Nontrivial Phases
in
Quantum Mechanics

by

Michael Randall Ringor

A Thesis
Submitted to the Faculty of Graduate Studies
in Partial Fulfillment of the Requirements
for the Degree of

Master of Science

Department of Physics
University of Manitoba
Winnipeg, Manitoba

ISBN 0-315-71880-3

NONTRIVIAL PHASES IN QUANTUM MECHANICS

BY

MICHAEL RANDALL RINGOR

A thesis submitted to the Faculty of Graduate Studies
of the University of Manitoba in partial fulfillment of the
requirements of the degree of

MASTER OF SCIENCE

To Aja

Abstract

In certain dynamical systems there exists nonintegrable or path dependent phases associated with the quantum evolution of the system. These phases indicate a nontrivial component in the underlying topological structure of the system. In some sense these phases record the history of the system during the evolution.

In this work, a cohesive presentation is given on the nature of nontrivial or geometrical phases; and an attempt is made to clarify and enhance the present literature. A spin system is examined to illustrate the significance of nontrivial phases in quantum physics.

Who said Berry's phase is trivial?

Acknowledgements

I would like to thank my advisor, Dr. B.S. Bhakar for many thought provoking discussions and constructive criticism of the thesis. I am also thankful for his encouragement and advice throughout my tenure. The support of the University of Manitoba in the form of teaching assistantships is gratefully acknowledged.

My deepest gratitude goes to my family and friends for their unfailing support throughout this endeavor.

Contents

Chapter 1

Introduction

This thesis is essentially concerned with the quantum evolution of composite systems consisting of two subsystems. Denote the Hilbert space of subsystems 1 and 2 by $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Then the Hilbert space of the composite system is the product space

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2.$$

A Hamiltonian for a composite system is given by

$$\mathbf{H} = H_1 + H_2 + V$$

where H_1 and H_2 are the Hamiltonians for subsystems 1 and 2, respectively. The operator V represents the interaction between the two subsystems.

Suppose the various operators in H_1, H_2 and V can be grouped so that

we obtain the formal expression

$$\mathbf{H} = H(\mathbf{P}, \mathbf{X}(t)) + h(\mathbf{q}, \mathbf{p}; \mathbf{X}(t)). \tag{1.1}$$

In equation (1.1), the Hamiltonian h depends parametrically on $\mathbf{X}(t)$, and the momenta $\mathbf{P}$ and $\mathbf{p}$ are conjugate to $\mathbf{X}$ and $\mathbf{q}$, respectively. To be physically meaningful, we require that H be self adjoint, and h be symmetric and relatively bounded with respect to H so that $\mathbf{H}$ is self adjoint[1]. We redefine the previous subsystems so that now, subsystem 1 corresponds to H, and subsystem 2, with h. We shall also call H the *external Hamiltonian*, and h the *internal Hamiltonian*. These labels are purely arbitrary. However, when the composite system is a molecule, we may label the nuclear constituent the external system, while the electronic constituent, the internal system. Throughout this thesis we will consider Hamiltonians of the type given in equation (1.1).

Before continuing further we shall first clarify by what is meant by an evolution of a quantum system. In the case where the quantities $\{\mathbf{X}\}$ in the Hamiltonian (1.1) are slow changing with time[2], the evolution generated by $\mathbf{H}$ is *adiabatic*. Furthermore, if at time T we have $\mathbf{X}(\mathbf{0}) = \mathbf{X}(T)$, the adiabatic evolution is *cyclic*. Evolution may also be viewed as a transport of the system in some topological space, or a continuous change in the topological structure of the system. Such an evolution will be called *geometric evolution*.

[1] See [Ka], theorem 4.3.

[2] A precise statement will be given in chapter 2

The time evolution of the composite system is determined once we solve the Schrödinger equation[3] with its associated Cauchy condition

$$i\hbar\frac{d\psi}{dt} = \mathbf{H}\psi \qquad \psi(0) = \psi_0. \tag{1.2}$$

Here ψ is a vector in $\mathcal{H}$ belonging to the domain of $\mathbf{H}$. Unfortunately, there exists no general method of obtaining pointwise solutions to equation (1.2). Inevitably, some approximation has to be made. In recent years there has been considerable interest in the adiabatic and the related Born-Oppenheimer approximations (see, for example [M]). In such schemes certain dynamical degrees of freedom are assumed fixed in time; their roles being reduced to that of parameters in the Hamiltonian $\mathbf{H}$ of the system. Such a procedure causes phase factors to appear in the approximate solution. Berry's contribution had been in realizing that these phases are nontrivial and play a significant role in quantum and classical physics [B], [B2]. Specifically, these phases are *path dependent*, or nonintegrable.

The concept of a nonintegrable phase factor is not entirely new. Earlier, Wu and Yang employed the concept of nonintegrable phase factors in their examination of the Aharonov-Bohm effect and gauge fields [WY]. Shortly after, Mead and Truhlar, also noted similar structures in their application of the Born-Oppenheimer approximation to molecular systems [MT]. Until Berry's realization, the ramifications of nontrivial phase factors were not fully explored.

[3]Equation (1.2) is the abstract Schrödinger equation

There are several ways of showing how a nontrivial phase can arise. In this thesis it is obtained in a manner which is different from what is presented in the literature. The point of departure is a comment made by Schiff that, in the adiabatic approximation, one can globally[4] fix the phase of the eigenfunction corresponding to a Hamiltonian H [S]. By assuming the contrary, a formula for the nontrivial phase can be deduced. Since this phase owes its existence to the adiabatic approximation, it is called the adiabatic phase[5].

The adiabatic evolution of a quantum system is characterized by a curve on a manifold whose local coordinates parametrize the Hamiltonian H of the system. In a cyclic evolution, this curve is closed. The adiabatic phase depends on this path and therefore on the properties of the parameter manifold. An interesting feature is that the adiabatic phase manifests itself as a gauge field in the parameter manifold. Moreover, in the presence of degeneracies[6], a monopole structure is induced. In this sense, the adiabatic phase behaves like the the Wess-Zumino-Witten term[7]. This suggests a rich geometric substratum. Indeed, Simon first gave the interpretation that the adiabatic phase is a consequence of a holonomy transformation on a Hermitian line bundle [Si]. This interpretation forms the basis for a geometric theory of nontrivial phases. It turns out that the nontrivial phases can be

[4]i.e once a specific choice of phase is made, that choice remains for all time.

[5]The nontrivial phase is to be distinguished from the adiabatic phase. The latter is a special case of the former.

[6]These are degeneracies which occur for some value of the parameter $X(t)$

[7]A magnetic monopole-type term in an effective Lagrangian.

completely described in a differential geometric way, without invoking any adiabatic assumptions.

The geometrical foundation of the theory lies in the fibre bundle structures in the topology of the system; structures induced by an equivalence class on the space of square integrable (or L^2) functions. The space P of L^2 functions by an equivalence relation forms the $P(M, U(1))$ principal fibre bundle with structure group[8] $U(1)$, and base space M. This fibre bundle admits a natural connection[9], the integral of which is identified as a nontrivial phase. The Hermitian bundle which Simon uses is the induced bundle on a finite dimensional parameter space mapped injectively into the base space M. One can define other bundle structures whose natural connection gives rise to a nontrivial phase. The Hopf bundle has as its base space, a complex projective space. The evolution curve in the Hopf bundle is always closed. Hence, an evolution which gives rise to a nontrivial phase can be viewed as a holonomy on the fibre bundle. The nontrivial phase is often referred to as the *geometrical or topological phase* because of this intimate connection with geometry.

Cyclic evolution is not a necessary condition for the existence of nontrivial phases. A noncylic evolution, as in the case where repeated measurements are performed, can exhibit a geometrical phase. Although the natural connections no longer support the existence of the geometrical phase, it is possible to define a connection called the Pancharatnam connection so that

[8]The Abelian group of unitary gauge transformation.

[9]A geometric structure relating the various equivalence classes.

a nontrivial phase appears in noncyclic evolution. The necessary conditions for the existence of a nontrivial phase decribed in this thesis are reminiscent of the mathematically rigorous conditions put forward by Kiritsis in his topological investigation of the adiabatic phase [Ki]. In that paper, existence of the adiabatic phase depends on the possibility or impossibility of lifting the map $f : M \rightarrow CP^1$, where f is defined by the Hamiltonian, to $\tilde{f} : M \rightarrow S^3$. Here M is a compact manifold coordinated by a set of parameters $\{X\}$, and CP^1 is the complex projective space of 2-dimensional complex vectors of unit modulus, topologically equivalent to the 3-sphere. The conditions stated in the thesis are not on the same mathematical level as those given by Kiritsis, but the prevailing idea is the same: the classification of nontrivial phases amounts to topologically classifying their respective bundles.

To recapitulate, let us put the concept of nontrivial phases in its proper perspective in the Hamiltonian formalism. As the system evolves, the topological structure of the system changes. In certain cases the geometric evolution is such that the system develops a nontrivial topology. This happens in much the same way a Mobius topology can be induced in a euclidean strip by making a half twist and joining the ends together. This "twisting" of topological structures in the system manifests itself as a nontrivial phase. In order for this twisting to occur, it is necessary that $\mathbf{H}$ be time dependent. However, time dependence is not sufficient. There are systems whose Hamiltonian is time dependent but do not display a nontrivial phase; for example the forced harmonic oscillator. One means of introducing time dependence

in the Hamiltonian is through the time variation of a set of variables $\{\mathbf{X}\}$ which parametrize the Hamiltonian. This is the case in adiabatic evolution. The set $\{\mathbf{X}\}$ is a set of degrees of freedom of the external system, but from the point of view of the internal system, these external dynamical variables are merely slowly varying parameters.

In the Lagrangian picture, the nontrivial phase appears as an additional term in the action functional. This is explicit in the path integral formulation. We construct the effective propagator

$$\langle X, t; n | e^{-iHt/\hbar} | Y, t_0; m \rangle$$

which describes the evolution from the space-time point (Y, t_0) and state m, to the point (X, t) and eigenstate n. Taking the system around a closed circuit, yields a topological term in the action integral. The phase space formulation can be extended using the coherent state representation to include systems having a curved phase space. This extended formulation can be generalized further, eliminating the adiabaticity requirement. Berry's phase can be easily obtained from the generalized path integral formula by taking the adiabatic limit. In any case, the action functional includes a term such that

$$S^{eff} = S + \hbar\gamma$$

where S is the usual action integral $\int L dt$. Besides giving a different perspective of the nontrivial phase, the Langrangian picture has the novelty of

providing a field theoretic realization of nontrivial phases.

There has been a plethora of phenomena where nontrivial phases arise. Experimental and theoretical consequences of these phase have been observed in condensed matter and nuclear physics, optical and molecular physics [FS],[B],[WeZe],[Za],[Ha],[J],[BP],[TC],[CW]. The theory of nontrivial phases provides new insights to old problems and raise intriguing questions both in classical and quantum mechanics.

The aim of this thesis to to give a clear presentation of the fundamental nature of nontrivial phases in quantum theory. An attempt is made to clarify and hence enhance the present literature. The adiabatic phase is derived in chapter 2. In chapter 3, the connection between nontrivial phases and gauge structures is established; thus providing a motivation towards a geometric description. We examine in, chapter 4, spin-field interactions in the context of nontrivial phases. Finally, in chapter 5, we examine the classical analogue of the nontrivial phase and briefly discuss the connection between nontrivial phases and anomalies which can arise during quantization.

Chapter 2

Adiabatic Evolution

2.1 Introduction

In this chapter we examine in some detail how a nontrivial phase may arise in quantum systems undergoing cyclic adiabatic evolution. In this investigation the implications of the quantum adiabatic theorem are exploited to extract an explicit formula for such a phase. The case where the Hamiltonian exhibits a nondegenerate spectrum is examined, then generalized to the case where the spectrum is degenerate. We first employ the Schrödinger formalism and then use the path integral approach to gain further insight into cyclic quantum evolution.

2.2 The Adiabatic Phase

First we state the quantum adiabatic theorem [M] and use it to demonstrate the existence of a nontrivial phase. Consider a Hamiltonian h which depends continuously on a set of time dependent parameters, $\{\mathbf{X}(t)\}$. In what follows

we shall sometimes use the notation $h(t)$ to denote $h(\mathbf{p}, \mathbf{q}; \mathbf{X}(t))$. Suppose that by slowly varying these parameters, the Hamiltonian changes continuously from an initial value h_0 at time t_0 to a final value h_1 at time t_1. Define

$$T = t_1 - t_0 \qquad s = (t - t_0)/T$$

and let $h(s)$ be the value of the Hamiltonian at $t = t_0 + sT$; $h(s)$ being a continuous function of $s \in [0,1]$ with initial and final values given by $h(0) = h_0$, $h(1) = h_1$. In this parametrization, the Schrödinger evolution of a system depends on the parameter T which measures the rate of passage $h_0 \to h_1$.

Theorem 2.2.1 *Let $h(s)$ have an entirely discrete spectrum. Denote the j^{th} eigenvalue of $h(s)$ by ε_j, and the projectors onto the respective subspaces by $P_j(s)$. Both ε_j and P_j are assumed to be continuous functions of s. Suppose that throughout the interval $[0,1]$ the eigenvalues remain distinct, i.e $\varepsilon_j(s) \neq \varepsilon_k(s)$ whatever j, k and the derivatives dP_j/ds d^2P_j/ds^2 are well defined and piece-wise continuous in $[0,1]$. Then the evolution operator $U(t, t_0) \equiv U_T(s)$ has the asymptotic property*

$$\lim_{T\to\infty} U_T(s)P_j(0) = P_j(s) \lim_{T\to\infty} U_T(s).$$

proof:see [M]

This is the quantum adiabatic theorem. Consequently, if ϕ_j is an eigenvector of h_0 with eigenvalue $\varepsilon_j(0)$, then $P_j(0)\phi_j = \phi_j$; and the adiabatic theorem

gives

$$\lim_{T\to\infty} U_T(s)\phi_j = P_j \lim_{T\to\infty} U_T(s)\phi_j.$$

Thus we see that if the system is initially in an eigenstate of h_0 it will, at time t_1, have passed continuously into the eigenstate of h_1. Suppose that the evolution is cyclic so that $h_1 = h_0$ then the adiabatic theorem implies that the wave functions of the initial and final states differ only in phase. This phase, previously ignored, is physically significant and therefore nontrivial. This nontrivial phase is known as the *adiabatic* or *Berry's phase.*

Having examined the quantum adiabatic theorem, we next discuss how the nontrivial phase may arise. Since the external system only provides the internal system with a set of parameters $\{\mathbf{X}\}$, we are not concerned specifically with the external Hamiltonian. Instead we are interested in the internal Hamiltonian h which depends parametrically on the set $\{\mathbf{X}\}$. In what follows, we have tacitly assumed the adiabatic approximation. Consider the time independent Schrödinger equation

$$h(\mathbf{X}(t))\phi_n(\mathbf{q}, \mathbf{X}(t)) = \varepsilon_n(\mathbf{X}(t))\phi_n(\mathbf{q}, \mathbf{X}(t)). \tag{2.1}$$

Let equation(2.1) be solved exactly for the case where $\mathbf{X}$ is a constant. In general parameters $\mathbf{X}$ are changing with time, and a closed form solution may not be possible. Therefore, we assume that the evolution of $\mathbf{X}(t)$ is sufficiently slow such that the conditions of the adiabatic theorem are satisfied. In this case the internal system will remain in the same energy level throughout

the evolution. In other words, the slow variation of $\mathbf{X}$ with time does not induce energy transitions between quantum levels in the internal system. Let $\{\phi_n(\mathbf{q}, \mathbf{X})\}$ be a set of nondegenerate eigenfunctions, then the wavefunction for the system can be written as

$$\psi = \sum_n a_n(t)\phi_n(t)e^{-\frac{i}{\hbar}\int_0^t \epsilon_n(t')dt'}. \tag{2.2}$$

The wavefunction (2.2) satisfies the Schrödinger equation

$$i\hbar\frac{d\psi}{dt} = h(t)\psi \tag{2.3}$$

where for brevity we write $h(\mathbf{p}, \mathbf{q}; \mathbf{X}(t)) \equiv h(t)$ and $\phi_n(\mathbf{q}, \mathbf{X}(t)) \equiv \phi_n(t)$. Upon substituting (2.2) into (2.3) we obtain, after some algebra

$$\sum_n (\dot{a}_n + a_n\frac{\partial\phi_n}{\partial t})e^{-\frac{i}{\hbar}\int_0^t \epsilon_n(t')dt'} = 0. \tag{2.4}$$

In the above expression $\dot{a}_n = da_n/dt$. Multiplying (2.4) by $\bar{\phi}_k$ (complex conjugation ϕ_k) and integrating over all space yields,

$$\sum_n (\dot{a}_n\langle k|n\rangle + a_n\langle k|\dot{n}\rangle)e^{-\frac{i}{\hbar}\int_0^t \epsilon_n(t')dt'} = 0 \tag{2.5}$$

where $\langle l|m\rangle$ stands for the usual scalar product (ϕ_l, ϕ_m). Solving (2.5) for $\dot{a}_k(t)$ we obtain

$$\begin{aligned} \dot{a}_k(t) &= -\sum_n a_n \langle k|\dot{n}\rangle e^{-\frac{i}{\hbar}\int_0^t (\varepsilon_n - \varepsilon_k)dt'} \\ &= -a_k(t)\langle k|\dot{k}\rangle - \sum_{n;n\neq m} \langle k|\dot{n}\rangle e^{-\frac{i}{\hbar}\int_0^t w_{nk}dt'} \end{aligned} \tag{2.6}$$

where $w_{nk} = \varepsilon_n - \varepsilon_k$.

Suppose it is not possible to globally fix all the phases so that $\langle k|\dot{k}\rangle$ does not vanish, then for the n^{th} adiabatic level,

$$\psi = a_n(t) e^{-\frac{i}{\hbar}\int_0^t \varepsilon_n(t')dt'}, \tag{2.7}$$

and equation (2.6) reduces to (on replacing k by n)

$$\dot{a}_n(t) = -a_n(t)\langle n|\dot{n}\rangle \tag{2.8}$$

which is a first order linear differential equation. Under the adiabatic approximation, the system remains in the n^{th} eigenstate and hence equation (2.8) is easily solved to yield

$$a_n(t) = a_0 e^{i\int_0^t i\langle n|\dot{n}\rangle dt'}. \tag{2.9}$$

Recalling that the time dependence of the various quantities in equation (2.9) being due solely to the time variation of the parameters $\mathbf{X}(t)$, we can express

the argument of the exponential as an integral in the parameter space. Let us introduce the notation

$$\begin{aligned}\gamma_n(t) &\equiv i\int_0^t \langle n|\dot{n}\rangle dt' \\ &= i\int_0^t \langle n|\partial_\nu n\rangle \dot{X}^\nu(t')dt'\end{aligned}$$

where $\partial_\nu n \equiv \partial\phi_n/\partial X^\nu$. In the cyclic evolution with time period T, $X_i(T) = X_i(0)$, and $h(T) = h(0)$. Thus,

$$\gamma_n(C) = i\oint \langle n|\partial_\nu n\rangle dX^\nu. \tag{2.10}$$

Therefore in a cyclic evolution $\gamma_n(C)$ is a line integral along a closed curve C in parameter space. Using (2.10) and substituting (2.9) into (2.7) yields

$$\psi(T) = \phi_n(T)e^{-i\gamma_n(C)}e^{-\frac{i}{\hbar}\int_0^t \epsilon_n(t')dt'}. \tag{2.11}$$

Thus we see that if it is not possible to globally define all the phases then there is, in addition to the dynamical phase, a nontrivial phase $\gamma_n(C)$ associated with the adiabatic evolution.

The phase $\gamma(C)$ has some interesting properties. This phase is nonintegrable and multivalued under continuation around a circuit C: $\gamma_n(T) \neq \gamma_n(0)$. Moreover, for a particular level, it depends only on the parameters $\mathbf{X}(t)$ and not on any other aspects of the Hamiltonian $h(\mathbf{p}, \mathbf{q}; \mathbf{X})$. Observe

that

$$\begin{aligned}\langle n|\partial_\nu n\rangle &= \int \bar{\phi}_n(X)\partial_\nu\phi_n(X)d^3r \\ &= \partial_\nu\int \bar{\phi}_n\phi_n d^3r - \int(\partial_\nu\bar{\phi}_n)\phi_n d^3r \\ &= -\overline{\int \bar{\phi}_n\partial_\nu\phi_n d^3r} \\ &= -\overline{\langle n|\partial_\nu n\rangle}.\end{aligned}$$

Hence $\langle n|\partial_\nu n\rangle$ is purely imaginary so that $\gamma_n(C)$ is real. These properties give rise to remarkable physical consequences which will be examined in chapters 3 and 4.

