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# Introduction

Condensed matter physics deals with the behavior of particles at finite density and at low temperatures, where, depending on factors such as applied pressure, doping, spin of the particles, etc., matter can reorganize itself in different phases. Classically, we learn of phases such as liquid, crystal, or vapor, but the quantum world holds many more fascinating mysteries. Quantum theory predicts the existence of myriad states of matter, such as superconductors, charge density waves, Bose-Einstein condensates, ferromagnets and antiferromagnets, and many others. In all these states, the underlying principle for characterizing the state is that of symmetry breaking. An order parameter with observable consequences acquires an expectation finite value in the state of matter studied and differentiates it from others. For example, a ferromagnet has an overall magnetization, which breaks the rotational symmetry of the spin and picks a particular direction of the north pole. An antiferromagnet does not have an overall magnetization but develops a staggered-order parameter at some finite wavevector. Landau's theory of phase transitions provides the phenomenological footing on which symmetry-broken states can be explained. In this theory, a high-temperature symmetric phase experiences a phase transition to a low-temperature, less-symmetric, symmetry-broken state. The theory has very general premises, such as the possibility of expansion of the free energy in the order parameter: when close to a phase transition, this is likely to be possible because the order parameter is small. The transition can be first, second, or higher order, depending on the vanishing of the coefficient of the second, third, or higher coefficient of the expansion of the free energy in the order parameter. However, the major limitation of Landau's theory of phase transitions is that it is related to a *local* order parameter. In the past decade it has become clear that a series of phases of matter with so-called topological order do not have a local order parameter. For some (most) of them, a (highly) nonlocal order parameter can be defined, but it is unclear how a Landau-like theory of this order parameter can be developed. Among these phases, which boast excitations with fractional statistics, the experimentally established ones are the fractional quantum Hall (FQH) states. It has been shown that FQH phases have a nonlocal order parameter, which corresponds to annihilating an electron at a position and, crucially, unwinding a number of fluxes (for an Abelian state). The flux unwinding is highly nonlocal, and it is not clear if a true Ginzburg-Landau theory can be written for this order parameter. States with nonlocal order parameters could be called topologically ordered; more generally, however, the definition of a topological phase is a phase of matter whose low-energy field theory is a topological field theory. Recently, topological phases have been pursued because of their potential practical applications: it has been proposed that a topological quantum computer could employ the 2-D quasi-particles of non-Abelian FQH states (called non-Abelian anyons), whose world lines cross over one another to form braids [1]. These braids form the logic gates that make up the computer. A major advantage of a topological quantum computer over one using trapped quantum particles is that the former encodes information nonlocally and hence is less susceptible to local decoherence processes [1, 2]. Although the concept of topologically ordered phases has been around for more than a decade, most examples involved complicated states of matter, such as the FQH, quantum double models, doubled Chern-Simons theories, and others. The topologically ordered states that have been experimentally realized and theoretically investigated up to now have involved strong electron-electron interactions.

States of matter formed out of free fermions have been deemed to be topologically "trivial" in the past, mostly because the Hamiltonian spectrum is exactly solvable. However, a subset of such states, which we call *topological insulators*, have interesting properties, such as gapless edge states, despite being made out of noninteracting fermions. The paradigm example of such a state is the integer quantum Hall effect, which requires an applied magnetic field on a semiconductor sample. More recently, examples of topological phases that do not require external magnetic fields have been proposed, the first being Haldane's Chern insulator model [3]. Although this state has not been experimentally realized, a time-reversal-invariant (TR-invariant) version has been proposed and discovered [4, 5, 6, 7, 8, 9, 10]. The term *topological* (attached to phases or insulators) implies the existence of a bulk invariant (usually an integer or a rational number or set of numbers) that differentiates between phases of matter having the same symmetry. In the field of topological insulators, topological is usually associated with the existence of gapless edge modes when a system is spatially cut in two, but this is not the generic situation; topological phases or even insulators can exist without the presence of gapless edge modes.

Despite the fact that the field of band theory has been around since the foundations of quantum mechanics almost a century ago, it was realized only in 2006 that there exists an enhanced band theory, called *topological band theory* which takes into account concepts such as Chern numbers and Berry phases. It is quite remarkable and exciting that the theory we have used to understand insulators and semiconductors for almost a century is incomplete and that the underpinnings of the new theory, which includes topological effects, is being worked out during our lifetimes. In this book, we provide a foundation for understanding and beginning research in the field of topological insulators. We aim to provide the reader with both physical understanding and the mathematical tools to undertake high-level research in this emerging field. Recent work in the theory of insulators [4, 5, 6] showed that an important consideration is not only which symmetries the state breaks, but which symmetries must be preserved to ensure the stability of the state. A series of symmetries, the most important of which are time-reversal and charge conjugation, can be used to classify insulating states of matter. The trivial insulator is differentiated from the nontrivial, topological insulator, which (in most, but not all, cases) exhibits gapless surface or boundary gapless states protected from opening a gap.

