First-order topological quantum phase transitions

With Vladimir Juričić and Sasha Balatsky

Topological materials

Quantum Hall effect:

\[ \mathbb{Z}_2 \] topological insulators:

\[ \nu \in \{1, 0, 0\} \]

[Image of Bi\(_2\)Se\(_3\) band structure]

\[ E_{B}(eV) \]

\[ k_x (\text{Å}^{-1}) \]

\[ k_y (\text{Å}^{-1}) \]

M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010).

Topological crystalline insulators:


Quantum spin-Hall effect:

[Image of band structure]

M. Z. Hasan et al., Rev. Mod. Phys. 82, 3045 (2010).
The canonical understanding:
The canonical understanding:

- Topological phase transition can only occur when accompanied by a closing of the gap.
The canonical understanding:

- Topological phase transition can only occur when accompanied by a closing of the gap.
The canonical understanding:

- Topological phase transition can only occur when accompanied by a closing of the gap.
- Second-order phase transition
Contradicting experiments?

**ARPES** data on topological crystalline insulators.

Lead-doped tin selenide:

![Graph](image)

Contradicting experiments?

ARPES data on topological crystalline insulators.

Lead-doped tin selenide:


Tin-doped lead telluride:

B. A. Assaf et al., NPJ Quantum Materials 2, 26 (2017).
Contradicting experiments?

**ARPES data on topological crystalline insulators.**

**First-order phase transition**

**Lead-doped tin selenide:**


**Tin-doped lead telluride:**

Bernevig-Hughes-Zhang (BHZ) model:

\[ H(k) = v_F \Gamma \cdot k + (M - Bk^2) \Gamma_0 \]

with spectrum:

\[ \epsilon(k) = \sqrt{M^2 + (1 - 2MB)k^2 + B^2k^4} \]

- **$B$** is the band curvature (linked to doping).
- **$M$** is the band gap.
- \( \text{signum}(MB) > 0 \Rightarrow \text{topological phase.} \)
Thermodynamic analysis of BHZ model

- Bernevig-Hughes-Zhang (BHZ) model:
  \[ H(k) = v_F \Gamma \cdot k + (M - Bk^2) \Gamma_0 \]
  with spectrum:
  \[ \epsilon(k) = \sqrt{M^2 + (1 - 2MB)k^2 + B^2k^4} \]

- Compute the free energy at zero temperature:
  \[ F_0 = \int \frac{d^3k}{(2\pi)^3} \epsilon(k) \]

- \( B \) is the band curvature (linked to doping).
- \( M \) is the band gap.
- \( \text{signum}(MB) > 0 \Rightarrow \) topological phase.
Thermodynamic analysis of BHZ model

- Bernevig-Hughes-Zhang (BHZ) model:
  
  \[ H(\mathbf{k}) = v_F \mathbf{\Gamma} \cdot \mathbf{k} + \left( M - Bk^2 \right) \Gamma_0 \]

  with spectrum:

  \[ \epsilon(\mathbf{k}) = \sqrt{M^2 + (1 - 2MB)k^2 + B^2k^4} \]

- Compute the free energy at zero temperature:

  \[ F_0 = \int \frac{d^3k}{(2\pi)^3} \epsilon(k) \]

- \( B \) is the band curvature (linked to doping).
- \( M \) is the band gap.
  
  \[ \rightarrow \text{Treat as variational parameter.} \]

- \( \text{signum}(MB) > 0 \Rightarrow \text{topological phase.} \)
Thermodynamic analysis of BHZ model

- Bernevig-Hughes-Zhang (BHZ) model:

\[ H(\mathbf{k}) = v_F \mathbf{\Gamma} \cdot \mathbf{k} + \left( M - Bk^2 \right) \mathbf{\Gamma}_0 \]

with spectrum:

\[ \epsilon(\mathbf{k}) = \sqrt{M^2 + (1 - 2MB)k^2 + B^2k^4} \]

- Compute the free energy at zero temperature:

\[ F_0 = \int \frac{d^3k}{(2\pi)^3} \epsilon(k) \]

- Critical \( B \approx 0.23 \) where first-order phase transition occurs

- \( B \) is the band curvature (linked to doping).
- \( M \) is the band gap.
  \( \rightarrow \) Treat as variational parameter.
- \( \text{signum}(MB) > 0 \Rightarrow \) topological phase.

What is a TPT in these materials?

Topological phase transition $\Rightarrow$ rearrangement of electron wave function.

Size of red dot is fraction of electron charge on Te atom.

Interlude: 2D vs 3D materials

Does this also work for 2D TIs?

Full expression for $F_0$ in 3D is:

$$F_0(M, B) = \sum_n \frac{M^4}{D_n} [A_n(MB) + C_n(MB) \log M^2]$$

- In 2D, the log term does not appear,
- This means only one minimum,
- Which moves smoothly through $M = 0$
- $\Rightarrow$ Second-order phase transition.
Finite temperature phase diagram

Include entropic contribution at finite temperature:

\[ F = F_0 + F_S = \int \frac{d^3k}{(2\pi)^3} \epsilon(k) + \int \frac{d^3k}{(2\pi)^3} \log \left( 1 + e^{-\epsilon(k)/T} \right) \]

- \( B \) can vary with \( T \):
  \[ B = B_0 - B_1 T. \]
- \( B_0 \) is doping contribution,
- \( B_1 \) is thermal expansion coefficient.


\[ B(T) < 0 \]

Increasing doping \( (x) \) \( \Rightarrow \) increasing \( B_0 \).


Experimental interpretation


Experimental interpretation


Re-entrant behaviour at (very?) high $T$?

- First-order topological phase transitions are possible.
- Qualitative agreement with experiments.


Reference:

✉️ david.abergel@nordita.org
🐦 @David_Abergel