

Berry and Pancharatnam Topological Phases of Atomic and Optical Systems

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Abstract Theoretical and experimental studies of Berry and Pancharatnam phases are reviewed. Basic elements of differential geometry are presented for understanding the topological nature of these phases. The basic theory analyzed by Berry in relation to magnetic monopoles is presented. The theory is generalized to nonadiabatic processes and to noncyclic Pancharatnam phases. Different systems are discussed including polarization optics, n -level atomic system, neutron interferometry and molecular topological phases.

1 Introduction

There is a large interest in topological phases which lead to interesting physical phenomena in quantum-mechanics and optics. Although the appearance of geometrical phases was known quite a long time ago from Aharonov-Bohm (AB) effect [1] and molecular spectroscopy [2,3], the general context in which such phases appear has been analyzed by Berry [4].

Berry [4] analyzed the problem of a quantum-mechanical state developing adiabatically in time under a slowly varying parameter-dependent Hamiltonian. He has shown that when the parameters return to their initial values after traversing a closed path, the wavefunction acquires a 'geometric' phase factor, dependent on the path, in addition to the well-known 'dynamical' phase factor $\exp\left[-\frac{i}{\hbar} \int E dt\right]$. The geometry underlying Berry's phase has been reformulated in terms of fibre-bundle theory [5-9] by Simon [10]. Aharonov and Anandan [11] removed the adiabatic restriction and replaced the notion of parameter space by the notion of projective space of rays in Hilbert space. Generalizations of the Berry's phase analysis to degenerate states have been analyzed by Wilczek and Zee [12].

Non-abelian gauge potentials were introduced in Yang-Mills theory already in 1954 [13]. In this theory [14] a generalization of electromagnetism was made in which the complex wavefunction of a charged particle is replaced by a wavefunction with two components, $\psi = \psi^i(x)$, $i = 1, 2$.

Following Wilczek and Zee article [12] many investigations have been made on non-abelian topological phases [15-21] and this area became of spe-

cial interest due to the possibility to use non-abelian topological phases in quantum computation [22-26].

Classical analogies to the quantum Berry's phase have been treated by Hannay [27]. He has treated a classical Hamiltonian which depends on parameters which are changed very slowly, then the adiabatic theorem states that the action variable I of the motion is conserved. By treating the change in the angle variable, holonomy has been made [27,28]. Application of the analysis to generalized harmonic oscillators, with and without the adiabatic approximation, have been analyzed [27-30]. Relations between geometric quantum phases and angles have been also analysed [31,32].

There are two basic kinds of topological phases which have been studied experimentally for polarized light: a) The phase acquired by a light wave when its polarization state undergoes a sequence of unitary transformations. This phase is equal to *half the solid angle* subtended by the circuit traced by the state on the *Poincare Sphere*. This case is similar to the doubly degenerate case treated by Berry [4], as will be described in Section (3.1). The similarity between the two cases including the factor half follows from the isomorphism of the problem with spin- $\frac{1}{2}$ system. b) Topological phases acquired by a light wave when its *direction of propagation* is slowly cycled along a closed path on the sphere of directions in real space. This topological phase is equal to the *solid angle of the circuit in the space of directions of the wavevector*. This case is similar to the case treated by Berry [4] (See Section 3.1) of a spinning particle in a magnetic field \vec{B} which is slowly

varied. Jordan has shown [33] that the Berry phases for spins or helicities is a general property of the spin states rather than that of the Hamiltonian.

The fundamental article, which led to various experiments on topological phases in momentum space was published by Chiao and Wu in 1986 [34], and immediately after that it was realized experimentally by Tomita and Chiao [35].

Many experimental and theoretical studies analysed noncyclic topological phases by following Pancharatnam [36-37] definition of phase. The use of Berry and Pancharatnam phases to noncyclic evolution raises the problem of gauge invariance which have been treated in various works [38-42]. It has been suggested to treat open cycles by closing the end points of the open cycles by geodesic lines [38,39]. Although this approach has some interesting implications, it is possible to avoid the use of this 'trick' by following the kinematical approach [40,41].

Bhandari and Samuel [43], and Bhandari in series of papers [44,45], have studied, experimentally and theoretically, interference effects of polarized light. The mathematical isomorphism between polarization of light and the two-state quantum system has been exploited. It has been shown [43-45] that for the appearance of topological phases the evolution of the state needs to be neither unitary nor cyclic and can be interrupted by measurements. Some new effects have been shown: a) In contradiction to the $U(1)$ group by which phases is defined only module 2π , the phases obtained by the $SU(2)$ group are unbounded and can have arbitrary values if the Poincare sphere is traversed more than once. b) Phase shifts defined by Pancharatnam criterion

can have discontinuous jumps and can change sign for small variations in the parameters near singular points. Singularities occur *around or through* points where the two interfering beams become orthogonal and for which Pancharatnam phase is undefined. The phase jumps are always related to the geometric phases which have global properties in contrast to the dynamical phases which are changing continuously.

The acquisition of a geometric phase in neutron spin rotation has been verified experimentally by Bitter and Dubbers [46] for the special case of adiabatic evolution. Nonadiabatic geometric phase was observed by Suter et al. [47], using NMR techniques and also it has been shown by Simon et al. [48] that evolving geometric phase can introduce frequency shifts. The idea of obtaining Lorentz-group Berry's phases [49] in squeezed light has been suggested by Chiao and Jordan [50]. Lorentz-group Berry's phases have been observed in polarization optics [51]. Geometric phase observations have been made at the single photon level [52,53], and in two photon interference experiments [54,55]. Berry's topological phases have been measured by using optical fibre interferometers [56,57].

There are many experimental and theoretical works studying the geometric phases in neutron interferometry [58] including among others the studies of Wagh and his colleagues [59-61]. In Section 3.4.3 we will analyze some of these experiments and in Section (4.3) we will review some other works in this field.

Most of the observations of Berry's phases are related to $SU(2)$ and Lorentz groups. Geometric phases for $SU(3)$ representations and three-level

quantum systems have been treated in some articles [62-65].

There is much interest in the use of Berry's phases to quantum computation [22-26]. There are different problems which have been treated for the abelian phases, including: a) topological phases for entangled states [66-68]. b) Generalization of topological phases to mixed states and decoherence [69-72]. c) Geometric quantum computation implemented in NMR [73-74]. The present article emphasizes only basic properties of topological Berry's and Pancharatnam phases. The present Review does not discuss the literature on AB and quantum Hall effects, or other specific problems (see, e.g., in the book Shapere and Wilczek [75]) in order not to widen too much the scope of the present Review. We would like, however, to refer here to an interesting discussion on Berry's phase in quantum Hall effect given in the book of Yoshioka [76]. Also of special interest in the present Review are the works discussing the relations between topological phases and Riemannian metric [40,77-81].

A deep understanding of topological phases can be achieved by the use of fibre-bundle theories. Following this idea the present Review is arranged as follows: In Chapter 2 basic elements of topology are summarized. This chapter is divided into three Sections: (3.1) Manifolds and Lie groups; (3.2) Cartan exterior algebra; (3.3) Fibre-bundles and differential geometry. In Chapter 3 general theories of topological phases are discussed. This chapter is divided into 4 sections: (3.1) Berry's phases for Schrodinger equation under the adiabatic approximation; (3.2) Generalization of Berry's phases

to nonadiabatic processes and its relation to fibre-bundle theory; (3.3) Description of Berry's phases for n -level atomic system by the use of Kahler potentials; (3.4) Generalization of Berry's phases to noncyclic processes by the use of Pancharatnam phase.

In Chapter 4 we review some experimental measurements of Berry's phases. This chapter is divided into 4 sections: (4.1) Topological phases in molecular spectroscopy; (4.2) Topological phases in polarization optics; (4.3) Geometric phases in neutron interferometry; (4.4) Berry's phases related to Lorentz group. In Chapter 5 we summarize our results and conclusions.

Chapter 2. Basic Theory of Topology

We use in the present Review the Einstein summation convention in which there is an implicit sum over each pair of repeated indices. We use overbar to indicate the complex conjugate (The asterisk is used later to denote cotangent space).

2.1 Manifolds and Lie groups

Assuming that the reader has a basic knowledge of group theory we discuss only certain relations between Lie groups and manifolds.

2.1.1 Definition of a Manifold

A real (or complex) n dimensional *manifold* M^n looks like Euclidean space \mathbb{R}^n (or \mathbb{C}^n) around each point. We introduce a certain '*neighborhood*' O_i covering a part of M^n , where each O_i is a subspace of \mathbb{R}^n (or \mathbb{C}^n). It is possible to

determine from a manifold of dimension n another manifold of dimension $n - 1$ by taking the ‘*boundary*’ of an n manifold. For example the boundary of a disc is a circle. We denote the boundary of a manifold M as ∂M . The boundary of a boundary is always empty, $\partial\partial M = 0$.

Suppose we have covering $\{O_i\}$ of a manifold M and a mapping ϕ_i from O_i to \mathbb{R}^n , then in the overlapping $O_i \cap O_j$ the transformation from the coordinate system ϕ_i to the coordinate system ϕ_j is given by the transition function

$$\phi_{ij} = \phi_j \phi_i^{-1} \quad (2.1)$$

In equation (2.1) the coordinates \mathbb{R}^n of the neighborhood O_i are transformed back to the manifold and then the overlapping neighborhood O_j is projected to its coordinates in \mathbb{R}^n .

2.1.2 Complex projective n -space $\mathbb{C}P^n$

$\mathbb{C}P^n$ is defined to be the space of complex lines through the origin of \mathbb{C}^{n+1} . Thus the point z_0, z_1, \dots, z_n is equivalent to the point $\mu z_0, \mu z_1, \dots, \mu z_n$ for all $\mu \in \mathbb{C} - 0$. If $z_i \neq 0$ on this line, we may associate to this line the coordinates $z_0/z_i, z_1/z_i \dots z_n/z_i$ with z_i/z_i omitted.

In quantum-mechanics $\mathbb{C}P^n$ describes the *rays* of the wavefunctions

$$|\psi\rangle = z_0|0\rangle + z_1|1\rangle + \dots z_n|n\rangle \quad (2.2)$$

where $|0\rangle, |1\rangle \dots |n\rangle$ is an orthogonal basis function. The coordinates z_j/z_i ($j \neq i, z_i \neq 0$) describe the space of rays, e.g., in the solution of Schrodinger equation for n -level atomic system.

2.1.3 SO(3) Manifold

The rotations of a vector $\vec{r}(t)$ in \mathbb{R}^3 space are described by the SO(3) group. for a 1 parameter group with angular velocity $\vec{\omega}$ we get

$$\left. \frac{d\vec{r}(t)}{dt} \right|_{t=t_0} = \vec{\omega} \times \vec{r}(t_0) \quad (2.3)$$

Starting from a vector in \mathbb{R}^3 given by (0,0,1), the development of this vector by the SO(3) group will lead to a vector (x, y, z) with a norm 1 ($x^2 + y^2 + z^2 = 1$). The tip of this vector is moving on the surface of a sphere which is defined as the *Poincare sphere*. An important example which is related to the SO(3) group is given by the *Two-Level System* (TLS) described by the wavefunction

$$|\psi\rangle = C_1|\psi_1\rangle + C_2|\psi_2\rangle, \quad (2.4)$$

where C_1 and C_2 are complex numbers. The components of the *Bloch vector* are given by

$$r_1 = \frac{C_1\bar{C}_2 + \bar{C}_1C_2}{\sqrt{2}}; r_2 = \frac{C_1\bar{C}_2 - \bar{C}_1C_2}{\sqrt{2}i}; r_3 = \bar{C}_1C_1 - \bar{C}_2C_2 \quad (2.5)$$

r_1 and r_2 are defined as the components of the complex dipole vector while r_3 is defined as the inversion. The interaction (without any losses) between TLS and resonant (or nearly resonant) em field leads (usually in a rotated system) to rotation of the Bloch vector on the Poincare sphere.

