Quantum anomalous Hall and antiferroelectric topological insulators

David Vanderbilt
Rutgers University
Brief history of TIs

Quantum Anomalous Hall Effect

- Proposed: 1988
- Discovered: 2013

Haldane, 1988

Quantum Spin Hall Effect

- Discovered: 2007

3D Topological Insulators

- Discovered: 2008

Physics World, IOP

Bi$_2$Se$_3$
This talk

Quantum Anomalous Hall Effect

$E = -\Delta$

$E = +\Delta$

Haldane, 1988

3D Topological Insulators

$Bi_2Se_3$

Part I

Part II

ES17, Princeton, June 26, 2017
Outline

Part I
• QAH from La/Lu on CrSi(Ge)Te$_3$
• “Flux state” in hybrid-functional calculations

Part II
• Antiferroelectric topological insulators
• Switch topological state by E-field ?
Collaborators

Part I
QAH: Lu/CrGeTe$_3$

Jianpeng Liu
*(now at UCSB)*

Se Young Park

Kevin Garrity

Part II
Antiferroelectric TIs

Tomeu Monserrat
*(moving to U. Cambridge)*

Joe Bennett

Karin Rabe

NSF DMR-1408838

ONR N0014-16-1-2591

Rutgers
Ordinary Hall conductivity

Measure $\sigma_{xy}$ in presence of $B$-field
Anomalous Hall conductivity (AHC)

Measure $\sigma_{xy}$ in **absence** of $B$-field
Quantum Hall effect

$\sigma_{xy} = 2 \frac{e^2}{h}$

~ 1980
Hall effects: The big picture

- Induced by B-field
  - Ordinary Hall
  - Quantum Hall
- Ferromagnetic sample
  - Anomalous Hall
  - Quantum Anomalous Hall

Metal
Topological insulator
Quantum anomalous Hall (QAH) effect

Ferromagnetic insulator

\[ \sigma_{yx} = \frac{e^2}{h} \]

Like integer quantum Hall, but no \( B_{\text{ext}} \)
QAH state has chiral edge channels

Dissipationless edge currents

Potential applications
2D: String Berry phases in QAH band

\[ \phi(k_x) = -\text{Im} \ln \left[ \langle u_1 | u_2 \rangle \langle u_2 | u_3 \rangle \cdots \langle u_{n-1} | u_n \rangle \right] \]
2D: String Berry phases in QAH band

\[ \phi(k_x) = -\text{Im} \ln \left[ \langle u_1 | u_2 \rangle \langle u_2 | u_3 \rangle \cdots \langle u_{n-1} | u_n \rangle \right] \]
Hybrid Wannier centers: $y_c$ vs. $k_x$

At each $k_x$, find 1D WF along $y$, and their centers

$$y_c(k_x) = \langle w_n,k_x | \hat{y} | w_n,k_x \rangle$$
Wannier centers in $y_c$ vs. $k_x$

At each $k_x$, find 1D WF along $y$, and their centers

\[ u_n(k_x) = \langle \hat{y}_y | w_{n,k_x} \rangle \]

\[ \sigma_{yx} = C \frac{e^2}{\hbar} \]

\[ E = C = 1 \]
Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the “Parity Anomaly”

F. D. M. Haldane

Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance $\sigma^{xy}$ in the absence of an external magnetic field. Massless fermions without spectral doubling occur at critical values of the model parameters, and exhibit the so-called “parity anomaly” of (2+1)-dimensional field theories.
Discovery of QAH (2013)

Experimentally observed quantum anomalous Hall effect in a magnetic topological insulator.

Cr-doped (Bi,Sb)$_2$Te$_3$ films

98% of $e^2/h$ at 30mK
Slightly Higher $T$

High-precision realization of robust quantum anomalous Hall state in a hard ferromagnetic topological insulator

Cui-Zu Chang†, Weiwei Zhao‡, Duk Y. Kim§, Haijun Zhang∥, Badih A. Assaf‡, Don Heiman¶, Shou-Cheng Zhang∥, Chaoxing Liu‡, Moses H. W. Chan‡ and Jagadeesh S. Moodera†

V-doped (Bi,Sb)$_2$Te$_3$ films

97% of $e^2/h$ at 200mK
99.98% of $e^2/h$ at 25mK

March 2015

5K
0K
High-\( T_c \) QAH?

