Majorana stripe order on the surface of a three-dimensional topological insulator

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Talk plan

• Brief introduction

• Model of *interacting* Majorana fermions
  — Symmetry considerations at the noninteracting level
  — Map to a quantum spin model in the special “neutrality” condition
  — Application of the world-line QMC methods
  — Further duality mapping to a quantum compass model
  — Away from the neutrality condition: mean-field theory

• Summary
Majorana zero modes (MZMs)

• (Generalized) bulk-boundary correspondence

  topological class of the bulk

  number of gapless edge states

  number of zero modes bound to topological defects (e.g., vortices)

  topo.
  trivial
  gapless edge state
  topo. SC
  vortex
  Majorana zero mode bound to a vortex
  Teo and Kane, PRB 2010

• Effect of interactions on the edge/vortex states?
Setup for a Majorana lattice

- Surface of a 3D TI subject to a SC proximity effect
  - Topological surface state resembling 2D $p+ip$ SC
  - Majorana zero modes (MZMs) bound to vortices
  - Introduce Abrikosov vortex lattice (Chiu et al, PRB 2015)

Figure credit: C.-K. Chiu et al.
Vortex state in the Fu-Kane model

Fu and Kane, PRL 2008
cf. Symposium talk by Hiroki Isobe (Nov. 9)

\[ \hat{H}_{FK} = \frac{1}{2} \int d^2r \hat{\Psi}^\dagger \mathcal{H}_{FK}(r) \hat{\Psi} ; \quad \hat{\Psi} = (\psi_{r}, \psi_{\downarrow r}, \psi_{\downarrow r}^\dagger, -\psi_{\uparrow r}^\dagger)^T \]

\[ \mathcal{H}_{FK} = \tau^z \left( -i v_F \sigma \cdot \nabla - \mu_F \right) + \text{Re} \Delta(r) \tau^x + \text{Im} \Delta(r) \tau^y, \]

\( \tau^{x,y,z} \) (\( \sigma^{x,y,z} \)) \cdots Pauli matrices in the Nambu (spin) basis

\( \Delta(r) \) \cdots proximity-induced pair potential

\( v_F \) \cdots velocity of the surface Dirac mode for \( \Delta = 0 \)

• Solution in the presence of a vortex \( \Delta(r) = \Delta_0(r) e^{-i(n\varphi+\vartheta)} \)

\[ \hat{\gamma} = \int d^2r \left( u(r) \psi_{\downarrow r} + u^*(r) \psi_{\downarrow r}^\dagger \right) = \hat{\gamma}^\dagger \]

\[ u(r) = u(r) = \mathcal{N}^{-1} e^{i\left(\frac{\vartheta}{2} - \frac{\pi}{4}\right)} \exp \left( -\int_0^r \Delta_0(r')dr' \right) \]

MZM
Symmetry considerations

• Different sym. classes for $\mu_F = 0$ and $\mu_F \neq 0$  
  Chiu et al., PRB 2015

  $$\mathcal{H}_{FK} = \tau^z \left(-i v_F \sigma \cdot \nabla - \mu_F \right) + \text{Re} \, \Delta(r) \tau^x + \text{Im} \, \Delta(r) \tau^y,$$

  $$\hat{\Psi}_r = (\hat{\psi}^\dagger_r, \hat{\psi}_r, \hat{\psi}^\dagger_r, -\hat{\psi}^\dagger_r)^T$$

— General case ($\mu_F \neq 0$) : symmetry class D

  1. Time-reversal symmetry is absent due to the applied magnetic field

  2. Only particle-hole symmetry $\Xi = \sigma^y \tau^y K$

— “neutrality condition” ($\mu_F = 0$) : symmetry class BDI

  3. Additional artificial time-reversal symmetry $\Theta_{\text{eff}}$

  $$\Theta_{\text{eff}} = \sigma^x \tau^x K, \quad \Theta_{\text{eff}}^2 = 1$$
Important consequences of $\Theta_{\text{eff}}$

- MZM for a vortex is a spin-down state

\[ \hat{\gamma} = \int d^2 r \left( u(r) \psi_{\downarrow r} + u^*(r) \psi_{\uparrow r}^\dagger \right) \]