Remark 2.2.1 In his paper Berry arrives at the adiabatic phase by inserting the ansatz

$$\psi = e^{i\gamma_n(t)}e^{-\frac{i}{\hbar}\int_0^t \varepsilon_n dt'}|n(\mathbf{X}(t))\rangle$$

into the Schrödinger equation (2.3) [B]. $\diamond$

Next we cast the adiabatic phase in the langauge of forms (see for example [F]). In equation (2.10), the quantity $i\langle n|\partial_\nu n\rangle dX^\nu$ can be written as a differential 1-form

$$w = i\langle n|\partial_\nu n\rangle dX^\nu = i\langle n|dn\rangle$$

where d is the exterior differential operator in parameter space. Equation (2.10) can therefore be written as

$$\gamma_n(C) = \oint w. \tag{2.12}$$

To continue further we recall a few basic facts from the theory of differential forms.

Lemma 2.2.1 (Poincaré) *Let w be any $(n-1)$-form. Then*

$$d(dw) = 0.$$

*proof:*see [Ru].

Theorem 2.2.2 (Stoke) *Let S be an oriented n-manifold and ∂S be its boundary. Then for any $(n-1)$ - form w*

$$\int_S dw = \oint_{\partial S} w.$$

*proof:*see [AMR]

If S is a bounded region in parameter space, then by Stoke's theorem, equation (2.12) can be written as

$$\begin{aligned} \gamma_n(C) &= i \int_{\partial S \equiv C} \langle n|dn\rangle \\ &= i \int_S d\langle n|dn\rangle. \end{aligned}$$

By Poincaré's lemma we have finally

$$\gamma_n(C) = i \int_S \langle dn|dn\rangle. \tag{2.13}$$

In local coordinates (2.13) reads

$$\gamma_n(C) = i \oint \langle \partial_j n|\partial_k n\rangle dX^j \wedge dX^k.$$

Note that $w = \langle n|dn\rangle$ is sensitive to the choice of phase[1]. Specifically, if $\phi_n \rightarrow e^{i\alpha}\phi_n$ then w transforms inhomogeneously: $w \rightarrow w - d\alpha$. Although w is not phase invariant the intergral $\oint w$ is invariant. In writing γ as a surface integral we obtain the 2-form $dw = i\langle dn|dn\rangle$. Unlike w this quantity is phase invariant. To show this let $\tilde{\phi}_n = e^{i\alpha}\phi_n$ then

$$\begin{aligned}
\langle d\tilde{n}|d\tilde{n}\rangle &= \langle \partial_\mu e^{i\alpha}\phi_n|\partial_\nu e^{i\alpha}\phi_n\rangle dX^\mu \wedge dX^\mu \\
&= [-\partial_\mu\alpha\partial_\nu\alpha + i(\partial_\mu\alpha)\langle\phi_n|\partial_\nu\phi_n\rangle + i(\partial_\nu\alpha)\langle\partial_\mu\phi_n|\phi\rangle \\
&\quad + \langle\partial_\mu\phi_n|\partial_\nu\phi_n\rangle]dX^\mu \wedge dX^\nu \\
&= d^2\alpha + id\alpha \wedge [\langle\phi_n|d\phi_n\rangle + \langle d\phi_n|\phi_n\rangle] + \langle d\phi_n|d\phi_n\rangle.
\end{aligned}$$

The first term in the last inequality is zero by Poincaré's lemma, and the term in the brackets vanishes by normalization. Thus $\langle dn|dn\rangle$ is phase invariant *although not manifestly so.*

[1]The phase referred to here is the arbitrary phase to within which a wavefunction ϕ is defined. This phase is not the same as the nontrivial phase.

A manifestly invariant formula for the phase can be obtained using equation (2.13). Define V as

$$V \equiv i\langle dn|dn\rangle$$

so that the phase is written

$$\gamma_n(C) = \oint_S V$$

then

$$\begin{aligned} V &= i\langle\partial_\mu n|\partial_\nu n\rangle dX^\mu \wedge dX^\nu \\ &= i[\langle\partial_\mu n|\partial_\nu n\rangle - \langle\partial_\nu n|\partial_\mu n\rangle]dX^\mu \wedge dX^\nu \\ &= -2Im\sum_{\mu<\nu}\langle\partial_\mu n|\partial_\nu n\rangle dX^\mu \wedge dX^\nu \\ &= -2Im\sum_{\mu<\nu}\sum_{m;m\neq n}\langle\partial_\mu n|m\rangle dX^\mu \wedge \langle m|\partial_\nu n\rangle dX^\nu. \end{aligned} \tag{2.14}$$

The term in which $m = n$ vanishes since we take only the imaginary parts (recalling that $\langle n|dn\rangle$ is purely imaginary). Intuitively if we imagine that $\langle n|\partial_j m\rangle$ are vectors and set $m = n$, we have a vector product of parallel vectors in equation (2.14). Hence the term for which $m = n$ is to be excluded from the summation. Now applying ∂_μ to the time independent Schrödinger

equation we get, upon multiplying by the bra $\langle m|$ and simplifying,

$$\langle m(X)|\partial_\mu n(X)\rangle = \frac{\langle m(X)|(\partial_\mu h)n(x)\rangle}{(\varepsilon_n - \varepsilon_m)}. \tag{2.15}$$

Using (2.15) in (2.14) we have

$$\begin{aligned} V &= -Im \sum_{\mu<\nu} \sum_{m;m\neq n} \frac{\langle n|(\partial_\mu h)m\rangle dX^\mu \wedge \langle m|(\partial_\nu h)n\rangle}{(\varepsilon_n - \varepsilon_m)^2} \\ &= -Im \sum_{m;m\neq n} \frac{\langle n|(dh)m\rangle \wedge \langle m|(dh)n\rangle}{(\varepsilon_n - \varepsilon_m)^2}. \end{aligned} \tag{2.16}$$

Since the formula (2.16) does not depend on the choice of phase, it is clear that it is manifestly phase invariant. An alternative formula is given by Avron, Seiler, and Simon [ASS]:

$$V = -iTr(dP_j P_j dP_j)$$

where P_j is the projector onto the j^{th} eigenspace having the representation $P_j(X) = |\phi_j\rangle\langle\phi_j|$; and d is the exterior derivative. Equation (2.16) shows explicity that if h is real we can choose all the eigenfunctions to be real; consequently $V = 0$, and hence $\gamma_n(C)$ vanishes. Therefore, systems for which there is a Berry phase must have nonreal Hamiltonians; or if h is real, magnetic fields must be present. Although (2.16) implies that $\gamma_n(C)$ depends on the details of the Hamiltonian h, it must be emphasized that the adiabatic phase reflects the properties of the parameter space and not of the

Hamiltonian.

We have thus far developed the theory of the adiabatic phase with the assumption that the eigenstates of the quantum system are nondegenerate. It is possible that the system posseses certain symmetries reflected by the symmetry group of the Hamiltonian. In such cases the energy spectrum is degenerate. In this section we remove the restriction that the eigenstates be nondegenerate. The adiabatic theorem implies that the subspaces of the degenerate spectrum are mapped into each other throughout the evolution.

As before, we suppose that the time independent Schrödinger equation (2.1) can be solved, with ϕ_n now being degenerate. We renormalize the energies so that $\varepsilon = 0$, and hence

$$h(\mathbf{p}, \mathbf{q}; \mathbf{X})\phi_n = 0.$$

Consider a single degenerate level n with multiplicity μ_n. As in degenerate perturbation theory we seek an orthonormal set $\{\xi_{n,i}\}_{i=1}^{\mu_n}$, $\langle \xi_{n,i} | \xi_{n,j} \rangle = \delta_{ij}$ in which each element $\xi_{n,i}$ is a linear combination of the n^{th} level degenerate eigenfunctions

$$\xi_{n,i} = \sum_{j}^{\mu_n} b_j^{(i)} \phi_{n,j}.$$

If the $\xi_{n,i}$'s are not orthonormal, they can always be made so by the Graham-Schmidt process [AG]. It will be understood that we are considering the n^{th} level; henceforth the subscript n will be omitted and the remaining subscript will identify a particular linear combination. Suppose the system is initially

in the state ξ_i. Then the wave function is

$$\psi = U(t)\xi_i, \tag{2.17}$$

$U(t)$ being a time dependent coefficient. Inserting (2.17) into the Schrödinger equation (2.3), multiplying by $\bar{\xi}_k$ (complex conjugation ξ_k) and integrating over all space we have,

$$\dot{U}(t)\langle\xi_k|\xi_j\rangle + U(t)\langle\xi_k|\dot{\xi}_j\rangle = 0;$$

or

$$\dot{U}(t) + U(t)A_{jk} = 0 \tag{2.18}$$

where we have used orthonormality of the ϕ's and defined A_{jk} to be

$$A_{jk} \equiv \langle\phi_k|\dot{\phi}_j\rangle. \tag{2.19}$$

Equation (2.18) is similar to equation (7) in Wilczeck and Zee's paper [WZ]. The standard solution to equation (2.18) is the product (or path ordered) integral

$$\begin{aligned} U &= Pe^{\int_0^t A(\tau)d\tau} \\ A(\tau) &= \langle\phi|\dot{\phi}\rangle. \end{aligned}$$

Note that A_μ is an antihermitian $\mu_n \times \mu_n$ matrix, therefore $U(t)$ must be also a $\mu_n \times \mu_n$ matrix. From the normalization condition it also follows that the matrix U is unitary.

Let the spanning set of the parameter manifold be $\mathbf{X} = (X_1, \ldots, X_n)$ then

$$\begin{aligned} A_\mu &= \langle \phi | \partial_\mu \phi \rangle \frac{dX^\mu}{d\tau} \\ (A_\mu)_{ij} &= \langle \phi_j | \partial_\mu \phi_i \rangle \frac{dX^\mu}{d\tau}. \end{aligned}$$

We may express the product integral as

$$U(t) = P \exp \int A_\mu d\tau.$$

Since the evolution is cylcic, the path in parameter space is closed and we can write

$$U = P e^{\oint \langle \phi | \partial_\mu \phi \rangle dX^\mu}.$$

Recalling that

$$w = \langle \phi | \partial_\mu \phi \rangle dX^\mu$$

the last equation can be written as

$$U = P e^{\oint w}. \tag{2.20}$$

Equation (2.20) is the "nonabelian" generalization of the adiabatic phase.

We have shown, in the context of the adiabatic theorem, that if the phase of the wave function cannot be globally fixed then there appears a nontrivial phase. This phase displays the nontrivial properties of the parameter space. The approach in developing the theory has been in the Schödinger formalism. To use the molecule model, the electronic degrees of freedom are of interest while the nuclear degrees of freedom are reduced to a set of slowly changing parameters. If we now consider the parameters as *dynamical variables*, again in the Schrödinger picture, it appears that a sort of gauge potential is induced in the parameter space [A],[J]. However, a more fruitful approach is to examine this problem in the path integral formalism. This is the content of the next section.

2.3 The Path Integral Formulation

In the last section, it had been pointed out that the adiabatic phase depends on the properties of the parameter space. This observation suggests an inherent topological structure. In using the differential approach to develop the theory of the adiabatic phase, only local aspects of the system are described. Global features manifest themselves only in the boundary conditions to be imposed on the differential equation. On the other hand, the (path) integral approach provides a global description of quantum mechanics. This point of view is only natural when describing nontrivial phases. In this approach, the parameter space is treated as a dynamical object, an aspect not present in the Scrödinger formalism. Thus it would be informative to reformulate the

theory in the path integral formalism so that topological features of a system may be revealed. This is the aim of this section.

Briefly we discuss the connection between the differential and integral formulations. In the Schrödinger picture, the dynamical evolution of a quantum system is governed by the differential equation with initial condition

$$\begin{aligned} i\hbar\frac{d\psi}{dt} &= H(t)\psi \\ \psi(t_0) &= \psi_0. \end{aligned} \tag{2.21}$$

Equation (2.21) generates an evolution $U(t,t_0)$ which can be defined as a linear map

$$\begin{aligned} \psi(t_0) &\rightarrow \psi(t) \\ \psi(t) &= U(t,t_0)\psi(t_0) \end{aligned}$$

and is associated with the elements of the 1-parameter group $\{e^{-\frac{i}{\hbar}Ht}\}$. The related quantum propagator is the kernel of the evolution operator and satisfies, for f,g bounded in $L^2(R^d)$

$$(f,U(t,t_0)g) = \int_{R^d\times R^d} \bar{f}(x)K(x,t;y,t_0)g(y)dxdy.$$

In the coordinate basis $\{|x\rangle\}$, the propagator $K(\cdot,t;\cdot,t_0)$ may be written as

$$K(x,t;y,t_0) = \langle x|e^{-\frac{i}{\hbar}Ht}|y\rangle$$

which may be interpreted as a transition amplitude which gives the probability that a system prepared at the spacetime point (y, t_0) will be observed at the point (x, t). Having briefly described the propagator we now turn to the global description of the adiabatic phase [KI1].

Suppose we have an interacting system whose Hamiltonian is given by

$$\mathbf{H} = H(\mathbf{P}, \mathbf{X}) + h(\mathbf{q}; \mathbf{X})$$

where, as before H and h are the external and internal Hamiltonians, respectively. We assume h depends only on the internal coordinate q and parametrically on the external coordinates X. The variables q, P, X are the eigenvalues of the operators $\mathbf{q}, \mathbf{P}, \mathbf{X}$:

$$\begin{aligned} \mathbf{q}|q\rangle &= q|q\rangle \\ \mathbf{P}|P\rangle &= P|P\rangle \\ \mathbf{X}|X\rangle &= X|X\rangle. \end{aligned} \tag{2.22}$$

Here $\{|q\rangle\}$ and $\{|X\rangle\}$ are coordinate bases and $\{|P\rangle\}$, a momentum basis. Denote the complete set of discrete and nondegenerate eigenfunctions of the internal Hamiltonian h by $\{\phi_n(X) \equiv |n(X)\rangle\}$. Using these bases we construct the following

$$\begin{aligned} |n(X), X\rangle &\equiv |n(X)\rangle \otimes |X\rangle \\ |n(X), P\rangle &\equiv |n(X)\rangle \otimes |P\rangle. \end{aligned}$$

Orthonormalization is given by

$$\langle n(X), Y | m(X), X \rangle = \delta_{mn} \delta(X - Y). \tag{2.23}$$

The propagator for a transition from the spacetime point (X_0, t_0) and quantum state $|m\rangle$ to the point (X, t) and state $|n\rangle$ is then

$$K(n, X, t; m, X_0, t_0) = \langle n(X), X | e^{-\frac{i}{\hbar}\mathbf{H}t} | m(X), X_0 \rangle. \tag{2.24}$$

If in equation (2.24) we set $|m(X), X_0\rangle = |n(X), X\rangle$, with $X = X_0$ and sum over n and X we have the space integral

$$G(t) = \sum_n \int \langle n(X_0), X_0 | e^{-\frac{i}{\hbar}\mathbf{H}t} | n(X_0), X_0 \rangle dX. \tag{2.25}$$

We shall call $G(t)$ the effective propagator.

Remark 2.3.1 In their paper, Kuratsuji and Iida derive the effective propagator by taking the trace of the time evolution operator [KI1], [KI2]. This is somewhat misleading since such a step is not valid until it is known that the evolution is such that it admits a trace-class operator $U(t, t_0)$.$\diamond$

In view of the interpretation that the propagator is a transition amplitude, equation (2.25) implies a quantum process starting in the initial state $|n(X_0), X_0\rangle$ and returning, after a time T, to the same state which we denote by $|n(X(T)), X_0(T)\rangle$ to distinquish it from the original state. The motivation in constructing the integral (2.25) is clear. The integral allows

us to obtain information on the energy spectrum of the system. Indeed if we take the Fourier-Laplace transform of $G(t)$, we get an equation similar to the energy-Green's function

$$\tilde{G}(E) = -i \int_0^\infty G(t) e^{\frac{i}{h}Et} dt.$$

This can serve as a basis for an experimental verification of the adiabatic phase.

We now construct the phase space path integral for the effective propagator. Recalling that $\mathbf{H} = H + h$, equation (2.25) can be written in the following way

$$G(t) = \sum_n \int \langle n(X_0(T)), X_0(T) | (e^{-\frac{i}{h}Ht/N} e^{-\frac{i}{h}ht/N})^N | n(X_0), X_0 \rangle dX_0. \quad (2.26)$$

We have used the fact that (see [Sc])

$$e^{-\frac{i}{h}(H+h)t/N} = e^{-\frac{i}{h}Ht/N} e^{-\frac{i}{h}ht/N} + O\left(\frac{t^2}{N^2}\right).$$

For $O(1/N^2)$ well behaved and for sufficiently large N the latter may be replaced by

$$e^{-\frac{i}{h}\mathbf{H}t/N} = e^{-\frac{i}{h}Ht/N} e^{-\frac{i}{h}ht/N}.$$

Using the Trotter product formula and alternately inserting the completeness relations $\sum_{m'} \int |m', P\rangle\langle m', P| dP$ and $\sum_m \int |m, X\rangle\langle m, X| dX$ into (2.26) we

obtain

$$
\begin{aligned}
G(T) \;=\; & \lim_{N\to\infty}\sum_{n}\int dX_0 \sum_{m_{N-1},m'_{N-1}} \cdots \sum_{m_1,m'_1}\int \prod_{k=1}^{N-1} dX_k \prod_{k=0}^{N-1} dP_k \\
& \langle n(X_0(T)), X_0(T)|m'_{N-1}, P_{N-1}\rangle \\
& \times \langle m'_{N-1}, P_{N-1}|e^{-\frac{i}{\hbar}Ht/N}e^{-\frac{i}{\hbar}ht/N}|m_{N-1}, X_{N-1}\rangle \\
& \times \langle m_{N-1}, X_{N-1}|m'_{N-2}, P_{N-2}\rangle \\
& \times \langle m'_{N-2}, P_{N-2}|e^{-\frac{i}{\hbar}Ht/N}e^{-\frac{i}{\hbar}ht/N}|m_{N-2}, X_{N-2}\rangle \\
& \vdots \\
& \times \langle m_1, X_1|m'_0, P_0\rangle \\
& \times \langle m'_0, P_0|e^{-\frac{i}{\hbar}Ht/N}e^{-\frac{i}{\hbar}ht/N}|n(X_0), X_0\rangle
\end{aligned}
$$

where the notation $|m_j\rangle \equiv |m(X_j)\rangle$ is used to denote the system at state m and position X_j. Considerable simplification is attained upon noting that

$$
\langle m_j, X_j|m'_{j-1}, P_{j-1}\rangle = \delta_{m_j m'_{j-1}}\frac{e^{\frac{i}{\hbar}P_{j-1}X_j}}{(2\pi\hbar)^{1/2}}
$$

and using the adiabatic approximation that only transitions between states of the same quantum number occur. Hence the sums $\sum_{m'}, \sum_{m}$ collapse and only the summation over n remains. Thus

$$
G(T) \;=\; \sum_{n}\int \prod_{k=0}^{N-1} d\mu(P_k, X_k) \prod_{j=0}^{N-1}\left[\frac{e^{\frac{i}{\hbar}P_j X_{j+1}}}{(2\pi\hbar)^{1/2}}\right]
$$

$$\times \prod_{j=1}^{N} \langle n(X_j), P_{j-1}|e^{-\frac{i}{\hbar}Ht/N}e^{-\frac{i}{\hbar}ht/N}|n(X_{j-1}), X_{j-1}\rangle \quad (2.27)$$

where $d\mu(P_k, X_k) = dP_k dX_k$.

