Title: Disorder and interaction effects in topological insulators

Abstract

Topological phases of matter are conventionally characterized at the non-interacting level through global invariants, whose evaluation relies on tracking the evolution of occupied single-particle states across the Brillouin zone. However, this paradigm becomes inadequate in the presence of disorder, which breaks translational symmetry, or strong electron–electron interactions, which invalidate the single-particle description. In such regimes, new theoretical and computational approaches are required to properly characterize topological properties. At the same time, the interplay between band topology, disorder, and correlations is expected to give rise to a rich and unconventional phenomenology, including disorder-induced topological phases and exotic states emerging from interaction.

This thesis investigates the effects of non-perturbative disorder and strong correlations in topological insulators, combining methodological developments with numerical simulations. A central theme is the extension of topological concepts beyond crystalline and non-interacting framework, with particular emphasis on real-space formulations and many-body diagnostics.

In the first part, disorder is addressed from a methodological perspective by introducing a suite of techniques for detecting topological phases in non-crystalline systems. In particular, we consider single-point topological invariants defined within the framework of very large supercells, and topological local markers applicable to both finite and extended systems. A key conceptual result is the demonstration that these space-resolved topological markers can serve as genuine local order parameters for topological phases in disordered systems, thereby challenging the conventional view that topological phase transitions can only be described in terms of global quantities. Using tight-binding models—specifically the Haldane model for quantum anomalous Hall insulators and the Kane–Mele model for quantum spin Hall insulators—extensive numerical simulations are performed in the presence of different types of disorder. The analysis reveals that topological local markers exhibit spatial fluctuations with well-defined statistical properties. These fluctuations are short-ranged and vanish under coarse-graining, except at the phase transitions, where they persist over large scales. By introducing a topological correlation function, correlation lengths and scaling behavior are extracted at criticality. In particular, at phase transitions this topological correlation function is characterized by universal critical exponents that appear independent of the type of disorder, while remaining sensitive to the nature of the transition and the symmetry class of the model. From an applicative perspective, these methods are further employed to study realistic systems showing topological phases, such as a monolayer of Jacutingaite, in the presence of vacancies, using effective Wannier Hamiltonians derived from first-principle calculations.

The second part focuses on the role of strong electron–electron interactions in topological insulators, treated within the variational Monte Carlo framework. Topological properties in interacting systems are identified using many-body markers derived from the modern theory of polarization, here applied in a novel way to large system sizes. The main achievement is the study of a one-dimensional two-orbital fermionic model with on-site (intra-band Hubbard U) and nearest-neighbor (V) interactions, described using a multi-orbital Jastrow–Slater variational wavefunction. The results reveal that electronic correlations do not simply renormalize the non-interacting picture but instead give rise to new emergent phases. In particular, the transition between trivial and topological phases becomes non-direct at finite U, with the emergence of an intermediate insulating phase exhibiting signatures of gapless spin excitations, which cannot be simply described within either the weak- or strong-coupling limits. A small-V interaction further stabilizes this intermediate insulator, while a sufficiently large value of nearest-neighbor repulsion gives rise to two different charge-density wave insulators. This approach is extended to the two-dimensional version of the model, namely the Bernevig–Hughes–Zhang (BHZ) model for quantum spin Hall insulators, in the presence of both intra- and inter-orbital interactions. In this setting, an antiferromagnetic phase can be stabilized in the regime of strong intra-band interaction, while the inclusion of inter-orbital coupling provides evidence for the emerging of an excitonic insulating phase in the strong-coupling regime. These results further highlight the richness of correlation-driven topological phenomena in higher-dimensional systems.

UNIVERSITÀ DEGLI STUDI DI TRIESTE

Disorder and interaction effects in topological insulators

PhD Candidate Roberta Favata

Supervisors: Federico Becca and Antimo Marrazzo.

Dr. Favata presented a twofold study investigating the effects of interaction and disorder in low-dimensional topological insulators. Regarding the former one, a variational quantum Monte Carlo approach was applied to the Bernevig-Hughes-Zhang (BHZ) model. In one dimension, a systematic analysis revealed an unexpected intermediate phase situated between the topological and trivial insulators; this phase is characterized by an insulating gap in the charge sector but gapless spin excitations. Furthermore, the study demonstrated that sufficiently large nearest-neighbor interactions stabilize charge-density-wave states. In two dimensions, the results confirmed the existence of an excitonic insulator, previously suggested in the limit of infinite dimensions. In the second part of the presentation, Dr. Favata investigated non-crystalline systems, by developing and applying novel tools to characterize topological phase transitions driven by disorder. In particular, real-space local markers have been introduced, showing that they can act as local order parameters with meaningful spatial fluctuations and correlation functions. These methods are also applied to realistic materials, such as a monolayer of Jacutingaite with vacancies, using Wannier Hamiltonians derived from first-principles calculations.

