14

The Pancharatnam-Berry Phase: Theoretical and Experimental Aspects

Francisco De Zela
Departamento de Ciencias, Sección Física
Pontificia Universidad Católica del Perú, Apartado, Lima
Peru

1. Introduction

In 1984 Berry addressed a quantum system undergoing a unitary and cyclic evolution under the action of a time-dependent Hamiltonian (M. V. Berry, 1984). The process was supposed to be adiabatic, meaning that the time scale of the system's evolution was much shorter than the time scale of the changing Hamiltonian. Until Berry's study, it was assumed that for a cyclic Hamiltonian the quantum state would acquire only so-called dynamical phases, deprived of physical meaning. Such phases could be eliminated by redefining the quantum state through a "gauge" transformation of the form $|\psi\rangle \rightarrow e^{i\alpha} |\psi\rangle$. However, Berry discovered that besides the dynamical, there was an additional phase that could not be "gauged away" and whose origin was geometric or topological. It depended on the path that $|\psi\rangle$ describes in the parameter space spanned by those parameters to which the Hamiltonian owed its time dependence. Berry's discovery was the starting point for a great amount of investigations that brought to light topological aspects of both quantum and classical systems. Berry's phase was soon recognized as a special case of more general phases that showed up when dealing with topological aspects of different systems. For example, the Aharonov-Bohm phase could be understood as a geometric phase. The rotation angle acquired by a parallel-transported vector after completing a closed loop in a gravitationally curved space-time region, is also a geometric, Berry-like phase. Another example is the precession of the plane of oscillation of a Foucault pendulum.

Berry's original formulation was directly applicable to the case of a spin-1/2 system evolving under the action of a slowly varying magnetic field that undergoes cyclic changes. A spin-1/2 system is a special case of a two-level system. Another instances are two-level atoms and polarized light, so that also in these cases we should expect to find geometric phases. In fact, the first experimental test of Berry's phase was done using polarized, classical light (A. Tomita, 1986). Pancharatnam (S. Pancharatnam, 1956) anticipated Berry's phase when he proposed, back in 1956, how to decide whether two polarization states are "in phase". Pancharatnam's prescription is an operational one, based upon observing whether the intensity of the interferogram formed by two polarized beams has maximal intensity. In that case, the two polarized beams are said to be "in phase". Such a definition is analogous to the definition of distant parallelism in differential geometry. Polarized states can be subjected to different transformations which could be cyclic or not, adiabatic or not, unitary or not.

And in all cases Pancharatnam's definition applies. Pancharatnam's phase bore therefore an anticipation and – at the same time – a generalization of Berry's phase. Indeed, Berry's assumptions about a cyclic, adiabatic and unitary evolution, turned out to be unnecessary for a geometric phase to appear. This was made clear through the contributions of several authors that addressed the issue right after Berry published his seminal results (Y. Aharonov, 1987; J. Samuel, 1988).

Pancharatnam's approach, general as it was when viewed as pregnant of so many concepts related to geometric phases, underlay nonetheless two important restrictions. It addressed nonorthogonal and at the same time pure, viz totally, polarized states. Here again the assumed restrictions turned out to be unnecessary. Indeed, it was recently proposed how to decide whether two orthogonal states are in phase or not (H. M. Wong, 2005). Mixed states have also been addressed (A. Uhlmann, 1986; E. Sjöqvist, 2000) in relation to geometric phases which – under appropriate conditions – can be exhibited as well-defined objects underlying the evolution of such states.

The present Chapter should provide an overview of the Pancharatnam-Berry phase by introducing it first within Berry's original approach, and then through the kinematic approach that was advanced by Simon and Mukunda some years after Berry's discovery (N. Mukunda, 1993). The kinematic approach brings to the fore the most essential aspects of geometric phases, something that was not fully accomplished when Berry first addressed the issue. It also leads to a natural introduction of geodesics in Hilbert space, and helps to connect Pancharatnam's approach with the so-called Bargmann invariants. We discuss these issues in the present Chapter. Other topics that this Chapter addresses are interferometry and polarimetry, two ways of measuring geometric phases, and some recent generalizations of Berry's phase to mixed states and to non-unitary evolutions. Finally, we show in which sense the relativistic effect known as Thomas rotation can be understood as a manifestation of a Berry-like phase, amenable to be tested with partially polarized states. All this illustrates how – as it has often been the case in physics – a fundamental discovery that is made by addressing a particular issue, can show afterwards to bear a rather unexpected generality and applicability. Berry's discovery ranks among this kind of fundamental advances.

2. The adiabatic and cyclic case: Berry's approach

Let us consider a non-conservative system, whose evolution is ruled by a time-dependent Hamiltonian $H(t)$. This occurs when the system is under the influence of an environment. The configuration of the environment can generally be specified by a set of parameters $(R_1, R_2, \ldots)$. For a changing environment the R_i are time-dependent, and so also the observables of the system, e.g., the Hamiltonian: $H(R(t)) \equiv H(R_1(t), R_2(t), \ldots) = H(t)$. The evolution of the quantum system is ruled by the Schrödinger equation, or more generally, by the Liouville-von Neumann equation (in units of $\hbar = 1$):

$$i\frac{d\rho(t)}{dt} = [H(R(t)), \rho(t)] \,. \tag{1}$$

Here, the density operator ρ is assumed to describe a pure state, i.e., to be of the form $\rho(t) = |\psi(t)\rangle \langle\psi(t)|$. An "environmental process" is given by $t \to R(t)$, the curve described by the vector R in parameter space. To such a process it corresponds a curve described by $|\psi(t)\rangle$ in the Hilbert space $\mathcal{H}$ to which it belongs, or by the corresponding curve $\rho(t) = |\psi(t)\rangle \langle\psi(t)|$

in the "projection space" $\mathcal{P}(\mathcal{H})$ to which ρ belongs. We will assume that for all R there is an orthonormal basis $|n;R\rangle$ such that

$$H(R)\,|n;R\rangle = E_n(R)\,|n;R\rangle\,. \tag{2}$$

An environmental process $R(t)$ is called periodic with period T, whenever $R(T) = R(0)$, $E_n(R(T)) = E_n(R(0))$, and $|n;R(T)\rangle\,\langle n;R(T)| = |n;R(0)\rangle\,\langle n;R(0)|$. Of course, we can change the eigenbasis according to $|n;R\rangle \rightarrow |n;R\rangle' = e^{i\alpha_n(R)}\,|n;R\rangle$, which is called a gauge transformation. When the adiabatic approximation was first studied, people assumed that it would be always possible to get rid of phase factors by simply performing a gauge transformation, if necessary (A. Bohm, 2003). Berry's discovery made clear that this is not always the case. The point is that we are not always totally free to choose the required phase factors when performing gauge transformations. Let us see why it is so. To this end, we consider first two simple cases in which phase factors appear that can be eliminated. A first case is a conservative system ($\partial H/\partial t = 0$). The initial condition $|\psi(0)\rangle = |n;R\rangle$ leads to $|\psi(t)\rangle = \exp(-iE_n t)\,|n;R\rangle$. In this case the phase factor can be gauged away. A second case is a non-conservative system whose Hamiltonian is such that $[H(t), H(t')] = 0$ for all t and t'. In this case $|\psi(t)\rangle = \exp(-i\int_0^t dt' E_n(t'))\,|n;R(0)\rangle$ and the phase factor can again be gauged away. Now, if $[H(t), H(t')] \neq 0$ the evolution is given by $|\psi(t)\rangle = \mathcal{T}\left[\exp(-i\int_0^t dt' E_n(t'))\right]|n;R(0)\rangle$, where $\mathcal{T}$ means the time-ordering operator. In this case, the phase-factor cannot generally be gauged away. To see why is this the case, let us first restrict ourselves to a slowly evolving Hamiltonian and to an *approximate* solution of Eq.(1), the so-called adiabatic approximation:

$$\rho(t) = |\psi(t)\rangle\,\langle\psi(t)| \approx |n;R(t)\rangle\,\langle n;R(t)|\,. \tag{3}$$

When $R(t)$ describes a closed path ($R(T) = R(0)$) so also does $\rho(t)$ under the adiabatic approximation, because the eigenprojectors are single-valued: $|\psi(T)\rangle\,\langle\psi(T)| \approx |n;R(T)\rangle\,\langle n;R(T)| = |n;R(0)\rangle\,\langle n;R(0)|$. However, the state $|\psi(t)\rangle$ may acquire a phase. Note that $|\psi(t)\rangle\,\langle\psi(t)| \approx |n;R(t)\rangle\,\langle n;R(t)|$ cannot be upgraded to an equality. This follows from observing that $H(R(t))$ and $|n;R(t)\rangle\,\langle n;R(t)|$ commute, so that for $|\psi(t)\rangle\,\langle\psi(t)| = |n;R(t)\rangle\,\langle n;R(t)|$ to satisfy Eq.(1), it must be stationary. Let us see under which conditions the adiabatic approximation applies. Writing $|\psi(t)\rangle = \sum_k c_k(t)\,|k;R(t)\rangle$, the adiabatic approximation means that $|\psi(t)\rangle \approx c_n(t)\,|n;R(t)\rangle$, with $c_n(0) = 1$, because $|\psi(0)\rangle = |n;R(0)\rangle$. By replacing such a $|\psi(t)\rangle$ in the Schrödinger equation one easily obtains the necessary and sufficient conditions for the validity of the adiabatic approximation (A. Bohm, 2003):

$$\frac{dc_n}{dt}\,|n;R(t)\rangle \approx -c_n\left[iE_n(t)\,|n;R(t)\rangle + \frac{d}{dt}\,|n;R(t)\rangle\right]. \tag{4}$$

Multiplying this equation by $\langle k;R(t)|$ it follows that

$$\langle k;R(t)|\,\frac{d}{dt}\,|n;R(t)\rangle \approx 0, \quad \text{for all } k \neq n. \tag{5}$$

By deriving Eq.(2) with respect to t this condition can be brought, after some calculations, to the form

$$\frac{\langle k; R(t)|\, dH(t)/dt\, |n; R(t)\rangle}{E_n(R) - E_k(R)} \approx 0, \quad \text{for all } k \neq n. \tag{6}$$

Hence, the energy differences $E_n(R) - E_k(R)$ – or correspondingly, the transition frequencies of the evolving system – set the time scale for which the variation of $H(t)$ can be considered "adiabatic", and $|\psi(t)\rangle \approx c_n(t)\,|n; R(t)\rangle$ a valid approximation. Next, we multiply Eq.(4) by $\langle n; R(t)|$ and obtain

$$\frac{dc_n}{dt} = -c_n \left[iE_n(t) + \langle n; R(t)|\, \frac{d}{dt}\, |n; R(t)\rangle \right], \tag{7}$$

whose solution is

$$c_n(t) = \exp\left[-i \int_0^t E_n(s) ds \right] \exp\left[-\int_0^t \langle n; R(s)|\, \frac{d}{ds}\, |n; R(s)\rangle\, ds \right] \equiv \exp\left(-i\Phi_{dyn}(t) \right) \exp\left(i\gamma_n(t) \right). \tag{8}$$

Here,

$$\gamma_n(t) = i \int_0^t \langle n; R(s)|\, \frac{d}{ds}\, |n; R(s)\rangle\, ds \tag{9}$$

is the geometric phase, which is defined modulo 2π. We see that it appears as an additional phase besides the dynamical phase Φ_{dyn}. We have thus,

$$|\psi(t)\rangle \approx c_n(t)\,|n; R(t)\rangle = \exp\left(-i\Phi_{dyn}(t) \right) \exp\left(i\gamma_n(t) \right) |n; R(t)\rangle. \tag{10}$$

The geometric phase γ_n can also be written in the following way, to make clear that it does not depend on the parameter s:

$$\gamma_n(t) = i \int_{R(0)}^{R(t)} \langle n; R|\, \frac{\partial}{\partial R_k}\, |n; R\rangle\, dR_k \equiv \int_{R(0)}^{R(t)} \mathbf{A}^{(n)} \cdot d\mathbf{R}. \tag{11}$$

