11 Condensed matter theory group

Titus Neupert, Ashley Cook, Seulgi Ok, and Frank Schindler

The condensed matter theory group studies topological phenomena in electronic systems. Numerical and analytical tools are used to model phases of matter and understand their unique physical properties. The term topology refers to a field of mathematics that is concerned with the relations of objects to each other if one allows for smooth deformations of these objects. Objects that can be transformed into each other by smooth deformations are said to be topologically equivalent. For example, one can smoothly deform a donut into a coffeecup but not a donut into a muffin. Thus a donut and a muffin are topologically different. Applying the same concepts to phases of quantum matter yields phenomena that are universal and surprisingly robust to perturbations. They are often related to measurable observables which are universally quantized, such as the Hall conductivity in the integer quantum Hall effect.

Topological systems can be strongly interacting, in which case we are often interested in phenomena related to so-called topological orders. Topologically ordered phases of matter are best understood in quasi two-dimensional systems with an energy gap at zero temperature, and are characterized by emergent fractionalized excitations. These so-called anyons could be used in future quantum computing devices. Our research group is mostly interested in a conceptual understanding of topological order and its generalization, for example to three dimensions. One of the projects completed this year [1] is concerned with possible phase transitions in topologically ordered states with anyonic excitations. In particular we showed that in many cases anyons with bosonic self-statistics cannot undergo a Bose-Einstein condensation transition. This results hints at a certain phase stability of states with uncondensable bosons.

We also study weakly or non-interacting systems, in which case interesting topological phenomena result from the band theory of solids. Such topological band characterizations were first discovered for insulating systems. The classic example in this category is the integer quantum Hall effect with its quantized topological Hall conductivity. It was recently joined by time-reversal symmetric insulators with topological properties. All of these systems are defined by the existence of boundary modes which cannot be removed by boundary perturbations that respect the symmetries protecting the topological character, such as time-reversal symmetry. Time-reversal symmetric topological insulators exist in two and three spatial dimensions and are characterized by a single Kramers pair of edge modes and a single, non-degenerate Dirac surface state, respectively.

More recently, the notion of topological band structures was extended from insulators to metals and semimetals. This direction of research characterizes symmetry-protected degeneracies in momentum space by topological numbers, showing that they are generic and can be robust against a large class of perturbations. The degeneracies can be point-like, giving rise to so-called Weyl or Dirac semimetals, or line-like, resulting in so-called nodal-line semimetals. Below we discuss in more detail a project [2] which defined a new class of such topological semimetals.

We have also entertained a series of experimental collaborations over the last year [3], [4], [5], of which the study of spin-polarized channels on the surface step edges of a so-called crystalline topological insulator stands out [5]. These one-dimensional edge channels are well localized, extremely robust against disorder, elevated temperatures, and magnetic fields.

[1] T. Neupert *et al.*, *No-Go Theorem for Boson Condensation in Topologically Ordered Quantum Liquids*, New Journal of Physics **18**, 123009 (2016).

[2] L. Muechler, A. Alexandradinata, T. Neupert, R. Car, *Topological Nonsymmorphic Metals from Band Inversion*, Phys. Rev. X **6**, 041069 (2016).

[3] D. Sutter *et al.*, *Hallmarks of Hund's coupling in the Mott insulator Ca_2RuO_4*, Nature Comm. (2017).

[4] P. K. Biswas *et al.*, *Suppression of magnetic excitations near the surface of the topological Kondo insulator SmB_6*, Phys. Rev. B **95**, 020410(R) (2016).

[5] P. Sessi *et al.*, *Robust spin-polarized midgap states at step edges of topological crystalline insulators*, Science **354**, 1269-1273 (2016).

[6] M. Laubach *et al.*, *Density wave instabilities and surface state evolution in interacting Weyl semimetals*, Phys. Rev. B **94**, 241102(R) (2016).

