Correlation effects in 2-D topological insulators

Journal Club

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OUTLINE

- General approach to study correlation effects
- Theoretical model
- Noninteracting quantum spin Hall insulator
- Bulk correlation effects

General approach to study correlation effects

The Research of TI

- Some examples of TI: QSHE in graphene, HgTe quantum well, BiSb alloys, and Bi_2Te_3 and Bi_2Se_3 crystals.
- TI, without the e-e interactions, can be understood in terms of single-particle Hamiltonians, allowing a full classification based on time-reversal, particle=hole, chiral symmetry and crystal symmetry.
- TI, with electron- electron interaction.

The approach to study correlation effects

- Consider the impact of the electron-electron interaction

non-interacting QSH state w/ SO coupling + interaction

  - good for the materials with significant S-O and e-e interaction
  - ex: transition-metal oxide Na_2IrO_3

- Consider the impact of the electron-electron interaction

non-interacting QSH state w/ weak SO coupling + strong interaction via a dynamically generated SO coupling

  - Topological Mott insulators: the gap is generated by interaction.
  - Ex: Sr_2IrO_4

The approach to study correlation effects

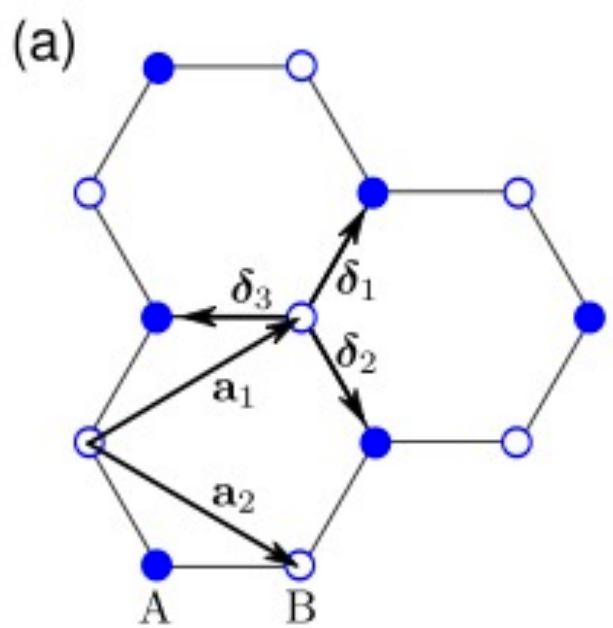
- Fractional topological insulators. With strong electronic interction and fractional charge and fractional statistics

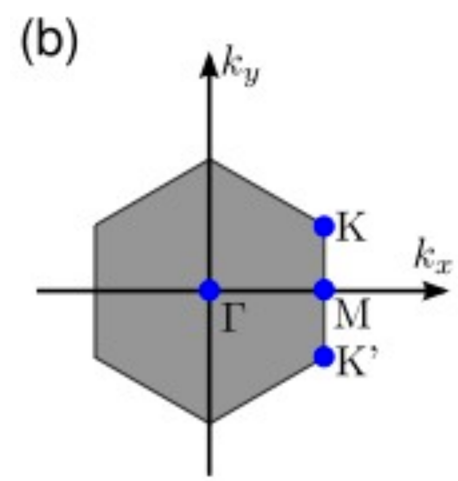
Theoretical Model

Theoretical Model

- Kane-Mele model

$$H_{\rm KM} = -t\sum_{\langle i,j\rangle}\hat{c}_i^\dagger\hat{c}_j + \mathrm{i}\,\lambda_{\rm SO}\sum_{\langle\langle i,j\rangle\rangle}\hat{c}_i^\dagger\,(\boldsymbol{\nu}_{ij}\cdot\boldsymbol{\sigma})\,\hat{c}_j + \mathrm{i}\,\lambda_{\rm R}\sum_{\langle i,j\rangle}\hat{c}_i^\dagger\,(\boldsymbol{s}\times\hat{\boldsymbol{d}}_{ij})_z\,\hat{c}_j\,.$$





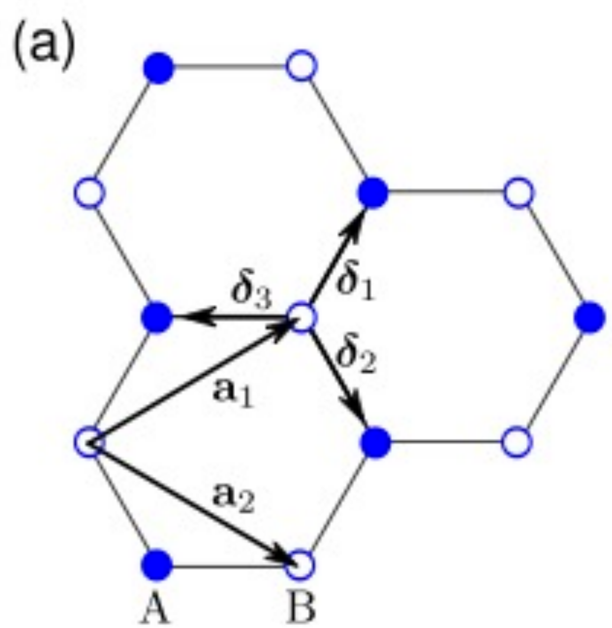
energy for hopping term

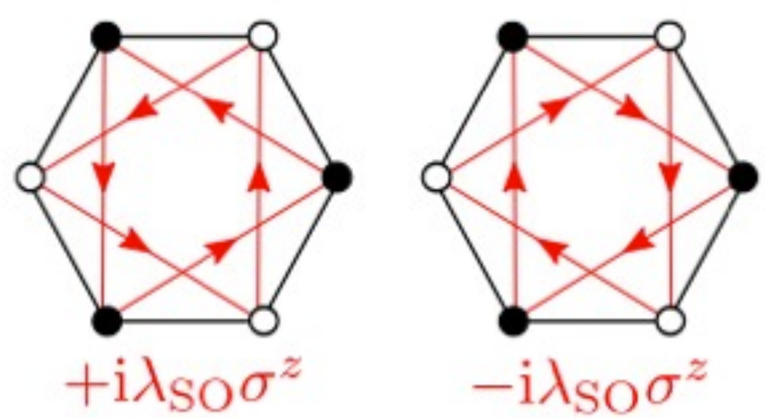
$$\pm t\left[3 + 2\cos(\sqrt{3}k_y) + 4\cos(3k_x/2)\cos(\sqrt{3}k_y/2)\right]^{1/2}$$

