Exotic Topological Phase Transitions in Correlated SOC Systems

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New Phases and Emergent Phenomena in

Correlated Materials with Strong Spin-Orbit Coupling

Sep. 2015, KITP

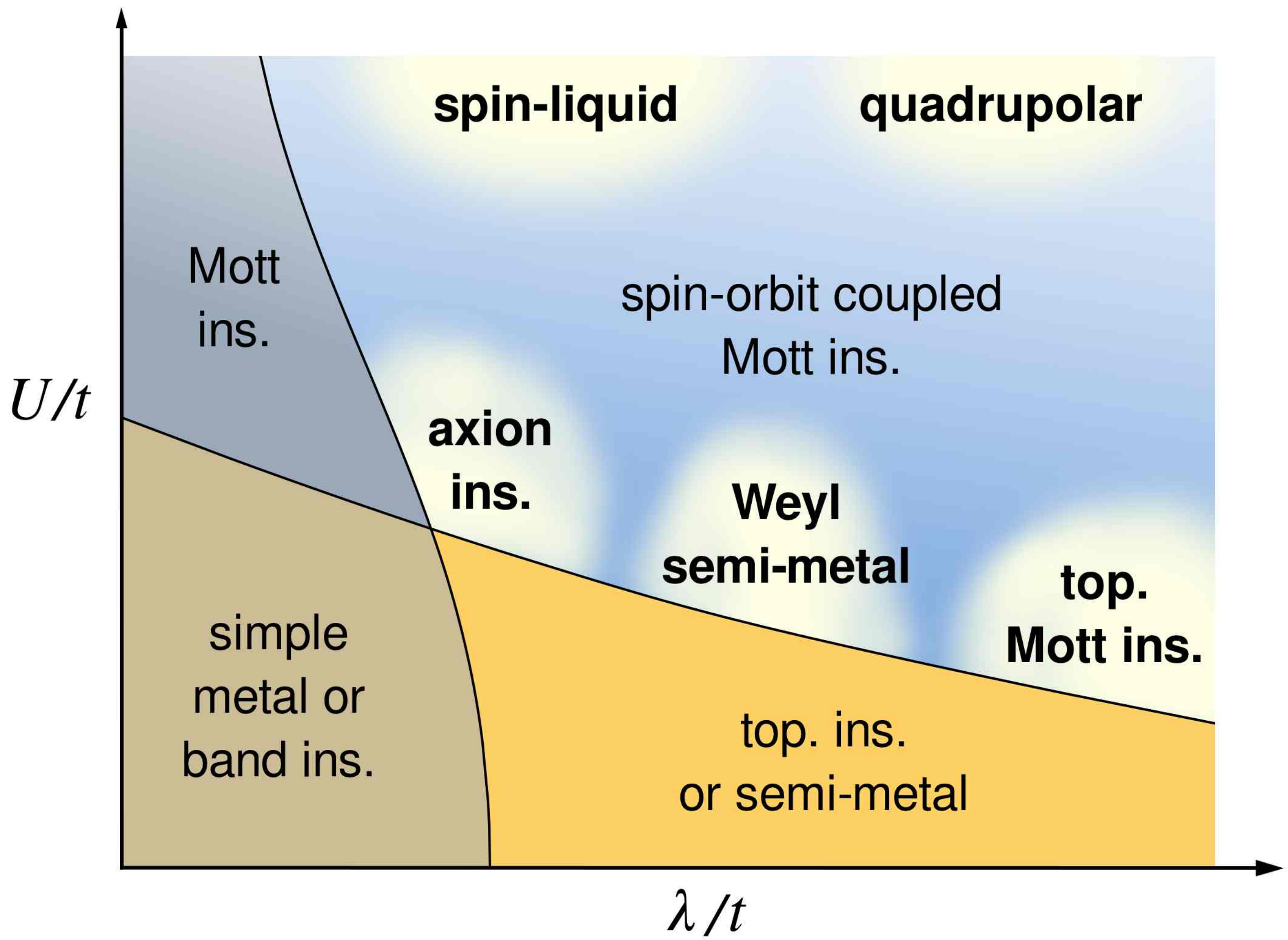
Outline

- Exotic topological phase transitions in (2+1)D
  - Bilayer QSH, by Quantum Monte Carlo (QMC)
  - **QSH-Mott** transition: **O(4) NLSM**
    with exact SO(4) symmetry, and topological Θ-term
  - **Semimetal-Mott** transition: $\mathbb{Z}_{16}$ classification of ^{3}He B
- Characterize topological transitions by **strange correlator**.
  - Decode the boundary feature from bulk wave function.
  - Tested on the single-layer QSH, matches **Luttinger liquid** theory of edge states.

- Collaborators
  - **UCSB**
    Cenke Xu
    Kevin Slagle
    Zhen Bi
    Jeremy Oon
    Alex Rasmussen
  - **Institute of Physics, China**
    Zi-Yang Meng
    Han-Qing Wu
    Yuan-Yao He
  - **Tsinghua University, China**
    Zhong Wang
- Fundings / Supports

NSF
the David & Lucile Packard FOUNDATION
UCSB CSC
ALFRED P. SLOAN FOUNDATION 1934
NSFC 国家自然科学基金委员会 National Natural Science Foundation of China

Quantum Matter with SOC



Witczak-Krampa, Chen, Kim, Balents (2013)

- Weak Correlation
  - Gapped Phase (SPT) TI, TSC,TCI…
  - Gapless Phase Weyl SM…
  - Well described by **band theory** on the free fermion / mean-field level
- Strong Correlation
  - SSB order, topological order (spin liquid)…
  - Interacting SPT

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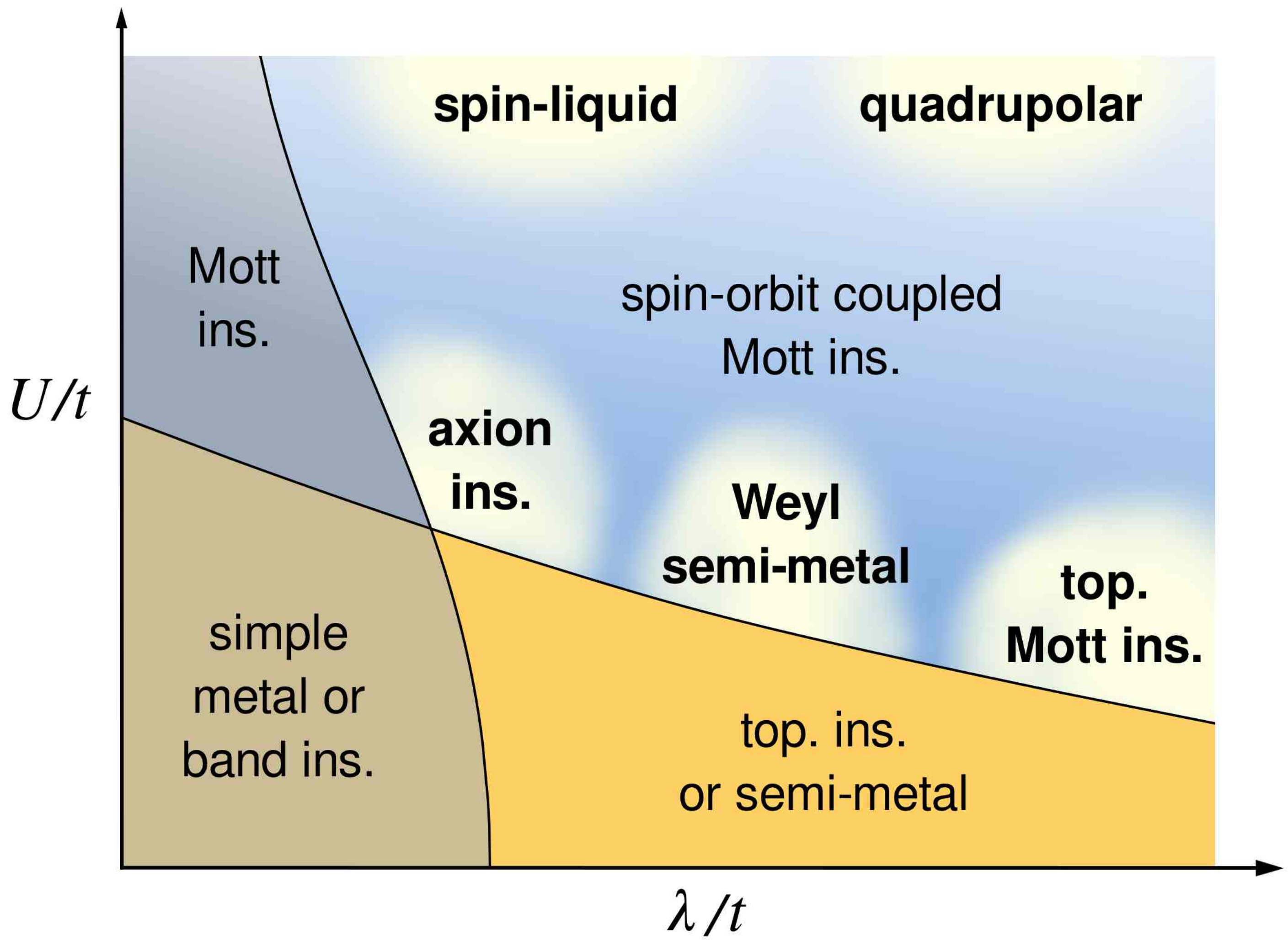

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Fermionic SPT States

- Fermionic **Symmetry Protected Topological (SPT)** States   Gu, Wen (2009) …
  - **Bulk**: fully gapped and non-degenerated.
  - **Boundary**: gapless or degenerated, symmetry protected.
- Within the **free** fermion band theory:
  - **Bulk**: separated from trivial phase by fermion gap closing.
  - **Boundary**: can not gap out, unless breaking the symmetry.
- With **interaction**, the story can be modified.
  - **Bulk**: Topological transition without closing fermion gap.
    - Interaction can drive the fermionic system to a **spin** (**bosonic**) system.
  - **Boundary**: Gap out fermions without breaking symmetry.
    - Interaction can introduce **surface topological order**.   Vishwanath, Senthil (2013) …
    - Interaction can **reduce SPT classifications**.   Fidkowski, Kitaev (2010) …
- Interaction can also lead to new SPT states …

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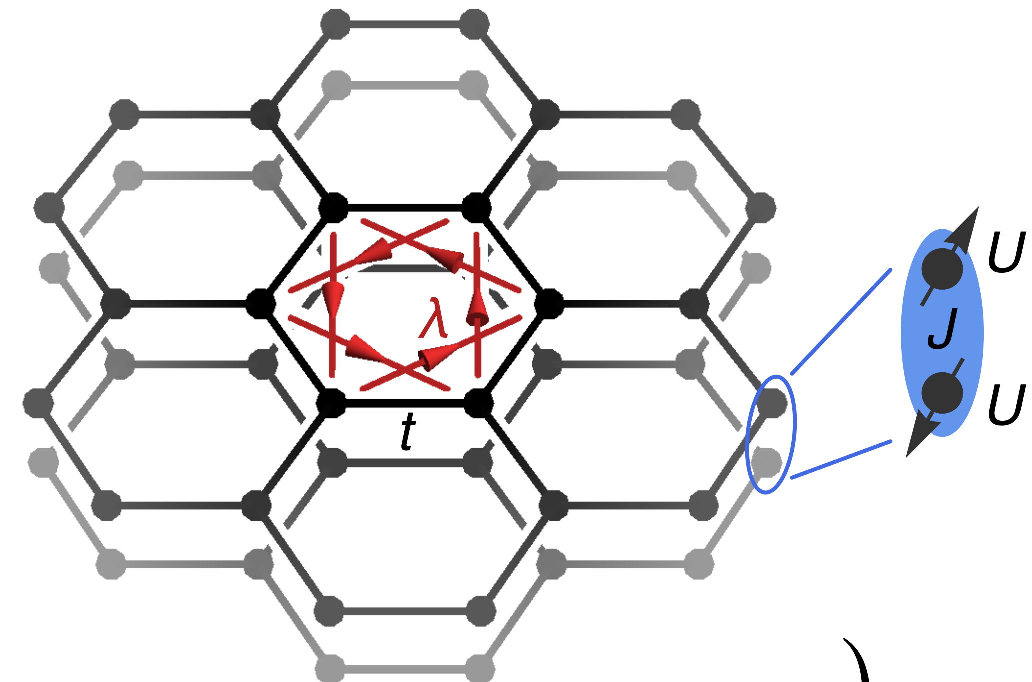
Bilayer Kane-Mele-Hubbard-Heisenberg Model



- Spin-1/2 fermions on a **bilayer** honeycomb lattice.
- Model Hamiltonian

$$H = H_{\text{band}} + H_{\text{int}}$$

- Bilayer Kane-Mele model

$$H_{\text{band}} = \sum_{\ell=1,2} \left(-t \sum_{\langle ij \rangle} c^{\dagger}_{i\ell}\, c_{j\ell} + \sum_{\langle\langle ij \rangle\rangle} i\, \lambda_{ij}\, c^{\dagger}_{i\ell}\, \sigma^{z}\, c_{j\ell} + H.c. \right)$$

