

BERRY PHASES IN ELECTRONIC STRUCTURE THEORY

Over the past 25 years, mathematical concepts associated with geometric phases have come to occupy a central place in our modern understanding of the physics of electrons in solids. These “Berry phases” describe the global phase acquired by a quantum state as the Hamiltonian is changed. Beginning at an elementary level, this book provides a pedagogical introduction to the important role of Berry phases and curvatures, and outlines their great influence upon many key properties of electrons in solids, including electric polarization, anomalous Hall conductivity, and the nature of the topological insulating state. It focuses on drawing connections between physical concepts and provides a solid framework for their integration, enabling researchers and students alike to explore and develop links to related fields. Computational examples and exercises throughout provide an added dimension to the book, giving readers the opportunity to explore the central concepts in a practical and engaging way.

DAVID VANDERBILT is Board of Governors Professor of Physics at Rutgers University, where he has made significant contributions to computational condensed-matter physics. He is a fellow of the American Physical Society and a member of the National Academy of Sciences, and was awarded the prestigious Rahman Prize in Computational Physics of the American Physical Society in 2006.

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“This book brings together almost forty years of progress in understanding how the wavefunctions of electrons in a crystal, and in particular their continuous evolution with momentum, determine important physical properties. David Vanderbilt is one of the creators of this field, and nearly every chapter includes topics where his contributions were decisive. In addition to its scope, one way in which this book differs from others on related topics is the clear path from physical insight, through theoretical understanding, to practical methods for specific materials. This book can be read profitably by those interested in the fundamental theory of topological phases as well as those seeking to understand modern electronic structure approaches.”

Joel Moore
Chern-Simons Professor of Physics, UC Berkeley

“The geometric phase and related concepts provide a unified framework for describing many fundamental properties of electrons in solids, from electric polarization to quantized effects in topological materials. Readers wishing to become familiar with these notions will find David Vanderbilt’s excellent book to be an invaluable resource.”

Ivo Souza
University of the Basque Country, San Sebastián

“Berry phases and associated geometric and topological concepts have transformed our understanding of electronic properties. This book provides a much needed pedagogical exposition with computational instructions which will be very valuable for students and researchers in solid state physics and materials science.”

Qian Niu
University of Texas

“David Vanderbilt explicates a new exciting frontier in solid state physics and materials theory, and does so in a clear and interesting to read way. Not only does he cover every nook and cranny of this new area, but in the process clearly explains the basics of electronic structure theory, such as density functional theory (DFT) and tight-binding, that will be extremely useful and important to any student of condensed matter theory. The subject of the book is how the phases of the wave functions, neglected for decades, effects important measurable properties of materials. He covers everything from the mathematical theory of geometric phases, applications to polarization and orbital magnetism, all the way to complex applications such as three-dimensional topological insulators and beyond. To be able to write about such seemingly esoteric matters in such a clear and gripping way is the mark of a great teacher. I look forward to my second reading of the book!”

Ronald Cohen
Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science

“For anyone who wants to learn about Berry phases in electronic structure and the exciting recent developments in topological insulators, I heartily recommend this book. David Vanderbilt is uniquely poised to present the concepts and practical developments in this field that has revolutionized our understanding of condensed matter. He has made some of the most important advances in electronic structure theory in the last 20 years, including the original work that has made Berry phases a central part the field, and he is known for lucid presentations. In this book Vanderbilt introduces the concepts in a way that is accessible to a nonexpert, with clear explanations and instructive examples, and yet he presents the material in the depth that it deserves. The book provides the reader with the background that is needed to understand each aspect: an excellent introduction to Berry phases and aspects of topology relevant to electrons in crystals, and the needed background in electronic structure theory. To give just one example, Wannier functions have become increasingly important in many ways, and this book provides an elegant way to understand their properties. The last three chapters are a coordinated presentation of the three most important roles of Berry phases: electric polarization, topological insulators and Weyl semimetals, and orbital magnetization. Each of these has aspects that were completely unknown or not understood only a few years ago, but now have elegant, simple explanations in terms of Berry phases. I recommend this book for anyone who wants to be a part of condensed matter theory in the twenty-first century or just to appreciate the basic ideas and phenomena of this exciting field.”

Richard M. Martin
University of Illinois Urbana Champaign

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DAVID VANDERBILT

Rutgers University



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Preface

This book introduces a class of mathematical methods connected with geometric phases, also known as Berry phases, and the important role that these have come to play in recent years in the band theory of electrons in crystals. The “Berry phase” terminology derives from the seminal papers of Michael Berry in the mid-1980s, in which he highlighted the importance of geometric phases in a wide range of physical contexts and advocated for a recognition of geometric phases as representing a new paradigm in theoretical physics. These concepts rapidly came to play a central role in aspects of atomic, molecular, nuclear, and optical physics, but were initially rather slow to enter into the theory of the electron bands in crystalline materials, commonly known as electronic structure theory.