Theoretical Model

- Kane-Mele model

$$H_{\mathrm{KM}} = -t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{SO}} \sum_{\langle\langle i,j \rangle\rangle} \hat{c}_i^\dagger \left(\boldsymbol{\nu}_{ij} \cdot \boldsymbol{\sigma}\right) \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{R}} \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \left(\boldsymbol{s} \times \hat{\boldsymbol{d}}_{ij}\right)_z \hat{c}_j \,.$$





Theoretical Model

- Kane-Mele model

$$H_{\mathrm{KM}} = -t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{SO}} \sum_{\langle\langle i,j \rangle\rangle} \hat{c}_i^\dagger \left(\boldsymbol{\nu}_{ij} \cdot \boldsymbol{\sigma}\right) \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{R}} \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \left(\boldsymbol{s} \times \hat{\boldsymbol{d}}_{ij}\right)_z \hat{c}_j .$$

Rashba coupling

- breaks z inversion symmetry because of purely off-diagonal
- when $\lambda_{SO} \neq 0$, The KM model describes a QSH insulator as long as

$$\lambda_R < 2\sqrt{3}\lambda_{SO}$$

- symmetry-protected crossing at k=0 (k=π) for armchair (zigzag) edge.

Theoretical Model

- KM-Hubbard model

$$H_{\mathrm{KMH}} = -t\sum_{\langle i,j\rangle} \hat{c}_i^\dagger \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{SO}} \sum_{\langle\langle i,j\rangle\rangle} \hat{c}_i^\dagger \left(\boldsymbol{\nu}_{ij}\cdot\boldsymbol{\sigma}\right)\hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{R}} \sum_{\langle i,j\rangle} \hat{c}_i^\dagger \left(\boldsymbol{s}\times\hat{\boldsymbol{d}}_{ij}\right)_z \hat{c}_j \,.$$

$$+\tfrac{1}{2}U\sum_i (\hat{c}_i^\dagger \hat{c}_i - 1)^2$$

  - compare to Hubbard model, the symmetry is reduced.
    SO coupling reduce the rotation symmetry C_6 to C_3 and spin rotation symmetry SU(2) to U(1) (w.o/ Rashba) or to Z_2(w/ Rashba)

  - can be investigated with exact quantum Monte Carlo.

Theoretical Model

- Haldane-Hubbard model - breaks TRS, doesn’t not describe QSH state.

$$H_{\mathrm{HH}} = -t_1 \sum_{\langle ij \rangle} c_i^\dagger c_j - t_2 \sum_{\langle\langle ij \rangle\rangle} \mathrm{e}^{\mathrm{i}\phi_{ij}} c_i^\dagger c_j + V \sum_{\langle ij \rangle} \widehat{n}_i \widehat{n}_j$$

SO coupling
with fixed spin
direction

Theoretical Model

- Haldane-Hubbard model - breaks TRS, doesn't not describe QSH state.

$$H_{\mathrm{HH}} = -t_1 \sum_{\langle ij \rangle} c_i^\dagger c_j - t_2 \sum_{\langle\langle ij \rangle\rangle} \mathrm{e}^{\mathrm{i}\phi_{ij}} c_i^\dagger c_j + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

nearest neighbor repulsion

- can be studied in the context of topological quantum phase transition
- V=0 realized the integer quantum anomalous Hall effect.
- Large V will cause a quantum phase transition to CDW state.

Theoretical Model

- BHZH model

$$H_{\rm BHZ} = \sum_{\boldsymbol{i}} \sum_{\alpha} \sum_{\sigma} \epsilon_\alpha c^\dagger_{\boldsymbol{i},\alpha,\sigma} c_{\boldsymbol{i},\alpha,\sigma} - \sum_{\boldsymbol{i},\boldsymbol{\delta}} \sum_{\alpha\beta} \sum_{\sigma} c^\dagger_{\boldsymbol{i}+\boldsymbol{\delta},\alpha,\sigma} [t^\sigma_{\boldsymbol{\delta}}]^{\alpha\beta} c_{\boldsymbol{i},\beta,\sigma} ,$$

  - Derive from HgTe quantum well
  - Consider s and p orbitals on 2D square lattice.

$$t^\sigma_{\pm x} = \begin{pmatrix} t_{\rm ss} & \pm t_{\rm sp} \\ \mp t_{\rm sp} & -t_{\rm pp} \end{pmatrix} ,$$

$$t^\sigma_{\pm y} = \begin{pmatrix} t_{\rm ss} & \pm {\rm i}\,{\rm sgn}(\sigma) t_{\rm sp} \\ \pm {\rm i}\,{\rm sgn}(\sigma) t_{\rm sp} & -t_{\rm pp} \end{pmatrix} .$$

Theoretical Model

- BHZH model

$$H_{\mathrm{BHZ}} = \sum_{\boldsymbol{i}} \sum_{\alpha} \sum_{\sigma} \epsilon_{\alpha} c^{\dagger}_{\boldsymbol{i},\alpha,\sigma} c_{\boldsymbol{i},\alpha,\sigma} - \sum_{\boldsymbol{i},\boldsymbol{\delta}} \sum_{\alpha\beta} \sum_{\sigma} c^{\dagger}_{\boldsymbol{i}+\boldsymbol{\delta},\alpha,\sigma} [t^{\sigma}_{\boldsymbol{\delta}}]^{\alpha\beta} c_{\boldsymbol{i},\beta,\sigma} ,$$

  - set $\varepsilon_s = -\varepsilon_p = \varepsilon / 2$, $t_{ss} = t_{pp} = t$
    There are three phases in this model.
    - For $-8t < \varepsilon < 0$, QSH phase(Γ phase).
    - For $0 < \varepsilon < 8t$, QSH phase(M phase).
    - Else trivial.

can be observed in HgTe quantum wells

Only in T-B model

Theoretical Model

- BHZH + Hubbard interaction

$$U \sum_{\boldsymbol{i}\alpha} \widehat{n}_{\boldsymbol{i}\alpha\uparrow} \widehat{n}_{\boldsymbol{i}\alpha\downarrow}$$