- The usual quadratic hybridization term is prohibited

\[ \hat{\Theta}_{\text{eff}} \hat{\gamma} \hat{\Theta}_{\text{eff}}^{-1} = \hat{\gamma} \]

\[ \hat{\Theta}_{\text{eff}} i \hat{\Theta}_{\text{eff}}^{-1} = -i \]

- Consequently, the corresponding interacting model must be in the strong coupling limit under the neutrality condition.

\[ \hat{H}_{\text{int}} = \sum_{i>j} i t_{ij} \hat{\gamma}_i \hat{\gamma}_j + \sum_{i>j>k>\ell} g_{ijk\ell} \hat{\gamma}_i \hat{\gamma}_j \hat{\gamma}_k \hat{\gamma}_\ell + \ldots \]

\[ \text{kinetic energy completely suppressed} \]
Square-lattice Majorana model

Simplest local interactions in the neutrality condition ($\mu_F = 0$)

\[
\hat{H}_g = g \sum_{\square} \hat{\gamma}_{\square_1} \hat{\gamma}_{\square_2} \hat{\gamma}_{\square_3} \hat{\gamma}_{\square_4}
\]

\[
\hat{\gamma}_r^\dagger = \hat{\gamma}_r, \quad \{\hat{\gamma}_r, \hat{\gamma}_{r'}\} = 2\delta_{r,r'}
\]

— Assume a square-lattice Abrikosov vortices (e.g., due to an array of pinning impurities and/or lattice anisotropies)

Additional term for $\mu_F \neq 0$

\[
\hat{H}_t = it \sum_r \left[ \hat{\gamma}_r \hat{\gamma}_{r+b} + (-1)^{r_y} \hat{\gamma}_r \hat{\gamma}_{r+a} \right]
\]

— $\pi$-flux due to underlying vortices  

cf. LuNi$_2$B$_2$C (De Wilde et al., PRL 1997)
Mapping to a spin model at $\mu_F = 0$

1. Introduce pairings

$$\hat{c}_{r_{\sigma}} = \frac{1}{2}(\hat{\gamma}_{r_{\sigma},1} + i\hat{\gamma}_{r_{\sigma},2})$$

complex fermion “bottom” “top”

2. Jordan-Wigner transformation (assuming OBC in the $b$ direction)

$$\hat{c}_{r_{\sigma}}^\dagger \hat{c}_{r_{\sigma}} = \frac{1}{2} \left(1 + \hat{\sigma}_{r_{\sigma}}^z\right)$$

$$\hat{c}_{r_{\sigma}}^\dagger = \frac{1}{2} \left(\prod_{n_{CM}(r'_{\sigma}) < n_{CM}(r_{\sigma})} \hat{\sigma}_{r_{\sigma}}^z\right) (\hat{\sigma}_{r_{\sigma}}^x + i\hat{\sigma}_{r_{\sigma}}^y)$$

$$\hat{H}_{g,\sigma} = -J \sum_{r_{\sigma}} \hat{\sigma}_{r_{\sigma}}^z \hat{\sigma}_{r_{\sigma} + a}^z - P \sum_{\square_{\sigma}} \left(\prod_{r_{\sigma} \in \square_{\sigma}} \hat{\sigma}_{r_{\sigma}}^x\right), \quad J = P = g$$

Faithful spin representation with only local interactions
Application of (bosonic) QMC

- The spin representation for $\mu_F = 0$ does not have the sign problem in the world-line QMC simulation.

- Thermodynamic properties can be investigated in an unbiased way!

- Broad peak in the specific heat at around $T \sim g$

- Additional divergent peak at $T \sim 0.25 \ g$, indicating a finite-temperature transition

- Inconsistent with the previous conjecture of QCP by Chiu et al. (PRB, 2015)

- What’s the nature of the low-$T$ phase?
Possibility of usual order of “spins”?  

