Strong correlation effects in 2D topological quantum phase transitions

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Introduction.

Ginzburg-Landau theory: *symmetry breaking* classification of matter phases

key concept: *local order parameter*

- **Magnetism**
  - magnetization $M$
- **Liquid-gas**
  - density difference $n(L) - n(G)$
- **“Superconductivity”**
  - pair amplitude $\psi$

Experimental detectability!
Introduction.

TOPOLOGICAL INSULATORS
quantum materials eluding the G-L paradigm!

bulk (band) insulator + with *gapless* edge modes.

*Dirac semi-metal* + *Spin-Orbit Coupling*

States classified in terms of the *Topological Properties* of the Hilbert space of Bloch functions:

key concept: *global topological invariant*
The quantum spin-Hall insulator

Initial focus on graphene but small SOC \((\text{gap} \sim 10^{-3}\text{meV})\)

**Idea:** look for systems with a larger SOC.

**BHZ model:** \(2\ QHI + \ \text{Time Reversal Symmetry.}\)

\[
H = \begin{pmatrix}
\hbar(k) & 0 \\
0 & \hbar^*(-k)
\end{pmatrix}
\]

\[
\hbar(k) = \mathbf{d}(k) \cdot \boldsymbol{\tau}
\]

Orbital pseudo-spin structure

\[
\mathbf{d}(k) = \begin{bmatrix}
\lambda \sin k_x, \lambda \sin k_y, M - \varepsilon(k)
\end{bmatrix}
\]

\(\text{CdTe/HgTe quantum wells.}\)

\(\text{Kane,Mele PRL 2005}\)

\(\text{Bernevig et al Science 2006}\)

\(\text{Konig et al Science 2007}\)
Topological QPT

BHZ description of topological transition:

\[ h(k) = d(k) \cdot \tau \]

Continuous Topological Quantum Phase Transition

Band structure evolves smoothly with control parameters...

trivial band insulator
Topological QPT

BHZ description of topological transition:

\[ h(k) = d(k) \cdot \tau \]

Continuous Topological Quantum Phase Transition

 bande structure evolves smoothly with control parameters...

Dirac cone semi-metal
Topological QPT

BHZ description of topological transition:

\[ h(k) = d(k) \cdot \tau \]

Continuous Topological Quantum Phase Transition

`band structure evolves smoothly with control parameters...`
What about the interaction?

Quest for larger **SOC**...heavy elements compounds (5d/4,5f)

Hexaborides **Sm/PuB$_6$**, Ir-based pyrochlores: **Sr$_2$Ir$_2$O$_7$**, etc..

Dzero et al. PRL 2010
D. Pesin, L. Balents, NP 2010
Deng et al PRL 2013

New materials?

Engineering correlated TI: **Transition Metal Oxides Heterostructures**

DMFT solution

Dynamical Mean-Field Theory
non-perturbative solution of the interacting problem

Idea: Reduce the interacting lattice problem to a self-consistent impurity problem

Advantages:
+ local quantum physics (beyond Hartree-Fock).
+ non-perturbative in the interaction
+ access to topological invariant

Drawbacks:
- neglects spatial fluctuations
- computational demanding...

solve using Exact Diagonalization & CTQMC

Obtain dynamical (non-scalar) self-energy. Describes the effects of interaction.
\[ \hat{\Sigma}(\omega) = \text{Re} \Sigma(\omega) \tau_z + \text{Im} \Sigma(\omega) \tau_0 \]
BHZN - Interaction

BHZN effective minimal model + multi-orbital interactions

LOW-SPIN  HIGH-SPIN

\[ H_I = (U - J_H) \frac{N(N - 1)}{2} - J_H \left( \frac{N^2}{4} + \frac{S_z^2}{2} - 2T_z^2 \right) \]

Effective reduction of the Mass term: 
\[ M_{\text{eff}} = M + \text{Tr} [\tau_z \hat{\Sigma}(0)] / 2 \]

Interaction driven TI

Mott phase at large U
Correlated QSHI

Phase diagram M-U (flipped view).

Weak coupling: Continuous \( \sim U=0 \)

Strong coupling: 1st order TQPT correlated many-body character
Correlated QSHI

A clear picture from the iso-U curves

\[ \Delta M_{\text{eff}} = M_{\text{eff}}(BI) - M_{\text{eff}}(QSH) \]

Metastable states hallmark of 1\textsuperscript{st} transition.

Diverging orbital compressibility at \( U=U_c \)

\[ \kappa = \partial \langle T_z \rangle / \partial M \]

Experimental accessible quantities marking the TQPT.
Absence of gap closure

The transition to a topological state occurs thru band-gap closing. 

$\mathbf{U < U_c}$
The transition to a topological state occurs thru band-gap closing. 

$\mathbf{Dirac \ cone \ formation.}$

$\mathbf{U > U_c}$
No gap-closing

No suppression of any symmetries protecting the topological state.

**Breakdown of the gap-less TQPT paradigm…**

弱耦合

$\Gamma$ $k$

$P(k)$

$M=3.22$ $M=3.23$ $M=3.24$ $M=3.251$ $M=3.26$ $M=3.27$ $M=3.28$

$\mathbf{U=2}$

带隙

强耦合

$\Gamma$ $k$

$P(k)$


$\mathbf{U=11}$

带隙
Correlated edge states

Consider a 2D stripe.

\[ H = \sum_{k_x y y'} \Psi_{k_x y}^+ M(k_x) \delta_{y y'} \Psi_{k_x y'} + \sum_{k_x y y'} \left( \Psi_{k_x y}^+ T \delta_{y+1 y'} \Psi_{k_x y'} + H.c. \right) \]

\[ M = [M - 2t \cos k_x] \Gamma_5 + \lambda \sin k_x \Gamma_x \]

\[ T = -t \Gamma_5 + i \frac{\lambda}{2} \Gamma_y \]

Helical gapless states localized at the edges.

What’s the effects of strong correlation on the 2D stripe?
Correlated edge states

Sequence of transitions to reach the Mott state.

$U_{c1}$, $U_{c2} \ldots U_c$

$y=1$, $y=2$, $y=3$, $y=4$, $y=5$

AA et al. PRB 2017
Correlated edge states

What's the fate of the edge states?

Bulk compression $\rightarrow$ Edge state reconstruction

Topological properties with OBC:

Local Chern Marker

$$C_\sigma(r) = 2\pi i \langle r | \hat{x}_P \hat{y}_Q - \hat{y}_P \hat{x}_Q | r \rangle$$

$$\mathbb{Z}_2 = (C_\uparrow - C_\downarrow)/2$$
Conclusions.

• Topological States can be favoured by strong interaction.
• Emergent thermodynamic character: 1\textsuperscript{st} order transition.
• New paradigm for TQPT: no gap closing but no symmetry breaking!
• Correlation driven edge states reconstruction.

Outlook...

• Break TRS or IS: correlation effects in Weyl SM.
• Interplay of strong interaction and SOC: from models to real materials.
• Topological Mott Insulators.
• Condensed matter realization of excitations beyond “standard model”