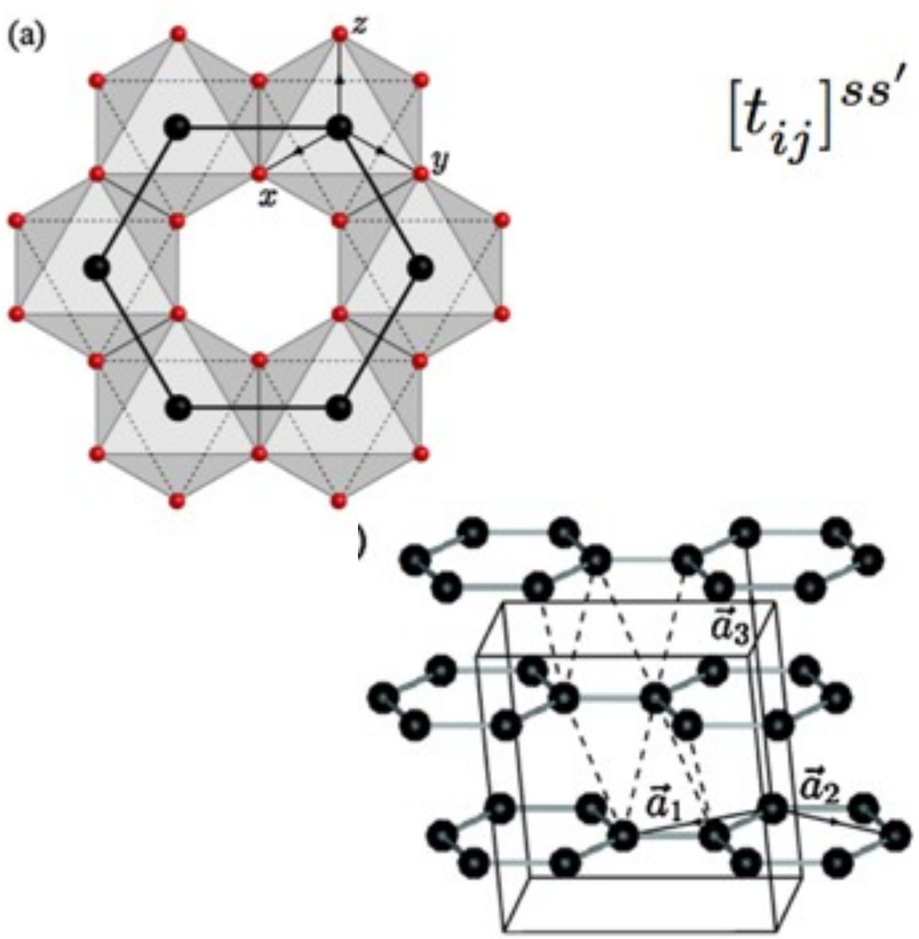
$$U \sum_{\boldsymbol{i}} \widehat{n}_{\boldsymbol{i}} (\widehat{n}_{\boldsymbol{i}} - 1)$$

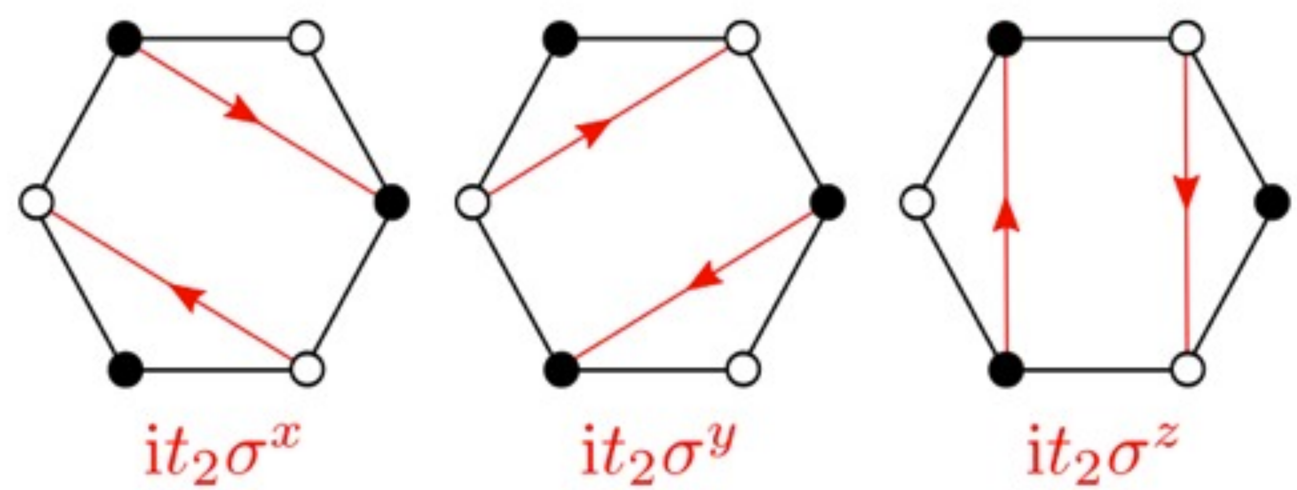
Theoretical Model

- Sodium iridate model. QSH phase in the transition-metal oxide Na_2IrO_3.

$$H_{\mathrm{SI}} = -t\sum_{\langle ij\rangle}\sum_{\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{\langle\langle ij\rangle\rangle}\sum_{ss'} c^{\dagger}_{is}[t_{ij}]^{ss'}c_{js'} + U\sum_{i}\widehat{n}_{i\uparrow}\widehat{n}_{i\downarrow}\,.$$

$$[t_{ij}]^{ss'} = -t_1\delta_{ss'} + \mathrm{i}t_2\sigma^{w}_{ss'}\,,$$





Theoretical Model

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$$H_{\mathrm{SI}} = -t\sum_{\langle ij\rangle}\sum_{\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{\langle\langle ij\rangle\rangle}\sum_{ss'} c^{\dagger}_{is}[t_{ij}]^{ss'}c_{js'} + U\sum_{i}\widehat{n}_{i\uparrow}\widehat{n}_{i\downarrow}\,.$$

  - Only one parameter t_2, that determines the strength of both spin-conserving and nonconserving hopping process. (note: two parameters in KM model)

  - Has helical edge states cross at k=0 (k=π) for armchair (zigzag) edge.

  - Strong e-e interacions are generical in Na_2IrO_3.

