Interaction effects in topological systems: helical Luttinger edge liquid and Majorana flat band

Congjun Wu University of California, San Diego

Selected Reference

- 1. C. Wu, B. Andrei Bernevig, and S. C. Zhang, Phys. Rev. Lett. 96, 106401(2006).
- 2. Dong Zheng, Guang-Ming Zhang, C. Wu, Phys. Rev. B 84, 205121 (2011).
- 3. Da Wang, Zhou-Shen Huang, Congjun Wu, Phys. Rev. B 89, 174510 (2014).
- 4. Yi Li, Da Wang, Congjun Wu, New J. Phys 15, 085002(2013)

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Collaborators:

Dong Zheng Yi Li Da Wang Zhousheng Huang

Guangming Zhang Shoucheng Zhang (Tsinghua/UCSD \rightarrow industry) (UCSD \rightarrow Princeton \rightarrow Johns Hopkins) (UCSD \rightarrow Nanjing Univ.) (UCSD \rightarrow Los Alamos)

(Tsinghua) (Stanford)

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Outline

• Introduction.

Quantum anomalous Hall \rightarrow topological insulators (TI) \rightarrow topological superconductor

• Stability criterial of interacting edge states of 2D TIs, and QMC study of interacting 2D TIs.

Helical Luttinger liquid and its stability against strong interactions.

• Spontaneous time-reversal symmetry breaking in Majorana flat-bands.

2D quantum hall systems

• Chiral edge modes responsible for quantized transverse charge transport; stable against disorder and interactions.

• Magnetic band-structure characterized by the topological TKNN (Chern) number.





Honeycomb lattice system (graphene)





В

• 2-component spinor: A-B \rightarrow two-level with a pseudo-B field.

$$H(\vec{k}) = \vec{h}(\vec{k}) \cdot \vec{\tau}$$

• h(k) is planar.

$$h_x(\vec{k}) = \sum_{i=1}^3 \cos \vec{k} \cdot \hat{e}_i \quad h_y(\vec{k}) = \sum_{i=1}^3 \sin \vec{k} \cdot \hat{e}_i$$

• Gapless Dirac cones $\leftarrow \rightarrow$ vanishing of h(k); protected by symmetry and topology.

 $A \qquad B \\ \hat{e}_3 \qquad B \\ 5$

The Haldane model – complex NNN hopping

TR breaking → Mass term flips the sign at K and K'.
 Work at UCSD!



Anomalous Hall effect (AHE) and its quantization

В

• Berry phase and curvature in momentum space.

$$\vec{A}(k) = \left\langle \psi_{L,k} \mid i \vec{\partial}_k \mid \psi_{L,k} \right\rangle, \qquad \Omega_z(\vec{k}) = \partial_{k_x} A_{k_y} - \partial_{k_y} A_{k_x}$$

• Anomalous velocity.

$$\dot{\vec{r}} = \nabla_k \varepsilon(\vec{k}) - \dot{\vec{k}} \times \vec{\Omega}(\vec{k})$$
$$\dot{\vec{k}} = q\vec{E} + q\vec{r} \times \vec{B}(\vec{r})$$

 Inter-band Van Vleck type response.

$$\boldsymbol{\sigma}_{xy} = \frac{e^2}{h} \int \frac{dk_x dk_y}{2\pi} \boldsymbol{\Omega}_z(\vec{k}) n_f(\vec{k})$$

Luttinger, PR, 112 793 (1958), Xiao, Chang, Niu, RMP 82, 1959 (2010).

$$\Omega_z(K) = \Omega_z(K')$$



Hall conductance as topological Chern (TKNN) number

• Brillouin zone has no boundary – torus.

$$v = \oint \frac{d^2 \vec{k}}{2\pi} \Omega_z(\vec{k}) = \oint \frac{d^2 \vec{k}}{2\pi} (\nabla \times \vec{A}(\vec{k})) = \pm 1$$

• Topology in the Kubo formula (linear response).

$$\sigma_{xy} = \lim_{\omega \to 0} \lim_{q \to 0} \frac{1}{\omega} \operatorname{Im} \langle j_x(q, \omega) j_y(-q, -\omega) \rangle$$
$$= \frac{e^2}{8\pi^2 \hbar} \iint dk_x dk_y \hat{h} \cdot (\partial_{k_x} \hat{h} \times \partial_{k_y} \hat{h}) =$$
$$= \frac{e^2}{2\pi \hbar} \int \frac{d^2 \vec{k}}{2\pi} \Omega_z(\vec{k}) = v \frac{e^2}{\hbar}$$

Thouless, Kohmoto, Nightingale, den Nijis, PRL 49, 405 (1982) Exp: C. Z. Chang et al, Science 340, 167 (2013)





Graphene as a 2D QSH or topo-insulator (TI): tiny gap

• Kane-Mele model: spin-orbit (SO) coupling = two copies of Haldane model.