2.1.4 SU(2) Manifold

SU(2) algebra consists of 2×2 Hermitian matrices with trace zero where the basis of these matrices is given by Pauli matrices σ_1, σ_2 and σ_3 . From

the connection between the Lie algebra of SU(2) and SO(3) one can find the correspondence between these groups. Assuming, for example, 1-parameter subgroup of SU(2):

$$\exp \left[\left(\frac{\sigma_3}{2i} \right) \theta \right] = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}, \quad (2.6)$$

it corresponds to the 1 parameter subgroup of rotation of \mathbb{R} in SO(3)

$$\exp [E_3\theta] = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.7)$$

where

$$E_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad E_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}; \quad E_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad (2.8)$$

More generally the correspondence follows from the fact that the commutation relations (CR) for $\frac{\sigma_1}{2i}$, $\frac{\sigma_2}{2i}$ and $\frac{\sigma_3}{2i}$ are equal to the corresponding CR of E_1 , E_2 and E_3 .

We find that for a change of θ in the range $0 \leq \theta \leq 2\pi$ equation (2.7) describes a closed rotation around the z axis. For the same change of θ the corresponding curve for SU(2) described by equation (2.6) is not a closed curve as it starts at I and ends in $-I$. Only two full rotations of SO(3) will correspond to a full rotation of SU(2). The change in sign of a spin or wavefunction $\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$ under a SU(2) 2π rotation is an important observable effect (see Section (3.1)) for spin- $\frac{1}{2}$ particles.

2.1.5 Cosets of Lie Groups

Let G be a Lie group with an algebra of g elements and $H \in G$ a subgroup. Denoting the algebra elements of H by $e, H_2 \dots H_h$ we form the product $ae = a, aH_2, \dots aH_h$. This aggregate of products is denoted simply as aH . The group elements of G can be given as a finite number g/h of distinct sets of h elements $H, aH, bH \dots$. These sets of elements are defined as the *left cosets* of H in G , and the division of the g elements into these left cosets is defined as G/H . We have shown that $SU(2)$ is the *double covering* of $SO(3)$, so that $SO(3)$ can be written as $SO(3) = SU(2)/Z_2$, where Z_2 is the group with the two elements ± 1 .

2.1.6 $SU(1,1)$ Manifold

The generators $K_1, K_2, K_3 = J_3$ of the $SU(1,1)$ group obey the CR[82]:

$$[K_i, K_j] = i\tilde{\epsilon}_{ijk}K_k . \quad (2.9)$$

Here $\tilde{\epsilon}_{ijk}$ is the Ricci tensor of a non-Euclidean space:

$$\tilde{\epsilon}_{ijk} = (-1)^{\delta_{k,3}}\epsilon_{ijk} [\tilde{\epsilon}_{123} = -1, \tilde{\epsilon}_{231} = 1, \tilde{\epsilon}_{312} = 1], \quad (2.10)$$

where $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$ and δ is the Kronecker symbol. ϵ with noncyclic transformations of the indices 1,2,3 gives -1, and all other components of ϵ_{ijk} (where two or three indices are equal) vanish. An important example describing $SU(1,1)$ manifold appears in the treatment of squeezed em fields. For a single mode of the em field with creation and annihilation operators a^\dagger

and a , respectively, where $[a, a^\dagger] = 1$, the generators K_1, K_2 and K_3 can be given as [50]:

$$K_1 = -i(aa - a^\dagger a^\dagger)/4; K_2 = (aa + a^\dagger a^\dagger)/4; K_3 = J_3 = \frac{aa^\dagger + a^\dagger a}{4} \quad (2.11)$$

Squeezed em field are produced by the unitary operator

$$S = \exp[ir(K_1 \cos \theta + K_2 \sin \theta)] \quad (2.12)$$

operating on the Fock state $|n\rangle$ or the coherent state $|\alpha\rangle$.

Let us consider a Hamiltonian given as [82]

$$H = \tau_1 K_1 + \tau_2 K_2 + \tau_3 K_3 . \quad (2.13)$$

The Bloch equations for $\vec{K} = (K_1, K_2, K_3)$ are given by

$$\frac{d\langle \vec{K} \rangle}{dt} = \vec{\tau} \tilde{\times} \langle \vec{K} \rangle \quad (2.14)$$

where the $SU(1, 1)$ vector product $\tilde{\times}$ is defined as [82]

$$\vec{\tau} \tilde{\times} \langle \vec{K} \rangle = \tilde{\epsilon}_{ijk} \tau_i \langle K_j \rangle . \quad (2.15)$$

During the evolution $\langle \vec{K} \rangle \cdot \langle \vec{K} \rangle = -\langle K_1 \rangle^2 - \langle K_2 \rangle^2 + \langle K_3 \rangle^2$ is conserved and the vector $\langle \vec{K} \rangle$ which starts from $\langle \vec{K}(0) \rangle = (0, 0, 1)$ stays on the unit hyperboloid, i.e. on the *Poincare hyperboloid*. Due to this conservation law one can specify the vector $\langle \vec{K} \rangle$ by its coordinates $\langle K_1 \rangle, \langle K_2 \rangle$.

2.2 Cartan Exterior Algebra

2.2.1 Tangent and Cotangent Space

Let us consider a point p on n -dimensional manifold surface M with coordinates x^i . A basis for the *tangent vector space* T_p of M at p is given by $(\partial/\partial x^i)$. For a differential dx^i of a coordinate x^i we use the definition

$$\langle dx^i \frac{\partial}{\partial x^j} \rangle = \frac{\partial x^i}{\partial x^j} = \delta_j^i. \quad (2.16)$$

For a vector $(v^j \partial/\partial x^j)$ belonging to the tangent vector space T_p we get

$$\langle dx^i \sum_j v^j \frac{\partial}{\partial x^j} \rangle = v^i \quad (2.17)$$

dx^i or a linear combination $\sum_i a_i dx^i$ is defined as a *differential form*. The differential forms on the manifold at point p are defined as the *cotangent space* T_p^* .

We can generalize the basic element of $T_p(M)$ and $T_p^*(M)$ to tensor fields over M [5-9].

2.2.2 Cartan's Wedge Product

The Cartan's product defined as *wedge product* or as *exterior product* is the antisymmetric tensor product of cotangent space basis elements. For example

$$dx \wedge dy = \frac{1}{2}(dx(\times)dy - dy(\times)dx) = -dy \wedge dx \quad (2.18)$$

where (\times) denotes here an oriented two-dimensional multiplication surface instead of ordinary multiplication and \wedge denotes exterior product. By definition

$$dx \wedge dx = dy \wedge dy = 0. \quad (2.19)$$

The differential elements dx and dy are *differential 1-forms*. The wedge product is a rule for constructing *2-forms* out of *1-forms*. A j -form on a manifold at a point p is given as

$$\omega^j(p) = f_{i_1, i_2 \dots i_j}(p) dx^{i_1} \wedge dx^{i_2} \wedge \dots \wedge dx^{i_j} \quad (2.20)$$

where the antisymmetric tensor $f_{i_1, i_2 \dots i_j}(p)$ having j indices is contracted with the wedge product of j differentials

2.2.3 Exterior Derivative and Stokes Formula

Exterior derivative, takes the j forms into $j + 1$ forms according to the rule

$$\begin{aligned} d(f(x)) &= \frac{\partial f}{\partial x^i} dx^i, \\ d(f_j(x) dx^j) &= \frac{\partial f_j}{\partial x^i} dx^i \wedge dx^j, \\ d(f_{jk}(x) dx^j \wedge dx^k) &= \frac{\partial f_{jk}}{\partial x^i} dx^i \wedge dx^j \wedge dx^k, \text{ etc} \end{aligned} \quad (2.21)$$

We use the convention that new differential line element is always inserted before any previously existing wedge product.

The exterior derivative on any form ω_j gives zero when applied twice

$$d\omega_j(p) = 0. \quad (2.22)$$

The rule for differentiating the wedge product of a j -form α_j and a q -form β_q is given by

$$d(\alpha_j \wedge \beta_q) = d\alpha_j \wedge \beta_q + (-1)^j \alpha_j \wedge d\beta_q. \quad (2.23)$$

In an oriented manifold two coordinate systems ϕ_i and ϕ_j in the overlapping $O_i \cap O_j$ are related by positive definite Jacobians.

If M is a j -dimensional oriented manifold with a boundary ∂M , then *Stokes theorem* says that for any $(j - 1)$ -form ω_{j-1}

$$\int_M d\omega_{j-1} = \int_{\partial M} \omega_{j-1} . \quad (2.24)$$

For further explanations about this theorem and applications see Refs. 5-9.

2.2.4 Homology and Cohomology

For a smooth connected manifold we define a *j-chain* a_j as a formal sum $\sum_i c_i N_i$ where the N_i are smooth p -dimensional oriented submanifolds of M . If the coefficient c_i are real (complex) then a_j is a real (complex) j chain; if the coefficients c_i are integers a_j is an integer chain.

We define ∂ as the operation of taking the oriented boundary, i.e., $\partial a_j = \sum_i c_i \partial N_i$ is a $j - 1$ chain. The set of *cycles* is defined as the set of a_k chains for which $\partial a_j = 0$, i.e. cycles are chains with no boundaries. *Boundaries* B_j are defined as chains which can be written as $B_j = \partial a_{j+1}$. The *simplicial homology* of M is defined as

$$H_j = Z_j / B_j \quad (2.25)$$

H_j is the set of equivalence classes of cycles Z_j which differ only by boundaries, i.e., $z'_j \simeq z_j$ if $z'_j - z_j = \partial a_{j+1}$.

We have exterior differential forms on M^n :

$$\begin{aligned} A^j &:= \text{all smooth } j\text{-forms on } M \\ Z^j &:= \text{all forms } \omega_j \text{ which are } \textit{closed}, \text{ i.e., for which } d\omega_j = 0. \\ B^j &:= \text{all forms which are } \textit{exact}, \text{ i.e., where } \omega_j = d\alpha_{j-1} \end{aligned} \quad (2.26)$$

de Rham cohomology is defined as

$$H^j = Z^j / B^j, \text{ i.e., closed forms modulo exact forms} \quad (2.27)$$

$$\omega_j \simeq \omega'_j \text{ iff } \omega_j = \omega'_j + d\alpha_{j-1} \text{ for some } \alpha_{j-1} . \quad (2.28)$$

We define

$$b_j = \dim H_j = \dim H^j \quad (2.29)$$

as the j 'th Betti number, i.e., it is equal to the dimension of H_j which is dual to H^j . The alternating sum of the Betti numbers for a smooth manifold with n dimensions is *Euler characteristic* given as

$$\chi(M) = \sum_{j=0}^n (-1)^j b_j . \quad (2.30)$$

One can find in the literature relations between Euler characteristic and Gauss-Bonnet theorems [5-9] representing integrations over all the manifold giving certain integers.

