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Quantum Spin Hall Effect and Topological Insulators

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Topological insulators (TIs), which exist in two and three dimensions, represent a new electronic phase stemming from the topological character of the bulk wave functions of certain materials and compounds. Unlike most other electronic states of matter, topological insulating phases were first proposed theoretically and then observed experimentally, although they can be found in highly common semiconductors and thermoelectric materials. These phases can emerge as a result of spin–orbit interaction and can be described within the framework of the band theory of solids. They manifest in the electronic structure of TIs, which are insulating in the bulk but conducting at their boundaries. The corresponding boundary states are protected by time-reversal symmetry (TRS) and the carriers at these states arrange in such a way that there is spin-momentum locking, that is, the direction towards which the carriers are traveling determines univocally the direction of the spin, thus resulting in intrinsic spin currents (see Chapter 2).

In the past, electronic phases have been classified, for example, as insulating, conducting, magnetic, or superconducting. In 1980, the integer quantum Hall (QH) phase was discovered [1], and it was quickly realized that it was topologically distinct from other electronic phases studied before, leading to a new classification paradigm based on the notion of topology [2]. The description using topological invariants readily showed that the QH conductance can take only precise values that are integers of e^2/h, thus imposing a severe constraint on the motion of the charge carriers. Such conductance quantization was later predicted for the spin degree of freedom in 2D TIs (Chapters 2 and 3). Indeed, TIs in two dimensions are closely related to the integer QH phase: they can be viewed as two superimposed QH phases in which the spin–orbit interaction takes the role of an effective magnetic field that acts in opposite directions for opposite spins. For this reason, 2D TIs are also described as a *quantum spin Hall* (QSH) phase and, in contrast to the QH phase, which is observed only when a strong magnetic field is applied, QSH phases (and in general all TIs) exist in the absence of a magnetic field, where TRS is preserved.

Historically, the QSH phenomenon was first described in graphene in a seminal paper by Kane and Mele [3] shortly after graphene caught the attention of the

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scientific community following the first transport experiments in 2004, via exfoliation of graphite, and the measurement of the QH effect in 2005 [4]. This first proposal for the existence of a QSH state followed an earlier model for graphene introduced by F.D.M. Haldane [5], where a periodic magnetic field with no net flux led to a quantized Hall effect. The Kane–Mele model [3] indeed describes two copies of the (spin-less) Haldane model such that spin-up electrons exhibit a chiral integer QH effect while spin-down electrons exhibit an anti-chiral integer QH effect. The QSH effect shows a quantized spin-Hall conductance and a vanishing charge-Hall conductance, although the conductance is not strictly quantized because the spin is usually not a conserved quantity in a real experimental system (see Chapter 3). Additionally, the degree of spin polarization is susceptible to disorder [6].

A very important point was the understanding that the QSH phase is nontrivial. In that context, Kane and Mele further introduced a topological Z_2-invariant which characterizes a state as a trivial or nontrivial band insulator [7]. Further studies of the robustness of the formed edge state proved both analytically and numerically that the nontrivial state is robust to both weak interactions [8] and the extra spin–orbit coupling terms that mix spin-up and spin-down electrons.

Although since its discovery graphene has demonstrated outstanding electrical, thermal, and mechanical properties [9, 10], as well as very long spin diffusion lengths in the high-temperature regime [11, 12], it was not graphene in which the QSH effect was first measured. Unfortunately, at temperatures achievable with today's technologies, the formation of spin-polarized counterpropagating currents at opposite edges of a clean graphene (ribbon) is out of experimental reach, owing to the vanishingly weak spin–orbit coupling in the order of microelectronvolts. The deposition of certain types of heavy atoms (such as thallium and indium) onto graphene could be a means of considerably enhancing local spin–orbit coupling and thus improving the observability of the topological phase [13–15] – a result that has triggered intense activity but still posing important challenges [16, 17].