The vector potential $\mathbf{A}^{(n)} \equiv i\,\langle n; R|\, \nabla\, |n; R\rangle$ is known as the *Mead-Berry vector potential*. Eq.(11) makes clear that γ_n depends only on the path defining the environmental process, i.e., the path joining the points $R(0)$ and $R(t)$ in parameter space. This highlights the geometrical nature of γ_n. Now, one can straightforwardly prove that a gauge transformation $|n; R\rangle \to |n; R\rangle' = e^{i\alpha_n(R)}\,|n; R\rangle$ causes the vector potential to change according to

$$\mathbf{A}^{(n)} \to \mathbf{A}'^{(n)} = \mathbf{A}^{(n)} - \nabla\alpha_n(R). \tag{12}$$

As a consequence, the geometric phase transforms as

$$\gamma_n(t) \to \gamma_n'(t) = \gamma_n(t) - \left[\alpha_n(R(t)) - \alpha_n(R(0)) \right]. \tag{13}$$

At first sight, gauge freedom seems to be an appropriate tool for removing the additional phase factor $\exp(i\gamma_n)$ in Eq.(10). Indeed, we can repeat the calculations leading to Eq.(10) but now using $|n; R\rangle' = e^{i\alpha_n(R)}\,|n; R\rangle$ instead of $|n; R\rangle$. We thus obtain an equation like Eq.(10) but with primed quantities. We could then choose $\alpha_n(R(t)) = -\gamma_n'(t)$ (modulo 2π) and so obtain

$$|\psi(t)\rangle \approx \exp\left(i\Phi_{dyn}(t) \right) |n; R(t)\rangle. \tag{14}$$

This is what V. Fock made when addressing adiabatic quantal evolutions (A. Bohm, 2003), thereby exploiting the apparent freedom one has for choosing $\alpha_n(R)$ when defining the eigenvectors $|n;R\rangle' = e^{i\alpha_n(R)}|n;R\rangle$. However, when the path C is closed, a restriction appears that limits our possible choices of phase factors. This follows from the fact that $R(T) = R(0)$ implies that $|n;R(T)\rangle = |n;R(0)\rangle$, because eigenvectors are single-valued (something we can always assume when a single patch is needed for covering our whole parameter space; otherwise, trivial phase factors are required). The eigenvectors $|n;R\rangle'$ are also single-valued, so that $|n;R(T)\rangle' = e^{i\alpha_n(R(T))}|n;R(T)\rangle = e^{i\alpha_n(R(0))}|n;R(0)\rangle = |n;R(0)\rangle' = e^{i\alpha_n(R(0))}|n;R(T)\rangle$. We have thus the restriction $\exp(i\alpha_n(T)) = \exp(i\alpha_n(0))$, which translates into $\alpha_n(T) = \alpha_n(0) + 2\pi m$, with m integer. Hence, because of Eq.(13),

$$\gamma_n(T) \longrightarrow \gamma_n'(T) = \gamma_n(T) - 2\pi m, \tag{15}$$

and we conclude that $\gamma_n(T)$ is *invariant*, modulo 2π, under gauge transformations. Thus, it cannot be gauged away, as initially expected. According to Eq.(11) γ_n is independent of the curve parameter (t), so that we should write $\gamma_n(C)$ instead of $\gamma_n(T)$. We have, finally,

$$|\psi(T)\rangle = \exp\left(-i\Phi_{dyn}(T)\right)\exp\left(i\gamma_n(C)\right)|\psi(0)\rangle\,, \tag{16}$$

with

$$\Phi_{dyn}(T) = \int_0^T E_n(t)dt, \tag{17}$$

$$\gamma_n(C) = \oint_C \mathbf{A}^{(n)} \cdot d\mathbf{R}. \tag{18}$$

This is Berry's result (M. V. Berry, 1984). The vector potential $\mathbf{A}^{(n)}$ behaves very much like an electromagnetic potential. The phase factors $\exp(i\alpha_n(R))$ belong to the group $U(1)$, hence the name "gauge transformations" given to the transformations $|n;R\rangle \to |n;R\rangle' = e^{i\alpha_n(R)}|n;R\rangle$. As in electromagnetism, we can also here introduce a field tensor $\mathbf{F}^{(n)}$ whose components are

$$F_{ij}^{(n)} = \frac{\partial}{\partial R_i}A_j^{(n)} - \frac{\partial}{\partial R_j}A_i^{(n)}. \tag{19}$$

Geometrically, $\mathbf{F}^{(n)}$ has the meaning of a "curvature". In differential geometry, where the language of differential forms is used, $\mathbf{A}^{(n)}$ is represented by a one-form, and $\mathbf{F}^{(n)}$ by a two-form. When the parameter space is three-dimensional, Eq.(19) can be written as

$$\mathbf{F}^{(n)} = \nabla \times \mathbf{A}^{(n)}. \tag{20}$$

Eq.(18) can then be written as

$$\gamma_n(C) = \int_S \mathbf{F}^{(n)} \cdot d\mathbf{S}, \tag{21}$$

with the surface element $d\mathbf{S}$ directed normally to the surface S, whose boundary is the curve C.

A paradigmatic case corresponds to a spin-1/2 subjected to a variable magnetic field $\mathbf{B}(t)=B\mathbf{n}(t)$, with $\mathbf{n}(t).\mathbf{n}(t) = 1$, see Fig.(1). The time-dependent Hamiltonian is then

$H(t) = -B(e/2mc)\mathbf{n}(t) \cdot \vec{\sigma}$, with $\vec{\sigma}$ the triple of Pauli matrices. The parameter space has the topology of the unit sphere S^2. It is not possible to assign coordinates to all point in S^2 with a single patch. One needs at least two of them, which requires introducing two vector potentials, one for each patch. They are related to one another by a gauge transformation, i.e., their difference is a gradient. The corresponding curvature three-vector $\mathbf{F} = \nabla \times \mathbf{A}$ is given by $\mathbf{F} = -\mathbf{e}_r/2r^2$, with $\mathbf{e}_r$ the unit radial vector. We note in passing that $\mathbf{F} = -\mathbf{e}_r/2r^2$ looks like a Coulomb field, while $\mathbf{F} = \nabla \times \mathbf{A}$ looks like a magnetic field. This hints at a formal connection between Berry's phase and Dirac's magnetic monopoles. In this case, $\gamma_n(C) = \int_S \mathbf{F} \cdot d\mathbf{S} = \int_S F_r r^2 \sin\theta d\theta d\varphi = -\int_S d\Omega/2$, so that

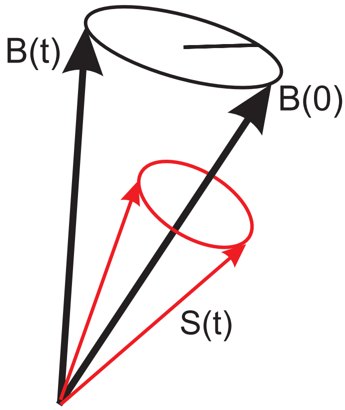


Fig. 1. A spin-1/2 subjected to a variable magnetic field $\mathbf{B}(t)$ that describes a closed trajectory. When the field changes slowly in the time scale of the spin dynamics, then the spin $\mathbf{S}$ can follow the field adiabatically. After a period, the spin state has accumulated a geometric phase in addition to the dynamical one.

$$\gamma_n(C) = -\Omega(C)/2, \tag{22}$$

$\Omega(C)$ being the solid angle enclosed by C. This important result can be generalized to arbitrary dimensions, as we shall see below.

We have introduced Berry's phase by considering a unitary, cyclic and adiabatic evolution. This was Berry's original approach. It was generalized to the non-adiabatic case by Aharonov and Anandan (Y. Aharonov, 1987), as already said, and by Samuel and Bhandari (J. Samuel, 1988) to the noncyclic case. A purely kinematic approach showed that it is unnecessary to invoke unitarity of the evolution. Such an approach was developed by Mukunda and Simon (N. Mukunda, 1993) and is the subject of the next Section.

3. The kinematic approach: total, geometric, and dynamical phases

Let us start by considering a Hilbert space $\mathcal{H}$. We define $\mathcal{H}_0 \subset \mathcal{H}$ as the set of normalized, nonzero vectors $|\psi\rangle \in \mathcal{H}$. A curve C_0 in $\mathcal{H}_0$ is defined through vectors $|\psi(s)\rangle$ that continuously depend on some parameter $s \in [s_1, s_2]$. Because $|\psi(s)\rangle$ is normalized, $\langle\psi(s)|\dot{\psi}(s)\rangle + \langle\dot{\psi}(s)|\psi(s)\rangle = 0$. Then, $Re\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, and

$$\langle\psi(s)|\dot{\psi}(s)\rangle = iIm\langle\psi(s)|\dot{\psi}(s)\rangle. \tag{23}$$

Now, consider the initial $|\psi(s_1)\rangle$ and the end point $|\psi(s_2)\rangle$ of $\mathcal{C}_0$. Following Pancharatnam, we define the total phase between these states as $\Phi_{tot}(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle$. Under a gauge transformation $|\psi(s)\rangle \rightarrow |\psi'(s)\rangle = \exp(i\alpha(s))\,|\psi(s)\rangle$, we have that $\mathcal{C}_0 \rightarrow \mathcal{C}_0'$, $\Phi_{tot}(\mathcal{C}_0) \rightarrow \Phi'_{tot}(\mathcal{C}_0) = \Phi_{tot}(\mathcal{C}_0) + \alpha(s_2) - \alpha(s_1)$ and $Im\langle\psi(s)|\dot{\psi}(s)\rangle \rightarrow Im\langle\psi'(s)|\dot{\psi}'(s)\rangle = Im\langle\psi(s)|\dot{\psi}(s)\rangle + \dot{\alpha}(s)$. From these properties it is easy to see that we can construct the following quantity, the "geometric phase", which is gauge-invariant:

$$\Phi_g(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle - Im\int_{s_1}^{s_2}\langle\psi(s)|\dot{\psi}(s)\rangle ds. \tag{24}$$

Besides being re-parametrization invariant, $\Phi_g(\mathcal{C}_0)$ is, most importantly, also gauge invariant. This means that despite being defined in terms of $|\psi(s)\rangle$ and $\mathcal{C}_0$, Φ_g effectively depends on equivalence classes of $|\psi(s)\rangle$ and $\mathcal{C}_0$, respectively. Indeed, the set $\{|\psi'\rangle = \exp(i\alpha)\,|\psi\rangle\}$ constitutes an equivalence class. The space spanned by such equivalence classes is called the "ray space" $\mathcal{R}_0$. Instead of working with equivalence classes we can work with projectors: $|\psi\rangle\langle\psi|$. The set $\{|\psi'\rangle = \exp(i\alpha)\,|\psi\rangle\}$ projects onto the object $|\psi\rangle\langle\psi|$ by means of a projection map $\pi : \mathcal{H}_0 \rightarrow \mathcal{R}_0$. In particular, the curves $\mathcal{C}_0$, $\mathcal{C}_0'$ which are interrelated by a gauge transformation, are also members of an equivalence class. Under π, they project onto a curve $C_0 \subset \mathcal{R}_0$. What we have seen above is that Φ_g is in fact a functional not of $\mathcal{C}_0$, but of C_0, the curve defined by $|\psi(s)\rangle\langle\psi(s)|$. This is the reason why we call Φ_g the "geometric phase" associated with the curve $C_0 \subset \mathcal{R}_0$. We should then better write $\Phi_g(C_0)$, though its actual calculation requires that we choose what is called a "lift" of C_0; that is, any curve $\mathcal{C}_0$ such that $\pi(\mathcal{C}_0) = C_0$. Thus, $\Phi_g(C_0)$ is defined in terms of two phases, see Eq.(24):

$$\Phi_{tot}(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle, \tag{25}$$

$$\Phi_{dyn}(\mathcal{C}_0) = Im\int_{s_1}^{s_2}\langle\psi(s)|\dot{\psi}(s)\rangle ds. \tag{26}$$

$\Phi_{tot}(\mathcal{C}_0)$ is, as already said, the *total* or the Pancharatnam phase of $\mathcal{C}_0$. It is the argument α of the complex number $\langle\psi(s_1)|\psi(s_2)\rangle = |\langle\psi(s_1)|\psi(s_2)\rangle|\,e^{i\alpha}$. Later on, we will discuss the physical meaning of this phase in the context of polarized states, the case addressed by Pancharatnam. $\Phi_{dyn}(\mathcal{C}_0)$ is the *dynamical phase* of $\mathcal{C}_0$. We see that even though both $\Phi_{tot}(\mathcal{C}_0)$ and $\Phi_{dyn}(\mathcal{C}_0)$ are functionals of $\mathcal{C}_0$, their difference Φ_g is a functional of $C_0 = \pi(\mathcal{C}_0)$:

$$\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0) - \Phi_{dyn}(\mathcal{C}_0). \tag{27}$$

