Mathematics of topological insulators

organized by
Daniel Freed, Gian Michele Graf, Rafe Mazzeo, and Michael I Weinstein

Workshop Summary

Final report on AIM Workshop on the Mathematics of Topological Insulators – Dec. 7-11, 2020

Organizers: D. Freed, G. M. Graf, R. Mazzeo and M. I. Weinstein

Overview

Topological Insulators is a field at the intersection of Mathematics and Physics, which emerged from two recent scientific revolutions in condensed matter physics and materials science: the recognition of the role of topology in characterizing materials and in the prediction of their physical properties, and the fabrication of and experimentation in two-dimensional materials, such as graphene, which are one-atom-thick monolayers that extend in-plane to the macro-scale.

This workshop's goal was to establish a stronger connection between analytical and topological researchers in the field of Topological Insulators. There was broad representation among speakers and participants coming from a range of communities in: mathematical physics, theoretical physics, PDE analysts, topologists and computational physics.

To facilitate interactions across disciplines, speakers were exhorted to devoted a significant part of their talks to communicating the basic ideas and research agenda / perspective with mathematicians in other areas.

Breakout working groups

Afternoon breakout working groups were formed around the following questions:

(1) Do edge states localize about irrational edges? ; Section .
(2) Long time behavior of topological edge modes in the presence of nonlinearity, e.g. as modeled by the nonlinear Schroedinger equation; Section .
(3) Lower bound on gap in fractional quantum Hall effect, especially for "conformal block" toy models; question proposed by participant Duncan Haldane; Section .
(4) Edge state propagation along non-straight edges; Section
(5) The "no-fold" (semi-metallic) condition, which relates leakage of edge state energy into the bulk by resonance processes; see Fefferman, Lee-Thorp and Weinstein (Annals of PDE, 2017), Drouot-Weinstein (Advances in Math. 2020) Section .
(6) The effect of randomness on Dirac (2D) and Weyl (3D) points
(7) Constructing microscopic systems and computing correlation functions in both microscopic and low energy effective field theory
(8) The spectral localizer in the strongly disordered regime
(9) For a class of two-scale Schroedinger Hamiltonians: understand the group velocity of edge currents and characterize the set on which they concentrate.

(10) Tutorial on the subjects of D. Freed's lecture on *Field theory as an invariant of quantum systems*

Working group reports.

Do edge states localize along irrational edges?.

The group focused on the problem of proving or disproving existence of edge states for a standard. discrete model of graphene sharply terminated along an edge having irrational slope with respect to the bulk structure. We discussed how the problem might be reduced to understanding rational edges with slopes p/q as q tends to infinity, and we started analyzing general rational edges. It has been asserted that index theory establishes that edge states exist; the relevant paper is complicated and not yet refereed. We plan to continue studying the problem from an analytic viewpoint, to obtain a concrete picture of edge states. A mailing list and Google drive have been set up for continued collaboration using *sococo.*

Topological edge modes and nonlinearity.

The nonlinear group focused on the effects of nonlinearity on topological models with an emphasis on edge effects (physically most interesting right now) and bulk effects, which are harder to realize experimentally with current technology but still have a number of open problems. We will focus our discussion on these two directions below.

The edge mode question originally posed by M. Rechtsman is best posed in terms of a next order correction and rigorous control on coupling to the bulk for a (strongly) nonlinear wave packet building off recent work of Ablowitz-Curtis-Ma (PRA, 2014) in the case of the honeycomb lattice. The physics requires an understanding of lifespans of nonlinear edge states currently not achieved as recently such states were observed experimentally by Mukherjee-Rechtsman (Science, 2020) but at higher power regimes than the asymptotic models really fit. Both corrections at higher power and coupling to the bulk would also be interesting to model for other topological lattice models as well. A related nonlinear edge model was proposed by G. Bal based upon a Dirac edge model he has studied lately that has a spatially dependent mass term grows linearly. This given an infinite mass boundary condition. This model is has isolated band structure very similar to the harmonic oscillator, hence the model spectrum is exact and one may be able to construct stationary states that have very long lifespans in a robust fashion. In 1d topological models such as the SSH model, it is easy to construct genuine nonlinear states that are edge localized, but this may be an interesting model for testing nonlinear coupling to the bulk as well.

The bulk nonlinear problem contains a number of fascinating mathematical questions. The problem of existence and structure for band gap solitons in topological lattice models was recently explored by Lumer et al (PRL, 2013) using a Floquet model and by Bandres-Marzuola-Osting-Rechtsman (preprint, 2020) for tight binding models, where the authors explored numerically the structure of the nonlinear gap states, their dynamics and bifurcation properties. The tight binding analysis allowed B-M-O-R to give continuum Dirac models that demonstrate similar phenomena numerically to the lattice solitons computed numerically, but variational arguments for existence and stability need to be properly done from a mathematics perspective. For existence, the variational techniques of for instance Esteban-Serre for nonlinear Dirac models should be adaptable to the case of a saturating nonlinearity, but modifications of recent work of Borelli may be required to observe structural symmetries in the solutions. The structure of the gap soliton appears strongly related to the Berry curvature at the band edge and very interesting things happen when there are degenerate band edges in the lattice. But doing more sophisticated pseudo-arc-length bifurcation methods on the lattice models should be undertaken to understand how nonlinear branching occurs deeper into the gap. In addition, the tight binding models demonstrated an orbitally stable regime of states in the setting of saturating nonlinearities, hence analysis of linear stability in topological lattice and Dirac models is a natural next step in non-self-adjoint spectral theory as an extension of the tremendous work undertaken to analyze the JL operator inherent to Nonlinear Schroedinger equations. Similarly, the dynamics at low power of these bulk states in an electric field seem to fit well the semi classical anomalous velocity dynamics predicted for wave packets at the band edge, but with oscillations stemming from coupling to the top band that takes the form of the Zitterbewegung predicted by Dirac. However, at high power these topological gap solitons experience very anomalous dynamics in an electric field and a particle model that is strongly different from the standard Newtonian soliton dynamics in a background need to be developed.