Now

$$\begin{aligned}
&\prod_{j=1}^{N} \langle n(X_j), P_{j-1}|e^{-\frac{i}{\hbar}Ht/N}e^{-\frac{i}{\hbar}ht/N}|n(X_{j-1}), X_{j-1}\rangle \\
&= \prod_{j=1}^{N} [\langle n(X_j)|n(X_{j-1})\rangle e^{-\frac{i}{\hbar}\epsilon_n(X_{j-1})t/N}\langle P_{j-1}|X_{j-1}\rangle e^{-\frac{i}{\hbar}H(P_{j-1},X_{j-1})t/N}] \\
&= \prod_{j=1}^{N} \left[\frac{\langle n(X_j)|n(X_{j-1})\rangle}{(2\pi\hbar)^{1/2}}\right] \\
&\quad \times \exp\left\{-\frac{i}{\hbar}\sum_{j=1}^{N}\left[\epsilon_n(X_{j-1}) + \frac{P_{j-1}X_{j-1}}{t/N} + H(P_{j-1}, X_{j-1})\right] t/N\right\} \\
&= \prod_{j=0}^{N-1} \left[\frac{\langle n(X_{j+1})|n(X_j)\rangle}{(2\pi\hbar)^{1/2}}\right] \\
&\quad \exp\left\{-\frac{i}{\hbar}\sum_{j=0}^{N-1}\left[\epsilon_n(X_j) + \frac{P_j X_J}{t/N} + H(P_j, X_j)\right] t/N\right\}. \qquad (2.28)
\end{aligned}$$

Each term $\langle n(X_{j+1})|n(X_j)\rangle$ denotes a *connection* between two infinitesimally separated points X_{j+1}, X_j. The connections here are analogous to the affine connections Γ^k_{ij} in Riemannian geometry. Taylor expansion gives

$$\begin{aligned}
\langle n(X_{j+1})|n(X_j)\rangle &= \langle n(X_{j+1})|n(X_{j+1} - dX_{j+1})\rangle \\
&\approx \langle n(X_{j+1})|(|n(X_{j+1})\rangle - \partial_k|n(X_{j+1})\rangle dX^k)
\end{aligned}$$

$$= 1 - \langle n(X_{j+1})|\partial_k n(X_{j+1})\rangle dX^k. \qquad (2.29)$$

The second term in (2.29) gives the adiabatic phase; and so

$$\begin{aligned}\prod_{j=0}^{N-1}\langle n(X_{j+1})|n(X_j)\rangle &= \prod_{j=0}^{N-1}\exp[\ln\langle n(X_{j+1})|n(X_j)\rangle] \\ &\approx \exp\sum_{j=0}^{N-1}\ln[1-w(X_j)] \\ &\approx \exp\sum_{j=0}^{N-1} iw(X_j). \qquad (2.30)\end{aligned}$$

where $w(X_j) = i\langle n(X_{j+1})|\partial_k n(X_{j+1})\rangle dX^k$ as before. Using (2.30) and (2.28) in (2.27), we have for the effective propagator

$$\begin{aligned}G(T) &= \lim_{N\to\infty}\sum_n \int\prod_{k=0}^{N-1}\frac{d\mu(P_k,X_k)}{(2\pi\hbar)^N}\exp i\sum_{j=0}^{N-1} w(X_j) \\ &\quad\times\exp\left\{\frac{i}{\hbar}\left[\sum_{j=0}^{N-1}\frac{P_j(X_{j+1}-X_j)}{t/N} - H(P_j,X_j)\right]\frac{t}{N}\right\} \\ &\quad\times\exp\left[-\frac{i}{\hbar}\sum_{j=0}^{N-1}\varepsilon_n(X_j)\frac{t}{N}\right]\end{aligned}$$

which in the continuum limit becomes

$$G(T) = \sum_n \int D(P,X)e^{i\gamma(C)}\exp\frac{i}{\hbar}\left[\int_0^T (P\dot{X} - H - \varepsilon_n(X(t)))dt\right]. \qquad (2.31)$$

Let $S_0 = \int(P\dot{X} - H)dt$ and define the adiabatic action as

$$S_n^{ad} = S_0 - \int_0^T \varepsilon_n dt.$$

then for the effective propagator we have the formal expression

$$G(T)^{eff} = \sum_n \int D(P,X) e^{\frac{i}{\hbar}[S_n^{ad} + \hbar\gamma_n(C)]}. \tag{2.32}$$

From equations (2.31) and (2.32) we find, in addition to the usual dynamical action, the object $\hbar\gamma_n(C)$ which could be called the topological action. The effective action, given by

$$S_n^{eff} = S_n^{ad} + \hbar\gamma_n(C)$$

may be interpreted as the action for a system in the effective "gauge field" described by the "potential" $w = i\langle n|\partial_j n\rangle dX^j$.

In the path integral formulation, we have integrated out some degrees of freedom associated with the internal system. This procedure is somewhat opposite to that adopted in chapter 2 where some degrees of freedom of the external system were suppressed. Integrating out some degrees of freedom gives an effective action with an added term arising from the topology of the integrated space. In effective field theories, such quantities are known as Wess-Zumino-Witten, Chern-Simons, or in general, topological terms. Clearly, there is an explicit analogy between nontrivial phases in

quantum mechanics and topological terms in field theory.

In the previous development we have assumed that the external system is described by the canonical pair (P, X). The formulation can be extended so that systems defined on general Lie algebraic manifolds can be treated. Such an extension is easily achieved in the coherent state representation. This is examined in the next section.

2.4 The Coherent State Representation

In this section we generalize the integral formulation of Berry's phase to the case of a spin system described by the internal coordinate q and the external variable S which satisfies the SU(2) algebra: $[S_i, S_j] = i\hbar\epsilon_{ijk}S_k$ [KI2]. Here we now consider a system where the phase space is noneuclidean and whose spanning set is a noncommutative set. We will call such systems *noncommuting*. The Hamiltonian is assumed to have the form

$$\mathbf{H} = H(S) + h(q; S) \tag{2.33}$$

Before continuing with the main objective, we briefly recall the definition and properties of *generalized coherent states* [P1],[P2],[R]. We will then specialize to SU(2) coherent states (henceforth SU(2)-CS).

Coherent states are an overcomplete, nonorthogonal system connected with the irreducible representation of Lie groups. The following definition is similar to that given in [P1].

Definition 2.1 *Let $G = g$ be an arbitrary Lie group with an irreducible unitary representation T acting in a Hilbert space $\mathcal{H}$. For a fixed vector $|\psi_0\rangle \in \mathcal{H}$, the set $\{|\psi_g\rangle : |\psi_g\rangle = T(g)|\psi_0\rangle\}$, where g runs over G, forms a set of states. Further let $R = \{r\}$ be a subgroup of G such that $T(r)|\psi_0\rangle = e^{i\alpha(r)}|\psi_0\rangle$. Then each $|\psi_0\rangle$, for all $g \in gR$, determine the same state, i.e they differ only by a phase $e^{i\alpha}$. In each coset $x = gR$, select a representative $g(x)$ of the group G to obtain the states $\{|\psi_{g(z)}\rangle \equiv |z\rangle\}$. Thus for each point $z \in G/R$ corresponding to g, the generalized coherent state is determined:*

$$|\psi_g\rangle = e^{i\alpha(g)}|\psi_{g(z)}\rangle. \tag{2.34}$$

Although the set of coherent states is overcomplete, the notion of completeness can nevertheless be defined by the so called partition of unity

$$\frac{1}{\beta}\int dz|z\rangle\langle z| = 1. \tag{2.35}$$

The constant β differs for each Lie group and is given by

$$\beta = \int |\langle z'|z\rangle|^2 dz.$$

The scalar product gives the reproducing relation

$$\langle z_1|z_2\rangle = e^{i[\alpha(g_1)-\alpha(g_2)]}\langle\psi_0|T(g_1^{-1}g_2)|\psi_0\rangle. \tag{2.36}$$

Given a Lie group, we can construct a set of generalized coherent

states. If G is the Heisenbeg-Weyl group, we obtain the set of ordinary coherent states which are closely related to the boson creation and annihilation operators $a^\dagger$ and a. Let G be the group SU(2). Let the states $|j,m\rangle$ be a basis for the representation space in which the irreducible unitary representation $T(g)$ of the group SU(2) acts. The infinitesimal generators $J_\pm = J_1 \pm iJ_2, J_3$ of $T(g)$ satisfy $[J_3, J_\pm] = \pm J_\pm, [J_-, J_+] = -2J_3$. The fixed vector $|\psi_0\rangle$ is chosen to be the minimal state $|j,-j\rangle$ so that $J_-|j,-j\rangle = 0$. The quotient space G/H is the 2-sphere S^2; a point being specified by the unit vector $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. Choose $g(\hat{n})$ so that $T(g) = e^{-i\phi J_3}e^{-i\theta J_2}e^{-i\psi J_3}$. Applying the definition, we obtain the system of SU(2)-CS

$$|n\rangle = e^{i\alpha(\hat{n})}e^{-i\phi J_3}e^{-i\theta J_2}|j,-j\rangle \tag{2.37}$$

where $\alpha(\hat{n}) = \psi j$. If the manifold S^2 is mapped onto the complex z-plane using the stereographic projection

$$z = -\tan\frac{\theta}{2}e^{-i\phi}$$

we can write

$$\begin{aligned} \mathcal{D} &\equiv e^{i\alpha(\hat{n})}e^{-i\phi J_3}e^{-i\theta J_2} = e^{zJ_+}e^{\beta J_3}e^{-\bar{z}J_-} \\ \beta &= \ln(1+|z|^2). \end{aligned} \tag{2.38}$$

Applying $\mathcal{D}$ to $|j,-j\rangle$, another form of SU(2)-CS is obtained

$$|z\rangle = (1+|z|^2)^{-j} e^{zJ_+}|j,-j\rangle. \tag{2.39}$$

In this parametrization, the partition of unity (2.35) is

$$\begin{aligned} \int d\mu(z)|z\rangle\langle z| &= 1 \qquad (2.40)\\ d\mu(z) &= \frac{2j+1}{\pi(1+|z|^2)} d\bar{z}dz. \end{aligned}$$

And the reproducing relation (2.36) is

$$\langle z|z'\rangle = \frac{(1+\bar{z}z)^{2j}}{[(1+|z|^2)(1+|z'|^2)]^j}. \tag{2.41}$$

Having defined generalized coherent states and identified some of their properties, we now turn to the task of constructing the effective propagator for the noncommuting system whose Hamiltonian is given by (2.33). This amounts to slightly modifiying the construction process for the phase space path integral. We construct the basis

$$|n(z),z\rangle = |n(z)\rangle \otimes |z\rangle. \tag{2.42}$$

Orthonormalization is given by

$$\langle n(z'),z'|n(z),z\rangle = \langle n(z')|n(z)\rangle\langle z|z'\rangle.$$

We should write $|n\rangle = |n(S)\rangle$, but in the basis $\{|z\rangle\}$ S can be expressed in terms of z; hence $|n(S)\rangle \rightarrow |n(z)\rangle$. Using the basis (2.42) along with the partition of unity (2.40) we obtain

$$\begin{aligned} G(T) &= \sum_n \int \langle n(z_0(T)), z_0| \left[e^{-\frac{i}{\hbar}Ht/N} e^{-\frac{i}{\hbar}ht/N} \right]^N |n(z_0), z_0\rangle d\mu(z_0) \\ &= \lim_{N\to\infty} \sum_n \int d\mu(z_0) \int \prod_{k=1}^{N-1} d\mu(z_k) \\ &\quad \times \prod_{k=1}^{N} \langle n(z_k), z_k| e^{-\frac{i}{\hbar}Ht/N} e^{-\frac{i}{\hbar}ht/N} |n(z_{k-1}), z_{k-1}\rangle. \end{aligned} \tag{2.43}$$

The integrand in (2.43) is approximated as follows:

$$\begin{aligned} &\prod_{k=1}^{N} \langle n(z_k), z_k| \left\{ 1 - \frac{i}{\hbar}[H(S) + h(q,S)]\frac{t}{N} + O\left(\frac{t^2}{N^2}\right) \right\} |n(z_{k-1}, z_{k-1})\rangle \\ &\approx \prod_{k=1}^{N} \left\{ \langle n(z_k), z_k | n(z_{k-1}), z_{k-1}\rangle - \frac{i}{\hbar}\langle n(z_k), z_k | H(S) | n(z_{k-1}), z_{k-1}\rangle \frac{t}{N} \right. \\ &\quad \left. -\frac{i}{\hbar}\langle n(z_k), z_k | h(q;S) | n(z_{k-1}), z_{k-1}\rangle \frac{t}{N} \right\} \\ &= \prod_{k=1}^{N} \langle n(z_k) | n(z_{k-1})\rangle \langle z_k | z_{k-1}\rangle \\ &\quad \times \left[1 - \frac{i}{\hbar} \left(\frac{\langle z_k | H(S) | z_{k-1}\rangle + \langle z_k | \varepsilon_n(S) | z_{k-1}\rangle}{\langle z_k | z_{k-1}\rangle} \right) \frac{t}{N} \right] \\ &= \prod_{k=1}^{N} \langle n(z_k) | n(z_{k-1})\rangle \langle z_k | z_{k-1}\rangle \\ &\quad \times \left[1 - \frac{i}{\hbar} \left(H(\bar{z}_k, z_{k-1}) + \lambda_n(z_{k-1}) \right) \frac{t}{N} \right] \end{aligned}$$

$$\approx \exp[\ln\langle n(z_k)|n(z_{k-1})\rangle + \ln\langle z_k|z_{k-1}\rangle]$$
$$\times \exp\left[-\frac{i}{\hbar}\sum_{k=1}^{N}[H(\bar{z}_k, z_{k-1}) + \lambda_n(z_{k-1})]\frac{t}{N}\right]. \tag{2.44}$$

In deriving (2.44) we have used

$$H(\bar{z}_k, z_{k-1}) = \frac{\langle z_k|H|z_{k-1}\rangle}{\langle z_k|z_{k-1}\rangle} \quad \lambda_n(z_{k-1}) = \frac{\langle z_k|\epsilon_n(S)|z_{k-1}\rangle}{\langle z_k|z_{k-1}\rangle}.$$

Next we examine the various quantities in (2.44)

$$1: \quad \prod_{k=1}^{N}\exp[\ln\langle n(z_k)|n(z_{k-1})\rangle \approx \exp i\sum_{k=1}^{N} w(z_k). \tag{2.45}$$

This result is shown in the following.

$$\begin{aligned}\text{LHS} &\approx \prod_{k=1}^{N}\exp\ln[1-\langle n(z_k)|dn(z_k)\rangle] \\ &\approx \exp\sum_{k=1}^{N} i[i\langle n(z_k)|dn(z_k)\rangle] \\ &= \exp\sum_{k=1}^{N} iw(z_k).\end{aligned}$$

Note that the operator d is defined on a complex manifold, therefore the 1-form w is written as

$$w = i\langle n(z_k)|dn(z_k)\rangle$$

$$= \quad i\left[\langle n(z_k)|\frac{\partial n(z_k)}{\partial z^l}\rangle dz^l + \langle n(z_k)|\frac{\partial n(z_k)}{\partial \bar{z}^l}\rangle d\bar{z}^l\right]. \qquad (2.46)$$

$$2: \qquad \prod_{k=1}^{N} \exp\ln\langle z_k|z_{k-1}\rangle \approx \exp\sum_{k=1}^{N}\frac{j}{1+|z_k|^2}(z_k\triangle\bar{z}_k - \bar{z}_k\triangle z_k). \qquad (2.47)$$

To show this define $\triangle z_k = z_k - z_{k-1}$, then

$$\begin{aligned}
LHS &= \prod_{k=1}^{N}\exp\ln\left\{\frac{[1+\bar{z}_k(z_k-\triangle z_k)]^{2j}}{[(1+|z_k|^2)(1+|z_k-\triangle z_k|^2)]^j}\right\} \\
&= \prod_{k=1}^{N}\exp j\left\{2\ln\left[(1+|z_k|^2)\left(1-\frac{\bar{z}_k\triangle z_k}{1+|z_k|^2}\right)\right]\right. \\
&\quad \left. -\ln\left[(1+|z_k|^2)^2\left(1-\frac{\bar{z}_k\triangle z_k - z_k\triangle\bar{z}_k}{1+|z_k|^2}\right)+O((\triangle z_k)^2)\right]\right\} \\
&= \prod_{k=1}^{N}\exp j\left\{2\ln\left(1-\frac{\bar{z}_k\triangle z_k}{1+|z_k|^2}\right)\right. \\
&\quad \left. -\ln\left[(1+|z_k|^2)^2\left(1-\frac{\bar{z}_k\triangle z_k - z_k\triangle\bar{z}_k}{1+|z_k|^2}\right)\right]+O((\triangle z_k)^2)\right\} \\
&= \prod_{k=1}^{N}\exp j\left\{-2\frac{\bar{z}_k\triangle z_k}{1+|z_k|^2}+\frac{\bar{z}_k\triangle z_k + z_k\triangle\bar{z}_k}{1+|z_k|^2}+O'((\triangle z_k)^2)\right\} \\
&\approx \exp\sum_{k=1}^{N}\frac{j}{1+|z_k|^2}(z_k\triangle\bar{z}_k - \bar{z}_k\triangle z_k).
\end{aligned}$$

Substituting (2.45), (2.47) into (2.44) we have, in the continuum limit, the expression for the effective propagator (2.43)

$$G(T) = \sum_n \int D(z)e^{i\gamma(C)}e^{\frac{i}{\hbar}\int_0^T\left[\frac{j\hbar}{1+|z|^2}(z\dot{\bar{z}}-\bar{z}\dot{z})-H(\bar{z},z)-\lambda_n(z)\right]dt}. \qquad (2.48)$$

The adiaatic action is identified to be

$$S_n^{ad} = \frac{i}{\hbar}\int_0^T \left[\frac{j\hbar}{1+|z|^2}(z\dot{\bar{z}} - \bar{z}\dot{z}) - H(\bar{z},z) - \lambda_n(z)\right] dt \qquad (2.49)$$

and we write (2.48) as

$$G(T) = \sum_n \int D(z) e^{\frac{i}{\hbar}[S_n^{ad} + \hbar\gamma_n(C)]} \qquad (2.50)$$

where $\gamma(C)$ is given by the integral of (2.46).

Thus in the SU(2)-CS representation, we arrive to a conclusion similar to that obtained in the phase-space formulation. The explicit formulas for the adiabatic phase and action function differ from their phase space counterparts but the difference vanishes by choosing the appropriate coherent state representation. Generalized coherent states for Lie groups other than SU(2) can be constructed along similar lines to treat various dynamical systems.

2.5 Discussion

In this chapter, we have shown how nontrivial phases arise in the context of the quantum adiabatic theorem. In the development of the theory, two approaches were taken: the differential and integral formalisms. In the Schrödinger approach it had been shown that, if the phase of eigenfunction cannot be globally fixed, then the adiabatic phase appears. When the theory is reformulated in the path integral formalism, the nontrivial phase

manifests itself in the form of an additional action term. This term is just $\hbar$ times Berry's phase, and has the interpretation of the action related to an induced "vector potential". This interpretation is valid since it can be shown that the adiabatic phase can be expressed as a surface integral of a "magnetic field" $V = i\langle dn|dn\rangle$ whose "vector potential" is $w = i\langle n|dn\rangle$. That the objects w and V so defined can be likened to gauge structures will be shown in the next chapter.

A question remains. In the differential formulation the adiabatic phase is developed on the premise that the phase cannot be globally removed. What then is the machinery giving existence to a nontrivial phase in the path integtral formalism? It cannot arise as a direct consequence of the adiabatic theorem; that theorem merely serves as a mechanism of transporting the eigenstate around a closed loop in parameter space. The global viewpoint of the path integral approach seems to indicate an underlying topological structure which expresses itself as a nontrivial phase when some degrees of freedom are integrated out. In this light the adiabatic approximation is secondary to the fact that one must take into account the topology of the integrated out system. The appearance of a 'magnetic vector potential' which behaves like a gauge object suggests a geometrical nature. Since such gauge objects are closely related to the rich geometry of fibre bundles and other differential structures [WY], we find motivation to probe into the underlying geometry of the adiabatic phase. This leads to a greater understanding of nontrivial phases and how they arise in more general contexts, not just via

the adiabatic mechanism. In chapter 3, the geometrical nature of nontrivial phases in quantum mechanics will be examined.

Chapter 3

Geometric Formulation

3.1 Introduction

Motivated by the geometrical features of the path integral formalism and by the appearance of gauge structures in the theory, we examine the topological phase using the tools of differential geometry. A subsidiary goal of this endeavour is to give a description which is independent of the adiabaticity condition. We thus obtain a generalization of the theory presented in chapter 2. The most important feature of the geometrical description is that it is unnecessary for the Hamiltonian to depend on a set of slowly varying parameters. *The only requirement for the Hamiltonian is to generate evolutions such that a connection can be defined on the fibre bundle structures associated with the evolution.* These concepts will be developed in the forthcoming sections.

3.2 Appearance of Gauge Structures

In this section we make explicit the analogy between the phase 1-form w and gauge potentials. This leads naturally to a geometric description of nontrivial phases, since it is known that the geometrical nature gauge theories lies in the theory of fibre bundles [WY], [BMSS]. We shall show that the 1-form w transforms like a gauge potential and derive from it, gauge fields over some manifold. Thus we generalize Berry's ideas and extend the analysis given by Wilczek and Zee [WZ].