Kane and Mele, PRL95, 146802(2005); PRL 95, 226801(2005).

• Helical edge states.



Instability: the single-particle back-scattering

$$H_0 = v_f \int dx (\psi_{R\uparrow}^+ i\partial_x \psi_{R\uparrow} - \psi_{L\downarrow}^+ i\partial_x \psi_{L\downarrow})$$

• Kane and Mele : The non-interacting helical systems remain gapless against disorder and impurity scatterings.



• Single particle backscattering term breaks TR symmetry (T²=-1).

$$H_{bg} = \psi_{R\uparrow}^{+} \psi_{L\downarrow} + \psi_{L\downarrow}^{+} \psi_{R\uparrow} \quad T^{-1} H_{bg} T = -H_{bg}$$

• How about interacting effects?



C.-R. Hu, Phys. Rev. Lett. 72, 1526 (1994) L. H. Greene, et al, PRL 89, 177001 (2002)

Majorana boundary zero modes

• Single-component fermion p-wave pairing in 1D – Kitaev 2001.





$$\gamma = \int dx \, u_0(x)\psi(x) + v_0(x)\psi^+(x)$$
$$u_0(x) = v_0^*(x)$$

Spin-orbit coupled superconducting wire under magnetic field – in debate.

P. A. Lee, arxiv 0907.2681 Sau, Lutchyn, Das Sarma PRL 2010. Liu, Potter, Law, Lee, PRL 109, 267002 (2011);

He, Ng, Lee, Law, PRL (2014).

L. P. Kouwenhouven, et al, Science 336 1003 (2012);

C. M. Marcus et al, PRB 87, 241401 (2013).

Observation of the Majorana mode



H. H. Sun, et al, PRL 116, 257003(2016)

<u>Majorana edge modes in quasi-1D Topo</u> <u>superconductors</u>

And reev bound states localized at ends z_0 with energy zero.



$$\gamma_{i} = \int dx \{ u_{0}(x) e^{-i\frac{\theta_{l}}{2} - i\frac{\pi}{4}} \psi_{i}(x) + v_{0}(x) e^{i\frac{\theta_{l}}{2} + i\frac{\pi}{4}} \psi_{i}^{\dagger}(x) \},$$

$$\dots$$

$$u_{0}(x) = v_{0}(x) \approx e^{-\frac{L-x}{\xi_{x}}} \sin k_{\xi} x$$

v

Dispersionless in k_x and k_y

And reev Bound States \rightarrow 1D or 2D Majorana fermions lattices.

Yi Li, Da Wang, Congjun Wu, New J. Phys 15, 085002(2013)

Kitaev, 2000; Tewari, et al, 2007; Alicea, et al, 2010; etc ...

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Interacting 2D TI edges: helical Luttinger liquid (HLL)



• Helical Luttinger liquid is special.

- 1. chiral Luttinger liquids in quantum Hall edges break TR symmetry;
- 2. spinless non-chiral Luttinger liquids: T²=1;
- 3. non-chiral spinful Luttinger liquids have an even number of branches of TR pairs.

Kane et al., PRL 2005, C. Wu et al., PRL 2006.

The "no-go" theorem for helical Luttinger liquids

• 1D HLL with an odd number of components can NOT be constructed in a purely 1D lattice system.



- Double degeneracy occurs at k=0 and π .
- Periodicity of the Brillouin zone.
- HLL with an odd number of components can appear as the edge states of a 2-D system.

Helical edge modes are stable under weak interactions, but can be destabilized by strong interactions!

C. Wu, B. A. Bernevig, S. C. Zhang, PRL 96, 1060401 (2006); C. Xu, J. Moore, PRB 2006.

Two-particle correlated back-scattering

• TR symmetry allows two-particle correlated back-scattering.