A periodic table classifying the topological insulators and superconductors has been created. The table organizes the possible topological states according to their space-time dimension and the symmetries that must remain protected: TR, charge-conjugation, and/or chiral symmetries [11, 12, 13]. The most interesting entries in this table, from a practical standpoint, are the 2-D and 3-D TR-invariant topological insulators, which have already been found in nature [7, 8, 9, 10]. These are insulating states classified by a $Z_2$ invariant that requires an unbroken TR symmetry to be stable. There are several different methods to calculate the $Z_2$ invariant [5, 9, 13, 14, 15, 16, 17, 18], and a nontrivial value for this quantity implies the existence of an odd number of gapless Dirac fermion boundary states as well as a nonzero [13] magnetoelectric polarization in three dimensions [13, 19]. The current classification of the topological insulators covers only the TR, charge-conjugation, or chiral symmetries and does not exhaust the number of all possible topological insulators. In principle, for every discrete symmetry, there must exist topological insulating phases with distinct physical properties and a topological number that classifies these phases and distinguishes them from the "trivial" ones. This is the point of view taken in this book.

So far, in our discussion we have used the term *topological* cavalierly. In this book, we also hope to clarify what makes an insulator topological. We should start by first defining a trivial insulator: this is the insulator that, upon slowly turning off the hopping elements and the hybridization between orbitals on different sites, flows adiabatically into the atomic limit.

In most of the existent literature on noninteracting topological insulators, it is implicitly assumed that nontrivial topology implies the presence of gapless edge states in the energy spectrum of a system with boundaries. However, it is well known from the literature on topological phases that such systems can theoretically exist without exhibiting gapless edge modes [20]. Hence, the edge modes cannot be the only diagnostic of a topological phase; consequently, the energy spectrum alone, with or without boundaries, is insufficient to determine the full topological character of a state of matter. In the bulk of an insulator, it is a known fact that the topological structure is encoded in the eigenstates rather than in the energy spectrum. As such, we can expect that entanglement—which depends only on the eigenstates—can provide additional information about the topological nature of the system. However, we know that topological entanglement entropy (or the subleading part of the entanglement entropy) [21, 22], the preferred quantity used to characterize topologically ordered phases, does not provide a unique classification and, moreover, vanishes for any noninteracting topological insulator, be it time-reversal breaking Chern insulators or TR-invariant topological insulators. However, careful studies of the full entanglement spectrum [23] are useful in characterizing these states [23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34].

This book covers most introductory concepts in topological band theory. It is aimed at the beginning graduate student who wants to enter quickly the research in this field. The philosophy behind the writing of this book is to mix physical insight with the rigorous computational details that would otherwise be time consuming to derive from scratch. The book starts with a review of the most important concept—that of Berry phases in chapter 2.

In chapter 3, we show how measurable quantities, such as Hall conductance, are related, through linear response, to Berry curvature and Chern numbers on both periodic and disordered systems, with and without applied magnetic field. We introduce the flat-band limit of an insulator, which simplifies tremendously the calculation of topological quantities. We present the Chern number as an obstruction in the full Brillouin zone (BZ) and as an integral of the Berry curvature over the full BZ of an insulator.

In chapter 4, we introduce the concept of TR symmetry for both spinless and spinful particles and show the vanishing of the Chern number in the presence of TR symmetry. We show that time reversal is an antiunitary operator and that its presence requires, for half-integer spin particles, the existence of doubly-degenerate states—a theorem known as Kramers' theorem. We then focus on the case of Bloch Hamiltonians in translationally invariant crystals and derive the conditions under which a Bloch Hamiltonian is TR invariant.

In chapter 5, we introduce and analyze the problem of 2-D lattice electrons in a magnetic field, with emphasis on the Chern numbers of the bands. We analyze the magnetic translation group on the lattice and explain the magnetic unit cell, showing that even though the magnetic field is uniform, translational invariance with the original unit cell is broken. We then obtain the spectrum of the 2-D nearest-neighbor-hopping Hamiltonian with rational flux $p/q$ per unit cell, where both $p$ and $q$ are integers. We present the spectrum of the Harper equation and the Hofstadter butterfly, analyze its symmetries, and show the presence of an index theorem that guarantees the existence of Dirac fermions. To obtain the Chern number of the bands, we perform the explicit calculation of the Hall conductance, starting from the anisotropic 1-D limit, and analyze the gap openings upon reducing the amount of anisotropy to make the system 2-dimensional. We then prove the equivalence of this method with the Diophantine equation method, which allows for the determination of the Hall conductance through simple methods. All these were bulk calculations, but in chapter 6 we begin to investigate the intimate relationship between Hall conductance and edge modes. We present the bulk-edge correspondence, Laughlin's gauge argument, and the transfer matrix method for calculating the edge modes and the bulk bands of a system with open boundary conditions in an applied magnetic field.

In chapter 7, we start the discussion of graphene, a single layer of carbon atoms in a hexagonal lattice, which has created a tremendous amount of research in the past few years. We analyze the symmetries of the graphene lattice and show that the local stability of the Dirac nodes present in this material is guaranteed by TR and inversion symmetries. We then show that these Dirac nodes are also influenced by the $C_3$ symmetry present in the hexagonal lattice. This symmetry forces the Dirac nodes to stay at particular points in the BZ and makes them globally stable. We then move to analyzing graphene in an open-boundary geometry and show that the system has edge modes, even though it is not a bulk insulator but a semimetal. We show the different possibilities for the evolution of these edge modes when the system opens a gap and argue for the existence of topological insulators on simple, physical grounds, purely on the basis of the existence of these edge modes.

