10 Condensed matter theory group

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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 interested in a conceptual understanding of topological order and its generalization, for example to three dimensions as well as in the question how such states can be realized and manipulated. One of the projects completed this year [1] is concerned with this latter problem: we pioneered the numerical study of heterostructures that combine a fractional quantum Hall state with a superconducting state. We showed that topological degrees of freedom emerge at the interface between the two. In another numerical study [2] we investigate the nature of phase transitions between two-dimensional topologically ordered states and trivial ones, relating them to accidental degeneracies in band structures.

The iconic model for strongly interacting phases of matter (topological or not) is the Hubbard model. Over the past year, we studied numerically its topological aspects [3]. In an experimental collaboration the effects of spin-orbit coupling for excitations of a Mott insulating state [4] were investigated.

We are also interested in 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 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 give rise to so-called Weyl or Dirac semimetals on which we have devoted a series of works over the past years. We highlight below one paper in which the annihilation of Weyl nodes is observed when the material is exposed to a strong magnetic field [5].

Finally, our research group is always interested in pioneering new methods to study phases of matter theoretically. An emergent direction in condensed matter physics is to employ machine learning algorithms in various contexts. We contributed to this effort with a study that uses an artificial neural network for phase classification based on numerical data [6], which we discuss in detail below.

[1] C. Repellin *et al.*, *Numerical investigation of gapped edge states in fractional quantum Hall-superconductor heterostructures*, npj Quantum Materials **3**, 14 (2018).

[2] S. Kourtis *et al.*, *Weyl-type topological phase transitions in fractional quantum Hall like systems*, Phys. Rev. B **96**, 205117 (2017).

[3] W.-L. Tu *et al.*, *Competing orders in the Hofstadter t-J model*, Phys. Rev. B **97**, 035154 (2017).

[4] L. Das *et al.*, *Spin-Orbital Excitations in Ca_2RuO_4 Revealed by Resonant Inelastic X-ray Scattering*, Phys. Rev. X **8**, 011048 (2018).

[5] C.-L. Zhang *et al.*, *Magnetic-tunnelling-induced Weyl node annihilation in TaP*, Nature Physics **13**, 979986 (2017).

[6] F. Schindler *et al.*, *Probing many-body localization with neural networks*, Phys. Rev. B **95**, 245134 (2017).

10.1 Simulation of parafermion heterostructures

While the fractional quantum Hall (FQH) effect remains of tremendous interest for realizing myriad phases ranging in complexity from Laughlin states all the way to states with non-Abelian quasiparticles such as Majorana fermions and Fibonacci anyons, experimental exploration of these systems has remained limited. The challenges are two-fold in experimentally confirming states with non-Abelian quasiparticles. First, these states can only be accessed under extreme experimental conditions, as they are protected by very small energy gaps. Second, the topological information is encoded in degenerate ground states or the state of quasiparticles, making it intrinsically hard to measure and manipulate.

To address these challenges, we undertook extensive numerical calculation of a FQH system that is coupled to a superconductor using exact diagonalization. More explicitly, we consider a bilayer FQH system, with magnetic field perpendicular to the layers, where the orientation of the field for one layer is opposite to that for the other layer, a construction that permits gapping out of the edge states with an interlayer superconducting pairing.

Our calculations are performed on a cylinder geometry in which the bilayer FQH droplet has two edges (Fig. 10.1). To make numerics feasible, we restricted our study to the subspace of zero energy bulk and edge excitations of the Laughlin $\nu = 1/3$ state in each layer. We find a three-fold ground state degeneracy of the gapped edge states, which can be understood as follows: By introducing a gap, the superconducting coupling turns the bilayer quantum Hall state with edges into a single-layer quantum Hall state on a manifold without boundary. This manifold is topologically equivalent to a torus, where the space between the two layers becomes the interior of the torus (Fig. 10.1 c)). On the torus, a Laughlin state at filling $\nu = 1/3$ has a three-fold ground state degeneracy, which is topologically equivalent to the three ground states we observe in the superconducting bilayer system.

As we demonstrate in this work, charge pumping can permute these ground states and provide evidence of their topological nature. Suppose we start with a state $|\Psi_0\rangle$ that has charge 0 on both edges. As unit ϕ_0 spin flux is adiabatically inserted, charge is transferred from the left to the right edge, so that the resulting state is $|\Psi_+\rangle$. The other ground states are expected to transform into one another analogously: $|\Psi_+\rangle \rightarrow |\Psi_-\rangle$, $|\Psi_-\rangle \rightarrow |\Psi_0\rangle$. Thus, after insertion of a quantum of spin flux, we expect to obtain a permutation of the three ground states.

