The Quantum Phase *

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The geometrical nature of the quantum phase is introduced. This phase is shown to originate from the non-trivial geometry of the fiber bundle: Hilbert space → space of states. The analysis is performed working in the general non-adiabatic setting.

1. Introduction

The first evidence of the quantum phase was seen as early as 1963 when sign ambiguities were discovered in the electronic wavefunctions of molecules [1]. This effect was later described by introducing a vector potential into the Schrödinger equation for the slow nuclear motion [2], and was referred to as the "molecular Aharonov-Bohm" effect. It was not until 1984 when Berry wrote his paper considering a general quantum system undergoing adiabatic time evolution, that widespread popularity in the quantum phase occurred [3]. The geometry of the phase was immediately cast into the language of fiber bundles attracting many mathematical physicists [4]. Aharonov and Anandan considered the more general case of non-adiabatic time evolution in 1987 [5]. They showed that the quantum phase originates from the geometry of projective Hilbert space [6].

2. The Geometry of the Quantum Phase

We will denote state vectors by $|\psi(t)\rangle$ which are elements of an $N+1$ dimensional complex vector space, $|\psi(t)\rangle \in \mathscr{C}^{N+1}$. We have in mind a finite dimensional Hilbert space with dimension $N+1$. For the infinite dimensional case we can take the limit $N \to \infty$. The set of normalized state vectors is given by

$$S^{2N+1} \approx \{|\psi\rangle \in \mathscr{C}^{N+1} : \langle\psi|\psi\rangle = 1\}. \quad (1)$$

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We see that this set is in one-to-one correspondence with the $2N+1$ real dimensional sphere S^{2N+1} which is embedded in $\mathscr{C}^{N+1}$. Two normalized state vectors which differ by a phase represent the same physical state. Mathematically this statement is called an equivalence relation

$$|\psi\rangle' \sim |\psi\rangle$$

if

$$|\psi\rangle' = e^{i\theta}|\psi\rangle. \quad (2)$$

This equivalence relation induces equivalence classes on the space S^{2N+1}. The set of all such classes forms a subspace of S^{2N+1} which is given by

$$\mathscr{C}\mathscr{P}^N \approx \frac{S^{2N+1}}{U(1)}, \quad (3)$$

where $\mathscr{C}\mathscr{P}^N$ is the complex projective space of dimension N.

The above construction defines a principal fiber bundle over $\mathscr{C}\mathscr{P}^N$ with group $U(1)$ [7]. We will denote this bundle in the following way:

$$U(1) \to S^{2N+1} \to \mathscr{C}\mathscr{P}^N, \quad (4)$$

where $U(1)$ is the fiber (phase), S^{2N+1} the total space (normalized vectors), and $\mathscr{C}\mathscr{P}^N$ the base space (physical states). We can visualize a local neighborhood of $\mathscr{C}\mathscr{P}^N$, where at each point in this neighborhood a fiber is attached. We can then imagine extending this picture globally, twisting the fibers together in some complicated way to obtain the total bundle space.

The geometry of the bundle is determined by specifying a connection. Since the bundle we have constructed is imbedded in a complex vector space, a natural connection can be defined using the scalar product. At each point in the bundle there exists a tangent space. This tangent space can be decomposed

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into two subspaces; a vertical subspace and a horizontal subspace. The vertical subspace consists of all tangent vectors which are tangent to the fiber. The horizontal subspace is a matter of choice, and specifying this subspace defines the connection. The natural choice is to use the scalar product and choose the horizontal subspace to be orthogonal to the vertical subspace. To see this more explicitly, consider a curve $|\tilde{\psi}(t)\rangle$ in the bundle space S^{2N+1}. This curve projects down onto a curve in $\mathscr{C}\mathscr{P}^N$ which is given by the projection operator $\tilde{\pi}(t) = |\tilde{\psi}(t)\rangle\langle\tilde{\psi}(t)|$. The tangent vectors to $|\tilde{\psi}(t)\rangle$ are given by $|\dot{\tilde{\psi}}(t)\rangle$ and can be decomposed in the following way [8]:

$$|\dot{\tilde{\psi}}(t)\rangle = \langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle\rangle + |h_{\tilde{\psi}}(t)\rangle\,, \tag{5}$$

where $|h_{\tilde{\psi}}(t)\rangle$ satisfies

$$\langle\tilde{\psi}(t)|h_{\tilde{\psi}}(t)\rangle = 0\,. \tag{6}$$

Equation (5) is a standard orthogonal decomposition of the vector $|\dot{\tilde{\psi}}(t)\rangle$. The component proportional to $|\tilde{\psi}(t)\rangle$ is the vertical part, and the orthogonal component $|h_{\tilde{\psi}}(t)\rangle$ is the horizontal part. Recall that two normalized state vectors which differ by a phase belong to the same fiber. These two vectors point in the same direction. This direction is the fiber direction or vertical direction. Equation (6) defines horizontal vectors as being orthogonal to vertical vectors and represents the choice of a connection (horizontal subspace).