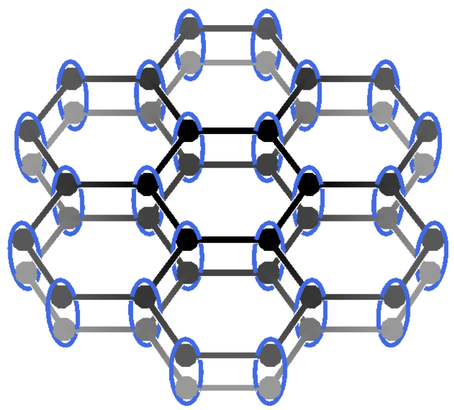
- λ - Kane-Mele SOC

- Hubbard-Heisenberg interaction

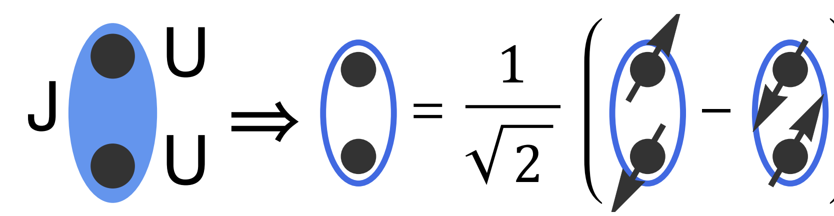
$$H_{\text{int}} = \frac{U}{2} \sum_{i,\ell} (n_{i\ell} - 1)^2 + J \sum_{i} \left(\boldsymbol{S}_{i1} \cdot \boldsymbol{S}_{i2} + \frac{1}{4} (n_{i1} - 1)(n_{i2} - 1) - \frac{1}{4} \right)$$

- U - on-site Hubbard
- J - interlayer Heisenberg

Phase Diagram

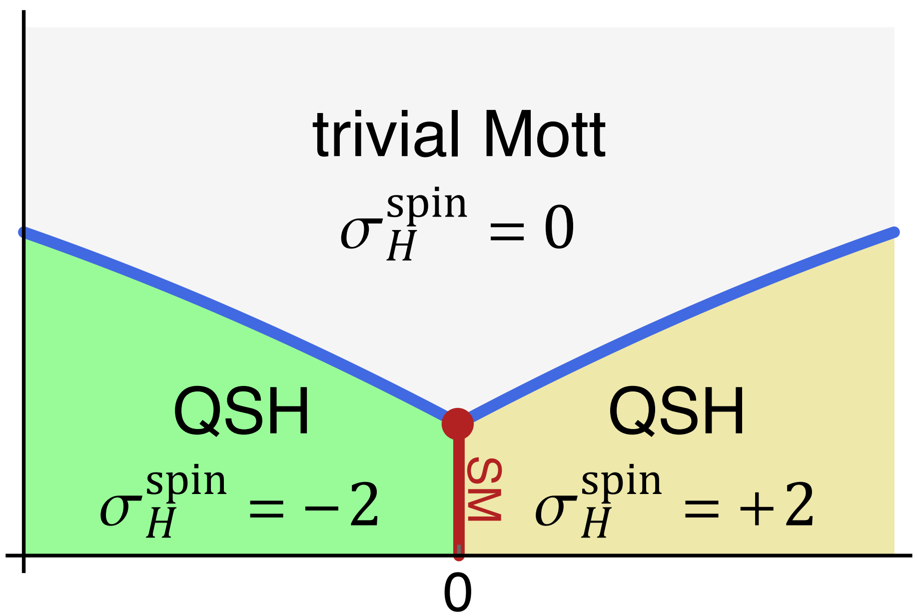


- Strong interaction limit
  Hubbard + Heisenberg interaction
  → interlayer spin-singlet (dimer)
  → trivial Mott

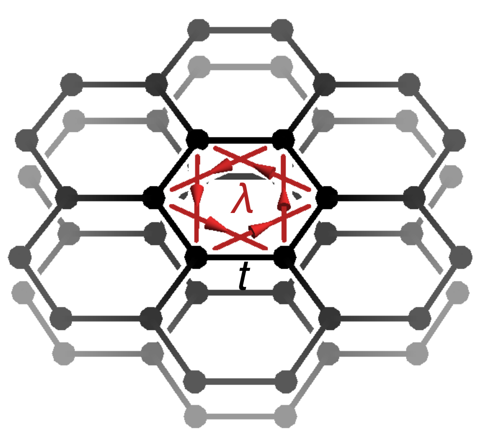


Slagle, You, Xu.
PRB **91**, 115121

U, J interaction

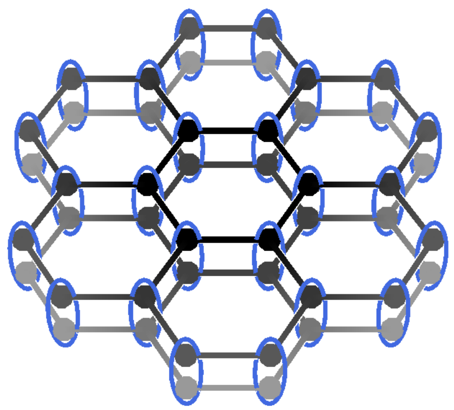


λ SOC



- Weak interaction limit
  Kane-Mele model x 2
  → spin Hall conductance ± 2
- $\mathbb{Z}$ classification $U(1)_{\text{spin}} \times [U(1) \times U(1)]_{\text{charge}} \times Z_2^T$

Phase Diagram



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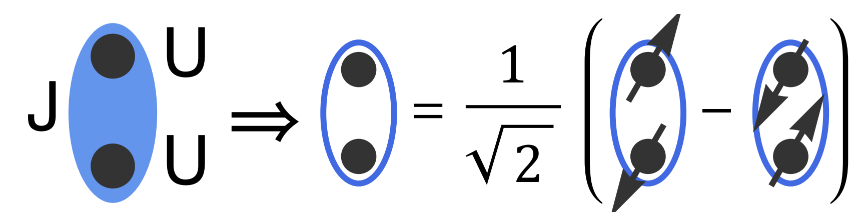

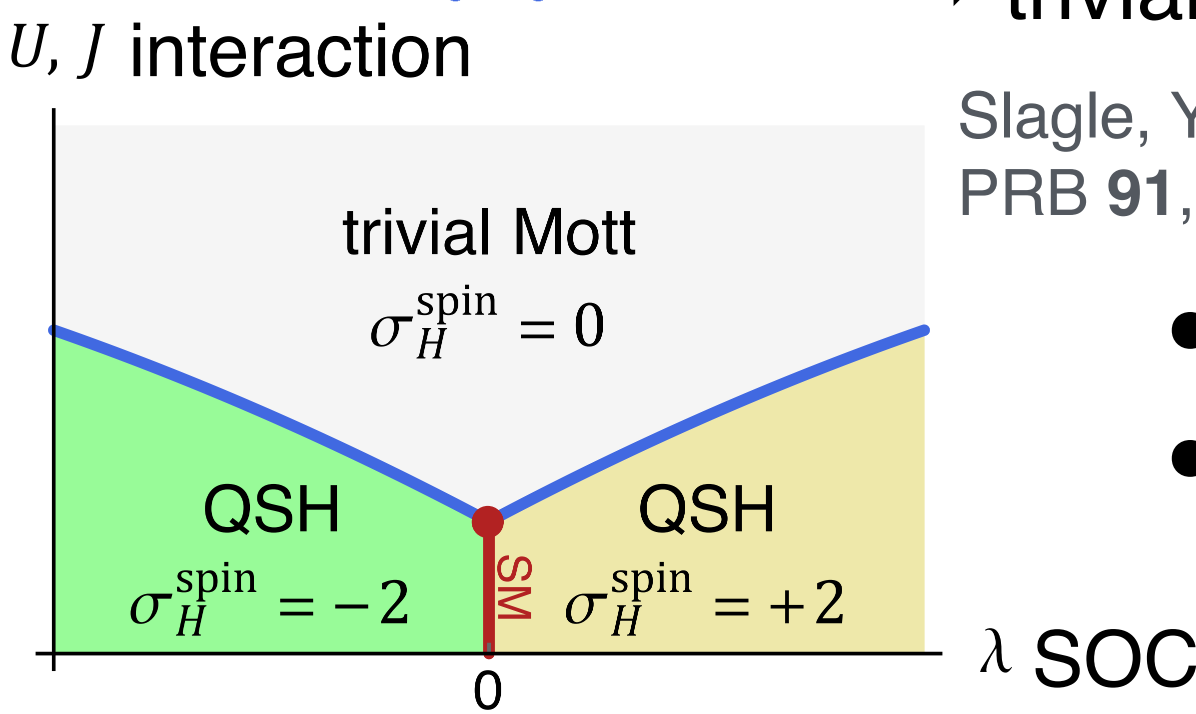

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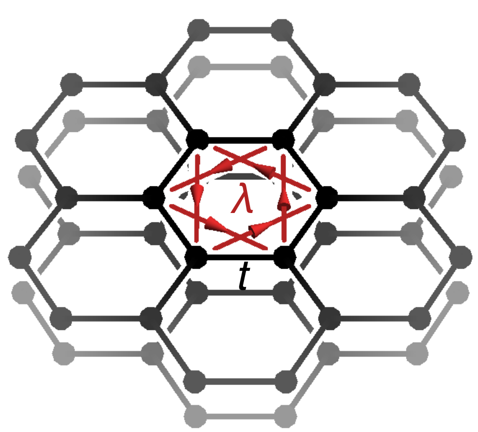
- QSH-QSH: **gapless fermion**
- QSH-Mott: gapped fermion + **gapless collective boson**



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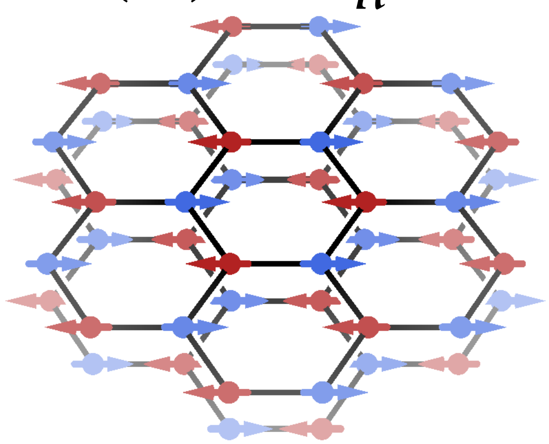
SO(4) Symmetric Point

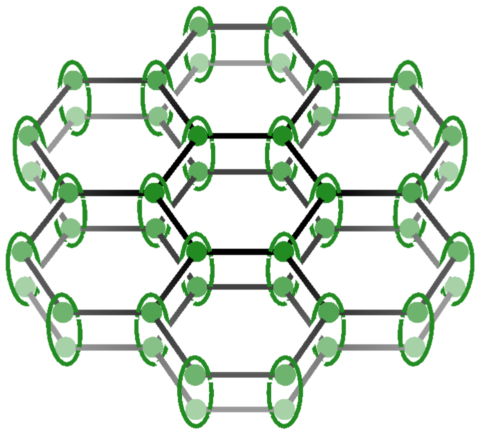
- At U = 0, the model has an exact SO(4) symmetry
  - SDW (XY-AFM)

$$S^+ = (-)^{i+\ell}\, c^\dagger_{i\ell}\, \sigma^+\, c_{i\ell}$$



  - SC (inter-layer singlet)