To further support our claim that the heterostructure realizes the desired topological superconducting edges, we calculated the spectral flow that corresponds to the 6π Josephson effect. In the thermodynamic limit, in which the three ground states of interest are degenerate, the *ground state* of the system does not return to itself when φ is advanced by 2π. Rather, it evolves into another degenerate ground state and

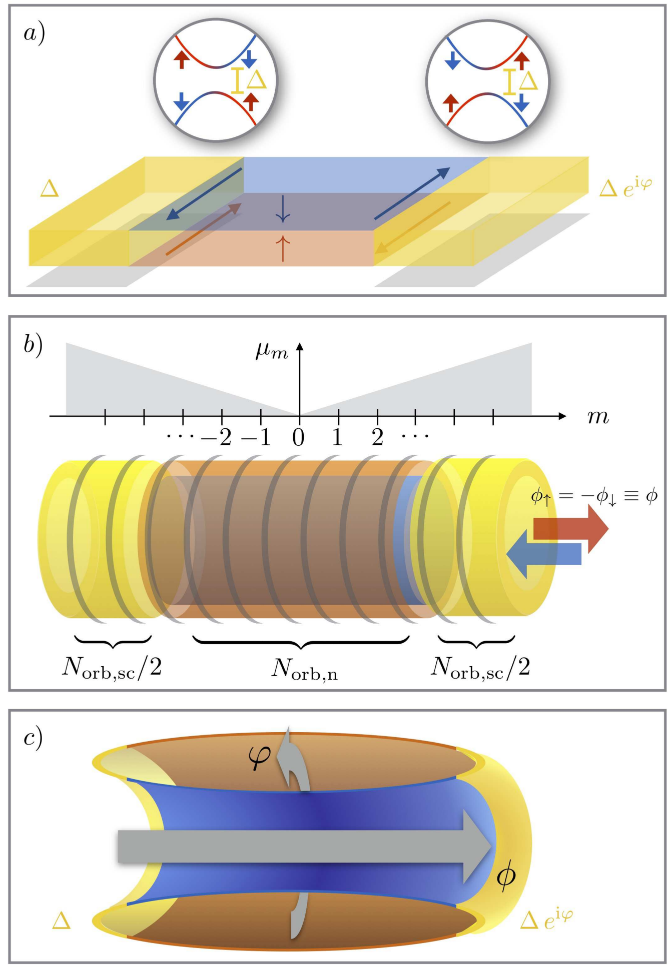

Fig. 10.1 – Schematics of the physical geometry and the one used for the numerical investigation.
a) Fractional topological insulator heterostructure in which carriers with spin up and down (red and blue) form a fractional quantum Hall state with opposite chirality. Proximity to superconducting reservoirs (yellow) induces a superconducting gap in their edge channels. To study the Josephson effect, arelative phase φ between the left and right superconducting order parameter is included.
b) When imposing periodic boundary conditions along the edges, resulting in a cylinder geometry, each edge carries a topological degree of freedom. The boundary conditions can be twisted by inserting a flux ϕ into the cylinder for spin up electrons and $-\phi$ for spin down electrons. In the Landau gauge orbitals are localized along the cylinder, where we consider $N_{\mathrm{orb,n}}$ and $N_{\mathrm{orb,sc}}$ normal and superconducting orbitals, respectively. The typical separation between orbitals is $2\pi\ell_B^2/L_y$, where L_y is the cylinder perimeter. The droplet is confined by a linear potential μ_m.
c) With the counter-propagating edges gapped out, the bilayer FQH state on the cylinder is topologically equivalent to a single layer FQH state on a torus, where the fluxes ϕ and φ run through its two noncontractible cycles and can be used to explore its topological ground state degeneracy. It is thus topologically equivalent to the ground state degeneracy of the gapped edge modes.

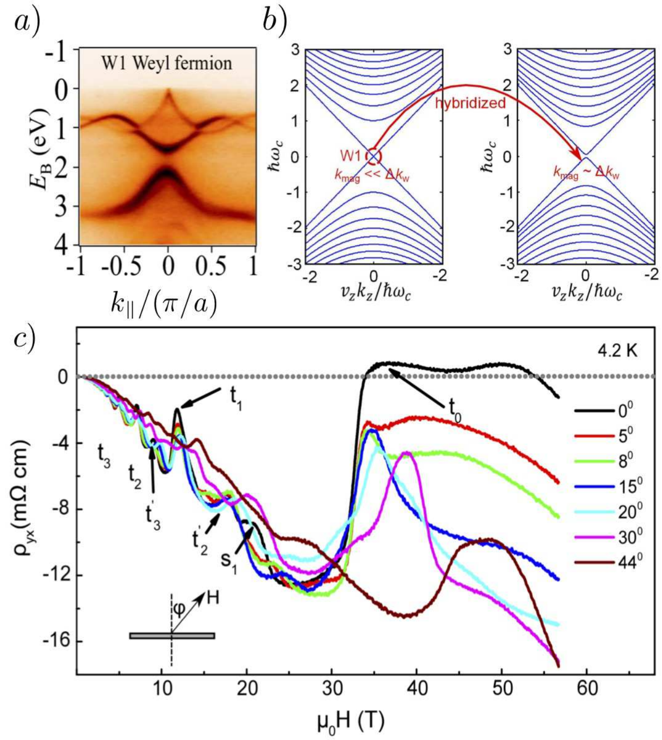

FIG. 10.2 – Magnetic field induced annihilation of Weyl fermions in the band structure of TaP.

