

**Springer Theses**

Recognizing Outstanding Ph.D. Research

Ryuji Takahashi

# Topological States on Interfaces Protected by Symmetry



Springer

# **Springer Theses**

Recognizing Outstanding Ph.D. Research

## **Aims and Scope**

The series “Springer Theses” brings together a selection of the very best Ph.D. theses from around the world and across the physical sciences. Nominated and endorsed by two recognized specialists, each published volume has been selected for its scientific excellence and the high impact of its contents for the pertinent field of research. For greater accessibility to non-specialists, the published versions include an extended introduction, as well as a foreword by the student’s supervisor explaining the special relevance of the work for the field. As a whole, the series will provide a valuable resource both for newcomers to the research fields described, and for other scientists seeking detailed background information on special questions. Finally, it provides an accredited documentation of the valuable contributions made by today’s younger generation of scientists.

### **Theses are accepted into the series by invited nomination only and must fulfill all of the following criteria**

- They must be written in good English.
- The topic should fall within the confines of Chemistry, Physics, Earth Sciences, Engineering and related interdisciplinary fields such as Materials, Nanoscience, Chemical Engineering, Complex Systems and Biophysics.
- The work reported in the thesis must represent a significant scientific advance.
- If the thesis includes previously published material, permission to reproduce this must be gained from the respective copyright holder.
- They must have been examined and passed during the 12 months prior to nomination.
- Each thesis should include a foreword by the supervisor outlining the significance of its content.
- The theses should have a clearly defined structure including an introduction accessible to scientists not expert in that particular field.

More information about this series at <http://www.springer.com/series/8790>

Ryuji Takahashi

# Topological States on Interfaces Protected by Symmetry

Doctoral Thesis accepted by  
Tokyo Institute of Technology, Tokyo, Japan

*Author*

Dr. Ryuji Takahashi  
Department of Physics  
Tokyo Institute of Technology  
Tokyo  
Japan

*Supervisor*

Prof. Shuichi Murakami  
Department of Physics  
Tokyo Institute of Technology  
Tokyo  
Japan

ISSN 2190-5053

Springer Theses

ISBN 978-4-431-55533-9

DOI 10.1007/978-4-431-55534-6

ISSN 2190-5061 (electronic)

ISBN 978-4-431-55534-6 (eBook)

Library of Congress Control Number: 2015934436

Springer Tokyo Heidelberg New York Dordrecht London

© Springer Japan 2015

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made.

Printed on acid-free paper

Springer Japan KK is part of Springer Science+Business Media ([www.springer.com](http://www.springer.com))

**Parts of this thesis have been published in the following journal articles:**

- R. Takahashi and S. Murakami, “Interfacial Fermi Loops from Interfacial Symmetries”, *Phys. Rev. Lett.*, **113**, 256406 (2014).
- R. Takahashi and S. Murakami, “Completely Flat Bands and Fully Localized States on Surfaces of Anisotropic Diamond-Lattice Models”, *Phys. Rev. B*, **88**, 235303 (2013).
- R. Takahashi and S. Murakami, “Gapless Interface States between Topological Insulators with Opposite Dirac Velocities”, *Phys. Rev. Lett.*, **107**, 166805 (2011).

# Supervisor's Foreword

Interfaces between two solids often exhibit exotic phenomena that are absent in either of the two parental materials. Interfaces have a number of degrees of freedom such as a combination of two materials, crystallographic orientations of the interface, and even the quality of the interface. Interface electronic states are often quite sensitive to these factors. This sensitivity to a number of factors, some of which cannot be controlled easily, causes various difficulties in theoretical research on interface electronic states and comparison with experiments. Theories on electronic states on interfaces are often restricted to first-principle calculations and phenomenological theories, because simplified effective models may not capture basic properties of interface states.

Historically, surface physics had had a similar aspect. Nevertheless, the discovery of topological insulators has added a renewed interest in the surface physics. It is qualitatively new that some surface electronic properties are robust and are determined by bulk topological properties. Furthermore, such proposals have been confirmed experimentally in various materials.

This book is concerned with theoretical pursuit of such topological phenomena in interface physics. This book, based on the dissertation of Dr. Ryuji Takahashi, theoretically explores possibilities of novel interface states from an interplay between topology and symmetry. Because the topics in this book are based on topology and symmetry, even simplified models with required properties of topology and symmetry turn out to be powerful in predicting new interface phenomena, which is in contrast with conventional interface phenomena. Various predictions in this book are yet to be observed experimentally, but the above-mentioned varieties of interfaces suggest that there is much room for future experimental and theoretical investigations.

Tokyo, Japan  
January 2015

Prof. Shuichi Murakami

# Acknowledgments

I would like to thank my Ph.D. advisor, Professor Shuichi Murakami, for his patient supervision. I gained knowledge from him about various subjects in condensed matter physics. He taught me how to tackle research. Without his support, I could not have accomplished this work. I am also very grateful for his support for my travels and participation in many conferences and workshops.