$$\Delta = c_{i1}{}^{\mathrm{T}}\, i\, \sigma^y\, c_{i2}$$

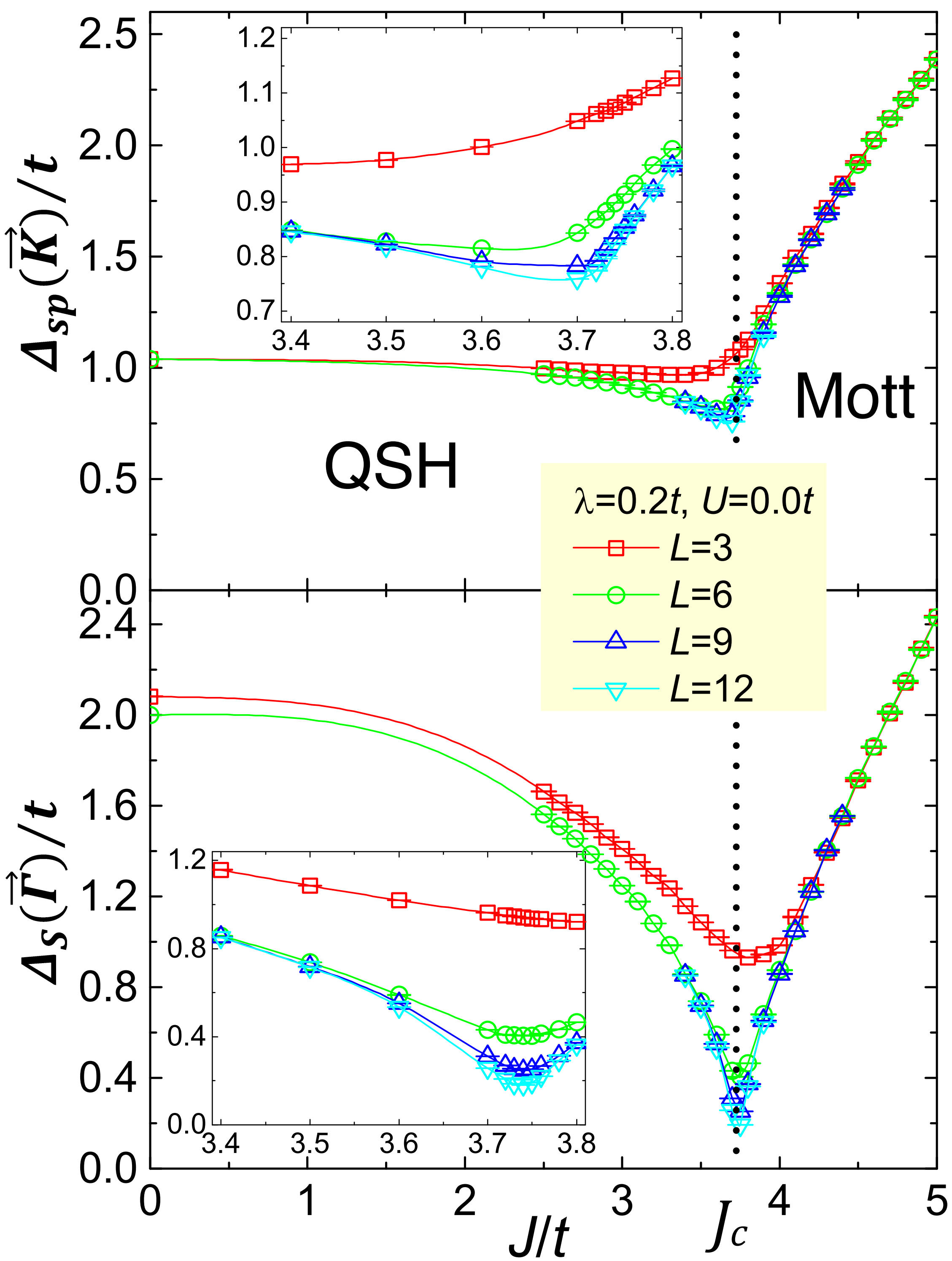


  - New fermions: $f_{i\uparrow} = \begin{pmatrix} c_{i1\uparrow} \\ (-)^i\, c^\dagger_{i2\uparrow} \end{pmatrix}$, $f_{i\downarrow} = \begin{pmatrix} (-)^i\, c_{i1\downarrow} \\ c^\dagger_{i2\downarrow} \end{pmatrix}$ $\mathrm{SO}(4) \simeq \mathrm{SU}(2)_\uparrow \times \mathrm{SU}(2)_\downarrow$
  - O(4) vector $(S^x,\ \mathrm{Im}\,\Delta,\ \mathrm{Re}\,\Delta,\ S^y) = f^\dagger_{i\downarrow}\left(\tau^0,\ i\tau^1,\ i\tau^2,\ i\tau^3\right) f_{i\uparrow} + h.c.$
  - Model Hamiltonian

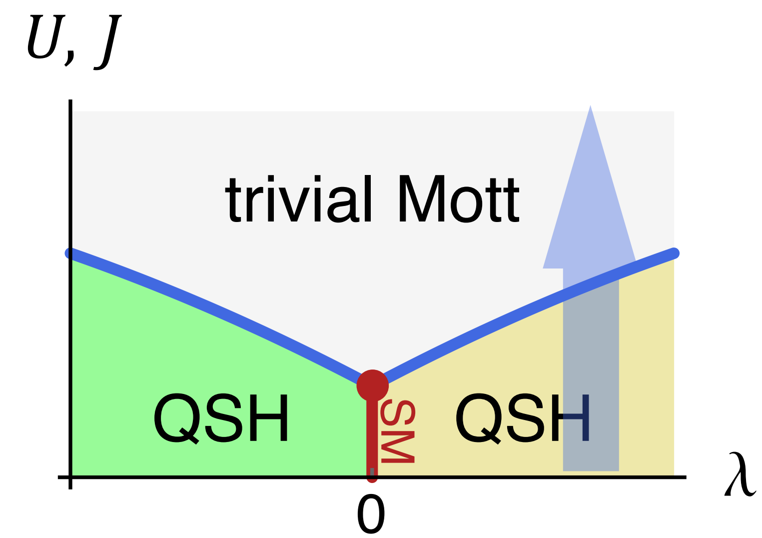
$$H = \sum_{i,j,\sigma} (-)^\sigma\, f^\dagger_{i\sigma}(-t_{ij} + i\lambda_{ij})\, f_{j\sigma} + h.c. - \frac{J}{16} \sum_i \left(D_i\, D_i^\dagger + D_i^\dagger\, D_i\right)$$

$$D_i = \sum_\sigma f_{i\sigma}\, i\tau^2\, f_{i\sigma}$$

Quantum Spin Hall → Trivial Mott



Y-Y He, et.al., arXiv:1508.06389



Slagle et. al. (2014)

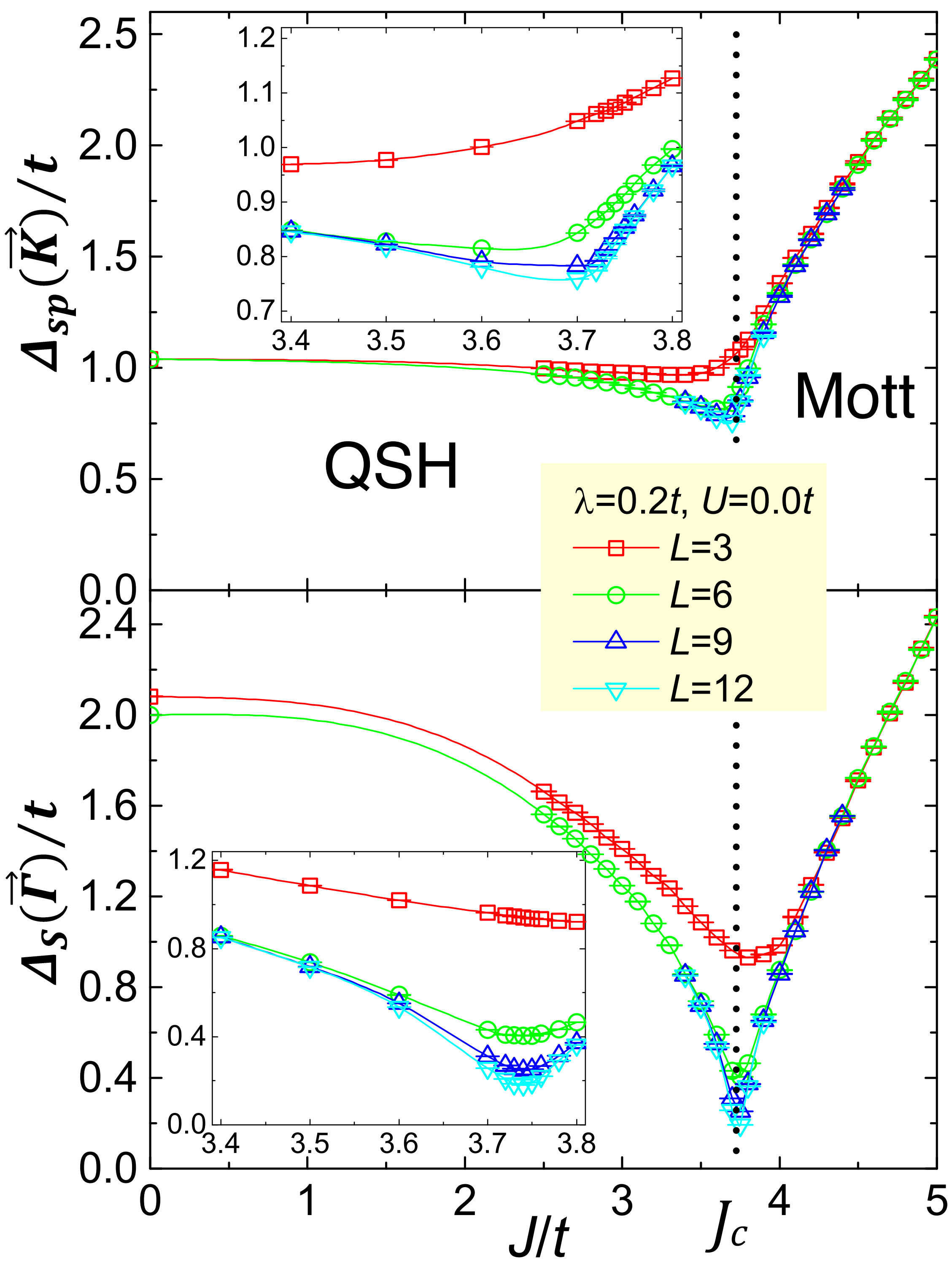
- Topological-Trivial Transition
  - Driven by interaction
  - Fermion: **gapped**
  - Spin/charge: **gapless**

$$\left\langle c^{\dagger}(\tau)\, c(0)\right\rangle \sim e^{-\Delta_{\mathrm{sp}}\,\tau}$$

$$\left\langle S^{+}(\tau)\, S^{-}(0)\right\rangle \sim e^{-\Delta_{S}\,\tau}$$

$$\left\langle \Delta^{\dagger}(\tau)\, \Delta(0)\right\rangle \sim e^{-\Delta_{D}\,\tau}$$

Quantum Spin Hall → Trivial Mott



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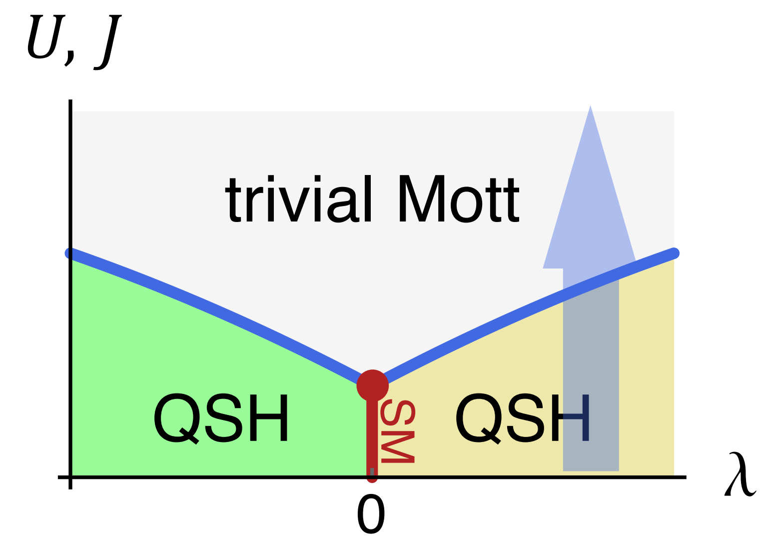


Slagle et. al. (2014)

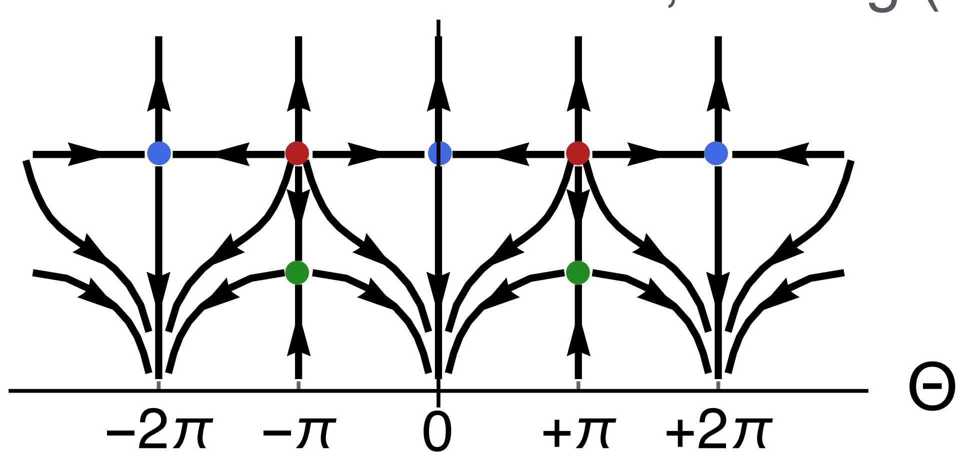
- Fermions are gapped → only bosonic d.o.f. involved → Bosonic SPT transition
- Bilayer QSH + Interaction → **Bosonic SPT**
  - Boundary: interaction marginally relevant → gaps out all fermion edge modes

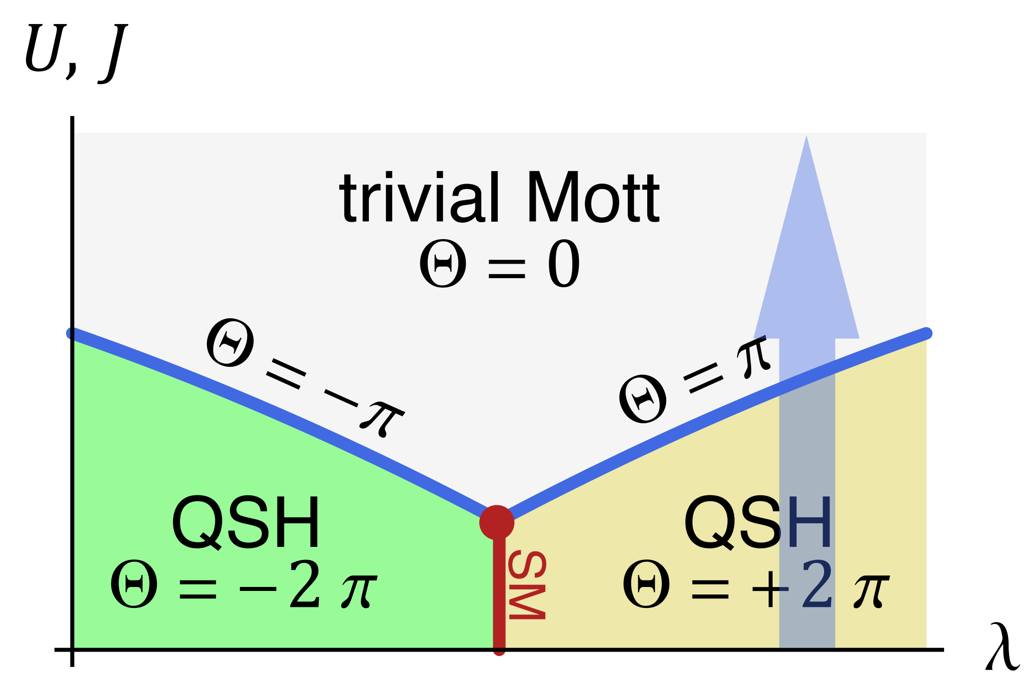
Bosonic SPT Transition

- Effective field theory: non-linear σ model (bosonic SPT)
  - O(4) vector $\boldsymbol{n}$: $n_1\, S^x + n_2\, S^y + n_3\, \mathrm{Re}\,\Delta + n_4\, \mathrm{Im}\,\Delta$

$$S = \int d^2x\, d\tau\, \frac{1}{g}\left(\partial_\mu \boldsymbol{n}\right)^2 + \frac{\Theta}{2\pi^2}\, \epsilon^{abcd}\, n_a\, \partial_\tau n_b\, \partial_x n_c\, \partial_y n_d$$