$$G_2(t,0) = \left\langle \psi_{R\uparrow 1}(t)\psi_{R\uparrow 2}(t) \; \psi_{L\downarrow 2}^+(0)\psi_{L\downarrow 1}^+(0) \right\rangle_{connected} \neq 0$$

$$H_{um} = \sum_{\langle ij \rangle} s_x(i) s_x(j) - s_y(i) s_y(j),$$

or $\sum_{\langle ij \rangle} s_x(i) s_y(j) + s_y(i) s_x(j)$

- Microscopically, this Umklapp process can be generated from anisotropic spin-spin interactions.
- Effective Hamiltonian: $H_{um} = g_u \int dx \, e^{i4k_f} \psi_{R\uparrow}^+(x) \psi_{R\uparrow}^+(x+\varepsilon) \psi_{L\downarrow}(x+\varepsilon) \psi_{L\downarrow}(x) + h.c.$
- U(1) rotation symmetry $\rightarrow Z_2$. $s_x \rightarrow -s_x$, $s_y \rightarrow -s_y$, $s_z \rightarrow s_z$

Bosonization+Renormalization group

• Sine-Gordon theory at $k_f = \pi/2$.

$$\psi_{R\uparrow} \propto e^{i\sqrt{4\pi\phi_{R\uparrow}}}, \ \psi_{L\downarrow} \propto e^{-i\sqrt{4\pi\phi_{L\downarrow}}}; \ \phi(\theta) = \phi_{R\uparrow} \pm \phi_{L\downarrow}$$
$$H_0 = \int dx \frac{v}{2} \{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \} + \frac{g_u}{2(\pi a)^2} \cos\sqrt{16\pi\phi}$$

• The scaling dimension:

$$\Delta_{g_u} = \frac{(\sqrt{16\pi K})^2}{4\pi} = 4K$$

$$\frac{dg_u}{d\ln L} = (2 - \Delta_{g_u})g_u$$



Bosonization+Renormalization group

• The cosine term is relevant at K<1/2 (strong repulsion); gap opens with

$$g_u \rightarrow \pm \infty \qquad \left\langle \cos \sqrt{16\pi} \phi \right\rangle \neq 0 \qquad \Delta \approx a^{-1} (g_u)^{\frac{1}{4(1/2-K)}}$$

• Order parameters $2k_f$ SDW orders N_x ($g_u < 0$) or N_y at ($g_u > 0$).

$$N_{_X} \propto \cos \sqrt{4\pi}\phi, \qquad N_{_Y} \propto \sin \sqrt{4\pi}\phi$$

• TR symmetry is spontaneously broken in the ground state.

• At $\Delta >> T > 0$ K, TR symmetry must be restored by thermal fluctuations and the gap \rightarrow pseudo gap.

Random two-particle back-scattering

• Scattering amplitudes $g_u(x)e^{i\alpha(x)}$ are quenched Gaussian variables.

$$H_{\text{int}} = \int dx \frac{g_u(x)}{2(\pi a)^2} \cos(\sqrt{16\pi}\phi + \alpha(x))$$

$$\left\langle g_u(x)e^{i\alpha(x)}\ g_u(y)e^{-i\alpha(y)}\right\rangle = D\delta(x-y) \quad \frac{dD}{d\ln t} = (3-8K)D$$

Giamarchi, Quantum physics in one dimension, oxford press (2004).

• If K<3/8, gap D opens. SDW order is spatially disordered but static in the time domain.

• At small but finite temperatures, gap remains but TR is restored by thermal fluctuations.

Single impurity scattering

• Boundary Sine-Gordon equation.

$$H_{\text{int}} = \int dx \frac{g_u}{2(\pi a)^2} \delta(x) \cos(\sqrt{16\pi}\phi) \qquad \frac{dg_u}{d\ln t} = (1 - 4K)g_u$$

C. Kane and M. P. A. Fisher, PRB 46, 15233 (1992).

• If K<1/4, g_u term is relevant. 1D line is divided into two segments.





Kondo problem: magnetic impurity scattering

$$H_{K} = \int dx \,\delta(x) \{ \frac{J_{//}}{2} (\sigma_{-} \psi_{R\uparrow}^{+} \psi_{L\downarrow} + \sigma_{+} \psi_{L\downarrow}^{+} \psi_{R\uparrow}) + J_{z} \sigma_{z} (\psi_{R\uparrow}^{+} \psi_{R\uparrow} - \psi_{L\downarrow}^{+} \psi_{L\downarrow}) \}$$

- Poor man RG: critical coupling J_z is shifted by interactions.
- If K<1 (repulsive interaction), the Kondo singlet can form with ferromagnetic couplings.



Instability criterial for helical Luttinger liquid

• Two-particle correlated back-scattering is allowed by TR symmetry, and becomes relevant at:

 $K_c < 1/2$ for Umklapp scattering at commensurate fillings. $K_c < 3/8$ for disordered two-particle scattering. $K_c < 1/4$ for a single impurity two-particle scattering.