I would also like to thank the faculty members, secretaries, and colleagues in the theoretical condensed matter physics groups in the Department of Physics at the Tokyo Institute of Technology, and Dr. Daniel Gosálbez-Martínez in the Universidad de Alicante in Spain.

Among Assistant Professors, I would especially like to thank Dr. Takehiko Yokoyama, Dr. Ryuichi Shindou, and Dr. Kiyomi Okamoto. Dr. Yokoyama gave me critical comments about my research. Through his work, I became interested in the finite-size effect in topological insulators. Dr. Shindou has great knowledge of many fields in physics. From him, I learned approaches for solving problems in physics. Dr. Okamoto and I worked in the same office for 5 years, and sometimes I had helpful discussions with him.

This work has been supported by the Global Center of Excellence Program of the Ministry of Education, Culture, Sports, Science, and Technology of Japan (“MEXT”), through the “Nanoscience and Quantum Physics” Project of the Tokyo Institute of Technology.

Finally, I would like to express my deep appreciation to my family, including my cousins.



# Contents

<b>1</b>	<b>Introduction</b> . . . . .	1
1.1	Topological Phase of Matters . . . . .	1
1.2	Organization of the Dissertation . . . . .	3
	References . . . . .	4
<b>2</b>	<b>Topological Invariant and Topological Phases</b> . . . . .	5
2.1	Integer Quantum Hall Effect . . . . .	5
2.1.1	Integer Quantum Hall Effect as a Topological Insulator . . . . .	7
2.1.2	Adiabatic Charge Polarization by the Berry Phase . . . . .	9
2.1.3	Laughlin’s Gedanen Experiment . . . . .	11
2.1.4	Physical Picture of the Edge State . . . . .	14
2.1.5	Berry Curvature in Systems with Broken Time-Reversal Symmetry . . . . .	16
2.2	Topological Insulator . . . . .	16
2.2.1	Topological Invariant Under Time-Reversal Symmetry . . . . .	18
2.2.2	Surface Effective Hamiltonian . . . . .	24
2.3	Topological Flat-Band States in Honeycomb Lattice . . . . .	25
2.3.1	Dispersion of the Honeycomb Lattice Model . . . . .	25
2.3.2	Topological Explanation for Existence of the Flat-Band States . . . . .	29
2.3.3	Completely Localized Edge States . . . . .	30
	References . . . . .	33
<b>3</b>	<b>Gapless Interface States Between Two Topological Insulators</b> . . . . .	35
3.1	Refractive Phenomena of the Surface States at the Boundary of Two Topological Insulators . . . . .	35
3.2	Gapless Interface States Between Two TIs . . . . .	39
3.2.1	Paradox in the Refractive Phenomena . . . . .	39
3.2.2	Gapless States from the Surface Effective Model . . . . .	40

3.2.3	Proof for the Existence of the Gapless States by the Mirror Chern Number . . . . .	43
3.3	Gapless Interface States in a Lattice Model . . . . .	46
3.3.1	Model . . . . .	46
3.3.2	Calculation of the Mirror Chern Number for the Model . . . . .	47
3.3.3	Gapless Interface States . . . . .	53
3.4	Interfacial Fermi Loops and Interfacial Symmetries . . . . .	55
3.4.1	Interfacial Fermi Loops in the FKM Model. . . . .	55
3.4.2	Interfacial Fermi Loops from Interfacial Symmetries . . . . .	59
3.4.3	Interfacial Fermi Loops in the $\pi$ -junction Interface. . . . .	61
	References . . . . .	62
<b>4</b>	<b>Weyl Semimetal in a Thin Topological Insulator</b> . . . . .	<b>63</b>
4.1	Gapless States Protected by Mirror Symmetry in a Topological Insulator . . . . .	63
4.1.1	Weyl Semimetal Under Broken Inversion Symmetry . . . . .	67
4.2	Weyl Semimetal Phase in a Lattice Model . . . . .	68
4.3	Estimation of the Magnetization at the Phase Transition . . . . .	70
	References . . . . .	71
<b>5</b>	<b>Summary and Outlook</b> . . . . .	<b>73</b>
<b>6</b>	<b>Properties of the Chern Numbers</b> . . . . .	<b>77</b>
6.1	Chern Number. . . . .	77
6.1.1	Berry Curvature with Time-Reversal Symmetry. . . . .	78
6.2	Kramers Theorem . . . . .	79
6.3	Berry Curvature and Chern Number. . . . .	80
6.3.1	Change of the Chern Number . . . . .	81
	Reference . . . . .	83
<b>7</b>	<b>Calculation for the Interface Fermi Loops</b> . . . . .	<b>85</b>
7.1	Classification of Interfacial Systems . . . . .	85
7.2	Fermi Loop for the IPHS . . . . .	86
	Reference . . . . .	88
	<b>Curriculum Vitae</b> . . . . .	<b>89</b>