Define the 1-form w to be

$$w = i\langle\xi|d\xi\rangle \tag{3.1}$$

whose matrix elements are given by

$$w_{ij} = \langle\xi_j|d\xi_i\rangle.$$

The set $\{|\xi_k\rangle\}$ is a degenerate set. Although equation (3.1) is obtained in chapter 2 by adiabaticity arguments, we assert here that the definition given here is independent of adiabaticity.

Let $\mathbf{U}$ be the group of unitary tranformations. For $\Omega \in \mathbf{U}$ the 1-form w transformes according to

$$w' = (d\Omega)\Omega^{-1} + \Omega w \Omega^{-1}. \tag{3.2}$$

This is easily proven: let $\xi' = \Omega\xi$

$$\begin{aligned} w'_{ij} &= \langle \xi'_j | d\xi'_i \rangle \\ &= \langle \Omega_{jl}\xi_l | d\Omega_{im}\xi_m \rangle \\ &= \bar{\Omega}_{jl}\langle \xi_l | \xi_m \rangle d\Omega_{im} + \bar{\Omega}_{jl}\langle \xi_l | d\xi_m \rangle \Omega_{im} \\ &= \bar{\Omega}_{jm} d\Omega_{im} + \bar{\Omega}_{jl} w_{ml} \Omega_{im} \\ &= (d\Omega_{im})\bar{\Omega}_{mj} + \Omega_{im} w_{ml} \bar{\Omega}_{lj} \\ &= [(d\Omega)\Omega^{-1} + \Omega w \Omega^{-1}]_{ij} \end{aligned}$$

where $\bar{\Omega}_{lm}$ is the complex conjugate of Ω_{lm}. Next we calulate dw. In local coordinates this is written

$$dw_{ij} = [\langle \partial_\mu \xi_j | \partial_\nu \xi_i \rangle - \langle \partial_\nu \xi_j | \partial_\mu \xi_i \rangle] dX^\mu \wedge dX^\nu. \tag{3.3}$$

Now

$$\begin{aligned} \partial_\mu \langle \xi_j | \partial_\nu \xi_i \rangle &= \langle \partial_\mu \xi_j | \partial_\nu \xi_i \rangle + \langle \xi_j | \partial_\mu \partial_\nu \xi_i \rangle \\ \partial_\nu \langle \xi_j | \partial_\mu \xi_i \rangle &= \langle \partial_\nu \xi_j | \partial_\mu \xi_i \rangle + \langle \xi_j | \partial_\nu \partial_\mu \xi_i \rangle. \end{aligned}$$

Using these in (3.3) along with the completeness relation $\sum_k |\xi_k\rangle\langle\xi_k| = 1$, yields

$$dw_{ij} = \{\partial_\mu \langle \xi_j | \partial_\nu \xi_i \rangle - \partial_\nu \langle \xi_j | \partial_\mu \xi_i \rangle$$

$$- [\langle \xi_j | \partial_\mu \xi_k \rangle \langle \xi_k | \partial_\nu \xi_i \rangle - \langle \xi_j | \partial_\nu \xi_k \rangle \langle \xi_k | \partial_\mu \xi_i \rangle]\} dX^\mu \wedge dX^\nu$$

$$= \{\partial_\mu (w_\nu)_{ij} - \partial_\nu (w_\mu)_{ij} - [w_\mu w_\nu - w_\nu w_\mu]_{ij}\} dX^\mu \wedge dX^\nu.$$

Finally

$$dw = \{\partial_\mu w_\nu - \partial_\nu w_\mu - [w_\mu, w_\nu]\} dX^\mu \wedge dX^\nu \tag{3.4}$$

where $w_\nu = \langle \xi | \partial_\nu \xi \rangle$ and $[\cdot, \cdot]$ is the commutator bracket. It is evident from (3.4) that the nonabelian gauge field G appears:

$$G \equiv \partial_\mu w_\nu - \partial_\nu w_\mu - [w_\mu, w_\nu]. \tag{3.5}$$

The remarks made in chapter 2, that w and dw are gauge-like objects, now have a firm basis.

Consider the case where $\mathbf{U} = U(1)$. Then $\Omega = e^{i\alpha(x)}$. Equation (3.2) then gives the transformation law for a vector potential

$$w' = w + id\alpha.$$

Since $U(1)$ is abelian, the commutator in (3.4) vanishes and we are left with what looks like the electromagnetic field

$$F_{\mu\nu} = \partial_\mu w_\nu - \partial_\nu w_\mu.$$

Nonrelativistically, we cannot completely identify $F_{\mu\nu}$ with the electromagnetic field, for the the object $F_{\mu\nu}$ above exists in a parameter manifold and not

on a space-time manifold. That is, *if the parameter manifold is Minkowski then* $F_{\mu\nu}$ is *the electromagnetic field.* If we assume the parameter manifold to be isomorphic to $\mathbf{R}^n$, so that the indices μ and ν refer to space components, then the diagonal components of $F_{\mu\nu}$ cannot be associated with electric field components. In this sense the analogy is imperfect. Nevertheless, in the present case $V = dw = \langle n|dn\rangle$ acts like a magnetic field on some manifold.

We have shown the striking similarities between w and dw with gauge potentials and fields. Although they are not true gauge objects, they give validity in associating them with differential structure. Specifically, w is a *connection* (since gauge potentials are labelled thusly), and dw is its *curvature.* The terminology comes not from gauge theory itself, but from differential geometry which puts gauge theory on a geometric footing. On this note we investigate next the geometry of nontrivial phases.

3.3 The Geometric Phase

The mathematical apparatus for this section is given in the appendix at the end of this chapter. Note particularly propositions 3.6.1 and 3.6.2; definitions 3.6.4, 3.6.5 and 3.6.7.

Let us now discuss how the nontrivial phase arises from natural geometric structures associated with quantum evolution. A salient feature of a differential-theoretic description is that the theory is set free from the adiabatic restriction. Moreover, it is not necessary that the evolution of the system be cyclic or unitary [SB]. If the evolution *is* cyclic by some defini-

tion, then the nontrivial phase may be viewed as a holonomy transformation [Si],[AA],[AA2],[An]. We first identify the natural geometric structures and then discuss the nontrivial phase in cyclic and noncyclic evolution.

Denote the set of normalizable states in the Hilbert space $\mathcal{H}$ of L^2 functions by P

$$P = \{\psi \in \mathcal{H} : \langle\psi|\psi\rangle \neq 0\}.$$

Define a *ray* in $\mathcal{H}$ to be an equivalence class

$$[\psi] = \{\psi' \in P|\psi' = e^{i\alpha}\psi\}, \quad \alpha \in \mathbf{R},$$

i.e states differing in phase only. Clearly the equivalence relation $\psi' \sim \psi$ defined above is induced by the abelian group U(1). Define the manifold M to be the quotient space of P by the equivalence relation $\sim$ induced by U(1): $M = P/\sim$. Thus the manifold M, which we call the ray-space, is the set of rays of $\mathcal{H}$; and the manifold P is the disjoint union of its equivalence classes(rays). There is a natural projection $\pi : P \rightarrow M$ which assigns each element ψ of P to a ray which contains ψ. The geometric structures just described form a principal fibre bundle $P(M, U(1))$ over the ray-space M. We will sometimes write P instead of $P(M, U(1))$.

On $P(M, U(1))$, there exists a natural connection Γ whose origin is in the Schrödinger equation. Let the state vector evolve according to

$$i\frac{d\psi}{dt} = h\psi \quad \hbar = 1$$

Here the Hamiltonian h is not necessarily self-adjoint; the consequence of which means the evolution may not be unitary. In any case, the evolution defines a curve in P which projects to a curve in M under the projection map π. We normalize the state vector so that the dynamical phase remains zero during the course of evolution. Define

$$\tilde{\phi} = \exp\left(i\int^t \frac{\langle\psi|h\psi\rangle}{\langle\psi\psi\rangle}dt'\right)\psi. \tag{3.6}$$

Inserting (3.6) into the Schrödinger equation above yields

$$i\frac{d\tilde{\phi}}{dt} = 0,$$

from which we obtain

$$\langle\tilde{\phi}|i\frac{d\tilde{\phi}}{dt}\rangle = 0. \tag{3.7}$$

With equation (3.7), we can define a connection Γ on P.

The evolution of the system defines a curve $\varphi(t)$ in P which projects to a curve $\phi(t)$ in M via π. Denote the vectors tangent to $\varphi(t)$ by $v_{\varphi_t} = (d\varphi(t)/dt)|_{\varphi_t}$, where φ_t is a point on the curve $\varphi(t)$. Then the set of all tangent vectors v forms the tangent space $T_{\varphi_t}P$. Let $H_{\tilde{\varphi}_t}$ be the set of tangent vectors in $T_{\varphi_t}P$ whose statefunctions $\tilde{\phi}$ satisfy equation (3.7) . Given a Hamiltonian h, the set $H_{\tilde{\varphi}_t}$ is uniquely determined by the Schrödinger equation. Observe that $H_{\tilde{\varphi}_t} \subseteq T_{\varphi_t}P$. Denoting the complement $T_{\varphi_t}P\backslash H_{\tilde{\varphi}_t}$

by $V_{\tilde{\varphi}_t}$, we have the decomposition

$$T_{\varphi_t}P = H_{\tilde{\varphi}_t} \oplus V_{\tilde{\varphi}_t}. \tag{3.8}$$

This decomposition of the tangent space $T_{\varphi_t}P$ defines a connection Γ in $P(M, U(1))$. By proposition (3.6.1), there then exists a connection 1-form which we define to be

$$w = i\langle \phi^{\times} | \frac{d\phi^{\times}}{dt} \rangle \tag{3.9}$$

where $\phi^{\times} \in P$ and $(d\phi^{\times}/dt) \in T_{\varphi_t}P$. Equation (3.8) implies that $\phi^{\times} = \tilde{\phi} + \phi_V$, where $\tilde{\phi} \in H_{\tilde{\varphi}_t}$ and $\phi_V \in V_{\tilde{\varphi}_t}$, so that

$$w = i\langle \phi_V | \frac{d\phi_V}{dt} \rangle.$$

Here we have made use of part 1 of proposition 3.6.1. Note that w in equation (3.9) vanishes if the tangent space $T_{\varphi_t}P$ cannot be decomposed according to the splitting (3.8). If $T_{\varphi_t}P = H_{\tilde{\varphi}_t} \oplus O$, where O is the zero subspace, then $\phi^{\times} = \tilde{\phi} \in H_{\tilde{\varphi}_t}$. Consequently $w = 0$. Having shown the existence of a nonvanishing connection 1-form w, we now proceed to relate w and the nontrivial phase.

Suppose the system undergoes a cyclic evolution where the state vector returns to the initial ray at some time τ, i.e, the endpoints of the curve $\varphi(t)$ lie in the same fibre. However, the endpoints $\varphi(0)$ and $\varphi(\tau)$ are not necessarily the same point in the fibre(ray). In any case the projected curve $\phi(t)$ in M

is closed. Given the curve $\phi(t)$ and an arbitrary point $\varphi_0 = \varphi(0)$ in P such that $\pi(\varphi_0) = \phi_0 = \phi(0)$, there exists a unique lift, which we shall denote by $\tilde{\phi}(t)$, starting from φ_0, by proposition 3.6.2. We may then define parallel translation as in definition 3.6.7. In the geometrical picture, evolution is viewed as the transport of the state vector ψ along a curve in the bundle space P of a pricipal fibre bundle; or alternatively as the transport of fibres along the curve $\phi(t)$ by parallel translation defined by

$$\tilde{\phi}_T : \pi^{-1}(\phi_0) \to \pi^{-1}(\phi_\tau) \tag{3.10}$$

Now the condition of parallel translation, definition 3.6.7, gives (with subscripts suppressed)

$$\partial\tilde{\phi} + w\tilde{\phi} = 0$$

which upon integrating yields the formal expression

$$\tilde{\phi} = e^{\oint w}\tilde{\phi}_0$$

where the integral is along a path in M. We thus obtain the familiar result that a nontrivial phase $\gamma = \oint w$ appears during the (cyclic) evolution.

Next we consider the conditions under which a nontrivial phase appears. Given a closed curve $\phi(t)$ in M, then there is a unique horizontal lift $\tilde{\phi}(t)$, a segment of which coincides with the curve representing the actual evolution of the system. The lifting of the closed curve $\phi(t)$ to P yields a

curve $\tilde{\phi}(t)$ which is not necessarily closed. If the Hamiltonian is such that the evolution allows a connection to be defined in the pricipal bundle, then the lift $\tilde{\phi}(t)$ is closed under the following conditions

1. the endpoints of $\tilde{\phi}(t)$ coincide: $\tilde{\phi}(\tau) = \phi(0)$
2. if $\tilde{\phi}(\tau) \neq \tilde{\phi}(0)$, then $\tilde{\phi}(t)$ is closed by the vertical curve which joins $\tilde{\phi}(\tau)$ and $\tilde{\phi}(0)$.

If $\tilde{\phi}(t)$ is closed according to the first condition, then w vanishes by (3.7). On the other hand, if $\tilde{\phi}(t)$ is closed according to condition 2, then $w = 0$ along the segment $[\tilde{\phi}(0), \tilde{\phi}(\tau)]$ (since this is the actual path of evolution). But along the vertical curve $w \neq 0$, as the tangent vectors to this curve are elements of the vertical subspace $\mathbf{V}$ (cf. proposition 3.6.1, property 1). When the evolution admits no connection, the horizontal lift is not connected by a vertical, and again the connection 1-form vanishes; consequently a nontrivial phase does not appear. Thus fibre bundles can be classified according to conditions 1 and 2.

We now explain how the nontrivial phase factor can be interpreted as a holonomy transformation. Define the loop space C_{x_0} to be the set of loops of M passing through the point $x_0 \in M$. On C_{x_0} there is a well defined multiplication law. The mapping (3.10) is then a diffeomorphism of the fibre $\pi^{-1}(x_0)$ onto itself. The set of all such diffeomorphisms $\{\tilde{\phi}_T\}$ forms a group called the *holonomy group* of a given connection Γ with reference point x_0. The holonomy group is a Lie group (see [KN]), whose elements induce

transformations on M. Thus the phase factor $\exp \oint w$ can be viewed as a holonomy transformation on M.

It is evident in the above analysis that the nontrivial phase is geometrical in nature. The geometrical phase depends only on the curve $\phi(t)$ and, more importantly, does not depend on the rate of transversal around $\phi(t)$. The adiabatic theorem, therefore, is not a necessary condition for the appearance of a nontrivial phase, but merely a means to an end.

Thus far we have discussed cyclic evolution in the sense that the curve traced out in P projects to a closed curve in ray-space. It may happen that the evolution is such that the state vector does not return to the initial ray. Consequently the curve $\phi(t)$ in M is open, and the evolution is noncyclic. The natural connection in $P(M, U(1))$ no longer provides a way of comparing the states; the vertical vectors, which are tangent to the fibre, lie on different fibres and cannot join the endpoints of the curve. However, there is a connection, called the *Pancharatnam connection* that will allow the comparison of states on different rays [SB], [AA2]. We examine this next.

Let $\tilde{\phi}_1, \tilde{\phi}_2 \in P$ be nonorthogonal states. The superposition of these two states gives

$$\|\tilde{\phi}_1 + \tilde{\phi}_2\| = \langle\tilde{\phi}_1|\tilde{\phi}_1\rangle + \langle\tilde{\phi}_2|\tilde{\phi}_2\rangle + 2Re\langle\tilde{\phi}_1|\tilde{\phi}_2\rangle$$

The term $\langle\tilde{\phi}_1|\tilde{\phi}_2\rangle$ represents the interference between $\tilde{\phi}_1$ and $\tilde{\phi}_2$. If $\langle\tilde{\phi}_1|\tilde{\phi}_2\rangle$ is real and positive, the modulus is already a maximum; and so $\tilde{\phi}_1$ and $\tilde{\phi}_2$ are "in phase". In general $\langle\tilde{\phi}_1|\tilde{\phi}_2\rangle$ is complex and we write the polar

form $r \exp i\beta$, $r > 0$. Where β is the phase difference between $\tilde{\phi}_1$ and $\tilde{\phi}_2$ and represents the Pancharatnam connection. There exists an intimate relationship between the phase difference and the connection 1-form w. To this end we examine the notion of geodesic curves in the ray space M.

We can define a metric on M by means of the positive definite inner product $\langle \cdot | \cdot \rangle$ on the Hilbert space $\mathcal{H}$. Let $\tilde{\phi}(s)$ be a curve in P and $\phi' = d\tilde{\phi}(s)/ds + w\tilde{\phi}(s)$ its covariant derivative. It is easy to show that the inner product $\langle \phi' | \phi' \rangle$ transforms covariantly under the transformation $\phi' \rightarrow e^{i\alpha(s)}\phi'$:

$$\begin{aligned}
\langle \phi' | \phi' \rangle \quad \rightarrow \quad & \left[-\left(\frac{d\alpha}{ds}\right)^2 + 2iw\frac{d\alpha}{ds} + w^2 \right] \langle \tilde{\phi} | \tilde{\phi} \rangle + \langle \frac{d\tilde{\phi}}{ds} | \frac{d\tilde{\phi}}{ds} \rangle \\
& + \left(w + i\frac{d\alpha}{ds} \right) \langle \frac{d\tilde{\phi}}{ds} | \tilde{\phi} \rangle + \left(w + i\frac{d\alpha}{ds} \right) \langle \tilde{\phi} | \frac{d\tilde{\phi}}{ds} \rangle \\
= \quad & \langle \frac{d\tilde{\phi}}{ds} | \frac{d\tilde{\phi}}{ds} \rangle + \tilde{w} \left[\langle \frac{\tilde{\phi}}{ds} | \tilde{\phi} \rangle + \langle \tilde{\phi} | \frac{d\tilde{\phi}}{ds} \rangle \right] + \tilde{w}^2 \langle \tilde{\phi} | \tilde{\phi} \rangle
\end{aligned}$$

where $\tilde{w} = w + id\alpha/ds$. Since the inner product $\langle \phi' | \phi' \rangle$ is covariant, it can be used to define a metric on M. Hence the distance squared between $\pi(\tilde{\phi}(s))$ and $\pi(\tilde{\phi}(s + ds))$ is given by

$$dl^2 = \langle \phi' | \phi' \rangle ds^2.$$

The variational principle applied on $\int \langle \phi' | \phi' \rangle dl$, where l is an affine parameter,

yields the geodesic equation

$$\frac{d\phi'}{dl} + w\phi' = 0.$$

Curves in P satisfying the geodesic equation project to geodesics in M. Geodesic curves in M allow the Pancharatnam phase difference to be expressed as a line integral of the connection 1-form.

Proposition 3.3.1 *Let $\tilde{\phi}_1, \tilde{\phi}_2 \in P$ be nonorthogonal and differing in phase β according to the Pancharatnam connection. Let $\tilde{\phi}(s)$ be any geodesic curve such that $\tilde{\phi}(\tau) = \tilde{\phi}_2$, $\tilde{\phi}(0) = \tilde{\phi}_1$ Then*

$$\beta = \int w(s)ds$$

proof: Let $r(t)$ be a geodesic in the rayspace M. The horizontal lift of this curve is a geodesic $\phi^{\star}(s)$ in P. The geodesics $\tilde{\phi}(s)$ and $\phi^{\star}(s)$ are related by a gauge transformation

$$\tilde{\phi}(s) = e^{i\alpha}\phi^{\star}(s).$$

Since $\tilde{\phi}_1$ and $\tilde{\phi}_2$ differ in phase β choose $\alpha(0) = 0, \alpha(\tau) = -\beta$. Integrating the 1-form w along the geodesic curve $\tilde{\phi}(s)$, noting that $w(s)$ tranforms inhomogeneously under gauge transformation, yields

$$\int_0^{\tau} w(s) \longrightarrow \int_0^{\tau} \left[w + \frac{d\alpha(s)}{ds} \right] ds.$$

Along the horizontal curve ϕ^*,$w = 0$ and we obtain immediately

$$\int_0^\tau \left(\frac{d\alpha(s)}{ds}\right) ds = \beta$$

q.e.d.