Let us stress that this definition of the geometric phase does not rest on the assumptions originally made by Berry. $\Phi_g(C_0)$ has been introduced in terms of a given evolution of state vectors $|\psi(s)\rangle$. This evolution does not need to be unitary, nor adiabatic. Furthermore, the path $\mathcal{C}_0$ could be open: no cyclic property is invoked. Given a $C_0 \subset \mathcal{R}_0$, we may choose different lifts to calculate $\Phi_g(C_0)$ and exploit this freedom to express $\Phi_g(C_0)$ according to our needs. For example, we can always make $\Phi_{tot}(\mathcal{C}_0) = 0$, by properly choosing the phase of, say, $|\psi(s_2)\rangle$. In that case, $\Phi_g(C_0) = -\Phi_{dyn}(\mathcal{C}_0)$. Alternatively, we can make $\Phi_{dyn}(\mathcal{C}_0) = 0$, so that $\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0)$, by choosing a so-called "*horizontal lift*", one which satisfies

$Im\langle\psi(s)|\dot{\psi}(s)\rangle = 0$. Because $Re\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, in this case $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$. In order to obtain a horizontal lift we can submit, if necessary, any lift $|\psi(s)\rangle$ to a gauge transformation: $|\psi(s)\rangle \to |\psi'(s)\rangle = \exp(i\alpha(s))\,|\psi(s)\rangle$, so that $Im\langle\psi(s)|\dot{\psi}(s)\rangle \to Im\langle\psi'(s)|\dot{\psi}'(s)\rangle = Im\langle\psi(s)|\dot{\psi}(s)\rangle + \dot{\alpha}(s)$. We then require $Im\langle\psi'(s)|\dot{\psi}'(s)\rangle = 0$, which yields

$$\alpha(s) = -Im\int_{s_1}^{s}\langle\psi(s)|\dot{\psi}(s)\rangle ds, \tag{28}$$

assuming $\alpha(s_1) = 0$, i.e., fixing $|\psi'(s_1)\rangle = |\psi(s_1)\rangle$ by proper choice of the initial phase.
As $\Phi_g(C_0)$ depends only on ray-space quantities, it should be possible to get an expression reflecting this fact. Such an expression can be obtained by considering the operator $K(s) = \dot{\rho}(s) = d(|\psi(s)\rangle\langle\psi(s)|)/ds$, whose action on $|\psi(s)\rangle$ gives

$$K(s)|\psi(s)\rangle = |\dot{\psi}(s)\rangle - \langle\psi(s)|\dot{\psi}(s)\rangle|\psi(s)\rangle. \tag{29}$$

$K(s)$ is obviously gauge invariant; hence, Eq.(29) holds also for gauge-transformed quantities. By choosing a horizontal lift, $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, Eq.(29) reads

$$\frac{d}{ds}|\psi(s)\rangle = \dot{\rho}(s)|\psi(s)\rangle. \tag{30}$$

The solution of Eq.(30) can be formally given as a Dyson series: $|\psi(s)\rangle = P\left(\exp\int_{s_1}^{s}\dot{\rho}(s)ds\right)|\psi(s_1)\rangle$, with P the "parameter-ordering" operator: it rearranges a product of parameter-labelled operators according to, e. g., $P\left(\dot{\rho}(s_1)\dot{\rho}(s_2)\dot{\rho}(s_3)\right) = \dot{\rho}(s_3)\dot{\rho}(s_2)\dot{\rho}(s_1)$, for $s_3 \geq s_2 \geq s_1$. Having a horizontal lift, the geometric phase reduces to $\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle$. Now, $\langle\psi(s_1)|\psi(s_2)\rangle = Tr\,|\psi(s_2)\rangle\langle\psi(s_1)|$, so that setting $|\psi(s_2)\rangle = P\left(\exp\int_{s_1}^{s_2}\dot{\rho}(s)ds\right)|\psi(s_1)\rangle$ we have

$$\Phi_g(C_0) = \arg Tr\left\{P\left(\exp\int_{s_1}^{s_2}\dot{\rho}(s)ds\right)\rho(s_1)\right\}. \tag{31}$$

Eq.(31) gives the desired expression of $\Phi_g(C_0)$ in terms of ray-space quantities. C_0 is any smooth curve in ray space. If C_0 is closed, $\rho(s_2) = \rho(s_1)$, and $|\psi(s_2)\rangle$ must be equal to $|\psi(s_1)\rangle$ up to a phase factor: $|\psi(s_2)\rangle = e^{i\alpha}\,|\psi(s_1)\rangle$, with $\alpha = \arg\langle\psi(s_2)|\psi(s_1)\rangle$. For the horizontal lift we are considering, $\alpha = \arg\langle\psi(s_2)|\psi(s_1)\rangle = \Phi_g(C_0)$, and we can thus write

$$|\psi(s_2)\rangle = P\left(\exp\int_{s_1}^{s_2}\dot{\rho}(s)ds\right)|\psi(s_1)\rangle = \exp\left(i\Phi_g(C_0)\right)|\psi(s_1)\rangle, \tag{32}$$

in accordance with our previous results.

3.1 Geodesics

We introduce now the concept of geodesics in both Hilbert-space and ray-space, with the help of Eq.(29). Notice that $K(s)\,|\psi(s)\rangle$ is orthogonal to $|\psi(s)\rangle$, that is, $\langle\psi(s)|\,K(s)\,|\psi(s)\rangle = 0$. In general, $\langle\psi(s)|\dot{\psi}(s)\rangle \neq 0$; i.e., the curve $\mathcal{C}_0 = \{|\psi(s)\rangle\}$ has a tangent vector $|\dot{\psi}(s)\rangle$ which is generally not orthogonal to $\mathcal{C}_0$. By letting $K(s)$ act on $|\psi(s)\rangle$ we get the component of $|\dot{\psi}(s)\rangle$ that is orthogonal to the curve. Such a component is obtained from $|\dot{\psi}(s)\rangle$ by subtracting its projection on $|\psi(s)\rangle$, i.e., we construct $|\dot{\psi}(s)\rangle - |\psi(s)\rangle\langle\psi(s)|\dot{\psi}(s)\rangle$. Let us denote this component by $|\dot{\psi}(s)\rangle_\perp = K(s)|\psi(s)\rangle$. Under a gauge transformation, $|\psi(s)\rangle \to |\psi'(s)\rangle = \exp(i\alpha(s))\,|\psi(s)\rangle$ and because $K'(s) = K(s)$, it follows $|\dot{\psi}'(s)\rangle_\perp = \exp(i\alpha(s))\,|\dot{\psi}(s)\rangle_\perp$. The modulus of $|\dot{\psi}(s)\rangle_{\perp}$ is the quantity in terms of which we can define the "length" of a curve. To make our definition parameter invariant, we take the square root of said modulus and define the length of C_0 as

$$\mathcal{L}(C_0) = \int_{s_1}^{s_2} \sqrt{{}_{\perp}\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle_{\perp}}ds. \tag{33}$$

Geodesics are defined as curves making $\mathcal{L}(C_0)$ extremal. By applying the tools of variational calculus one obtains (N. Mukunda, 1993)

$$\left(\frac{d}{ds} - \langle\psi(s)|\dot{\psi}(s)\rangle\right) \frac{|\dot{\psi}(s)\rangle_{\perp}}{\sqrt{{}_{\perp}\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle_{\perp}}} = f(s)|\psi(s)\rangle, \tag{34}$$

with $f(s)$ an arbitrary, real function. Although Eq.(34) depends on the lifted curve $\mathcal{C}_0$, it must be gauge and re-parametrization invariant, because it follows from Eq.(33). We may therefore change both the lift and the parametrization in Eq.(34). We choose a horizontal lift: $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, which implies that $|\dot{\psi}(s)\rangle_{\perp} = |\dot{\psi}(s)\rangle$. Furthermore, because of re-parametrization freedom we may take s such that $\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle$ is constant along $\mathcal{C}_0$. This fixes s up to linear inhomogeneous changes, i.e., up to affine transformations. Then, Eq.(34) reads

$$\frac{d^2}{ds^2}|\psi(s)\rangle = \sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle} f(s)|\psi(s)\rangle. \tag{35}$$

Now, by deriving twice the equation $\langle\psi(s)|\psi(s)\rangle = 1$, we obtain $\sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle} f(s) + \langle\dot{\psi}(s)|\dot{\psi}(s)\rangle = 0$, which fixes $f(s)$ to

$$f(s) = -\sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle}. \tag{36}$$

Thus, Eq.(35) reads finally

$$\frac{d^2}{ds^2}|\psi(s)\rangle = -\omega^2|\psi(s)\rangle, \tag{37}$$

with $\omega^2 \equiv \langle\dot{\psi}(0)|\dot{\psi}(0)\rangle$. This equation holds for geodesics that are horizontal lifts from the geodesic C_0 in ray space, and with s rendering $\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle$ constant. Eq.(37) is thus of second order and its general solution depends on two vectors. It can be solved, e.g., for the initial conditions $|\psi(0)\rangle = |\phi_1\rangle$ and $|\dot{\psi}(0)\rangle = \omega|\phi_2\rangle$, i.e., $\langle\phi_1|\phi_1\rangle = 1$, $\langle\phi_1|\phi_2\rangle = 0$, and $\langle\phi_2|\phi_2\rangle = 1$. The solution reads

$$|\psi(s)\rangle = \cos(\omega s)\,|\phi_1\rangle + \sin(\omega s)\,|\phi_2\rangle. \tag{38}$$

We see that $\langle\psi(0)|\psi(s)\rangle = \langle\phi_1|\psi(s)\rangle = \cos(\omega s)$. Because s has been fixed only up to an affine transformation, we can generally choose it such that $\cos(\omega s) \geq 0$ for $s \in [s_1, s_2]$, so that $\arg\langle\psi(0)|\psi(s)\rangle = 0$. But because our lift is horizontal, $\Phi_g(C_0) = \arg\langle\psi(0)|\psi(s)\rangle$, so that

$$\Phi_g(C_0) = 0 \quad \text{for a geodesic } C_0. \tag{39}$$

Eq.(38) shows that geodesics are arcs of circles in a space with orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle\}$. We are thus effectively dealing with a two-level system. The geodesic $|\psi(s)\rangle$ of Eq.(38) projects onto a geodesic in ray-space $\rho(s) = |\psi(s)\rangle\langle\psi(s)|$. Last one can be mapped onto the unit sphere in a well-known manner. Indeed, for a two-level system, $\rho(s)$ has the form

$$\rho(s) = \frac{1}{2}\left(I + \overrightarrow{n}(s)\cdot\overrightarrow{\sigma}\right), \tag{40}$$

with I the identity matrix and $\overrightarrow{n} = Tr(\rho\overrightarrow{\sigma})$. Now, any two unit vectors, $|\psi_1\rangle$ and $|\psi_2\rangle$, can always be connected by a geodesic. To show this, we need only note that for any two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ there are two corresponding vectors $\overrightarrow{n}_1$ and $\overrightarrow{n}_2$ on the unit sphere. These points can be joined by the shortest of the two arcs conforming a great circle. This is the geodesic arc joining ρ_1 and ρ_2 that can be lifted to a geodesic arc joining $|\psi_1\rangle$ and $|\psi_2\rangle$. If necessary, we can submit this curve to a gauge transformation, thereby generally destroying its horizontal but not its geodesic property. Let us discuss this procedure in more detail. Consider two nonparallel vectors $|\psi_1\rangle$, $|\psi_2'\rangle$. They span a two-dimensional subspace in which we can consider an orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle\}$. For example, $|\phi_1\rangle = |\psi_1\rangle$ and $|\phi_2\rangle = \left(|\psi_2'\rangle - |\phi_1\rangle\langle\phi_1|\psi_2'\rangle\right)/\sqrt{1-|\langle\phi_1|\psi_2'\rangle|^2}$. In such a basis, we can express $|\psi_2'\rangle$ in the form $|\psi_2'\rangle = e^{i\alpha}|\psi_2\rangle \equiv e^{i\alpha}\left[\cos(\theta/2)|\phi_1\rangle + e^{i\varphi}\sin(\theta/2)|\phi_2\rangle\right]$. We start by considering first the case in which the initial and final vectors are $|\phi_1\rangle = |\psi_1\rangle$ and $|\psi_2\rangle$, respectively. Thereafter, we deal with the more general case: $|\psi_2'\rangle = e^{i\alpha}|\psi_2\rangle$. The corresponding projectors $\rho_1 = |\psi_1\rangle\langle\psi_1|$ and $\rho_2 = |\psi_2\rangle\langle\psi_2|$ are given by expressions of the form of Eq.(40) with $\overrightarrow{n}_1 = (0,0,1)$ and $\overrightarrow{n}_2 = (\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$. That is, $\overrightarrow{n}_1$ is the North pole (of the "Bloch sphere") and $\overrightarrow{n}_2$ has coordinates (θ,φ). In order to bring $\overrightarrow{n}_1$ to $\overrightarrow{n}_2$ along a great circle we can submit $\overrightarrow{n}_1$ to a rotation around $\overrightarrow{n} = \overrightarrow{n}_1 \times \overrightarrow{n}_2/\sin\theta$. The rotation from $\overrightarrow{n}_1$ to $\overrightarrow{n}_2$ takes $|\psi_1\rangle$ to $|\psi_2\rangle$ by a $SU(2)$ transformation: $U(\theta,\varphi)\,|\psi_1\rangle = |\psi_2\rangle$, with

$$U(\theta,\varphi) = \exp\left(-i\frac{\theta}{2}\overrightarrow{n}\cdot\overrightarrow{\sigma}\right) = \cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)\overrightarrow{n}\cdot\overrightarrow{\sigma} = \cos\left(\frac{\theta}{2}\right)I - i\frac{\overrightarrow{n}_1\times\overrightarrow{n}_2}{2\cos(\theta/2)}\cdot\overrightarrow{\sigma}. \tag{41}$$

