Functional spin textures in novel materials

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Introduction

The question on how much technology and computational power our society needs is one that is best answered in abroad public debate, or over a good glass of wine. However, regardless of the outcome of such a discussion, the need for more efficient technology is self-evident. Lower power consumption of computing systems can have a significant impact on the world wide energy usage, but more importantly it will increase the lifetime of stand-alone solutions.

However, more efficient does not only mean lower power consumption, it also has other aspects. Other goals are to increase the speed, reduce the size, allow for extra flexibility beyond the binary system, and to replicate, or at least understand, the immense parallel processing capability of the human brain.

A promising pathway to achieve these goals lies in the field of *spintronics*. In this novel electronics design the goal is to use the spin, i.e. the intrinsic magnetic moment, of the electron rather than its charge. The main advantage is that a spin state can be transported without necessarily moving the charge. For logic, or computational, elements this field is still under development and more work is required. On the other hand, for data storage the use of spintronics principles has greatly enhanced the storage density and efficiency. This is based on the giant magneto resistance (GMR) effect discovered independently by Albert Fert and Peter Grünberg, for which they received the 2007 Nobel prize.

There are two main pathways to achieve spintronics applications, and any final application will probably rely on a combination of both. The first is based on magnetic materials, and the other on materials with large spin-orbit interaction (SOI). The advantage of magnetic materials is that this is based on a well established field with enormous amounts of experience. The disadvantage is that magnetic fields are non-local and changes are relatively slow. The study of systems with large SOI is, on the other hand, relatively new, but rapidly expanding. The advantage lies in the fact that SOI is local and instantaneous.

In either case novel materials are needed and my main contribution to the field lies in the role I played in the discovery of one class and the increased understanding of another class with functional large SOI properties. These two material classes are *topological insulators* and *Rashba systems*. In the following they will be shortly introduced and our main findings will be indicated.

This text is not meant as a scientific manuscript and therefore lacks proper referencing. More information, including well referenced articles and review articles, can be found on sois.epfl.ch. If necessary I would also be happy to guide any reader to more appropriate scientific literature. Furthermore, in the discussion many concepts are introduced in a non-rigourous way, and should thus be used to replace a proper scientific discussion. Most importantly this text inherently fails to acknowledge the crucial contribution of a large number of excellent scientist working in the field. This in no way reflects any lack of appreciation for the great work many people have done.

Topological Insulators

Currently the study of topological phases and their spin structure is one of the hottest topics in condensed matter physics and I am proud to say that we stood at the basis of this field. The main reasons for this interest is that topological insulators (TI) form in a sense a new phase of matter, which in turn has very peculiar spin properties.

Topology is the study similarities and differences between objects, but to fully appreciate the properties of TIs and the physics behind them, it is useful to start from the origin of the study of topology. Many argue that the basis of the study of topology lies in the Köningsberg bridge problem. The question was whether it was possible to cross all bridges of the city, and cross them only once, and return to the same place. In 1736 Leonhard Euler showed that whether this is possible does not depend on the starting

place or where the bridges lie, but only on whether there is any part of the city which has an odd number of bridges connecting it with the rest of the city. If this is the case a so-called Euler route is not possible, but if every part of the city has an even number of bridges the closed path is possible. This allows us to classify all cities into two distinct topological classes based on the number of bridges. Exactly the same can be done for materials as will be explained below.

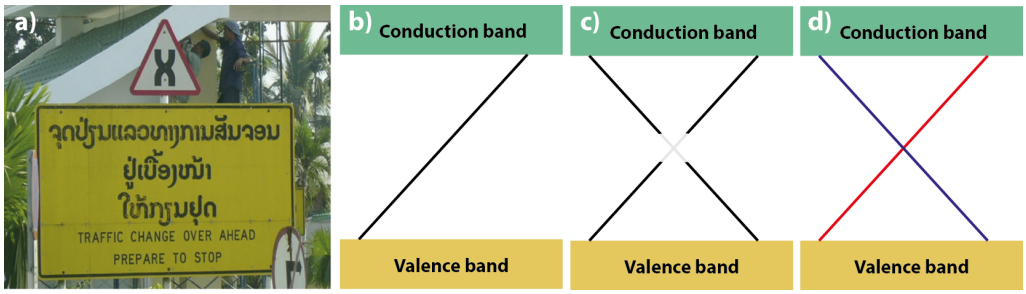

Figure 1: Illustration of the required band structure to form a topologically protected state. Only if the states are spin polarised as in d) they are protected from opening a gap.