Using proposition 3.6.1, we obtain the geometrical phase for a noncyclic evolution. Let $\tilde{\phi} \in P$ evolve from $\tilde{\phi}_0$ to $\tilde{\phi}_\tau$ with $\tilde{\phi}_\tau$ lying on a different fibre. Under π, $\tilde{\phi}_0, \tilde{\phi}_\tau$ project to the points $\pi(\tilde{\phi}_0), \pi(\tilde{\phi}_\tau) \in M$ respectively. Let $\pi(\tilde{\phi}_0)$ and $\pi(\tilde{\phi}_\tau)$ be joined by a geodesic curve $r(t)$. Then the curve $c = \phi(t) \bigcup r(s)$ is a closed curve in M. Here $\phi(t)$ is the projection of the curve $\tilde{\phi}(t)$ in P into M. The horizontal lift of c gives the curve $\tilde{c} = \tilde{\phi}(t) \bigcup g(s)$; where $\tilde{\phi}(t)$ is the evolution curve whose endpoints $\tilde{\phi}_0$ and $\tilde{\phi}_\tau$ are connected by a geodesic curve $g(s)$ in P. Suppose $\tilde{\phi}_0$ and $\tilde{\phi}_\tau$ are nonorthogonal, then their phase difference is given by the Pancharatnam connection. The condition of parallel transport along $\tilde{c}$ gives

$$\tilde{\phi}_\tau = \exp\left[\int_{\tilde{\phi}(t)} w(s)ds + \int_{g(s)} w(s)ds\right] \tilde{\phi}_0.$$

Along the curve $\tilde{\phi}(t)$, the connection 1-form w vanishes and the latter equation can be written as

$$\tilde{\phi}_\tau = e^{\oint_{\tilde{c}} w} \tilde{\phi}_0 = e^{\int_{g(s)} w(s)ds} \tilde{\phi}_0.$$

Thus the nontrivial phase can also arise in a noncyclic evolution.

When the Hamiltonian exhibits a degenerate spectrum, then the states form a degenerate subspace V_n of $\mathcal{H}$. In this case we examine the evolution of the n-dimensional subspace $V_n(t)$ whose elements are obtained from the vectors in V_n via the Schrödinger evolution in the time interval $[0,t]$. The geometric structure is not the principal bundle $P(M,U(1))$ but the *vector bundle* E_n over the Grassmann manifold G_n [An]. In contrast to $P(M,G)$, a vector bundle consists of essentially a union of (local) product spaces with a projection into a manifold; and whose fibres are vector spaces.

Let B be a Banach space such that $B = V \oplus F$. Denote the set of all split subspaces of B by $G(B)$, called the Grassmann manifold. If the subspaces V and F have dimension n and m respectively, $G(B)$ is denoted as $G_{nm}(B)$. We consider the space

$$E_n(B) = \{(V,v)|V \text{is an n-dimensional subspace of} B, v \in V\}$$

since the subspace of interest is $V_n(t)$ and not the cospace F. Now there is a projection $\rho : E_n(B) \to G_n(B)$ which allows a vector bundle structure in $E_n(B)$ (see [AMR]). Given this structure, let $E_n(B)$ be a Hilbert space $\mathcal{K}$ of $n+m$-dimension whose time dependent decomposition is $\mathcal{K} = V_n(t) + F_m(t)$. Suppose $V_n(\tau) = V_n(0)$ for some $\tau \in [0,t]$, then $V_n(t)$ undergoes cyclic evolution in the interval $[0,\tau]$. The group acting on $\mathcal{K}$ is the unitary group $U(n,m)$ which leaves the quantity $\sum_{i=n+1}^{n+m} x^i\bar{x}^i - \sum_{i=1}^{n} x^i\bar{x}^i$ in $\mathbf{C}^{n+m}$ invariant. The subgroup of $U(n,m)$ which leaves $V_n(t)$ invariant is $U(n) \times U(m)$, so the manifold $G_n(B)$ is given by $U(n,m)/U(n) \times U(m)$. Having established the

vector bundle structures analogous to those of the principal fibre bundle, it follows immediately from the nondegenerate case, the connection in $E_n(B)$ is given by the matrix- valued 1-form w_{ij}:

$$w_{ij} = \langle \psi_j | \frac{d\psi_i}{dt} \rangle$$

where $\psi_i \in \{\psi_j, j = 1, \ldots, n\}$, the orthonormal basis of $V_n(t)$. By parallel transport we have

$$\psi = Pe^{\int_0^t w dt} \psi_0.$$

We have thus uncovered the geometric substratum of the nontrivial phase for both degenerate and nondegenerate cases. In doing so we we obtain a description in which the adiabaticity condition is in no way essential; moreover we have a vastly richer description of the nontrivial phase.

3.4 Generalizing The Effective Propagator

We complete the geometric description of the nontrivial phase by extending the coherent state path integral to the case where the Hamiltonian is a function of the generators of an arbitrary Lie group G [K].

The set of generalized coherent states $\{|Z\rangle\}$, $Z \in \mathbf{C}$, along with the partition of unity form a Hilbert space. These states are obtained according to

$$|Z\rangle = T(g)|0\rangle$$

with g running over G. And $T(g)$ is defined as before. Let R be a subgroup of G. Then G can be regarded as a fibre bundle over the quotient space $G/R = M$, with structure group R. The parameter Z is then an element of M, and the vectors $|Z\rangle$ form a local cross section of the fibre bundle $G(M, R)$. A sequence of states

$$S = \{|Z^0\rangle, |Z^1\rangle, \ldots, |Z^\alpha\rangle, \ldots\}$$

is obtained by various choices of initial states $|0\rangle$. This sequence can be grouped into classes where any two vectors belonging to the same class are compatible.

Definition 3.4.1 *Let $|Z^\alpha\rangle$, $|Z^\beta\rangle$ be two vectors belonging to class α, β, respectively. For a given generator Q of a Lie group G, corresponding to $|Z^{(\cdot)}\rangle$, the vectors $|Z^\alpha\rangle$, $|Z^\beta\rangle$ are compatible if*

$$\langle Z^\alpha | Q | Z^\beta \rangle \neq 0.$$

Suppose the Hamiltonian is given by a function of the generators of G only: $H = f(Q)$. The effective propagator is

$$G(T) = \lim_{N\to\infty} \int d\mu(Z_0) \langle Z_0 | \exp(-\frac{i}{\hbar} Ht/N)^N | Z_0 \rangle$$

where $|Z_0\rangle$ is assumed to belong to a specific class α_0 of S. Inserting the

partition of unity, as before, gives

$$G(T) = \lim_{N\to\infty} \int d\mu(Z_0^{\alpha_0}) \int \prod_{k=1}^{N-1} d\mu(Z_k^{\alpha_k}) \langle Z_k^{\alpha_k} | \exp(-\frac{i}{\hbar} Ht/N) | Z_{k-1}^{\alpha_{k-1}} \rangle .$$

The integrand represents the probability amplitude for transitions from a coherent state of class α_{k-1} to a state of class α_k. Only classes for which $\alpha_{k-1} = \alpha_k$ do transitions occur, by compatibility. Assuming this, the labels α_{k-1}, α_k etc., are thus redundant, and henceforth, will be omitted. We have

$$\begin{aligned}
\text{integrand} &\approx \prod_{k=1}^{N-1} \langle Z_k | (1 - \frac{i}{\hbar} Ht/N) | Z_{k-1} \rangle \\
&= \prod_{k=1}^{N-1} \langle Z_k | Z_{k-1} \rangle \left(1 - \frac{i}{\hbar} \frac{\langle Z_k | H | Z_{k-1} \rangle}{\langle Z_k | Z_{k-1} \rangle} \frac{t}{N} \right) \\
&\approx \prod_{k=1}^{N-1} \exp(\ln \langle Z_k | Z_{k-1} \rangle) \exp \left(-\frac{i}{\hbar} \frac{\langle Z_k | H | Z_{k-1} \rangle}{\langle Z_k | Z_{k-1} \rangle} \frac{t}{N} \right) \\
&\approx \prod_{k=1}^{N-1} \exp \frac{i}{\hbar} \left[\frac{\langle Z_k | i\hbar \triangle Z_k \rangle}{t/N} - \frac{\langle Z_k | H | Z_{k-1} \rangle}{\langle Z_k | Z_{k-1} \rangle} \right] \\
&= \exp \frac{i}{\hbar} \left[\langle Z_k | \left(\frac{i\hbar \triangle}{t/N} - \frac{H}{\langle Z_k | Z_{k-1} \rangle} \right) | Z_k \rangle \right] .
\end{aligned}$$

In the above, $\triangle$ is the difference operator, and we have tacitly assumed that $\langle Z_k | Z_{k-1} \rangle \approx 1$. Thus in the continuum limit we have

$$G(T) = \int D(Z) \exp \frac{i}{\hbar} \int_0^T \langle Z | (i\hbar\partial_t - H) | Z \rangle dt. \qquad (3.11)$$

The first term in the exponent gives the general form for the geometric phase for the present case, and the second term is the dynamical phase. It is important to note that the above result is obtained without recourse to the adiabatic theorem.

The adiabatic phase can be recovered from (3.11) by assuming the Hamiltonian to be $\mathbf{H} = H(\zeta)+h(q;\zeta)$, and that ζ is slow changing. Then $\psi = |Z\rangle \approx |\zeta\rangle \otimes |n(\zeta)\rangle$ where $|n(\zeta)\rangle$ is an eigenstate of the internal Hamiltonian $h(q;\zeta)$. The adiabatic phase then follows.

The path integral formula (3.11) also reveals an interesting feature. The argument of the exponential remarkably resembles the Jackiw-Kerman formula for the effective action with Lagrangian $L = \langle Z|(i\hbar\partial_t - H)|Z\rangle$. Consequently it can be shown that the geometrical phase can be written as an integral of a symplectic 1-form [Ko].

3.5 Discussion

The appearance of gauge structures associated with the nontrivial phase indicates that such phases have a topological basis. Much of the differential-geometric machinery of gauge theory could be carried over to the description of nontrivial phases.

We have identified the principal fibre bundle $P(M, U(1))$ as the geometrical structure on which to describe the geometry of nontrivial phases. It is also feasible to use the Hopf-fibration $\mathcal{H} - \{0\}$ where the base manifold is the complex projective space $\mathcal{P} = (\mathcal{H} - \{0\})/C^*$ whose natural metric is

the Fubini-Study metric (see [EGH]). The structure group $C^\times$ is the group of multiplication by complex numbers. The Hopf-bundle is used in [AA1], [AA2], [An], and [Pa]. In this geometry, nontrivial phases can always be expressed as a holonomy transformation. However, by choosing to work in $P(M, U(1))$, we demonstrate that the geometric phase can also arise in non-cyclic evolution. Certainly there is no fundamental reason why nontrivial phases should be confined to cyclic evolution.

In this chapter, several facts were established. One, the adiabaticity condition is not essential for the existence of a nontrivial phase. Another is that the evolution is no longer required to be cyclic. Under certain conditions, nontrivial phases may arise in noncyclic evolution through the Pancharatnam connection.

3.6 Appendix

We review some basic facts from the theory of fibre bundles (see for example [KN], [EGH], [vW], [DM]). The theory of fibre bundles is intricably linked with modern gauge theories; it is also the basis for a geometric description of nontrivial phases.

Before giving a precise definition of a fibre bundle, we examine first the geometric edifice that surrounds its construction. The first is the concept of a manifold. Roughly, a manifold is a topological space which can support the process of differentiation; it is the underlying continuum on which to describe phenomena. We shall employ the following definition.

Definition 3.6.1 *A differentiable manifold M is a Hausdorff space which is locally homeomorphic to $\mathbf{R}^n$. This homeomorphism allows a differential structure of class C^r to be defined on M so that M is analytic.*

Throughout this chapter we shall assume that M is a C^∞- manifold. Associated with a manifold M is the tangent space. Let $c : [a,b] \in \mathbf{R} \to M$ be a differentiable curve of class C^1 such that $c(t_0) = x \in M$ for $t_0 \in [a,b]$. Let $\mathcal{F}(x)$ be the algebra of C^1 functions defined in a neighborhood of some point $p \in M$. The vector tangent to the curve $c(t)$ at p is the mapping $\chi : \mathcal{F}(p) \overset{into}{\to} \mathbf{R}$. For $f \in \mathcal{F}(X)$, this map is given by $\chi f = (df(c(t))/dt)_{t_0}$. Thus we have the definition

Definition 3.6.2 *The set of tangent vectors χf defines a linear space called the tangent space T_xM of M at x. The disjoint union $TM = \bigcup_{x\in M} T_xM$ is called the tangent bundle of M.*

We can then define a mapping which assigns to each point $x \in M$, a vector $\phi \in TM$. This assignment is called a vector field on M. Let $\mathcal{X}(M)$ be the set of vector fields on M; it is a real vector space under the operation of addition and scalar multiplication.

Next, we define a Lie group, which is of paramount importance in constructing the principal fibre bundle.

Definition 3.6.3 *A Lie group G is a structure which is simultaneously a group and a differentiable manifold such that the group operations $(a,b) \in G \times G \longmapsto ab \in G$ and $a \in G \longmapsto a^{-1} \in G$ are C^∞-maps.*

Let $g \in G$. The maps $L_g a = ga$ and $R_g a = ag$ for every $a \in G$ denote the left(respectively right) translations of G by an element g. The left(right) translations are diffeomorphism of G. A vector field $X \in \mathcal{X}(G)$ on G is left invariant if

$$dL_g X(a) = X(L_g a) = X(ga) \qquad \forall a, g \in G.$$

Here $dL_g \equiv (L_g)_*$ is an isomorphism of the tangent spaces $T_a(G), T_{ga}(G) \forall g \in G$. Similarly for right invariance

$$dR_g X(a) = X(R_g a) = X(ag)$$

where $dL_g \equiv (L_g)_*$ is an isomorphism between $T_a(G)$ and $T_{ag}(G)$ $\forall g \in G$. The set of left invariant vector fields on G form a vector space which is isomorphic to the tangent space $T_e(G)$ at the identity e; its dimension being equal to the order of the group G. We then define the *Lie algebra* $\mathcal{G}$ of G to be the set of all left invariant vector fields on G endowed with the Lie product (commutator) along with the operation of addition and scalar multiplication. The set $\mathcal{G}$ may be viewed as a Lie subalgebra of the Lie algebra $\mathcal{A}$ of vector fields $\mathcal{X}(G)$, i.e, $\mathcal{G}$ is a subspace of $\mathcal{A}$ for which the Lie product $[a, b]$ is an element of $\mathcal{G}$ for $a, b \in \mathcal{G}$.

Given a manifold M and a Lie group G, we define how G acts on M. The group G is a *Lie transformation group* of M if

1. Every element g of G induces a transformation of M: $x \to xg$ $x \in M$.

2. There is a differentiable mapping $(g, x) \in G \times M \rightarrow xg \in M$ such that $x(g_1 g_2) = (xg_1)g_2$ for $x \in M$ and $g_1, g_2 \in G$.

If $R_g x = x \ \ \forall x \in M$ implies $g = e$, then G acts *effectively* on M. For the stronger condition that if $R_g x = x$ for *some* $x \in M$, then $g = e$, we then have G acting *freely* on the right. We may define a Lie transformation group using left translation L_g in a similar fashion.

Preliminaries aside, we turn to the definition of a principal fibre bundle. A principle fibre bundle extends the notion of the topological product of a Lie group G and a manifold M.

Definition 3.6.4 *Let M be a differentiable manifold and G a Lie group. A differentiable principal fibre bundle over M with group G consists of a differentiable manifold P and an action of G on P satisfying the following conditions.*

1. *G acts freely on P on the right $(u, g) \in P \times G \longmapsto ug = R_g u \in P$.*

2. *M is the quotient space of P by the equivalence relation $\sim = \{(u_1, u_2) \in P \times P | \exists g : u_1 g = u_2\}$ induced by G. The natural projection $\pi : P \rightarrow M$ which assigns to each point $u \in P$, an equivalence class containing u, i.e, $[u] = \{u' \in P | u' \sim u\}$, is differentiable.*

3. *P is locally trivial, i.e, every point $x \in M$ has a neighborhood U and a diffeomorphism $\psi : \pi^{-1}(U) \rightarrow U \times G$ such that $\psi(u) = (\pi(u), \phi(u))$ where ϕ is a mapping of $\pi^{-1}(u)$ into G satisfying $\phi(ug) = (\phi(u))g$ for all $u \in \pi^{-1}(u)$ and $g \in G$.*

We shall denote the principal fibre bundle by $P(M,G)$, where P is the bundle or total space, M the base space, and G the structure group. We call the $\pi^{-1}(x) = \{ug | g \in G, \ \pi(u) = x\}$ the fibre over $x \in M$ through u. Each fibre is diffeomorphic to G and coincides with an equivalence class containing u; and each fibre is a point in M. A local cross section on P is a C^∞-map $\sigma : A \to P$; A being an open set of M such that $\pi \circ \sigma = 1$. If $A = M$, then σ is the global cross section. In terms of the cross section, a vector field may be alternatively defined as a local cross section of the tangent bundle TM.

Having established the geometrical foundation, we next examine the geometric machinery that gives rise to the nontrivial phase: the concept of a connection in a principal fibre bundle. There are many equivalent definitions for the connection (see for example [EGH]), however, for the purpose at hand, we shall use as a working definition, the following

Definition 3.6.5 *A connection in a principal fibre bundle $P(M,G)$ is a linear mapping $\Gamma_u : T_xM \to T_uP$ of the tangent space T_xM at x into the tangent space T_uP at $u \in \pi^{-1}(x)$ with the following properties*

1. *$\Gamma_u(T_xM) = H_u$ is the horizontal subspace of $T_u(P)$ such that $T_uP = H_u \oplus V_u$ where V_u is the vertical subspace of T_uP*

2. *$d\pi \circ \Gamma_u = 1$*

3. *If $u' = R_g u = ug, \ \ g \in G$ then $\Gamma_{u'} = \Gamma_{ug} = dR_g \Gamma_u$*

Thus a connection is essentially a splitting of the tangent space T_uP into a horizontal subspace H_u and a vertical subspace V_u. The space V_u is the

tangent space to the fibre at u

$$V_u = T_u(\pi^{-1}(x)).$$

Hence under the projection $d\pi$, $d\pi(V_u) = 0$ and $d\pi(H_u) = T_xM$. Any vector in T_uP can be uniquely decomposed into horizontal and vertical components (fig. 3.1) The subspace V_u is isomorphic to the Lie algebra $\mathcal{G}$ of G. This

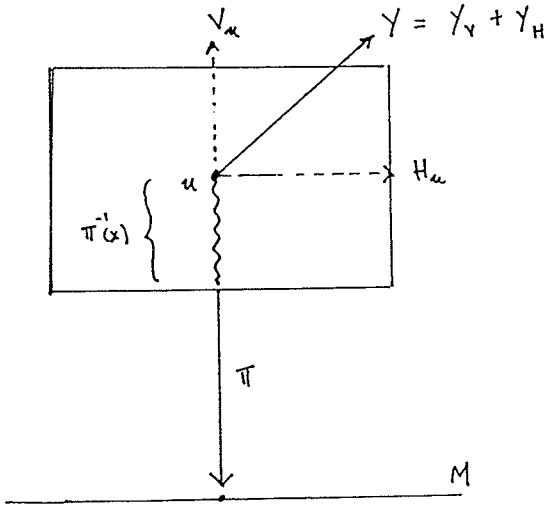

fig. 3.1

isomorphism gives rise to a $\mathcal{G}$-valued differential form w on P called the *connection 1-form*, mapping $T_uP \to \mathcal{G}$:

$$T_uP \xrightarrow{v} T_u(\pi^{-1}(x)) \overset{i}{\cong} \mathcal{G}(G)$$
$$\underbrace{\qquad\qquad\qquad\qquad}_{w}$$

Here v is a linear map induced by the isomorphism i and takes vectors in T_uP to the vertical subspace V_u.

It turns out that a connection and the 1-form w are intimately associated. We have

Proposition 3.6.1 *Given a connection Γ in $P(M,G)$. Then there exists a connection 1-form with values in the Lie algebra $\mathcal{G}$ of G having the properties*

1. $w(udg) = g^{-1}dg,\ u \in P,\ g \in G$ *i.e* $w(Y) = w(Y_V) = \tilde{Y}_V,\ Y_V \subset T_uP,\ \tilde{Y}_V \in \mathcal{G}$ *and* $w(Y) = 0$ *for* $Y \in H_u$

2. $w(dR_gY) = g^{-1}w(Y)g$

Conversely, given w on P satisfying conditions (1)-(2), there is a unique connection Γ in P whose connection 1-form is w. Proof: Refer to [KN], proposition 1.1

In condition (1) $dg \in T_gG$ and $g^{-1}dg \in T_eG = \mathcal{G}(G)$; the vertical udg is mapped into the element of the Lie algebra corresponding to dg. Condition (2) says that under right translation w transforms according to the inverse adjoint representation of the group G in $\mathcal{G}$.

Closely related to the 1-form w is the curvature 2-form.

