Correlation Effects in Quantum Spin Hall Insulators

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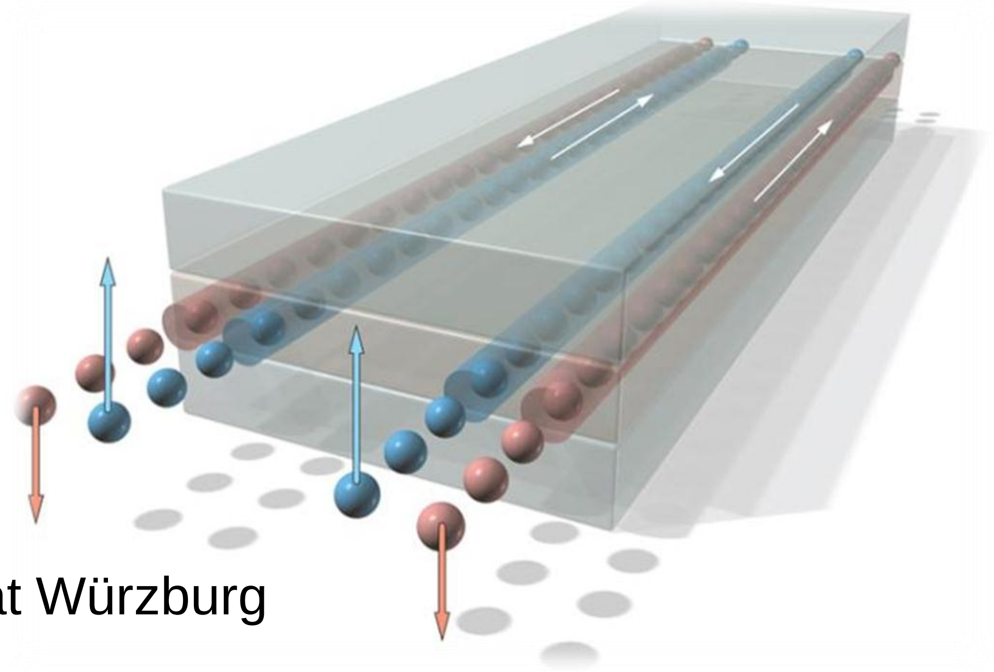


- Martin Hohenadler Universität Würzburg
- Fakher F. Assaad

- Thomas C. Lang RWTH Aachen University
- Stefan Wessel

- Alejandro Muramatsu Universität Stuttgart

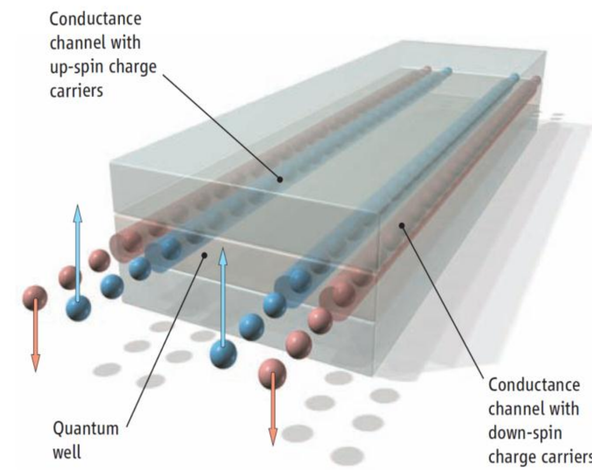
- Z. Y. Meng et al., Nature 464, (2010)
- M. Hohenadler et al., PRL 106, (2011)
- Z. Y. Meng et al., in preparation

Motivation

Topological / Quantum spin-Hall insulators

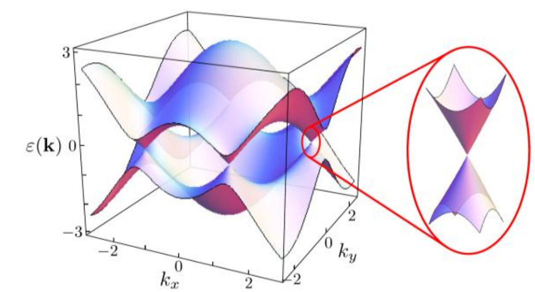
- New state of matter from strong spin-orbit (SO) coupling.
- Predicted and realized in HgTe QWs.