  - $\Theta = 2\pi$: spin-1 ~ 2π vortex of Δ = π-flux of fermion → QSH insulator with $\sigma_H^{\mathrm{spin}} = 2$
  - $\Theta = 0$: trivial insulator

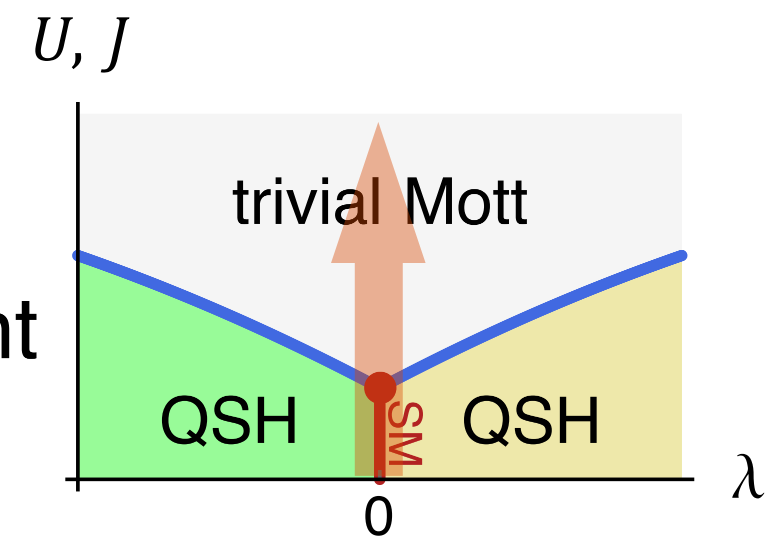




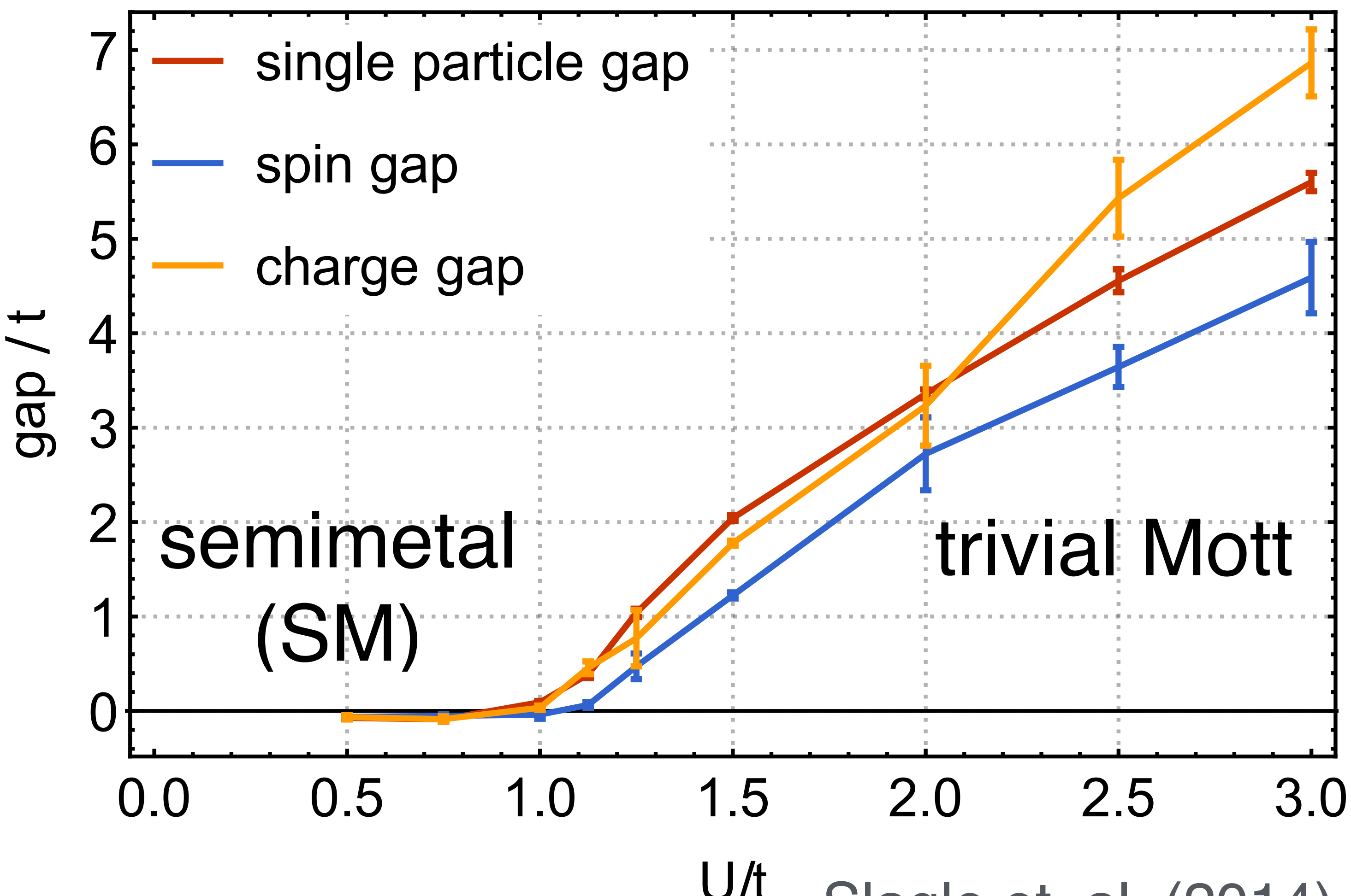
- Sign-free QMC for O(4) NLSM and 2d bosonic SPT's.

Semimetal → Trivial Mott (λ = 0)

- **Continuous** phase transition
  - At J=2U, the model has SO(5) symmetry
  - Gaps open continuously at the same point → No symmetry breaking

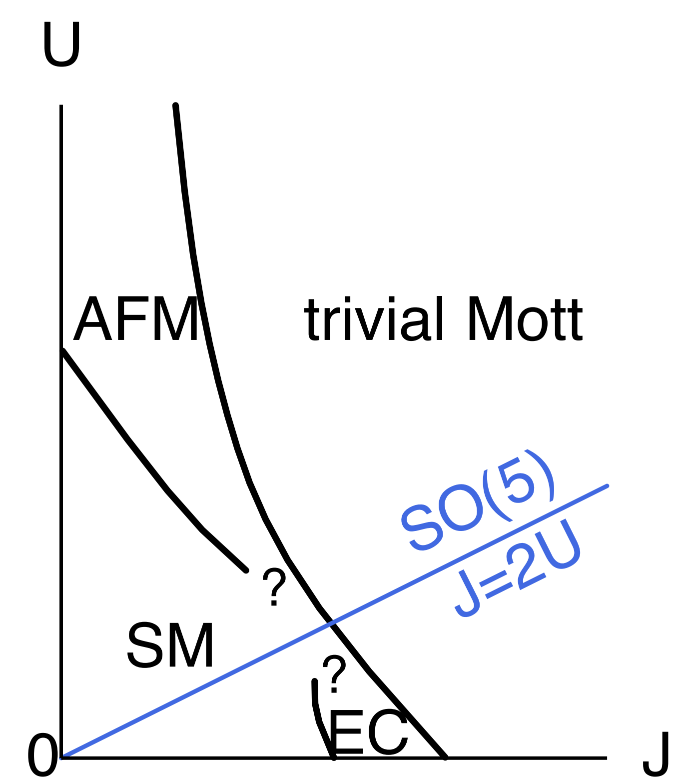


gaps with λ =0



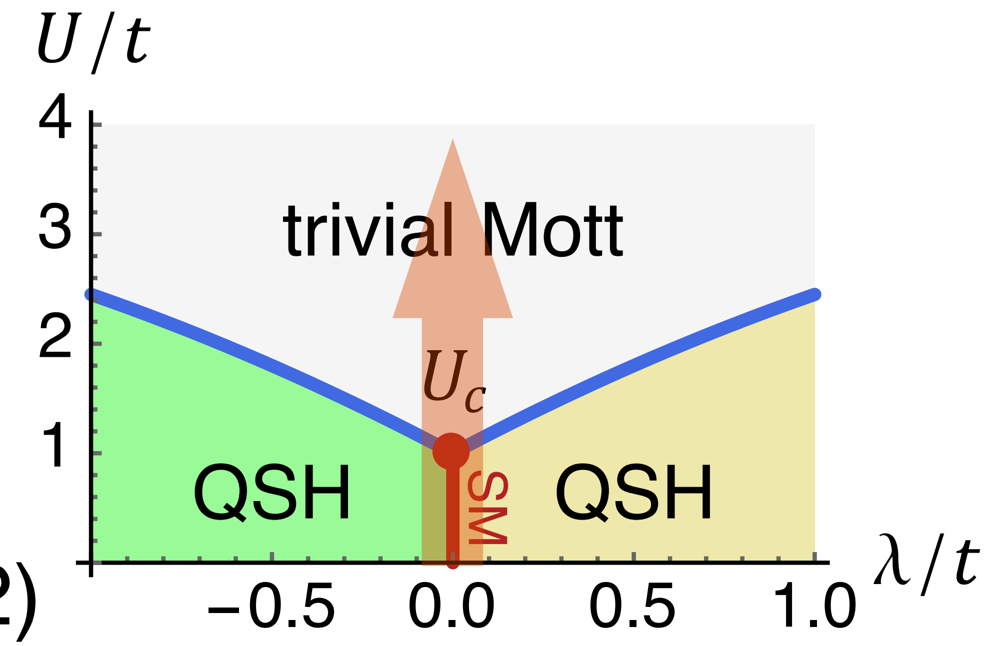
Slagle et. al. (2014)

- In general, SSB phases may set in.



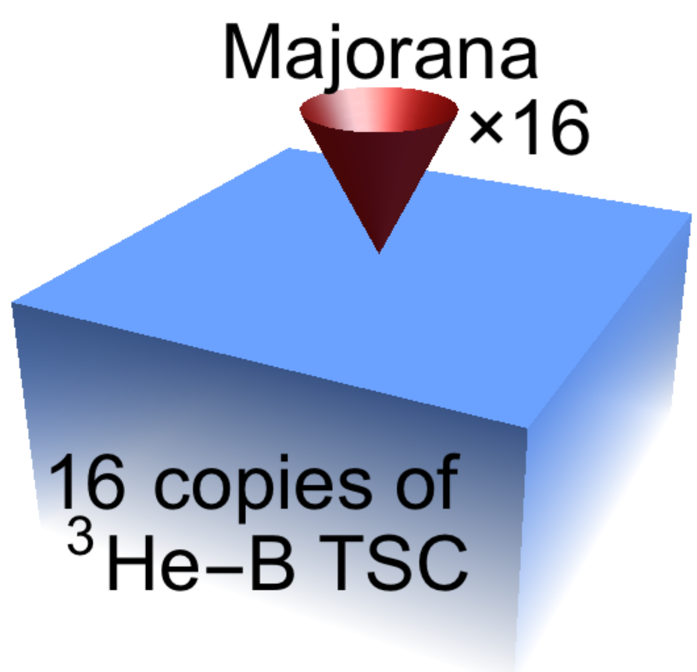
Interaction Reduced SPT Classification

- **Continuous** phase transition
  - There must be a field theory
  - Semimetal ~ 16 Majorana cones
    - layers (×2)
    - valleys (×2)
    - spins (×2)
    - particle-hole (×2)



  - Same as the boundary of 16 copies of ^{3}He B-phase TSC.
  - Gapped out by interaction without breaking symmetry.
  - Beyond Landau's paradigm.
  - Consistent with the $\mathbb{Z}_{16}$ classification of ^{3}He-B TSC.

Wang, Senthil (2014).
Fidkowski, Chen, Vishwanath (2013).