Noninteracting Quantum Spin Hall System

Noninteracting quantum spin Hall insulator

- Consider a KM model.
  - Time reversal symmetry. $H(-\boldsymbol{k}) = \hat{\Theta} H(\boldsymbol{k}) \hat{\Theta}^{-1}$
  - KM model w.o Rashba coupling = 2 copies of Haldane model. (like QSHE ~ 2 copies of QHE).
  - In Haldane model, the Hall conductivity is $\sigma_{xy} = \pm e^2/h$
    In KM model, the Hall conductivity $\sigma_{xy}^{\uparrow} = -\sigma_{xy}^{\downarrow}$.
    The total Hall conductivity = 0.
    The spin Hall conductivity $\sigma_{xy}^{\mathrm{s}} = (\hbar/2e)(\sigma_{xy}^{\uparrow} - \sigma_{xy}^{\downarrow})$

Noninteracting quantum spin Hall insulator

- Topological invariant

  - For a noninteracting IQH system, the chern number is

    $$C_m = \frac{1}{2\pi} \int \mathrm{d}^2\boldsymbol{k}\, \mathcal{F}_m(\boldsymbol{k})$$

    for 2*2 Hamiltonian $H^\sigma(\boldsymbol{k}) = \boldsymbol{h}^\sigma(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$, it can be further simplified to

    $$C^\sigma = \frac{1}{4\pi} \int \mathrm{d}^2\boldsymbol{k} \left[\partial_{k_x} \hat{\boldsymbol{h}}^\sigma(\boldsymbol{k}) \times \partial_{k_y} \hat{\boldsymbol{h}}^\sigma(\boldsymbol{k})\right] \cdot \hat{\boldsymbol{h}}^\sigma(\boldsymbol{k}).$$

  - In QSH system, Chern number =0 and the spin Chern number is $C^{\mathrm{s}} = (C^\uparrow - C^\downarrow)/2 = \pm 1$,and the corresponding z2 topological invariant can be defined by $\nu = C^{\mathrm{s}} \bmod 2$
    (note: it's only true when spin is conserved.)

Noninteracting quantum spin Hall insulator

- It is the special form of the S-O cause the existence of a topological state.

  Counter-ex: adding a staggered sublattice potential can also open a gap, which preserve TRS but breaks inversion symmetry. But it leads to a trivial insulator.

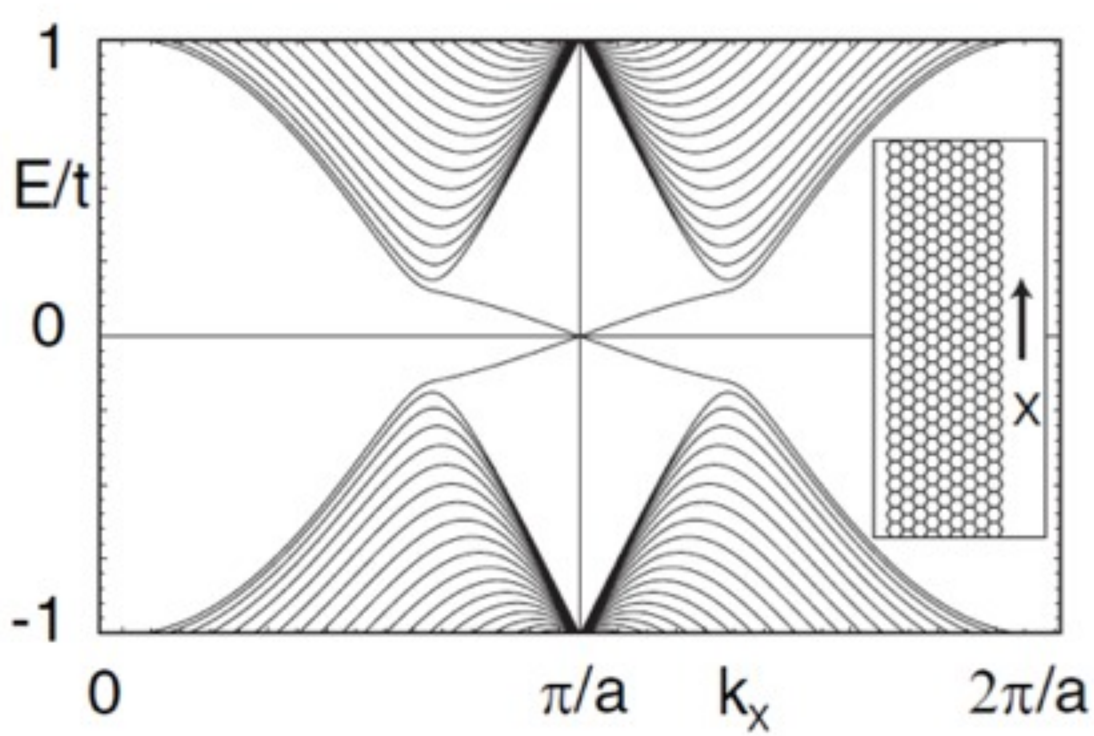
- the gap can be closed by Rashba coupling.

- bulk-boundary correspondence - thee existence of edge states is guaranteed by the topological nature of the bulk system.

- the topological phase can't be adiabatically connected to trivial phase. The transition can occur either via a closing of the bulk band gap, or via the breaking of TRS