a) Angle-resolved photoemission spectroscopy image of a Weyl node in TaP, visible as a linear band crossing near the Fermi level.

b) Schematic of how a strong magnetic field hybridizes two Weyl nodes in the Landau level band structure in TaP: The two Weyl nodes are at the same momentum k_z and have opposite chirality. Thus they come with linearly and oppositely dispersing Landau levels which cross each other at small fields. As the inverse magnetic length becomes of the same scale as the transverse Weyl node separation in momentum space, the linear Landau levels hybridize. The transport properties of the material change drastically.

c) Hall conductivity as a function of magnetic field. The critical field where the Weyl node Landau levels annihilate is manifest via a drastic jump and sign reversal of the Hall conductivity (0° trace).

only after φ is advanced by 6π does the system return to its initial state, because the elementary excitations of the superconducting edge are Cooper-paired quasiparticles of charge $2e/3$, delocalized along the cylinder perimeter, which tunnel across the bulk gap.

System sizes in this work were limited, but we were nevertheless able to demonstrate four key features: (i) the edges develop a spectral gap induced by the superconducting coupling, (ii) the expected number of three nearly degenerate ground states without any charge imbalance between the two halves of the system, (iii) charge pumping can permute the ground states, and (iv) the system exhibits a 6π-periodic Josephson effect. For each signature, we discussed the suitable parameter regime. Our work provides the first quantitative study of fractional edge modes coupled to superconducting leads in a fully microscopic model and should serve as an important foundation for future work.

10.2 Annihilating Weyl fermions with a magnetic field

Weyl semimetals display the most elementary topological band degeneracies [7]: two bands in a three-dimensional band structure are degenerate in an isolated point in momentum space. Away from this singular point, the bands generically disperse linearly. Quasi-particle excitations near the degeneracy point (Weyl node) are described by the Weyl equation, hence the name. These quasiparticles have a number of unique properties when it comes to their electromagnetic response. In some precise sense, they can be regarded as magnetic monopoles in momentum space and are associated with a topological charge ± 1.

In the most widely studied class of Weyl semimetals, the Weyl nodes arise from spin-orbit coupling which can be thought of as a perturbation to a more symmetric band structure. As a result, Weyl nodes of opposite charge come in pairs that in many cases are separated by a small distance Δk_{W} in momentum space.

When the material is exposed to an strong external magnetic field, Weyl fermions generate a very distinct quasi-one-dimensional band structure of dispersing Landau levels. Apart from two sets of Landau levels above and below the Weyl node, respectively, there is a single 'chiral' Landau level that disperses linearly across the energy of the Weyl node. The sign of the associated velocity is given by the topological charge of the Weyl node. Because of this chiral Landau level, a single Weyl fermion cannot become insulating when exposed to a magnetic field.

Tantalum phosphide (TaP) is a Weyl semimetal [8] with two relevant features: Its Weyl nodes are very close to the Fermi level and their separation in momentum Δk_{W} is rather small as shown in Fig. 10.2 a). We studied the transport properties of TaP when exposed to a strong magnetic field. The field orientation was chosen such that the Weyl nodes are separated in momentum space perpendicular to the magnetic field B, this corresponds to 0° in Fig. 10.2 c). In this configuration, the chiral Landau levels of the two Weyl nodes with opposite velocity cross as shown in Fig. 10.2 b). For small fields, this crossing is only hybridizing by an exponentially small amount in the ratio of $\Delta k_{\mathrm{W}}^{-1}$ and the magnetic length $\ell \propto 1/\sqrt{B}$. The magnetic length is the typical length scale on which the magnetic field breaks the translational symmetry of the system. As the field is increased, a noticeable hybridization appears as soon as $\ell^{-1} \sim \Delta k_{\mathrm{W}}$ and the system turns into an insulator.

In the transport measurement, this change in the electronic structure manifests itself in a dramatic change and sign reversal in the Hall conductivity at around $B = 30$ T as shown in Fig. 10.2 c). This field scale is in very good agreement with the expectation from our theoretical calculations.

The residual conductivity for $B > 30$ T comes from other Fermi pockets in the Brillouin zone that are unrelated to the Weyl node.