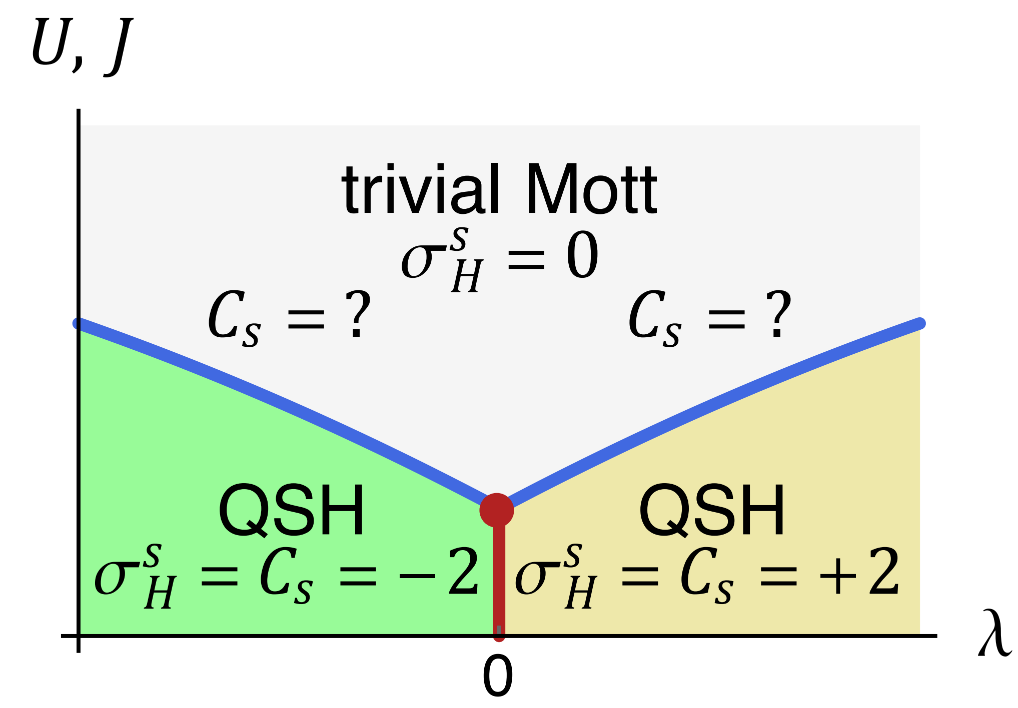
Spin Chern Number ≠ Spin Hall Conductance

- Spin Chern number

$$C_s = \frac{1}{48\,\pi^2} \int d^3 k\, \epsilon^{\mu\nu\lambda}$$

$$\mathrm{Tr}\left(-\sigma^z\, G\, \partial_\mu G^{-1}\, G\, \partial_\nu G^{-1}\, G\, \partial_\lambda G^{-1}\right)$$

Green's function $G(k) = -\left\langle c_k\, c_k^\dagger \right\rangle$



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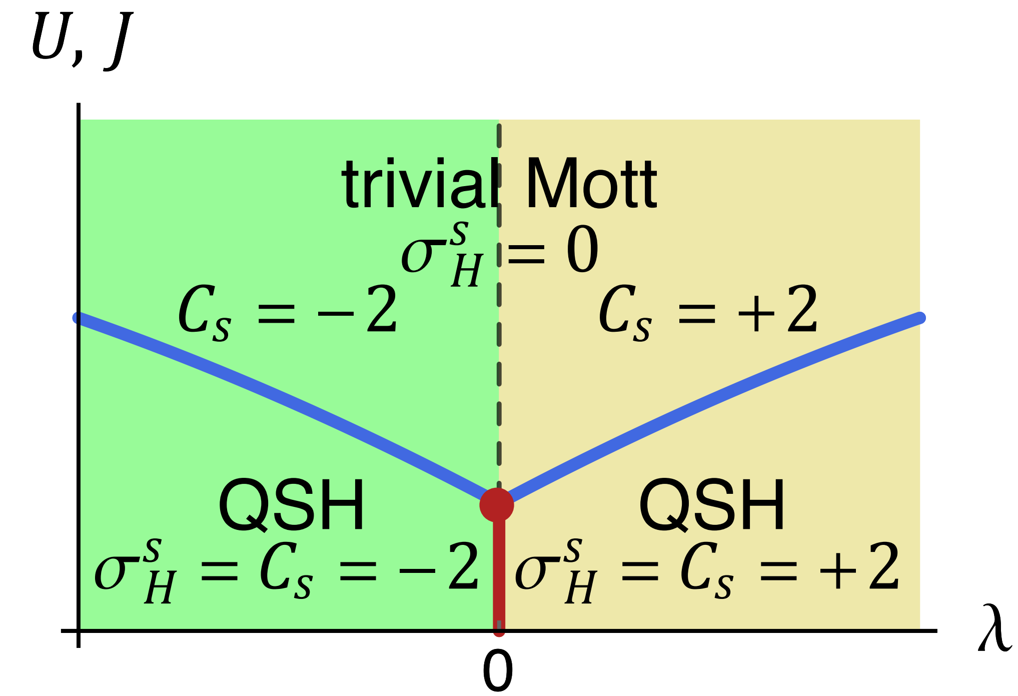

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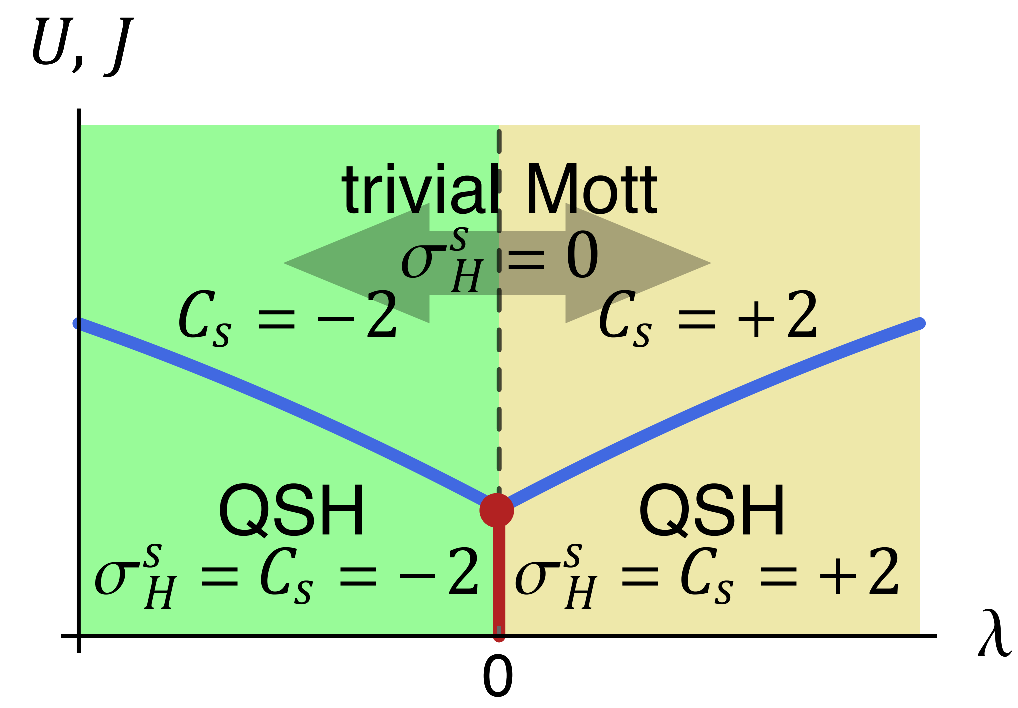
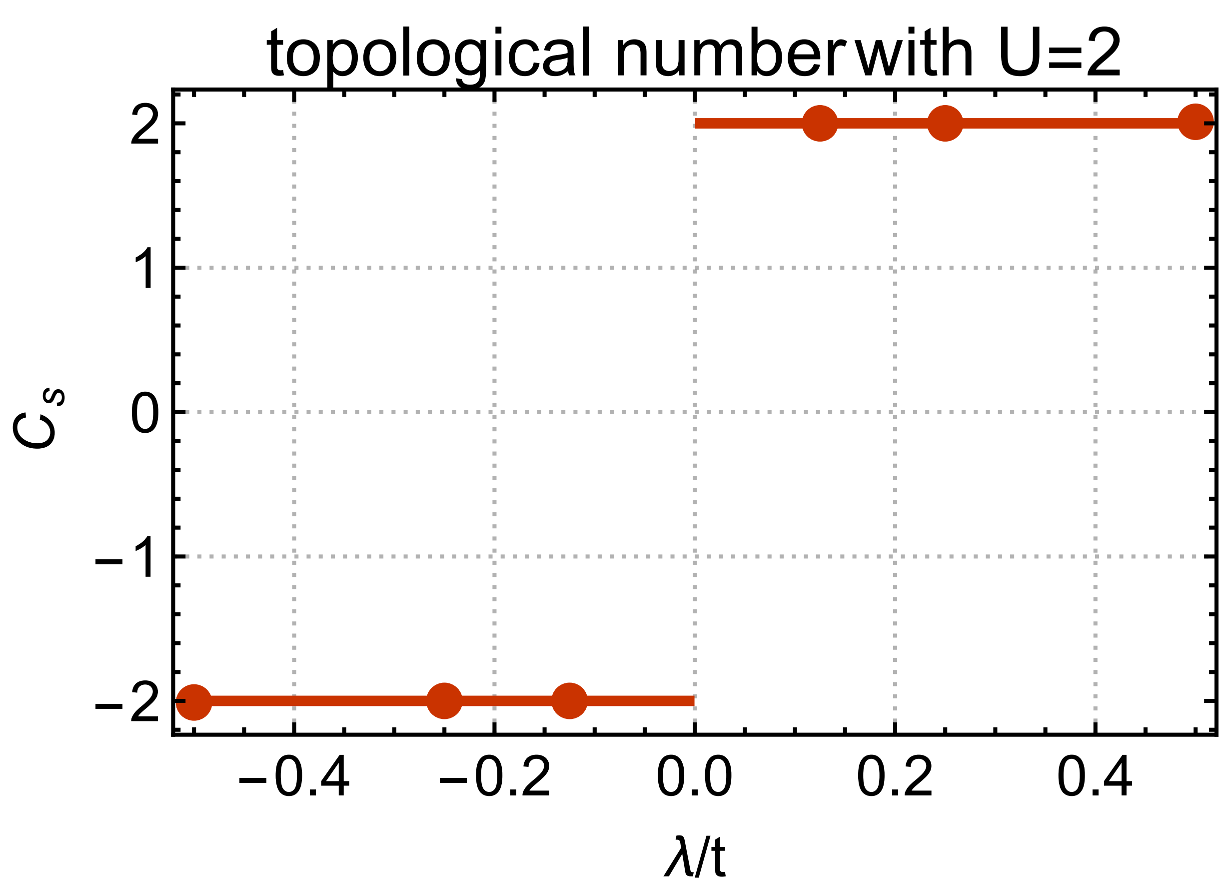


- QMC Result



- Not a phase transition
- Transition of C_s via zeros of G at zero frequency
- Pole of G^{-1}= Zero of G
- Fermions are **gapped** → no poles, only zeros

You, Wang, Oon, Xu,
PRB **90**, 060502

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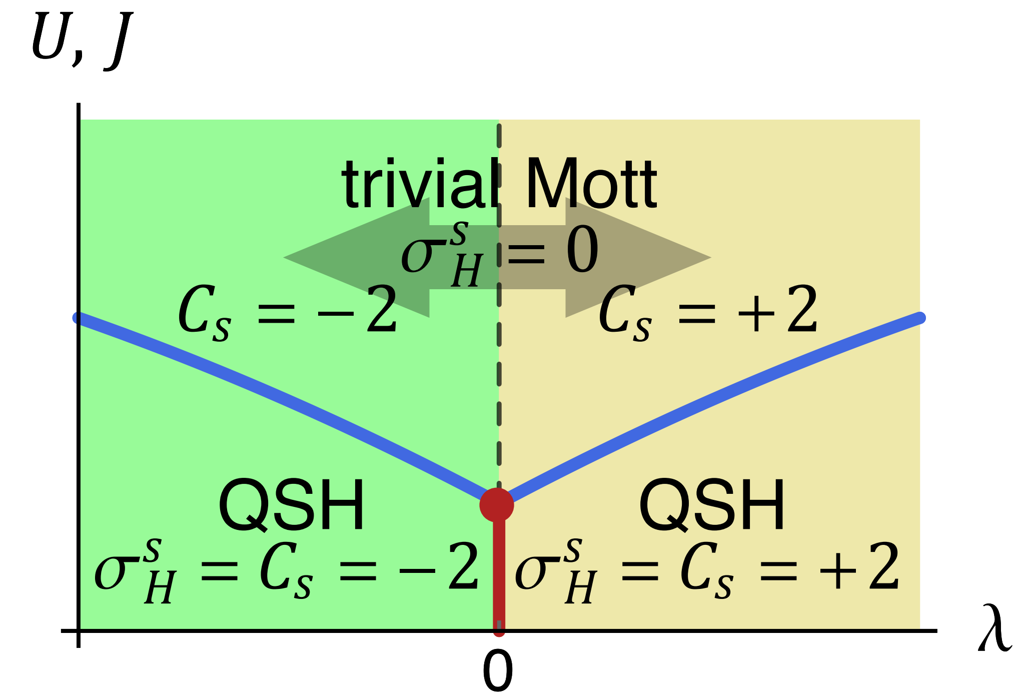