Bernevig et al., Science 2006; König et al., Science 2007



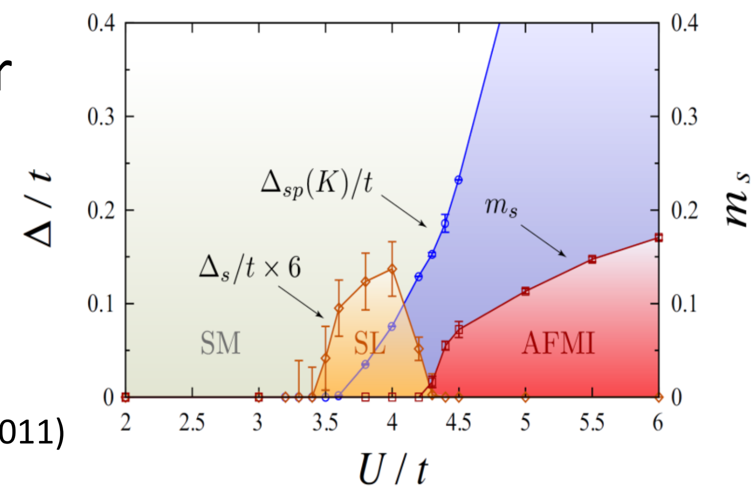
Correlated Dirac fermions

- Hubbard model on the honeycomb lattice,
  Quantum spin liquid phase.
  Meng et al., Nature (2010)
- Massless Dirac fermions in Graphene with SO coupling.
  Kane and Mele, Phys. Rev. Lett. (2005)

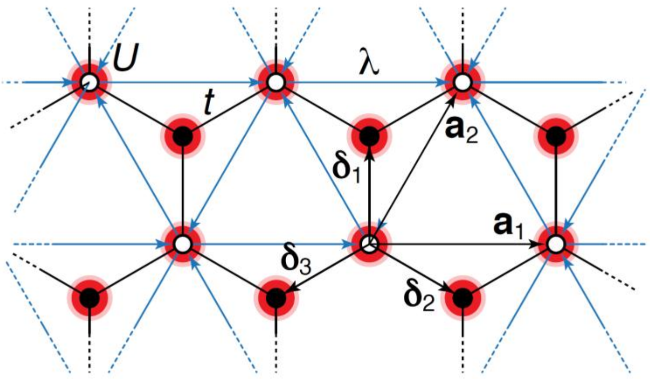


Topological / Quantum spin-Hall insulator
+ Interactions

Hasan and Kane, Rev. Mod. Phys. (2010)
Pesin and Balents, Nature Physics (2010)
Rachel and Le Hur, Phys. Rev. B (2010)
D. Zheng et al., arXiv:1011.5858 (2010)
S.-L. Yu et al., Phys. Rev. Lett. (2011)
D.-H. Lee, arXiv:1105.4900 (2011); Griset and Xu, arXiv:1107.1245 (2011)



Kane-Mele-Hubbard Model

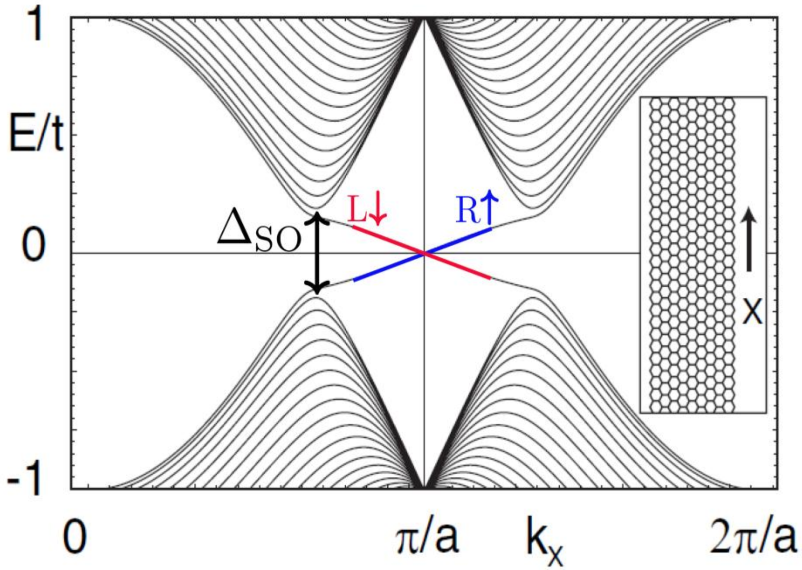


$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i\lambda \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j + \frac{U}{2} \sum_i (c_i^\dagger c_i - 1)^2$$

$$c_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$$

$$\nu_{ij} = \pm 1$$

- Nearest-neighbor hopping t
- Spin-orbit coupling λ
- Coulomb repulsion U
- $\lambda \neq 0$: SU(2) → U(1), $C_6 \rightarrow C_3$