To overcome the limitations imposed by the low spin–orbit interaction in graphene, the QSH phase was early on proposed by Bernevig and Zhang in intricate strain architecture promoted by strong spin–orbit coupling [18]. Bernevig, Hughes, and Zhang (BHZ) further suggested another model of TIs, which was easier to achieve experimentally, through the design of cadmium telluride/mercury telluride/cadmium telluride (CdTe/HgTe/CdTe) quantum wells in which a thin (~7 nm) sheet of HgTe is sandwiched between two sheets of CdTe [19]. The known inverted band structure in HgTe combined with confinement to open a gap in it resulted in the prediction of edge channels with quantized conductance, which were subsequently identified by the group of L. W. Molenkamp [20] through transport measurements (Figure 1.1). These measurements sparked considerable excitement and strongly increased the attention on this new class of materials. These developments, together with studies on other quantum well structures, are presented in Chapter 3.

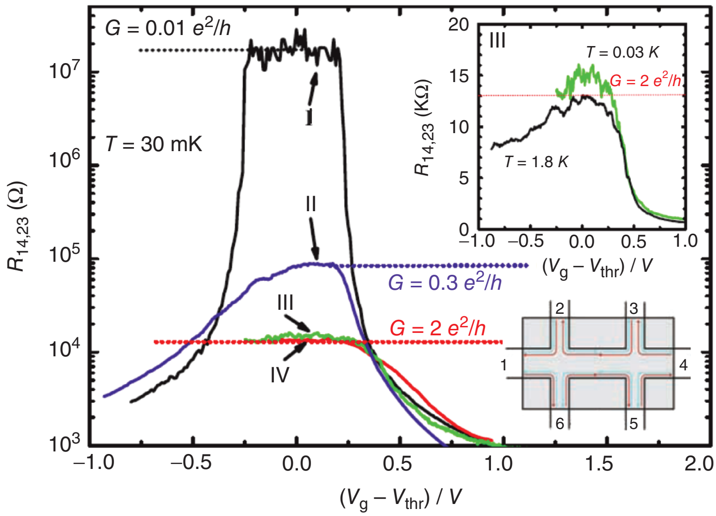

Figure 1.1 Longitudinal resistance of CdTe/HgTe/CdTe quantum wells of varying quantum well thickness showing conductance quantization of $G = 2e^2/h$ in the bulk gap region for samples in the topological nontrivial phase (for details please refer to Chapter 3).

In 2007, 3D bulk solids of binary compounds involving bismuth were predicted to belong to the TIs family [21]. The first experimentally realized 3D TI state was then discovered in bismuth antimonide [22], and shortly afterward in pure antimony, bismuth selenide, bismuth telluride, and antimony telluride using angle-resolved photoemission spectroscopy (ARPES) (see Chapters 4 and 8). The band structure and the absence of backscattering have also been reported with scanning tunneling microscopy and spectroscopy (see Chapter 9).

Three-dimensional TIs have several attributes in common with graphene, such as their low-energy electronic properties dominated by massless Dirac Fermion excitations, where the energy dispersion relations are described by a Dirac cone (see illustration in Figure 1.2). Differences lie in the parity of the number of Dirac cones emerging at surfaces and the spin–orbit interaction and TRS present in TIs, which result in the spin-momentum locking property, whereas clean graphene exhibits a pseudospin-momentum locking not related to TRS but with the internal symmetry of the honeycomb lattice.

The massless Dirac electronic structure allows an effective description in terms of the Dirac equation which identically writes as $v_F\ \boldsymbol{\sigma}.\mathbf{p}$, where $\boldsymbol{\sigma}$ is the vector of Pauli matrices related to the pseudospin quantum degree of freedom for graphene and the spin degree of freedom for TIs. For TIs, the spin vector always points in the $+\pi/2$ phase-shifted direction with respect to the momentum direction. As a result of such symmetry relation, a π-Berry's phase is obtained when rotating the wave function around the Dirac cone, and carriers are spin-polarized, mostly lying in the plane (see Figure 1.3).

