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Berry Phases in Electronic Structure Theory. Electric Polarization, Orbital Magnetization and Topological Insulators. By David Vanderbilt. Cambridge University Press, 2018. Hardback, pp. x+384. Price GBP 59.99. ISBN 9781107157651.

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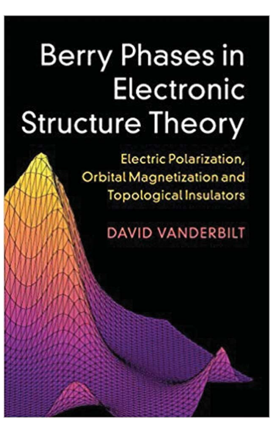
The book by David Vanderbilt, *Berry Phases in Electronic Structure Theory*, is a very pedagogical introduction to the role played by Berry phases in our understanding of the electronic properties of matter. It is indeed written by one of the prominent contributors to the field.

Since their discovery in 1984, Berry phases have been used to understand or reinterpret a variety of phenomena such as charge pumping, polarization, orbital magnetization and Hall effects, as well as topological insulators. They are all discussed in the book, step by step, from an elementary level to a more detailed understanding. Throughout the book a Python package, *PythTB*, is used to provide numerical examples that support the theory given in the book. The code of the examples is given in the appendices so that it can be investigated by the reader.

In the first chapter D. Vanderbilt gives an overview of the physics covered in the book, and explains on physical grounds several of the results obtained in later chapters.

The second chapter reviews elementary concepts in solid-state physics. A rather lucid and self-contained discussion of density functional theory, Bloch functions and tight-binding Hamiltonians is given. The *PythTB* package is also introduced. This package, developed at Rutgers University, allows one to build and solve tight-binding models and compute Berry phases related properties. It is most useful to understand the concepts newly introduced in later chapters.

From the mathematical point of view, the third chapter is the most important in the book. The Berry phase is first introduced as a Pancharatnam phase. A parameter space is considered, and the phase of a state vector is accumulated along a closed path which is covered in a finite number of steps. Later, the continuous limit is taken, and important concepts such as Berry connection and curvature are defined. The Chern theorem, which is that the integral of the Berry curvature on a 2-surface is quantized, is then stated. With regard to its importance for later applications, one may regret that a more mathematical derivation is not given, although convincing arguments are presented. After the discussion of Berry phases in general terms, several applications are considered. Adiabatic dynamics is reviewed, making apparent the role played by the Berry phase. Then, instead of considering a generic parameter space for a defined Berry phase, the Brillouin zone is chosen, and the parameters are the components of the electron wavevectors. This is used in most of the following chapters. Finally, the chapter is concluded with a discussion of Wannier functions. In particular, it is shown how the gauge freedom on the Bloch functions affects the average value of the position operator, the Wannier centres, and how they are related to Berry phases. This is very useful in later chapters to obtain a physical picture of the phenomenon under consideration.



Chapters 4, 5 and 6 are devoted to applications of the general concepts developed so far. The modern theory of polarization is presented in Chapter 4, a theory developed by David Vanderbilt himself in the 1990s. In insulators, the textbook approach to polarization is based on a separation of the charge into free and bound charges, which then define polarizable entities. In solids, the separation is far from obvious, and this approach prevented practical computations for many years. The arguments given in the first chapter of the book, advocating for a multivalued polarization, are derived here. To

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obtain this result, the time variation of the polarization is identified with the adiabatic current computed in Chapter 3. Then the polarization appears to be given by the integral of the Berry connection over the Brillouin zone. The multi-valuedness of the polarization is then a consequence of the modulo 2π invariance of the integral of the Berry connection under a gauge transformation. Later in the chapter, a link is made with the Wannier centres, expressing the polarization as a sum over Wannier centres, each of them being assigned with the elementary electronic charge. Somehow, this picture rescues the classical dipole picture, which was debated in the first chapter, and allows one to understand the multi-valuedness of the polarization as a cell assignment problem for the charges. The chapter ends with several surface and interface theorems, which relate surface and interface charges to bulk polarization.

Chapter 6 is devoted to orbital magnetization. The chapter begins with a discussion which is similar to the polarization problem. Indeed, its definition suffers from the same problems as polarization in the textbook definition. Later in the chapter, a special emphasis is given to the magnetoelectric coupling, which is the change of polarization when a magnetic field is applied, or, equivalently, the change of magnetization under an applied electric field. The focus is given to the frozen-lattice orbital contribution to the magnetoelectric coupling. At first it is shown to determine the surface anomalous Hall conductivity, as the polarization does determine surfaces charges, and must therefore be regarded as a multi-valued quantity, to be defined modulo a quantum of e^2/h. It is finally expressed using Berry phase formalism, as was the polarization. Part of this contribution, the itinerant contribution in non-zero electric field, which excludes the local contribution associated with the circulation of Wannier functions around the Wannier centres and the zero-field contribution, is found to be given by the Chern–Simons axion coupling. Therefore, the end of the chapter discusses axion electrodynamics.

Chapter 5 is devoted to topological insulators and semimetals. The chapter is rich in content, discussing several of the exotic phases that are currently topics of research. The beginning of the chapter is used to define classes of topological insulators as systems whose Hamiltonians can be continuously connected along a path without a closing of the gap. As explained by the author, this classification is very different from the one by Landau, which is based on order parameters. The sections following this introduction discuss several classifications. At first D. Vanderbilt discusses the Haldane model, which has a broken time-reversal symmetry, as the 'hydrogen atom of topological insulators', to evidence band inversion as a typical case of topological transition. As a result of integrating the Berry curvature over the Brillouin zone, the Chern number is shown to jump by an integer across the transition, as a consequence of gap closing. This example is used to define Chern insulators. The correspondence with edge states is then discussed, and related to the quantum anomalous Hall physics. After having shown that 2D insulators with broken time-reversal symmetry can be topologically classified using Chern numbers, the next section discusses quantum spin Hall insulators, 2D systems which are time-reversal invariant, as members of the Z_2-odd classes, as opposed to the Z classification of Chern insulators. In particular, the strategies used to compute the Z_2 invariant from *ab initio* calculations are discussed. The author also discusses the case of 3D Z_2 topological insulators.

In the 2D and 3D case, the author illustrates the classification of topological insulators using the flow of hybrid Wannier centres, which was introduced in Chapter 3. It is most useful to obtain a physical picture, since depending on whether the hybrid centres connect neighbouring cells or not when crossing the Brillouin zone in one direction, the value of the topological numbers can be inferred.

The discussion is not limited to insulators since Weyl semimetals are also considered. They are metals with a vanishing density of states at the Fermi level due to a conical intersection of bands around that energy, at the Weyl points. The chirality of the Weyl points is first related to the flux of the Berry curvature around a sphere surrounding those points, and later unusual transport properties resulting from that energy band configuration are discussed. In particular, we can mention the chiral anomaly and the chiral magnetic effect. The chapter ends with a review of other topological systems not discussed in the main part of the book.

Finally, I would like to recommend this book to crystallographers, and more generally to condensed-matter physicists who wish to learn about the physics of Berry phases. The pedagogical presentation used throughout will allow careful readers to start working on the more detailed literature with a solid basis and a clear view of recent results.