U=0 Kane-Mele Model

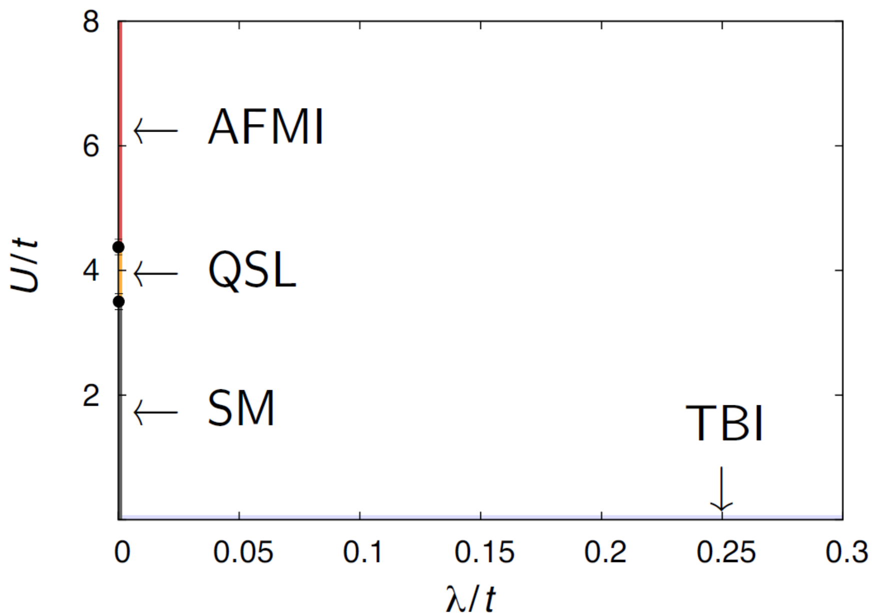
- Time reversal invariant QSH insulator
- Spin-orbital bulk gap $\Delta_{SO} = 3\sqrt{3}\lambda$
- Gapless, helical edge states (topologically protected)

Kane and Mele, Phys. Rev. Lett. (2005)
C. Wu et al., Phys. Rev. Lett. (2006)

Phase diagram of Kane-Mele-Hubbard Model

Limiting cases

- Dirac fermions ($\lambda = 0$)
  Semimetal (SM) → Quantum Spin Liquid (QSL) → Antiferromagnetic Mott Insulator (AFMI)
- Kane-Mele Model ($U = 0$)
  Topological Band Insulator (TBI)



- Magnetic transition at $\lambda > 0$?
- Effect of λ on QSL and SM ?
- Effect of U on the helical edge states ?

Method

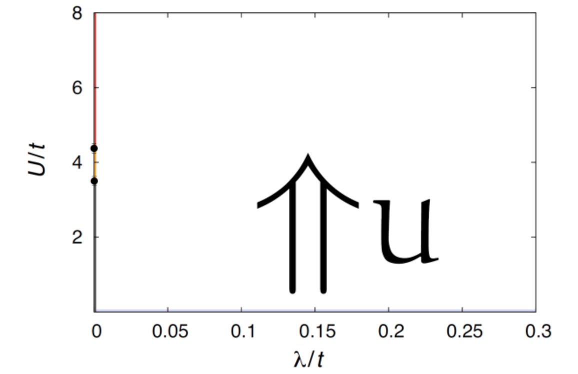
Projective (zero temperature) Determinantal Quantum Monte Carlo

- Hubbard-Stratonovich transformation, auxiliary field of integer spins
- Scales as $\sim N_\tau N^3$ (N_τ imaginary time slices, $N = 2L^2$ system size)
- Sign-problem free at half-filling

Magnetic transition at finite Spin-Orbit coupling

$\lambda = 0$: Heisenberg AFMI with $J = 4t^2/U$ at large U/t

$\lambda > 0$: z-direction frustrated, easy-plane XY order



Magnetic structure factor:

$$S^{xy}_{\mathrm{AF}} = \frac{1}{L^2}\sum_{i,j}(-1)^{i+j}\langle\Psi_0|S^+_i S^-_j + S^-_i S^+_j|\Psi_0\rangle$$

U(1) symmetry is spontaneously broken, expected (2+1)D XY universality class

D.-H. Lee, arXiv (2011); Griset and Xu, arXiv (2011)

Finite size scaling:

$$\frac{S^{xy}_{\mathrm{AF}}}{N} = L^{-2\beta/\nu} f_1[(U - U_c)L^{1/\nu}]$$

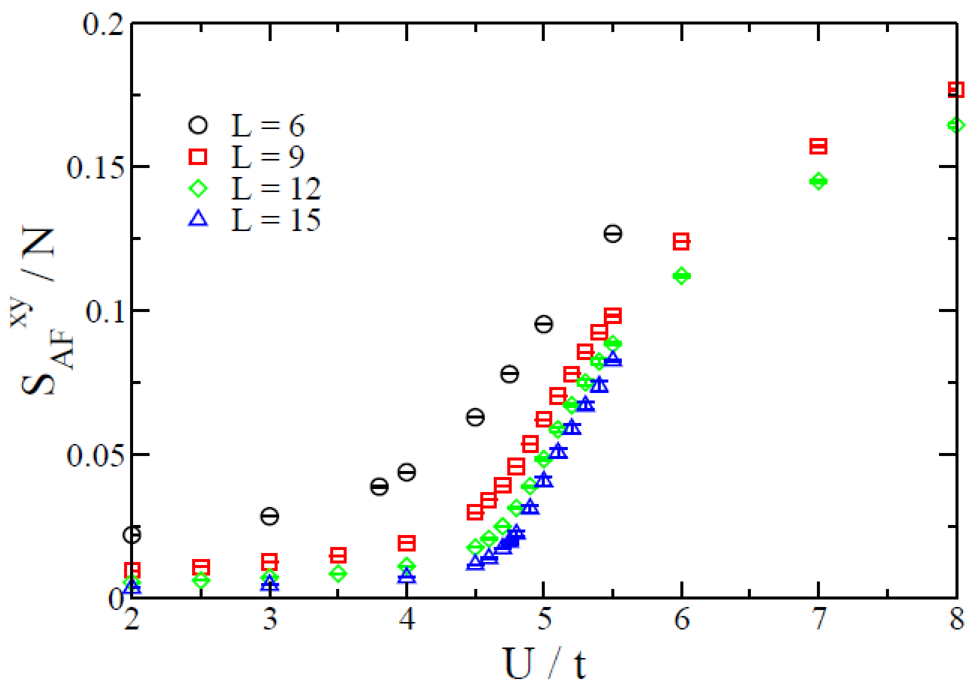
3D XY exponents:

