PHY

国外物理名著系列 26

（影印版）

# 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

A.Bohm A.Mostafazadeh
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科学出版社
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北京

**图字:01-2009-1136**



**图书在版编目(CIP)数据**

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 = The Geometric Phase in Quantum Systems: Foundations, Mathematical Concepts, and Applications in Molecular and Condensed Matter Physics:英文/(美)博赫姆(Bohm, A.)等著. —影印本. —北京:科学出版社,2009
(国外物理名著系列;26)
ISBN 978-7-03-024008-8

Ⅰ. 量… Ⅱ. 博… Ⅲ. 数学-应用-量子力学-研究生-教材-英文
Ⅳ. 0413.1

中国版本图书馆 CIP 数据核字(2009)第 019231 号

责任编辑:王飞龙 胡凯 鄢德平/责任印制:钱玉芬/封面设计:陈敬

科学出版社出版
北京东黄城根北街 16 号
邮政编码: 100717
http://www.sciencep.com

双青印刷厂印刷

科学出版社发行 各地新华书店经销

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2009 年 3 月第 一 版 开本:B5(720×1000)
2009 年 3 月第一次印刷 印张:28 3/4
印数:1~2 500 字数:579 600

**定价:86.00 元**

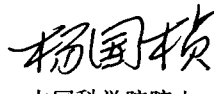
(如有印装质量问题,我社负责调换〈双青〉)

# 国外物理名著系列序言

对于国内的物理学工作者和青年学生来讲，研读国外优秀的物理学著作是系统掌握物理学知识的一个重要手段。但是，在国内并不能及时、方便地买到国外的图书，且国外图书不菲的价格往往令国内的读者却步，因此，把国外的优秀物理原著引进到国内，让国内的读者能够方便地以较低的价格购买是一项意义深远的工作，将有助于国内物理学工作者和青年学生掌握国际物理学的前沿知识，进而推动我国物理学科研和教学的发展。

为了满足国内读者对国外优秀物理学著作的需求，科学出版社启动了引进国外优秀著作的工作，出版社的这一举措得到了国内物理学界的积极响应和支持，很快成立了专家委员会，开展了选题的推荐和筛选工作，在出版社初选的书单基础上确定了第一批引进的项目，这些图书几乎涉及了近代物理学的所有领域，既有阐述学科基本理论的经典名著，也有反映某一学科专题前沿的专著。在选择图书时，专家委员会遵循了以下原则：基础理论方面的图书强调“经典”，选择了那些经得起时间检验、对物理学的发展产生重要影响、现在还不“过时”的著作（如狄拉克的《量子力学原理》）。反映物理学某一领域进展的著作强调“前沿”和“热点”，根据国内物理学研究发展的实际情况，选择了能够体现相关学科最新进展，对有关方向的科研人员和研究生有重要参考价值的图书。这些图书都是最新版的，多数图书都是2000年以后出版的，还有相当一部分是当年出版的新书。因此，这套丛书具有权威性、前瞻性和应用性强的特点。由于国外出版社的要求，科学出版社对部分图书进行了少量的翻译和注释（主要是目录标题和练习题），但这并不会影响图书“原汁原味”的感觉，可能还会方便国内读者的阅读和理解。

“他山之石，可以攻玉”，希望这套丛书的出版能够为国内物理学工作者和青年学生的工作和学习提供参考，也希望国内更多专家参与到这一工作中来，推荐更多的好书。



中国科学院院士
中国物理学会理事长

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.

## Acknowledgments

A. B. would like to express his gratitude to J. Anandan, M. V. Berry, B. K. Kendrick, L. Loewe and C. A. Mead for discussions on the subject of various chapters of this book. He is particularly grateful to C. A. Mead and A. Mondragon for reading parts of the earlier manuscript and for their comments and suggestions. He also thanks the participants and organizers of the NATO Advanced Study Institute and GIFT International Seminar Salamanca where some of the material of this book was first presented.

A. M. would like to thank his PhD advisor Bryce DeWitt and his teachers Can Delale, Metin Arik, Cecile DeWitt-Morette, and Gary Hamrick for their guidance and encouragement, his friends and colleagues Ertuğrul Demircan, Teoman Turgut, Bahman Darian, Rouzbeh Allahverdi, Luis Boya, Don Page, Mohsen Razavy, and graduate students of his mathematical physics course (taught at the Sharif University of Technology, Tehran, in the Spring of 1995) for fruitful discussions and comments. He would also like to acknowledge the financial support of the Killam Foundation of Canada and the hospitality of the Theoretical Physics Institute of the University of Alberta during the preparation of the first draft of the book.

Q. N. wishes to acknowledge his PhD and post-doctoral advisers David Thouless, Walter Kohn and Eduardo Fradkin for their mentorship, and his former students M. C. Chang and G. Sundaram and colleagues Ping Ao, L. Kleinman, and A. H. MacDonald for their close collaborations. He especially thanks Julie Zhu for her love, understanding, and care.

H. K. would like to thank I. B. Bersuker, J. E. Boggs, P. J. Rossky, J. F. Stanton, and R. E. Wyatt for their hospitality during his stay at the Institute of Theoretical Chemistry, the University of Texas at Austin, where a part of the manuscript was prepared. He also thanks K. Makoshi and N. Shima for making this extended stay possible, G. C. Schatz, V. Z. Polinger

and Y. Takada for helpful comments and discussions, and B. Kendrick for providing some of the figures.

J. Z. acknowledges many instructive interactions on the subject of geometric phases with E. R. Grant, A. Pines, and M. Bausch-Koenig. He also thanks A. Bohm for inviting him to participate in this project.

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.

We gratefully acknowledge support from the Welch Foundation.

Austin, *Arno Bohm, Qian Niu*
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Bloomington, *Josef Zwanziger*
March 2003

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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].

The fact that the geometric phase has important observable consequences in many areas of physics and chemistry is not the only reason why it has attracted so much attention. The geometric phase is also one of the most beautiful examples of what Wigner once called "the unreasonable effectiveness of mathematics in the natural sciences."

Immediately after Berry's introduction of the adiabatic geometric phase, Simon [230] noticed that it could be interpreted as the holonomy of a fiber bundle and that Berry's gauge potential played the role of a connection on this fiber bundle. It was this relation to the beautiful mathematics of fiber bundles that caused the geometric phase to become a fashion in mathematical physics. When the theory of fiber bundles was established and when the mathematics of the universal classifying bundles and connections was developed, no one could imagine that these would be directly related to a quantum mechanical phase factor which could be measured in say an interference experiment. The universal connection is the "natural" mathematical object which classifies the geometric structures on arbitrary (finite-dimensional) principal fiber bundles. It is incredible that this mathematical entity is exactly the gauge potential whose integral over a closed path of states gives the Aharonov–Anandan phase with Berry's gauge potential as its limiting case [44, 184], and that this connection is related to Mead's vector potential which was discovered in the study of molecular structure.