2.2.5 Complex Manifolds

For a manifold with n complex coordinates

$$z_k = x_k + iy_k \quad (k = 1, 2 \dots n) \quad (2.31)$$

$$\frac{\partial}{\partial z_k} = \frac{1}{2} \left(\frac{\partial}{\partial x_k} - i \frac{\partial}{\partial y_k} \right); \quad \frac{\partial}{\partial \bar{z}_k} = \frac{1}{2} \left(\frac{\partial}{\partial x_k} + i \frac{\partial}{\partial y_k} \right) \quad (2.32)$$

$$dz_k = dx_k + idy_k; \quad d\bar{z}_k = dx_k - idy_k \quad (2.33)$$

A function f of the manifold complex coordinates is *holomorphic* if

$$df = \sum_{k=1}^n \frac{\partial f}{\partial z_k} dz_k = \partial f \quad (2.34)$$

and for which

$$\bar{\partial}f = \sum_{k=1}^n \frac{\partial f}{\partial \bar{z}_k} d\bar{z}_k = 0 . \quad (2.35)$$

The *complex tangent and cotangent* spaces are defined as:

$$T_c(M) = \left\{ \frac{\partial}{\partial z_k} \right\} ; \quad \bar{T}_c = \left\{ \frac{\partial}{\partial \bar{z}_k} \right\} \quad (2.36)$$

$$T_c^*(M) = \{dz_k\} ; \quad \bar{T}_c^* = d\bar{z}_k . \quad (2.37)$$

The theory of complex manifolds will be used later in connection with Kahler manifolds.

2.3 Fibre-Bundles and Differential Geometry

In the present Section basic concepts of *differential geometry* in relation to *fibre-bundle* theories are explained [5-9].

2.3.1 Fibre-Bundle Definition and Properties

Fibre-bundle is defined by the following collection of requirements:

- a. We have a certain manifold M which is defined as the *basis space* X .
- b. We have another manifold F called the *fibre* which is defined over the space X .
- c. The total space E includes both the basis space X and the fibre F and a *projection* π of E onto $X : \pi E \rightarrow X$. A fibre-bundle E over M with a fibre F is covered with a set of *local neighborhoods* $\{U_i\}$ where in each U_i the bundle E is described by the product $U_i \times F$.

- d. The bundle E is specified by a set of *transition functions* $\{\phi_{ij}\}$ which transform the fibre manifolds between two neighborhoods $U_i \cap U_j$.
- e. There is a set of open coordinate neighborhoods U_α covering X where for each U_α

$$\pi^{-1}U_\alpha \rightarrow U_\alpha \times F \quad (2.38)$$

Although the *local topology* of the bundle is trivial the *global topology* of the *fibre-bundle* may be quite complicated as a consequence of nontrivial transition functions.

- f. If $x \in X$, i.e., if x is a certain element in the base space X , $\pi^{-1}(x)$ is the *fibre* f over x , i.e., f is the fibre corresponding to x . An element of the bundle E can be written as (x, f) , $f \in F$, $x \in U_\alpha$ where U_α is a certain neighborhood of X .
- g. If $(x, f) \in U_\alpha \times F$ and $(x', f') \in U_\beta \times F$ then $(x, f) \sim (x', f')$ if $x = x'$ and $\phi_{\alpha\beta}(x)f = f'$ where \sim denotes equivalence relation.

A *section* s of a fibre-bundle is given by a preferred point $s(x) \in f(x)$ on each fibre corresponding to a point x of the base manifold $X \equiv M$.

2.3.2 Connection on Riemannian Manifolds

For a Riemannian manifold and a local coordinate system $(U; u^i)$ the length ds of an *infinitesimal tangent vector* is given by

$$ds^2 = g_{ij} du^i du^j \quad (2.39)$$

where $g_{ij} = g_{ji}$. For the unit sphere, which is a special case of Riemannian manifold,

$$ds^2 = d\theta^2 + \sin^2 \theta d\phi \quad (2.40)$$

where θ and ϕ are the spherical angles.

In each neighborhood U of the basis manifold, the fibres which are expressed as $\pi^{-1}U$, can be given by a linear combination of the *local frame coordinates* $\{\hat{e}_1, \hat{e}_2 \dots \hat{e}_n\}$. A curve $\vec{x}(t)$ on the manifold which is a function of parameter t can be *lifted* to a *local section* in the fibre given as

$$s(\vec{x}) = \sum_{i=1}^n \hat{e}_i(\vec{x}) z^i(\vec{x}) \quad (2.41)$$

The local basis of coordinates of the tangent space $T(E)$ is given by $(\partial/\partial x^\mu, \partial/\partial z^i)$ and of the cotangent space is given by (dx^μ, dz^i) , where x^μ and z^i are the coordinate of the basis and the fibre, respectively. A curve $\vec{x}(t)$ in the basis M is *lifted* to a curve

$$C(t) = (x^\mu(t), z^i(t)) \quad (2.42)$$

in the total bundle. Differentiation along $C(t)$ is given by

$$\frac{d}{dt} = \dot{x}^\mu \frac{\partial}{\partial x^\mu} + \dot{z}^i \frac{\partial}{\partial z^i}, \quad (2.43)$$

where the transformation of the fibres obey the *parallel transport equation*

$$\dot{z}^i + \Gamma_{\mu j}^i \dot{x}^\mu z^j = 0 \quad (2.44)$$

and $\Gamma_{\mu j}^i$ are referred to as the *Levi-Civita connections* (or Christoffel symbols).

We get

$$\frac{d}{dt} = \dot{x}^\mu \left(\frac{\partial}{\partial x^\mu} - \Gamma_{\mu j}^i z^j \frac{\partial}{\partial z^i} \right) = \dot{x}^\mu D_\mu \quad (2.45)$$

where the operator in the brackets of equation (2.45) is defined as the *covariant derivative* D_μ . One should notice that the covariant derivative assumes the *parallel transport* of equation (2.44). The change in the total space E is split into *vertical* and *horizontal* components. The vertical components with basis $(\partial/\partial z^i)$ represent changes which are strictly in the fibre and are *not coupled* to changes in the manifold basis. Such *vertical* components have no effect on the physical state. Eq. (2.45), based on the parallel transport, describes the change in the physical state along the curve $\vec{x}(t)$. The first term in the brackets of this equation represents ordinary derivative while the second term represents changes in the fibre which are coupled to the manifold basis. The above equations have been used for Schrodinger equation [83] and were reduced to simple forms where the fibre was found to be the geometric Berry's phase. Under a change in frame we obtain

$$z'^i = \phi_{ij}(\vec{x})z^j, \quad e'_j = e_i\phi_{ij}^{-1}(\vec{x}) \quad (2.46)$$

where these sections are invariant

$$s(\vec{x}) = e_i z^i = e'_i z'^i = s'(\vec{x}) . \quad (2.47)$$

Curvature measures the extent to which parallel transport is path dependent and it is given by the commutators of D_μ and D_ν . The calculations of the connections Γ_{jk}^i and the curvatures might be quite complicated for general cases and the reader is referred to the literature [5-9]. Also one finds equations relating the connections to the metric coefficients g_{ik} . [5-9]

2.3.3 Connections of Vector Bundles

Tangent bundle TM^n to a manifold is defined for each patch of the manifold by a corresponding set of coordinates u tangent to the manifold. the vector field \vec{Q} tangent to the manifold is given by (See Section 2.2.1)

$$\vec{Q} = \left(Q_1 \frac{\partial}{\partial u^1}, Q_2 \frac{\partial}{\partial u^2} \cdots Q_n \frac{\partial}{\partial u^n} \right) \quad (2.48)$$

where $\frac{\partial}{\partial u^1}, \frac{\partial}{\partial u^2} \dots \frac{\partial}{\partial u^n}$ is the basis for the vector bundle and $Q_1, Q_2 \dots Q_n$ are the components of the vector field. The *cotangent bundle* T^*M^n is a *covector* field where the basis for the cotangent bundle is given by $du^1, du^2 \dots du^n$ and the covector field components are given by A_1, A_2, \dots, A_n . In the overlap between the two patches U_1 and U_2 the same vector fields can be transformed from one patch U_1 to another U_2 by transition functions [5-9]. The *connections* on a surface M^2 in \mathbb{R}^3 of a vector-bundle have special simple forms. (A nice exercise which derives the Levi Civita connections on the manifold M^2 can be found in Ref. 5.)

Let us assume that we have a manifold surface M^2 in the space \mathbb{R}^3 and let \vec{v} be a vector field that is tangent to M at a point p . Let us assume also that we have a curve on the surface M which is a function of *parameter* t and whose tangent at p is the vector \vec{x} . We define the *covariant differentiation* $\nabla_{\vec{x}}\vec{v}$ of a vector field \vec{v} at the point p as the projection of the ordinary derivative $\frac{d\vec{v}}{dt}$ on the vector \vec{x} . The covariant differentiation is obtained by throwing away the normal component of the ordinary partial derivative. The covariant differentiation differs from the ordinary partial derivative and the quantity

that measures this difference is called the *connection*. The components of the covariant differentiation of the vector \vec{v} can be written as [6]:

$$(\nabla_{\dot{x}}\vec{v})^\alpha = \frac{dv^\alpha}{du^\beta}x^\beta + \Gamma_{\beta\gamma}^\alpha v^\gamma x^\beta \quad (2.49)$$

The first term on the right side of Eq.(2.49) represents the ordinary derivative while the second term represents the connection. We say that $\vec{v}(t)$ is *parallel transported* along the curve which is a function of parameter t

$$\nabla_{\dot{x}}\vec{v} = 0 , \quad (2.50)$$

i.e., the covariant differentiation along the tangent \dot{x} to the curve vanishes.

A geodesic curve is defined by

$$\nabla_{\dot{x}}(\dot{x}) = 0 \quad (2.51)$$

so that the covariant differentiation of \dot{x} has only a component normal to the surface, and the geodesic equation obtains the form [5-9]:

$$\frac{d^2x^\mu}{dt^2} + \Gamma_{\lambda\sigma}^\mu \frac{dx^\lambda}{dt} \frac{dx^\sigma}{dt} = 0 \quad (2.52)$$

The change in angle of the vector \vec{v} when it is parallel transported along a closed circuit on the manifold basis is called the *holonomy angle*. The *holonomy matrix* is the matrix which rotates the vector \vec{v} for this closed parallel transportation. For vector \vec{v} in \mathbb{R}^3 and a manifold M^2 one gets a 3×3 holonomy matrix. The set of all holonomy matrices form a group called the *holonomy group*.

2.3.4 Connections on Principal Bundles

A *principal bundle* is a fibre-bundle where the fibre is a Lie group G acting on a manifold. Both the transition functions and the fibres belong to g algebra and act on G by left multiplication. The Maurer-Cartan form $g^{-1}dg$ is a matrix of one-forms belonging to the Lie algebra g . The coordinates of the principal bundle P are given by (x, g) where $g \in G$. A *local section* of P is a map from a neighborhood U of the manifold basis to G . Connection on a principal bundle provides a rule for the parallel transport of sections.