$$\beta = 0.3486(1)$$

$$\nu = 0.6717(1)$$

$$z = 1$$

Campostrini et al., PRB 74 (2006)



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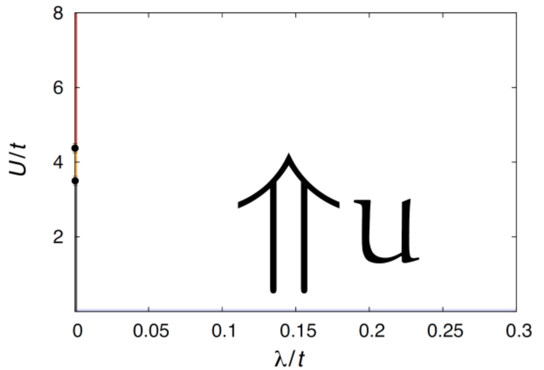

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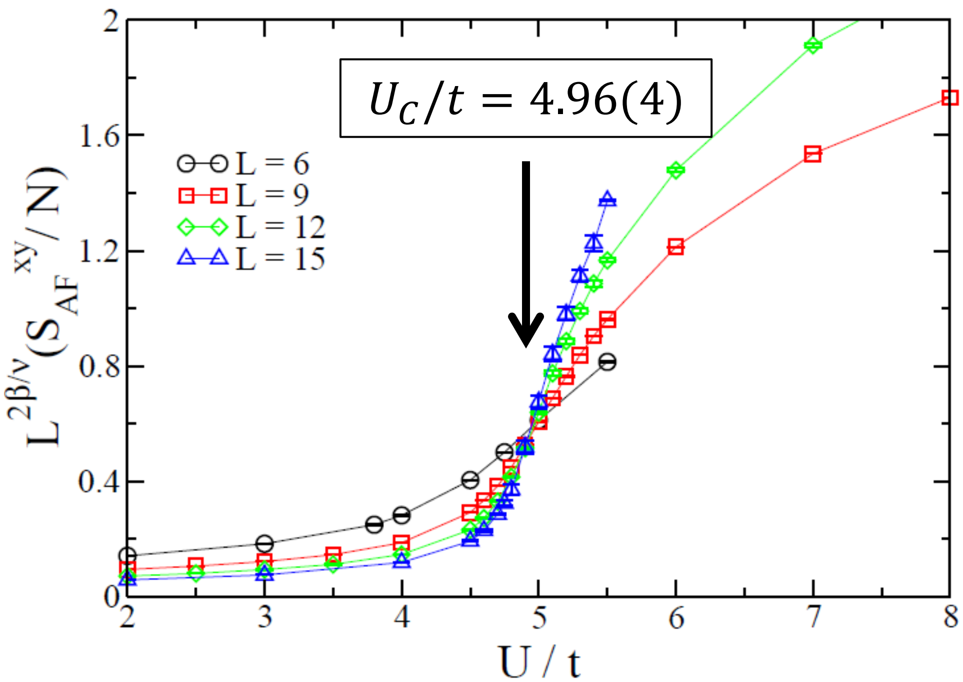

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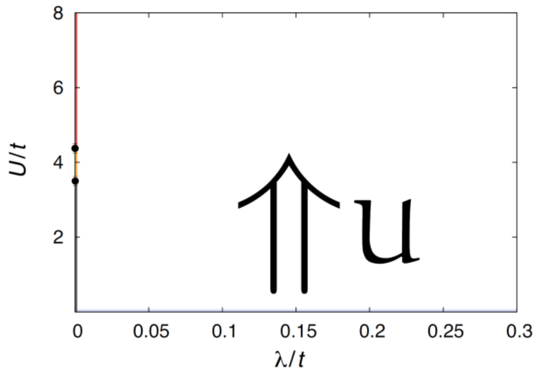

