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Colin Howard

Measuring, Interpreting and Translating Electron Quasiparticle – Phonon Interactions on the Surfaces of the Topological Insulators Bismuth Selenide and Bismuth Telluride

Doctoral Thesis accepted by Boston University, Boston,
Massachusetts, USA

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ISSN 2190-5053

Springer Theses

ISBN 978-3-319-44722-3

DOI 10.1007/978-3-319-44723-0

ISSN 2190-5061 (electronic)

ISBN 978-3-319-44723-0 (eBook)

Library of Congress Control Number: 2016950525

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The registered company is Springer International Publishing AG

The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

*For my parents and María, without whom
I would not have been able to do this*

Supervisor's Foreword

The new class of materials coined topological insulators (TIs) has been the subject of extensive studies over the past 5 years and continues to be one of the most active research areas of condensed matter physics. The main attraction in studying these materials, from both fundamental and technological perspectives, has been the presence of chiral Dirac fermion quasiparticles (DFQs) that define a robust metallic surface state protected against backscattering by time-reversal symmetry. Strong spin-orbit interactions lock the Dirac fermion quasiparticles' (DFQs) spin to the state wave vector in a mutually perpendicular configuration, giving the Dirac cone a definite chirality. Consequently, DFQs on the surface cannot backscatter from lattice vacancies, grain boundaries, phonons, etc. into their time-reversed counterparts. Technical improvements may minimize defects, but phonons are always present. Despite these constraints, it was recently found that the DFQs strongly interact with surface boson excitations, especially phonon and coupled plasmon-spin excitations. Consequently, DFQ-phonon interaction should be a dominant scattering mechanism for Dirac fermions on these surfaces at finite temperatures. Hence, the electron-phonon interaction is of exceptional importance when assessing the feasibility of promising applications in technologies such as spintronics and quantum computing.

Most of the reported studies adopted a noninteracting, single-particle approach to the DFQ system. However, recently, there have been several experimental and theoretical reports on the interaction of the DFQs with surface phonons. Prior to Dr. Howard's thesis work, there has been little consensus about the magnitude of this coupling as evidenced by widely varying values of the electron-phonon coupling parameter λ appearing in the literature.

Dr. Howard's thesis presents experimental and theoretical results about the surface dynamics and the surface Dirac fermion (DF) spectral function of strong topological insulators Bi_2Te_3 , and Bi_2Se_3 , and describes the corresponding techniques used. The experimental results, employing inelastic helium atom-surface scattering techniques, reveal the presence of a prominent Kohn anomaly in the measured surface phonon dispersion of a low-lying optical mode and the absence of surface Rayleigh acoustic phonons. With the aid of fitting the experimental data to theoretical models employing phonon Matsubara functions, he was able

to extract the matrix elements of the coupling Hamiltonian and to determine the modifications to the surface phonon propagator encoded in the phonon self-energy. This, in turn, allowed him to calculate, for the first time, the phonon mode-specific electron-phonon coupling $\lambda(\mathbf{q})$ from experimental data and to obtain an average coupling significantly higher than typical values obtained for metals, underscoring the strong interaction between optical surface phonons and surface Dirac fermions in topological insulators. Finally, to connect to experimental λ values obtained from photoemission spectroscopy, he constructed an electronic DFQ Matsubara function using the determined electron-phonon matrix elements and the optical phonon dispersion. Dr. Howard was then able to extract the DFQ spectral function and the density of states for comparison with angle-resolved photoemission (ARPES) and scanning tunneling spectroscopy results. The ensuing spectral function revealed several important features. First, the footprints of phonon interactions occur on an energy scale of the order of 1 meV, which sets a necessary energy resolution of that magnitude or better to observe these features and extract a reliable value for λ . Second, he found that the electron-phonon coupling parameter extracted from the spectral function was strongly temperature dependent, which invalidates extraction methodologies that assume a temperature-independent λ and a linear temperature dependence of the corresponding spectral linewidth.

I hope that the methodology and techniques presented in Dr. Howard's thesis could hold promise for determining how EPC, as well as other quasiparticle interactions, modifies the electronic structure in a variety of condensed matter systems. I also hope that the entire work would be useful for students and researchers.

Boston, MA, USA
May 2016

Michael El-Batanouny

Abstract

The following dissertation presents a comprehensive study of the interaction between Dirac fermion quasiparticles (DFQs) and surface phonons on the surfaces of the topological insulators Bi_2Se_3 and Bi_2Te_3 . Inelastic helium atom surface scattering (HASS) spectroscopy and time of flight (TOF) techniques were used to measure the surface phonon dispersion of these materials along the two high-symmetry directions of the surface Brillouin zone (SBZ). Two anomalies common to both materials are exhibited in the experimental data. First, there is an absence of Rayleigh acoustic waves on the surface of these materials, pointing to weak coupling between the surface charge density and the surface acoustic phonon modes and potential applications for soundproofing technologies. Secondly, both materials exhibit an out-of-plane polarized optical phonon mode beginning at the SBZ center and dispersing to lower energy with increasing wave vector along both high-symmetry directions of the SBZ. This trend terminates in a V-shaped minimum at a wave vector corresponding to $2k_F$ for each material, after which the dispersion resumes its upward trend. This phenomenon constitutes a strong Kohn anomaly and can be attributed to the interaction between the surface phonons and DFQs.

