CHAPTER I

INTRODUCTION

The Geometrical Phase

In quantum mechanics, we are struck by the peculiar fact that an equation of physics contains imaginary quantities. The time dependent Schrödinger equation

$$\hat{H}|\psi\rangle = i\hbar|\dot{\psi}\rangle \tag{1}$$

involves i (the square root of negative unity) both in its time derivative and possibly in the Hamiltonian operator $\hat{H}$. The solutions of Eq.(1) are consequently complex.

It is said that the phases of wave functions ψ that solve Eq.(1) do not matter, because physical quantities are determined by the absolute value squared, which is real. But this is only true if ψ describes the entire system is described. Since in practice and perhaps even in principle we cannot construct the wave functions for everything that might interest us, we must deal with wave functions that describe only a part of the entire system, and then interference experiments between different parts allow determination of the relative phase.

During the last few years, considerable interest has been focused on a complex of physical ideas that share a common mathematical theme (Shapere and Wilczek, 1989), the concept of holonomy. The recent flurry of activity began in 1984 with a paper by Michael Berry (Berry, 1984). He showed that the adiabatic evolution of energy eigenfunctions, with respect to a time-dependent quantum

Hamiltonian $\widehat{H}(t)$, contains a phase of deeply geometrical origin (now known as "Berry's phase" or "Geometrical phase", γ) in addition to the familiar dynamical phase $\exp[-iEt/\hbar]$. The additional phase approaches a finite, non-zero limit as the Hamiltonian is taken more and more slowly around a closed path in its parameter space **R**. Berry's observation, although basically elementary, seems to be quite profound. Multiplicative phases or more generally group transformations with similar mathematical origins have been identified and found to be important in a startling variety of physical contexts. Examples of geometrical phases abound in many areas of physics. Many familiar problems that we do not ordinarily associate with geometrical phases may be phrased in terms of them. Often, the result is a clearer understanding of the structure of the problem and an elegant expression of its solution.

Consider, for example, the precession of a Foucault pendulum. Standard treatments (Symon, 1980) calculate the rate of precession of a pendulum in a frame rotating with the surface of the earth in terms of the Coriolis force, but a much simpler and more geometric explanation may be given as follows. Suppose a pendulum is transported along a closed loop C, in the gravitational field of a point mass, and that the period and amplitude of its swing are small compared to the typical time and distance scales of the transport motion. We may assume that the loop lies on the surface of a sphere concentric with the mass, although this assumption is not necessary. Now, when the pendulum returns to its initial position, its invariant plane will have rotated by some angle. For example, for transport around a sphere at a constant latitude (relative to the north pole) , a straightforward calculation shows that the net rotation will be $2\pi \cos\theta$ radians. A remarkable feature of this result is that it is independent of the rate at which different parts the loop are traversed (provided that the traversal is slow). This is a consequence of the fact that the Coriolis force is proportional to the velocity of transport, so that its integrated effect is invariant under rescaling of time. (Velocity-dependent forces, like the magnetic force on a moving charge, tend to be associated with geometric phases.) For transport along the equator, the pendulum will not precess. This may be seen from a symmetry argument. The rate of precession does not depend on the direction of the pendulum's swing, so we may assume that the invariant plane lies in a north-south direction. Then any precession would break the reflection symmetry between the northern and southern hemispheres, so that the pendulum must not precess at all. (Alternatively, the Coriolis force at the equator always points vertically, and cannot torque the pendulum's invariant plane.) Now if C is made up of geodesic segments, the precession will all come from the angles where the segments meet; the total precession is equal to the net deficit angle, which in turn equals the solid angle enclosed by C modulo 2π. Finally, we can approximate any loop by a sequence of geodesic segments, so that the most general result (on or off the surface of the sphere) is that the net precession is equal to the enclosed solid angle. This result may seem rather esoteric, but its generality and geometric nature suggest its depth. In fact, the mathematics describing it is essentially identical to that describing the motion of a charged particle in the field of a magnetic monopole. The most famous example of a physical phase is the one given by Aharonov and Bohm thirty three years ago (Aharonov and Bohm, 1959). They considered the motion of a charged particle around a magnetic flux tube from which the particle is excluded. Although the particle remains in a region free of any electromagnetic fields, its wave function acquires a phase given by the line integral around the closed particle path of the vector potential A describing the magnetic field B. Alternatively, by Stoke's law, the phase is the magnetic flux through any surface enclosed by the path.