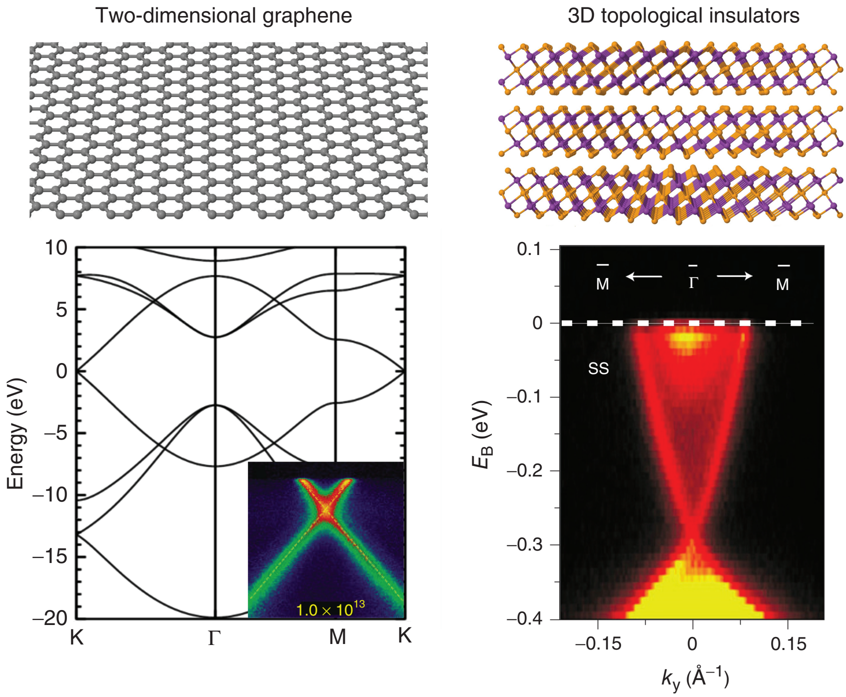

Figure 1.2 Ball-and-stick models of graphene and three dimensional topological insulators, together with energy dispersion relation in vicinity of charge neutrality point, exhibiting Dirac cone structures (Graphene ARPES from [54] TI ARPES from [55]). Reprinted by permission from Macmillan Publishers Ltd, copyright (2009).

Such Berry-phase effects are also studied in relation to the quantum anomalous Hall effect (QAHE), which is a manifestation of the above-mentioned QH physics in absence of external magnetic fields. This is of particular interest because it could be useful to exploit such transport phenomena in applications without the need to produce high magnetic fields. Here, TIs are believed to play a major role (see Chapter 14).

Many semiconductors within the large family of Heusler materials are now believed to exhibit topological surface states [23–25]. Unlike graphene, where the Fermi level ideally coincides with the Dirac point, this is not necessarily the case for 3D TIs. In some of these materials, the Fermi level falls in either the conduction band or the valence band, and its position can strongly vary because of naturally occurring defects. Therefore, the carrier concentration must be controlled via gating or doping to tune the Fermi level into the bulk bandgap [26, 27]. This limitation has triggered an intense search for clean TIs with the Fermi level occurring in the gap. The experimental characterization of such materials using molecular beam epitaxy, modified Bridgman techniques, and vapor- or solid-phase growth is described in Chapters 10–12, respectively.

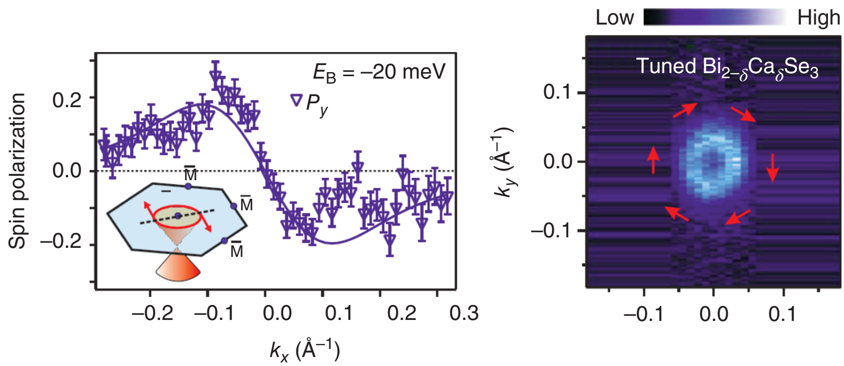

Figure 1.3 ARPES data from Bi2Se3. Spin polarization showing spin-momentum locking effect (from [56]). Reprinted by permission from Macmillan Publishers Ltd, copyright (2009).