Fractional Quantum Hall Effect.

Duncan Haldane began by giving a general introduction about the Fractional Quantum Hall Effect, namely the phenomenon by which interacting electrons in the plane, that are subject to a transversal magnetic field, exhibit a quantization of the Hall conductance at values that are rational fractions of the quantum of resistance, provided their density is close to an alike fraction of the particle density of a filled Landau level.

Key items of the introduction were (i) the Laughlin wave-function and its relatives (conformal blocks), (ii) the picture of flux attachment and its more modern understanding as "orbital attachment", (iii) the pseudo-potentials as a means to describe interactions, (iv) the emergent non-commutative geometry, (v) the role of the guiding center as opposed to that of the particle position, and (vi) the competing roles of two geometries provided by the effective mass tensor and the magnetic field, respectively.

The main focus though was on the problem of the gap. More precisely, there are pseudo-potentials for which the Laughlin (or related) wave-functions are seen to be groundstates, and the task is to establish the existence of a gap above them. That task is made more difficult by the fact the gap is actually supposed to exist only in infinite volume limit, given that otherwise gapless edge excitations are present. The discussion turned around the question of characterizing the spurious kernel states (Jack polynomials), as well as low lying excited states. Also discussed was the possibility of an infinite-volume formulation of the problem, as well as similarities and differences to the AKLT spin model.

Edge state propagation along non-straight edges.

Experiments demonstrate, see e.g. [L16], that energy propagates along boundaries of topological insulators. This manifests through space-localized states that occur at the edges of topological insulators. When the boundary is commensurate with a periodic atomic structure, the material admits edge states (time-harmonic waves localized along the boundary), whose characteristics (profile, speed) can be detailed relatively well. Although impressive general existence results exist for edge states [GP,AHV,BKR], the quantitative description of currents breaks down. This research group focused on models where the edge is not exactly translation invariant but one can nonetheless precisely describe the structure of the edge state. This research group aimed to construct and study models where the the edge is not translation invariant but one can nonetheless precisely describe energy propagation.

Problems and outcomes. In our discussion we studied three different models: (i) an edge with a slowly-varying (but not necessarily small) defect
(ii) a sharp edge that remains close to a straight line, and
(iii) a weakly bent edge.
In the first two settings, we found an ansatz which yields wavepacket solutions propagating uni-directionally along the edge, with a phase affected by the defect. In the third case, we found wavepackets that propagate in both directions. Uni-directional propagation, on the other hand, seems to occur along the nodal set of the domain wall. This requires to go beyond a standard adiabatic approximation that takes into account eigenvalue crossings. The discussion during the AIM workshop initiates possible collaborations for further investigating such issues.

Bibliography

[AHV] Avila, J.C., Schulz-Baldes, H. and Villegas-Blas, C. *Topological invariants of edge states for periodic two-dimensional models.* Math. Phys., Anal. Geom., 16:136170, 2013.

[BKR]Bourne, C., Kellendonk, J. and Rennie, A. The K-Theoretic BulkEdge Correspondence for Topological Insulators. Ann. Henri Poincar 18, 1833–1866 (2017).

[GP] Graf, G.M., Porta, M. Bulk-Edge Correspondence for Two-Dimensional Topological Insulators. Commun. Math. Phys. 324, 851895 (2013).

[L16] Li, X. et al. .*Experimental Observation of Topological Edge States at the Surface Step Edge of the Topological Insulator* $ZrTe_5$, Phys. Rev. Lett., 116, 17, 176803, 2016.

The "no-fold" condition.

There was a short discussion of the "no folds" or "no dipping" condition. In particular, Peter Kuchment explained the significance of the condition, I briefly surveyed the results of arXiv:2004.12931 ("A local test for global extrema in the dispersion relation of a periodic graph" by Gregory Berkolaiko, Yaiza Canzani, Graham Cox, Jeremy L. Marzuola) and Ralph explained some results from arXiv:1807.05751 ("Local models and global constraints for degeneracies and band crossings", by Ralph M. Kaufmann, Sergei Khlebnikov, Birgit Wehefritz-Kaufmann). It was felt that constructing a Morse theory for eigenvalues of families of Hamiltonians (including the non-smooth points of band crossings) might be a way forward.

Other

Among other notable influences of the workshop was that Peter Kuchment will lead a two-semester graduate course on Topological Insulators at Texas A&M University with contributions by Eric Rowell (Topological phases of matter), Gouliang Yu (Noncommutative geometry and K-theory) and Gregory Berkolaiko (Tight-binding model examples).