Noninteracting quantum spin Hall insulator

- The edge state



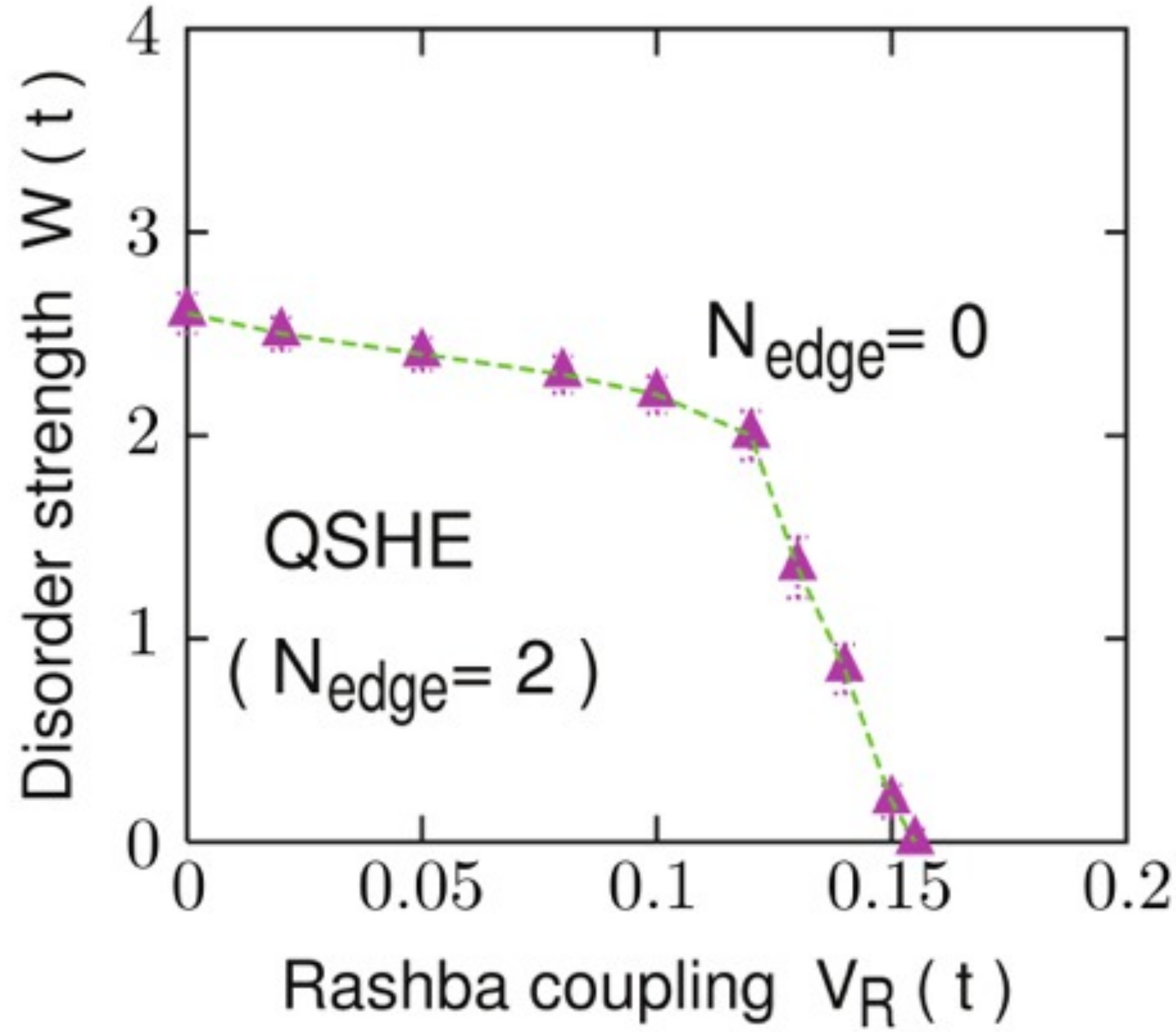
for the zigzag case

It is protected by TRS

The single-particle backscattering is not allowed in a helical liquid, because the two states are orthogonal. However, if even number of edge states exist for each spin direction, single-pparticle backscattering is allowed.

Noninteracting quantum spin Hall insulator

The stability of edge state are respect to disorder and Rashba spin-orbit coupling.



Noninteracting quantum spin Hall insulator

- An alternative approach to study the topological states of matter is based on Chern-Simons field theory - a low-energy theory of gauge fields that is applicable to interacting and even fractional states.

  - Example: IQHE.

    - Start from simple noninteracting Haldane model

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j$$

    - Coupled to EM field,

$$H(A^\mu) = \sum_{ij} t_{ij} c_i^\dagger c_j \exp\left[\frac{2\pi \mathrm{i}}{\Phi_0} \int_i^j \mathbf{A}(\mathbf{l}, t) \cdot \mathrm{d}\mathbf{l}\right] + ec \sum_i A_0(i, t) c_i^\dagger c_i \,.$$

Noninteracting quantum spin Hall insulator

- Write down the partition function

$$Z(A_\mu) = \int \prod_i \mathrm{d}c_i^\dagger \mathrm{d}c_i \, \mathrm{e}^{\mathrm{i}S(A_\mu)}$$

with action

$$S(A_\mu) = \int \mathrm{d}t \left\{ \sum_i c_i^\dagger(t) \left[\delta_{ij} \mathrm{i}\partial_t - t_{ij} \right] c_j(t) + \sum_i j^\mu(i,t) A_\mu(i,t) \right\} .$$

- Integrate out the fermion operator to get

$$S_{\mathrm{eff}}^{\mathrm{CS}}(A_\mu) = C \frac{e^2}{4\pi} \epsilon^{\mu\nu\rho} \int \mathrm{d}^2x \int \mathrm{d}t A_\mu \partial_\nu A_\rho$$

- Using $j_\mu = \delta S_{\mathrm{eff}}^{\mathrm{CS}} / \delta A_\mu$, we can get the response function, familiar quantized Hall response

