

TOPOLOGICAL PHASES IN TWO-DIMENSIONAL QUANTUM MATERIALS

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A DISSERTATION
PRESENTED TO THE FACULTY
OF PRINCETON UNIVERSITY
IN CANDIDACY FOR THE DEGREE
OF DOCTOR OF PHILOSOPHY

RECOMMENDED FOR ACCEPTANCE BY
THE DEPARTMENT OF
PHYSICS

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May 2026

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Abstract

Two-dimensional crystals can host electronic phases whose defining properties are topological: they are fixed by integers that survive any smooth deformation of the material. This dissertation studies how such phases arise in layered transition-metal compounds, and how they can be identified from transport measurements that are available in practice. Chapter 2 reviews the band-theory description of the quantum spin Hall insulator. Chapter 3 develops a tight-binding model for a strained monolayer and computes its $\mathbb{Z}_2$ invariant as a function of strain and spin-orbit coupling. Chapter 4 compares the predicted phase diagram with edge-conductance data from four devices and finds a transition near 1.8% biaxial strain, where the edge conductance approaches the quantized value $2e^2/h$.

Acknowledgements

I thank my adviser, Professor Daniel S. Okafor, for teaching me to trust a calculation only after it has been done two different ways. I am grateful to the members of the condensed matter group for many discussions at the blackboard, and to the staff of the device fabrication facility for their patience with my first samples. My family made the long winters shorter.

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Chapter 1

Introduction

The integer quantum Hall effect showed that a measured conductance can be quantized with astonishing precision because it is fixed by a topological invariant of the electronic bands [5]. Haldane then showed that no external magnetic field is needed: a lattice model with broken time-reversal symmetry can realize the same physics [2]. Kane and Mele extended the idea to systems that preserve time reversal, predicting the quantum spin Hall insulator [4], which was soon observed in HgTe quantum wells [1].

Layered materials offer a new setting for these ideas, because strain, twist angle and gating can tune a single monolayer across a topological transition. This dissertation asks two questions: where in parameter space does the transition occur for a realistic monolayer, and what signature of it survives in imperfect devices?

Chapter 2

Topological Band Theory

For a two-dimensional insulator with time-reversal symmetry, the relevant invariant is a $\mathbb{Z}_2$ index ν . In the presence of inversion symmetry it can be computed from the parities $\xi_m(\Gamma_i)$ of the occupied bands at the four time-reversal invariant momenta,

$$(-1)^\nu = \prod_{i=1}^4 \prod_{m=1}^N \xi_{2m}(\Gamma_i). \quad (2.1)$$

A non-trivial index, $\nu = 1$, guarantees a pair of helical edge states that cross the bulk gap [3].

Each contributes one conductance quantum, so a clean sample with two edges has a two-terminal conductance of $2e^2/h$.

Chapter 3

A Strained Monolayer Model

We describe the monolayer by a four-band tight-binding Hamiltonian with nearest- and next-nearest-neighbour hopping and intrinsic spin-orbit coupling λ . Biaxial strain ϵ enters through the hopping amplitudes, which scale as

$$t_{ij}(\epsilon) = t_{ij}^{(0)} \exp[-\beta \epsilon], \quad (3.1)$$

with a Grüneisen-like parameter β fitted to first-principles bands. Tensile strain narrows the gap at Γ until the bands invert, at which point the parities in Equation (2.1) change and the index becomes non-trivial.

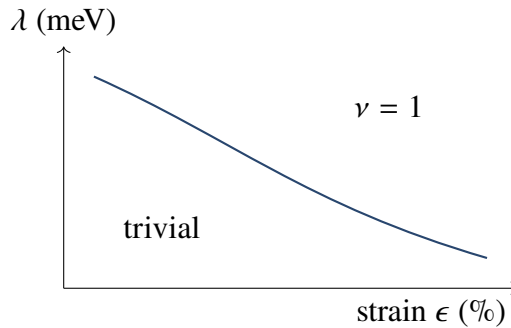


Figure 3.1: Schematic phase diagram of the model: the transition line separates the trivial insulator from the quantum spin Hall phase.

Chapter 4

Edge Transport in Strained Devices

Four devices were strained on a flexible substrate and measured at 1.6 K. Table 4.1 lists the strain at which each device first showed a conductance plateau within 10% of $2e^2/h$.

Table 4.1: Onset of the edge-conductance plateau in four devices.

Device	Channel length (μm)	Onset strain (%)	Plateau (e^2/h)
D1	0.8	1.7	1.94
D2	1.2	1.8	1.91
D3	2.0	1.9	1.83
D4	4.5	2.1	1.62

The plateau degrades with channel length, as expected when backscattering between the two edges becomes possible through puddles in the bulk. Extrapolating to short channels gives a transition strain of $1.8 \pm 0.1\%$, in agreement with the model of Chapter 3.

Chapter 5

Conclusion

A single strained monolayer can be tuned across a topological transition, and the transition is visible in edge transport when channels are short compared with the distance between charge puddles. The combination of a calibrated model and a short-channel extrapolation gives a practical way to locate the transition in new materials.

Appendix A

Parity Eigenvalues of the Four-Band Model

At each time-reversal invariant momentum the Hamiltonian commutes with the inversion operator, so the occupied Bloch states can be chosen with definite parity. The parities at Γ change sign when the two central bands exchange order, while those at the three M points remain fixed across the strain range studied, so the product in Equation (2.1) flips exactly once.

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