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The Geometric Phase in Quantum Systems

Foundations, Mathematical Concepts, and Applications in Molecular and Condensed Matter Physics

量子系统中的几何相位

基本原理、数学概念及其在分子物理和凝聚态物理中的应用

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To our wives

Preface

Since Berry's introduction of the adiabatic geometrical phase, a large number of articles have appeared on the theoretical foundations, physical applications, and experimental manifestations of geometric phases. Although there are by now several review articles on geometric phases, there have been no comprehensive books or monographs on the subject. The present volume is intended to fill this gap in the literature. It is aimed at a diverse audience of advanced undergraduate as well as graduate students of physics and chemistry.

Due to their general nature, geometric phases have found applications in several different areas of physics and chemistry. Their theoretical basis has been shown to be related to the most basic concepts of modern mathematics. These make a complete treatment of the subject in a single volume a quite impossible task. We have included in this book an introductory part which offers an elementary discussion of the basic concepts and is based on our graduate level courses and summer school lectures. In the later part of the book we present more advanced subjects on the mathematical foundations of the geometric phase and the applications of the geometric phase in molecular and condensed matter physics. In the preparation of this book priority was given to the clarity of the exposition. We have also made every attempt to make the book as self-contained as possible.

A student with a good understanding of basic quantum mechanics should be able to learn the contents of the book at a reasonable pace. Although we have not assumed a knowledge of differential geometry, familiarity with manifolds and differential forms will certainly facilitate a quick reading. Readers with limited mathematical background should consult Appendix A. Here we offer a discussion of the most basic mathematical concepts together with worked examples. Appendix B provides an overview of the point group theory needed to understand many of the molecular examples of geometric phases.

Chapter 1 includes an introduction to the importance of geometric phases as well as a short historical survey of the developments which led to their discovery. Chapter 2 introduces Berry's adiabatic geometrical phase. This is followed by a discussion of the topological phase of Aharonov and Bohm. Chapter 3 is devoted to a detailed treatment of the quantum dynamics of a magnetic dipole in a precessing magnetic field. This is used as the motivation

for the introduction of the non-adiabatic geometric phase of Aharonov and Anandan in Chap. 4. This chapter also discusses the connections between the geometric phase and the theory of fiber bundles. Chapter 5 offers a more detailed introduction to fiber bundles and gauge theories. Chapter 6 includes a thorough discussion of different holonomy interpretations of the geometric phase and their relation to universal classifying bundles and connections. Chapter 7 treats the non-Abelian generalization of the ordinary geometrical phase. Chapters 8 and 9 discuss the emergence and importance of the Abelian and non-Abelian geometric phases in molecular physics. Chapters 10 and 11 provide a wealth of experimental examples in which the geometric phase has been detected and for which knowledge of the geometric phase greatly enhances understanding. The final three chapters survey various manifestations and applications of the geometric phase in condensed matter systems.

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The quantum geometric phase has been a research topic in many areas of science: theoretical amd mathematical physics, condensed matter theory, theoretical and experimental chemistry. This book is a collaboration of these diverse areas of physics and chemistry.

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1. Introduction

Today quantum mechanics forms an important part of our understanding of physical phenomena. Its consequences both at the fundamental and practical levels have intrigued mathematicians, physicists, chemists, and even philosophers for the past seven decades. A quantum system is usually described in terms of certain vector spaces and linear operators acting on these spaces. The vector spaces and their operators represent the states and the observables of the quantum system. The dynamics of a quantum system is determined by dynamical differential equations, the Schrödinger or the Heisenberg equations, which involve a linear operator called the Hamiltonian.

The Hamiltonian operator yields the energy levels and more importantly describes the evolution of the states of the physical system in time. Standard textbooks on quantum mechanics discuss almost exclusively the properties of quantum systems whose Hamiltonian does not depend on time. In many practical situations, however, the physical parameters which occur in the expression for the Hamiltonian are determined by time-dependent external or environmental factors. The study of time-dependent Hamiltonians is therefore very important in modeling real physical systems. One of the most interesting aspects of a quantum system with a time-dependent Hamiltonian is the occurrence of the geometric phase.

The geometric phase had been ignored in quantum physics for more than half a century. It had not been forgotten, but was thought to be unimportant. In 1928, Fock [82] showed that such a phase could be set to unity by a redefinition of the phase of the initial wave function. Although Fock's proof was limited to non-cyclic evolutions only, his conclusion was generally accepted until around 1980 when Mead and Truhlar [167] and Berry [31] reconsidered cyclic evolutions.

A cyclic evolution is an evolution in which the initial quantum state evolves periodically in time. For a pure cyclic state, this means that the state operator returns to the initial operator after each period while the corresponding state vector evolves into a vector which agrees with the initial vector only up to a phase factor. This phase factor contains, in addition to the usual dynamical phase, a purely geometric part which does not depend on the duration of the evolution.

Cyclic evolutions play an important role in the description of quantum systems in a periodically changing environment. The environment can be either classical such as a magnetic dipole in a precessing external magnetic field, or quantal such as an electron in the changing quantal environment of the collective motion of a molecule.