To quantify the coupling between the optical phonons experiencing strong renormalization and the DFQs at the surface, a phenomenological model was constructed based within the random phase approximation. Fitting the theoretical model to the experimental data allowed for the extraction of the matrix elements of the coupling Hamiltonian and the modifications to the surface phonon propagator encoded in the phonon self energy. This allowed, for the first time, calculation of phonon mode-specific quasiparticle-phonon coupling $\lambda_v(\mathbf{q})$ from experimental data. Additionally, an averaged coupling parameter was determined for both materials yielding $\bar{\lambda}^{\text{Te}} \approx 2$ and $\bar{\lambda}^{\text{Se}} \approx 0.7$. These values are significantly higher than those of typical metals, underscoring the strong coupling between optical surface phonons and DFQs in topological insulators.

In an effort to connect experimental results obtained from phonon and photoemission spectroscopies, a computational process for taking coupling information from the phonon perspective and translating it to the DFQ perspective was derived. The procedure involves using information obtained from HASS measurements

(namely the coupling matrix elements and optical phonon dispersion) as input to a Matsubara Green function formalism, from which one can obtain the real and imaginary parts of the DFQ self energy. With these at hand it is possible to calculate the DFQ spectral function and density of states, allowing for comparison with photoemission and scanning tunneling spectroscopies. The results set the necessary energy resolution and extraction methodology for calculating $\tilde{\lambda}$ from the DFQ perspective. Additionally, determining $\tilde{\lambda}$ from the calculated spectral functions yields results identical to those obtained from HASS, proving the self-consistency of the approach.

Acknowledgments

First and foremost, I would like to thank the most important person in my life, María Jorgelina González, who was crazy enough to become my wife during this whole ordeal. Without her, this dissertation would definitely not have been written. A constant source of inspiration and support, I will never be able to thank her enough nor express how important she is for my life. That being said, I can still try. So, María, I offer you my deepest and most sincere thanks for being the perfect companion over these past 5 years. I cannot wait to see where our journey takes us.

Second, I would like to thank my parents, Gail, Judd and Lori. Ever since I was young, both my father and mother instilled a great wonderment of the unknown in me. I feel that my passion for physics and desire to delve into the frontiers of knowledge are at least partly due to them. They also taught me the value of hard and honest work, whether it be physical or mental, and for that lesson, I am eternally grateful. It sometimes pains me to think about the sacrifices they all made in their own lives so that I had the opportunity at an education. I hope that this dissertation will, in some small way, show that those sacrifices were not in vain.

Of course, a proper acknowledgment would not be complete without thanking those in the Boston University physics department who touched my life, through physics or otherwise. I would like to thank Mirtha Cabello, for always being so helpful, practicing Spanish with me, and helping María and I find a place to live upon moving to Boston. I would also like to sincerely thank Sidney Redner for being perhaps the most lucid and kind professor of my graduate school tenure. Finally, I am extremely grateful to Claudio Chamon. My respect for him stems not only from his teaching ability but also his humility and profound guidance on my own research.

Finally, I owe an enormous debt of gratitude to my advisor and mentor Michael El-Batanouny. I often smile thinking that much of what I know about the finer details of our physical world is due to a man who started his own journey halfway across the world in a completely different culture. He has accomplished so much in his own life that it is often difficult to imagine where he found time to do it all, but I

look at that as a source of inspiration rather than intimidation. I thank him for his endless patience, profound insight, and occasional history lesson! I thank him for the thorough conversations, long experiments, and countless Skype calls. Perhaps, they were not all enjoyable at the time, but they have made me the scientist that I am today, and for that, I am forever grateful.

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List of Abbreviations

2D	Two dimensional
ARPES	Angle-resolved photoemission spectroscopy
BZ	Brillouin zone
DFQ	Dirac fermion quasiparticle
EPC	Electron-phonon coupling
FPGA	Field programmable gate array
FWHM	Full width at half maximum
HASS	Helium atom-surface scattering
MCPEM	Multichannel plate electron multiplier
QHE	Quantum hall effect
QSHE	Quantum spin hall effect
RGA	Residual gas analyzer
SBZ	Surface Brillouin zone
TCI	Topological crystalline insulator
TI	Topological insulator
TOF	Time of flight
TRS	Time-reversal symmetry
UHV	Ultra-high vacuum