• The Kondo critical point is shifted by interaction.

The Kane-Mele-Hubbard (KMH) model

 Double of the Haldane's model quantum anomalous Hall model: spin up and down components with opposite flux patterns.

$$H_{NN} = -t \sum_{\vec{r} \in A} \{ c_{\alpha}^{+}(\vec{r}_{A}) c_{\alpha}(\vec{r}_{B}) + h.c. \}$$

$$H_{NNN} = \sum_{\vec{r}\vec{r}'} t' e^{i\delta} \{ c_{\uparrow}^{+}(\vec{r}_{A}) c_{\uparrow}(\vec{r}_{A}') + c_{\uparrow}^{+}(\vec{r}_{B}) c_{\uparrow}(\vec{r}_{B}') \}$$

+
$$\sum_{\vec{r}\vec{r}'} t' e^{-i\delta} \{ c_{\downarrow}^{+}(\vec{r}_{A}) c_{\downarrow}(\vec{r}_{A}') + c_{\downarrow}^{+}(\vec{r}_{B}) c_{\downarrow}(\vec{r}_{B}') \} + h.c.$$



The Hubbard interaction.

$$H_{U} = U \sum_{\vec{r}} (n_{\uparrow}(\vec{r}) - \frac{1}{2}) (n_{\downarrow}(\vec{r}) - \frac{1}{2})$$



<u>Monte-Carlo (Aesthetics of brutal force: 大巧不工)</u>

• Probability distribution:

$$w(\{\sigma_i\}) = \exp[-\beta H(\{\sigma_i\})]/Z$$

$$H=-J\sum_{\langle ij
angle}\sigma_{i}^{z}\sigma_{j}^{z}$$

• Observables: magnetization and susceptibility.

$$M = \frac{1}{N} \sum_{\{\sigma\}} w\{\sigma\} (\sum_{i} \sigma_{i}) \qquad \chi = \frac{1}{N^{2}} \sum_{\{\sigma\}} w\{\sigma\} (\sum_{i} \sigma_{i})^{2}$$

- Importance sampling and detailed balance (Metropolis):
 - Start from a configuration {s} with probability w({s}). Get a trial configuration by flipping a spin.
 - 2. Calculate acceptance ratio: $r = w(\{\sigma_{trial}\}) / w(\{\sigma\})$.
 - 3. If r>1, accept it; If r<1, accept it wit the probability of r.

Auxiliary field QMC for fermions

Blankenbecler, Scalapino, and Sugar. PRD 24, 2278 (1981)

• Using path integral formalism, fermions are represented as Grassmann variables.

• Transform Grassmann variables into probability.



• Decouple interaction terms using Hubbard-Stratonovich (H-S) bosonic fields.

• Integrate out fermions and the resulting fermion functional determinants work as statistical weights.

The sign (phase) problem!!!

• Generally, the fermion functional determinants are not positive definite. Sampling with the absolute value of fermion functional determinants.

$$\langle O \rangle = \langle \langle \operatorname{sign} \times O \rangle \rangle / \langle \langle \operatorname{sign} \rangle \rangle$$

• Huge cancellation in the average of signs.

• Statistical errors scale exponentially with the inverse of temperatures and the size of samples.

• Finite size scaling and low temperature physics inaccessible.

Absence of the sign problem in the KMH model

- Projector method (T=0K).
- H-S decomposition. P-h transf. one spin component.

$$\langle \hat{O} \rangle = \frac{\langle \psi_0 | \hat{O} | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} = \frac{\langle \psi_T | e^{-\Theta H} \hat{O} e^{-\Theta H} | \psi_T \rangle}{\langle \psi_T | e^{-2\Theta H} | \psi_T \rangle}$$

$$e^{-\Theta H} = \sum_{\{l\}} \{ \prod_{p=M}^{1} e^{-\Delta \tau \sum_{i,j} c_{i\uparrow}^{+} K_{ij}^{\uparrow} c_{j\uparrow}} e^{i\sqrt{\Delta \tau U/2} \sum_{i} \eta_{i,p} (c_{i\uparrow}^{+} c_{i\uparrow} - 1/2)} \prod_{p=M}^{1} e^{-\Delta \tau \sum_{i,j} d_{i\downarrow}^{+} K_{ij}^{\downarrow} d_{j\downarrow}} e^{-i\sqrt{\Delta \tau U/2} \sum_{i} \eta_{i,p} (d_{i\downarrow}^{+} d_{i\downarrow} - 1/2)} \prod_{i,p} \gamma_{i,p} (l) \}$$

• Determinants factorize into complex conjugate pairs \rightarrow positive definite statistical weight.

$$\operatorname{Det}(\uparrow) = \operatorname{Det}^*(\downarrow)$$

The global phase diagram of KMH model at half-filling





Dong Zheng, Guang-Ming Zhang, C. Wu, Phys. Rev. B 84, 205121 (2011).