In any matrix group G , $g^{-1}dg$ is a matrix with left invariant 1-form entries. For example, in $SO(2)$, for

$$g(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad (2.53)$$

we have

$$g^{-1}dg = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} (\times)d\theta \quad (2.54)$$

and $d\theta$ is a rotation invariant 1-form on the circle $SO(2)$. Let h be a given (*fixed*) group element then $(hg)^{-1}d(hg) = g^{-1}h^{-1}hdg = g^{-1}dg$, as claimed.

The connection on P is 1-form ω in $T^*(P)$ whose vertical component is the Maurer-Cartan form $g^{-1}dg$, and it can be written as

$$\omega = g^{-1}Ag + g^{-1}dg \quad (2.55)$$

where

$$A(\vec{x}) = A_\mu^a(\vec{x}) \frac{\lambda_a}{2i} dx^\mu \quad (2.56)$$

satisfy

$$\left[\frac{\lambda_a}{2i}, \frac{\lambda_b}{2i} \right] = f_{abc} \left(\frac{\lambda_c}{2i} \right) \quad (2.57)$$

where f_{abc} are the structure constants.

If $\vec{x}(t)$ is a curve in M , the sections $g_{ij}(t)$ are defined to be parallel transported along $\vec{x}(t)$ if the following matrix differential equation is satisfied

$$g^{-1} \frac{dg}{dt} + g^{-1} \left(A_{\mu}^a(\vec{x}) \left(\frac{\lambda_a}{2i} \right) \frac{dx^{\mu}}{dt} \right) g = 0. \quad (2.58)$$

The curvature is *Lie algebra matrix 2-form* given by [5-9]:

$$\Omega = d\omega + \omega \wedge \omega = g^{-1} F g \quad (2.59)$$

where

$$F = dA + A \wedge A \quad (2.60)$$

Let us consider two overlapping neighborhoods U and U' and a transition function ϕ relating the local fibre coordinates g and g' , respectively, in U and U' , then [5-9]:

$$g' = \phi g . \quad (2.61)$$

In the overlapping region $U \cap U'$, A transforms as

$$A' = \phi A \phi^{-1} + \phi d\phi^{-1} \quad (2.62)$$

while F transforms as

$$F' = \phi F \phi^{-1} \quad (2.63)$$

The above equations for *Principal Bundles* are especially important for the use of non-abelian geometric phases in holonomic quantum computation [22-26].

2.3.5 Chern Classes

The use of *characteristic polynomial* has been developed extensively in the literature [5-9] for various *classes*. We give here short explanation about *Chern Classes*, in relation to integration over manifolds [5-9].

Let α be a complex $k \times k$ matrix and $P(\alpha)$ a polynomial in the components of α . Then $P(\alpha)$ is called *invariant polynomial* or *characteristic polynomial* if

$$P(\alpha) = P(g^{-1}\alpha g) \quad (2.64)$$

for all $g \in GL(k, \mathbb{C})$. An example of invariant polynomial is given by $\text{Det}(I + \alpha)$ which is used to define the Chern classes. The total *Chern form* is defined as:

$$C(\Omega) = \text{Det} \left(I + \frac{i}{2\pi} \Omega \right) = C_0 + C_1(\Omega) + C_2(\Omega) + \dots \quad (2.65)$$

where

$$C_0 = 1; \quad C_1 = \frac{i}{2\pi} \text{Tr}(\Omega); \quad C_2 = \frac{1}{8\pi^2} \{ \text{Tr}(\Omega \wedge \Omega) - \text{Tr}(\Omega) \wedge \text{Tr}(\Omega) \}, \quad (2.66)$$

etc.

If we integrate $C_j(\Omega)$ over any $2j$ cycle in M with integer coefficients, we obtain an integer! The *Chern numbers* [5] of a bundle are the numbers which result from integration characteristic polynomials over the entire manifold. An example of Chern number will be described later (see Section 2.2.4 for the definitions of *cycles* and *cohomology groups*, and see the relations between Chern numbers and cohomology groups as analyzed in Refs. [5-9].)

Chapter 3. General Theories of Topological Phases

3.1 Berry's Phases for Schrodinger Equation under the Adiabatic Approximation

In the present Section we summarize the main results obtained by Berry in his paper of 1984 [4]. Although there is no experimental evidence for the existence of magnetic charges or monopoles, the interest in such monopoles arose in the scientific area of Berry's phases due to the fact that *formally* certain Berry's phases systems have the same *mathematical structure* as the Dirac magnetic monopole [84-88].

3.1.1 Magnetic Monopole

We give here only a short description of the fibre-bundle structure of magnetic monopole [Ref. 75, p. 119].

For a single monopole at the origin it is convenient to describe the gauge potential by spherical coordinates.

$$A_r = A_\theta = 0, \quad A_\phi = \left(\frac{n}{2}\right)(1 - \cos\theta) \quad (3.1)$$

A_ϕ has a 'Dirac string' singularity along the line $\theta = \pi$; there the magnitude of A_ϕ

$$g^{\phi\phi} A_\phi A_\phi = \frac{n(1 - \cos\theta)^2}{2 \sin^2\theta}. \quad (3.2)$$

The string can be moved around by means of a gauge transformation

$$A \rightarrow A - \nabla\Lambda \quad (3.3)$$

but it cannot be removed.

In order to avoid singular gauge potential, Wu and Yang [87] introduced the following construction. They covered S^2 with two patches S^+ and S^- :

$$\begin{aligned} S^+ &\equiv \left\{ \theta, \phi; 0 \leq \theta < \frac{\pi}{2} + \epsilon \right\}, \\ S^- &\equiv \left\{ \theta, \phi; \frac{\pi}{2} - \epsilon < \theta \leq \pi \right\}, \end{aligned} \quad (3.4)$$

two open sets that respectively contain the northern and southern hemispheres and whose intersection is an open set containing the equator. Over each patch, the restricted bundle is isomorphic to the trivial bundle $S^\pm \times U(1)$. We break S^2 into the two hemispherical neighborhoods

$$\begin{aligned} S^+ \times U(1), & \text{ coordinates } \theta, \phi, e^{i\psi_+} \\ S^- \times U(1), & \text{ coordinates } \theta, \phi, e^{i\psi_-}. \end{aligned} \quad (3.5)$$

The transition functions must be function of ϕ along $S^+ \cap S^-$ and must be elements of $U(1)$ to give a *principal bundle*. We therefore choose to relate the S^+ and S^- fibre coordinates as follows

$$e^{i\psi_-} = e^{in\phi} e^{i\psi_+}. \quad (3.6)$$

The *winding number* n must be integer for the resulting structure to be a manifold, i.e., the fibres must fit together exactly when we complete a full rotation around the equator in ϕ . This is a topological version of the Dirac monopole *quantization condition*.

Using the above construction we can specify a non-singular gauge potential for the magnetic monopole field. One choice is

$$A_\phi^+ = \left(\frac{n}{2}\right)(1 - \cos \theta) \text{ over } S^+; \quad A_\phi^- = \left(\frac{n}{2}\right)(-1 - \cos \theta) \text{ over } S^-. \quad (3.7)$$

After straightforward calculations one finds [5] that the curvature of the magnetic monopole is given by

$$F = \left(\frac{n}{2}\right) \sin \theta d\theta \wedge d\phi \quad (3.8)$$

The total Chern class of U(1) bundle is given by [5]

$$C(P) = 1 + C_1(P) = 1 - \frac{F}{2\pi} . \quad (3.9)$$

The integral of C_1 for the Dirac monopole U(1) bundle, over S^2 is integer giving the monopole charge

$$\int_{S^2} \frac{F}{2\pi} = -n . \quad (3.10)$$

3.1.2 Berry's Treatment of Geometrical Phases Related to Magnetic Monopole Formalism

Due to the importance of Berry's article of 1984 [4], which led to a breakthrough in this field, we summarize here some of its essential results.

Using the adiabatic approximation Berry assumed physical systems which are transported around a closed path in parameter space $\vec{R}(t)$, with Hamiltonian $H(\vec{R}(t))$ such that $\vec{R}(T) = \vec{R}(0)$, and for simplicity \vec{R} was assumed to be three dimensional. The path is called circuit and denoted by C . In addition to the dynamical phase, a geometrical phase is obtained. After some calculations and using Stokes theorem a special form for the geometric phase was obtained [4]

$$\gamma_n(C) = - \int \int_C d\vec{S} \cdot \vec{V}_n(\vec{R}) \quad (3.11)$$

where $d\vec{S}$ denotes area element in \vec{R} space, n denotes a certain nondegenerate eigenstate of the Hamiltonian and $\vec{V}_n(\vec{R})$ is given as [4]

$$\vec{V}_n(\vec{R}) \equiv \text{Im} \sum_{m \neq n} \frac{\langle n(\vec{R}) | \vec{\nabla}_{\vec{R}} H(\vec{R}) | m(\vec{R}) \rangle \times \langle m(\vec{R}) | \vec{\nabla}_{\vec{R}} H(\vec{R}) | n(\vec{R}) \rangle}{[E_m(\vec{R}) - E_n(\vec{R})]^2}. \quad (3.12)$$

Berry treated the case in which the circuit C lies close to a point \vec{R}^* in parameter space at which the state n is *involved in degeneracy*. He considered the most common situation, where the degeneracy involves only two states denoted by $+$ and $-$, and where $E_+(\vec{R}) \geq E_-(\vec{R})$. For a circuit which starts at $+$ state, he obtained after some calculations

$$V_+(\vec{R}) = \frac{\vec{R}}{2R^3} \quad (3.13)$$

where by using equation (3.13) for $V_n(\vec{R}) = V_+(\vec{R})$ in equation (3.11), the phase change $\gamma_+(C)$ is equal to the flux through C of the magnetic field of a monopole with strength $-\frac{1}{2}$ located at the degeneracy $\vec{R} = 0$. Obviously $V_-(\vec{R}) = -V_+(\vec{R})$ so that $\gamma_-(C) = -\gamma_+(C)$. The geometric phase factor associated with C is then given by

$$\exp\{i\gamma_{\pm}(C)\} = \exp\left[\pm\frac{1}{2}\Omega(C)\right] \quad (3.14)$$

where $\Omega(C)$ is the *solid angle* that C subtends at the degeneracy.

Berry [4] treated the case of a particle with spin S (integer or half integer) interacting with a magnetic field \vec{B} via the Hamiltonian

$$H(\vec{B}) = \kappa\hbar\vec{B} \cdot \vec{S} \quad (3.15)$$

where κ is a constant involving the gyromagnetic ratio and \vec{S} is the vector spin operator with $2S + 1$ eigenvalues n that lie between $-S$ and $+S$. The eigenvalues are

$$E_n(\vec{B}) = \kappa \hbar B n \quad (3.16)$$

and so there is a $2S + 1$ -fold degeneracy when $\vec{B} = 0$. The components of \vec{B} correspond to the parameters \vec{R} used in the previous analysis. The phase change $\gamma_n(C)$ has been calculated [4] for the case in which \vec{B} is slowly varied (and hence the spin rotated) round a circuit C in the *direction* along \vec{B} .