Definition 3.6.6 *Let Γ be a connection on $P(M,G)$ whose associated connection 1-form is w. The $\mathcal{G}$-valued 2-form*

$$\Omega = \nabla w = dw \circ p$$

is the curvature 2-form of the connection. Here p is the projection $p : T_uP \rightarrow H_u$

Recapitulating, a connection exists on $P(M, G)$ if T_uP has the direct sum decomposition $T_uP = V_u \oplus H_u$. The set of horizontal vectors connect neighboring points of P so that if one point is on a fibre then so is the neighboring point. This process is characterized by a differential 1-form describing the connection. Conversely, a connection 1-form w implies a connection Γ. Finally, we make the remark that any principal fibre bundle admits a connection if the base manifold is paracompact (cf. [KN], Theorem 2.1)

Given that a connection Γ is defined on $P(M, G)$, we introduce the notion of parallel translation of fibres along a curve in the base manifold M. For this concept, we shall need the idea of a *horizontal lift* of a vector field X on M. The horizontal lift of the vector field X is that unique vector field $\tilde{X}$ on P which is horizontal, and projects according to $d\pi(\tilde{X}(u)) = X(\pi(u))$-the value of X at u. Similarly, we can define the horizontal lift of a piece-wise differentiable curve $c(t)$ in M to be the horizontal curve $\tilde{c}(t)$ in P such that $\tilde{c}$ is piece-wise differentiable and whose tangent vectors are horizontal. Under the projection π

$$\pi(\tilde{c}) = c.$$

Let c be a curve (assumed to be C^1) in M. Then there is an associated curve in P.

Proposition 3.6.2 *For an arbitrary point* $u_0 \in \pi^{-1}(x_0) \subset P$ *with* $\pi(u_0) =$

$c(t_0)$, *there exists a unique lift* $\tilde{c}$ *of* c *beginning at* u_0. *proof:*see [KN], proposition 3.1

The proof outlined in [KN] can be extended to give a sufficiency condition for a curve $\tilde{c}$ to be horizontal. In that proof the lift $\tilde{c}$ must have the form

$$\tilde{c}(t) = u(t)g(t)$$

where $g(t)$ is a curve in G, and $u(t)$ a curve in P. The curve $g(t)$ must be such that $\tilde{c}$ is a horizontal curve. Differentiating with respect to t gives

$$\dot{\tilde{c}}(t) = \dot{u}(t)g(t) + u(t)\dot{g}(t)$$

Here $\dot{u}$ and $\dot{g}$ are tangent vectors at the points u and g in their respective spaces. If w is the connection form in $P(M, G)$, then properties (1)-(2) in proposition 3.3.1 implies

$$w(\dot{\tilde{c}}(t)) = g^{-1}(t)w(\dot{u}(t))g(t) + g^{-1}\dot{g}(t)$$

where $g^{-1}(t)\dot{g}(t)$ is a curve in the Lie algebra $\mathcal{G} = T_eG$ of G. So that the curve $\tilde{c}(t)$ is horizontal, we impose the condition $w(\tilde{c}(t)) = 0$ giving

$$g^{-1}(t)\dot{g}(t) = -g^{-1}(t)w(\dot{u}(t))g(t)$$

or

$$w(\dot{u}(t)) = \dot{g}(t)g^{-1}(t)$$

Thus $\tilde{c}$ is horizontal if the latter holds true; and a unique curve $g(t)$ in G with $g(0) = e$ can be obtained by integration.

Finally, using proposition 3.6.2 we come to the definition of parallel translation along a curve $\tilde{c}$ in $P(M, G)$ which projects onto a curve c in M.

Definition 3.6.7 *Let $c(t)$ join two points X_0 and X_1 in M. Let $u_0 \in \pi^{-1}(x_0) = F_{x_0}$ be an arbitrary point in the fibre over x_0. Let $\tilde{c}$ be the unique lift of c starting from u_0, and let the endpoint of $\tilde{c}$ $u_1 \in F_{x_1} = \pi^{-1}(x_1)$. By varying the value of u_0 in the fibre F_{x_0} we get a mapping $\mathcal{C} : F_{x_0} \to F_{x_1}$. This mapping defines the parallel translation of fibres of $P(M, G)$ along $c(t)$ with respect to a given connection w. The map $\mathcal{C}$ is provided by an element $g \in G$ which is uniquely associated with the path $c(t)$ in M, furthermore $\mathcal{C}$ is a diffeomorphism for every c.*

A condition for parallel translation may be established using the covariant derivative. The covariant derivative may be defined as the operator ∇_μ in the tangent bundle TM:

$$\nabla_\mu = \partial_\mu + w_\mu$$

Here the subscript μ denotes the direction of a tangent (basis) vector b_μ to the curve $c(t)$ at some point in M, i.e, $\mu \leftrightarrow b_\mu = \frac{dc}{dt}\Big|_{x_0 \in M}$. If u is a vector in P, then $\nabla_\mu u$ denotes the covariant derivative of u in the direction of μ. Thus a vector u is parallel translated along a curve $c(t)$ if

$$\nabla_\mu u = 0.$$

Chapter 4

An Application to Spin Systems

4.1 Introduction

Up to this point, our considerations had been purely academic. In the following presentation, the concept of the nontrivial phase is applied to a simple quantum system. In particular, a spin system in an external magnetic field. This will demonstrate that geometric phases are physically nontrivial.

4.2 Spin-1/2 Particles in a Magnetic Field

Consider two coupled spin-1/2 particles in an external magnetic field $\vec{B}$. A Hamiltonian for such a system is

$$H = \lambda \sigma_1 \cdot \sigma_2 - (\mu_1 \sigma_1 + \mu_2 \sigma_2) \cdot \vec{B} \tag{4.1}$$

where σ_i are the Pauli matrices; and λ, μ_1, μ_2 are coupling constants. The Hamiltonian (4.1) could describe a hydrogen atom in a magnetic field, or approximate a positronium system.

Without loss of essential generality, we choose the direction of $\vec{B}$ to be along the z-axis. Let the basis be the set $\{\phi_{kl}\}$ where $\phi_{kl} = \phi_k \otimes \phi_l$. The indices $(k,l) \leftrightarrow (\pm,\pm)$ denote the spin states of particles 1 and 2, respectively. Spin up will be denoted by '+' and spin down by '$-$'. In the basis $\{\phi_{kl}\}$, σ^2 and σ_z commute. Define the Pauli spin exchange operator $\mathbf{P}$ by its action on the set $\{\phi_{kl}\}$

$$\begin{aligned} \mathbf{P}\phi_{\pm\pm} &= \phi_{\pm\pm} \\ \mathbf{P}\phi_{\pm\mp} &= \phi_{\mp\pm} \end{aligned}$$

It is straightforward to verify the identity

$$\sigma_1 \cdot \sigma_2 = 2\mathbf{P} - \mathbf{1}.$$

The Schrödinger operator can therefore be written as

$$\lambda(2\mathbf{P} - \mathbf{1}) - (\mu_1\sigma_{1z} + \mu_2\sigma_{2z})B - i\hbar\frac{d}{dt}. \tag{4.2}$$

Since the set $\{\phi_{kl}\}$ is a complete orthonormal set, we can express the

state function ψ as the linear combination

$$\psi = C_1\phi_{++} + C_2\phi_{+-} + C_3\phi_{-+} + C_4\phi_{--} \tag{4.3}$$

where the coefficients C_i are time dependent. Applying the operator (4.2) to the state function (4.3) leads to the linear system

$$i\hbar \begin{pmatrix} \dot{C}_1 \\ \dot{C}_2 \\ \dot{C}_3 \\ \dot{C}_4 \end{pmatrix} = \begin{pmatrix} \lambda + \mu B & 0 & 0 & 0 \\ 0 & -\lambda + \mu' B & 2\lambda & 0 \\ 0 & 2\lambda & -\lambda + \mu' B & 0 \\ 0 & 0 & 0 & \lambda - \mu B \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix}$$

or

$$i\hbar \frac{d\mathbf{C}}{dt} = \tilde{\mathbf{M}}\mathbf{C}. \tag{4.4}$$

In the above we have defined

$$\begin{aligned} \mu &= -(\mu_1 + \mu_2) \\ \mu' &= -(\mu_1 - \mu_2). \end{aligned}$$

Substituting $\mathbf{C} = \zeta e^{-i\varepsilon t/\hbar}$ into the linear system yields

$$\mathrm{M}\zeta = \varepsilon\zeta. \tag{4.5}$$

Here ζ is a constant 4-component column vector.

Solving the linear system (4.5) can be facilitated using the following

Lemma 4.1 *Let H be a 2×2 Hermitian matrix. Define the angles θ and α in terms of the elements of H:*

$$\begin{aligned} \tan\theta &= \frac{2|H_{21}|}{H_{11} - H_{22}} \quad 0 \leq \theta < \pi \\ H_{21} &= |H_{21}|e^{i\alpha} \quad 0 \leq \alpha < 2\pi. \end{aligned} \tag{4.6}$$

Then the eigenvalues of H are

$$\begin{aligned} \epsilon_1 &= \frac{1}{2}(H_{11} + H_{22}) + \frac{1}{2}[(H_{11} - H_{22})^2 + 4H_{12}H_{21}]^{1/2} \\ \epsilon_2 &= \frac{1}{2}(H_{11} + H_{22}) - \frac{1}{2}[(H_{11} - H_{22})^2 + 4H_{12}H_{21}]^{1/2}. \end{aligned}$$

Furthermore, in any basis $\{\phi_j\}_{j=1,2}$, the corresponding eigenvectors are

$$\begin{aligned} \Psi_1 &= \cos\frac{\theta}{2}e^{-i\alpha/2}\phi_1 + \sin\frac{\theta}{2}e^{i\alpha/2}\phi_2 \\ \Psi_2 &= -\sin\frac{\theta}{2}e^{-i\alpha/2}\phi_1 + \cos\frac{\theta}{2}e^{i\alpha/2}\phi_2 \end{aligned}$$

*proof:*see [CBF], complement B1V.

In the linear system (4.4), the components C_1 and C_2 can be easily solved to yield[1]

$$\begin{aligned} \psi_1 &= \phi_{++} \quad \varepsilon = \lambda + \mu B \\ \psi_4 &= \phi_{--} \quad \varepsilon = \lambda - \mu B \end{aligned}$$

[1]We have omitted the phase factor $e^{-i\varepsilon t/\hbar}$

The linear system (4.5) therefore reduces to

$$\begin{pmatrix} -\lambda + \mu' B & 2\lambda \\ 2\lambda & -\lambda - \mu' B \end{pmatrix} \begin{pmatrix} \zeta_2 \\ \zeta_3 \end{pmatrix} = \varepsilon \begin{pmatrix} \zeta_2 \\ \zeta_3 \end{pmatrix} \tag{4.7}$$

The coefficient matrix M in (4.7) is a 2×2 symmetric matrix. By lemma (4.1) we obtain

$$\begin{aligned} \psi_2 &= \cos\frac{\theta}{2}\phi_{+-} + \sin\frac{\theta}{2}\phi_{-+} \qquad (4.8) \\ \varepsilon_2 &= \lambda[-1 + 2(1 + \mu'^2 B^2/4\lambda)^{1/2}] \\ \psi_3 &= -\sin\frac{\theta}{2}\phi_{+-} + \cos\frac{\theta}{2}\phi_{-+} \\ \varepsilon_3 &= -\lambda[1 + 2(1 + \mu'^2 B^2/4\lambda^2)^{1/2}] \qquad (4.9) \end{aligned}$$

where

$$\begin{aligned} \tan\theta &= \frac{2\lambda}{\mu' B} \qquad (4.10) \\ e^{i\alpha} &= 1 \end{aligned}$$

To determine w, it is sufficient to calculate the quantity

$$\langle \psi_l | i \frac{\partial}{\partial B} \psi_l \rangle \quad l = 1 \sim 4. \tag{4.11}$$

Using the expression for θ in (4.10), the operator $\partial/\partial B$ can be written in

terms of θ:

$$\frac{\partial}{\partial B} = K\frac{\partial}{\partial \theta} \tag{4.12}$$

where

$$K = -\frac{2\mu'\lambda}{(\mu' B)^2 + (2\lambda)^2}.$$

Applying the operator (4.12) to the statefunctions in (4.8), we find that the quantity (4.11) is identically zero for all ψ_l. Consequently a nontrivial phase does not arise. This is what we obtain mathematically. Physically the situation is different.

In an experimental setting, the physical system is prepared and then injected into some registration apparatus. A magnetic field is turned on and slowly increased while the effects of the field are monitored. Suppose the magnetic field is increased to the point where $\mu' B/\lambda \gg 1$ and then decreased to its original intensity. At low magnetic field strength, we essentially have Zeeman splitting of the energy levels. The states ψ_1, ψ_2, ψ_4 are the triplet states, and ψ_3 is the singlet state. However, as the intensity of B increases we find that

$$\begin{aligned} \varepsilon_2 &\simeq -\lambda + \mu' B \\ \varepsilon_3 &\simeq -\lambda - \mu' B \end{aligned}$$

and

$$\frac{\cos\theta/2}{\sin\theta/2} \gg 1.$$

Thus for large magnetic fields

$$\begin{aligned} \psi_2 &\sim \cos\frac{\theta}{2}\phi_{+-} \\ \psi_3 &\sim \cos\frac{\theta}{2}\phi_{-+}. \end{aligned} \tag{4.13}$$

Therefore, to calculate the nontrivial phase we consider a sequence of statefunctions so that we obtain the set $\{w_0, w_1, \ldots, w(t), \ldots\}$ where $w_l(t) = \langle\psi_l|i(\partial/\partial B(t))\psi_l\rangle dB(t)$, $l = 2, 3$. Initially $w_l = 0$ but as $t \to \infty$,w becomes increasingly nonvanishing. The history of the system as the magnetic field is changed is then given by the path integral

$$\oint w_l = \int_0^{\mu' B/2\lambda} \langle\psi_l|i\frac{\partial}{\partial B}\psi_l\rangle dB + \int_{\mu' B/2\lambda}^0 \langle\psi_l|i\frac{\partial}{\partial B}\psi_l\rangle d(-B).$$

In terms of θ, the last equation can be written formally as

$$\oint w = 2\int_0^{\pi/2} \langle\psi_l|\tilde{K}\frac{\partial}{\partial\theta}\psi_l\rangle d\theta \tag{4.14}$$

where $\tilde{K} = i(\partial B/\partial\theta)K$. The largest contribution in (4.14) is from the pure states given in (4.13). Assuming $\tilde{K}$ to be constant, we obtain

$$\langle\psi_l|\tilde{K}\frac{\partial}{\partial\theta}\psi_l\rangle \sim \frac{\tilde{K}}{4}(\pm)\sin\theta$$

where '+'or'−' is taken if $l = 2, 3$, respectively. Therefore the nontrivial

phase is

$$\gamma_l = \pm\frac{\tilde{K}}{2}. \tag{4.15}$$

Thus as the magnetic field is increased, the spins become increasingly uncoupled; that is, the topological structure of the system changes. That such an event occurs is indicated by the presence of a geometrical phase (4.15).

It is important to note that the parameter manifold in the present situation is 3-dimensional. The evolution, however, takes place on a 1-dimensional subset-the real line $\mathbf{R}$. We have shown that a nontrivial phase can arise from a geometric evolution on a 1-dimensional manifold.

The previous considerations can be generalized to the case where particles 1 and 2 have spins j_1, j_2[2] respectively, and in a magnetic field pointing in an arbitrary direction. The Hamiltonian for this system is

$$H = \mathbf{J}_2 \cdot \mathbf{J}_2 - (\mu_1 \mathbf{J}_1 + \mu_2 \mathbf{J}_2) \cdot \vec{B}$$

where $\mathbf{J}_i$ is the spin-j operator for particle i. This Hamiltonian arises in the study of spin-chain systems with local fields at each spin site [Bh]. Conceptually, the problem is not difficult. The analysis on the other hand, is quite lengthy and nontrivial. If the coupling constants μ_1, μ_2 are equal, then the general problem is tractible but physically uninteresting. We shall, therefore not discuss the general problem. We will instead take a reductionistic approach.

[2]j integral or half-integral

When the magnetic field is increased, the spin-spin interaction between particles 1 and 2 is dominated by the magnetic field interaction. The problem then is essentially one of a spin-j particle interacting with a magnetic field. We consider this problem in the next sequel. In doing so, we will obtain a deeper understanding of the 2-particle system considered earlier.

4.3 The Basic Spin System

Let the Hamiltonian be given by

$$H = \mathbf{J} \cdot \mathbf{B} \tag{4.16}$$

where $\mathbf{J}$ is a spin-j operator with $2j+1$ eigenvalues. The Hamiltonian (4.16) depends on time dependent parameters $\{B_i\}_{i=1,2,3}$ which form a local coordinate for a manifold M. If $B = 0$, then the eigenstates of the Hamiltonian are $2j+1$ degenerate. Therefore let $B \neq 0$. Then on the manifold $M_0 = R^3 - \{0\}$, the set of eigenvalues are nowhere degenerate. Let the system undergo cyclic evolution. This is characterized by a closed curve $\mathcal{C}$ in M_0.

We now calculate the geometric phase. This is easily accomplished by using the SU(2)-coherent state given by

$$|z\rangle = \frac{1}{(1+|z|^2)^j} e^{zJ_+} |j, -j\rangle$$

with parametrization (via stereographic projection)

$$z = -\tan(\theta/2)e^{-i\phi} \tag{4.17}$$

In this representation, the connection 1-form $w = i\langle z|z\rangle$ has the form (see appendix)

$$w = i\frac{j}{1+|z|^2}(\bar{z}dz - zd\bar{z}).$$

Using parametrization (4.17), we obtain

$$\begin{aligned} w &= i\frac{j}{1+\tan^2(\theta/2)}\left\{\tan\frac{\theta}{2}e^{i\phi}\, d(\tan\frac{\theta}{2}e^{-i\phi}) \right. \\ &\quad \left. - \tan\frac{\theta}{2}e^{-i\phi}d(\tan\frac{\theta}{2}e^{i\phi})\right\} \\ &= 2\frac{j\tan^2\theta/2}{1+\tan^2\theta/2}d\phi \\ &= j(1-\cos\theta)d\phi. \end{aligned}$$

The geometric phase is thus

$$\begin{aligned} \gamma &= \oint_{\partial S} j(1-\cos\theta)d\phi \\ &= 2\pi j(1-cos\theta). \end{aligned}$$

By Stoke's Theorem, this can be written as

$$\gamma = j\oint_S \sin\theta d\theta \wedge d\phi = j\Omega \tag{4.18}$$

where $\Omega = \oint_S \sin\theta d\theta \wedge d\phi$ is the solid angle subtended by the closed curve C.

Remark 4.1 Berry [B] and several others (such as [Si], [KI]) have investigated the basic spin system. Berry in particular obtains the formula

$$V_n(B) = n\frac{\vec{B}}{B^3}$$

for the 2-form $V = dw$. Here n is the eigenvalue of J_z. We point out that n in the above equation is to be distinguished from j in equation (4.18). The quantum number j represents the minimal value of n. The nontrivial phase factor is

$$e^{i\gamma_n(C)} = e^{in\Omega(C)}$$

where $\Omega(C)$ is the solid angle that the circuit C subtends at the point $B = 0$ in the magnetic field space. The nontrivial phase is the flux of a magnetic-like field generated by a monopole with strength n located at the point of degeneracy $B = 0$.$\diamond$

However, there is an ambiguity. The surface bounded by the closed curve C is not specified in (4.18). There are two possible choices for surface; denote this by S^+ and S^-. Both surfaces are joined together along the curve C (fig.4.2) Since C is traversed in a specified direction, the surfaces S^+, S^- are oppositely oriented. The geometric phase factor, with this ambiguity is given by

$$e^{i\gamma} = \begin{cases} e^{i\oint_{S^+} dw} \\ e^{-i\oint_{S^-} dw} \end{cases}$$

To be consistent, we require

$$e^{i\oint_{S^+} dw} = e^{-i\oint_{S^-} dw}.$$

This implies

$$\oint_{S^+} dw = -\oint_{S^-} dw + 2\pi n$$

and therefore

$$\oint_S dw = 2\pi n,$$

where n is an integer. Thus we arrive at a topological quantization similar to the Dirac quantization.