Setting $|\psi(s)\rangle = U(\theta s,\varphi)|\phi_1\rangle$ we have $|\psi(0)\rangle = |\psi_1\rangle$, $|\psi(1)\rangle = |\psi_2\rangle$, and the curve $|\psi(s)\rangle$, $s\in[0,1]$, is a horizontal geodesic. Indeed, by explicitly writing $U(\theta s,\varphi)$ as

$$U(\theta s,\varphi) = \cos\left(\frac{\theta}{2}s\right)I - i\sin\left(\frac{\theta}{2}s\right)\overrightarrow{n}_\varphi\cdot\overrightarrow{\sigma}, \tag{42}$$

with $\overrightarrow{n}_\varphi = (-\sin\varphi, \cos\varphi, 0)$, we can straightforwardly verify that $|\psi(s)\rangle$ fulfills the defining properties of horizontal geodesics, namely $\langle\psi(s)|\dot\psi(s)\rangle = 0$, and

$$\frac{d^2}{ds^2}|\psi(s)\rangle = -\langle\dot\psi(s)|\dot\psi(s)\rangle|\psi(s)\rangle = -\frac{\theta^2}{4}|\psi(s)\rangle. \tag{43}$$

Hence, we have proved that for $|\psi_1\rangle = |\phi_1\rangle$ and $|\psi_2\rangle = \cos(\theta/2)|\phi_1\rangle + e^{i\varphi}\sin(\theta/2)|\phi_2\rangle$, there is a horizontal geodesic $|\psi(s)\rangle = U(\theta s,\varphi)|\phi_1\rangle$ joining these vectors, with $U(\theta s,\varphi)$ as in Eq.(42). Next, we consider a general final vector $|\psi_2'\rangle = e^{i\alpha}|\psi_2\rangle$. In this case we need only change $U(\theta s,\varphi)$ by $e^{-i\alpha s}U(\theta s,\varphi)$ and it follows that the curve $|\psi'(s)\rangle = e^{-i\alpha s}U(\theta s,\varphi)|\phi_1\rangle$, with $|\psi'(0)\rangle = |\psi_1\rangle$, $|\psi'(1)\rangle = |\psi_2'\rangle$, is still a geodesic; that is, it satisfies Eq.(34) (with $f(s) = \theta/2$) though it is no longer horizontal: $\langle\psi'(s)|\dot\psi'(s)\rangle = -i\alpha$. In summary, we have proved that any two vectors, $|\psi_1\rangle$ and $|\psi_2\rangle$, can be connected by a geodesic $\mathcal{C}_0$. If this geodesic happens to be horizontal, then its dynamical phase vanishes and so does its total phase $\arg\langle\psi_1|\psi_2\rangle$, see

Eq.(38). Hence, $\Phi_g(C_0) = 0$. This last property is gauge independent. However, if $\mathcal{C}_0$ is not horizontal, then $\Phi_{dyn}(C_0) \neq 0$ and $\arg\langle\psi_1|\psi_2\rangle \neq 0$, but $\Phi_g(C_0) = 0$ anyway.
Eq.(39) leads to an alternative formulation of the geometric phase. It rests upon the concept of Bargmann invariants, for which Eq.(39) plays a central role, together with the total phase $\arg\langle\psi_1|\psi_2\rangle$. When $\arg\langle\psi_1|\psi_2\rangle = 0$ we say that $|\psi_1\rangle$ and $|\psi_2\rangle$ are "in phase". This generalizes Pancharatnam's definition for polarization states to the quantal case. As we have seen, $|\psi_1\rangle$ and $|\psi_2\rangle$ are "in phase" when these two vectors can be joined by a horizontal geodesic. Consider a third vector $|\psi_3\rangle$, joined to $|\psi_2\rangle$ by a horizontal geodesic, so that $\arg\langle\psi_2|\psi_3\rangle = 0$ too. Our three vectors are thus joined by a curve made of two geodesic arcs. Can we conclude that $|\psi_3\rangle$ and $|\psi_1\rangle$ are "in phase"? The answer is generally on the negative. Being "in phase" is not a transitive property. The following discussion illustrates this point.

3.2 Bargmann invariants

Consider N points in ray space: $\rho_1, \rho_2, \ldots, \rho_N$. As we have seen, each pair can be connected by a geodesic arc. Let us denote by C_0 the curve formed by the $N-1$ geodesic arcs joining the N points. Let us assume that any two neighboring points are nonorthogonal. That is, for any lift $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle$, it holds $\langle\psi_i|\psi_{i+1}\rangle \neq 0$, for $i = 1, \ldots, N-1$. The geometric phase $\Phi_g(C_0)$ is given by

$$\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0) - \Phi_{dyn}(\mathcal{C}_0) = \arg\langle\psi_1|\psi_N\rangle - \sum_{k=1}^{N-1} \Phi_{dyn}^{(k,k+1)}, \tag{44}$$

where $\Phi_{dyn}^{(k,k+1)}$ is the dynamical phase for the geodesic joining $|\psi_k\rangle$ with $|\psi_{k+1}\rangle$. Because $\Phi_g^{(k,k+1)} = 0$, we can write $\Phi_{dyn}^{(k,k+1)} = \Phi_{tot}^{(k,k+1)} - \Phi_g^{(k,k+1)} = \arg\langle\psi_k|\psi_{k+1}\rangle$. Now, $\sum_{k=1}^{N-1} \arg\langle\psi_k|\psi_{k+1}\rangle = \arg\prod_{k=1}^{N-1}\langle\psi_k|\psi_{k+1}\rangle$, and $\arg\langle\psi_1|\psi_N\rangle = -\arg\langle\psi_N|\psi_1\rangle$, so that

$$\Phi_g(C_0) = \arg\langle\psi_1|\psi_N\rangle - \arg\prod_{k=1}^{N-1}\langle\psi_k|\psi_{k+1}\rangle = -\arg\left(\prod_{k=1}^{N-1}\langle\psi_k|\psi_{k+1}\rangle\right)\langle\psi_N|\psi_1\rangle, \tag{45}$$

and we can finally write

$$\Phi_g(C_0) = -\arg\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\ldots\langle\psi_N|\psi_1\rangle. \tag{46}$$

Although $\Phi_g(C_0)$ has been derived by joining $|\psi_1\rangle, \ldots, |\psi_N\rangle$ with geodesic arcs, the final expression does not depend on these arcs, but only on the vectors they join. Quantities like $\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_1\rangle$ are called "Bargmann invariants". They generalize $|\langle\psi_1|\psi_2\rangle|^2$, which is invariant under simultaneous $U(1)$ transformations: $|\psi_1\rangle \to |\psi_1'\rangle = \exp(i\alpha_1)|\psi_1\rangle$ and $|\psi_2\rangle \to |\psi_2'\rangle = \exp(i\alpha_2)|\psi_2\rangle$. Quantities that are invariant under $U(1) \otimes U(1) \otimes \ldots$ were introduced by Bargmann for studying the difference between unitary and anti-unitary transformations.
The curve C_0 in Eq.(45) was assumed to be open: $\rho_N \neq \rho_1$. However, we can close the curve to $\widetilde{C}_0$, by completing the $N-1$-sided polygon C_0 with a geodesic arc connecting ρ_N with ρ_1. By repeating the steps leading to Eq.(45), though taking into account that now $\Phi_{tot}(\widetilde{\mathcal{C}}_0) = 0$ because the final point $|\psi_{N+1}\rangle = |\psi_1\rangle$, we see that $\Phi_g(\widetilde{C}_0) = -\Phi_{dyn}(\widetilde{C}_0) = -\arg\prod_{k=1}^{N}\langle\psi_k|\psi_{k+1}\rangle$, so that $\Phi_g(\widetilde{C}_0)$ is given again by Eq.(46). In other words, $\Phi_g(\widetilde{C}_0) = \Phi_g(C_0)$.

Starting from Eq.(46) it is possible to recover the results previously found for general open curves (N. Mukunda, 1993). One proceeds by approximating a given curve by a polygonal arc made up of $N \to \infty$ geodesic arcs. By a limiting procedure one recovers then $\Phi_g(\mathcal{C}_0) = \Phi_{tot}(\mathcal{C}_0) - \Phi_{dyn}(\mathcal{C}_0)$ with $\Phi_{tot}(\mathcal{C}_0)$ and $\Phi_{dyn}(\mathcal{C}_0)$ given by Eqs.(25) and (26), respectively. Also Eq.(31) can be recovered in a similar fashion (N. Mukunda, 1993).
The quantity $\langle\psi_1|\psi_3\rangle\langle\psi_3|\psi_2\rangle\langle\psi_2|\psi_1\rangle$, the three-vertex Bargmann invariant, can be identified as the basic building block of geometric phases. It can be seen as the result of two successive filtering measurements, the first projecting $|\psi_1\rangle$ on $|\psi_2\rangle$, followed by a second projection on $|\psi_3\rangle$. The phase of the final state with respect to the first one is $\Phi_g^{\triangle} = -\arg\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_1\rangle = -\arg Tr\rho_1\rho_2\rho_3$. It can be proved (A. G. Wagh, 1999) that $\Phi_g^{\triangle} = -\Omega_p^{\triangle}/2$. Here, $\Omega_p^{\triangle}$ is the solid angle subtended by the spherical triangle formed by shorter geodesics between $|\psi_2\rangle$, $|\psi_3\rangle$ and the projection $|\psi_1\rangle^p$ of $|\psi_1\rangle$ on the subspace spanned by the other two vectors. Now, given a closed curve $\widetilde{C}_0$, by triangulation with infinitesimal geodesic triangles it is possible to express $\Phi_g(\widetilde{C}_0)$ as (A. G. Wagh, 1999)

$$\Phi_g(\widetilde{C}_0) = -\frac{1}{2}\int_S d\Omega_p, \tag{47}$$

thereby generalizing Eq.(22).