Now that a connection has been specified, we can define the notion of a horizontal lift. The horizontal lift is defined by lifting the tangent vectors to the curve $\tilde{\pi}(t)$ in $\mathscr{C}\mathscr{P}^N$ up along the fibers orienting them such that they are horizontal. We see from (5) that in order for $|\tilde{\psi}(t)\rangle$ to be a horizontal lift, the vertical part of $|\dot{\tilde{\psi}}(t)\rangle$ must vanish:

$$\langle\tilde{\psi}(t)|\dot{\tilde{\psi}}(t)\rangle = 0\,. \tag{7}$$

Equation (7) is called the horizontal lift equation or the equation for parallel transport.

We are now prepared to define the quantum phase. Consider a closed path in $\mathscr{C}\mathscr{P}^N$ denoted by $\mathscr{C}$. This closed path is given by the projection operator $\tilde{\pi}(t)$ where $\tilde{\pi}(0) = \tilde{\pi}(T)$. The horizontal lift $|\tilde{\psi}(t)\rangle$ of this closed path starts in the fiber above $\tilde{\pi}(0)$ and at time T returns to a *different* point in this same fiber. The difference between the initial and final horizontal lift vector is a phase

$$|\tilde{\psi}(T)\rangle = e^{i\beta}|\tilde{\psi}(0)\rangle\,. \tag{8}$$

The phase factor $e^{i\beta}$ is the quantum phase (or holonomy). An explicit expression for β can be found by introducing a local section. A local section maps a local neighborhood of $\mathscr{C}\mathscr{P}^N$ into the bundle space above this neighborhood. It therefore maps the closed path $\mathscr{C}$ onto a closed path in S^{2N+1}. The closed path in S^{2N+1} will be denoted by $|\phi(t)\rangle$ where $|\phi(0)\rangle = |\phi(T)\rangle$. We can express $|\tilde{\psi}(t)\rangle$ in terms of $|\phi(t)\rangle$:

$$|\tilde{\psi}(t)\rangle = e^{ig(t)}|\phi(t)\rangle\,, \tag{9}$$

where $g(t)$ is some real function of t. Substituting the expression of (9) into the horizontal lift equation (7) and integrating over the time period T, we find

$$\beta = g(T) - g(0) = i\int_0^T \langle\phi(t)|\dot{\phi}(t)\rangle\,\mathrm{d}t\,. \tag{10}$$

We can express β more geometrically by introducing coordinates x of the local neighborhood in $\mathscr{C}\mathscr{P}^N$, and defining a connection one-form A given by

$$A \equiv i\langle\phi(x)|\mathrm{d}|\phi(x)\rangle\,. \tag{11}$$

The operator d is the exterior derivative with respect to the coordinates x. The curvature two-form F is given by $F = \mathrm{d}A$. Using (11) in (10) and applying Stoke's theorem, we find

$$\beta = \oint_{\mathscr{C}} A = \int_{\mathscr{S}} F\,, \tag{12}$$

where $\mathscr{S}$ is the surface enclosed by the path $\mathscr{C}$. Equation (12) shows that the quantum phase originates from the curvature of projective Hilbert space.

The physical situation that we have in mind is an interference experiment. A typical example of such an experiment consists of a beam which at time $t = 0$ is split into two beams. One beam goes through an apparatus and the other beam goes around the apparatus. At time $t = T$ the beams are recombined and the interference pattern is observed. The state vector for the beam which goes through the apparatus will denoted by $|\psi(t)\rangle$. The physical state of this beam is given by $\pi(t) = |\psi(t)\rangle\langle\psi(t)|$. The Hamiltonian which represents the apparatus will be denoted by $H(t)$ and is chosen to produce cyclic evolution, $\pi(0) = \pi(T)$. The measured relative phase between the two beams is given by $|\psi(T)\rangle = e^{i\alpha}|\psi(0)\rangle$, which can be found by performing a similar analysis that led to (10). In place of (7) we have the equation

$$\langle\psi(t)|\dot{\psi}(t)\rangle = -i\langle\psi(t)|H(t)|\psi(t)\rangle\,, \tag{13}$$

which is obtained by contracting $\langle\psi(t)|$ with the Schrödinger equation for $|\psi(t)\rangle$. A straightforward calculation shows that [5]

$$\alpha = i\int_0^T \langle\phi(t)|\dot{\phi}(t)\rangle\,\mathrm{d}t - \int_0^T \langle\psi(t)|H(t)|\psi(t)\rangle\,\mathrm{d}t\,. \quad (14)$$

We recognize the first term on the r.h.s. of (14) as the quantum (or geometrical) phase. The second term depends explicitly on the Hamiltonian. This term is the dynamical (or energy) phase. Equation (14) shows that a general quantum mechanical system which undergoes cyclic time evolution acquires both a geometrical and dynamical phase.

In the past the geometrical phase was not properly taken into account. It was believed that this phase factor could be gauged away. However, from (12) it is clear that the geometrical phase can not be gauged away. Hence, the geometrical phase could lead to interesting physical effects in many time dependent quantum mechanical systems.

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