In chapter 8, we start the presentation of the simplest topological insulator, the Chern insulator, in two spatial dimensions. This insulator has a phase that exhibits a nonzero Hall conductance, so it breaks TR symmetry without having a net magnetic flux per unit cell (quantum Hall with zero applied field). We derive the physics of this insulator by looking at the physics of the closing and reopening of the Dirac fermion gap at points in the BZ. We analyze the behavior of the Berry potential on the lattice and point out, through an explicit calculation, the absence of a smooth gauge in cases where the Chern number does not vanish. We present Haldane's model of a Chern insulator on the graphene lattice and analyze its properties. We then end the chapter with an analysis of the physical properties of a Chern insulator in a magnetic field and of the edge modes that appear in a mass domain wall of the Dirac equation.

In chapter 9 we begin the subject of TR topological insulators by presenting the Kane and Mele model—the first model exhibiting such phase in two space dimensions. We analyze its symmetries and show that, in its simplest form, it is equivalent to two copies of Haldane's Chern insulator, for spin ↑ and spin ↓ with opposite Chern numbers. We then couple the two spins and show that the topological phase survives perturbations. We physically argue that there are two types of TR-invariant topological insulators, differentiated by the number of pairs of edge modes that they consider. If the number of pairs of edge states is odd, the topological phase is protected against small perturbations, whereas if the number of pairs is even, the insulator is not protected against perturbations and is adiabatically connected to a trivial one. We end the chapter by presenting the theoretical model and experimental predictions for mercury telluride (HgTe) quantum wells, which is the first experimentally observed topological insulator.

Chapter 10 is devoted to the introduction of $Z_2$ invariants for TR-invariant topological insulators. These invariants are used to characterize whether a TR-insulator is a nontrivial topological or a trivial one. There exist several equivalent formulations of these invariants in two dimensions. We adopt a chronological viewpoint and first present the initial invariants before moving to the modern description of the $Z_2$ invariant through sewing matrices. We introduce and expand on the modern theory of charge polarization (used to define the Chern number) before presenting its generalization to the theory of TR polarization used to define the $Z_2$ invariant. We show the intimate link between the TR polarization and the presence of pairs of edge modes and physically define the 2-D topological insulator even in the presence of interactions. We show that a trivial generalization of the $Z_2$ invariant from two to three dimensions allows us to define a 3-D topological insulator class of materials.

In chapter 11, we show how to understand topological insulators through simple band-crossing arguments in different dimensions. We supplement the Wigner–von Neumann classification of degeneracies with requirements such as TR and inversion symmetry and show how a trivial insulator can be transformed into a nontrivial one through a series of gap-closing-and-reopening transitions.

In chapter 12, we analyze insulators with inversion symmetry, with and without time reversal. When both inversion and TR symmetry are present, we give a simple expression of the $Z_2$ invariant, which can and has been used extensively to distinguish nontrivial topological insulators.

In chapter 13, we start analyzing the field theory of topological insulators by the procedure of dimensional reduction. We show that integer quantum Hall effects (Chern insulators) exist in any even space dimension, derive their response to magnetic and electric fields, and show that they are classified by an integer called $n$th Chern number, where $n$ is an integer. We relate their response to electromagnetic fields with the existence of gapless surface states.

In chapter 14, we show how, by dimensional reduction, the 3-D TR-invariant topological insulator can be obtained from a four-space-dimensional topological insulator. We obtain the field theory of three-space-dimensional topological insulators and show that they can be described by a magnetoelectric polarization—the generalization to 3 space dimensions of the 1-D charge polarization. We analyze the magnetoelectric polarization and show that in the presence of TR symmetry (or inversion), it can be quantized to take two values.

In chapter 15, we discuss several experimental predictions of the physics of the topological insulators.

In chapter 16, we introduce the concept of topological superconductors via standard models of spinless fermions in 1 and 2 dimensions with $p$-wave superconductivity. These superconductors exhibit topological states that are stable even without conserving any special symmetries. These superconductors have unique properties, one example being the non-Abelian statistics of vortices in the 2-D chiral topological superconductor.

In chapter 17 we move on to study topological superconductors, which require time-reversal symmetry to be stable. These states are similar in nature to the 2-D quantum-spin Hall effect and the 3-D strong topological insulator discussed in the earlier chapters, but with some notable differences. Perhaps the most interesting distinction is that the 3-D superconductor states are classified by an integer instead of a $Z_2$ quantity, as in the insulator case.

Finally, in chapter 18, we capitalize on all the previous discussions to show how hybrid topological insulator and superconductor states can be created from time-reversal invariant topological insulators in proximity to magnets, superconductors, or both. Such composite structures lead to experimentally viable proposals to create exotic phenomena, such as Majorana fermion-bound states (the simplest non-Abelian anyon).

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