This began to change in the 1990s with the introduction of the “modern theory of polarization,” and then in the early 2000s with developments in the theory of Wannier functions and the emergence of a proper theory of orbital magnetization. However, the pace accelerated greatly with the exciting developments in the theory of topological insulators in the mid- to late 2000s, and by 2010 it was clear that the role of Berry phases in the electronic structure of crystalline materials had become very topical. In the years since then, the field has been advancing rapidly, with the interest in topological states of crystalline materials developing in many directions.

These advances convinced me of the need for a pedagogical text that could capture and synthesize the core of these developments. With this in mind, I began the process of turning some informal lecture notes, prepared earlier for a graduate-level special-topics course, into a proper text. The opportunity to teach this course again in 2016 provided a further impetus to continue the writing, and also to develop an accompanying set of computational examples and exercises. The scientific understanding of topological phases continued to develop rapidly during the course of the writing, with topological semimetals and other novel topological states attracting much attention. Where possible, I have expanded the later chapters to reflect some of this recent progress as well.

This book is the result.

I owe a debt of gratitude to a large number of individuals who provided invaluable comments and suggestions as this book developed. First, I warmly acknowledge the feedback offered by the students in the special-topics courses I taught on this subject, as well as other students and postdocs who were at Rutgers during those years. Among those who notably contributed useful ideas, comments, and corrections are Victor Aleksandrov, Sinisa Coh, Philipp Eck, Qiang Han, Wenshuo Liu, Jisoo Moon, Alexey Soluyanov, Maryam Taherinejad, Nicodemos Varnava, Wenhan Wu, and Tahir Yusufaly. Others who gave a careful reading to some sections and provided me with especially valuable feedback and corrections include Heung-Sik Kim, Se Young Park, and Shuchen Zhu. I also wish to thank Barry Bradlyn, Charlie Kane, Joel Moore, and Qian Niu for assistance in clarifying some subtle points of physics, and for helping me to understand how best to present certain topics that lie somewhat outside the scope of my own expertise.

Special thanks are due to Sinisa Coh for his role as the prime developer and maintainer of the PYTHTB code package, which plays such an important part in the scheme of this book.

I wish to thank the Simons Foundation for providing a Simons Fellowship in Theoretical Physics in 2014, which funded a sabbatical extension during which the first part of this book was written. In addition, I thank the Department of Chemistry at Princeton University for providing a visiting appointment that allowed me to devote some quiet days to writing away from the distractions of my office at Rutgers. I would also like to acknowledge the importance of research funding from the National Science Foundation and the Office of Naval Research, which provided resources in support of the research conducted in my group on the topics discussed here.

I would especially like to thank my colleagues in the Department of Physics and Astronomy at Rutgers University for providing a consistently supportive intellectual environment over the course of my career at Rutgers.

Three other individuals deserve special mention. Richard Martin, who provided valuable comments on pedagogical approaches to the material presented here, has been a constant source of inspiration and support over the course of my professional career. Raffaele Resta, who likewise provided important feedback on the structure of the book, is perhaps the person whose scientific career most closely parallels the topics addressed here. Our interactions over the years have been deeper and more pervasive than the occasional formal collaborations might suggest, and his scientific impact on me and on the field has been profound. Finally I must acknowledge Ivo Souza, with whom I have collaborated frequently over the years on topics connected with the themes of this book. Ivo has been the most conscientious reader of my draft chapters as they have developed. He has frequently suggested ways of

improving or extending a line of argument, and has been relentless in finding errors and inconsistencies in the text. His assistance has been inestimable, and I thank him profoundly.

I am deeply grateful to my wife Roslyn, whose love and encouragement have been a great source of support in the course of writing this book.

Lastly, I would like to thank all of the graduate students and postdocs who have worked with me over the years. We have shared the excitement and joy of developing some of the concepts discussed in this book, designing computational schemes to implement them, and exploring their physical consequences. It has been a great journey, and a pleasure to have all of them along for the ride.

Acronyms

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
4D	four-dimensional
AHC	anomalous Hall conductivity
ARPES	angle-resolved photoemission spectroscopy
bcc	body-centered cubic
BZ	Brillouin zone
CS	Chern–Simons
DFT	density-functional theory
fcc	face-centered cubic
GGA	generalized gradient approximation
HWF	hybrid Wannier function
IC	itinerant circulation
LC	local circulation
LCAO	linear combination of atomic orbitals
LDA	local-density approximation
LSDA	local spin-density approximation
ME	magnetoelectric
MLWF	maximally localized Wannier function
QAH	quantum anomalous Hall
QSH	quantum spin Hall
SI	international system of units
SOC	spin-orbit coupling
SVD	singular value decomposition
TB	tight binding
TI	topological insulator
TR	time reversal
TRIM	time-reversal invariant momentum (or momenta)