Part of the definition of different topological classes, be it cities, knots, or rubber band versus Mbius strip, is that it is not possible to smoothly transform one class into another. This transformation can only be achieved by some drastic measure that changes the symmetry of the system, or by going through a singularity. What such a singularity can look like when changing from the pseudo-topological class of left-hand to right-hand traffic is illustrated in Figure 1a).

So what does this have to do with special materials and spin? In any material the energy levels are determined first by the atomic levels of the elements in the material, then by the formation of bonds between these elements, then by the formation of bands in a crystal, and finally by the the spin-orbit interaction. At each of these steps the energy levels shift up or down depending on their parity and symmetry. If we now look at the Fermi level (the highest occupied energy in a material) and count the number of parity inversions throughout the whole of momentum space, this can either be even or odd, whereby zero is considered even.

The spin-orbit interaction will furthermore cause a hybridisation of states, opening up an energy gap whenever two states meet. Combined with the odd number off crossings of the Fermi level this causes a SOI-induced gap rendering the material an insulator.

Similar to the case of the number of bridges above, this allows us to distinguish all materials into two distinct topological classes. One with an even number of parity inversions ($\nu = 0$) and one with an odds number of parity inversions ($\nu = 1$). The latter defines the so-called $\mathbb{Z}_2$ topological insulator class.

At the interface of materials with different topology of their band structure, the electronic structure will have to go through a singularity to connect the two systems. Such a singularity results in a state which must exist at the interface, which is referred to as topological protection. The question now arises how this topological protection is reflected in the electronic structure of the interface. To make sure the state crosses the gap level, and its existence is thus guaranteed, it needs at least to reach from the valence to the conduction band as illustrated in Figure 1b). However, in this case the symmetry parallel to the interface appears broken, and it thus can't be the correct solution. Therefore we need to include a second band that is a mirror image of the first one around the Brillouin zone centre (Figure 1c)). But now the two bands would be able to hybridise and open up a gap, therefore lifting the protection. The only way to resolve this is by requiring that the bands have opposite spin polarisation (Figure 1d)). In this case time reversal symmetry, $E(k,\uparrow) = E(-k,\downarrow)$, dictates that the bands have to cross at zero momentum and thus a gap can't open up.

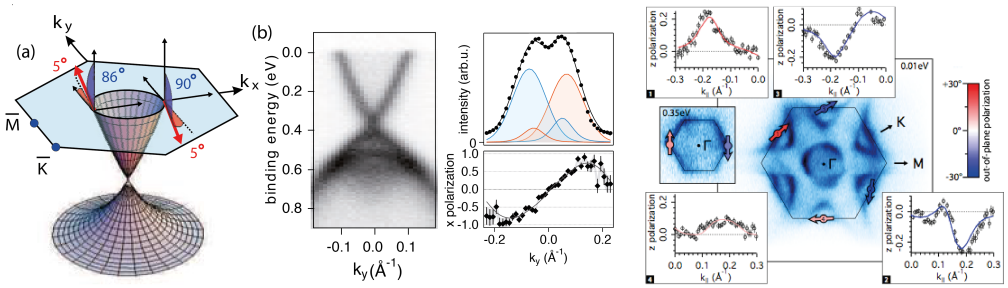

Figure 2: Schematic drawing and experimental results for some representative topological insulators.

Although bands can be spin-polarised for different reasons, this means that the details of the spin texture are the ultimate means to identify a topological insulator. To be more precise, there needs to be an odd number of spin-polarised states encircling so-called time-reversal invariant momenta. Thus measuring the number of spin polarised states is the true, and at that moment, only proof a material is a topological insulator. We were the first

in the world to perform these measurements and thus identify a TI, and the results are reproduced in Figure 2 for a variety of materials.

These results explain the topological protection mechanism in reciprocal space, but they don't explain what happens in real space. In order to explore this we took a closer look at $TlBiSe_2$, which we had previously identified as a topological insulator. For this material all possible theory approaches predicted also the existence of trivial, unprotected, surface states besides the topologically protected surface states. However, in no experiment these trivial states were observed. By looking at the surface structure on an atomic level we could determine that the top layer of the crystal has become too disordered by the cleaving process to host any dispersing states. This suppresses the trivial surface states, but the topological state shifts away from the disordered surface more into the bulk of the crystal.

The explanation for this behaviour is rather simple. The disordered or damaged surface becomes topologically trivial ($\nu = 0$) and the interface between the two topologies thus shifts down. We have been able to verify this for other samples where by sputtering we could change the topology of the top layer.

Rashba systems

Although topological insulators have very promising spin properties, the currently known topological phases consist of materials which are not easy to handle. An important alternative is provided by the so-called Rashba effect. This effect primarily relies on broken symmetry and can in principle be induced in any material.