$$\exp\left[\frac{ie}{\hbar c}\oint \mathbf{A}(\mathbf{R})\cdot d\mathbf{R}\right] = \exp\left[\frac{ie}{\hbar c}\oint d\mathbf{S}\cdot\mathbf{B}\right] \quad ; \quad \mathbf{B} = \nabla\times\mathbf{A}$$

As is well-known, this Aharonov-Bohm phase has been experimentally observed.

Berry's original paper on the quantal adiabatic phase, elegantly presents the key concepts surrounding what we have come to know as Berry's phase, the gauge invariance of the adiabatic phase, the expression of the phase as the integral of the magnetic field from a monopole over an enclosed surface, and the theorem on degeneracies of a complex Hamiltonian. The example of a spin in a slowly changing field, which has become a paradigm to studies (and measurements) of geometrical phase, is shown to lead to a magnetic-monopole-like effect. Berry proposes an experiment to measure the phase, by splitting a beam of coherently polarized electrons in a magnetic field, rotating the field around one of the beams, and measuring the resulting phase difference by interference.

His purpose here is to explain how the phase factor contains a circuit-dependent component $\exp[i\gamma_n(t)]$ in addition to the familiar dynamic component $\exp[-iEt/\hbar]$ which accompanies the evolution of any stationary state. A general formula for the geometrical phase in terms of the eigenstates of $\hat{H}$ will be obtained in the next section.

<u>General Formula for Phase Factor</u>

Let the Hamiltonian $\hat{H}(\mathbf{R})$ be changed by varying parameters $\mathbf{R} = (X, Y, \cdots)$ on which it depends. Then the excursion of the system between times t = 0 and t = T can be pictured as transport around a closed path $\mathbf{R}(t)$ in parameter space, with a Hamiltonian $\hat{H}(\mathbf{R}(t))$ such that $\mathbf{R}(T) = \mathbf{R}(0)$. The path will henceforth be called a circuit and denoted by C. For the adiabatic approximation to apply (Schiff, 1968), T must be large. The state $|\psi(t)\rangle$ of the system evolves according to Schrödinger's equation

$$\hat{H}(\mathbf{R}(t))|\psi(t)\rangle = i\hbar|\dot{\psi}(t)\rangle \tag{2}$$

At any instant, the natural basis consists of the eigenstates $|n(\mathbf{R})\rangle$ (assumed discrete) of $\hat{H}(\mathbf{R})$ for $\mathbf{R} = \mathbf{R}(t)$, that satisfy

$$\hat{H}(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle \qquad (3)$$

with energies $E_n(\mathbf{R})$. This eigenvalue equation implies no relation between the phases of the eigenstate $|n(\mathbf{R})\rangle$ at different $\mathbf{R}$. For present purposes any differentiable choice of phases can be made, provided $|n(\mathbf{R})\rangle$ is single valued in a parameter domain that includes the circuit C.