After some calculations Berry [4] got the result:

$$\vec{V}_n(\vec{B}) = \frac{n\vec{B}}{B^3} . \quad (3.17)$$

Now, the use of Eq. (3.13) shows that $\gamma_n(C)$ is the flux through C of the “magnetic field” of a monopole with strength $-n$ located at the origin of magnetic field space. Thus the geometric phase factor is given by

$$\exp \{i\gamma_n(C)\} = \exp \{-in\Omega(C)\} \quad (3.18)$$

where $\Omega(C)$ is the solid angle that C subtends at $\vec{B} = 0$.

3.2 Geometric Description of the Berry’s Phase without the Adiabatic Approximation

If a quantum system is initially in an eigenstate of the Hamiltonian and is changing with time, according to slowly varying parameters, the adiabatic conditions guarantee that it remains in an eigenstate of the instantaneous Hamiltonian. Assuming an initially eigenstate of the Hamiltonian

$$H(\vec{R})|n, \vec{R}\rangle = E_n(\vec{R})|n, \vec{R}\rangle, \quad (3.19)$$

and parameters \vec{R} , which are slowly varying along a closed curve C in parameter space in time T , the geometrical phase factor is given by [4]:

$$\gamma_n(C) = i \oint d\vec{R} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle . \quad (3.20)$$

This phase is given in addition to the dynamical phase given by

$$\phi_{\text{dyn}} = - \int_0^T E_n(\tau) d\tau . \quad (3.21)$$

Considering the state vector $|\psi(t)\rangle$, Aharanov and Anandan [11] removed its dynamical phase factor, by defining a new state:

$$|\phi(t)\rangle = \exp \left[i \int_0^t h(t') \right] |\psi(t)\rangle , \quad (3.22)$$

where

$$h(t') = \langle \psi | \psi \rangle^{-1} \text{Re} \langle \psi(t') | H(t') | \psi(t') \rangle . \quad (3.23)$$

The geometrical phase factor is then given, without any adiabatic approximation, by

$$\gamma_{\text{geom.}} = i \oint d\vec{R} \cdot \langle \phi(\vec{R}, t) | \vec{\nabla}_{\vec{R}} | \phi(\vec{R}, t) \rangle . \quad (3.24)$$

The term $\langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle$ of equation (3.20), or the term $\langle \phi(\vec{R}, t) | \vec{\nabla}_{\vec{R}} | \phi(\vec{R}, t) \rangle$ of equation (3.24), is referred to as a vector potential.

Topological effects obtained from closed circuits are referred to in the literature as holonomy (like the present treatment of a change of phase in Schrodinger equation, a change of angle of polarization in optics, etc.). By using Stokes theorem, integration over a closed circuit can be transformed to integration over the closed surface. In topological theories $d\vec{R} \cdot \langle n \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle$

can be considered as ‘one form’ while the integration over the surface is considered as the integration over the ‘curvature two-form’.

As in electromagnetic theory the vector potential is defined up to a gauge transformation. By performing the transformation

$$|n, \vec{R}(t)\rangle' = \exp(i\alpha_n(\vec{R}))|n, \vec{R}(t)\rangle \quad (3.25)$$

we induce a “gauge transformation” on $\vec{A}_{\vec{R}}(n, t)$:

$$\vec{A}'_{\vec{R}}(n, t) = \vec{A}_{\vec{R}}(n, t) - \vec{\nabla}_{\vec{R}}(\alpha_n(\vec{R})) . \quad (3.26)$$

From the definition of Berry phase given by equation (3.20) it is clear that the Berry phase is gauge invariant for a closed circuit.

The same conclusion is obtained for the vector potential defined by equation (3.24).

The movement of the wavefunction $\phi(\vec{R}, t)$ as a function of the parameters \vec{R} is considered in fibre-bundle theories as a movement along the basis $\phi(\vec{R}, t)$. This movement can be ‘lifted’ to the ‘total space’ as the ‘section’ which includes the change of the ‘fibre’, i.e., the change in the geometric phase as a function of the change of the ‘fibre-bundle basis’. The use of equation (3.20) or (3.24) is explained in ‘fibre-bundle’ theories as parallel transport of the Schrodinger wavefunction [83,64-65]. An important point here is that the change of the fibre is given uniquely as a function of changes in the manifold basis. For many experiments on geometric phases the total space is given by the manifold SU(2) while the fibre is U(1) and the basis is SU(2)/U(1). However, other manifolds can be used with different fibres. In the above

treatment both the dynamical and geometrical phase are included in the fibre where the first part has local properties (depending on the wavefunction at a certain time) while the latter has global properties (depending on closed circuit in parameter space).

The Berry's geometric phase is similar to the geometric phase obtained in AB effect, in which electron acquires a topological phase shift after encircling a solenoid. Although such phase shift is calculated for a closed circuit [1], this phase can be observed by a shift in the interference pattern for electrons propagating from their source into two routes, to their final observation points. Mathematically, therefore, a closed circuit is obtained by reversing the propagation direction in one of the two electron routes. In order to obtain the topological phase one has to eliminate the dynamical contribution to the phase difference, which can follow from different optical paths in the two routes which interfere.

The advantage of using closed circuits for observing topological phases is that the results are gauge invariant and also that Stokes theorem can be used. The use of closed circuits shows the relation between topological phase and singular points. For vector bundles singularity is obtained at the point at which the vector field, e.g., the vector potential vanishes, as in this point the direction of the vector field is undefined. An important point in this connection is that geometric phases, as those defined by Berry [4,11] can be obtained only if the number of components of \vec{R} is larger than 1, so that it can encircle a singular point. In Section 3.4 we generalize, however, the use of

geometric phases to open circle by following the definition of Pancharatnam phase [36].

3.3 Berry's Phases for a n -Level Atomic Systems and Kähler Metric

3.3.1 Kahler Metric [5-9, 89-91]

We define *complex exterior form* $\Lambda^{p,q}$ which have basis containing p factors of dZ_k and q factors of $d\bar{Z}_j$ with corresponding wedge products [see the analysis and explanations given in Section (2.2)]. The operators ∂ and $\bar{\partial}$ act as:

$$\begin{aligned}\partial : \Lambda^{p,q} &\rightarrow \Lambda^{p+1,q} , \\ \bar{\partial} : \Lambda^{p,q} &\rightarrow \Lambda^{p,q+1}\end{aligned}\tag{3.27}$$

These operators satisfy the relations

$$\partial\partial\omega = 0 , \quad \bar{\partial}\bar{\partial}\omega = 0 , \quad \partial\bar{\partial}\omega = -\bar{\partial}\partial\omega\tag{3.28}$$

We have an *almost complex structure* if there exists a linear map J from $T(M)$ to $T(M)$ such that $J^2 = -1$. For example take a cartesian coordinate system (x, y) on \mathbb{R}^2 and define J by the 2×2 matrix

$$J \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \Rightarrow J^2 \begin{pmatrix} x \\ y \end{pmatrix} = - \begin{pmatrix} x \\ y \end{pmatrix} .\tag{3.29}$$

In this example J is equivalent to multiplication by $i = \sqrt{-1}$.

More generally operator J is defined as an operator which have eigenvalues $\pm i$. No J can be found on odd-dimensional manifold.

Let us consider a Hermitian metric on M given by

$$ds^2 = g_{a\bar{b}} dZ_a d\bar{Z}_b\tag{3.30}$$

where $g_{a\bar{b}}$ is a Hermitian matrix. We define the *Kähler form*

$$K = \left(\frac{i}{2}\right) g_{a\bar{b}} dZ_a \wedge d\bar{Z}_b . \quad (3.31)$$

It is easy to show that $K = \bar{K}$ [5].

A matrix is said to be a *Kähler metric* if $dK = 0$, i.e., if the Kähler form is *closed*.

The *Fubiny-Study metric* on $P_n(\mathbb{C})$ [see Section 2.1.2)] is given by

$$\begin{aligned} K &= \left(\frac{i}{2}\right) \partial\bar{\partial} \ln \left(1 + \sum_{\alpha=1}^n Z^\alpha \bar{Z}^\alpha\right) \\ &= \left(\frac{i}{2}\right) \left(\frac{dZ_\alpha \wedge d\bar{Z}^\beta}{(1 + \sum_\gamma Z_\gamma \bar{Z}^\gamma)^2}\right) \left\{ [\delta_{\alpha\beta} (1 + \sum_\gamma Z_\gamma \bar{Z}^\gamma)] - \bar{Z}_\alpha Z^\beta \right\} . \end{aligned} \quad (3.32)$$

This quite complicated equation has a simple form for the standard metric on S^2 with radius $\frac{1}{2}$ given in complex coordinates by

$$ds^2 = \frac{dx^2 + dy^2}{1 + x^2 + y^2} = \frac{dZ d\bar{Z}}{(1 + Z\bar{Z})^2} \quad (3.33)$$

and the Kähler form is given by

$$K = \left(\frac{i}{2}\right) \frac{dZ \wedge d\bar{Z}}{(1 + Z\bar{Z})^2} = \frac{dx \wedge dy}{(1 + x^2 + y^2)^2} = \left(\frac{i}{2}\right) \partial\bar{\partial} \ln(1 + z\bar{z}) . \quad (3.34)$$

The \ln terms in equations (3.32) and (3.34) are referred to as *Kähler potentials*. The integration of (3.34), multiplied by $\frac{1}{\pi}$, over all the manifold gives 1 (a special form of Gauss-Bonnet theorem with Chern number 1).

3.3.2 Berry's Phase for n -Level Atomic System [92]

Let us take a nondegenerate n -level atomic system so that the quantum system of this Hilbert space is given by $n + 1$ complex amplitudes Z^α where superscripts of Greek indices range from 0 to n

$$|\psi\rangle = |Z^0, Z^1, \dots, Z^n\rangle \quad (3.35)$$

For a normalized state

$$\langle \psi | \psi \rangle = \delta_{\alpha\beta} \bar{Z}^\alpha Z^\beta = \bar{Z}_\beta Z^\beta = 1 \quad (3.36)$$

and this lies on the unit sphere S^{2n+1} in \mathbb{C}^{n+1} .

For $Z^0 \neq 0$ $P_n(\mathbb{C})$ may be given by complex coordinates [see Section (2.1.2)]

$$W^i = Z^i / Z^0 \quad (3.37)$$

where Latin indices range from 1 to n . Using units in which $\hbar = 1$ and denoting time derivative by an overdot one may write the evolution of the quantum state by Hermitian Hamiltonian H as

$$|\dot{\psi}(t)\rangle = -iH(t)|\psi(t)\rangle \Rightarrow \dot{Z}^\alpha = -iH_\beta^\alpha Z^\beta . \quad (3.38)$$

If the evolution undergoes a circuit in ray space, the original state returns to itself up to a phase factor

$$|\psi(T)\rangle = e^{i\phi(T)} |\psi(0)\rangle . \quad (3.39)$$

Part of this phase $\phi(T)$ may be identified as a dynamical phase [see Section (3.2)]:

$$\epsilon(T) = - \int_0^T \frac{\langle \psi(t) | H(t) | \psi(t) \rangle}{\langle \psi(t) | \psi(t) \rangle} dt \quad (3.40)$$

but the remainder

$$\gamma(T) = \phi(T) - \epsilon(T) \quad (3.41)$$

is geometrical and depends purely on the closed path evolution of the ray in projective Hilbert space. After straightforward calculations one gets [92]:

$$\dot{\gamma}(t) dt = \left(\frac{i}{2} \right) \left(\frac{\bar{W}_i dW^i - W_i d\bar{W}^i}{1 + \bar{W}_k W^k} \right) = A , \quad (3.42)$$

so that

$$\gamma(T) = \oint A , \quad (3.43)$$

i.e., the Berry's phase is obtained by integral of the one-form A around the circuit in $P_n(\mathbb{C})$. So that A is the *connection for the geometrical phase*.