11.1 Nonsymmorphic topological metals

A large part of the activities in the condensed matter theory group was concerned with the exploration of new types of topological metals and semimetals over the past year. Topological metals display various intriguing physical properties, such as protected modes on the surface of the crystal and record-high changes in the resistivity when a magnetic field is applied ("titanic magnetoresistance") [7].

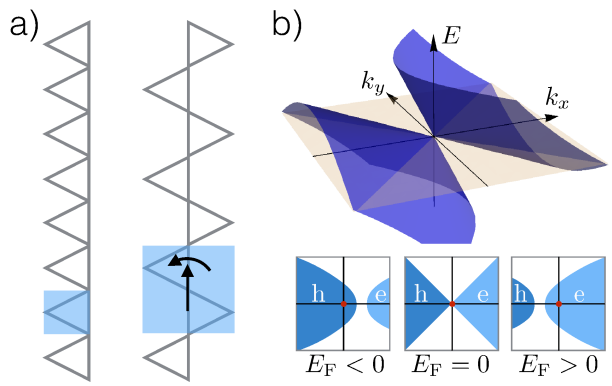

FIG. 11.1 – Nonsymmorphic semimetals. a) One-dimensional lattice with symmorphic (left) and nonsymmorphic (right) symmetry. The nonsymmorphic symmetry is a combination of translation and mirror reflection. b) Energy dispersion of a strongly Lorentz-violating Dirac fermion for which the velocity of both branches of the dispersion have the same sign for some direction of propagation. As a consequence, the Dirac point is a symmetry-protected touching point of a electron and a hole pocket (lower panels).

In a collaboration with researchers from Yale and Princeton, we proposed a new class of topological metals with a type of symmetry that is abundantly found in crystals, namely a nonsymmorphic symmetry [8]. This class of metals is topological in the sense of being robust to both deformations by the external environment, as well as to more microscopic deformations within the crystal itself.

A close look at the symmetries of a crystal, such as rotations, reflections, and translations, shows that crystals divide in two classes, called symmorphic and nonsymmorphic. Symmorphic crystals transform into themselves under discrete translations by the lattice period, rotations and reflections. Just as abundant in nature are nonsymmorphic crystals, which transform into themselves under symmetry operations that combine a rotation or a reflection with a translation by a fraction of the lattice period. As illustrated in Fig. 11.1 a), the left image has symmorphic symmetry, while the right image is nonsymmorphic, that is, under a reflection with respect to the horizontal bisecting line, combined with a translation by half the lattice period, the image returns to itself.

Nonsymmorphic symmetries lead to fundamentally different arrangements of the atoms in a crystal, which in turn have a profound influence on their electronic properties. Indeed, crystals with the nonsymmorphic symmetry of Fig. 11.1 a), and having an odd number of electrons per lattice period, are guaranteed to be metals [9]. For an even number of electrons, we find distinct phases of matter that exhibit either metallic or insulating behavior; a transition between an insulator and a metal is accompanied by a change in the symmetry properties. Such changes are discrete, in the sense of changing from one integer to another. In analogy to how there is no continuous way to change from integer into another, the metallic states of matter are profoundly robust and cannot easily be transformed into a different state of matter. Practically, these crystals are not as susceptible to impurities and defects as regular crystals, making them attractive candidates for electronic devices.

Using the language of topology, this new state is different from other electronic states that can exist in a nonsymmorphic crystal. In the present case it is the topology of the quantum-mechanical wavefunctions that distinguishes the electronic states. Electrons having the nonsymmorphic symmetry of Fig. 11.1 a) behave as if they had an additional degree of freedom that can only take two discrete values, analogous to the half-integer-spin degree of freedom in electrons. A unique property of spin, which has an analogy in the nonsymmorphic case, is that it does not return back to itself after a rotation of 360 degrees but only after a rotation of 720 degrees. This resembles walking around a Moebius strip, where one only returns to the starting point after going around the strip twice.