4. Pancharatnam-Berry phase and its measurement by polarimetry and interferometry

4.1 Interferometric arrangement

We introduced the total phase, $\arg\langle\psi_1|\psi_2\rangle$, as a generalization of Pancharatnam's definition for the relative phase between two polarized states of light. According to Pancharatnam's definition, we can operationally decide whether two nonorthogonal states are "in phase". Consider two nonorthogonal polarization states, $|i\rangle$ and $|f\rangle \neq |i\rangle$, and let them interfere. Due to the optical-path difference, there is a relative phase-shift ϕ giving rise to an intensity pattern

$$I = \left|e^{i\phi}|i\rangle + |f\rangle\right|^2 \propto 1 + |\langle i|f\rangle| \cos\left(\phi - \arg\langle i|f\rangle\right). \tag{48}$$

The maxima of I occur for $\phi = \arg\langle i|f\rangle \equiv \Phi_{tot}$, which is thereby operationally defined as the total (Pancharatnam) phase between $|i\rangle$ and $|f\rangle$. If $\arg\langle i|f\rangle = 0$, the states are said to be "in phase". Polarization states are two-level systems. When they are submitted to the action of intensity-preserving optical elements, like wave-plates, their polarization transformations belong to the group $SU(2)$ (modulo global phase factors). We can exhibit Φ_{tot} by submitting $|i\rangle$ to $U \in SU(2)$, thereby producing a state $|f\rangle = U|i\rangle$. Eq.(48) applies to, say, a Mach-Zehnder array. Alternatively, one could employ polarimetric methods. We will discuss both methods in what follows. Among the different parameterizations of U, the following one is particularly well suited for extracting Pancharatnam's phase:

$$U(\beta,\gamma,\delta) = \exp\left(i(\frac{\delta+\gamma}{2})\sigma_z\right)\exp\left(-i\beta\sigma_y\right)\exp\left(i(\frac{\delta-\gamma}{2})\sigma_z\right) = \begin{pmatrix} e^{i\delta}\cos\beta & -e^{i\gamma}\sin\beta \\ e^{-i\gamma}\sin\beta & e^{-i\delta}\cos\beta \end{pmatrix}. \tag{49}$$

Indeed, taking as initial state $|i\rangle = |+\rangle_z \equiv |+\rangle$, the eigenstate of σ_z for the eigenvalue $+1$, and setting $|f\rangle = U|+\rangle$, we obtain

$$\langle i|f\rangle = \langle +|\, U(\beta,\gamma,\delta)\, |+\rangle = e^{i\delta}\cos\beta. \tag{50}$$

Thus, $\Phi_{tot} = \arg\langle i|f\rangle = \delta + \arg(\cos\beta)$, for $\beta \neq (2n+1)\pi/2$. Because $\cos\beta$ takes on positive and negative real values, $\arg(\cos\beta)$ equals 0 or π, and Φ_{tot} is thus given by δ modulo π. In principle, then, we could obtain Φ_P (modulo π) by comparing two interferograms, one taken as a reference and corresponding to $\Phi_P = 0$ ($U = I$), and the other corresponding to the application of U. Their relative shift gives Φ_P. We can implement unitary transformations using quarter-wave plates (Q) and half-wave plates (H). These transformations are of the form $U(\xi,\eta,\zeta) = \exp\left(-i\xi\sigma_y/2\right)\exp\left(i\eta\sigma_z/2\right)\exp\left(-i\zeta\sigma_y/2\right)$. They can be realized with the following gadget (R. Simon, 1990), in which the arguments of Q and H mean the angles of their major axes to the vertical direction:

$$U(\xi,\eta,\zeta) = Q\left(\frac{-3\pi + 2\xi}{4}\right) H\left(\frac{\xi - \eta - \zeta - \pi}{4}\right) Q\left(\frac{\pi - 2\zeta}{4}\right). \tag{51}$$

The corresponding interferogram has an intensity pattern given by

$$I_V = \frac{1}{2}\left[1 - \cos\left(\frac{\eta}{2}\right)\cos\left(\frac{\xi+\zeta}{2}\right)\cos(\phi) - \sin\left(\frac{\eta}{2}\right)\cos\left(\frac{\xi-\zeta}{2}\right)\sin(\phi)\right]. \tag{52}$$

I_V refers to an initial state $|+\rangle_z$ that is vertically polarized. This result follows from the parametrization of U given by $U(\xi,\eta,\zeta)$. By using the relationship between this parametrization and that of Eq.(49), i.e., $U(\beta,\gamma,\delta)$, one can show that I_V can be written as

$$I_V = \frac{1}{2}\left[1 - \cos\beta\cos(\phi - \delta)\right]. \tag{53}$$

Pancharatnam's phase $\Phi_P = \delta$ is thus given by the shift of the interferogram I_V with respect to a reference interferogram $I = \left[1 - \cos\beta\cos\phi\right]/2$. By recording one interferogram after the other one could measure their relative shift. However, thermal and mechanical disturbances make it difficult to record stable reference patterns, thereby precluding accurate measurements of Φ_P. A way out of this situation follows from observing that the intensity pattern corresponding to an initial, horizontally polarized state $|-\rangle_z$ is given by

$$I_H = \frac{1}{2}\left[1 - \cos(\beta)\cos(\phi + \delta)\right]. \tag{54}$$

Hence, the relative shift between I_V and I_H is twice Pancharatnam's phase. If one manages to divide the laser beam into a vertically and a horizontally polarized part, the two halves of the laser beam will be subjected to equal disturbances and one can record two interferograms in a single shot. The relative shift would be thus easily measurable, being robust to thermal and mechanical disturbances. With such an array it is possible to measure Pancharatnam's phase for different unitary transformations. This approach proved to be realizable, using either a beam expander or a polarizing beam displacer (J. C. Loredo, 2009).

A similar approach can be used to measure the geometric phase $\Phi_g = \Phi_P(\mathcal{C}_0) - \Phi_{dyn}(\mathcal{C}_0)$. One can exploit the gauge freedom and choose an appropriate phase factor $\exp(i\alpha(s))$, so as to make $\Phi_{dyn}(\mathcal{C}_0) = 0$ along a curve $\mathcal{C}_0 : |\psi(s)\rangle\,,\ s \in [s_1, s_2]$ which is traced out by polarization states $|\psi(s)\rangle$ resulting from $U(s)$: $|\psi(s)\rangle = U(s)\,|\psi(0)\rangle$. Any $U(s)$ can be realized

by making one or more parameters in $U(\xi,\eta,\zeta)$ (see Eq.(51)) functions of s. Setting the corresponding QHQ-gadget on one arm of the interferometer, one lets the polarization state $|\psi(s)\rangle$ follow a prescribed curve. A second QHQ-gadget can be put on the other arm, in order to produce the factor $\exp(i\alpha(s))$ that is needed to make $\Phi_{dyn}(\mathcal{C}_0) = 0$. To fix $\alpha(s)$, one solves $Im\langle\psi(s)|\dot{\psi}(s)\rangle + \dot{\alpha}(s) = 0$. The corresponding interferometric setup is shown in Fig.(2). It is of the Mach-Zehnder type; but a Sagnac and a Michelson interferometer could be used as well. With the help of this array one can generate geometric phases associated to non-geodesic trajectories on the Poincaré sphere (J. C. Loredo, 2011). In this way, one is not constrained to use special trajectories, along which the dynamical phase identically vanishes (Y. Ota, 2009). The geometric phase is nowadays seen as an important tool for implementing robust quantum gates that can be employed in information processing (E. Sjöqvist, 2008). It appears to be noise resilient, as recent experiments seem to confirm (S. Fillip, 2009).
Ref.(J. C. Loredo, 2011) reports measurements that were obtained with a 30 mW cw He-Ne laser (632.8 nm) and the interferometric array shown in Fig.(2).The interferograms were

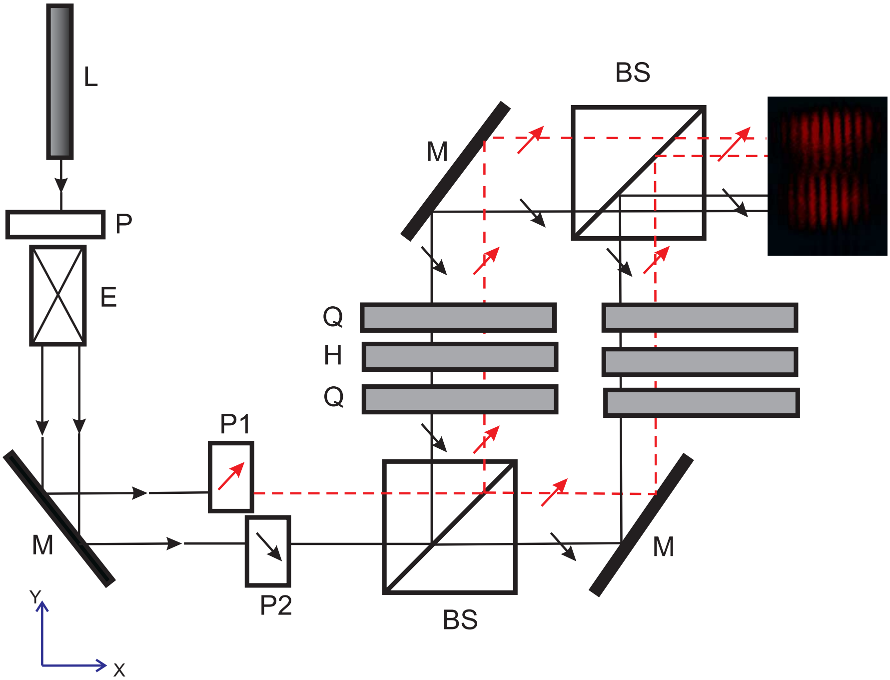


Fig. 2. Mach-Zehnder array for measuring the geometric phase. Quarter (Q) and half (H) wave plates are used for realizing the $SU(2)$ transformations. L: He-Ne laser, P, P_1, P_2: polarizers, E: beam expander, BS: beam-splitter, M: mirror.

recorded with the help of a CCD camera and evaluated using an algorithm that performs a column average of each half of the interferogram. The output was then submitted to a low-pass filter to get rid of noisy features. For each pair of curves the algorithm searches for relative minima and compares their locations. This procedure could be applied to a set of interferograms corresponding to different choices of $U(\xi,\eta,\zeta)$. Experimental results are shown in Fig. (3), corresponding to the trajectory on the Poincaré sphere shown in Fig. (4). As can be seen, they are in very good agreement with theoretical predictions.

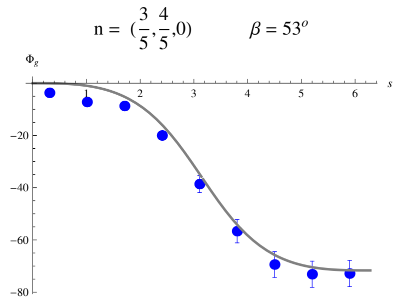


Fig. 3. Geometric phase for a non-geodesic trajectory on the Poincaré sphere. The trajectory is a circle resulting from intersecting a cone with the Poincaré sphere. It is fixed by the axis n of the cone and its aperture angle β.

4.2 Polarimetric arrangement

Some years ago, Wagh and Rakhecha proposed a polarimetric method to measure Pancharatnam's phase (A. G. Wagh, 1995;b). Such a method is experimentally more demanding than the interferometric one, but it was considered more accurate because it requires a single beam. Both methods were tested in experiments with neutrons (A. G. Wagh, 1997; 2000), whose spins were subjected to $SU(2)$ transformations by applying a magnetic field. Now, it is not obvious that one can extract phase information from a single beam. As we shall see, polarimetry can be understood as "virtual interferometry", in which a single beam is decomposed in two "virtual" beams.

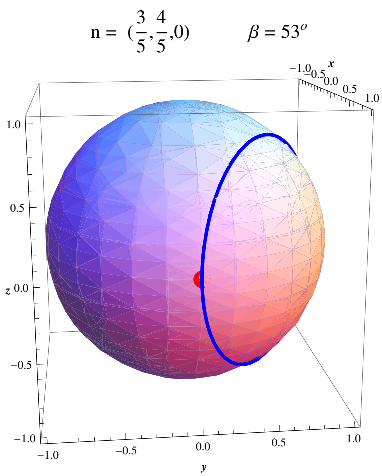


Fig. 4. The trajectory described on the Poincaré sphere. The dynamical phase is simultaneously cancelled by means of a QHQ gadget.

