Introduction

Two linked concepts have been central to the theory of quantum mechanics since its development nearly a century ago. One states that the probability of a measurement is given by the squared norm of the corresponding quantum amplitude, so that the *phase* of that amplitude has no importance to the final measurement. The other asserts that the interference phenomena associated with phase *differences* can modulate the amplitudes, thereby giving rise to measurable effects. One famous example of the latter is the double slit experiment. Another is the Aharonov–Bohm effect, in which the interference that occurs when a beam of charged particles is split and recombined is found to depend on the magnetic flux enclosed between the two legs of the path. Nevertheless, we tend to regard these as exceptional cases, and for most practical purposes we often think it is safe to ignore quantum phases.

Until recently, this has been the dominant point of view in solid state physics. In the theory of the electronic structure of crystalline systems, almost all quantities of interest can be expressed as Bloch-state expectation values, including the band energies, charge densities, spin densities, local densities of states, total energies, forces, stresses, spin magnetic moments, and so on. In computing such quantities, the overall phase in front of any given Bloch function plays no role.

In a paradigm shift that has occurred over the last 25 years, however, it has become clear that the phases of the electronic states are essential for the description of some properties of crystalline materials, including electric polarization, orbital magnetization, and anomalous Hall conductivity. In fact, the overall phase of a given Bloch function is still immaterial, but the *relative phase* between states at nearby times, or for nearby Hamiltonians, or for nearby wavevectors of Bloch functions, can have crucial physical consequences. In these cases, the appropriate formalism is that of a geometric phase, or Berry phase, which is defined in terms of a global phase difference that accumulates when tracing the evolution of a quantum state in time, or along a path in the parameter space of the Hamiltonian, or along a path in the space of Bloch wavevectors (i.e., the Brillouin zone) of a crystalline system.

In the last 15 years, a related paradigm shift has occurred with the discovery and development of the theory of topological insulators. Previously, the distinction between different phases of matter had almost always rested on Landau-theory concepts of symmetry and order parameters. By contrast, the topological insulator Bi_2Se_3 is known to be identical with its trivial analogue Sb_2Se_3 in all respects as far as symmetry is concerned, and no order parameter can be defined to distinguish them. The difference is that the Bloch functions in Bi_2Se_3 are twisted in a manner connected with their phase evolution across the Brillouin zone, while those of Sb_2Se_3 are not. Again, Berry phases and curvatures are at the heart of these developments.

The purpose of this book is to give a pedagogical introduction to the mathematics of Berry phases and the closely related concepts of Berry connections, Berry curvatures, and Chern numbers, and then explain how these concepts have come to play a central role in several aspects of electronic structure theory. In particular, they have come to underlie the modern theories of electric polarization, anomalous Hall conductivity, orbital magnetization, magnetoelectric coupling, and topological insulators and semimetals.

The intended audience is that of advanced graduate students and researchers in the fields of condensed matter and electronic structure theory. A solid background in quantum mechanics and solid state physics, preferably at the graduate level, is assumed. Virtually all of the concepts described in this book rely only on a description at the single-particle level, so that the formalisms and techniques of many-body physics are not essential here. A prior familiarity with electronic structure calculations in the density-functional context, or the simpler tight-binding formulation, will be useful but not essential. The book is intended to be accessible to both experimental and theoretical students, although the former may wish to skim over a few sections that have a more formal mathematical flavor.

The book is organized as follows. The first chapter provides a pedagogical introduction to the *physics* of the concepts and phenomena to be discussed in the book. That is, I explain why, on physical grounds, we might expect the electric polarization to be defined only modulo a quantum, or why the anomalous Hall conductivity of an insulator should be quantized. Since the proper introduction of the mathematical formalism needed to discuss these topics has been deferred to later chapters, this has entailed some compromises. Readers who find this chapter to be hard going are encouraged to skim or skip some sections, or the entire chapter, and then return to it later after working through some of the subsequent material.

The second chapter gives a brief review of the theory of electrons in crystalline solids. Most of this coverage should be familiar to the typical reader, but the chapter also provides an introduction to tight-binding theory and its implementation in the open-source PythTB package, which will be used for examples and exercises throughout the later chapters, and to linear response theory. The mathematical framework of the theory of Berry phases (also known as geometrical phases) and curvatures is then carefully introduced in Chapter 3. Initially this is done in the context of the ground state of a finite system whose Hamiltonian is undergoing an adiabatic deformation described by one or more external parameters. The same theory is then applied to crystalline solids in which the wavevector of the Bloch eigenstates serves as an internal parameter, possibly together with external parameters. The treatment here is primarily mathematical, but some hints will appear as to the physical significance of the Berry-related quantities.

The remainder of the book is devoted to developing those connections between the mathematics and physics. Chapter 4 is devoted to the Berry-phase theory of electric polarization, quantized adiabatic charge transport, and surface charge. The ability to compute the Berry-phase polarization is now a standard feature of almost all well-known electronic-structure code packages, but subtleties often arise in the interpretation of the results, and these are discussed at some length. Chapter 5 then introduces the theory of topological insulators and semimetals, starting with the 2D quantum anomalous Hall state (which we may regard as the "mother of all topological insulators"), and then discussing 2D quantum spin Hall insulators, 3D strong topological insulators, topological crystalline insulators, and Weyl semimetals. Our story then concludes in Chapter 6 with a discussion of orbital magnetization and magnetoelectric coupling, and especially the role of the Chern–Simons "axion" coupling, which is closely related to the theory of topological insulators.

The book is structured so that it can form the basis of an advanced special-topics course at the graduate level. It should also serve well for a motivated individual interested in learning the material in an independent context. Exercises are provided throughout, and in formulating these I have tried to strike a balance between theory and practice. Many of the exercises are of the traditional form where students are asked to complete a derivation, apply a theory to a special case, or extend some argument given in the text. The remainder are computational in nature and require that students familiarize themselves with the use of the PythTB code package, which is detailed in Appendix D. This open-source package is written in the Python programming language, and can be downloaded from standard Python repositories or from the Cambridge University Press website at http://minisites.cambridgecore.org/berryphases. An elementary knowledge of

PYTHON programming is required, but this is not hard to pick up with the aid of the examples given and the various PYTHON tutorials that can be found online. None of the calculations are computationally demanding, so any laptop or desktop computer with PYTHON installed can be used to complete these exercises. While it would be possible to teach this material without making use of the computational exercises, I believe that the ability to illustrate the formal theory by practical computations adds an important element to the learning experience.