The theory was applied to the material WTe_2 which has garnered attention for its highly unusual resistivity under the effect of a magnetic field. Recent photoemission experiments have also shown that the electrons in WTe_2 absorb right-handed photons differently than they would left-handed photons. The theory that was formulated showed that these experiments on WTe_2 can be understood based on the topological properties of this new class of metals. The topologically protected band crossing in these nonsymmorphic semimetals is of the form of a Dirac cone, i.e., resembling that of massless relativistic electrons. Such an electronic structure is already known from atomically thin carbon layers, i.e., graphene. However, our study uncovered that the monolayer of WTe_2 realizes an interesting twist to this electronic structure, in that the velocity of the Dirac electrons becomes very anisotropic. This anisotropy is so strong that the velocities of the two branches of the Dirac cone have the same sign in one direction of space, while they have opposite signs in another as seen in Fig. 11.1 b). This forces the Dirac cone to 'tilt over' and can be seen as a strong breaking of Lorentz symmetry [10] – a situation distinct from the Lorentz symmetric Dirac cones in graphene, for example.

[7] A. N. Mazhar *et al.*, *Large, non-saturating magnetoresistance in WTe_2*, Nature **514** 205 (2014).

[8] L. Muechler, A. Alexandradinata, T. Neupert, R. Car, *Topological Nonsymmorphic Metals from Band Inversion*, Phys. Rev. X **6**, 041069 (2016).

[9] H. Watanabe *et al.*, *Filling-Enforced Gaplessness in Band Structures of the 230 Space Groups*, Phys. Rev. Lett. **117**, 096404.

[10] H. Watanabe *et al.*, *Type-II Weyl semimetals*, Nature **527** 495 (2015).

11.2 No go theorem for Bose-Einstein condensation of anyons

Topologically ordered states of matter are realized in quasi two-dimensional systems, such as the fractional quantum Hall effect. The zero-temperature ground state of such a system is a gapped quantum liquid, i.e., it is a completely featureless state. What is most interesting are the elementary excitations above this liquid ground state. One can construct localized excitations that have particle-like character and striking universal properties and can move freely in the liquid (one says they are deconfined). The excitations have fractionalized quantum numbers with respect to those of the constituent particles out of which the quantum liquid is made (electrons), for example by carrying a sharply defined fraction of the elementary charge. More important, however, are the fractionalized quantum-statistical properties of these excitations. Free particles in nature come only in two species, fermions and bosons, depending on whether the quantum mechanical wave function acquires a minus sign when two of these particles are interchanged. The fractionalized particles in topologically ordered systems can change the phase of the quantum mechanical wave function by any (rational) amount when transported around one another (Fig. 11.2 a). They are thus called anyons. Even more strikingly, such anyons can entirely change the quantum mechanical state of the system when transported around one another. If this is the case, they are called non-Abelian anyons. Physicists have envisioned building a particularly robust quantum computer based on these exotic properties of non-Abelian anyons [11].

Of all these quantum mechanical particles, bosons stand out by their ability to undergo a Bose-Einstein condensation: They can coherently appear in large numbers in a quantum system, driving it into a new phase [12, 13]. This effect has been shown in cold atomic gases, for example, and is closely related to the phenomenon of superconductivity.

Our study shows that not all bosons can undergo a Bose-Einstein condensation transition [14]. We proved a no-go theorem by which the condensation of classes of non-Abelian *bosons*, which appear as excitations in topologically ordered quantum liquids, is forbidden. This is relevant because Bose condensation is a common mechanism by which phase transitions between topologically ordered phases are driven (Fig. 11.2 b). Roughly speaking, the theorem states that if the amount of quantum information carried by the non-Abelian boson is smaller than the quantum information carried by the particles it can branch into after the condensation transition, there is an obstruction against its condensation.