In 1956 Pancharatnam [208] discovered an analog of the quantum geometric phase in polarization optics. Three years later Y. Aharonov and D. Bohm published their findings on the significance of the electromagnetic vector potential in quantum mechanics [8]. They showed how the presence of a vector potential that did not produce an electric or magnetic field in the configuration space of free electrons could influence their interference pattern. The change in the interference pattern is due to the so-called Aharonov–Bohm phases which are special examples of the geometric phase. The Aharonov–Bohm phases received much attention in the 1960s, but it was not until the 1980s that the importance of the geometric phase was fully recognized.

The geometric phase in molecular systems appeared first in an implicit manner in the study of the $E \otimes e$ Jahn–Teller problem by Longuet-Higgins *et al.* [159] and by Herzberg and Longuet-Higgins [105]. They noticed that an electronic wave function that could be taken as real in all nuclear configurations behaved as a double-valued function that changed sign when the nuclear coordinates traversed a loop encircling a crossing point of the energy levels (potential energy surfaces) in the nuclear coordinate space.

The first concrete derivation of a geometric phase and the corresponding gauge potential was carried out in 1978 by Mead and Truhlar [167]. They considered the chemical reaction $H + H_2 \rightarrow H_2 + H$, which could be viewed as a wave packet motion from one minimum of the potential energy surface of the H_3 system to another. H_3 is an example of an $E \otimes e$ Jahn–Teller system, and the electronic wave function undergoes the sign changes found by Longuet-Higgins and his collaborators. Mead and Truhlar argued that the double-valuedness of the wave function caused by these sign changes could be avoided by including a vector potential in the electronic Hamiltonian.

This amounts to an improvement of the standard molecular Born–Oppenheimer approximation [48]. The latter is based on the observation that one can divide the motion of the constituents of a molecule into two "parts": the fast motion of the electrons and the slow collective rotations and vibrations of the molecule as a whole. One first investigates the dynamics of the fast variables while keeping the slow variables fixed, and then determines the dynamics of the slow variables. This means that in the Born–Oppenheimer approximation one treats the fast and the slow motions as two separate parts that do not influence each other. If, on the other hand, one does not consider the nuclear coordinates as fixed parameters but as quantum observables whose values change slowly in time, then the gauge potential underlying the geometric phase emerges naturally from the Born–Oppenheimer method.

Conceptually simpler than the gauge theory of the Born–Oppenheimer method is the investigation of quantum systems whose Hamiltonian depends on a set of slowly changing parameters. This was carried out in 1984 in a beautiful paper by Berry [31] who considered quite general quantum systems in a slowly changing classical environment. In this paper Berry derived the same gauge potential and the geometric phase that Mead and Truhlar had obtained from the Born–Oppenheimer method for the molecule. He further showed that indeed the celebrated Aharonov–Bohm phase was a special case of a geometric phase.

Berry's derivation of the adiabatic geometric phase – also known as the Berry phase – made use of the quantum adiabatic approximation which was only relevant for slowly changing Hamiltonians. However, it is easy to show that for a Hamiltonian with changing eigenvectors the adiabatic approximation of the dynamics of a cyclic evolution cannot be exact. Therefore Berry's phase could only be an approximation of the true quantum geometric phase. The latter was introduced for general unitary cyclic evolutions by Aharonov and Anandan in 1987 [7] and subsequently generalized to arbitrary (not necessarily unitary or cyclic) evolutions by Samuel and Bhandari [224].

Soon after the publication of Berry's paper, a number of experiments were performed to observe geometric phases. Among these are the nuclear magnetic resonance experiment by Suter *et al.* [239] and the nuclear quadrupole resonance experiment by Tycko [254]. A manifestation of the geometric phase in polarization optics was also observed in an experiment by Tomita and Chiao [250]. Today, there are many publications on various experimental studies of geometric phases in molecular physics. In particular, the geometric phase effect in the $E \otimes e$ problem was recently verified in a very convincing way by high-resolution spectroscopy of Na_3 and Li_3 [122, 259].

Geometric phases also play an important role in the study of condensed matter systems. One of the earliest results in this direction is due to Zak [281] who noticed that certain non-integrable phases of the Bloch wave function could be identified as a geometric phase. This was later related to the polarization of crystal insulators [124] and used to develop a practical method of calculating piezoelectric and ferroelectric properties [219]. Geometric phases in Bloch waves can also affect the semiclassical dynamics of electrons in metals and semiconductors [141, 237] and have important applications in the theory of the anomalous Hall effect [119]. More spectacularly, the quantized Hall conductance discovered in two-dimensional electron systems can be identified as a manifestation of certain geometric phases [23, 201, 247]. Adiabatic particle transport in Bloch bands and mesoscopic systems [245] may be most directly understood in terms of geometric phases as well. Some other applications of the geometric phase in condensed matter physics include a first-principles calculation of spin waves [198, 202], the dynamics of quantized vortices [249], and fractional statistics [18].