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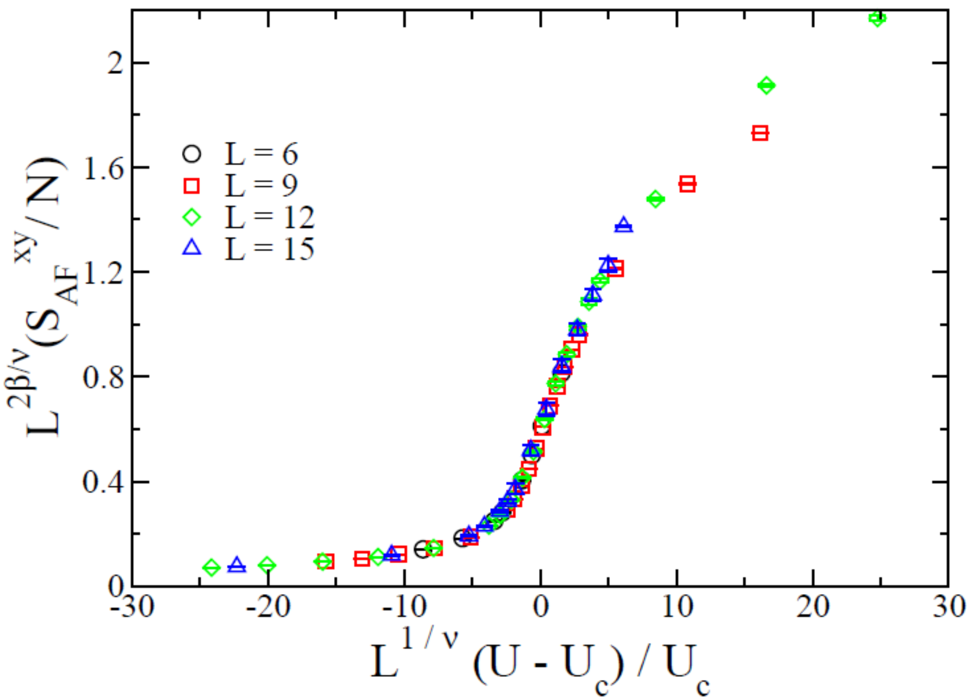

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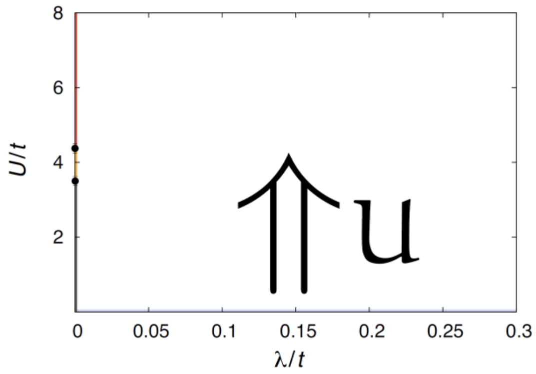

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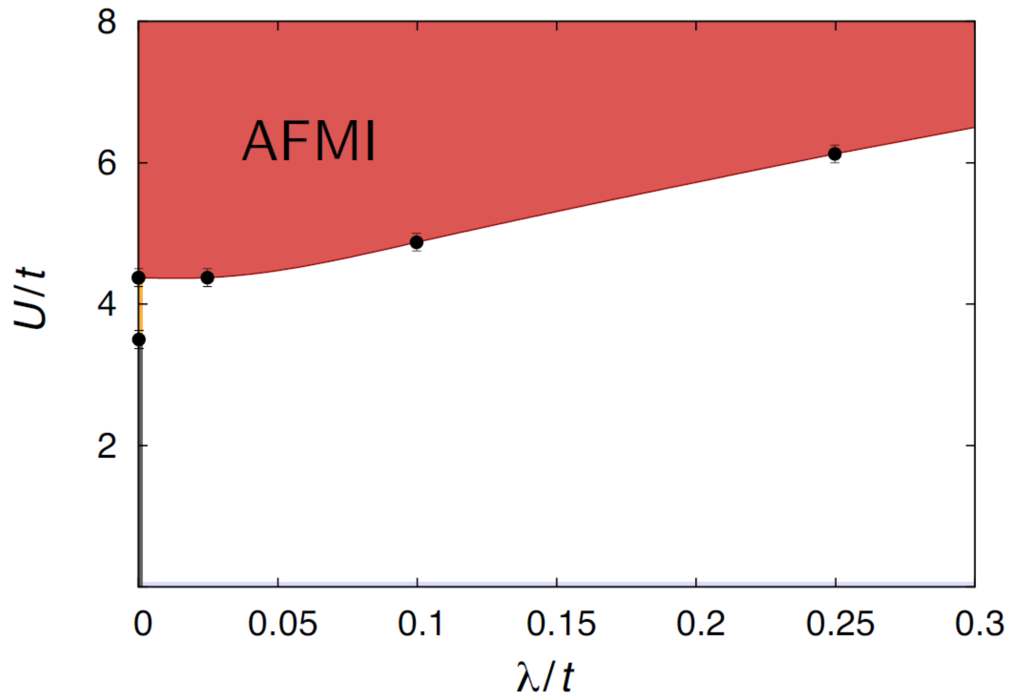
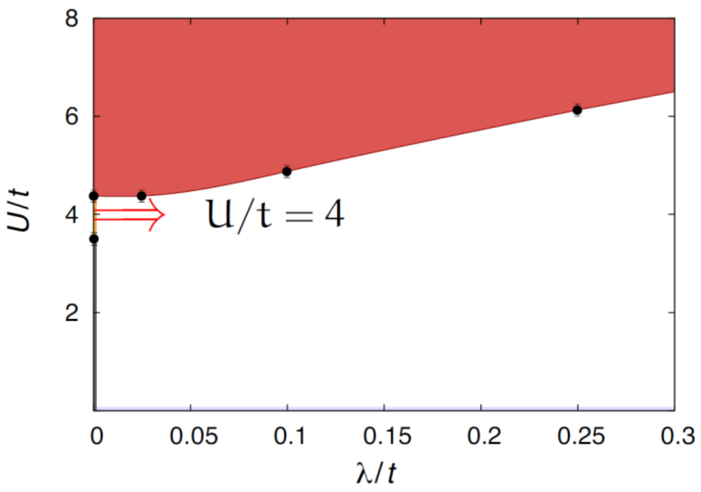
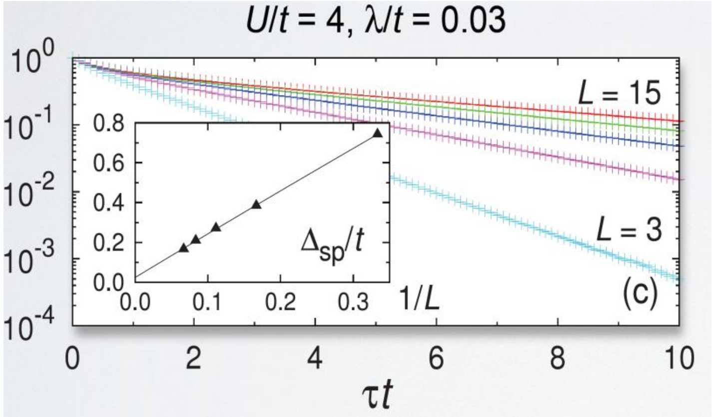