[7] B. Yan, *et al. Topological Materials: Weyl Semimetals*, Ann. Rev. Cond. Matt. Phys. **8**, 337-354 (2017).

[8] S.-Y. Xu, *et al. Experimental discovery of a topological Weyl semimetal state in TaP*, Science Advances **1**, e1501092 (2015).

10.3 Machine learning for detecting phase transitions

Artificial intelligence is widely employed in science and information technology whenever large amounts of data need to be analyzed or classified. Machine learning techniques and neural networks in particular are becoming a more and more widespread tool also in statistical and condensed matter physics. A typical class of tasks for neural networks are classification problems, for instance to identify whether images show cats or dogs. Classification, for instance that of phases of (quantum) matter based on various observables, is a prominent task in condensed matter physics.

In this project, which is our first venture into the field of machine learning, we used a neural network for exactly that task – a binary phase classification – based on numerically obtained data [9]. The two phases to be distinguished are a thermalizing and a localized phase of a Heisenberg spin chain in a random field. The Hamiltonian is strongly interacting and the phase with strong random field is called many-body localized. Many-body localization means that a system keeps a memory of its initial condition for arbitrary long times for states at high energies/temperatures [10]. The quantum entanglement is not scrambled as in a conventional, thermalizing system. As a consequence, many-body localized states do not follow the conventional rules of quantum statistical mechanics and in particular violate ergodicity. These properties and their potential for quantum information storage make them an important current research field.

However, there are many open questions about the properties of the many-body localized phase and the associated phase transition. It is not clear, which observable is best suited to detect the phase transition from numerical data on finite-size systems. This is where neural networks become useful. We taught a neural network and entanglement fingerprint of typical states well in the localized and well in the thermalizing phase of the spin chain and then asked it to classify the same entanglement fingerprint for states in the transition region to determine the phase boundary. The fingerprint we used is the so-called entanglement spectrum [11] (defined as the spectrum of the reduced density matrix when one half of the spin chain is traced over). The entanglement spectrum was shown to contain a lot of universal information about quantum phases via its level statistics, gaps between levels, degeneracies of levels and more.

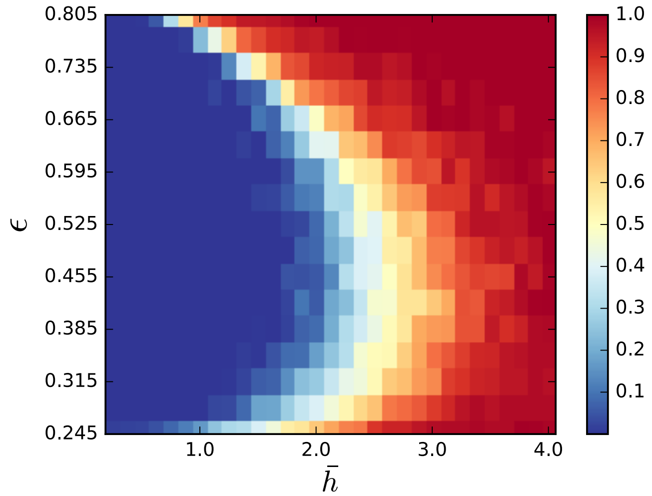

FIG. 10.3 – Phase diagram of a spin-1/2 Heisenberg chain in a random field obtained using a neural network. The horizontal axis is the strength of the disorder field, the vertical axis is energy density (the classification is valid for arbitrary excited states). The blue region is thermalizing, while the red region is in a many-body localized phase.

We did not teach the neural network which features in the entanglement spectrum of the spin chain are relevant for the classification. Rather, we later used the technique of hallucinogenic dreaming to determine what properties the network had learned. (This was the first time the technique was applied to condensed matter physics.) It turned out that the network had correctly learned a known power-law feature of the entanglement spectrum.

Most importantly, however, the neural network was able to pin down the phase transition very sharply, even by only looking at individual eigenstates of the spin-chain Hamiltonian. The phase boundary shown in Fig. 10.3 is in quantitative agreement with previous results, but needs much less numerical input to be computed. Our neural network approach is a combination of a so-called supervised and an unsupervised technique in that we do not a priori know where the phase transition is. To enhance the performance, we invented an algorithm called confidence optimization, which incentives the confident classification of the states near the phase transition. This work was an interesting first venture into the field of machine learning, on which we will follow up with diverse further projects.

[9] F. Schindler *et al.*, *Probing many-body localization with neural networks*, Phys. Rev. B **95**, 245134 (2017).

[10] A. Soluyanov *et al.*, *Type-II Weyl semimetals*, Nature **527**, 495-498 (2015).

[11] H. Li, *et al.*, *Entanglement Spectrum as a Generalization of Entanglement Entropy: Identification of Topological Order in Non-Abelian Fractional Quantum Hall Effect States*, Phys. Rev. Lett. **101**, 010504 (2008).