High-\( T_c \) superconductors

High-\( T_c \) QAH insulators
QAH insulators

• “QAH insulator” = “Chern insulator”

• Usefulness:
  – Precision measurement?
  – Dissipationless “wires” for microelectronics?
  – Magnetoelectric coupling?

• Needed:
  – 2D ferromagnetic insulator
  – Strong spin-orbit coupling
Idea #1: Heavy atoms on magnetic substrate

Top view

Side view

Pb  Mn  Te

Spins

Kevin Garrity
NIST
Washington, DC

ES17, Princeton, June 26, 2017
Honeycomb Pb on MnTe

- $E_F$ is in gap of 36 meV with $C=-1$
- This is a QAH insulator!
- Even larger minimum direct gap (>0.2 eV above)
Idea #2: Rocksalt EuO/GdN

Kevin Garrity and D.V.

*Chern insulators from a magnetic rocksalt interface*

Idea #2: Rocksalt EuO/GdN

$C = -1$    Gap = 130 meV
Idea #3: Adatoms on CrSiTe$_3$ or CrGeTe$_3$

$E_g \sim 1$ eV
FM, $T_c \sim 32$K
Magnetization $\perp$ surface
Non-polar surfaces
Adatoms on CrSiTe$_3$ or CrGeTe$_3$

Top view

Adatoms:
- Bi, Pb, Tl, Hg, Au, In, Sb, Sn
  - No luck
- Rare earths: La, Lu
  - Bizarre result:
    - Found QAH state
    - Turned off SOC
    - It survived!

Side view

Substrate:
Single-layer CrSiTe$_3$ or CrGeTe$_3$
Bizarre result for CrGeTe$_3$:Lu

Hybrid functional calculation (without SOC)

Blue: Majority spin
Red: Minority spin

Spontaneously broken time reversal!
Orbital currents: “Flux state”

Orbital currents and orbital moments for CrGeTe₃:Lu
QAH insulator, $C=-1$

Edge bandstructure and anomalous Hall conductivity for CrGeTe$_3$:Lu
Summary: QAH insulators

- Sponateous TR breaking in orbital sector
  - Lu on CrGeTe$_3$
  - La on CrSiTe$_3$
- Generates QAH insulating state
  - Within hybrid functional calculation
- Test with beyond-DFT methods?
Recent related preprint

Quantum anomalous Hall state from spatially decaying interactions on the decorated honeycomb lattice

Mengsu Chen, Hoi-Yin Hui, Sumanta Tewari, V. W. Scarola

(Submitted on 16 May 2017)
Outline

Part I:
• QAH from La/Lu on CrSi(Ge)Te$_3$
• “Flux state” in hybrid-functional calculations

Part II
• Antiferroelectric topological insulators
• Switch topological state by E-field (?)
Polarity of 3D topological insulators (TIs)

Centrosymmetric TIs
• Bi$_2$Se$_3$, Bi$_2$Te$_3$, etc.

Polar TIs
• BiTeI under pressure
• Polarization not switchable

Ferroelectric TIs
• Sb$_2$Te$_3$-GeTe$^1$; LiZnSb and CsPbI$_3^2$; KMgBi$^3$
• Polarization switching does not change topological state
• But it does reverse surface state chirality

$^1$Tominaga et al., Adv. Mater. Interfaces 1, 1300027 (2014)
Ferroelectrics and antiferroelectrics

Ferroelectric (FE)

Antiferroelectric (AFE)
AFE TIs

Type I

Type II

Type III

Topological insulator

Normal insulator
• Can AFE and TI coexist?
• TI: need strong SOC and small band gaps
• Oxides have large band gaps (>1 eV)
• New families of non-oxide AFEs could provide a good platform for materials search
ABC antiferroelectrics