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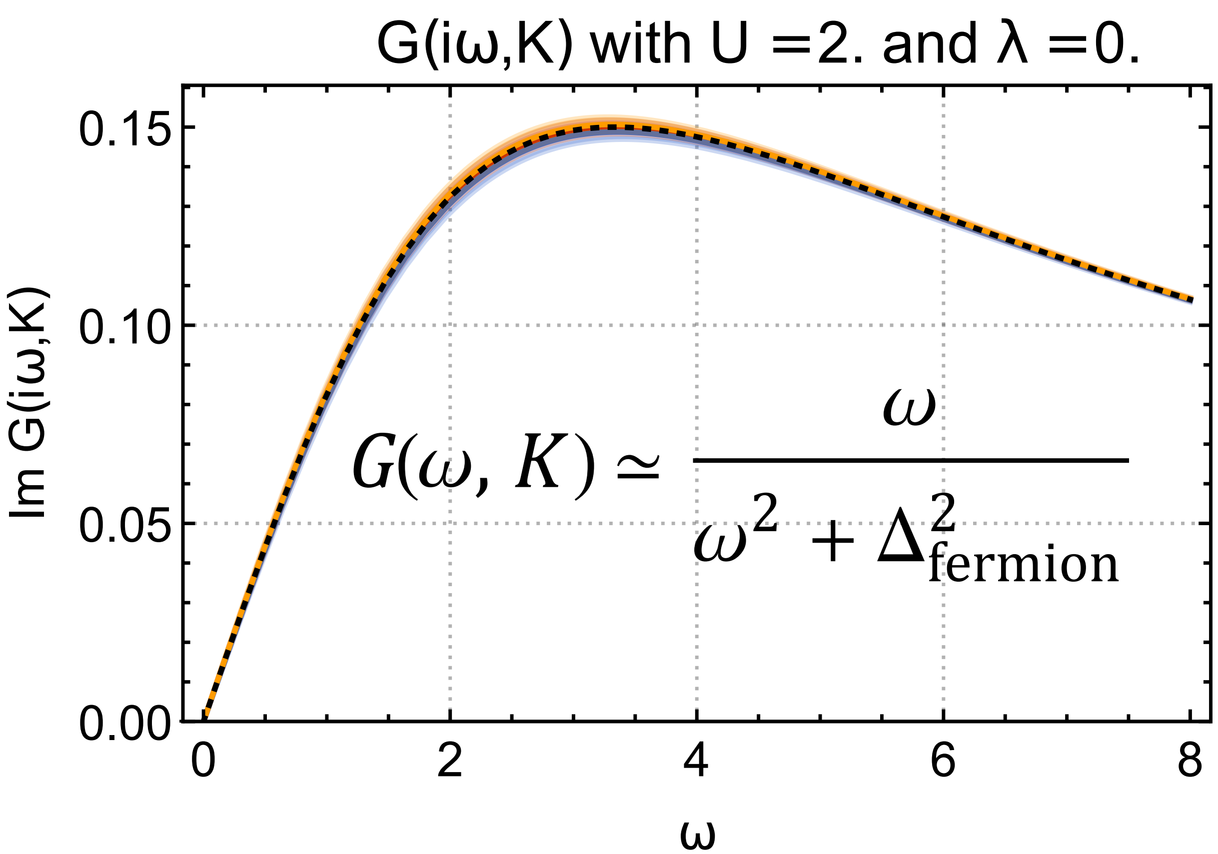

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Strange Correlator ~ Boundary Correlator

- Physical correlator: short-ranged

$$\frac{\langle \Psi|\phi(r)\phi(r')|\Psi\rangle}{\langle \Psi|\Psi\rangle} \sim e^{-|r-r'|/\xi}$$

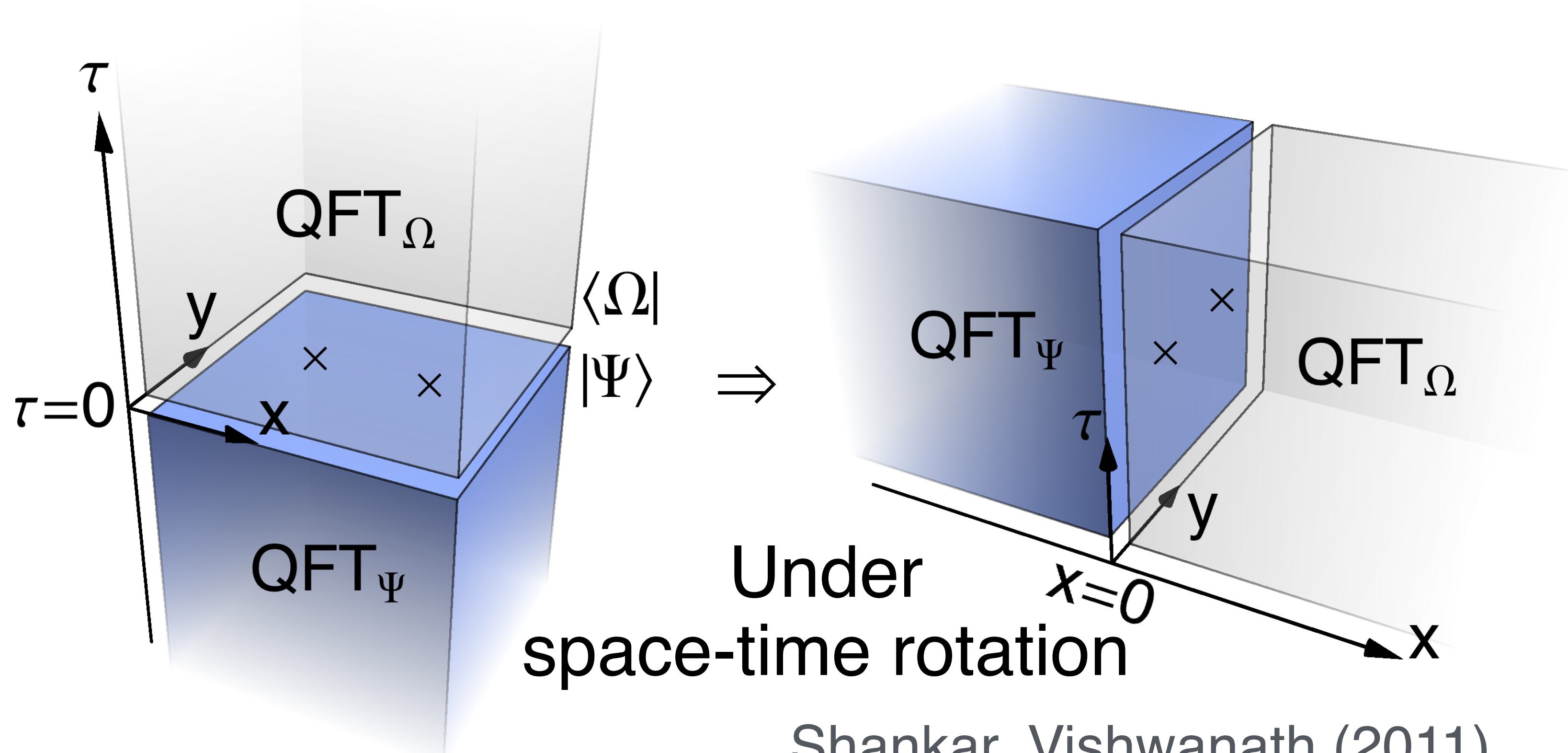
- **Strange correlator**: long-ranged or power-law (in 1d and 2d)

trivial direct product state

$$\frac{\langle \Omega|\phi(r)\phi(r')|\Psi\rangle}{\langle \Omega|\Psi\rangle} \sim |r-r'|^{-\eta} \text{ or const.}$$

non-trivial SPT (to probe)

You et. al., PRL **112**, 247202



Under space-time rotation

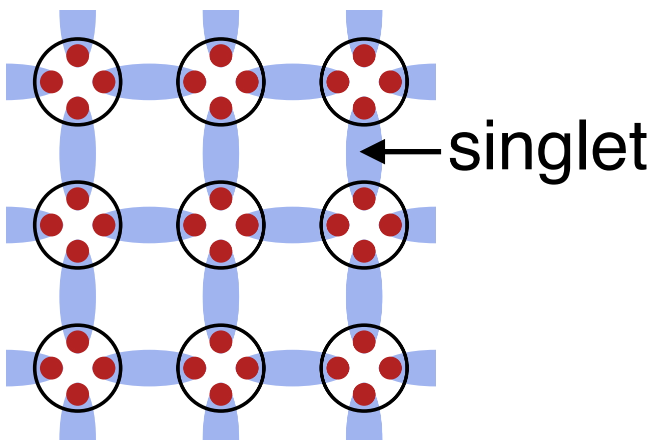
Shankar, Vishwanath (2011)

Examples of Strange Correlator

- Bosonic SPT: 2d AKLT

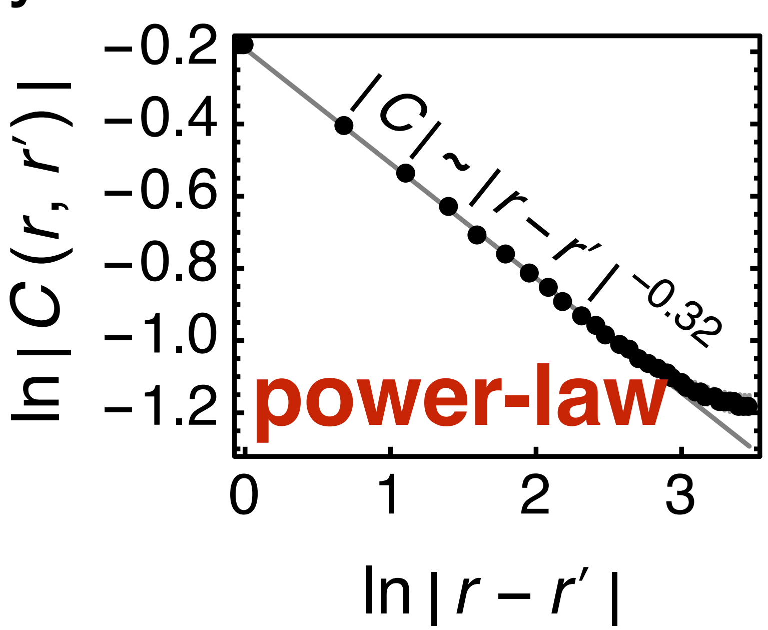
$$|\Omega\rangle = |000\cdots\rangle \quad S^z = 0$$

$$|\Psi\rangle =$$



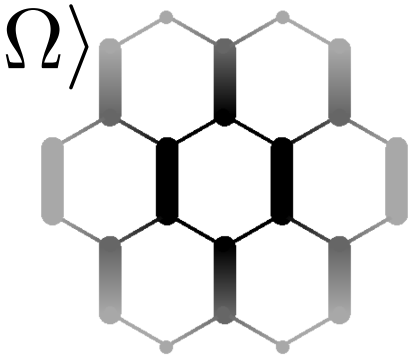
$$C(r,r') = \frac{\langle\Omega|S_r^+ S_{r'}^-|\Psi\rangle}{\langle\Omega|\Psi\rangle}$$

By DMRG:

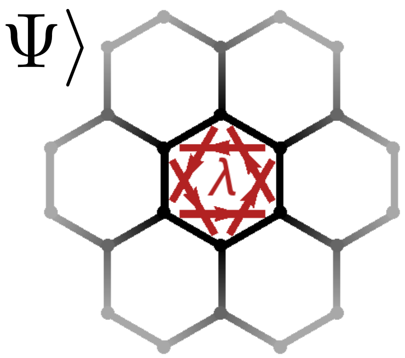


- Free fermionic SPT: 2d QSH

$|\Omega\rangle$

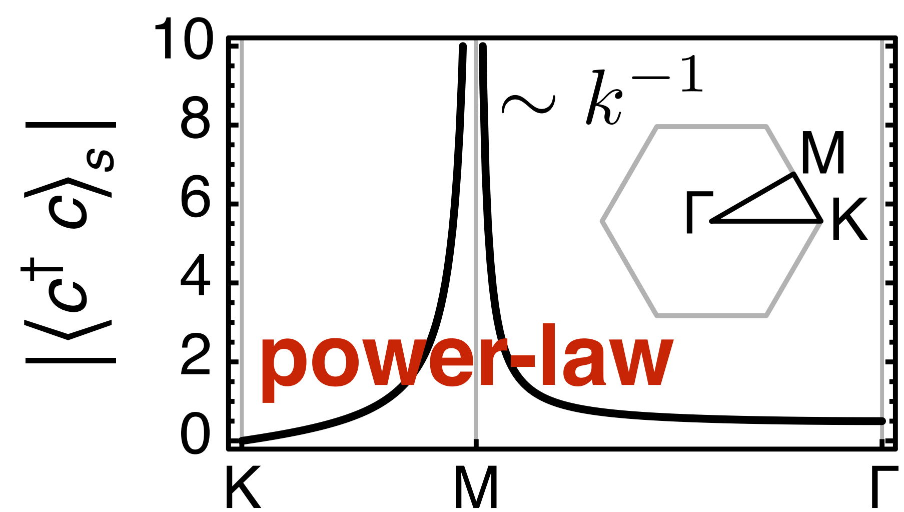


$|\Psi\rangle$



$$C(k) = \frac{\langle\Omega|\, c^\dagger_{kA\uparrow}\, c_{kB\uparrow}\, |\Psi\rangle}{\langle\Omega\,|\Psi\rangle}$$

$$C(k) \sim \frac{1}{k_x + i\, k_y} \Rightarrow C(r) \sim \frac{1}{x + i\, y}$$



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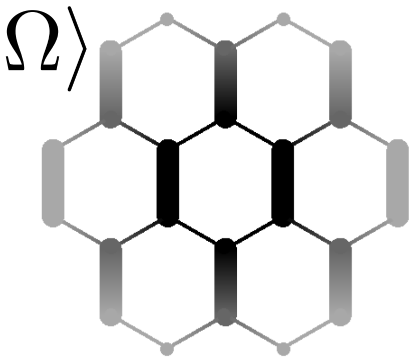
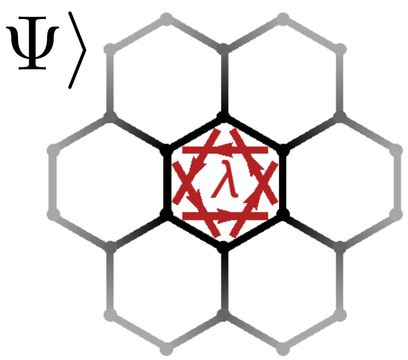
$|\Omega\rangle$  $|\Psi\rangle$ 