$$j_x = \sigma_{xy} E_y , \quad \sigma_{xy} = C \frac{e^2}{h} .$$

Bulk Correlation Effect

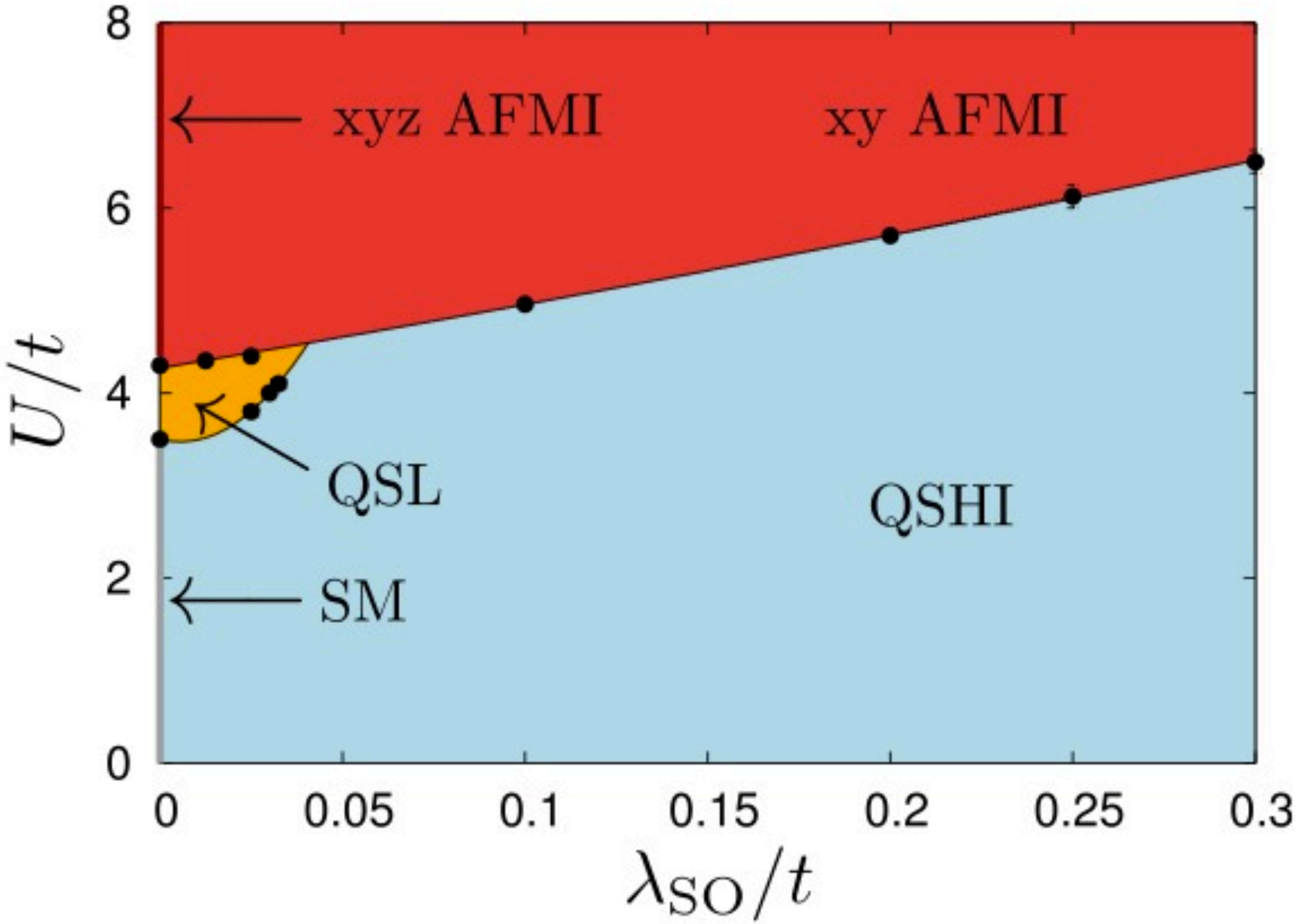
Bulk correlation effects

- Now let's consider the impact of electronic correlations.

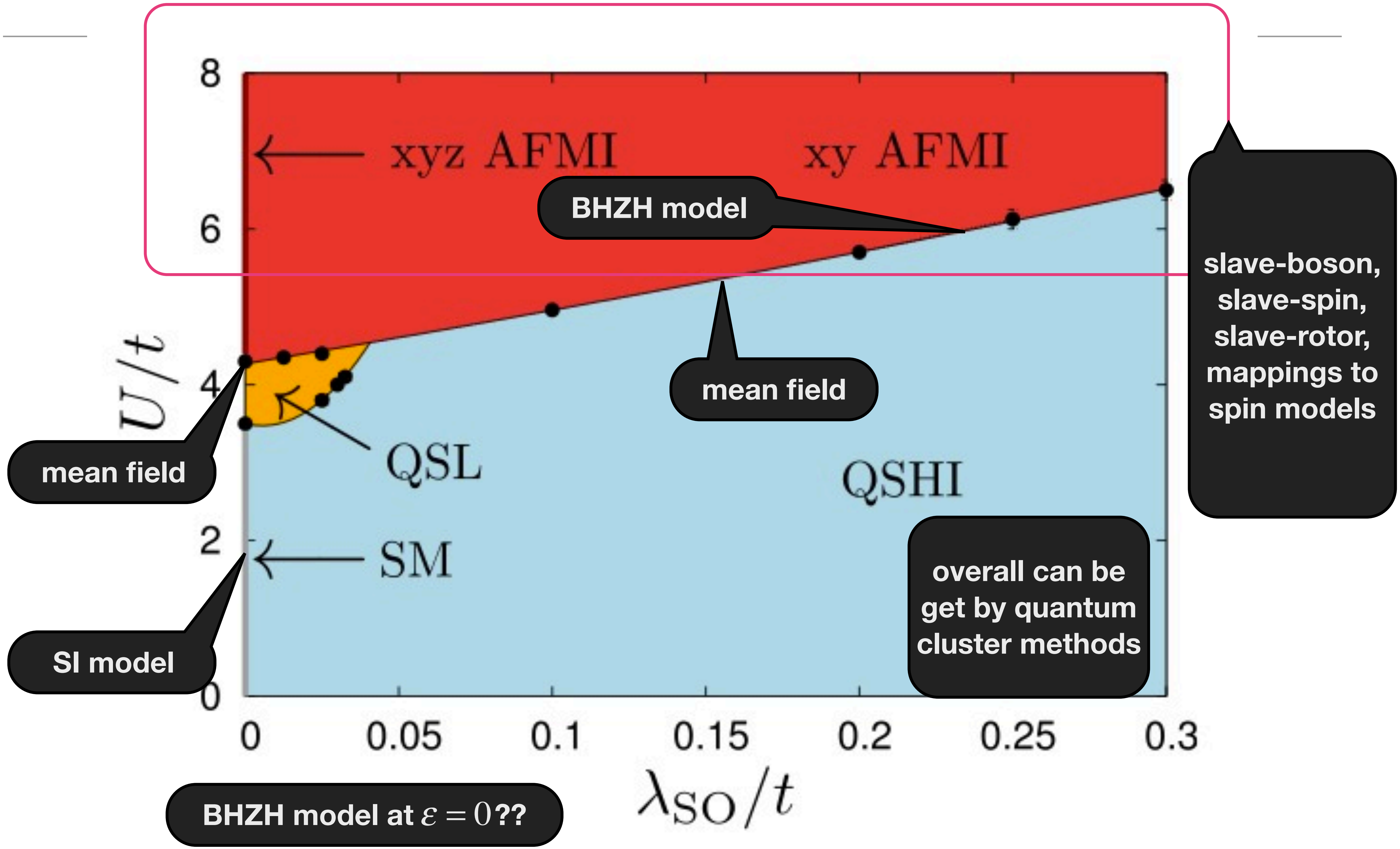
- Start from the KMH model.   We can see how the the phases change by the ration of SO/t coupling and electronic interaction U/t.

$$H_{\mathrm{KMH}} = -t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{SO}} \sum_{\langle\langle i,j \rangle\rangle} \hat{c}_i^\dagger \left(\boldsymbol{\nu}_{ij} \cdot \boldsymbol{\sigma}\right) \hat{c}_j + \mathrm{i}\,\lambda_{\mathrm{R}} \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \left(\boldsymbol{s} \times \hat{\boldsymbol{d}}_{ij}\right)_z \hat{c}_j \,. \\ + \tfrac{1}{2} U \sum_i (\hat{c}_i^\dagger \hat{c}_i - 1)^2$$