Consider an initial state $|+\rangle \equiv |+\rangle_z$ and let it be submitted to a $\pi/2$-rotation around the x-axis to produce the circularly polarized state $(|+\rangle - i|-\rangle)/\sqrt{2}$, which is in turn acted upon by $\exp(-\phi\sigma_z/2)$. The result is $V|+\rangle \equiv \exp(-i\phi\sigma_z/2)\exp(-i\pi\sigma_x/4)|+\rangle$, i.e., the state $\left(|+\rangle - ie^{i\phi}|-\rangle\right)/\sqrt{2}$, up to a global phase. We have thereby generated a relative phase-shift ϕ between $|+\rangle$ and $|-\rangle$, as in an interferometer. Applying $U \in SU(2)$ we obtain $UV|+\rangle = e^{-i\phi/2}\left(U|+\rangle - ie^{i\phi}U|-\rangle\right)/\sqrt{2} \equiv |\chi_+\rangle + |\chi_-\rangle$. From this state we will extract Pancharatnam's phase. To this end, we project with $V|+\rangle$, so that the intensity of the projected state is

$$I = \left|\langle +|V^\dagger(|\chi_+\rangle + |\chi_-\rangle)\right|^2. \tag{55}$$

Let us write $V|+\rangle = e^{-i\phi/2}\left(|+\rangle - ie^{i\phi}|-\rangle\right)/\sqrt{2} \equiv |\varphi_+\rangle + |\varphi_+\rangle$ and take U as given by Eq.(49). Calculating the amplitude $\langle +|V^\dagger(|\chi_+\rangle + |\chi_-\rangle) = (\langle\varphi_+| + \langle\varphi_-|)(|\chi_+\rangle + |\chi_-\rangle)$ we obtain, using $\langle\varphi_\pm|\chi_\pm\rangle = \exp(\pm i\delta)\cos(\beta)/2$, and $\langle\varphi_\mp|\chi_\pm\rangle = i\exp(\mp i(\gamma+\phi))\sin(\beta)/2$, that $(\langle\varphi_+| + \langle\varphi_-|)(|\chi_+\rangle + |\chi_-\rangle) = \cos(\beta)\cos(\delta) + i\sin(\beta)\cos(\gamma+\phi)$ and

$$I = \cos^2(\beta)\cos^2(\delta) + \sin^2(\beta)\cos^2(\gamma+\phi). \tag{56}$$

Eq.(56) contains Pancharatnam's phase $\delta = \Phi_{tot}$. It can be extracted from intensity measurements. Indeed, Eq.(56) yields the minimal and maximal intensity values of the pattern that arises from varying ϕ. They are given by $I_{\min} = \cos^2(\beta)\cos^2(\delta)$ and $I_{\max} = \cos^2(\beta)\cos^2(\delta) + \sin^2(\beta)$, respectively, so that Pancharatnam's phase follows from

$$\cos^2(\delta) = \frac{I_{\min}}{1 - I_{\max} + I_{\min}}. \tag{57}$$

In order to measure the geometric phase, we make $\Phi_{dyn} = 0$. As we saw before, this can be achieved by using in place of the gauge $|\psi(s)\rangle = U(s)|+\rangle$, the gauge $|\psi(s)\rangle = \exp[i\alpha(s)]U(s)|+\rangle$. In this way we get $\langle\psi(s)|d\psi(s)/ds\rangle = 0$, so that $\Phi_{tot} = \Phi_g$. To be specific, let us assume that we wish to generate circular trajectories corresponding to rotations by an angle s around $\vec{n}(\theta,\varphi)$. The corresponding unitarity is $U(\theta,\varphi,s) = \exp\left[-is\,\vec{n}(\theta,\varphi)\cdot\vec{\sigma}\right]$. In order to make $\Phi_{dyn}(\mathcal{C}_0) = 0$ in this case, we can take $\alpha(s) = \langle +|\,\vec{n}(\theta,\varphi)\cdot\vec{\sigma}\,|+\rangle s$.

In an optical arrangement we implement V and U with retarders. Simon and Mukunda (R. Simon, 1989) proposed a gadget realizing $U(\theta,\varphi,s)$, so that the circular trajectory is generated by rotating a single retarder (H) by the angle $s/2$, after having fixed θ and φ. This gadget is

$$U(\theta,\varphi,s) = Q\left(\frac{\pi+\varphi}{2}\right)Q\left(\frac{\theta+\varphi}{2}\right)H\left(\frac{-\pi+\theta+\varphi}{2}+\frac{s}{2}\right)Q\left(\frac{\theta+\varphi}{2}\right)Q\left(\frac{\varphi}{2}\right). \tag{58}$$

As for $V = \exp(-i\phi\sigma_z/2)\exp(-i\pi\sigma_x/4)$, we have $\exp(-i\pi\sigma_x/4) = Q(\pi/4)$ and $\exp(-i\phi\sigma_z/2) = Q(\pi/4)H((\phi-\pi)/4)Q(\pi/4)$. Using $Q^2(\pi/4) = H(\pi/4)$ and $\exp(+i\phi\sigma_z/2) = Q(-\pi/4)H((\phi+\pi)/4)Q(-\pi/4)$ we get

$$U_{tot} \equiv V^\dagger UV = H\left(-\frac{\pi}{4}\right)H\left(\frac{\phi+\pi}{4}\right)Q\left(-\frac{\pi}{4}\right)UQ\left(\frac{\pi}{4}\right)H\left(\frac{\phi-\pi}{4}\right)H\left(\frac{\pi}{4}\right). \tag{59}$$

Inserting for U the corresponding operator, which in the present case is $\exp[i\alpha(s)]U(\theta,\varphi,s)$, we obtain the full arrangement. Applying relations like $Q(\alpha)H(\beta) = H(\beta)Q(2\beta-\alpha)$,

$Q(\alpha)H(\beta)H(\gamma) = Q(\alpha + \pi/2)H(\alpha - \beta + \gamma - \pi/2)$, etc. (R. Simon, 1990), we can reduce the array from elf to seven retarders:

$$U_{tot}(\theta, \varphi, s, \gamma) = Q\left(\frac{\pi}{4} - \frac{\gamma}{2}\right) Q\left(-\pi - \frac{\varphi}{2} - \frac{\gamma}{2}\right) Q\left(\frac{\pi - \theta - \varphi}{2} - \frac{\gamma}{2}\right) \times \tag{60}$$
$$\times H\left(\frac{-s - \theta - \varphi}{2} - \frac{\gamma}{2}\right) Q\left(\frac{\pi - \theta - \varphi}{2} - \frac{\gamma}{2}\right) Q\left(\frac{\pi - \varphi}{2} - \frac{\gamma}{2}\right) Q\left(-\frac{\pi}{4} - \frac{\gamma}{2}\right),$$

with $\gamma \equiv \sigma + \alpha(s) = \sigma + s \sin\theta \cos\varphi$. For each fixed value of s – that is, for each point on the chosen trajectory – one generates an intensity pattern through variation of σ, i.e., by rotating the whole array σ radians over some interval, which should be large enough for recording several maximal and minimal intensity values. From these values one can obtain $\Phi_g(s)$. Indeed, the intensity is given by $I = |\langle + | U_{tot} | + \rangle|^2$, and it can be proved (J. C. Loredo, 2011) that in the present case $I = \cos^2(s) + \sin^2(s)\left[\cos(\theta)\cos(\sigma - \alpha(s)) - \sin(\theta)\sin(\varphi)\sin(\sigma - \alpha(s))\right]^2$. From this result one derives the following expression for the geometric phase (J. C. Loredo, 2011):

$$\Phi_g(s) = \arccos\left(\sqrt{I_{\min}}\right)\sqrt{\frac{1 - I_{\max}}{1 - I_{\min}}} - \arctan\left(\sqrt{\frac{1 - I_{\max}}{I_{\min}}}\right). \tag{61}$$

This result has been tested for various trajectories (J. C. Loredo, 2011), confirming theoretical predictions with the expected accuracy. Though all these experiments were performed with a cw He-Ne laser, an alternative setting using single-photon sources should produce similar results. This is so because all the aforementioned results have topological, rather than classical or quantal character.

5. Geometric phase for mixed states

Up to this point, the geometric phase refers to pure states $\rho = |\psi\rangle\langle\psi|$. It is natural to ask whether geometric phases can be defined for mixed states as well. Uhlmann addressed this question (A. Uhlmann, 1986) and introduced a phase based on the concept of parallel transport. When a pure state $|\psi(s)\rangle$ evolves under parallel transport, it remains in phase with $|\psi(s + ds)\rangle$, i.e., the system does not suffer local phase changes. After completing a closed loop, a state may acquire a nontrivial phase, stemming from the curvature of the underlying parameter space. This notion can be extended to mixed states. To this end, Uhlmann considered so-called "purifications" of mixed states. That is, one considers a mixed state as being part of a larger system, which is in a pure state. There are infinitely many possible purifications of a given mixed state. Hence, to a given cyclic evolution there correspond infinitely many evolutions of the purifications. However, one of these evolutions can be singled out as the one which is "maximally parallel" (A. Uhlmann, 1986), and this leads to a definition of geometric phases for mixed states.

An alternative approach was addressed more recently by Sjöqvist *et al*. (E. Sjöqvist, 2000). The starting point is Pancharatnam's approach; i.e., the interference between two states: $|i\rangle$, to which a phase-shift ϕ is applied, and $|f\rangle = U|i\rangle$, with U unitary. The interference pattern is given by

$$I = \left| e^{i\phi} \left| i \right\rangle + U \left| i \right\rangle \right|^2 = 2 + 2 \left| \langle i|U|i\rangle \right| \cos\left(\phi - \arg\langle i|U|i\rangle\right) = 2 + 2v \cos\left(\phi - \Phi_{tot}\right), \tag{62}$$

with $v = |\langle i|U|i\rangle|$ being the visibility and $\Phi_{tot} = \arg\langle i|U|i\rangle$ the total phase between $|i\rangle$ and $U|i\rangle$.

Consider now a mixed state $\rho = \sum_i w_i |i\rangle\langle i|$, with $\sum_i w_i = 1$. The intensity profile will now be given by the contributions of all the individual pure states:

$$I = \sum_i w_i \left| e^{i\phi} \left| i \right\rangle + U \left| i \right\rangle \right|^2 = 2 + 2 \sum_i w_i \left| \langle i|U|i\rangle \right| \cos\left(\phi - \arg\langle i|U|i\rangle\right). \tag{63}$$

We can write I in a basis-independent form as (E. Sjöqvist, 2000)

$$I = 2 + 2 \left| Tr\left(U\rho\right) \right| \cos\left[\phi - \arg Tr\left(U\rho\right)\right]. \tag{64}$$

It is then clear that $v = |Tr\,(U\rho)|$ and that the total phase can be operationally defined as $\Phi_{tot} = \arg Tr\,(U\rho)$, which is the value of the shift ϕ at which maximal intensity is attained. As expected, such a definition reduces to Pancharatnam's for pure states $\rho = |i\rangle\langle i|$.

Let us now address the extension of the *geometric* phase for mixed states. For pure states $|\psi(s)\rangle$ the geometric phase equals Pancharatnam's phase whenever $|\psi(s)\rangle$ evolves under parallel transport: $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$. We can try to extend the notion of parallel transport for mixed states by requiring $\rho(s)$ to be in phase with $\rho(s+ds) = U(s+ds)\,\rho_0 U^\dagger(s+ds) = U(s+ds)\,U^\dagger(s)\rho(s)U(s)U^\dagger(s+ds)$. According to our previous definition, the phase difference between $\rho(s)$ and $\rho(s+ds)$ is given by $\arg Tr\left(U(s+ds)U^\dagger(s)\rho(s)\right)$ in this case. We say that $\rho(s)$ and $\rho(s+ds)$ are in phase when $\arg Tr\left(U(s+ds)U^\dagger(s)\rho(s)\right) = 0$, i.e., $Tr\left(U(s+ds)U^\dagger(s)\rho(s)\right)$ is a positive real number. Now, because $Tr\,(\rho(s)) = 1$ and $\rho(s)^\dagger = \rho(s)$, the number $Tr\left(\dot{U}U^\dagger\rho\right)$ is purely imaginary. Hence, a necessary condition for parallel transport is

$$Tr\left(\dot{U}(s)U^\dagger(s)\rho(s)\right) = 0. \tag{65}$$

However, such a condition is not sufficient to fix $U(s)$ for a given $\rho(s)$. Indeed, considering any $N \times N$ matrix representation of the given ρ, Eq.(65) determines U only up to N phase factors. In order to fix these factors we must impose a more stringent condition:

$$\langle k(s)|\dot{U}(s)U^\dagger(s)|k(s)\rangle = 0, \quad k = 1, \ldots, N, \tag{66}$$

where $\rho(s) = \sum_k w_k |k(s)\rangle\langle k(s)|$. This gives the desired generalization of parallel transport to the case of mixed states. We can now define a geometric phase for a state that evolves along the curve $C : s \to \rho(s) = U(s)\rho_0 U^\dagger(s)$, with $s \in [s_1, s_2]$ and $U(s)$ satisfying Eqs.(65) and (66). The dynamical phase $\Phi_{dyn} \equiv -i \int_{s_1}^{s_2} ds Tr\left(U^\dagger(s)\dot{U}(s)\rho(0)\right) = 0$ and we define the geometric phase Φ_g for mixed states as