The presentation underscored the conceptual complexity of the problems and the technical details to assess the relevant physical aspects. The results achieved by the candidate are of high caliber and were presented with clarity. Furthermore, Dr. Favata demonstrated a profound mastery of the subjects, also addressing all questions with well-reasoned responses.

The committee recommends admitting her to the final presentation.

The Committee
Angelo Bassi
Federico Becca
Ugo Marzolino
Thomas Schäfer
Andrea Trombettoni

DOTTORANDO / *PHD STUDENT*	
COGNOME / *SURNAME* FAVATA	**NOME / *NAME*** ROBERTA
CORSO DI DOTTORATO / *PHD COURSE*	**CICLO / *CYCLE***
PHYSICS	38
SUPERVISORE (COGNOME, NOME) / *SUPERVISOR (SURNAME, NAME)*	
BECCA FEDERICO	
CO-SUPERVISORE (EVENTUALE) (COGNOME, NOME) / *CO-SUPERVISOR IF APPLICABLE (SURNAME, NAME)*	
MARRAZZO ANTIMO	

BREVE RELAZIONE SULL'ATTIVITÀ DI RICERCA / *CONCISE PROGRESS REPORT (RESEARCH ACTIVITIES)*

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My research has focused on topological phases of matter beyond the band-theory paradigm, addressing the effects of strong electronic correlations and disorder. Topological properties are commonly established at the non-interacting level in terms of global invariants computed from single-particle states defined in the Brillouin zone. However, when the translational symmetry is broken by disorder or strong correlations invalidate the single-particle picture, conventional tools fail and new strategies are needed to characterize topology. My work explores these regimes, where the interplay between band topology, interactions and disorder leads to novel and exotic phenomena.

The research developed along two main directions. One is the study of the effect of electronic interactions in topological insulators through a variational Monte Carlo (VMC) approach, by employing many-body markers in a novel way on large system sizes and finding very rich phase diagrams. The other is the investigation of disorder in topological insulators, first from a methodological perspective, by developing topological invariants for non-crystalline systems, and further from an applicative perspective, by proposing topological local order parameters to characterize disorder-driven phase transitions.

A major achievement is the study of a one-dimensional two-orbital fermionic model with on-site intra-band (U) and nearest-neighbor (V) interactions, using a Jastrow-Slater wavefuntion within VMC. The results, published in *PRB* ***111**, 155105 (2025)*, reveal that correlations induce emergent phases beyond the non-interacting picture. Notably, a spin-gapless insulating phase appears between the trivial and topological states, demonstrating that the transition is not direct. We extended this approach to the two-dimensional case with intra- and inter-band interactions, where signatures of excitonic insulating phases at strong coupling are observed.

In parallel, the PhD activity has addressed topological systems in the presence of disorder. Alongside the development of single-point invariants for disorder systems [*Electron. Struct.* ***5**, 014005 (2023)*], we argued that local topological markers can serve as local order parameters in disordered systems, against the common belief that topological phase transitions are only described in terms of global quantities. In *PRL* ***135**, 026603 (2025)*, we show that these markers exhibit meaningful fluctuations and correlation functions with a scaling behavior at criticality that is characterized by universal critical exponents. These contributions have been implemented in a Python package, freely available on Github and actively updated with new features. These methods are also applied to real systems which show topological phases, such as a monolayer of Jacutingaite in the presence of vacancies, by using Wannier Hamiltonians extracted from first-principle calculations.

ATTIVITÀ FORMATIVE / *TRAINING ATTENDED BY THE PHD STUDENT*			
TIPO / *TYPE* Corso/Seminario/Workshop/ Convegno/Stage/Altro (specificare) – *Course/Seminar/Workshop/ Conference/Stage/Other (specify)*	**TITOLO / *TITLE***	**SEDE / *LOCATION***	***PERIODO (DAL AL)* / TIME PERIOD (FROM TO)**
WORKSHOP	21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods https://indico.ictp.it/event/10056/	ICTP, Trieste (Italy)	11/01/2023-13/01/2023
CONFERENCE	CMT@BRIXEN: The meeting of the condensed matter theory Italian community https://cmtconference.it/	Università di Padova, Bressanone (Italy)	05/06/2023-07/06/2023
WORKSHOP	Workshop on Quantum Monte Carlo Methods at Work for Describing Novel States of Matter https://indico.ictp.it/event/10187/	ICTP, Trieste (Italy)	10/07/2023-14/07/2023
SCHOOL	Topological Matter School TMS23 https://tms-dipc.org/	University of Basque Country, Donostia-San Sebastian (Spain)	21/08/2023-25/08/2023
CONFERENCE	Conference on Fractionalization and Emergent Gauge Fields in Quantum Matter https://indico.ictp.it/event/10168/	ICTP, Trieste (Italy)	04/12/2023-08/12/2023