By the *Stokes theorem*, one gets

$$\gamma(T) = \int \int_S F \quad (3.44)$$

the integral, over a surface S bounded by the circuit of the *curvature 2-form*

$$F = dA = i \left\{ \frac{\bar{W}_i W_j - (1 + \bar{W}_k W^k) \delta_{ij}}{(1 + \bar{W}_\ell W^\ell)^2} \right\} dW^i \wedge d\bar{W}^j . \quad (3.45)$$

Thus F is an explicit realization of the 2-form given by Simon [10] in terms of the coordinates of $P_n(\mathbb{C})$.

3.4 Pancharatnam Phase and Noncyclic Evolution

Consider two normalized nonorthogonal Hilbert states $|A\rangle$ and $|B\rangle$, and assume further that $|A\rangle$ is exposed to U(1) shift $e^{i\phi}$ [36]. The resulting interference pattern is determined by

$$I = |e^{i\phi}|A\rangle + |B\rangle|^2 = 2 + 2|\langle A|B\rangle| \cos[\phi - \arg\langle A|B\rangle] \quad (3.46)$$

where its maximum is obtained at the Pancharatnam relative phase $\phi_0 \equiv \arg\langle A|B\rangle$. This phase is reduced to the U(1) case whenever $|B\rangle = e^{i\theta}|A\rangle$ as it yields $\arg\langle A|B\rangle = \theta$. In the original treatments of the Berry phase [4] one considers a quantal system evolving around a closed circuit, from an initial wavefunction $|A\rangle$ to a final wavefunction $|B\rangle$ where $|B\rangle$ is obtained

from $|A\rangle$ be a cyclic evolution, i.e., by multiplication with a $U(1)$ phase factor. Although the initial phase of the quantal state is defined arbitrarily, the phase difference between the state $|A\rangle$ and $|B\rangle$ is well defined and can be observed by interferometric methods. In a non-cyclic evolution if the final wave $|B\rangle$ is superimposed on the initial state $|A\rangle$ only the component $\langle A|B\rangle|A\rangle$ along $|A\rangle$ interferes with $|A\rangle$. All other components of $|B\rangle$ which are orthogonal to $|A\rangle$ merely add to the intensity, since their cross terms with $|A\rangle$ vanish. The ‘*Pancharatnam connection*’ defines the phase between $|B\rangle$ and $|A\rangle$ as $\phi_0 = \arg\langle A|B\rangle$. The interference amplitude $|\langle A|B\rangle|$ differs from unity if the evolution is non-cyclic [36] and this difference leads to reduction of the visibility in the interference pattern. The Pancharatnam phase is indeterminate if $|B\rangle$ is orthogonal to $|A\rangle$. The use of Pancharatnam phases to noncyclic evolution raises the problem of gauge invariance.

In order to treat this problem we introduce a more general definition of the geometric phase which is defined also for open circuits and is reduced to that described in the Sections (3.1-3.3) for closed circuits. In Section (3.4.1) we develop such definition and in Section (3.4.2) we apply it to neutron interferometry.

3.4.1 The Geometric Phase for Noncyclic Evolution

Let us assume that under adiabatic approximation the initial state $|n; \vec{R}(0)\rangle$ at time $t = 0$ develop after time t into the state $|n; \vec{R}(t)\rangle$ where this development is not cyclic, i.e. $\vec{R}(t) \neq \vec{R}(0)$. We define the geometric phase as

[93]:

$$\gamma_n(C) = \arg\langle n; \vec{R}(0)|n; \vec{R}(t)\rangle + i \int_{\vec{R}(0)}^{\vec{R}(t)} d\vec{R} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle \quad (3.47)$$

where now C is not a closed circuit. This equation reduces to equation (3.20) for a cyclic motion where the first term on the right side of equation (3.47) vanishes. We have the following relations:

$$R_e \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle = 0; \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle = i \text{Im} \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle . \quad (3.48)$$

Therefore we can write (3.47) as

$$\gamma_n(C) = \arg\langle n; \vec{R}(0)|n; \vec{R}(t)\rangle - \text{Im} \int_{\vec{R}(0)}^{\vec{R}(t)} d\vec{R} \cdot \langle n \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle . \quad (3.49)$$

The crucial point here is that $\gamma_n(C)$ is gauge invariant since the change in the two terms on the right side of equation (3.47) are equal in magnitude and opposite in sign. We can generalize the definition of geometric phase for open cycles without the adiabatic approximation as

$$\gamma_{\text{geom.}}(C) = \arg\langle \phi(\vec{R}, 0) | \phi(\vec{R}, t) \rangle - \text{Im} \int_{\vec{R}(0)}^{\vec{R}(t)} d\vec{R} \cdot \langle \phi(\vec{R}, t) | \vec{\nabla}_{\vec{R}} | \phi(\vec{R}, t) \rangle \quad (3.50)$$

where the function $\phi(\vec{R}, t)$ was defined in Section (3.2). The above equations are obtained after eliminating the dynamical phase from the time evolution and the definitions given here coincide with the definitions of geometric phases of Section (3.2) only for closed circuits.

If the wavefunction depends *only* on one parameter S then $\langle \psi(S) | \dot{\psi}(S) \rangle$ (where the derivative $\dot{\psi}$ is according to parameter S) might be defined as a dynamical phase [40]. For such cases we can define gauge invariant phases

for open circuits by subtracting this dynamical phase from $\langle n, S(0) | n, S(t) \rangle$ [or $\langle \phi(S(0)) | \phi(S(t)) \rangle$] [40]. We find that different definitions of geometric phases can be used, but any definition of geometric phase should be gauge invariant.

Samuel and Bhandari [39] and Jordan [38] solved the problem of gauge invariant geometric phases for open circuits by closing the end points of the open circuit by the shortest ‘geodesic’ line. Then the gauge invariant phase for the open circuit is equal to that obtained from the closed circuit for which one can use the definitions of Section (3.2). In order to explain this ‘trick’ let us use equation (3.47) for a geodesic line (for which $\gamma_n(C) = 0$), starting at $|n, \vec{R}(t)\rangle$ and ending at $|n, \vec{R}(0)\rangle$. For this geodesic line we get $\gamma_n(\text{geodesic}) = 0 = \arg \langle n, \vec{R}(t) | n, \vec{R}(0) \rangle + i \int_{\vec{R}(t)}^{\vec{R}(0)} d\vec{R}_{\text{geod.}} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle$ so that

$$\arg \langle n, \vec{R}(0) | n, \vec{R}(t) \rangle = i \int_{\vec{R}(t)}^{\vec{R}(0)} d\vec{R}_{\text{geod.}} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle \quad (3.51)$$

Substituting equation (3.51) in equation (3.47) we get

$$\gamma_n(C) = i \int_{\vec{R}(0)}^{\vec{R}(t)} d\vec{R} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle + i \int_{\vec{R}(t)}^{\vec{R}(0)} d\vec{R}_{\text{geod.}} \cdot \langle n, \vec{R} | \vec{\nabla}_{\vec{R}} | n, \vec{R} \rangle, \quad (3.52)$$

so that $\gamma_n(C)$ for open cycle given by (3.47) becomes equal to the geometric phase for the closed circuit of (3.52). Although the above analysis has been made by using equation (3.47) under the adiabatic approximation a straightforward analogous treatment can be made for the nonadiabatic case by the use of equation (3.50).

3.4.2 The Use of Pancharatnam Phase in Neutron Interferometry

We discuss here a special experiment in neutron interferometry. Using polarized neutrons Wagh et al. [60,61] have determined phases as well as interference amplitudes for *noncyclic* spinor evolution in *static magnetic fields*. Interferometrically, the noncyclic phase ought to be determined from the shift between U(1) interference without and with the Hamiltonian affecting the evolution [60]. Wagh et al. [61] have presented the first observation of the *noncyclic* phase for neutrons and the associated amplitude of interference. We review here the basic theory [60,37] on which these experiments are based.

The time development of the spin- $\frac{1}{2}$ particle which performs a precession in angle θ around a constant magnetic field $\vec{B} = B\hat{Z}$ is given at time t by the wavefunction

$$|\psi_t\rangle = e^{-i(\phi/2)} \cos\left(\frac{\theta}{2}\right) | + Z \rangle + e^{i(\phi/2)} \sin\left(\frac{\theta}{2}\right) | - Z \rangle \quad (3.53)$$

where the Larmor phase ϕ is given by

$$\phi = -2\mu Bt/\hbar, \quad (3.54)$$

and μ is the magnetic dipole of the particle. Here we assumed that at time $t = 0$ the wavefunction of the particle is given by

$$|\psi_0\rangle = \cos\left(\frac{\theta}{2}\right) | + Z \rangle + \sin\left(\frac{\theta}{2}\right) | - Z \rangle. \quad (3.55)$$

One should notice that after a full rotation ($\phi = 2\pi$) the wavefunction inverts its sign. This result is due to the nature of spin- $\frac{1}{2}$ particle.

The Pancharatnam phase difference between $|\psi_0\rangle$ and $|\psi_t\rangle$ is given after a straightforward calculation [37,60] as

$$\alpha = \arg\langle\psi_0|\psi_t\rangle = -\arctan\{\cos\theta\tan(\phi/2)\} . \quad (3.56)$$

The phase α can be tested in neutron interferometry by dividing the neutron beam into one beam which is exposed to the magnetic field \vec{B} while applying a variable U(1) phase χ to the other beam. The interference intensity measured by a detector in one output of the interferometer can be represented as

$$I \propto 1 + \nu \cos(\chi - \phi) \quad (3.57)$$

where

$$\nu = |\langle\psi_0|\psi_t\rangle| = [1 - \sin^2\theta \sin^2(\phi/2)]^{\frac{1}{2}} \quad (3.58)$$

In the above calculation we find that the time development of the wavefunction is a function of only one parameter. Therefore we can use the following form for the geometric phase [37,40,60]

$$\gamma_{\text{geom.}}(C) = \arg\langle\psi_0|\psi_t\rangle - \text{Im} \int_0^t \langle\psi_{t'}|\frac{d}{dt}|\psi_{t'}\rangle dt' \quad (3.59)$$

where the second term on the right side of equation (3.59) is the dynamical phase

$$\alpha_D = -\left(\frac{\phi}{2}\right) \cos\theta \quad (3.60)$$

and the geometrical phase for the noncyclic evolution is given by

$$\gamma_{\text{geom.}} = \alpha - \alpha_D \quad (3.61)$$

The above equations are reduced to simple forms for $\theta = 0, \pi$. Then we get

$$\nu = 1; \alpha_D = \pm(\phi/2); \alpha = \pm(\phi/2) \quad (3.62)$$

and for this case the geometric phase vanishes. For $\theta = \pi/2$ we find that $\langle \psi_0 | \psi_t \rangle$ is real and the Pancharatnam phase is undefined. Excluding these special cases, we find that for the general case both dynamical and geometrical phases are obtained by the use of equations (3.60-3.61).