$$\Phi_g = \arg Tr\left(U(s)\rho(0)\right). \tag{67}$$

Φ_g is gauge and parametrization invariant and has been defined for general paths, open or closed. In special cases, Φ_g can be expressed in terms of a solid angle, as it is the case with Berry's phase. For example, a two-level system can be described by

$$\rho = \frac{1}{2}\left(I + \overrightarrow{r}\cdot\overrightarrow{\sigma}\right) = \frac{1}{2}\left(I + r\overrightarrow{n}\cdot\overrightarrow{\sigma}\right), \tag{68}$$

with $\overrightarrow{n}\cdot\overrightarrow{n} = 1$ and r constant for unitary evolutions. For pure states $r = 1$, while for mixed states $r < 1$. The unitary evolution of $\rho(s)$ makes $\overrightarrow{n}(s)$ to trace out a curve C on the Bloch sphere. If necessary, we close C to $\widetilde{C}$ by joining initial and final points with a geodesic arc, so that $\widetilde{C}$ subtends a solid angle Ω. Then, the two eigenstates $|\pm; \overrightarrow{n}\cdot\overrightarrow{\sigma}\rangle$ of $\overrightarrow{n}\cdot\overrightarrow{\sigma}$ acquire geometric phases $\mp\Omega/2$. Both states have the same visibility $v_0 = \left|\langle\pm; \overrightarrow{n}\cdot\overrightarrow{\sigma}|U|\pm; \overrightarrow{n}\cdot\overrightarrow{\sigma}\rangle\right|$. The eigenvalues of ρ are $w_\pm = (1 \pm r)/2$. The geometric phase thus reads

$$\Phi_g = \arg\left(\frac{1+r}{2}e^{-i\Omega/2} + \frac{1-r}{2}e^{+i\Omega/2}\right) = -\arctan\left(r\tan\left(\frac{\Omega}{2}\right)\right). \tag{69}$$

and the visibility

$$v = v_0\left|\frac{1+r}{2}e^{-i\Omega/2} + \frac{1-r}{2}e^{+i\Omega/2}\right| = v_0\sqrt{\cos^2\left(\frac{\Omega}{2}\right) + r^2\sin^2\left(\frac{\Omega}{2}\right)}. \tag{70}$$

Eqs.(69) and (70) reduce for $r = 1$ to $\Phi_g = -\Omega/2$ and $v = v_0$, respectively, the known expressions for pure states. For maximally mixed states, $r = 0$, we obtain $\Phi_g = \arg\cos(\Omega/2)$, $v = |\cos(\Omega/2)|$, and Eq.(64) yields

$$I = 2 + 2\left|\cos(\Omega/2)\right|\cos\left(\phi - \arg\cos(\Omega/2)\right) = 2 + 2\cos(\Omega/2)\cos\phi. \tag{71}$$

We see that for $\Omega = 2\pi$ there is a sign change in the intensity pattern. This was experimentally observed in early experiments testing the 4π symmetry of spin-1/2 particles (H. Rauch, 1975). Much later, theoretical results like those expressed in Eqs.(69,70) have been successfully put to experimental test (M. Ericsson, 2005).

The above extensions of Pancharatnam's and geometric phases assume a unitary evolution $|i\rangle \to |f\rangle = U|i\rangle$. A non-unitary evolution – reflecting the influence of an environment – can be handled with the help of an ancilla; that is, by replacing the true environment by an environment simulator, a fictitious system being in a pure state $|0_e\rangle\langle 0_e|$, which is appended to the given system. The system plus the environment simulator are then described by $\widetilde{\rho} = \rho \otimes |0_e\rangle\langle 0_e|$ and evolve unitarily, $\widetilde{\rho} \to \widetilde{\rho}' = U\widetilde{\rho}U^\dagger$, in such a way that by tracing over the environment we recover the change of $\rho \to \rho' = Tr_e\widetilde{\rho}'$. Introducing an orthonormal basis $\{|k_e\rangle\}_{k=0,\ldots,M}$ for the environment, we can write $Tr_e\widetilde{\rho}' = \sum_k K_k\rho K_k^\dagger$, with $K_k \equiv \langle k_e|U|0_e\rangle$ being so-called Kraus operators (S. Haroche, 2007). Using these tools it is possible to extend total and geometric phases to non-unitary evolutions (J. G. Peixoto, 2002).

6. Thomas rotation in relativity and in polarization optics

In this closing Section we address a well-known effect of special relativity, Thomas rotation, and show its links to geometric phases. We recall that Thomas rotation is a rather surprising effect of Lorentz transformations. These transformations connect to one another the coordinates of two inertial systems, O and O', by $x^\mu \to x'^\mu = \Lambda^\mu_\nu x^\nu$, with $\Lambda^\mu_\nu \eta_{\mu\tau}\Lambda^\tau_\sigma = \eta_{\nu\sigma}$. Here, $\eta_{\mu\nu}$ denotes the Minkowsky metric tensor. Lorentz transformations form a six-parameter Lie group, whose elements can be written as (J. D. Jackson, 1975) $\Lambda = \exp L$, with $L = -\overrightarrow{\omega}\cdot\overrightarrow{S} - \overrightarrow{\zeta}\cdot\overrightarrow{K}$. The matrices $\overrightarrow{S}$ and $\overrightarrow{K}$ are the group generators, while

$\vec{\omega} = (\omega_1, \omega_2, \omega_3)$ and $\vec{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$ are six parameters, those required to fix any group element. The generators form an algebra, the Lie algebra of the group, which in the present case is defined through the following commutators:

$$\left[S_i, S_j\right] = \epsilon_{ijk} S_k, \tag{72}$$

$$\left[S_i, K_j\right] = \epsilon_{ijk} K_k, \tag{73}$$

$$\left[K_i, K_j\right] = -\epsilon_{ijk} S_k \tag{74}$$

In Eq.(72) we recognize the generators of the rotation group. On the other hand, the K_i are generators of "boosts" connecting two systems that move with uniform relative velocity and parallel axes. Intuitively, if O and O' are related by a boost, and so also O' and O'', then we expect that the same holds true for the transformation relating O and O''. The surprising discovery of Thomas was that this is not the case. Having parallel axes is not a transitive property within the framework of Lorentz transformations. The product of two boosts is not a boost, but it is instead a product of a boost by a rotation, the Thomas rotation. As almost all relativistic effects, in order to exhibit Thomas rotation we should consider systems whose relative velocity is near the velocity of light. Otherwise, the effect is too small to be observed. However, there is an equivalent effect that appears in the context of geometric phases, whose observation might be realizable with standard equipment. The root of Thomas rotation is the non-transitive property of boosts. As we have seen, Pancharatnam's connection relates also in a non-transitive way two polarization states. Intensity-preserving transformations of these states form a representation of the rotation group $SU(2)$. But these are only particular transformations among others, more general ones, which include intensity non-preserving transformations. The latter can be realized with the help of, e.g., polarizers, that is, *dichroich* optical elements. These elements provide us with the necessary tools for studying Thomas rotations.

Before we discuss the optical framework, we need some more algebra to build the bridge connecting Lorentz and polarization transformations. To this end, we recall the Dirac equation (J. D. Bjorken, 1964):

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0, \tag{75}$$

with $\psi(x)$ denoting a bi-spinor and the γ^μ being the Dirac matrices: $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}$. Bi-spinor space can be used as a representation-space for the Lorentz group. The Lorentz transformation $\Lambda = \exp L$, which acts in space-time, has a corresponding representation in bi-spinor space that is given by (J. D. Bjorken, 1964)

$$S(\Omega_{\mu\nu}) = \exp\left(-\frac{1}{4}\Omega_{\mu\nu}\gamma^\mu\gamma^\nu\right), \tag{76}$$

with $\Omega_{\mu\nu}(\Lambda) = -\Omega_{\nu\mu}(\Lambda)$ constituting six independent parameters. The commutation properties of the γ^μ allow us to write $S(\Omega_{\mu\nu})$ in terms of Pauli matrices $\vec{\sigma}$. This is so because $S(\Omega_{\mu\nu})$ contains only even products of the γ^μ matrices. Such products conform a subalgebra of the γ^μ, which is isomorphic to the Pauli-algebra. We can then map each 4×4 matrix $S(\Omega_{\mu\nu})$ into a 2×2 matrix

$$T(\overrightarrow{\alpha}, \overrightarrow{\beta}) = \exp\left[\left(\overrightarrow{\alpha} + i\overrightarrow{\beta}\right) \cdot \overrightarrow{\sigma}\right]. \tag{77}$$

We see that $T(\overrightarrow{\alpha}, \overrightarrow{\beta})$ is like an element of $SU(2)$, $\exp\left(i\overrightarrow{\delta} \cdot \overrightarrow{\sigma}\right)$, but with $\overrightarrow{\delta}$ being replaced by a complex three vector $\overrightarrow{\alpha} + i\overrightarrow{\beta}$ that entails the six real parameters of the Lorentz group. The representation of this group as in Eq.(77) is what we need to establish a connection with polarization optics.

A monochromatic, polarized, plane wave can be represented by Jones vectors with complex components: $|\pi\rangle = \left(\cos\chi, e^{i\phi}\sin\chi\right)^T$. Alternatively, polarization states can be represented by four-component Stokes vectors $(s_0, \overrightarrow{s})$, corresponding to a representation of pure states by density operators:

$$\rho = |\pi\rangle\langle\pi| = \frac{1}{2}\left(I + \overrightarrow{s} \cdot \overrightarrow{\sigma}\right). \tag{78}$$

In general, the Stokes four-vector $(s_0, \overrightarrow{s}) = (Tr\rho, Tr(\rho\sigma_1), Tr(\rho\sigma_2), Tr(\rho\sigma_3))$. The Stokes three-vector $\overrightarrow{s}$ that corresponds to the Jones vector $|\pi\rangle = \left(\cos\chi, e^{i\phi}\sin\chi\right)^T$ is given by $\overrightarrow{s} = (\cos(\phi)\sin(2\chi), \sin(\phi)\sin(2\chi), \cos(2\chi))$. Vectors $\overrightarrow{s}$ span the Poincaré-Bloch sphere.

Intensity preserving transformations, like those realized by wave plates, are represented by 2×2 matrices belonging to the $SU(2)$ group. The effect of such a matrix on $\overrightarrow{s}$ is to rotate this vector without changing its length. By applying $U = \exp\left(i\Phi\overrightarrow{n} \cdot \overrightarrow{\sigma}/2\right)$ to an input vector $|\pi_i\rangle$ we obtain an output vector $|\pi_o\rangle = U|\pi_i\rangle$. The corresponding Stokes vectors, $\overrightarrow{s}_i$ and $\overrightarrow{s}_o$, are related to one another by the well-known Rodrigues formula (H. Goldstein, 1980) that gives a rotated vector in terms of the rotation angle Φ and axis $\overrightarrow{n}$:

$$\overrightarrow{s}_o = \cos(\Phi)\overrightarrow{s}_i + [1 - \cos(\Phi)]\left(\overrightarrow{n} \cdot \overrightarrow{s}_i\right)\overrightarrow{n} + \sin(\Phi)\overrightarrow{s}_i \times \overrightarrow{n}. \tag{79}$$

Consider now dichroic optical elements, e.g., a non-ideal polarizer. To encompass optical conventions we use in what follows the Pauli matrices: $\rho_1 = \sigma_3$, $\rho_2 = \sigma_1$, $\rho_3 = \sigma_2$. In such a representation $|\pi\rangle = \left(\cos\chi, e^{i\phi}\sin\chi\right)^T$ is x-polarized when $\chi = 0$ and y-polarized when $\chi = \pi/2$. The matrix representing a non-ideal polarizer whose lines of maximal and minimal transmission are along the x- and y-polarization axes, respectively, is given by

$$J_{diag} = \begin{pmatrix} p_x & 0 \\ 0 & p_y \end{pmatrix}. \tag{80}$$

The eigenvectors of J_{diag}, $(1,0)^T$ and $(0,1)^T$, are thus polarization vectors along the x and $-x$ directions, respectively, on the Poincaré sphere. The corresponding matrix whose eigenvectors are $|\pi_1\rangle = \left(\cos\chi, e^{i\phi}\sin\chi\right)^T$ and its orthogonal $|\pi_2\rangle = \left(-e^{-i\phi}\sin\chi, \cos\chi\right)^T$, is given by

$$J = \left(\frac{p_x + p_y}{2}\right) I + \left(\frac{p_x - p_y}{2}\right)\left[(\cos 2\chi)\,\rho_1 + (\sin 2\chi\cos\phi)\,\rho_2 + (\sin 2\chi\sin\phi)\,\rho_3\right]. \tag{81}$$