What happens to QSL at finite at $\lambda > 0$?



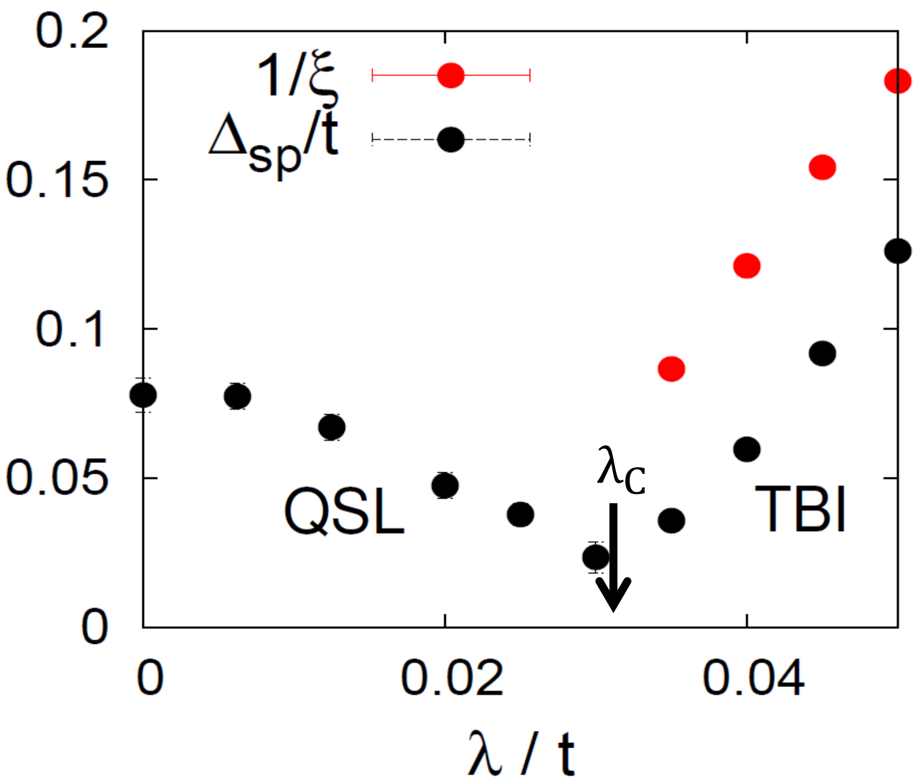
- No local order parameter in the QSL, nor TBI.
- Single particle gap at the Dirac point:

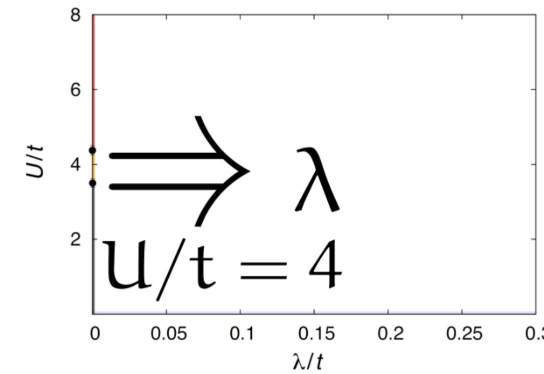
$$G(\mathbf{K},\tau) = \langle\Psi_0|\, c^\dagger_{\mathbf{K},\sigma}(\tau) c_{\mathbf{K},\sigma}\,|\Psi_0\rangle \approx Z \exp(-\tau\,\Delta_{sp})$$