Chapter 4. Measurements of Topological Phases

4.1 Topological Phases in Molecular Jahn-Teller System

General treatments of Topological phases in molecular spectroscopy are quite complicated [2-3,94-103] and needs expertise of this scientific area. We demonstrate basic concepts of molecular topological phases by giving here a simple analysis of Jahn-Teller effect [101-102].

We treat here a doubly degenerate molecular electronic states $|\psi_1\rangle$ and $|\psi_2\rangle$ where one needs to consider a combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ for their interaction with the molecular vibrations. Such interactions are beyond the Born-Oppenheimer approximation [101-102]. In Jahn-Teller system one considers, for example, triatomic molecules (ions) in which there is a coupling between the degenerate electronic states and the nuclear vibrations, or a group of atoms in crystals. For simplicity of the present treatment we consider a coupling between the degenerate electronic state and two normal coordinate vibrations Q_a and Q_b , which have the same frequency ω . We

consider interaction V_{in} which is linear in the Q_a and Q_b coordinates and in the form

$$V_{int} = -K \begin{pmatrix} -Q_a & Q_b \\ Q_b & Q_a \end{pmatrix}, \quad (4.1)$$

as required by the Jahn-Teller analysis. The constant K represents the strength of the coupling between the degenerate electronic states and the two normal vibration coordinates. The effective Hamiltonian of the normal vibration is given by

$$H_{\text{eff}} = \frac{P_a^2 + P_b^2}{2\mu} + \frac{\mu\omega^2}{2}(Q_a^2 + Q_b^2) - K \begin{pmatrix} -Q_a & Q_b \\ Q_b & Q_a \end{pmatrix} \quad (4.2)$$

where P_a and P_b are the conjugate momenta to Q_a and Q_b , respectively. μ is the effective mass of the normal vibration. The normal coordinates can be written

$$Q_a = \rho \cos \theta ; \quad Q_b = \rho \sin \theta \quad (4.3)$$

where ρ is a constant and θ is variable. The last term of equation (4.2) removes the degeneracy of the electronic energies ϵ_{\pm} which could be considered as effective vibrational potentials to be added to the vibrational potential of the double degenerate normal coordinate (Q_a, Q_b) :

$$V_{ab}^{\pm} = \left(\frac{\mu\omega^2}{2} \right) \rho^2 + \epsilon^{\pm} \quad (4.4)$$

The positive potential V_{ab}^+ and the negative one V_{ab}^- describe potential surfaces as a function of the coordinates Q_a, Q_b where near the degeneracy point these adiabatic surfaces are conical.

In order to find the eigenenergies ϵ_{\pm} and the electronic eigenkets $|+(\theta)\rangle$ and $|-(\theta)\rangle$, corresponding to these eigenenergies, we solve the equation

$$-K\rho \begin{pmatrix} -\cos\theta & \sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \epsilon \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} . \quad (4.5)$$

The electronic energies are given as

$$\epsilon_{\pm} = \pm K\rho , \quad (4.6)$$

and the calculation of the amplitudes C_1, C_2 give the corresponding eigenkets:

$$\begin{aligned} |+(\theta)\rangle &= \cos(\frac{\theta}{2})|\psi_1\rangle - \sin(\frac{\theta}{2})|\psi_2\rangle, \\ |-(\theta)\rangle &= \sin(\frac{\theta}{2})|\psi_1\rangle + \cos(\frac{\theta}{2})|\psi_2\rangle \end{aligned} . \quad (4.7)$$

Here we notice that electron kets change sign for rotation by 2π around the symmetry axis

$$|\pm(\theta = 2\pi)\rangle = (-1)|\pm\theta(0)\rangle . \quad (4.8)$$

Formally, this is the same as the rotation of a $\frac{1}{2}$ -spin system discussed in Section (2.1), since the sinusoidal dependence of the kets on the rotation is given by one-half of the rotation angle. One should notice, however, that it is the *orbital state* ket of the electron system that has changed sign and thus has nothing to do with spins. The factor -1 on the right side of equation (4.8) is shown to be related to Berry's phase factor. Since the eigenkets of equation (4.7) are not single valued one should find a phase factor that will make the kets single valued. For $|-(\theta)\rangle$, for example, define

$$|X_-\rangle = |-(\theta)\rangle e^{i\theta/2} . \quad (4.9)$$

The transformation (4.9) restores the single valuedness, but now there is a nonzero vector potential

$$A_\theta = \left(\frac{1}{i}\right)\langle X_- \left| \frac{d}{d\theta} \right| X_- \rangle = \frac{1}{2} . \quad (4.10)$$

The integration of the vector potential around a closed circuit which includes in the circuit the origin of the Q_a, Q_b plane (which is the degeneracy point of the electron system) gives Berry's phase factor π which change the sign of the wavefunction $|X_- \rangle$. It was noticed by molecular spectroscopists that restoration of the single valuedness of the electronic eigenstate leads to nonzero vector potentials [2,94-97].

The dynamical motion of the normal coordinates Q_a, Q_b (given by ρ, θ), under the potentials of equation (4.4), are obtained by solving the two-dimensional Schrodinger equation

$$\left\{ - \left(\frac{\hbar^2}{2\mu} \right) \left(\frac{\partial^2}{\partial \rho^2} + \left(\frac{1}{\rho} \right) \frac{\partial}{\partial \rho} + \left(\frac{1}{\rho^2} \right) \frac{\partial^2}{\partial \theta^2} \right) + V_{ab}^\pm(\rho) \right\} \psi(\rho, \theta) = E\psi(\rho, \theta) \quad (4.11)$$

$$\psi(\rho, \theta) = \begin{cases} \phi_+(\rho, \theta) | +(\theta) \rangle \\ \phi_-(\rho, \theta) | -(\theta) \rangle \end{cases} \quad (4.12)$$

Since equation (4.11) is a differential equation with separable variables we can solve it by choosing the nucleus wavefunction as

$$\phi_\pm(\rho, \theta) = f_\pm(\rho) e^{ij\theta} . \quad (4.13)$$

The state ket of the electron system changes sign when θ is rotated by 2π . Therefore in order to cancel this sign change, $\phi_\pm(\rho, \theta)$ must change its

sign to preserve the single valued nature of $\psi(\rho, \theta)$. From this requirement we conclude that $\exp(ij2\pi) = -1$. That is

$$j = \text{half integer, } (\ell = \text{integer}) . \quad (4.14)$$

The presence of the Berry's has changed the quantum number that characterized the rotation of atoms, from the usual integer number to half integer ones!

The low energy excitations in the potential as given by

$$E_{nj} \simeq (n + \frac{1}{2})\hbar\omega + \frac{\hbar^2(j^2 + \frac{1}{4})}{2\mu\rho_0^2} ; n \text{ integer; } j = \text{half integer} . \quad (4.15)$$

The result is given by the sum of the energies of vibration along the radial direction and those of rotation in the plane of the normal mode coordinates.

We should notice that the demand for single valuedness in the above treatment has been made for the total molecular wavefunction describing a *closed* system, i.e., a system for which the total Hamiltonian is conserved. In the treatments of Berry's phase given in Sections (3.1)-(3.3) we have assumed an Hamiltonian which is a function of time. For such *open* systems we have not the requirement of single valuedness which will be similar to that of molecular spectroscopy.

4.2 Measurements of Topological Phases with Polarized Light

4.2.1 Berry's Phases on Poincare Sphere

Let us give a simple explanation for the description of a Poincare sphere by Stokes parameters [104] which are equivalent to the Bloch vector. The em

field of a monochromatic plane polarized light propagating in the z direction can be given as

$$E_x = a_1 \cos(\tau + \delta_1) ; E_y = a_2 \cos(\tau + \delta_2) \quad (4.16)$$

where a_1 and a_2 are the amplitudes in the x and y directions. τ is the variable phase factor while δ_1 and δ_2 are constants. By using a simple algebra [104] one obtains the equation of an ellipse

$$\left(\frac{E_x}{a_1}\right)^2 + \left(\frac{E_y}{a_2}\right)^2 - 2\left(\frac{E_x}{a_1}\right)\left(\frac{E_y}{a_2}\right)\cos\delta = \sin^2\delta \quad (4.17)$$

where

$$\delta = \delta_1 - \delta_2 . \quad (4.18)$$

The ellipse will be reduced to *linearly polarized light* when $\delta = \delta_2 - \delta_1 = m\pi$ ($m = 0, \pm 1, \pm 2 \dots$). The ellipse is reduced to right-handed (left-handed) *circularly polarized wave* for $\delta = 2m\pi + \pi/2$ ($2m\pi - \pi/2$) [104]. Instead of using the real form of equation (4.16) it is more convenient to describe the em field as a complex Jones vector [105]

$$\begin{aligned} E_x(\text{complex}) &= a_1 e^{i(\tau + \delta_1)} = A_1 \\ E_y(\text{complex}) &= a_2 e^{i(\tau + \delta_2)} = A_2 \end{aligned} \quad (4.19)$$

Jones vector is described as a complex spinor vector $\begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$. The Stokes parameters of a plane monochromatic wave are described by the four quantities

$$\begin{aligned} S &= a_1^2 + a_2^2 = |A_1|^2 + |A_2|^2, \\ S_1 &= a_1^2 - a_2^2 = |A_1|^2 - |A_2|^2, \\ S_2 &= 2a_1 a_2 \cos(\delta) = A_1^* A_2 + A_1 A_2^*, \\ S_3 &= 2a_1 a_2 \sin\delta = (A_1 A_2^* - A_1^* A_2)/i . \end{aligned} \quad (4.20)$$

The parameter S is proportional to the intensity of the wave and this parameter can be normalized to 1 for unitary transformations. Then the Stokes parameters are equivalent *mathematically* to the Bloch vector components described in Section (2.1.3). For nonunitary transformations the magnitude of the Bloch vector, or equivalently the radius of the Poincare sphere, is decreasing then the parameters become important. However, by using the Pancharatnam phase approach the topological phase obtained for nonunitary transformations are similar to those of unitary transformations. Using Stokes parameters right-handed (left-handed) circular polarization is presented by the north (south) pole of the Poincare sphere. Linear polarization is represented by points in the equatorial plane [105].

Jones vectors for right and left polarized light waves are given by [105]:

$$\hat{R} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} ; \hat{L} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}. \quad (4.21)$$

These two circular polarizations are mutually orthogonal in the sense $\hat{R}^\dagger \hat{L} = 0$. Any pair of orthogonal Jones vectors can be used as a basis of the mathematic space spanned by the Jones vector. This description corresponds to spinors of two-level system where the two levels are here two orthogonal complex polarization states. Elliptic polarization can be represented as the following Jones vector

$$\hat{J} = \begin{pmatrix} \cos \psi & \psi \\ e^{i\delta} & \sin \psi \end{pmatrix}. \quad (4.22)$$

By operating on the polarization states with different optical apparatus (e.g., retardation waveplates, active rotating materials, polarizers, etc.) the two components of the Jones vector are transformed differently [105].