- There is a 1D “gauge-like” symmetry in the model for \( \mu_F = 0 \)

\[
[H_{g,\sigma}, \hat{O}^{\text{spin}}_h(y)] = 0, \quad \forall y
\]

\[
\hat{O}^{\text{spin}}_h(y) = \prod_{r_\sigma} \hat{\sigma}_{r_\sigma}^x (r_\sigma^x, y)
\]

Flipping the whole spins in a row

- These 1D symmetries cause a dimensional reduction from 2D to 1D for the order parameter field \( \sigma^z \)

- No long-range order of \( \sigma^z \) is possible at \( T > 0 \) at any momentum, as known as “generalized Elitzur’s theorem”

Batista and Nussinov, PRB 2005
Kramers-Wannier transformation

• To elucidate the nature of the low-$T$ phase, we invoke a two-step duality mapping

\[ P \text{ term: } \begin{bmatrix} \sigma \rightarrow \tau \end{bmatrix} \]

\[ J \text{ term: } \begin{bmatrix} \sigma \rightarrow \tau \end{bmatrix} \]

\[ K.-W. \text{ trans. } \#1 (\sigma \rightarrow \tau) \]

\[ \hat{\tau}_{r_\tau}^{z} = \hat{\sigma}_{r_\sigma}^{z} \hat{\sigma}_{r_\sigma}^{z} + a' \]

\[ \hat{\tau}_{r_\tau}^{x} = \prod_{n_{RM}(r'_\sigma) \leq n_{RM}(r_\sigma)} \hat{\sigma}_{r'_\sigma}^{x} \]

\[ \hat{H}_{g,\tau} = \hat{H}_{g,\tau}^{e} + \hat{H}_{g,\tau}^{o} \]

\[ \hat{H}_{g,\tau}^{e(o)} = \sum_{r_\tau \in \text{even (odd) columns}} \left( -J \hat{\tau}_{r_\tau}^{z} - P \hat{\tau}_{r_\tau}^{x} \hat{\tau}_{r_\tau}^{x} \hat{\tau}_{r_\tau}^{x} + 2a \hat{\tau}_{r_\tau}^{x} + 2b \hat{\tau}_{r_\tau}^{x} + 2a + 2b \right) \]
Finally, we obtain two decoupled copies of the quantum compass model.

K.-W. transformation #2 ($\tau \rightarrow \mu$)

$$\hat{\mu}^x_{\mu} = \hat{\tau}^x_{r_{\tau}} \hat{r}_{r_{\tau}} + 2b$$

$$\hat{\mu}^z_{\mu} = \prod_{\hat{n}_{CM}(r'_{\tau}) \leq \hat{n}_{CM}(r_{\tau})} \hat{r}'_{r_{\tau}}$$

$$\hat{H}_{g,\mu} = \hat{H}_{g,\mu}^c + \hat{H}_{g,\mu}^o$$

$$\hat{H}_{g,\mu}^{c(o)} = \sum_{r_{\mu} \in \text{even (odd) column}} \left(-P \hat{\mu}^x_{r_{\mu}} \hat{\mu}^x_{r_{\mu}+2a} - J \hat{\mu}^z_{r_{\mu}} \hat{\mu}^z_{r_{\mu}+2b}\right)$$
Correspondence of the interactions

\[ \hat{H}_g = g \sum_\square \hat{\gamma}_1 \hat{\gamma}_2 \hat{\gamma}_3 \hat{\gamma}_4 \]

1. Jordan-Wigner transformation
2. Duality transformation

\[ \hat{H}_{g,\mu} = \hat{H}_{g,\mu}^e + \hat{H}_{g,\mu}^o, \quad \hat{H}_{g,\mu}^{e(o)} = \sum_{\text{r}_\mu \in \text{even (odd) column}} \left( -P \hat{\mu}_{\text{r}_\mu}^x \hat{\mu}_{\text{r}_\mu}^x + 2a - J \hat{\mu}_{\text{r}_\mu}^z \hat{\mu}_{\text{r}_{\mu+2b}}^z \right) \]

- The even-odd decoupling of the compass model corresponds to the \textit{checkerboard decomposition} of the Majorana model
“Nematic” order of the compass model