M. Hohenadler et al., Phys. Rev. Lett. 106, (2011)

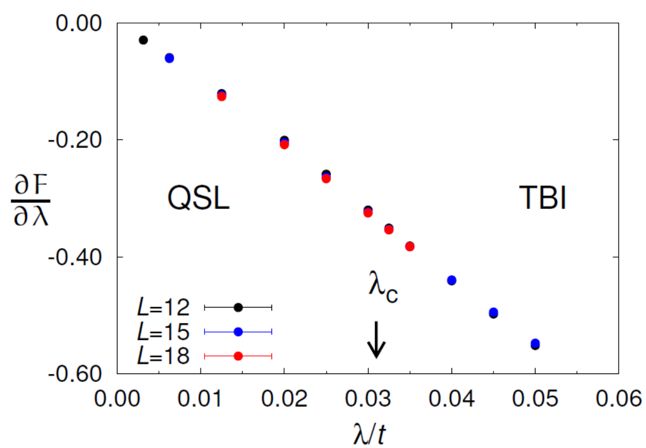
QSL to TBI transition with increasing λ





Extrapolated single particle gap:

- QSL – TBI transition at $\lambda_C \approx 0.03t$
- States not adiabatically connected



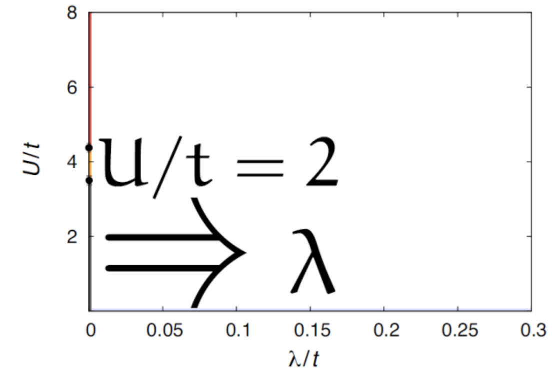
Free energy derivative:

$$\frac{\partial F}{\partial \lambda} = \langle i \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j \rangle$$

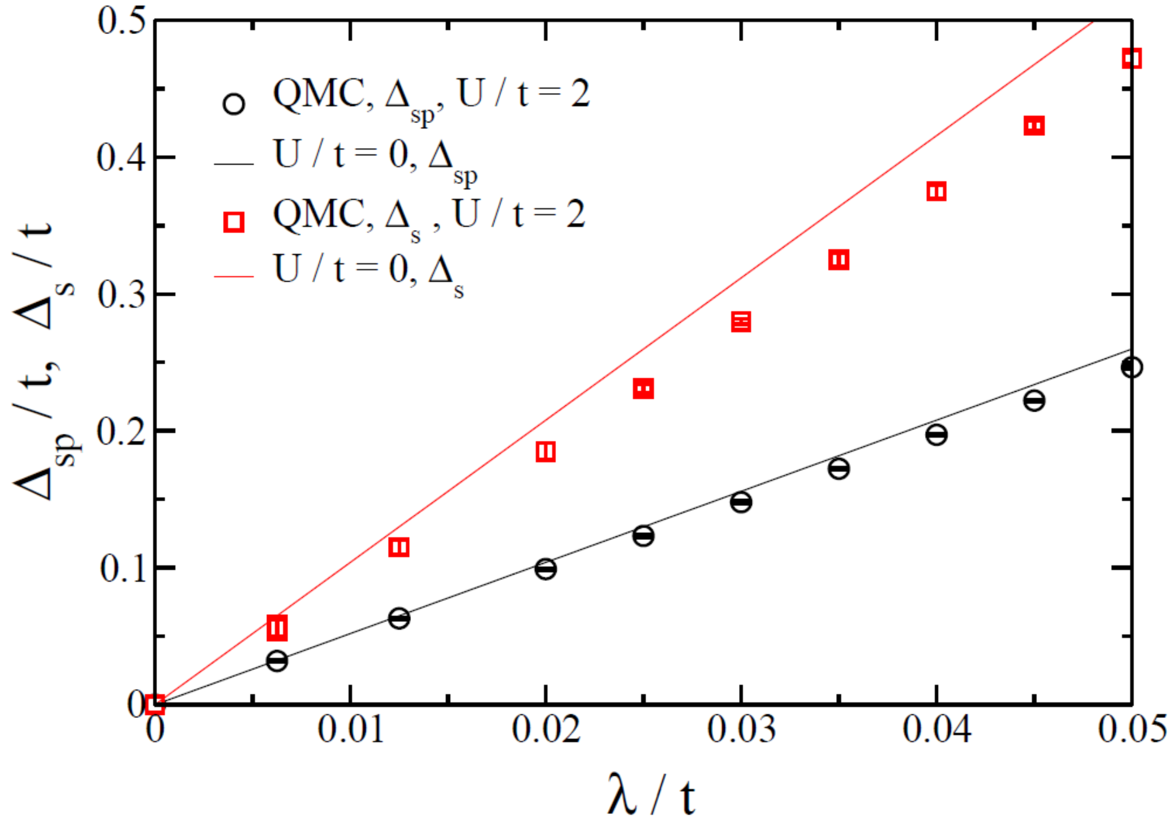
Transition appears to be continuous.
Predicted to be 1st order