WORKSHOP	Workshop on Twistronics and Moiré Materials: Bridging Theory and Experiments https://indico.ictp.it/event/10456/	ICTP, Trieste (Italy)	16/01/2024-19/01/2024
SCHOOL	2024 Arnold Sommerfeld School: Modeling strongly correlated electrons: Numerics, analytics, and quantum simulations https://www.theorie.physik.uni-muenchen.de/activities/schools/archiv/asc_school_2024/index.html	LMU, Munich (Germany)	16/09/2024-20/09/2024
CONFERENCE	Conference on Advances in Topological Condensed Matter https://indico.ictp.it/event/10518/	ICTP, Trieste (Italy)	11/11/2024-15/11/2024
CONFERENCE	APS Joint March Meeting: Global Physics Summit 2025 https://www.aps.org/events/2025/joint-meeting	Anaheim, CA (USA)	16/03/2025-21/03/2025
WORKSHOP	Topology and Geometry Beyond Perfect Crystals https://indico.fysik.su.se/event/8803/	NORDITA, Stockholm (Sweden)	08/06/2025-14/06/2025

ATTIVITÀ DI DIDATTICA E DI RICERCA / *TEACHING AND RESEARCH ACTIVITIES HELD BY THE PHD STUDENT*

TIPO / *TYPE*	**TITOLO / *TITLE***
ATTIVITÀ TUTORIALI E DIDATTICO INTEGRATIVE SVOLTE / *TUTORING ACTIVITIES*	• Co-supervision of a Master's student during their thesis project

SEMINARI TENUTI DAL DOTTORANDO / *SEMINARS HELD BY THE PHD STUDENT*	• Seminar to the CQSL group at EPFL (Lausanne, Switzerland, March 2026)
PUBBLICAZIONI SCIENTIFICHE / *SCIENTIFIC PUBLICATIONS* riferimenti bibliografici completi delle pubblicazioni presenti nel catalogo ArTS / *full bibliographic references of the publications submitted to the ArTS catalogue*	• R. Favata, and A. Marrazzo, *Single-point spin Chern number in a supercell framework*, Electron. Struct. **5** 014005 (2023) https://iopscience.iop.org/article/10.1088/2516-1075/acba6f/meta • R. Favata, D. Piccioni, A. Parola, and F. Becca, *Interaction-induced phases in the half-filled Bernevig-Hughes-Zhang model in one dimension*, Phys. Rev. B **111**, 155105 (2025) https://journals.aps.org/prb/abstract/10.1103/PhysRevB.111.155105 • R. Favata, N. Baù, and A. Marrazzo, *Fluctuations and correlations of local topological order parameters in disordered two-dimensional topological insulators*, Phys. Rev. Lett. **135**, 026603 (2025) https://journals.aps.org/prl/abstract/10.1103/h4d8-3lw1
PRESENTAZIONI A CONGRESSI, POSTER, ABSTRACT ETC / *PRESENTATIONS AT CONFERENCES, POSTERS,* ABSTRACTS, se pubblicato, riportare i riferimenti bibliografici / *if published provide full bibliographic references*	PRESENTATIONS AT CONFERENCES: • Fluctuations and correlations of topological local order parameters in 2D disordered topological insulators (APS March Meeting 2025, Anaheim) POSTERS: • Total Energy and Force Methods (ICTP, Trieste, Italy, January 2023) • CMT@BRIXEN (Bressanone, Italy, June 2023) • Topological Matter School TMS23 (San Sebastian, Spain, August 2023) • Workshop on Twistronics and Moiré Materials (ICTP, Trieste, Italy, January 2023): I was one of the winners of the poster session with the work ``Topological phase diagram of two-band fermionic chain in presence of Hubbard interaction" • 2024 Arnold Sommerfeld School (Munich, Germany, September 2024) • Conference on Advances in Topological Condensed Matter (ICTP, Trieste, Italy, December 2024): I received the APS poster prize for early career researcher with the work ``Topological phase diagram of two-band fermionic chain in presence of Hubbard interaction" • Topology and Geometry Beyond Perfect Crystals (Nordita, Stockholm, Sweden, June 2025)

Data compilazione /*Date,* 30/03/2026

Firma dottorando/*PhD student's signature*

Roberta Favata

Firma supervisore/*Supervisor's signature*

Federico Becca