Nussinov and van der Brink, RMP, 2015

• Any spin-spin correlation function is short-ranged at $T > 0$
• Breaking of the spin-lattice $\mathbb{Z}_2$ reflection symmetry

$$\begin{cases} a \leftrightarrow b \\ x \leftrightarrow z \end{cases}$$

Order parameter

$$\hat{D}_\mu (\mathbf{r}_\mu) = \hat{\mu}_x^{\mathbf{r}_\mu} \hat{\mu}_x^{\mathbf{r}_\mu} + 2a - \hat{\mu}_z^{\mathbf{r}_\mu} \hat{\mu}_z^{\mathbf{r}_\mu} + 2b$$

Figure credit: Wenzel and Janke, PRB (2008)
“Majorana stripe” order

\( \mu \) spin (even columns) \( \mu \) spin (odd columns) plaquettes with more energy gain plaquettes with less energy gain

A (even)

B (odd)

A \( \cup \) B
Confirmation by QMC

- The Majorana stripe order appears at $T \sim 0.25g$, consistent with the location of the divergent peak in the specific heat.

**Order parameter**

$$\hat{D}_\sigma(\mathbf{r}_\sigma) = \hat{\sigma}_\sigma^Z \mathbf{r}_\sigma + a \hat{\sigma}_\sigma^Z \mathbf{r}_\sigma + 2a - \hat{\sigma}_\sigma^x \mathbf{r}_\sigma + 2b \hat{\sigma}_\sigma^x \mathbf{r}_\sigma + a + 2b \hat{\sigma}_\sigma^x \mathbf{r}_\sigma + a$$

$$\left( \hat{D}_\mu(\mathbf{r}_\mu) = \hat{\mu}_\mu^x \mathbf{r}_\mu + 2a - \hat{\mu}_\mu^z \mathbf{r}_\mu + 2b \right)$$
Away from the neutrality condition

\[ \hat{H} = \hat{H}_g + \hat{H}_t \]

\[ \hat{H}_g = g \sum \gamma_{1234} \]

\[ \hat{H}_t = it \sum_r \left[ \gamma_r \gamma_{r+b} + (-1)^r \gamma_r \gamma_{r+a} \right] \]

- MF approximation \( \hat{H} \to \hat{H}_{MF} \)
Away from the neutrality condition

\[ \hat{H} = \hat{H}_g + \hat{H}_t \]

\[ \hat{H}_g = g \sum_\square \hat{\gamma}_1 \hat{\gamma}_2 \hat{\gamma}_3 \hat{\gamma}_4 \]

\[ \hat{H}_t = it \sum_\mathbf{r} \left[ \hat{\gamma}_r \hat{\gamma}_{r+b} + (-1)^{\gamma}\hat{\gamma}_r \hat{\gamma}_{r+} \right] \]

- MF approximation \( \hat{H} \rightarrow \hat{H}_{\text{MF}} \)

Gap closing induced by the Majorana hybridization
Phenomenology at $t = t_c$

- Gap closing
- Restoration of the broken translational & rotational symmetries

![Graphs showing order parameter change with $P/J$ at $t = 0.2$ and $t = 0.8$.]
Recent work by Affleck et al.

- Mean-field approx. (similar to ours)
- Low-energy effective model, RG analysis, etc.: weak-coupling instabilities

\[ \mathcal{L} = \bar{\psi} i \gamma^\mu \partial_\mu \psi + |\partial_\mu \phi|^2 - m^2 |\phi|^2 + g_1 (\psi_1^\dagger \psi_2^\dagger \phi + \text{H.c.}) - g_2 |\phi|^4 \quad (g > 0), \]

- The transition \( t = t_c \) is claimed to be SUSY.
  - Both fields are massless at \( t = t_c \), forming an emergent super-multiplet
Summary

• We studied the system of square-lattice Majorana fermions that may be realized at the TI-SC interface.

• Under the neutrality condition (i.e., $\mu_F = 0$), the minimal model can be faithfully mapped to a spin model. The spin representation has no sign problem in the world-line QMC.

• The ground state for $\mu_F = 0$ is a gapped (“Majorana stripe”) state, breaking the translational and rotational symmetries.

• The hybridization induces a quantum phase transition, which might belong to a SUSY universality class.

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