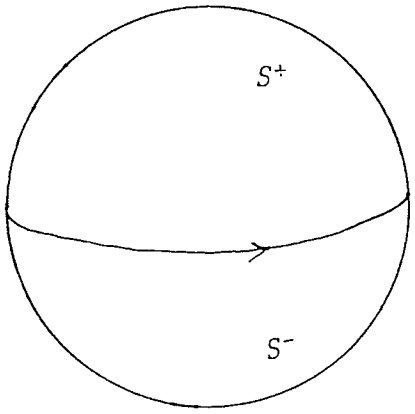

fig.4.2

The above considerations suggests that a monopole field structure has been induced on the manifold M_0. We show this explicitly. Consider the

standard expression for a Dirac monopole with strength j (see [A]):

$$\vec{A}(\vec{r}) = \frac{j}{r(z+r)}(-y, x, 0).$$

Transforming to spherical coordinates, the latter equation can be written as

$$\begin{aligned} \vec{A}(\vec{r}) \cdot d\vec{r} &= \frac{j}{r(z+r)}(x dy - y dx) \\ &= j(1 - \cos\theta) d\phi \end{aligned}$$

which is exactly w (see equation (4.18). Hence, w is the vector potential for a monopole of strength j. However, note that the parametrization (4.17) is ill defined for $\theta = \pi$. An alternative parametrization for the coherent state is

$$z' = \cot(\theta/2) e^{-i\phi} \tag{4.19}$$

which is defined for $\theta = \pi$ but not for $\theta = 0$. Using this parametrization, the connection 1-form w is

$$\begin{aligned} w' &= i\frac{j}{1+\cot^2\theta/2}\left\{\cot\frac{\theta}{2}e^{i\phi}d(\cot\frac{\theta}{2}e^{-i\phi}) - \cot\frac{\theta}{2}e^{-i\phi}d(\cot\frac{\theta}{2}e^{i\phi})\right\} \\ &= \frac{j\cot^2\theta/2}{1+\cot^2\theta/2}d\phi \\ &= -j(1+\cos\theta)d\phi. \end{aligned}$$

This is equivalent to the vector potential

$$\vec{A}'(\vec{r}) = \frac{j}{r(z-r)}(-y, x, 0).$$

We then have

$$\begin{aligned} \gamma &= j \oint (1 - \cos\theta) d\phi \\ \gamma' &= -j \oint (1 + cos\theta) d\phi. \end{aligned}$$

Comparing the last two equations indicates that there exists no unique, singularity free vector potential over the manifold $S^+ \bigcup S^-$. The choice $\vec{A}'(\vec{r})$ has a string singularity along $z = r$, or $\theta = 0$; whereas choosing $\vec{A}(\vec{r})$ gives a string singularity along $\theta = \pi$. Furthermore, observe that w' and w (hence $\vec{A}'$ and $\vec{A}$) differ by an exterior derivative $w' - w = d(j\phi)$. Therefore, w' and w are related by a gauge transformation. It is clear that a monopole structure is induced on the manifold M_0.

These conclusions follow from the nontrivial topology of M_0. Since $R^3 - \{0\}$ is topologically equivalent to $S^2 \times S^1$, the manifold M_0 is nontrivial due to the S^2 component. We choose a local coordinate system obtained by stereographic projection (equations (4.17) and (4.19)) since, in this case, only two charts S^+ and S^- are needed to cover S^2, unlike the spherical coordinates (θ, ϕ) which require more than two open subsets of R^2 to cover

the region $0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi$. Hence

$$S^2 = S^+ \bigcup S^-.$$

That we require two charts to cover S^2 explains the nonexistence of a singularity free vector potential on M_0.

Now the chart S^+ is coordinated by a set of complex parameters $\{z = \zeta + i\eta\}$ which are related to the coordinates (θ, ϕ) by $z = -\tan(\theta/2)e^{-i\phi}$, that is $(\zeta, \eta) \Longleftrightarrow (\tan(\theta/2)\cos\phi, -\tan(\theta/2)\sin\phi)$. Note that z is not defined for $\theta = \pi$, therefore S^+ is S^2 without the southpole-the point (π, ϕ). Similarly, S^- is coordinated by $\{z' = \zeta', \eta'\}$ where $z' = \cot(\theta/2)e^{-i\phi}$ so that $(\zeta', \eta') \Longleftrightarrow (\cot(\theta/2)\cos\phi, \cot(\theta/2)\sin\phi)$ and so it is S^2 without the northpole-the point $(0, \phi)$. The intersection $S^+ \bigcap S^- = \mathcal{C}_\phi$ is the curve characterizing the evolution, and is parametrized by ϕ.

Previously, it had been shown that the gauge group U(1) is acting on the manifolds S^+, S^- via $e^{i\gamma}, e^{i\gamma'}$, respectively. The set $\{\zeta, \eta; \zeta', \eta'; e^{i\gamma}, e^{i\gamma}\}$ form local coordinate systems on the product manifold $S^{\pm} \times U(1)$ (see [N]). One can then define transition functions which allow the patching of pairs of these product manifolds to form a fibre bundle $P(S^2, U(1))$-the so called monopole bundle (see [EGH]). A connection can be defined on this bundle. Integrating the connection 1-forms w' and w around the curve $\mathcal{C}$ gives the geometric phase. That there are two 1-forms w' and w, is a direct consequence of the fact that two charts are required to cover S^2 ; a singularity free 1-form cannot be defined on S^2.

4.4 Discussion

In this chapter we have given an example of a physical system where a geometrical phase arises. Others may be cited. Nontrivial phases have surfaced in 1 and 2-dimensional antiferromagnetic spin chains and lattices [FS], [WeZe], [H]. The problem considered in these papers is the question whether a Hopf term should appear in the nonlinear σ model for antiferromagnets. This question is resolved by looking how nontrivial phases and other topological terms arise in the model. No Hopf term appears. In the paper by Zak [Za], a Berry's phase is calculated for an electron moving in a periodic lattice. Usually, the parameter space is introduced by external means but in this case, the electron-lattice system has as its parameter manifold, the Brillouin zone of the solid. A system, analogous to the molecular system proposed in chapter 2, which also exhibits a notrivial phase is the $T_1 \otimes (\varepsilon_g \oplus \tau_{2g})$ Jahn-Teller system. The electronic and phonon states are coupled such that the total wavefunction is invariant under rotations in phonon space. This implies a concerted sign change in the total wavefunction constituents [COB]; a phenomenon explainable by the geometric phase [B]. Semenof and Sodana have found that nontrivial phases are related to the conductivity tensor, providing new insights into the fractional quantum Hall effect [SS]. In nuclear quadrupole resonance, nonabelian gauge structures similar to those examined in chapters 2 and 3 appear.

It is amazing that what was once ignored has become so useful in physics.

4.5 Appendix

In this appendix, we calculate in detail the quantity $i\langle z|dz\rangle$. The operator d is defined on a complex manifold coordinated by the set $\{z\}$; therefore

$$\langle z|dz\rangle = \langle z|\partial_z z\rangle dz + \langle z|\partial_{\bar{z}} z\rangle d\bar{z}.$$

The quantities $\langle z|\partial_z z\rangle$ and $\langle z|\partial_{\bar{z}} z\rangle$ can be evaluated explicitly by specifying the coherent state. We shall deal with (1) boson coherent states and (2) SU(2) coherent states.

Boson Coherent States These states are given by

$$|z\rangle = e^{-|z|/2} e^{za\dagger}|0\rangle$$

where $a\dagger$ is the creation operator and $|0\rangle$ is the minimal harmonic eigenstate. Two states $|z_1\rangle$ and $|z_2\rangle$ satisfy

$$\begin{aligned} \langle z_1|z_2\rangle &= \exp\left[-\frac{1}{2}(\bar{z}_1 z_1 + \bar{z}_2 - 2\bar{z}_1 z_2)\right] \\ \langle z|z\rangle &= 1. \end{aligned} \tag{4.20}$$

Differentiating the left side of (4.20) with respect to z_2 yields

$$\frac{d}{dz_2}\langle z_1|z_2\rangle = \langle z_1|\frac{d}{dz_2}\{\exp[-\bar{z}_2 z_2/2]\exp(z_2 a\dagger)\}|0\rangle$$

$$= -\frac{1}{2}\langle z_1|z_2\rangle\bar{z}_2 + \langle z_1|a\dagger z_2\rangle.$$

Doing likewise for the right hand side gives

$$\frac{d}{dz_2}\exp\left[-\frac{1}{2}(\bar{z}_1 z_1 + \bar{z}_2 z_2 - 2\bar{z}_1 z_2)\right] = (-\bar{z}_2/2 + 2\bar{z}_1)\langle z_1|z_2\rangle.$$

Therefore

$$-\frac{1}{2}\langle z_1|z_2\rangle\bar{z}_2 + \langle z_1|a\dagger|z_2\rangle = (-\frac{1}{2}\bar{z}_2 + \bar{z}_1)\langle z_1|z_2\rangle$$

or

$$\bar{z}_1 = \frac{\langle z_1|a\dagger|z_2\rangle}{\langle z_1|z_2\rangle}. \tag{4.21}$$

Now

$$\begin{aligned}\partial_z|z\rangle &= \partial_z\{e^{-\frac{1}{2}\bar{z}z}e^{za\dagger}|0\rangle\} \\ &= -\frac{1}{2}\bar{z}I|z\rangle + a\dagger|z\rangle\end{aligned}$$

from which, upon using (4.21),

$$\begin{aligned}\langle z|\partial_z z\rangle &= -\frac{1}{2}\bar{z} + \langle z|z\rangle \\ &= \frac{1}{2}\bar{z}.\end{aligned}$$

The dual calculation yields

$$\langle z|\partial_{\bar{z}} z\rangle = -\frac{1}{2}\bar{z}.$$

Hence

$$\langle z|dz\rangle = \frac{i}{2}(\bar{z}dz - zd\bar{z}).$$

SU(2) Coherent States The set of coherent states are given by

$$|z\rangle = \frac{1}{(1+|z|^2)^j} e^{zJ_+}|j,-j\rangle$$

and satisfy

$$\langle z_1|z_2\rangle = \frac{1}{[(1+|z_1|^2)(1+|z_2|^2)]^j}(1+\bar{z}_1 z_2)^{2j}.$$

Differentiating the latter equation as before yields for the left hand side

$$\begin{aligned}\frac{d}{dz_2}\langle z_1|z_2\rangle &= \langle z_1|\left[\frac{d}{dz_2}(1+|z_2|^2)^{-j}e^{z_2 J_+}\right]|j,-j\rangle \\ &= -j(1+|z_2|^2)^{-1}\langle z_1|z_2\rangle\bar{z}_2 + \langle z_1|J_+|z_2\rangle.\end{aligned}$$

And for the right hand side

$$\frac{d}{dz_2}\left\{\frac{(1+\bar{z}_1 z_2)^2}{(1+|z_1|^2)(1+|z_2|^2)}\right\}^j =$$

$$j\frac{(1+|z_1|^2)(1+|z_2|^2)\langle z_1|z_2\rangle}{(1+\bar{z}_1 z_2)^2(1+|z_1|^2)}$$

$$\times \left\{ \frac{2(1+\bar{z}_1 z_2)(1+|z_2|^2)\bar{z}_1 - (1+\bar{z}_1 z_2)^2 \bar{z}_2}{(1+|z_1|^2)^2} \right\}$$

$$= j\langle z_1|z_2\rangle \left\{ \frac{2\bar{z}_1}{1+\bar{z}_1 z_2} - \frac{\bar{z}_2}{1+|z_2|^2} \right\}.$$

Equating both sides gives

$$\langle z_1|J_+|z_2\rangle - \frac{j\langle z_1|z_2\rangle}{1+|z_2|^2}\bar{z}_2 = j\langle z_1|z_2\rangle \left\{ \frac{2\bar{z}_1}{1+\bar{z}_1 z_2} - \frac{\bar{z}_2}{1+|z_2|^2} \right\}.$$

Therefore

$$\frac{\langle z_1|J_+|z_2\rangle}{\langle z_1|z_2\rangle} = 2j\frac{\bar{z}_1}{1+\bar{z}_1 z_2}. \tag{4.22}$$

Taking partial derivatives as before, we have

$$\begin{aligned} \partial_z|z\rangle &= -j(1+|z|^2)^{-1}\bar{z}|z\rangle + J_+|z\rangle \\ \partial_{\bar{z}}|z\rangle &= -j(1+|z|^2)^{-1}z|z\rangle. \end{aligned}$$

With the help of (4.22), we have the following inner products:

$$\begin{aligned} \langle z|\partial_z z\rangle &= j\frac{\bar{z}}{1+|z|^2} \\ \langle z|\partial_{\bar{z}} z\rangle &= -j\frac{z}{1+|z|^2}. \end{aligned}$$

Finally we obtain

$$i\langle z|dz\rangle = i\frac{j}{1+|z|^2}(\bar{z}dz - zd\bar{z}).$$

Chapter 5

Classical and Quantum Holonomy

5.1 Introduction

We discuss in this chapter the role of nontrivial phases in quantization algorithms. First we discuss the modification of the semiclassical quantization rule by the inclusion of the nontrivial phase. Then the classical analogue of the the geometric phase is derived. This leads to a discussion of classical and quantum holonomy and its relation to anomalous terms which arise when one attempts to quantize certain classical systems [IK], [KI3], [NAG], [GT1], [GT2].

5.2 Semiclassical Quantization rule

We suppose the Hamiltonian is given by $H = H_1(\zeta) + h(q, \zeta)$, where ζ and q are the external and internal degrees of freedom, respectively. Then in the coherent state representation the state vector is the tensor product $|z\rangle =$

$|\zeta\rangle \otimes |n(\zeta)\rangle$. Here $|\zeta\rangle$ is associated with the Hamiltonian $H_1(\zeta)$ and $|n(\zeta)\rangle$ is the n^{th} adiabatic state of the internal Hamiltonian $h(q,\zeta)$ with energy λ_n. It remains to calculate $\langle z|(i\hbar\partial_t - H)|z\rangle$. Performing calculations identical to those of section 2.3, we obtain the effective propagator

$$G(T) = \sum \int \mathcal{D}(\zeta) e^{\frac{i}{\hbar} S_n^{ad} + \hbar\gamma_n}$$

where

$$\begin{aligned} S_n^{ad} &= \int_0^T [\langle\zeta|i\hbar\partial_t\zeta\rangle - H_1 - \lambda_n]dt \\ \hbar\gamma_n &= \int_0^T \langle n(\zeta)|i\hbar\partial_t n(\zeta)\rangle dt. \end{aligned}$$

Information on the energy spectrum of a physical system is obtained by studying the analytical properties of the energy Green's function $\tilde{G}(E)$, which is obtained from the Laplace-Fourier transform of the effective propagator $G(T)$:

$$\tilde{G}(T)(E) = -i \int_0^\infty G(T) e^{iEt/\hbar} dt. \tag{5.1}$$

The poles of $\tilde{G}(E)$ exhibit complete information on the energy spectrum.

Consider now a single adiabatic level (henceforth we omit the subscript n). The effective propagator $G(T)$ is first approximated by means of the stationary phase method (see,[Gu]), giving

$$G^{sc}(T) \sim \sum_c \exp\left[\frac{i}{\hbar} S^{ad} + i\hbar\gamma - \frac{i\pi\alpha}{2}\right] \tag{5.2}$$

where α is the Keller-Maslov index and $\sum_{\mathcal{C}}$ is the sum over classical trajectories (see [Gu]). Inserting (5.2) into (5.1) and again using the method of stationary phase yields

$$\tilde{G}(E) \sim \sum_{\mathcal{C}} \exp\left[\frac{i}{\hbar} W^{ad} + i\hbar\gamma - \frac{i\pi\alpha}{2}\right]. \tag{5.3}$$

Here the action integral W^{ad} is given by

$$W = S^{ad} + ET$$

and the period T satisfies

$$\partial_t(S^{ad} + ET) = 0.$$

This equation defines an energy surface $H_1 + \lambda = E$ which in turn determines (for some Hamiltonians) a single basic trajectory $\mathcal{C}$ with period $T(E)$. Assuming this and taking into account contributions from multiple m-transversals of the basic orbit so that $W^{ad} \to mW$,and $\gamma \to m\gamma$ then summing (5.3) yields

$$\tilde{G}_{sc}(E) \sim \sum_{m=1}^{\infty} \exp \frac{i}{\hbar} m(W^{ad} + \hbar\gamma - \alpha\pi\hbar/2)$$

which is just an infinite geometric series. It can be written as

$$\tilde{G}^{sc}(E) \sim \frac{\exp i(W^{ad} + \hbar\gamma - \alpha\pi\hbar/2)/\hbar}{1 - \exp i(W^{ad} + \hbar\gamma - \alpha\pi\hbar/2)/\hbar}. \tag{5.4}$$

The pole of equation (5.4) gives

$$W^{ad} + \hbar\gamma - \alpha\pi\hbar/2 = 2n\pi\hbar \tag{5.5}$$

where n is an integer.

Obtaining the semiclassical quantization rule requires an explicit form for W^{ad}. This is given by

$$\begin{aligned} W^{ad} &= \int_0^T (\langle\zeta|i\hbar\partial_t\zeta\rangle - H_1 - \lambda)dt + ET \\ &= \oint_C \langle\zeta|i\hbar d\zeta\rangle - \int_0^T (H_1 + \lambda)dt + ET \\ &= \oint_C \langle\zeta|i\hbar d\zeta\rangle. \end{aligned}$$

If we let $|\zeta\rangle$ be the boson coherent state, $|\zeta\rangle = e^{-|\zeta|^2/2}e^{\zeta a^\dagger}|0\rangle$ where $\zeta = (P + iQ)/\sqrt{2\hbar}$ then (see appendix)

$$\langle\zeta|d\zeta\rangle = \frac{1}{2}[\bar{\zeta}d\zeta - \zeta d\bar{\zeta}].$$

And so, with repeated application of Stoke's theorem

$$\begin{aligned} W^{ad} &= \frac{i\hbar}{2}\oint_{C=\partial S}\bar{\zeta}d\zeta - \zeta d\bar{\zeta} \\ &= -\frac{i}{\hbar}\oint_S d\zeta \wedge d\bar{\zeta} \\ &= -\frac{i}{2}\oint_S d(P+iQ)\wedge(P-iQ) \\ &= \frac{-i}{2}\oint_S d^2P + d^2Q - idP\wedge dQ + idQ\wedge dP \\ &= -i\oint_S idP\wedge dQ \\ &= \oint_{\partial S} PdQ. \end{aligned}$$

Thus from (5.5) we have

$$\oint PdQ = (n + \frac{\alpha}{4} - \frac{\gamma}{2})2\pi\hbar$$

which is the semiclassical quantization rule modified by the geometric phase γ.

The foregoing analysis can serve as a theoretical basis for the experimental investigation of the effects of nontrivial phases on the energy spectra of composite systems which are undergoing adiabatic evolution.

5.3 Geometrical angles

The appearance of topological terms is not solely a quantum phenomenon. There is at the classical level, a quantity completely analogous to the nontriv-

ial phase. By modifying the *classical* adiabatic theorem in a similar fashion to the quantum case, it can be shown, for integrable systems, that there is an additional term which appears with the usual angle variables [Ha], [B2]. This extra term, called Hannay's angle or adiabatic angle, is shown to be the classical analogue of the adiabatic phase [B2]. This adiabatic angle reflects the topological features of the system in much the same way the adiabatic phase does at the quantum level. In this section we derive an explicit formula which relates the geometrical angle and the nontrivial phase.

Consider a slowly cycled integrable system. As in the quantum case the Hamiltonian depends parametrically on the set $\{X(t)\}$. Let $S(q, I; X(t))$ be the multivalued generating function for the canonical transformation to action angle variables (see [Per]):

$$\begin{aligned} (q,p) &\longrightarrow (\theta, I) \\ p^{(\alpha)} &= \frac{\partial S^{(\alpha)}}{\partial q} \quad \theta^{(\alpha)} = \frac{\partial S^{(\alpha)}}{\partial q} \end{aligned}$$

The superscript α denotes the homomorphism between q and p on the phase space torus. Since the canonical transformation is time dependent through $X(t)$, the old and new Hamiltonians, H and K respectively, are related according to (see [G])

$$K(\theta, I, t) = H(q, p; X(t)) + \frac{\partial S^{(\alpha)}(q, I; X(t))}{\partial t}$$

where q and p are functions of θ, I and depend parametrically on $X(t)$.