Adiabatically, a system prepared in one of these states $|n(\mathbf{R}(0))\rangle$ will evolve with $\hat{H}$ and be in the state $|n(\mathbf{R}(t))\rangle$ at t. Thus $|\psi(t)\rangle$ can be written as

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_0^t dt' E_n\left(\mathbf{R}\left(t'\right)\right)\right]\exp[i\gamma_n(t)]|n(\mathbf{R}(t))\rangle \qquad (4)$$

The first exponential is the familiar dynamical phase factor. In this thesis the object of attention is the second exponential. The crucial point will be that its phase $\gamma_n(t)$ is non-integrable, γ_n cannot be written as a function of $\mathbf{R}$ and in particular is not single valued under continuation around the circuit, i.e. $\gamma_n(T) \neq \gamma_n(0)$

The function $\gamma_n(t)$ is determined by the requirement that $|\psi(t)\rangle$ satisfy Schrödinger's equation, and direct substitution of Eq. (4) into Eq. (2) leads to

$$\dot{\gamma}_n(t) = i\left\langle n(\mathbf{R}(t))\middle|\nabla_{\mathbf{R}}\, n(\mathbf{R}(t))\right\rangle \cdot \dot{\mathbf{R}}(t) \qquad (5)$$

The total phase change of $|\psi\rangle$ round C is given by

$$|\psi(T)\rangle = \exp[i\gamma_n(C)]\exp\left[-\frac{i}{\hbar}\int_0^T dt\, E_n(\mathbf{R}(t))\right]|\psi(0)\rangle \qquad (6)$$

where the geometrical phase change is

$$\gamma_n(C) = i\oint_C \langle n(\mathbf{R})|\nabla_{\mathbf{R}}\, n(\mathbf{R})\rangle \cdot d\mathbf{R} \tag{7}$$

The geometrical phase is a physical parameter can be further emphasized by expressing this result in the suggestive notation

$$\mathbf{A}_n(\mathbf{R}) = i\langle n(\mathbf{R})|\nabla_R\, n(\mathbf{R})\rangle \tag{8}$$

so that

$$\gamma_n(C) = \oint_C d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R}) \tag{9}$$

is written in terms of a "vector potential" like quantity $\mathbf{A}_n(\mathbf{R})$. If we choose to redefine the phase of the eigenstate by an arbitrary phase $\Lambda\,(\mathbf{R})$,

$$|n(\mathbf{R})\rangle \rightarrow \exp\left[i\,\Lambda(\mathbf{R})\right]|n(\mathbf{R})\rangle \tag{10}$$

then

$$\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) + \nabla_R\,\Lambda(\mathbf{R}) \tag{11}$$

which is analogous to a gauge transformation [Appendix A]. Obviously, an observable cannot depend upon the choice of gauge, and it is clear that geometrical phase obeys this property since, by Stokes' theorem, we can write

$$\gamma_n(C) = \oint_C d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R}) = \int d\mathbf{S} \cdot \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})$$

$$\rightarrow \int d\mathbf{S} \cdot \nabla_{\mathbf{R}} \times \left[\mathbf{A}_n(\mathbf{R}) + \nabla_{\mathbf{R}} \Lambda(\mathbf{R})\right] = \int d\mathbf{S} \cdot \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}) \qquad (12)$$

so that γ_n is unchanged.

The analogy with electromagnetic potentials and fields does not mean that the effects are necessarily of electromagnetic origin. Therefore, we shall use a mathematical terminology, which makes no reference to electrodynamics, and call the vector potential **A** a connection and the field $\mathbf{B} = \nabla \times \mathbf{A}$ a curvature. This terminology also highlights the fact that the phase arises from non-trivial topological properties of the space spanned by the parameter.

Outline of thesis

Generally, a critical step in solving quantum mechanical problems is to set up the Hamiltonian, or classically, the Lagrangian of the system. We thus begin the second chapter with a brief review of the Born-Oppenheimer approximation in molecular physics. In chapter III we will study the principal mathematical device used in this thesis, the path integration technique formulated by Feynman and Hibbs (Feynman and Hibbs, 1961). It has been used as an approach to the geometrical phase by Kuratsuji and Iida (Kuratsuji and Iida, 1985) as in Chapter IV. Chapter V is devoted to a study of magnetic monopoles and geometrical phases. Chapter VI will be a general discussion.