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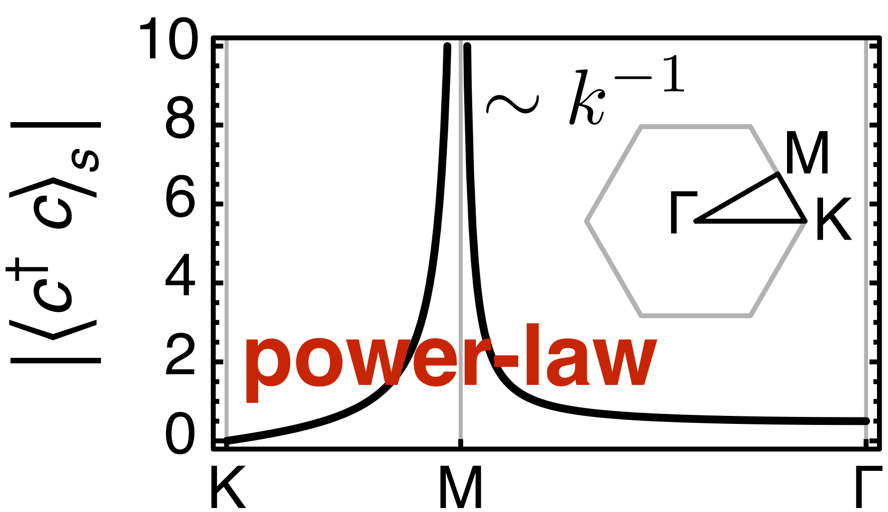
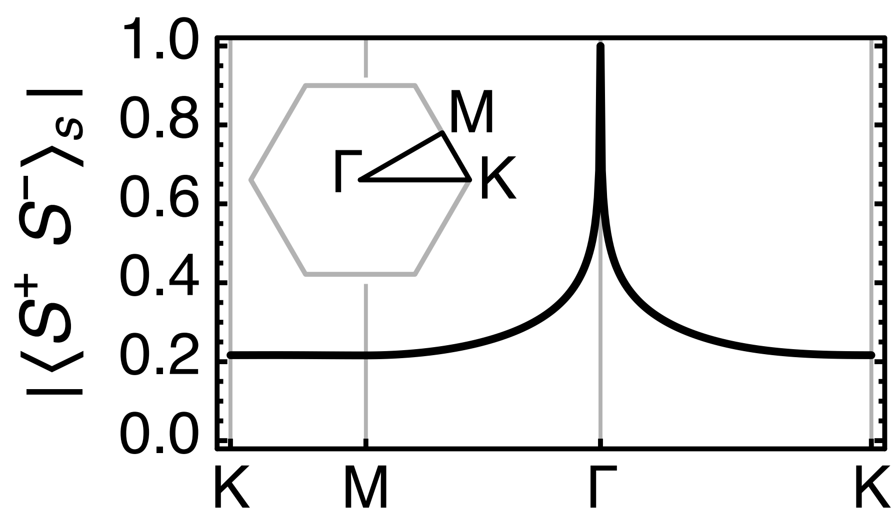


- Bosonic channels
  - Spin: $S^{+}_{A} = c^{\dagger}_{A\uparrow}\, c_{A\downarrow}$
  - Charge: $\Delta_A = c_{A\uparrow}\, c_{A\downarrow}$

$$S = \frac{\langle \Omega |\, S^{+}_{rA}\, S^{-}_{r'A}\, |\Psi\rangle}{\langle \Omega \,|\Psi\rangle} \quad D = \frac{\langle \Omega |\, \Delta^{\dagger}_{rA}\, \Delta_{r'A}\, |\Psi\rangle}{\langle \Omega \,|\Psi\rangle}$$

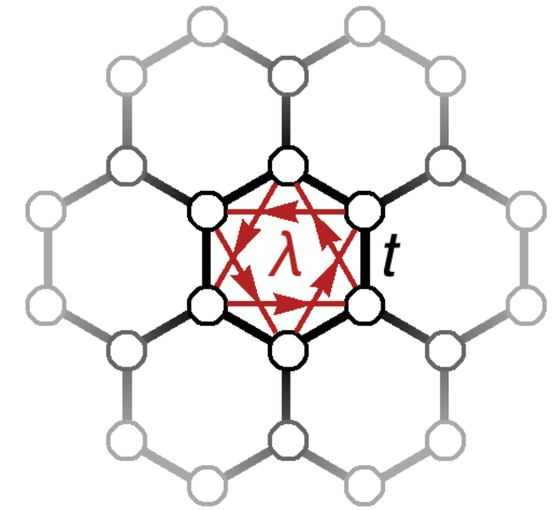
$$S(r) \sim r^{-2} \Rightarrow S(k) \sim -\ln k$$

$$D(r) \sim r^{-2} \Rightarrow D(k) \sim -\ln k$$

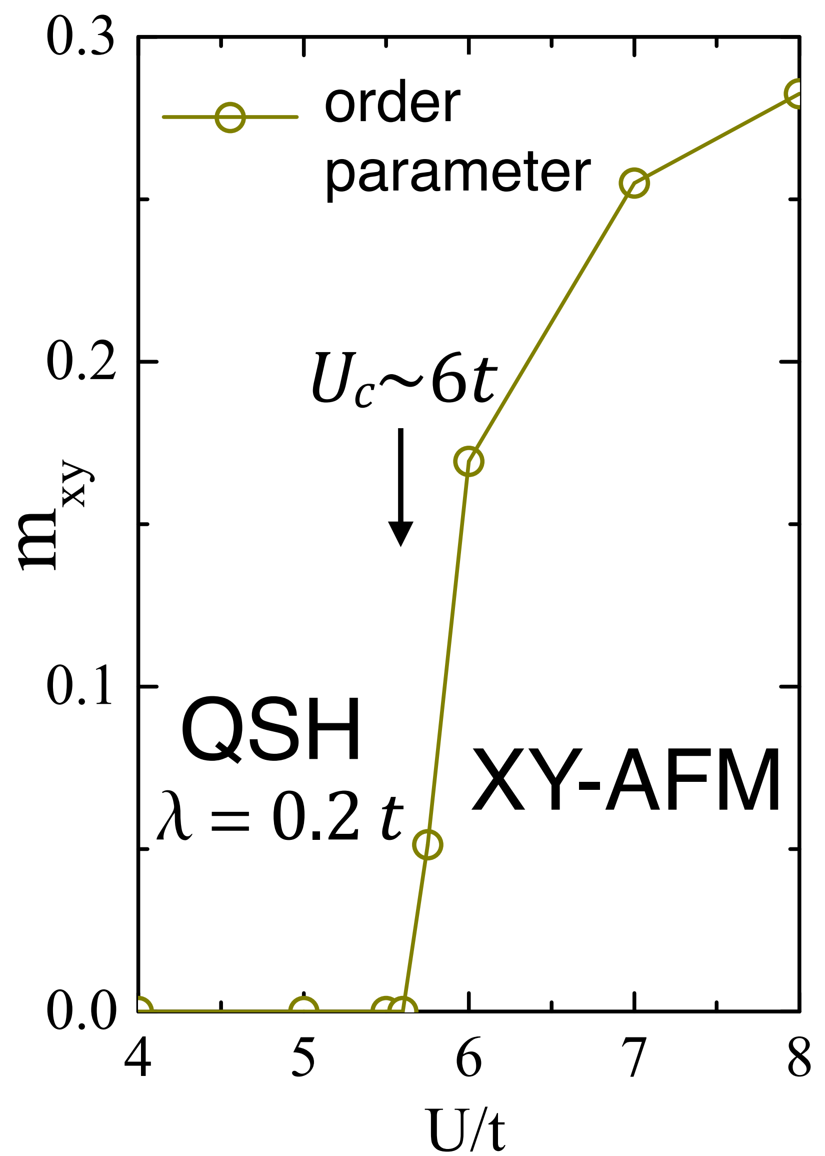


Single-Layer Kane-Mele-Hubbard Model

- Spin-1/2 fermion on **single-layer** honeycomb



$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_{\langle\langle ij \rangle\rangle} i\lambda_{ij}\, c_i^\dagger \sigma^z c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



- QSH (SPT nontrivial)

  $U(1)_{\text{charge}} \times U(1)_{\text{spin}} \times Z_2^T$ symmetry

  $\rightarrow$ $\mathbb{Z}$ classification (~ A class)

- AFM (SPT trivial)

  $U(1)_{\text{charge}} \rtimes Z_2^{T'}$ $\left(\mathcal{T}^2 = 1\right)$ symmetry

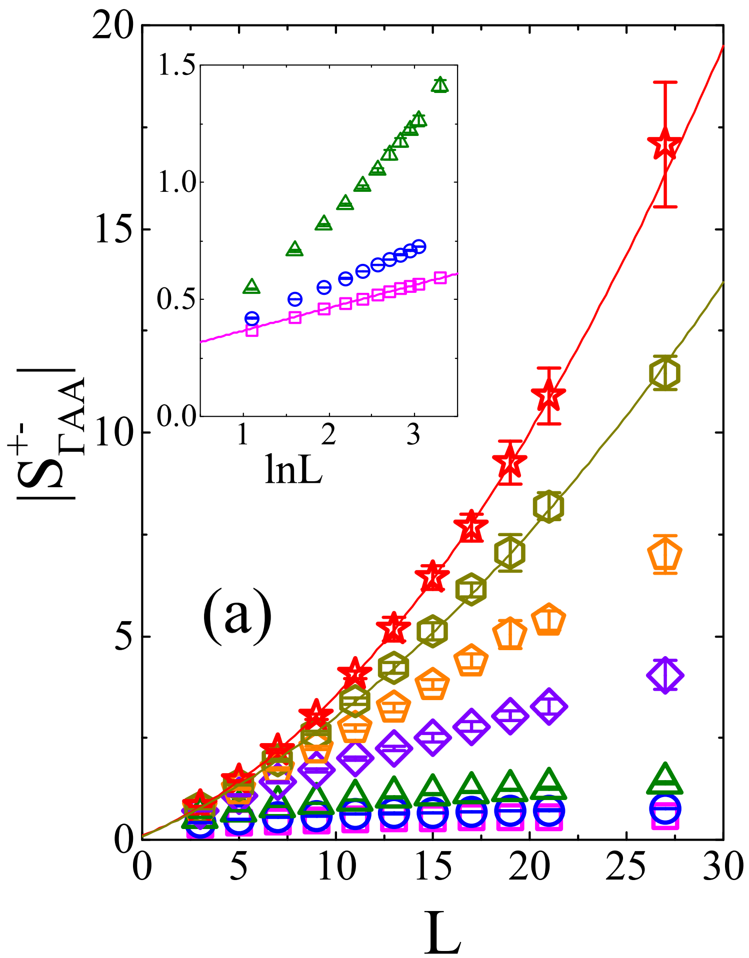
  $Z_2^{T'} : c_i \rightarrow \mathcal{K}\, \sigma^x\, c_i$

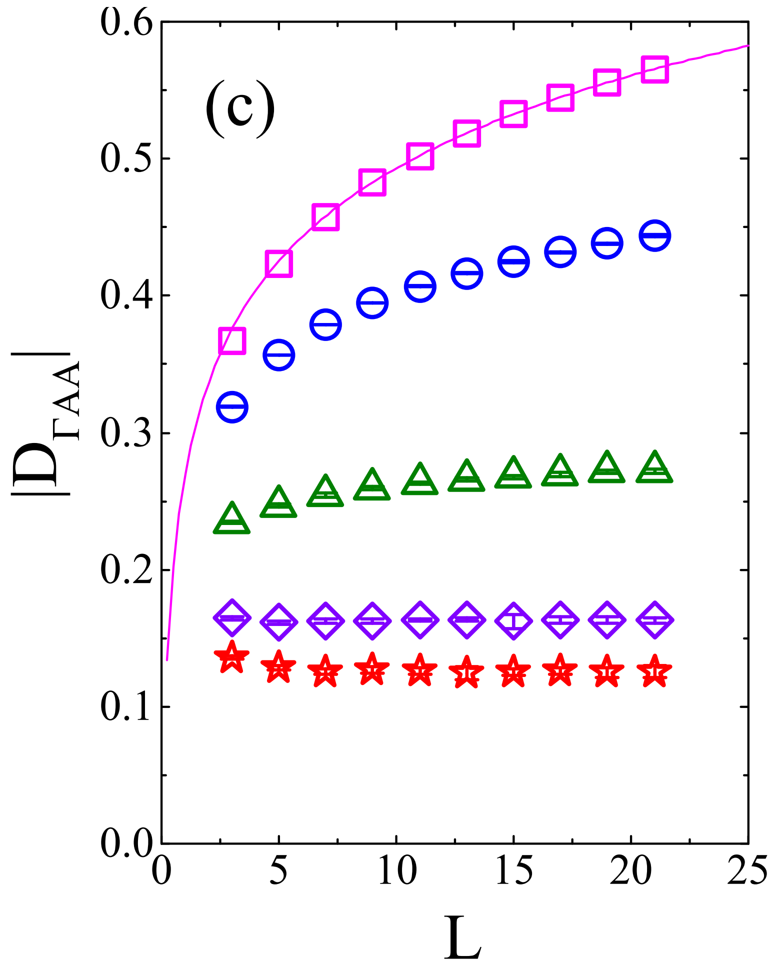
  $\rightarrow$ trivial classification (AIII class)

  - No protected gapless fermion edge mode.