In a simple picture the effect can be explained as follows. Any unidirectional symmetry breaking is on a microscopic level associated by a potential gradient. In the rest frame of an electron moving perpendicular to the related electric field, this field is transformed into a magnetic field. The magnitude and direction of this field directly depends on the momentum of the electron. In the magnetic field the energy levels of the electron state undergo a Zeeman splitting thus lifting the spin degeneracy. The resulting spin-resolved electronic structure is illustrated in Figure 3a).

If an electron with a given spin is injected in such a Rashba system, it's spinor will be decomposed in a coherent superposition of the spin eigenstates in the Rashba material. Because these states have a different momentum at the Fermi energy, a phase difference will occur between them for the moving spin state. After a certain distance a coherent summation of the

spinors will then result in a rotated spin orientation. Therefore the Rashba system can be used to rotate and manipulate spin states.

The above mentioned model is qualitatively correct, but quantitatively fails to reproduce observations by several orders of magnitude. It was already early on realised that one has to consider the atomic contribution to the potential gradient, and that thus spin-orbit interaction becomes the most important driving force. We performed spin-sensitive measurements on a variety of model systems to pin down all the possible influences. This lead us to realise that one of the most important aspects is the atomic corrugation and the consequent shift of the wave function away from the core.

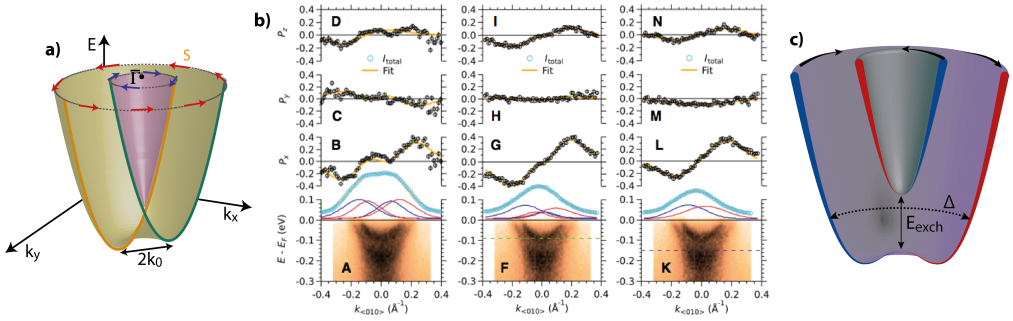

Figure 3: a) General electronic structure of a Rashba system. b) Experimental results for the 2DEG on the surface of $SrTiO_3$. c) Electronic structure of a Rashba system combined with magnetic order.

All these model systems had their problems for application because of a large metallic influence of spin degenerate states. However, the lessons learned from this allowed us to apply the same principle to insulating oxides. In $SrTiO_3$, a transparent wide band gap insulator, a structural rearrangement at the surface induces a two-dimensional electron gas (2DEG) there. The corrugation induced by this rearrangement is so large as to induce a large Rashba-type spin splitting in these states as shown in Figure 3b).

This giant spin splitting of a metallic state on a insulating background already has far reaching prospects for applications, but there is another feature in this system that makes it even more appealing. The atomic configuration at the surface of $SrTiO_3$ creates a magnetic order with an energy scale smaller than the spin-orbit interaction. This causes the opening of a gap at zero momentum as illustrated in Figure 3c). When the chemical potential is tuned inside this gap, which is easy because of the insulating

nature of bulk $SrTiO_3$, there is only one spin polarised Fermi contour, similar to what is found in topological insulators. Adding to this the fact that $SrTiO_3$ becomes superconducting at a temperature of 250 mK, this system combines all the properties for the formation of Majorana fermions.

Majorana fermions are fermions which are their own anti-particle and as such are intrinsically in a superposition of both states. This makes them an ideal candidate for qubits, the building blocks of a quantum computer. Up to now signatures of Majorana fermions have only been found in artificial structures that combine the SOI, magnetism, and superconductivity separately, with only very limited flexibility. The advantage of our finding is that it should be possible to etch nanostructures designed for manipulating Majorana fermions and showing their non-abelian statistics.

Outlook

The research presented here is of fundamental character and the application of any findings in everyday life is dependent on many factors. However, it shows that materials with suitable spintronics properties can be found by carefully considering what causes the required spin textures. Our current research aims at making these properties easily tuneable, one of the main requirements for any application.

Furthermore, new topological phases are currently being predicted each with more fascinating properties than the previous ones. This indicates that materials with novel spin properties are now within reach and can play an important role in future electronics.