• A large region with paramagnetic bulk but antiferromagnetic edge states.

Edge properties with non-magnetic bulk

- AF form factor for each zig-zag line from the edge to the center.
- AF is weakest in the middle and strongest at the edge.



8*8*2; x periodical; y: open

Zheng, G. M. Zhang, C. Wu PRB 84, 205121 (2011).

 $\lambda = 0.1, U_c \approx 5$

Index of zigzag rows

AF two-point correlations along the edge

$$S_{x} + iS_{y} = \psi_{R\uparrow}^{+}\psi_{L\downarrow} \propto e^{i\sqrt{4\pi}\phi}$$
$$\left\langle S_{x}(x)S_{x}(x')\right\rangle ^{\sim} 1 / | x - x' |^{-2K}$$



A narrow strip 34*4*2



• The two different phases according to K<(>) 1/2.

$$K = 0.8 \qquad U = 1$$

0.5
$$U = 1.5$$

0.4 U = 2

Large U: bulk antiferromagnetism (AF)

• Easy plane antiferromagnet.



0

2

3

4

U/t

5

6

7

8

34

Meng et al., Nature 2010. Hohenadler, Lang, and Assaad arxiv:1011.5063; Zheng, Wu, G. M. Zhang, arxiv:1011.5858.

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• Stability criterial of the interacting edge states of 2D TIs, and QMC study of interacting 2D TIs.

Strong interactions can gap out the helical edge states.

• Spontaneous time-reversal symmetry breaking in Majorana flat bands.

<u>Majorana edge modes in quasi-1D Topo</u> <u>superconductors</u>

And reev bound states localized at ends z_0 with energy zero.



$$\gamma_{i} = \int dx \{ u_{0}(x) e^{-i\frac{\theta_{l}}{2} - i\frac{\pi}{4}} \psi_{i}(x) + v_{0}(x) e^{i\frac{\theta_{l}}{2} + i\frac{\pi}{4}} \psi_{i}^{\dagger}(x) \},$$

$$\dots$$

$$u_{0}(x) = v_{0}(x) \approx e^{-\frac{L-x}{\xi_{x}}} \sin k_{\xi} x$$

v

Dispersionless in k_x and k_y

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Yi Li, Da Wang, Congjun Wu, New J. Phys 15, 085002(2013)

Kitaev, 2000; Tewari, et al, 2007; Alicea, et al, 2010; etc ...

Majorana Josephson coupling between chains



Superconducting phase – Majorana fermion coupling

$$H_t = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - i J_{majorana} \sum_{\langle i,j \rangle} \sin(\frac{\theta_i - \theta_j}{2}) \gamma_i \gamma_j$$

• Possibility (I): Uniform phase, TR symmetry maintained.

Majorana edge modes decouple – flat edge-bands.

But density of states diverges \rightarrow intrinsic instability!!

• Possibility (II): Spontaneous TR symmetry breaking.

Majorana modes coupled and develop dispersion – lowering energy.

A self-consistent calculation (B-de G)

$$H_{\rm mf} = -\sum_{i} \left\{ (t_x c_i^{\dagger} c_{i+\hat{e}_x} + t_y c_i^{\dagger} c_{i+\hat{e}_y} + \text{h.c.}) - \mu c_i^{\dagger} c_i \right\} - V \sum_{i} \left\{ \Delta_{i,i+\hat{e}_x}^* c_{i+\hat{e}_x} c_i + \text{h.c.} \right\}$$
$$+ V \sum_{i} \Delta_{i,i+\hat{e}_x}^* \Delta_{i,i+\hat{e}_x},$$

• Supercurrent distribution – nonquantized vortex-antivortex



• Superfluid phase distribution

Local Density of States (LDOS)



adapt LDOC analysis for the subtraction in form

<u>Summary</u>

• No-go theorem: HLL with odd number of components can not be constructed in a purely 1D lattice system.

• Helical edge states are stable at weak interactions but are gapped out with increasing interactions.

• Sign-problem free simulation on Kane-Mele-Hubbard model --

Magnetic fluctuations are strongest on the edge; bulk paramagnetism + edge AFM

• Spontaneous vortex-antivortex formation in Majorana edge flat bands.