Bhandari and Samuel [43] observed Poincare topological phases by moving the polarization state of a monochromatic field on the Poincare sphere. For this purpose they have used quarter phase plates (which produces a difference in phase which is a quarter of 2π between two orthogonal polarizations) and optical active medium (which causes a certain rotation of the plane of polarized light). They also exchanged the optical active material by polaroids and in this wave have shown that the Pancharatnam geometric phase can be obtained also for nonunitary transformations. In either case the beam comes back with an added topological phase which is equal to the *half the solid angle* subtended by the area of the circuit on the Poincare sphere. In principal due to a large dynamical phase it is very difficult to measure the topological phases. Therefore the real measurements [43] were obtained as the *difference in the topological phases* for two circuits which have the same dynamical phase. There are various articles reporting observations of polarization states on the Poincare sphere [43-45, 106].

4.2.2 Topological Phases of Photons in Momentum Space

There is an analogy between the change in direction $(\hat{k}_x, \hat{k}_y, \hat{k}_z)$ of the photon by using externally slowly varying parameters and by adiabatic change in the direction of the magnetic field (B_x, B_y, B_z) where the geometrical phase for the latter case has been treated by Berry, as presented in Section (3.1). If there is nothing to change the sign of the helicity of the photon the helicity quantum number is an adiabatic invariant.

When the photon propagates smoothly down a helical waveguide (or more practically through a fibre), \vec{k} is constrained to remain parallel to the local axis of the waveguide, since the momentum of the photon is in this direction. The geometry of a helical path of a waveguide (or fibre with a unity winding number) constrains \vec{k} to trace out a loop on the surface of a sphere in parameter space (k_x, k_y, k_z) where the origin $\vec{k} = 0$ of this space is singular [compare $\vec{k} = 0$ with the singular point $\vec{B} = 0$ for the case treated by Berry [4]]. Following Berry's argument [as presented in Section (3.1)] we obtain here a geometrical phase

$$\gamma(C) = -\sigma\Omega(C) \quad (4.23)$$

where $\sigma = \pm 1$ is the helicity number and $\Omega(C)$ is the solid angle subtended by the loop C with respect to $\vec{k} = 0$. For a circle one gets [4]:

$$\Omega(C) = 2\pi N(1 - \cos\theta) \quad (4.24)$$

where N is the winding number of the helix and θ is the angle between the local fibre axis and the axis of the helix (the 'pitch angle') of the helix.

In the experiment [35] a linearly polarized laser has been focused into a single-mode isotropic fibre which is wound into the shape of a helix. The fibre output points are at the same direction as the input. The output light is analyzed to determine its axis of linear polarizer relative to that of the input light.

Let the initial state be represented by

$$|X\rangle = 2^{-\frac{1}{2}}(|+\rangle + |-\rangle) \quad (4.25)$$

where $|\pm\rangle$ are the eigenstates of the helicity $\sigma = \pm 1$. After propagating through the helix, the final state at the output of the fibre, if we ignore dynamical and birefringence effects, is

$$|X'\rangle = 2^{-\frac{1}{2}}(\exp(i\gamma_+)|+\rangle + \exp(-i\gamma_+)|-\rangle) \quad (4.26)$$

Here γ_+ is the phase for $\sigma = +1$. Therefore $|\langle X|X'\rangle|^2 = \cos^2 \gamma_+$. By Malus law, this implies that the plane polarization has been rotated by an angle which is equal to γ_+ . Chiao and Wu [34] have discussed the validity conditions for the adiabatic approximation and have considered also other cases of polarized light by which Berry's geometric phase can be measured. The elimination of dynamical and other optical activities in the experiments have been discussed [34-35] including the role of geometric phase as a quantum or classical effect [33-35, 107-109].

The topological phases of photons in momentum space have been realized by various constructions of interferometers: 1) Non-planar Mach-Zehnder interferometers where the geometric phase is observed as fringe shift [110-111] In such interferometers additive effects of Poincare sphere and helicity momentum phase have been observed [112]. 2) Interferometers with fibre loops have been built into ring interferometer [56] and in Sagnac interferometer [57] and have been used by coincidence counters to determine the geometric phase for a single photon and of a photon pair from parametric down conversion [113]. 3) The effects of reflections on quantum phases have been discussed [114].

4.3 Neutron Interferometry

Berry's original idea to observe the geometric phase for a spin particle around the magnetic field *under the adiabatic approximation* has been realized experimentally by Bitter and Dubbers [46]. They have used polarized cold electrons ($\lambda = 8\text{\AA}$) propagating along a helical magnetic field which allows for an easy fulfillment of the adiabaticity conditions.

In the usual interferometry experiments with neutrons the adiabatic approximation is not valid [58,115]. There are various articles treating the phase shifts of spinor wavefunctions interacting with magnetic fields [116-122]. Phases in coupled neutron interference loops and off-diagonal geometric phases in polarized neutron interferometry have been observed [123-124].

An analysis of topological phases in neutron interferometry has been discussed in Section 3.4.3, where such analysis with the corresponding measurements have been related to Pancharatnam phase analysis, which is valid also for noncyclic geometric phase.

4.4 Observations of Lorentz-Group Topological Phases

Kitano and Yabuzaki (KY) [51] have described Lorentz-Group Berry's phases observations in polarization optics. They have used in their analysis nonunitary Lorentz-Group transformations which are different from the unitary transformations described by Chiao and Jordan (CJ) [50] for squeezed *em* fields [125] as those described in Section 2.1.6. The Lorentz-Group generators

used by KY are given by the matrices:

$$K_1 = i\sigma_z/2 = \begin{pmatrix} \frac{i}{2} & 0 \\ 0 & -\frac{i}{2} \end{pmatrix}; K_2 = i\sigma_x/2 = \begin{pmatrix} 0 & \frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix}; K_3 = J_3 = \sigma_y/2 = \begin{pmatrix} 0 & -\frac{i}{2} \\ \frac{i}{2} & 0 \end{pmatrix}. \quad (4.27)$$

The CR of these operators are the same like those of (2.9), but since here the generators K_1 and K_2 are non-hermitian the present classical polarization optics system is basically different from that of the quantized squeezed em fields.

KY have used the transformation

$$T = S_4 S_3 S_2 S_1 = \exp(irK_2) \exp(isK_1) \exp(-isK_2) \exp(-irK_1) \quad (4.28)$$

This transformation is the same as that suggested by CJ but here the operators S_1, S_2, S_3 and S_4 are not unitary. A straightforward calculation shows that

$$\exp(isK_1) = \begin{pmatrix} \exp(-\frac{s}{2}) & 0 \\ 0 & \exp(\frac{s}{2}) \end{pmatrix}; \exp(irK_2) = \begin{pmatrix} \cosh(\frac{r}{2}) & -\sinh(\frac{r}{2}) \\ -\sinh(\frac{r}{2}) & \cosh(\frac{r}{2}) \end{pmatrix}. \quad (4.29)$$

In order to realize the transformation given by equation (4.28) KY have squeezed the space of polarization states of light by linear polarizers. A linearly polarized light wave propagating along the z direction can be described by a pair of real components E_x and E_y arranged as a column vector. Then the effect of a linear polarizer whose optical axes are set parallel to the coordinate axes can be represented by the 2×2 matrix

$$S = \text{diag}(t_x, t_y) = t_a \begin{pmatrix} \kappa & 0 \\ 0 & \kappa^{-1} \end{pmatrix} \quad (4.30)$$

where $t_x(t_y)$ is the transmission coefficient for the $x(y)$ component of the field. We note that S is composed of two parts: the isotropic loss $t_a = (t_x t_y)^{\frac{1}{2}}$. Since KY were not interested in the absolute intensities but in the polarization states of light, they neglected the isotropic losses.

The realization of the T transformation has been obtained [51] by using a sequence of polarization squeezing. If the parameters are chosen so that $\tanh(r) = \sinh(s)$, then T leads to a cyclic transformation

$$T \propto \exp(-i\phi J_3) \quad (4.31)$$

where the rotation angle $\phi/2$ is given by the relation

$$\sin \phi = \tanh^2(r) \quad (4.32)$$

It has been shown that when the extinction ratio of each polarizer is adjusted properly the system becomes equivalent to a (lossy) polarization rotator.

The basic idea of Lorentz-Group Berry's topological phase is that such phase will be given by

$$\theta_B = \oint d\Omega \quad (4.33)$$

where the integral is over the area of the hyperboloid (Lorentz metric) enclosed by the loop [82]. Although the measurements of the phase shift ϕ measured by KY are in good agreement with their theoretical calculations, the phase ϕ measured by them includes the summation of geometrical and dynamical phases.

Quantum systems exhibiting SU(2) or SU(1,1) dynamical symmetry including theoretical calculations of geometrical and dynamical phases have

been analyzed by Cervero and Lejarreta [126-127]. Experimental observation of Berry's phases of the Lorentz group has been reported by Swensmark and Dimon [128]. They have analyzed a nonlinear system, which when tuned in the vicinity of an instability shows a response similar to a Lorentz group. They have used a number of successive transformations combined in such a way that they make a closed loop on the hyperboloid. Their measurements of the Berry's phase are in a good agreement with the use of equation (4.33).

Chapter 5. Summary and Discussion

Geometric phases are intrinsically related to fibre-bundle topological theories. Usually topology is considered as the mathematical basis for general relativity and for certain fields in high energy physics. However, deep understanding of geometric phases related to time development by Schrodinger equation and interference effects in optics needs also the use of these analytical methods. Following this idea basic elements of topology are explained in Chapter 2, including the description of various manifolds, Cartan exterior algebra, fibre-bundles theories and differential geometry basic concepts. The discussions presented in this chapter should be helpful in analyzing complicated topological phases, e.g., those related to quantum computation. Also we demonstrate close connections between topological phases and topological singularities.

In Chapter 3 we describe the fundamental analysis made by Berry for topological phases related to 'magnate monopoles'. Generalization of Berry's phases to nonadiabatic time development and their relation to fibre-bundle

theories are discussed. The analysis of Berry's phase for n -level atomic system is treated by the use of Kahler metric. The relation between rays in quantum mechanics and Berry's phase is explained by using fibre-bundle theory. The use of Pancharatnam phases for noncyclic quantum evolution and for optical systems in relation to geometrical phase is discussed. The problem of gauge invariance in relation to Pancharatnam phase is emphasized, and solutions for various systems are given.

In Chapter 4 various measurements of geometrical phases are described. The relation between deviation from Born-Oppenheimer approximations and geometric phases in molecular spectroscopy is emphasized. A simple analysis is described for a special system known as the Jahn-Teller effect. Although geometric phases appeared in molecular studies quite long ago they are basically different from those described by Berry.

The topological phases known as Berry's phases are for open systems (with time dependent Hamiltonian) while the molecular system of nuclei plus electrons is closed [total Hamiltonian is conserved]. Measurements of geometric phases in polarization optics related to $SU(2)$ group are described. The appearance of geometric phases in many experiments performed in this field are analysed both for closed circuits following Berry's approach and for nonclosed circuits following Pancharatnam formalism. Basic experiments in neutron interferometry are discussed. A short analysis of geometric phases which are related to the Lorentz group is given.

It is not possible in one Review to cover all the interesting theories and experiments which have been developed for analysing geometrical phases

phenomena. We have described here only some selected topics in this field. There are many other theoretical and experimental [129-186] articles in which different topics and/or different analysis of topological phases have been described.

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