**Polar**

$P6_3/mmc$ LiGaGe

**Nonpolar**

$P6_3/mmc$ ZrBeSi

**Antipolar**

$Pnma$ MgSrSi

1\textsuperscript{st} order phase transition
Previous high-throughput study

<table>
<thead>
<tr>
<th>ABC</th>
<th>$\Delta E_{sw}$ (meV)</th>
<th>$P$ (C/m²)</th>
<th>$\Gamma^+_5$</th>
<th>$M^-_2$ (meV)</th>
<th>$\Delta E$ (meV)</th>
<th>$\Delta V$ ($\text{Å}^3$)</th>
<th>$\Delta V/V$ (%)</th>
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<td>LiBeP</td>
<td>119</td>
<td>0.85</td>
<td>0.26</td>
<td>1.26</td>
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<td>20</td>
<td>0.38</td>
<td>0.41</td>
<td>1.28</td>
<td>230</td>
<td>0.49</td>
<td>1.1</td>
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<td>MgLiAs</td>
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<td>0.39</td>
<td>0.42</td>
<td>1.35</td>
<td>207</td>
<td>0.12</td>
<td>0.2</td>
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<td>CaLiSb</td>
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<td>0.18</td>
<td>0.19</td>
<td>1.17</td>
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<td>0.1</td>
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<td>CaLiBi</td>
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<td>0.19</td>
<td>0.20</td>
<td>1.16</td>
<td>80</td>
<td>-0.10</td>
<td>-0.1</td>
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<td>NaMgP</td>
<td>102</td>
<td>0.49</td>
<td>0.31</td>
<td>1.43</td>
<td>275</td>
<td>1.88</td>
<td>3.2</td>
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<tr>
<td>NaMgAs</td>
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<td>0.48</td>
<td>0.34</td>
<td>1.44</td>
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<td>NaMgSb</td>
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<td>0.43</td>
<td>0.40</td>
<td>1.51</td>
<td>154</td>
<td>0.93</td>
<td>1.2</td>
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<td>NaMgBi</td>
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<td>0.42</td>
<td>0.44</td>
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<td>1.4</td>
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<td>1.4</td>
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<td>KNaS</td>
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<td>2.7</td>
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<tr>
<td>KNaTe</td>
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<td>0.38</td>
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<td>NaAgSe</td>
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<tr>
<td>BaCaSi</td>
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<td>0.35</td>
<td>1.62</td>
<td>310</td>
<td>0.37</td>
<td>0.4</td>
</tr>
</tbody>
</table>


Also LiMgBi
DFT with spin-orbit

Type III

Polar P6\textsubscript{3}mc (P)

Non-polar Pnma (NP)

All six phases are TI under ambient conditions!

<table>
<thead>
<tr>
<th></th>
<th>$E_P - E_{NP}$</th>
<th>$E_g(P)$</th>
<th>$E_g(NP)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiMgBi</td>
<td>59</td>
<td>66</td>
<td>12</td>
</tr>
<tr>
<td>NaMgBi</td>
<td>122</td>
<td>85</td>
<td>22</td>
</tr>
<tr>
<td>KMgBi</td>
<td>239</td>
<td>96</td>
<td>16</td>
</tr>
</tbody>
</table>

(Units = meV)
Find Type-I or Type-II behavior?

Try modifying these compounds with

- Epitaxial strain
- Hydrostatic pressure
LiMgBi with epitaxial strain
LiMgBi with epitaxial strain

Energy (eV)

-1.0

0.0

0.5

1.0

K

Γ

AK

Mg

Bi

NI

-2.9%

TI

+0.3%
LiMgBi with epitaxial strain
Displacements of torsion can be decomposed into two modes: an antipolar mode (shifting of atoms along \( \text{mc} \)) that breaks the high-symmetry structure to \( /\text{C}0\text{mc} \)), followed by a nonpolar mode (shifting of \( /\text{mc} \)) that does not break any additional symmetry. A polar distortion specified by a Wyckoff position of \( 3d \) along \( /\text{mc} \)\) is obtained by a nonpolar distortion of \( /\text{C}0\text{mc} \), followed by a polar mode (shifting of \( 3d \) along \( /\text{mc} \)) that does not break any additional symmetry.

**FIG. 1 (color online).** Left panel: planar buckling distortions of the high-symmetry ZrBeSi structure type (center), as described in Ref. \([21]\) (previously referred to as the anti-ABC structure type relative to the high-symmetry ZrBeSi structure). Right panel: antipolar distortions of the MgSrSi structure relative to the LiGaGe-type structure. Finally, we included 20 compounds in the MgSrSi structure type. We identify 11 combinations drawn from the high-throughput study of Bennett et al.\([27]\) that are predicted to have the orthorhombic structure. These candidate antiferroelectrics \([28]\) in addition to being insulating, these compounds can have spontaneous polarization comparable to that of BaTiO\(_3\).

