar product or Hermitean metric. We want to consider normalized state vectors undergoing unitary evolution, namely all $\mid \psi\rangle$ such that $\langle\psi(t) \mid \psi(t)\rangle = 1$ for all time. Normalized state vectors are elements of the sphere S^{2N+1} or S^{∞}, which is a submanifold of $C^{N+1} - \{0\}$ or $\mathcal{H} - \{0\}$.

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

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 $\mid \psi(t)\rangle$ to the operator $\mid \psi(t)\rangle\langle\psi(t) \mid$ 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 $U(1)$ [4].

III. The Connection and Horizontal Lift

The geometry of the fiber bundle 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 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 with respect to a given connection defines the geometrical phase. The total phase can then be decomposed into a geometrical part and a remaining part called dynamical.

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 $\mid \dot{\phi}(t)\rangle$, the tangent vectors to the curve $\mid \phi(t)\rangle$ in E. These tangent vectors are in TE and can be decomposed into vertical and horizontal parts via the scalar product,

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

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

The horizontal component satisfies

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

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 $\mid \phi(t)\rangle$, and horizontal vectors are proportional to $\mid h_{\phi}(t)\rangle$.

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 $\mid \tilde{\psi}(t)\rangle$. By definition, the tangent vectors to the curve $\mid \tilde{\psi}(t)\rangle$ must be horizontal. From equation (1) this means

$$\langle\tilde{\psi}(t) \mid \dot{\tilde{\psi}}(t)\rangle = 0 \tag{3}$$

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

$$\mid \tilde{\psi}(t)\rangle = e^{if(t)} \mid \phi(t)\rangle \tag{4}$$

where $\mid \tilde{\psi}(T)\rangle = e^{i(f(T)-f(0))} \mid \tilde{\psi}(0)\rangle$ and $\mid \phi(T)\rangle = \mid \phi(0)\rangle$. The path $\mid \phi(t)\rangle$ represents a section which is a continuous mapping of a patch U on M into the region of E above U. A section maps a closed path in M onto a closed path in E. Choosing a different patch on M corresponds to choosing a different section or closed path in E. Different sections are related by the structure group,

$$\mid \phi'(t)\rangle = e^{i\theta(t)} \mid \phi(t)\rangle. \tag{5}$$

In order for $\mid \phi'(t)\rangle$ to be a closed path in E, $\theta(t)$ must satisfy $\theta(T) = \theta(0) + 2\pi n$ (n an integer). Equation (5) is called a gauge transformation.

Defining $\beta = f(T) - f(0)$, substituting equation (4) into (3) and integrating yields

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

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

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

where θ is the fiber coordinate and the X^{μ} are the coordinates of M. Contracting this equation with $i\langle\phi \mid$ from the left and integrating yields

$$\beta = i \int_0^T \dot{\theta}\langle\phi \mid \frac{\partial}{\partial\theta} \mid \phi\rangle dt + i \int_0^T \dot{X}^{\mu}\langle\phi \mid \frac{\partial}{\partial X^{\mu}} \mid \phi\rangle dt. \tag{6}$$

By considering a $U(1)$ action, it can be shown

$$\frac{\partial \mid \phi\rangle}{\partial\theta} = i \mid \phi\rangle. \tag{7}$$

Using equation (7) and $\langle \phi \mid \phi \rangle = 1$, equation (6) becomes

$$\beta = -\int_0^T \dot{\theta} dt + i \int_0^T \langle \phi \mid \frac{\partial}{\partial X^\mu} \mid \phi \rangle \dot{X}^\mu dt. \tag{8}$$

We define the connection form

$$\tilde{A} = i \langle \phi \mid \frac{\partial}{\partial X^\mu} \mid \phi \rangle dX^\mu. \tag{9}$$

Using equation (9), we can express the second term in equation (8) as

$$i \int_0^T \langle \phi \mid \frac{\partial}{\partial X^\mu} \mid \phi \rangle \dot{X}^\mu dt = \oint_c \tilde{A}.$$

The first integral in equation (8) 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. The holonomy (or geometric phase) $e^{i\beta}$ is independent of the choice of gauge

$$e^{i\beta} = e^{i \oint_c \tilde{A}} e^{-i2\pi n}$$
$$e^{i\beta} = e^{i \oint_c \tilde{A}}.$$

With this understanding we can choose a gauge and write

$$\beta = \oint_c \tilde{A}. \tag{10}$$

The phase angle β is the standard geometric phase angle. Equation (10) expresses β as a line integral of the connection form $\tilde{A}$ over a closed path C in M. We note that for unitary evolution $Re\langle \phi \mid \dot{\phi} \rangle = 0$ which implies that equation (9) can be written as

$$\tilde{A} = -Im \langle \phi \mid d \mid \phi \rangle$$

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

$$\tilde{F} = d\tilde{A}$$
$$\tilde{F} = -Im(d\langle \phi \mid) \wedge (d \mid \phi \rangle)$$

and by using Stoke's theorem we can express β as [5],[6]

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

where S is the two-dimensional surface enclosed by the path C in M.

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 non-trivial. 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.

Physical effects of non-trivial geometries appear in molecular physics [7]. These effects are described by the introduction of a vector potential (connection) into the molecular equations of motion [8]. The relative momenta coordinates $\vec{P}$ go into $\vec{P} - \vec{A}$. This change alters the canonical commutation relations [9], and may be of interest in a spectrum generating group approach [10].

References

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