Taking x as transmission axis ($p_x > p_y$), writing $p_x = e^{-\alpha_m}$, $p_y = e^{-\alpha_M}$ and setting $\overrightarrow{\Gamma} = (\cos 2\chi, \sin 2\chi\cos\phi, \sin 2\chi\sin\phi)$, we obtain, with $\alpha_s = \alpha_m + \alpha_M$ and $\alpha_d = \alpha_M - \alpha_m$,

$$J = \exp\left(-\frac{\alpha_s}{2}\right)\left\{\cosh\left(\frac{\alpha_d}{2}\right) I + \sinh\left(\frac{\alpha_d}{2}\right) \overrightarrow{\Gamma} \cdot \overrightarrow{\rho}\right\}. \tag{82}$$

We can show that Eq.(77) is just of this form. To this end, we write $T(\overrightarrow{\alpha}, \overrightarrow{\beta}) = \exp(-\overrightarrow{f} \cdot \overrightarrow{\rho})$, with $\overrightarrow{f} = \overrightarrow{\alpha} + i\overrightarrow{\beta}$, and observe that $\overrightarrow{f} \cdot \overrightarrow{\rho}$ has eigenvalues

$$\lambda_\pm = \pm\sqrt{\overrightarrow{\alpha}^2 - \overrightarrow{\beta}^2 + 2i\overrightarrow{\alpha} \cdot \overrightarrow{\beta}} \equiv \pm z. \tag{83}$$

Denoting by $|\mathbf{f}_\pm\rangle$ the eigenvectors of $\overrightarrow{f} \cdot \overrightarrow{\rho}$; that is, $\overrightarrow{f} \cdot \overrightarrow{\rho}\,|\mathbf{f}_\pm\rangle = \lambda_\pm |\mathbf{f}_\pm\rangle$, we have $I = |\mathbf{f}_+\rangle\langle\mathbf{f}_+| + |\mathbf{f}_-\rangle\langle\mathbf{f}_-|$ and $\overrightarrow{f} \cdot \overrightarrow{\rho} = \lambda_+ |\mathbf{f}_+\rangle\langle\mathbf{f}_+| + \lambda_- |\mathbf{f}_-\rangle\langle\mathbf{f}_-|$. Solving for $|\mathbf{f}_\pm\rangle\langle\mathbf{f}_\pm|$ we obtain

$$|\mathbf{f}_\pm\rangle\langle\mathbf{f}_\pm| = \frac{zI \pm \overrightarrow{f} \cdot \overrightarrow{\rho}}{2z}. \tag{84}$$

Using $\exp A = \sum_n \exp a_n |a_n\rangle\langle a_n|$ with $A = -\overrightarrow{f} \cdot \overrightarrow{\rho}$ and observing that $\exp\left(-\overrightarrow{f} \cdot \overrightarrow{\rho}\right)$ has eigenvectors $|\mathbf{f}_\pm\rangle$ and eigenvalues $\exp(\mp z)$, we get

$$\begin{aligned}
\exp(-\overrightarrow{f} \cdot \overrightarrow{\rho}) &= e^{-z}|\mathbf{f}_+\rangle\langle\mathbf{f}_+| + e^{z}|\mathbf{f}_-\rangle\langle\mathbf{f}_-| = \frac{e^{-z}}{2z}\left(zI + \mathbf{f} \cdot \overrightarrow{\rho}\right) + \frac{e^{z}}{2z}\left(zI - \overrightarrow{f} \cdot \overrightarrow{\rho}\right) \\
&= \left(\frac{e^z + e^{-z}}{2}\right) I - \left(\frac{e^z - e^{-z}}{2z}\right) \overrightarrow{f} \cdot \overrightarrow{\rho} \\
&= (\cosh z) I - \sinh z \left(\frac{\overrightarrow{f}}{z}\right) \cdot \overrightarrow{\rho}
\end{aligned} \tag{85}$$

It is easy to show from Eq.(85) that a Lorentz transformation $\exp(-\overrightarrow{f} \cdot \overrightarrow{\rho})$ can generally be written as a product of a boost by a rotation. It is clear from Eq.(77) that a rotation is obtained when $\overrightarrow{\alpha} = \overrightarrow{0}$ and a boost when $\overrightarrow{\beta} = \overrightarrow{0}$. A general rotation $U(\xi, \eta, \zeta) \in SU(2)$ can be implemented with the help of three wave-plates, see Eq.(51). A general boost can be implemented with dichroic elements realizing Eq.(82). The global factor there, $\exp(-\alpha_s/2)$, corresponds to an overall intensity attenuation. We can thus in principle realize any transformation of the form $\exp(-\overrightarrow{f} \cdot \overrightarrow{\rho})$ by using optical elements like wave-plates and dichroic elements. In particular, by letting a polarization state pass through two consecutive dichroic elements – each corresponding to a boost – we could make appear a phase between initial and final states. This is a geometric phase rooted on Thomas rotation, which can thus be exhibited by using the tools of polarization optics. Thus, we have here another example showing the topological root shared by two quite distinct physical phenomena.

7. Conclusion

Berry's phase was initially seen as a surprising result, which contradicted the common wisdom that only dynamical phases would show up when dealing with adiabatically evolving states. But soon after its discovery it brought to light a plethora of physical effects sharing a common topological or geometrical root. Once the initial concept was relatively well understood, people could recognize its manifestation in previously studied cases, like the Aharonov-Bohm effect and the Pancharatnam's prescription for establishing whether two polarization states of light are in phase. Thanks to the contributions of a great number of researchers, Berry's phase has evolved into a rich subject of study that embraces manifold aspects. There are still several open questions and partially understood phenomena, as well as promising approaches to implement practical applications of geometrical phases, notably those related to quantum information processing. The present Chapter can give but a pale portrait and a limited view of what is a wide and rich subject. However, it is perhaps precisely out of these limitations that it could serve the purpose of awaking the reader's interest for studying in depth such a fascinating subject-matter.

8. References

M. V. Berry, "Quantal phase factors accompanying adiabatic changes", *Proc. R. Soc. London Ser. A,* vol. 392, pp. 45-57, 1984.

A. Tomita and R. Y. Chiao, "Observation of Berry's Topological Phase by Use of an Optical Fiber", *Phys. Rev. Lett.*, vol. 57 pp. 937-940, 1986.

S. Pancharatnam, "Generalized theory of interference and its applications", *Proceedings of the Indian Academy of Science A,* vol. 44, pp. 247-262, 1956.

Y. Aharonov et al., "Phase change during a cyclic quantum evolution", *Phys. Rev. Lett.*, vol. 58, pp. 1593-1596, 1987.

J. Samuel and R. Bhandari, "General Setting for Berry's Phase", *Phys. Rev. Lett.*, vol. 60, pp. 2339-2342, 1988.

H. M. Wong et al., "Quantum Geometric Phase between Orthogonal States", *Phys. Rev. Lett.,* vol. 94, pp. 070406-1-070406-4, 2005.

A. Uhlmann, "Parallel transport and quantum holonomy along density operators", *Rep. Math. Phys.*, vol. 24, pp. 229-240, 1986.

E. Sjöqvist et al., "Geometric Phases for Mixed States in Interferometry", *Phys. Rev. Lett.,* vol. 85, pp. 2845-2849, 2000.

N. Mukunda and R. Simon, "Quantum Kinematic Approach to the Geometric Phase. I. General Formalism", *Ann. Phys. (N. Y.)*, vol. 228, pp. 205-268, 1993.

A. Bohm et al., *The Geometric Phase in Quantum Systems*, Springer, New York, 2003.

A. G. Wagh and V. C. Rakhecha, "Gauge-independent formalism for parallel transport, geodesics and geometric phase", *J. Phys. A: Math. Gen.,* vol. 32, 5167-5178, 1999.

R. Simon and N. Mukunda, "Minimal three-component SU(2) gadget for polarization optics", *Phys. Lett. A,* vol. 143, pp. 165-169, 1990.

J. C. Loredo et al., "Measurement of Pancharatnams phase by robust interferometric and polarimetric methods", *Phys. Rev. A* vol. 80, pp. 012113-1-012113-9, 2009.

J. C. Loredo et al., "Measurement of geometric phases by robust interferometric methods", *J. of Phys.: Conf. Ser.*, vol. 274, pp. 012140-1-012140-9, 2011.

Y. Ota et al. "Geometric quantum gates in liquid-state NMR based on a cancellation of dynamical phases", *Phys. Rev. Lett.,* vol. 80, pp. 052311-1-052311-4, 2009.

E. Sjöqvist, "A new phase in quantum computation", *Physics* 1, 35, 2008. Available: http://link.aps.org/doi/10.1103/Physics.1.35.

S. Fillip et al. "Experimental Demonstration of the Stability of Berry's Phase for a Spin-1/2 Particle", *Phys. Rev. Lett.,* vol. 102, pp. 030404-1-030404-4, 2009.

A. G. Wagh and V. C. Rakhecha, "On measuring the Pancharatnam phase. II. SU(2) polarimetry", *Phys. Lett. A,* vol. 197, pp. 112-115, 1995.

A. G. Wagh and V. C. Rakhecha, “On measuring the Pancharatnam phase. I. Interferometry”, *Phys. Lett. A*, vol. 197, pp. 107-111, 1995.

A. G. Wagh et al., “Experimental Separation of Geometric and Dynamical Phases Using Neutron Interferometry”, *Phys. Rev. Lett.*, vol. 78, pp. 755-759, 1997.

A. G. Wagh et al., “Neutron polarimetric separation of geometric and dynamical phases”, *Phys. Lett. A*, vol. 268, 209-216 (2000).

R. Simon and N. Mukunda, “Universal SU(2) gadget for polarization optics”, *Phys. Lett. A*, vol. 138, pp. 474-480, 1989.

J. C. Loredo, ”Geometric phase in photonics”, Master Thesis, Physics Section, Pontificia Universidad Católica del Perú, Lima-Peru, 2011.

H. Rauch et al., “Verification of coherent spinor rotation of fermions”, *Phys. Lett. A*, vol. 54, 425-427, 1975.

S. Haroche and J-M. Raimond, *Exploring the Quantum*, Oxford University Press, Oxford, 2007.

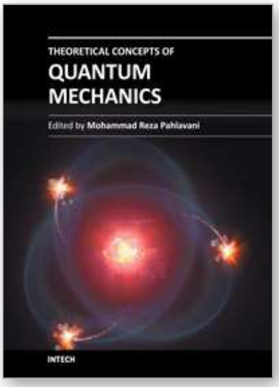
M. Ericsson et al. “Measurement of Geometric Phases for Mixed States Using Single Photon Interferometry”, *Phys. Rev. Lett.*, vol. 94, pp. 05041-1-04041-4, 2005.

J. G. Peixoto de Faria et al. “Phases of quantum states in completely positive non-unitary evolution”, *Europhys. Lett.*, vol. 62, pp. 782-788, 2002

J. D. Jackson, *Classical Electrodynamics*, 2nd. Ed., John Wiley and Sons, New York, 1975.

J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill, New York, 1964.

H. Goldstein, *Classical Mechanics*, 2nd. Ed., Addison-Wesley, Reading, Massachusetts, 1980.



Theoretical Concepts of Quantum Mechanics
Edited by Prof. Mohammad Reza Pahlavani

ISBN 978-953-51-0088-1
Hard cover, 598 pages
Publisher InTech
Published online 24, February, 2012
Published in print edition February, 2012

Quantum theory as a scientific revolution profoundly influenced human thought about the universe and governed forces of nature. Perhaps the historical development of quantum mechanics mimics the history of human scientific struggles from their beginning. This book, which brought together an international community of invited authors, represents a rich account of foundation, scientific history of quantum mechanics, relativistic quantum mechanics and field theory, and different methods to solve the Schrodinger equation. We wish for this collected volume to become an important reference for students and researchers.

InTech Europe
University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
Fax: +385 (51) 686 166
www.intechopen.com

InTech China
Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821