An interesting application of our theorem applies to bosons that appear in so-called Fibonacci topological order, which is of particular interest to the aim of building a topological quantum computer. We show that Fibonacci topological order cannot undergo any type of condensation transition.

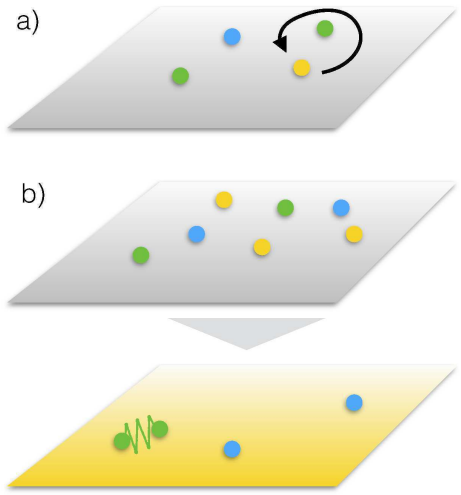

FIG. 11.2 – Two-dimensional topologically ordered states are characterized by several types of anyon quasiparticle excitations (colored dots). a) A key property of topologically ordered phases is that when anyons are adiabatically braided around one another, the quantum state of the entire system can change. b) A class of transitions between anyon theories can be described by the condensation of a bosonic anyon (here in yellow). The condensation changes the type of topological order, for instance by confining part of the anyons that are then not part of the low-energy excitations anymore, as depicted for the green anyon here.

This may point to a certain robustness of this topological order. More broadly, our results shed light on the rich mathematical structure behind topologically ordered states with anyons.

[11] C. Chamon, *et al. Topological Aspects of Condensed Matter Physics, Chapter 2*, Lecture Notes of the Les Houches Summer School: Volume 103, August 2014.

[12] F. A. Bais and J. K. Slingerland, *Condensate-induced transitions between topologically ordered phases*, Phys. Rev. B **79**, 045316 (2009).

[13] T. Neupert *et al. Boson condensation in topologically ordered quantum liquids*, Phys. Rev. B **93**, 115103 (2016).

[14] T. Neupert *et al. No-Go Theorem for Boson Condensation in Topologically Ordered Quantum Liquids*, New Journal of Physics **18**, 123009 (2016).

11.3 Spin-polarized step-edge states on the surface of topological crystalline insulators

Of the various collaborations that we have entertained with experimental groups, we want to highlight one that discovered a new type of one-dimensional conducting states on the surface of a very special crystal, as so-called topological crystalline insulator [15].

A topological crystalline insulator is an insulating three-dimensional crystal with gapless, i.e., conducting, electronic states on its surface. These surface states behave like relativistic Dirac electrons, just as in graphene, with the difference that they have a well-defined spin direction that is tied to their propagation direction (Fig. 11.3 b). The surface cannot be made insulating unless one breaks symmetries of the crystal such as certain mirror symmetries. In practice, these surface Dirac electrons are found to be a robust property of topological crystalline insulators, that is largely insensitive to imperfections of the surface [16].

Our experimental collaborators from the University of Wuerzburg, Germany, carefully examined the surface of the topological crystalline insulator (Pb,Sn)Se with a scanning-tunneling microscope and spectroscope. This device can resolve the topography and electronic structure of surfaces with atomic scale resolution and precision. Besides the expected surface states, they found one-dimensional conducting channels exactly at places of the surface where a step-edge is located. A step edge is the termination of extra layer(s) of atoms on the surface. Even more strikingly, these one-dimensional channels were only present if the step edge was an odd number of atomic layers thick (like one and three layers), while no extra states where found if the step was a even number of atomic layers high.