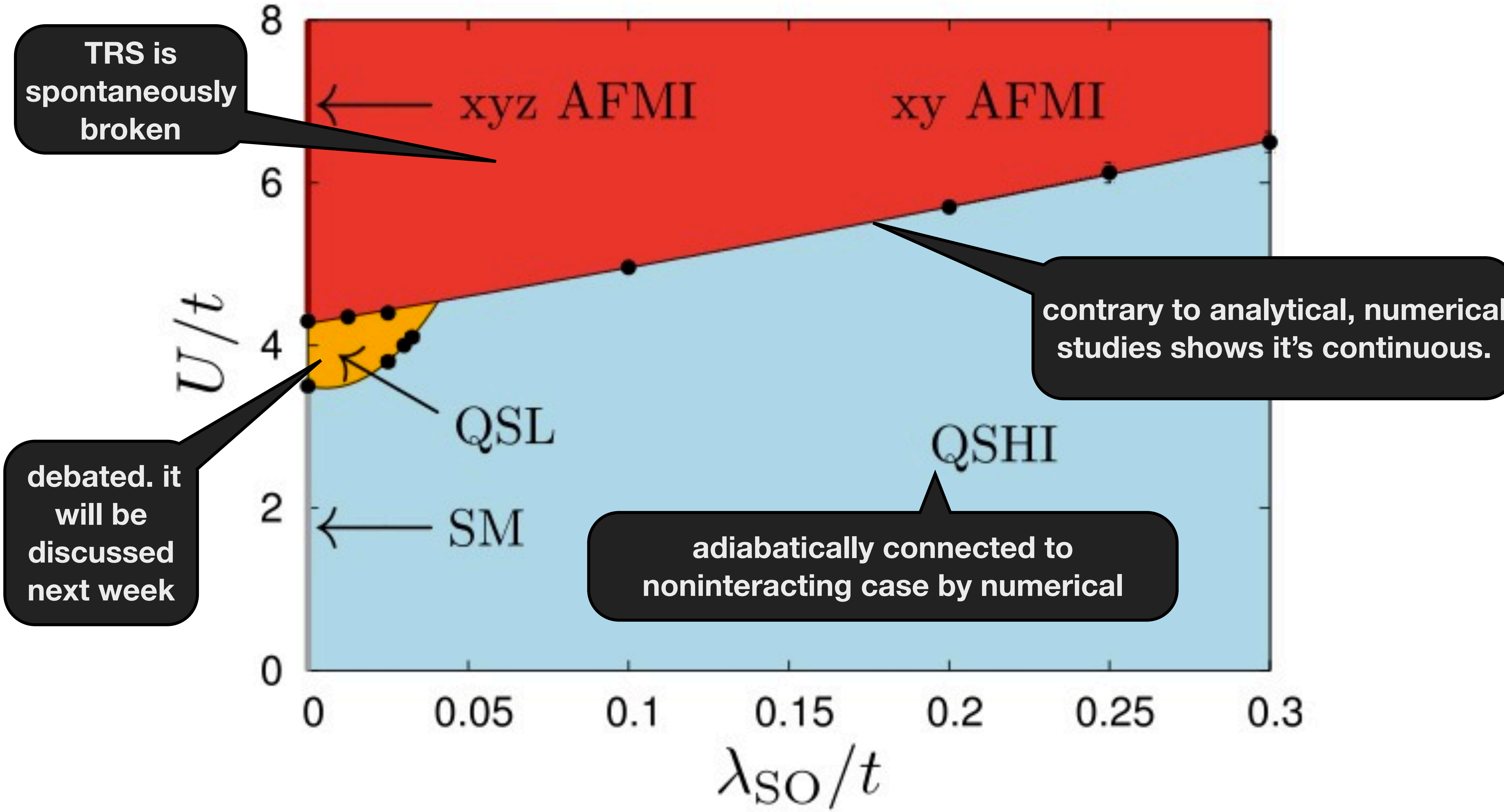
KMH model


8
6
4
2
0
U/t
xyz AFMI
xy AFMI
QSL
QSHI
SM
0
0.05
0.1
0.15
0.2
0.25
0.3
λ_{SO}/t

KMH model - quantum Monte Carlo simlation

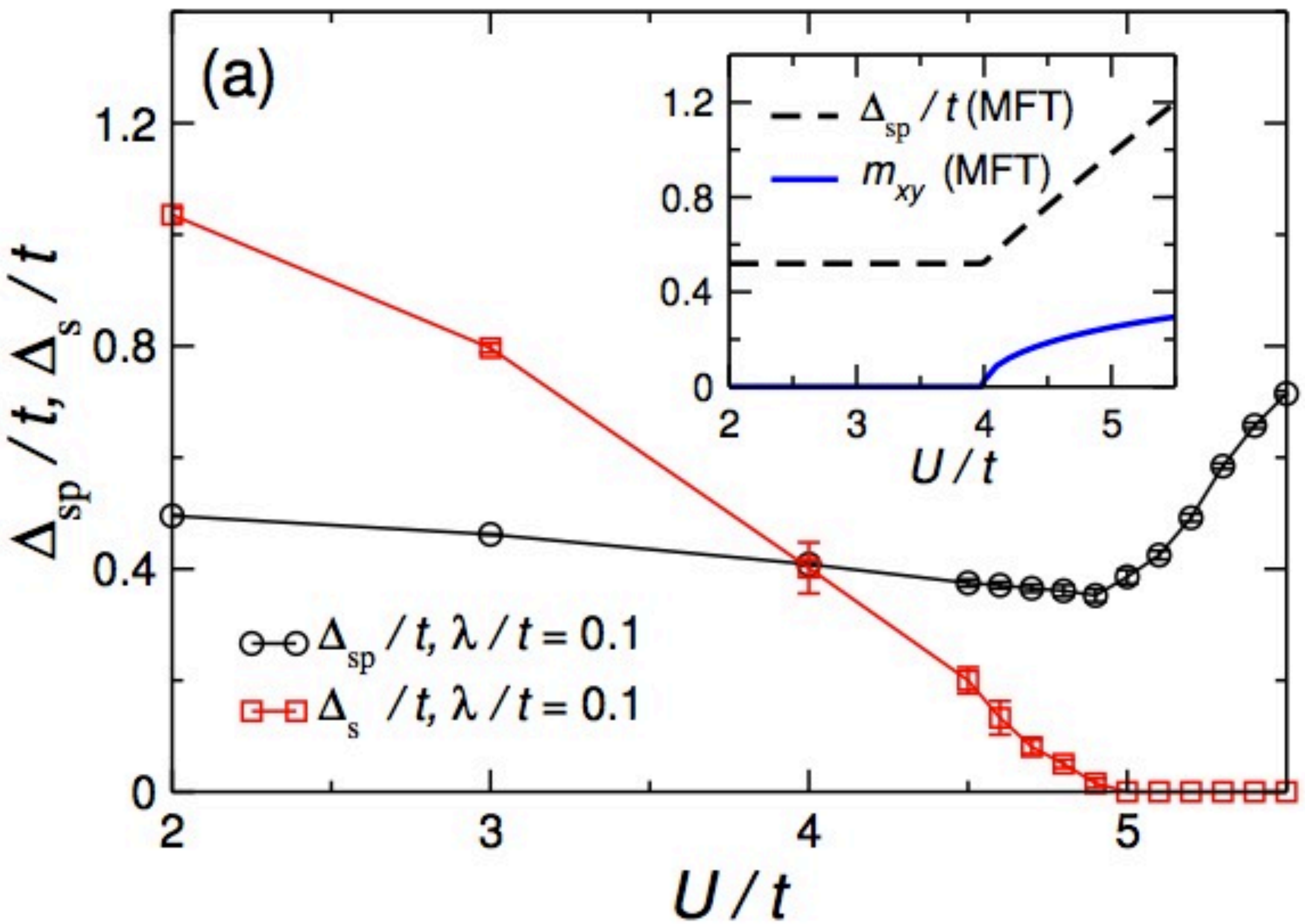


KMH model


TRS is spontaneously broken
xyz AFMI
xy AFMI
contrary to analytical, numerical studies shows it's continuous.
QSL
QSHI
debated. it will be discussed next week
SM
adiabatically connected to noninteracting case by numerical
8
6
4
2
0
U/t
0
0.05
0.1
0.15
0.2
0.25
0.3
λ_{SO}/t

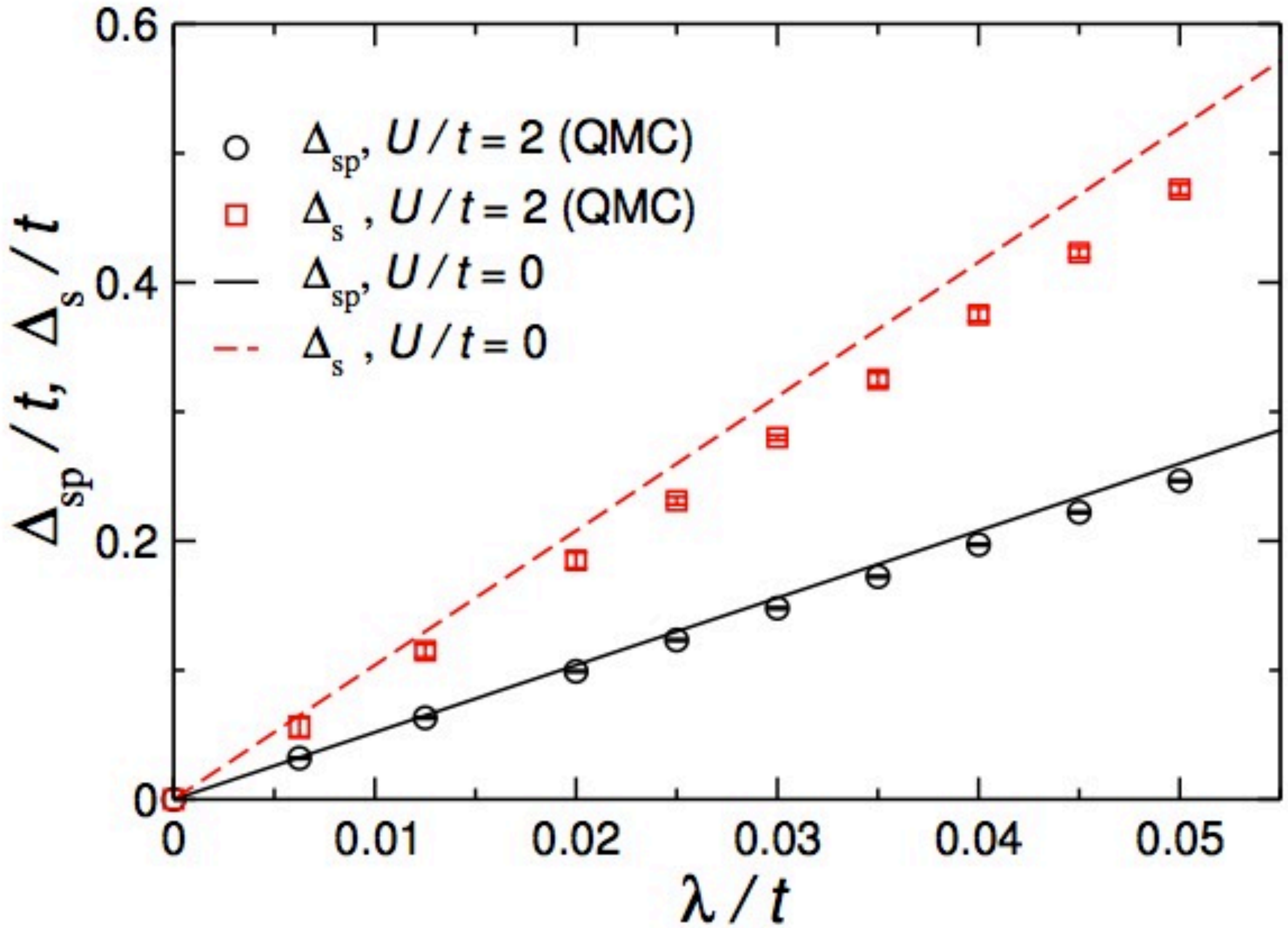
Bulk correlation effect

- The gap remains open in QSH phase.



Bulk correlation effect

- The interacting phase can be adiabatically relates to the noninteracting model. So to what extent this phase resembles the KM model?



Bulk correlation effect

- The topological invariant is still one.
- gapless helical edge states are observed even for substantial values of U/t. (But the spectral weight, edge transport and magnetic correlations would be modified.)
- Conclusion: the QSH phase is qualitatively unaffected by correlation up to the point where it breaks done.

END.....   GOOD NIGHT~