For each structural variant \( \text{ABC} \text{BC}\), we included 13 combinations studied, we find that the band gaps are in the range of 0.2 to 0.2 eV. For all insulating compounds for which both the FE and AFE phases are insulating and in addition to being insulating, these compounds can have an energy difference below 0.2 eV. For all insulating compounds, nonpolar distortions, band gaps, and structural parameters, nonpolar distortions, band gaps, and for the future development of new high-performance ferroelectrics offer promise for experimental investigation and for the future development of new high-performance ferroelectrics offer promise for experimental investigation.

Our search set of candidate MgSrSi-type antiferroelectrics \([30]\) was used to generate maxi-AB \( /\text{C}0\text{mc} \), where the underscore indicates a substitution of a block element for a f-block element from the high-throughput study of Zhang et al.\([31]\) that are predicted to have the orthorhombic structure. Finally, we included 20 compounds in the MgSrSi structure type. We identify 11 combinations drawn from the high-throughput study of Bennett et al.\([27]\) that are predicted to have the orthorhombic structure. These candidate antiferroelectrics \([28]\) in addition to being insulating, these compounds can have spontaneous polarization comparable to that of BaTiO\(_3\).

In this Letter, we use first-principles methods to establish a new class of antiferroelectrics in the MgSrSi structure. Finally, we included 20 compounds in the MgSrSi structure type. We identify 11 combinations drawn from the high-throughput study of Bennett et al.\([27]\) that are predicted to have the orthorhombic structure. These candidate antiferroelectrics \([28]\) in addition to being insulating, these compounds can have spontaneous polarization comparable to that of BaTiO\(_3\).

Orthorhombic: \( b/a \) changes by \( \sim8\% \) in LiMgBi.
LiMgBi with epitaxial strain
Find Type-I or Type-II behavior?

Try modifying these compounds with

- Epitaxial strain
  - LiMgBi: Type I from -1.3% to 0.4%
  - NaMgBi: Metal/TI at 0% (Type II at -4.5%)
  - KMgBi: Metal/TI at 0% (Type III below -1%)

- Hydrostatic pressure?
KMgBi under hydrostatic pressure

Diagram showing the band gap (meV) as a function of pressure (GPa). The graph is divided into regions labeled Ambient, Polar, TI, Metal, NI, and NP. The pressure axis ranges from 0 to 3 GPa. The diagram also includes a phase diagram with high pressure regions marked as Type I.
Find Type-I or Type-II behavior?

Try modifying these compounds with

- **Epitaxial strain**
  - LiMgBi: Type I from -1.3% to 0.4%
  - NaMgBi: Metal/TI at 0% (Type II at -4.5%)
  - KMgBi: Metal/TI at 0% (Type III below -1%)

- **Hydrostatic pressure**
  - LiMgBi: Becomes unstable rel. to MgLiBi
  - NaMgBi: Stays Type III to 2.1 GPa
  - KMgBi: Type I from 0.9 to 2.5 Gpa
Summary: AFE TIs

Type I
- P → TI
- strained LiMgBi
- pressurized KMgBi

Type II
- P → TI
- strained NaMgBi
- strained KMgBi

Type III
- P → TI
- equilibrium AMgBi
- A = Li, Na, K
Can Type-I AFE TI be switched?

Apply $E$

$E = 0 : NP + \text{Normal}$

Metallic !

Polar + TI

Short circuit: Collapse of $P$ ?
Proposal: AFE + TI can be realized in a class of ABC antiferroelectrics

Best candidates: $X\text{MgBi}, X=\text{Li, Na, K}$

Type I (polar state is TI) in LiMgBi under epitaxial strain conditions

Other cases possible with epi strain or hydrostatic pressure

Switchability raises interesting questions for Types I and II
Collaborators

Part I
QAH: Lu/CrGeTe₃

Jianpeng Liu
(now at UCSB)

Kevin Garrity
Se Young Park

Part II
Antiferroelectric TIs

Tomeu Monserrat
(See poster on temperature effects in TIs)

Joe Bennett
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