Define

$$\mathcal{S}(\theta, I; X) = S^{(\alpha)}(q, I; X) \quad 0 \leq \theta \leq 2\pi \tag{5.6}$$

so that $\mathcal{S}$ and hence K are single valued. Using (5.6) we obtain

$$\frac{\partial S^{(\alpha)}}{\partial X_l} = \frac{\partial \mathcal{S}}{\partial X_l} - p_i \frac{\partial q_i}{\partial X_l}.$$

In the last equation we have made use of the relation

$$p_i = \frac{\partial S^{(\alpha)}}{\partial q_i}.$$

The new Hamiltonian is therefore

$$K(\theta, I; t) = H(I, X(t)) + \left[\frac{\partial \mathcal{S}}{\partial X_l} - p_i \frac{\partial q_i}{\partial X_l}\right] \frac{dX_l}{dt}.$$

It is globally single valued since

$$\mathcal{S}(\theta + 2\pi, I; X) - \mathcal{S}(\theta, I; X) = \oint p dq = 2\pi I.$$

The equation of motion for the angle is

$$\dot{\theta}_m = \frac{\partial K}{\partial I_m} = \frac{\partial H}{\partial I_m} + \frac{\partial}{\partial I_m}\left[\frac{\partial \mathcal{S}}{\partial X_l} - p_i \frac{\partial q_i}{\partial X_l}\right] \frac{dX_l}{dt}$$

which, upon integrating, yields

$$\theta_m = \int_0^T \nu_m(I,X)dt + \int_0^T \frac{\partial}{\partial I_m}\left[\frac{\partial \mathcal{S}}{\partial X_l} - p_i\frac{\partial q_i}{\partial X_l}\right]\frac{dX_l}{dt}dt. \qquad (5.7)$$

The first term in (5.7) is the usual angle swept out in time T; whereas the second term is the classical adiabatic angle.

To make the connection between the classical and quantum holonomy, we make use of the averaging principle (see [Ar]). The second term in equation (5.7) can be thought of as a perturbation so that the averaging principle gives

$$\langle\theta_m\rangle = \oint dX_l \frac{1}{(2\pi)^N}\oint \mathcal{D}(\theta)\frac{\partial}{\partial I_m}\left[\frac{\partial \mathcal{S}}{\partial X_l} - p_i\frac{\partial q_i}{\partial X_l}\right]$$

where $\oint \mathcal{D}(\theta) = \int \prod_{k=1}^N d\theta_k$; or in differential form notation,

$$\langle\theta\rangle = \frac{\partial}{\partial I}\oint_{\partial A}\left\{\frac{1}{(2\pi)^N}\oint \mathcal{D}(\theta)[d\mathcal{S} - p\wedge dq]\right\}.$$

Applying Stoke's theorem to this equation gives the surface integral over a surface A.

$$\begin{aligned}\langle\theta\rangle &= -\frac{\partial}{\partial I}\oint_A \frac{1}{(2\pi)^N}\oint \mathcal{D}(\theta)dq\wedge dp \\ &= -\frac{\partial}{\partial I}\oint dW. \qquad (5.8)\end{aligned}$$

In equation (5.8) we have defined the angle 1-form W to be

$$W = \frac{1}{(2\pi)^N} \oint \mathcal{D}(\theta) p \wedge dq.$$

In the classical case W is the connection on the phase space bundle and dW is the assoctiated curvature. The behavior of W is completely analogous to w.

We go further and derive an equation which relates the phase 2-form and the angle 2-form [B2]. The phase 2-form is given by $V = d_X \langle n | i d_X n \rangle$, which in the position basis $\{q\}$ is

$$V = i \int dq \bar{\psi}_n(q; X) d_X \psi_n(q; X). \tag{5.9}$$

Semiclassically

$$\psi_n(q; X) = \sum_\alpha c_\alpha(q, I; X) e^{-iS^{(\alpha)}(q,I;X)/\hbar} \tag{5.10}$$

where

$$c_\alpha^2 = \frac{1}{(2\pi)^N} \left(\frac{d\theta^{(\alpha)}}{dq} \right).$$

Substituting (5.10) into (5.9) and exploiting the fact that products of the form $e^{-iS^{(\alpha)}/\hbar} e^{iS^{(\beta)}/\hbar}$ vanish by semiclassical cancellation, we arrive at

$$V = d_X \int \frac{1}{\hbar (2\pi)^N} \sum_\alpha \left(\frac{d\theta^{(\alpha)}}{dq} \right) d_X S^{(\alpha)}$$

$$
\begin{aligned}
&= \frac{d_X}{\hbar}\int dq \frac{1}{(2\pi)^N}\sum_{\alpha}\left(\frac{d\theta^{(\alpha)}}{dq}\right)(d_X\mathcal{S} - p_i d_X q_i) \\
&= -\frac{1}{\hbar}\oint \frac{\mathcal{D}(\theta)}{(2\pi)^N}(dp\wedge dq) \\
&= -\frac{1}{\hbar}W(I;X). \qquad (5.11)
\end{aligned}
$$

Comparing equations (5.8) and (5.11) we obtain an explicit relationship between the geometric phase and angle:

$$\langle\theta\rangle = -\hbar\frac{\partial}{\partial I}\gamma.$$

Using the Bohr-Sommerfeld quantization rule

$$I_j = (n_j + \sigma_j)\hbar \quad (\sigma = constant)$$

we get the expansion [GT1]

$$-\frac{\partial\gamma}{\partial n_j} = \langle\theta_j\rangle + f_1\mathcal{O}(\hbar) + f_2\mathcal{O}(\hbar^{3/2}) + \cdots. \qquad (5.12)$$

The functions $f_1, f_2, \cdots$ depend on I and the circuit C. Equation (5.12) shows that γ is nonvanishing to leading order in $\hbar$. This implies that a non-trivial phase will always develop in the quantized version of a classical system exhibiting a geometric angle. On the other hand, it is possible that $\gamma \neq 0$ while the zeroth order term vanishes. Therefore it is not necessary for the classical version to have a geometric angle despite the corresponding quan-

tum system displaying a nontrivial phase. Only for quadratic Hamiltonians does $\gamma \neq 0$ imply $\langle\theta\rangle \neq 0$, since in this case $f_1 = f_2 = \cdots = 0$ [B2], [GT1].

5.4 Anomalies

Quantum systems displaying a nontrivial phase and not necessarily developing a geometrical angle at the classical level is reminiscent of anomalies in field theory. It would be natural then to ponder if anomalies are connected with nontrivial phases and angles.

Anomalies occur when the full set of classical symmetries cannot be preserved under all possible quantization schemes. It was shown by Nelson and Alverez-Gaumé that systems with anomalies must develop a nontrivial phase when treated in the Hamiltonian formalism [NAG]. In their paper, they consider an SU(2) gauge theory with Weyl fermions and show that the adiabatic phase reflects the Mobius topology of the system. Kuratsuji and Iida have demonstrated that the symplectic structure of the phase space is modified by the presence of nontrivial phases. Such a modification changes the Poisson structure in that the degrees of freedom of the external system is reduced; the variables q, p become noncanonical. So when the Poisson brackets are replaced by commutators, anomalous terms appear in the quantum theory [IK],[KI3]:

$$\begin{aligned} [Q_i, Q_j] &= i\hbar E(Q_i, Q_j) + \cdots \\ [Q_i, P_j] &= i\hbar\delta_{ij} + i\hbar^2 E(P_i, Q_j) + \cdots \end{aligned}$$

$$[P_i, P_j] \;=\; -i\hbar E(Q_i, Q_j) + \cdots$$

where

$$E(A, B) = i[\langle n|\partial_A \partial_B|n\rangle - \langle n|\partial_B \partial_A|n\rangle.$$

A similar conclusion, using instead Grassmann variables, was reached by Gozzi and Thacker [GT2]. Something subtle is obviously going on when one switches from classical mechanics to quantum mechanics or vice versa; and a part of this subtlety is captured by the geometric angle and phase.

The *exact* role of nontrivial phases and angles in theory of anomalies is probably the least understood. There is much territory yet unexplored. At this point there are only speculations. It has been suggested that since $\langle\theta\rangle \neq 0$ implies $\gamma \neq 0$, the geometrical angle can serve as an indicator fortelling that anomalies may arise during quantization. One would then only examine the classical Hamiltonian [GT2]. At the classical level, quantities other than the symmetries of the system may not be preserved in the quantization process. This is perhaps indicated by the geometrical angle. We elaborate. Classically, a symmetry can always be effected by a symmetry transformation whose generators may or may not act globally. It is believed that presence of nonglobal generators is a necessary condition for the appearance of anomalies and hence nontrivial phases. There are certain regions in phase space where the symmetry transformation is no longer canonical. The 2-form $dp \wedge dq$ is not preserved, implying that a region of phase space can be arbitrarily shrunk. Now at the quantum level, such a transformation is

rejected by the Heisenberg uncertainty principle. And so anomalous terms arise.

Another point of view comes from linear programming (see for example [Mu]). In linear programming one optimizes an objective function subject to a host of constraints. Quite often some constraints are redundant for a particular objective function. Deleting redundant constraints do not change the optimum but merely change the geometry of a multidimensional polyhedron. That is the system has a trivial topology. However, suppose that the coefficients of the objective function is changed by some mechanism which we call a 'canonical transformation'. Then it is possible that some (or all) of the redundant constraints become active in the system; the consequence of which is that there may be no feasible, or unique solution to the system. The linear program has then reached a stage where 'anomalies' are present. The usual method of solving linear programs is the Simplex algorithm, a scheme which we metaphorically call the Hamiltonian formalism. Now the Simplex method has an inherent consistency check. At each stage of the iteration one can determine the status of the system; sensitivity analysis can determine if an anomaly will turn up. This seems to be the case with nontrivial phases and angles.

Suppose that Classical and Quantum mechanics is some sort of linear program. A set of constraints determines a classical program, while another set determines a quantum program. One of the fundamental constraints would be the Heisenberg uncertainty relation $\Delta x \Delta p \sim \hbar$. Let the quanti-

zation procedure be the transformation that changes the coefficients of the objective function in this fictitious linear program. Usually, quantization is straight forward so that no anomalous terms arise; that is, the Heisenberg relation is a redundant constraint. However, in some systems, the transformation causes the Heisenberg constraint to become active, thus changing the geometry of the system. This could lead to an anomaly. When an anomaly does arise, the simplex tableau for this linear program would display, through the dual variables (or shadow prices), the nontrivial topology of the multi-dimensional polyhedron. These dual variables behave like a nontrivial phase or geometrical angle, depending on the constraint configuration; classical or quantum mechanical. This analogy with linear programming offers a different perspective into the mechanisms of anomalies and their relation to nontrivial phases and angles.

Yet another avenue not fully explored is the possible connection of nontrivial phases and angles to quasi-invariance. Here we have a dynamical system described by a Lagrangian L, and on which a symmetry group G acts. Under the action of G, Lagrange's equation of motion remains unchanged but the Lagrangian changes by a total time derivative; L is quasi-invariant. The total time derivative is reminiscent of the additional term in the effective action. Recall that

$$S^{eff} = S + \hbar\gamma$$

Now in terms of the Lagrangian

$$S = \int L(q, \dot{q}) dt.$$

By quasi-invariance

$$\mathcal{L} = L + \frac{df}{dt}$$

where f is a function of $q, \dot{q}, t$. Therefore

$$\begin{aligned} \mathcal{S} &= \int L + \int \left(\frac{df}{dt}\right) dt \\ &= S + \int \left(\frac{df}{dt}\right) dt \end{aligned} \tag{5.13}$$

Clearly, we have shown similarities between the effective action and equation (5.13). The similarity may be trivial, but there is nothing to lose if one asks: is there *any possibility at all* that the second term in (5.13) is equivalent to a nontrivial phase?

In this chapter, we have shown that the geometrical phase has a classical counterpart. The remainder of the chapter is highly speculative but possible avenues of research are pointed out. We repeat what was stated at the end of chapter 4: it is amazing that these phases, previously regarded as trivial, has become very nontrivial.

References

[A] I.J.R. Aitchison, *Berry Phases, Magnetic Monopoles, and Wess-Zumino Terms or How the Skyrmion got its Spin* , Acta Physica Polonica B v.18(3), 207(1987).

[AA1] Y. Aharonov and J. Anandan,*Phase changes during Cyclic Quantum Evolution*, Phys. Rev. Lett. v.58(16) 1593(1987).

[AA2] J. Anandan and Y. Aharonov, *Geometric Quantum Phases and Angles*, Phys. Rev. D v.38(6) 1863(1988).

[AG] N.I.Akhiezer and I.M.Glazman, *Theory of Linear Operators in Hilbert space v.1*, (Ungar, New York, 1978).

[AMR] R. Abraham, J.E. Marsden and T. Ratui, *Manifolds, Tensor Analysis, and Applications, 2nd ed.*, (Springer-Verlag, New York, 1988).

[An] J. Anandan, *Nonadiabatic Nonabelian Geometric Phase* , Phys. Rev. Lett. A v.133(4,5) 171(1988).

[Ar] V.I Arnold, *Mathematical Methods of Classical Mechanics* ,Springer-Verlag, New York, 1978).

[ASS] J.E. Avron, R. Seiler, and B. Simon, *Homotopy and Quantisation in Condensed Matter Physics*, Phys. Rev. Lett. v.51 51(1983).

[B] M.V. Berry, *Quantal Phase factors Accompanying Adiabatic Changes*, Proc. Roy. Soc. Lond. A v.392 45(1984).

[B2] M.V. Berry, *Adiabatic Angles and Quantal Adiabatic Phases*, J. Phys. A: Math. Gen. v.18 15(1985).

[BD] D.M. Bird and A.R. Preston, *Observation of Berry's Geometrical Phase in Electron Diffraction from Screw Dislocation*, Phys. Rev. Lett. v.61(25) 2863(1988).

[Bh] B.S. Bhakar, private communication.

[BMSS] A.B. Balachandran, G. Marmo, B.S. Skagerstam, and A.S Stern, *Gauge Symmetries and Fibre Bundles* (Springer-Verlag, Berlin, 1983).

[CDL] C. Cohen-Tannoudji, B. Diu and F. Lalö, *Quantum Mechanics v.1* (Hermann and Wiley, Paris, 1977).

[COB] C.C. Chancy and M.C.M O'Brien, *Berry's Geometric Quantum Phase and the* $T_1 \otimes (\varepsilon_g \oplus \tau_{2g})$ *Jahn-Teller Effect*, J. Phys. A:Math. Gen. v.21 3347(1988).

[CW] R. Chiao and Y. Wu, *Manifestation of Berry's Topological Phase for the Photon*, Phys. Rev. Lett. v.57(8) 933(1986).

[DM] W. Drechsler and M.E Mayer,*Fibre Bundle Techniques in Gauge Theories* (Springer-Verlag, Berlin, 1977).

[EGH] T. Eguchi, P.B. Gilky and A.J. Hanson, *Gravitation, Gauge Theories and Differential Geometry*, Physics Reports v.66(9) 213(1980).

[F] H. Flanders, *Differential Forms with Applications to the Physical Sciences* (Dover, 1989).

[FS] E. Fradkin and M. Stone, *Topological Terms in 1 and 2 - Dimensional Quantum Heisenberg Antiferromagnets*, Phys. Rev. B v.38(10) 7215(1988).

[G] H. Goldstein, *Classical Mechanics 2nd ed.* Addison-Wesley, Phillipines, 1980).

[GT1] E. Gozzi and W. Thacker, *Classical Adiabatic Holonomy in a Grassmannian System*, Phys. Rev. D v.38(8) 2388(1987).

[GT2] E. Gozzi and W. Thacker, *Classical Adiabatic Holonomy and its Canonical Structure*, Phys. Rev. D v.38(8) 2398(1987).

[Gu] M.C. Gutzwiller, *Phase-Integral Approximation in Momentum Space and the Bound States of an Atom*, J. Math. Phys. v.8(10) 1979(1967).

[H] F. Haldane, *O(3) Nonlinear Model and the Topological Distinction Between Integer and Half Integer Spin Antiferromagnets in Two Dimensions*, Phys. Rev. Lett. v.61(8) 1029(1988).

[Ha] J.H Hannay, *Angle Variable Holonomy in Adiabatic Excursions of an Integrable Hamiltonian*, J. Phys. A: Math. Gen v.18 221(1985).

[IK] S. Iida and H. Kuratsuji, *Adiabatic Theorem and Anomalous Commutators*, Phys. Lett. B v.184(2,3) 242(1987).

[J] R. Jackiw, *Berry's Phase-Topological Ideas from Atomic, Molecular and Optical Physics*, Comm. Atomic and Molecular Physics v.21(2) 71(1982).

[K] H. Kuratsuji, *Geometrical Canonical Phase Factors and Path Integrals*, Phys. Rev. Lett. v.61(15) 1687(1988).

[Ka] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1976).

[KI1] H. Kuratsuji and S. Iida, *Effective Action for Adiabatic Processes*, Prog. Theor. Phys. v.74(3) 439(1985).

[KI2] H. Kuratsuji and S. Iida, *Dynamical Meaning of Quantum Adiabatic Phase: The Case of a Noncanonical System*, Phys. Rev. Lett. v.56(10) 1003(1986).

[KI3] H. Kuratsuji and S. Iida, *Deformation of Symplectic Structures and Anomalous Commutators in Field Theories*, Phys. Lett. B v.184(2.3) 242(1987).

[Ki] E. Kiritsis, *A Topological Investigation of the Quantum Adiabatic Phase*, Commun. Math. Phys. v.111 417(1987).

[Ko] A. Kovner, *Berry's Phase and Effective Action*, Phys. Rev A v.40(2) 545(1989).

[KN] S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry vols 1,2* (Wiley and Sons, New York, 1963).

[M] A. Messiah, *Quantum Mechanics v.2* (North-Holland, Amsterdam, 1966).

[MT] C.A. Mead and D.G. Truhlar, *On the Determination of Born-Oppenheimer Nuclear Motion Wavefunction Including Complications Due to Conical Intersections and Identical Nuclei*, J. Chem. Phys. v.70 2284(1979).

[Mu] K. Murty, *Linear Programming* (Wiley, New York, 1983).

[N] N. Nakagawa, *Geometrical Phase Factors and Higher Order Adiabatic Approximations*, An. of Physics v.179 145(1987).

[NAG] P. Nelson and L.A. Alvarez-Guame, *Hamiltonian interpretation of Anomalies*, Commun. Math. Phys. v.99 103(1985).

[P1] A.M. Perelomov, *Coherent States for Arbitrary Lie Groups*, Commun. Math. Phys. v.26 222(1972).

[P2] A.M. Perelomov, *Generalized Coherent States and Some of Their Applications*, Sov Phys. Usp v.20(9) 703(1977).

[Pa] D. Page, *Geometric Description of Berrys's Phase*, Phys.Rev. A v.36(7) 3479(1987).

[Per] I. Percival and D. Richards, *Introduction to Dynamics* (Cambridge Univ. Press, 1982).

[R] J.M. Radcliffe, *Some Properties of Coherent States*, J. Phys. A: Gen. Phys. v.4 313(1971).

[Ru] W. Rudin, *Principles of Mathematical Analysis* (McGraw-Hill,1976).

[S] L.I. Schiff, *Quantum Mechanics 3rd ed.*(McGraw-Hill 1960).

[SB] J. Samuel and R. Bhandari, *General Setting for Berry's Phase*, Phys. Rev. Lett. v.60(23) 2339(1988).

[Sc] L.S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981).

[Si] B. Simon, Holonomy, *The Quantum Adiabatic Theorem, and Berry's Phase*, Phys. Rev. Lett. v.51(24) 2167(1983).

[SS] G.N. Semenoff and P. Sodano, *Non-Abelian Adiabatic Phases and the Fractional Quantum Hall Effect*, Phys. Rev. Lett. v.57(10) 1195(1986).

[TC] A. Tomita and R. Chiao, *Observation of Berry's Topological Phase by Use of an Optical Fiber*, Phys. Rev. Lett. v.57(8) 937(1986).

[vW] C. van Westenholz, *Differential Forms in Mathematical Physics* (North-Holland, Amsterdam, 1978).

[WeZe] X.G. Wen and A. Zee,*Spin Waves and Topological Terms in the Mean-Field Theory of Two-Dimensional Ferromagnets and Antiferromagnets*, Phys. Rev. Lett. v.61(8) 1025(1988).

[WY] T.T. Wu and C.N. Yang, *Concept of Nonintegrable Phase Factors and Global Formulation of Gauge Fields*, Phys. Rev. D v.12(12) 3845(1975).

[WZ] F. Wilczek and A. Zee, *Appearance of Gauge Structures in Simple Dynamical Systems*, Phys. Rev. Lett. v.52(24) 2111(1984).

[Za] J. Zak, *Berry's Phase for Energy Bands in Solids*, Phys.Rev. Lett. v.62(23) 2747(1989).

[Ze] A. Zee, *Non-Abelian Gauge Structure in Nuclear Quadrupole Resonance*, Phys. Rev. A v.38(1) 1(1988).