Griset and Xu, arXiv (2011)

Effect of Spin-Orbit coupling on semi-metal



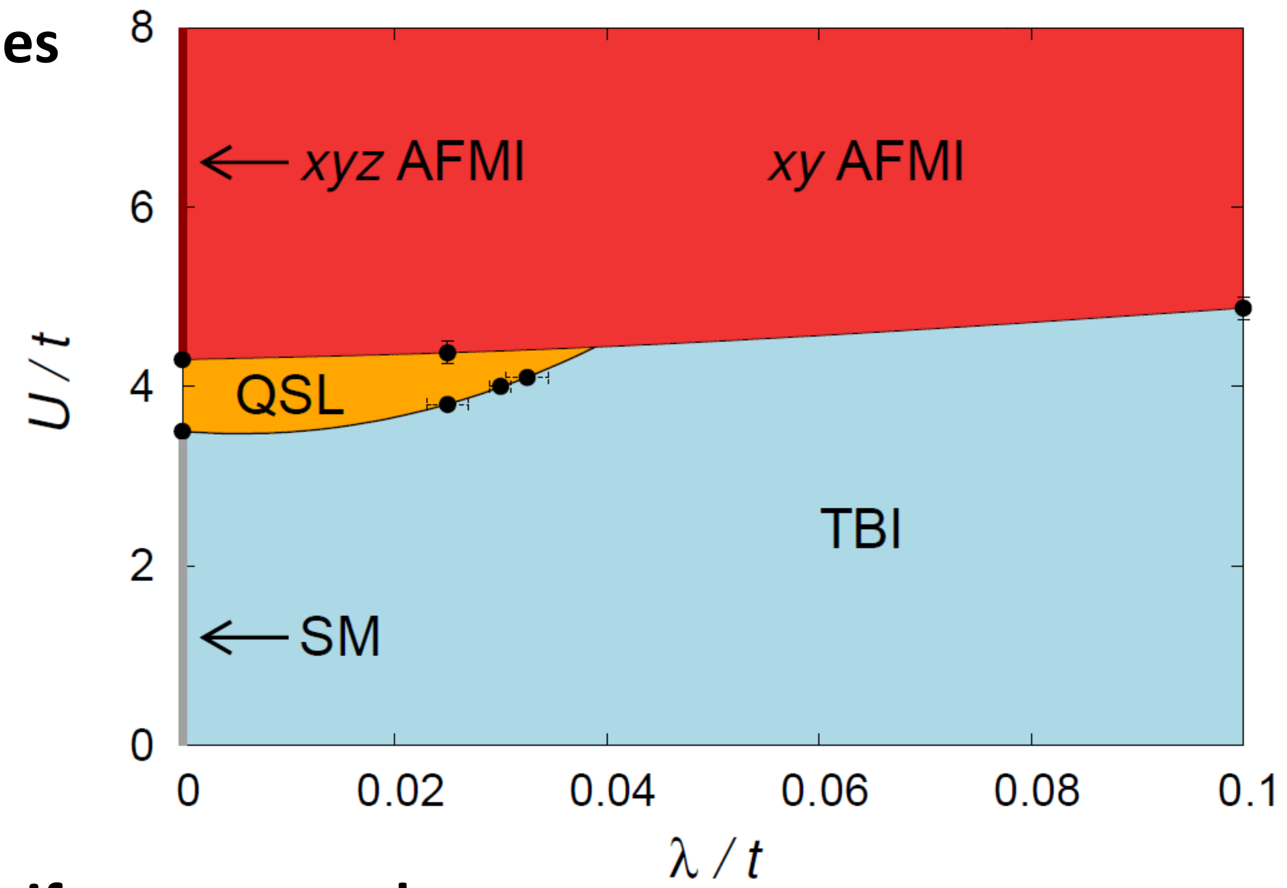
Extrapolated single particle gap Δ_{sp} and spin gap Δ_S



- Agree with U=0 results: $\Delta_{sp} = 3\sqrt{3}\lambda$, $\Delta_s = 6\sqrt{3}\lambda$.
- SM to TBI transition at $\lambda = 0^+$.

Phase diagram of Kane-Mele-Hubbard Model

5 different phases



Benchmark & unify recent works:

- Rachel and Le Hur, Phys. Rev. B (2010) (mean-field, slave rotor)
- D. Zheng et al., arXiv:1011.5858 (2010) (QMC)
- S.-L. Yu et al., Phys. Rev. Lett. (2011) (VCA)
- Yamaji and Imada, Phys. Rev. B (2011) (VMC)
- W. Wu et al., arXiv:1106.0943 (2011) (DMFT)
- D.-H. Lee, arXiv:1105.4900 (2011) (QFT)
- Griset and Xu, arXiv:1107.1245(2011) (QFT)