This systematic observation can be explained by the topological electronic structure of the surface, which can be seen as an exotic form of a Dirac semimetal [17]. In the rock salt lattice structure of (Pb,Sn)Se (the same structure as regular salt, NaCl, see Fig. 11.3 a), even and odd step edges can, when viewed from above, be distinguished as follows (see Fig. 11.3 c): For even steps, the lattice structure on either side looks exactly the same. For odd steps, the lattice structure on one side is translated by a fractional (half) lattice vector with respect to the other side. This fractional translation has nontrivial implications for the surface electronic states: The quantum mechanical wave functions acquire a nontrivial phase, so-called Berry phase, under such a translation. As a result the surface state Dirac electron wave functions cannot be phase-matched between both sides of the step edge everywhere. This interference or phase frustration results in the presence of extra electronic states which are bound to the step edge as observed in the experiment (Fig. 11.3 e).

The one dimensional channels bound to the odd step edges have remarkable properties. First, they seem to travel along the step edge almost unperturbed, i.e., with very little back scattering from impurities. Second, they are nearly dispersionless, meaning that they are found at the same energy independent of the momentum along the edge. Third, they were still observed at temperatures as high as 80 K and in magnetic fields of up to 11 T (the highest field accessible by the apparatus). Fourth, they are confined to a very narrow region of only about 10 nm. Together, these characteristics make them a promising platform to build electronics and quantum devices on the smallest scales.

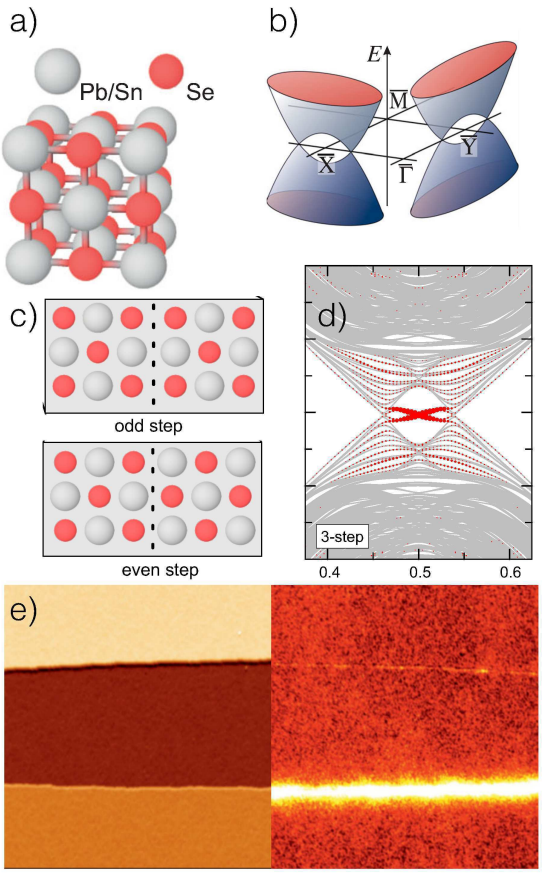

FIG. 11.3 – One-dimensional step-edge states on the surface of three-dimensional topological crystalline insulators. a) Rocksalt lattice structure of (Pb,Sn)Se. b) Four topologically protected non-spin-degenerate Dirac cones in the surface Brillouin zone of (Pb,Sn)Se. c) Difference between odd and even step edge when viewed from above. The lattice structure on the left and right of the odd step edge is related by a fractional lattice translation. d) Numerical simulation of the electronic structure of a three atoms high step edge (energy vs. momentum along the edge). Highlighted in red are the states localized along the step edge. e) Scanning tunneling microscope image of an even step edge (above) and an odd step edge (below). Left is the topography and right is the spectroscopy image, which clearly shows the one-dimensional channel bound to the odd step edge.

[15] P. Sessi *et al.*, *Robust spin-polarized midgap states at step edges of topological crystalline insulators*, Science **354**, 1269-1273 (2016).

[16] L. Fu, *Topological Crystalline Insulators*, Phys. Rev. B **106**, 106802 (2011).

[17] T. Hsieh *et al.*, *Topological crystalline insulators in the SnTe material class*, Nature Communications **3**, 982 (2012).