Strange Correlator of Interacting QSH

- Helical Luttinger Liquid
  - Fermion channel: $C(r)\sim r^{-g/2-1/2\,g} \Rightarrow C(k)\sim k^{g/2+1/2\,g-2}$
  - Spin channel: $S(r)\sim r^{-2\,g} \Rightarrow S(k=\Gamma)\sim L^{2-2\,g}$
  - Charge channel: $D(r)\sim r^{-2/g} \Rightarrow D(k=\Gamma)\sim L^{2-2/g}$

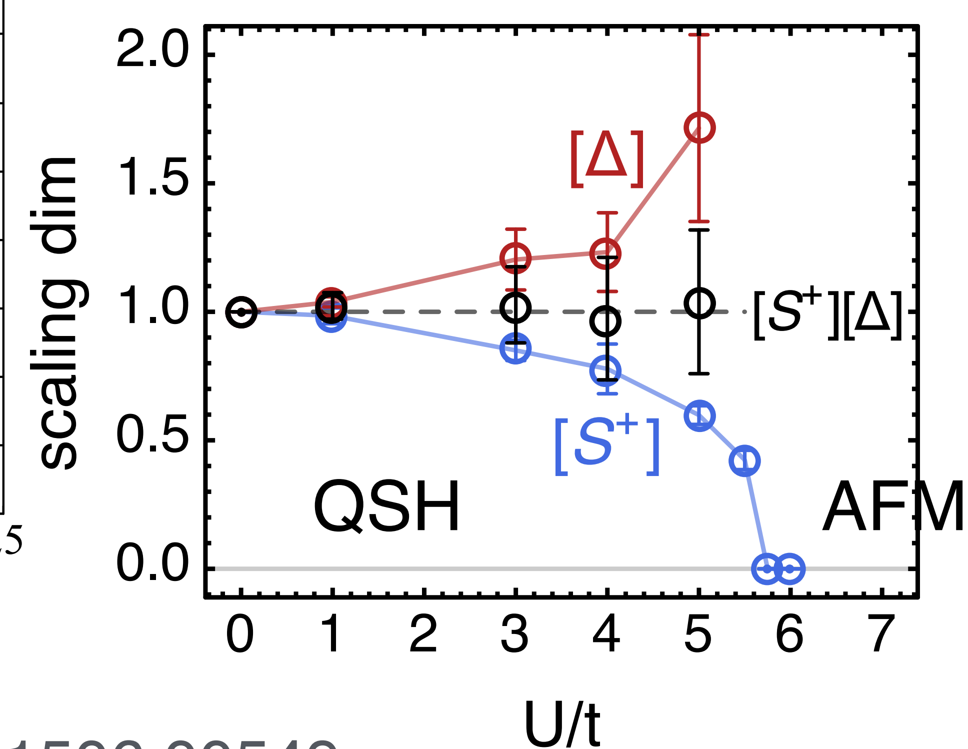




$U=0: g=1 \Rightarrow S,\, D\sim \ln L$

$U=U_c: g=0 \Rightarrow S\sim L^2,$

$D\sim L^{-\infty}\sim e^{-L}$



arXiv:1506.00549

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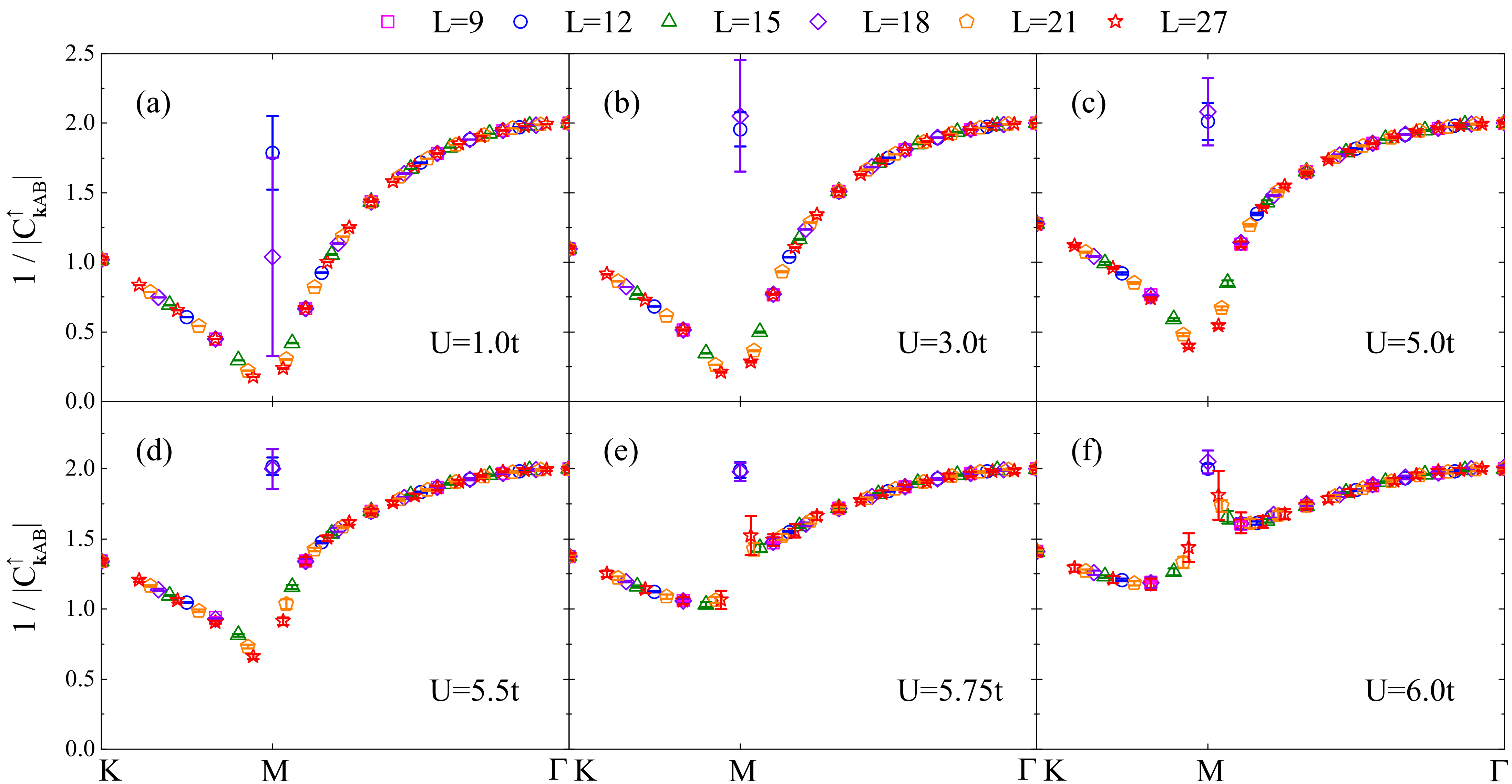

Wu et.al. arXiv:1506.00549

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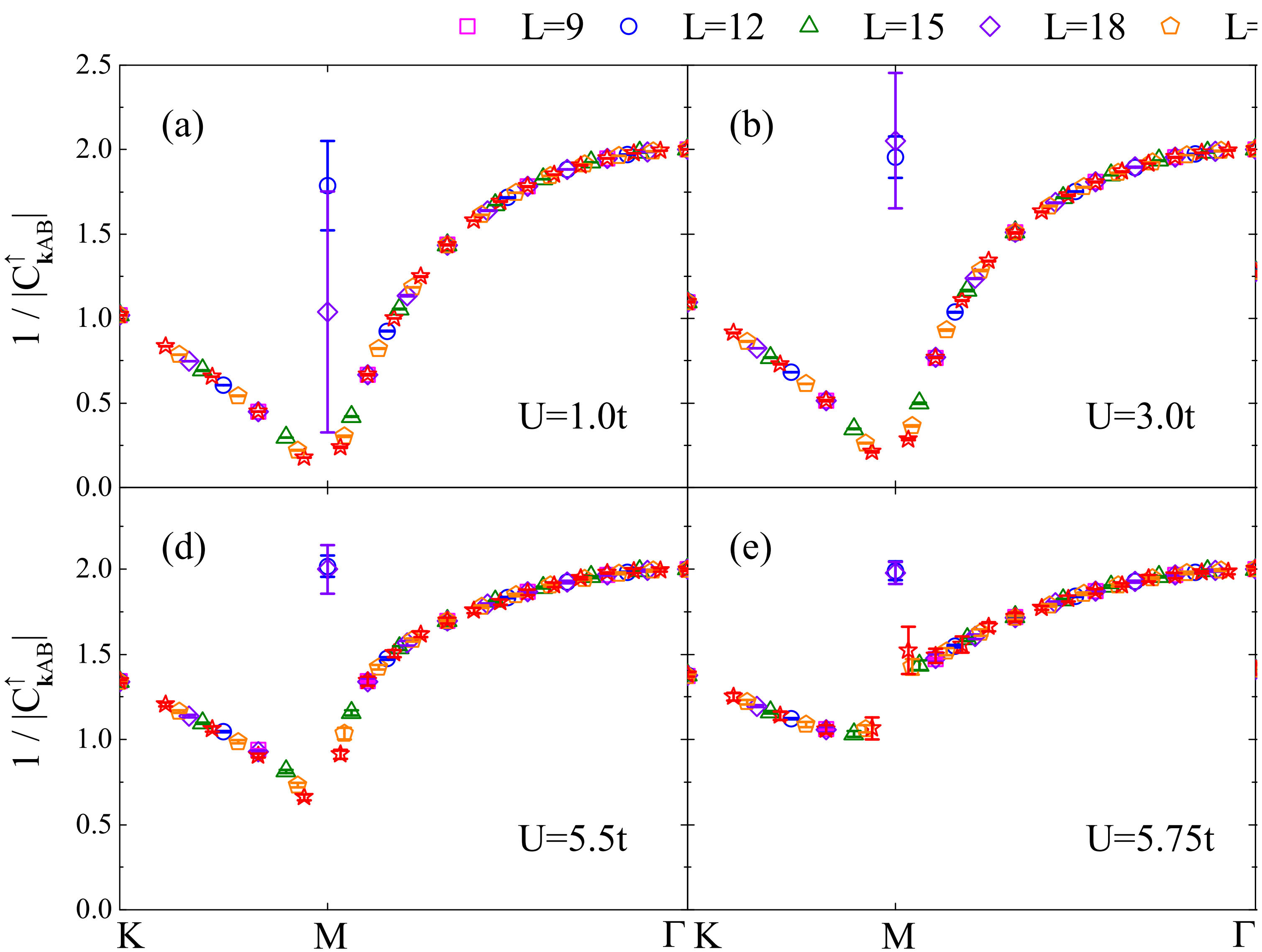
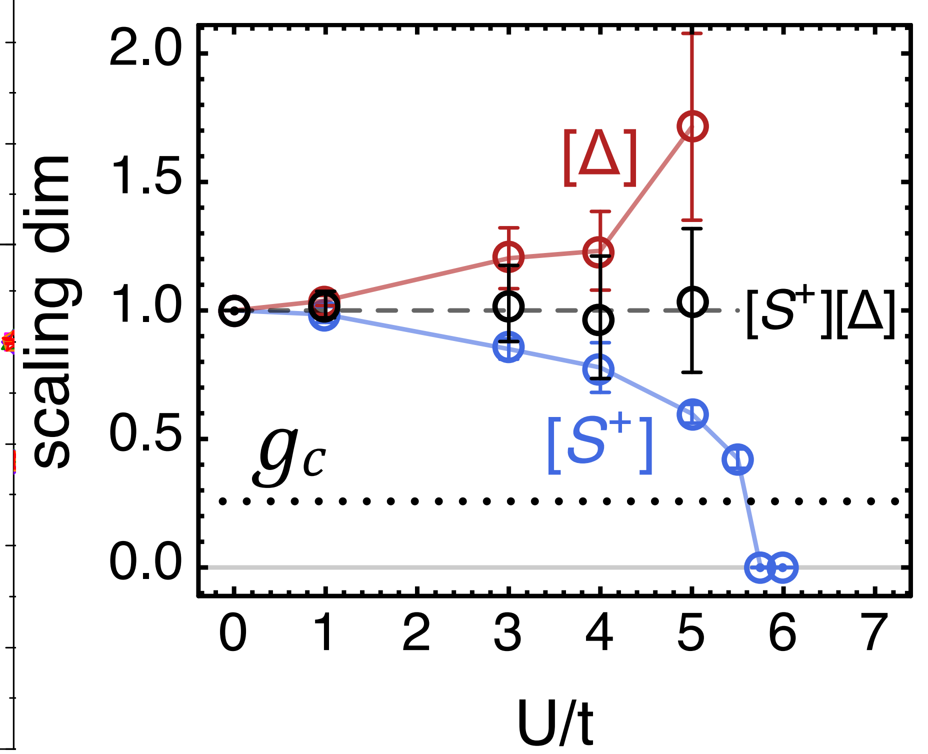


$$g/2 + 1/2g - 2 = 0$$
$$\Rightarrow g_c = 2 - 3^{1/2} \approx 0.27$$



Wu et.al. arXiv:1506.00549

Summary

- Topology + Interaction → Exotic quantum phase transitions:
  - Interaction can make a fermionic SPT state into a bosonic SPT state, such that the topological-trivial transition can happen by closing the boson gap only.
  - Interaction can gap out the Dirac / Majorana cones without generating any mean-field mass term, without breaking the symmetry.
- Strange correlator as a (numerical) diagnosis for SPT states based on bulk wave function, for both bosonic and fermionic systems, free and strong interacting.
- Outlook: QSH insulators may be realized in cold atom systems by shaking the optical lattice.

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Thanks for Your Attention!