The first results and confirmation of the existence of TIs generated great excitement; nevertheless, the dynamical aspects driven by spin–orbit coupling at the surface states remain largely unknown. The material quality of exfoliated or epitaxial grown TIs remains insufficient to avoid the dominant bulk states that severely complicate conventional transport measurements. The 3D TIs studied so far do not truly insulate [28, 29], and just a few transport experiments [30–34] have revealed convincing signatures of the exotic surface states, albeit indirect (see also Chapter 13). Besides, the surface states seem to be strongly sensitive to (optical) phonon modes, limiting the use of the material to relatively low bias and temperatures [35]. These effects underscore the importance of studying nanostructures to minimize the effect of the bulk carriers (see Chapter 11). Transport characterization of the most common materials is described in Chapters 3 and 10–12.

The quest for novel realizations of topological insulating phases is also driven by *ab initio* simulations of candidate materials. The small bulk bandgaps and associated energy scales (0.3 eV and smaller) demand high-quality theoretical predictions, as an incorrect description of the electronic structure might lead to an incorrect assignment to one phase or the other. Three chapters in this book (Chapters 5–7) are devoted to state-of-the art electronic structure theory and simulation comparing different approaches from density functional theory to many-body perturbation theory with the aim to be quantitative on such energy scales. The description of the spin–orbit coupling and the topological properties are central to these chapters. Nevertheless, many conceptual and technical hurdles will have to be overcome or circumvented, not least of which is the fact that, because chemical and structural modification of these materials destroy their “ideal” properties, the resulting modified forms are too complex to be studied by current theoretical methods. Thus, a more realistic approach is needed to model the essential physics of these complex and disordered materials, including descriptions of their spin transport and spin relaxation mechanisms, together with studies on the feasibility of controlled spin manipulation by external fields.

Despite all the unknowns, the world of TIs, with an insulating bulk phase together with robust conducting surface states, is clearly providing a fascinating class of new materials opening new horizons for harvesting the spin degree of freedom in future information processing technologies. Spin-polarized ARPES experiments have unambiguously confirmed peculiar spin-polarization features and, similar to graphene, spectroscopy has also confirmed that surface states of TIs are characterized by Dirac cones that dominate their low-energy excitation physics. The spin textures of TIs could be also used and tuned to design spintronics devices, including spin filtering, spin control, and magnetic recording technologies. Indeed, very large spin torques have been reported in bilayer TI/ferromagnet (FM) [36, 37], a promising result for memory devices. Advances in this field could pave the way to low power consumption as well as all-spin-based information processing technology with capabilities ranging from replacing conventional electronics to disruptive quantum computing. They could also lead to flexible electronic [38], nonlinear optical, and efficient thermoelectric materials. Several TIs are known for their thermoelectric properties, with some of the highest figures of merit [39]. Properly engineering the surface states to control heat and thermal transport independently might be a route to enhancing their efficiency [40].

Some of the challenges driven by spin manipulation in graphene and TIs (using external gating, laser illumination, or other means) could form the basis of new fields of research. Several possibilities for generating photoinduced bandgaps in graphene and the formation of states akin to those of TIs have been proposed theoretically, opening another field of research in which light illumination becomes an intriguing enabling tool to switch on and off the formation of the topological state [41–44]. Recently, a new type of QSH phase was proposed and discovered in graphene subjected to a very large magnetic field (tilted with respect to its surface) [45]. Unlike the case where TRS is preserved, such QSH phase is found to be protected by a spin-rotation symmetry that emerges as electron spins are polarized by the large in-plane magnetic field in a half-filled Landau level.

The discovery of TIs has also triggered fundamental questions regarding realizations of other topological phases in gapped systems, for example, topological crystalline insulators [46–50] or topological superconductors [51, 52]. Among other fundamental aspects, the observation of Majorana fermions (see Chapter 15) or magnetic monopoles in TIs covered by a thin ferromagnet and axion electrodynamics [53] are also important drivers in this nascent field.

To progress in this quest, the description of the foundations of the field of TIs is necessary. The aim of this book is to provide an overview of today's knowledge of this exciting field, pointing out to the frontline advances in experimental and theoretical studies, as well as perspectives for further work.

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