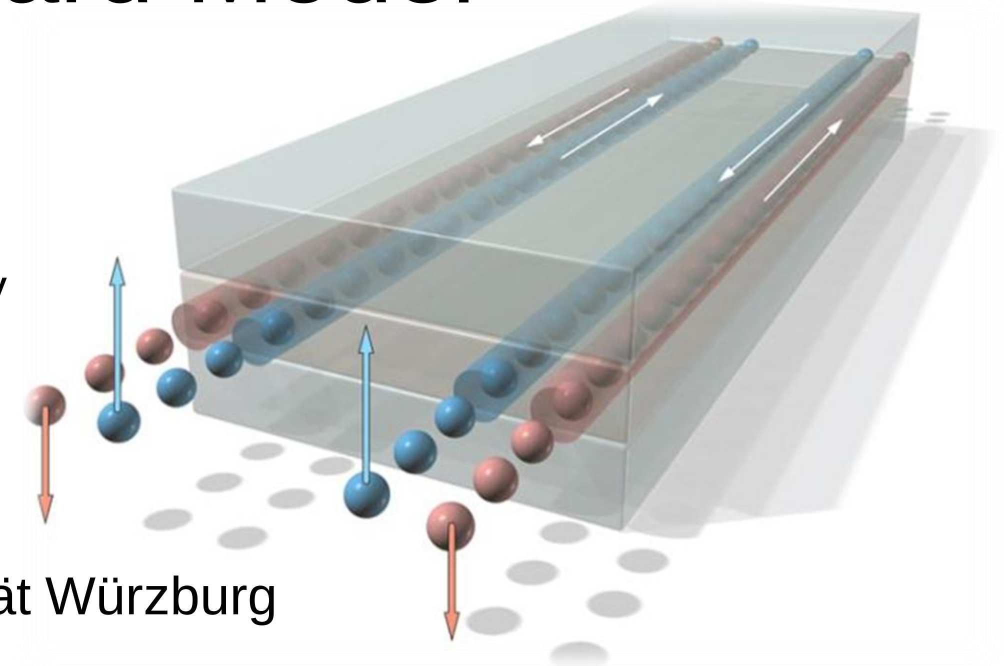
Quantum Phase Transitions in Kane-Mele-Hubbard Model



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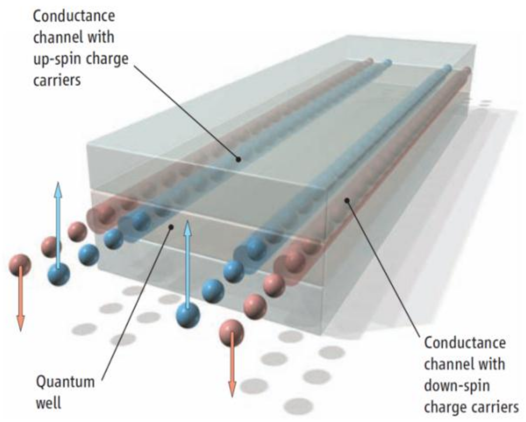
- Z. Y. Meng *et al*., Nature 464, (2010)
- M. Hohenadler *et al*., PRL 106, (2011)
- M. H., Z. Y. M., *et al*., PRB accepted

Motivation

Topological / Quantum spin-Hall insulator

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

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



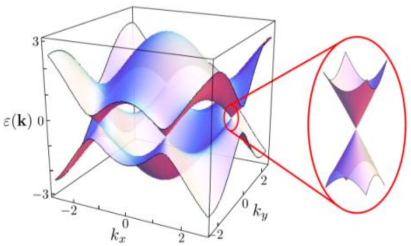
Graphene, Correlated Dirac fermions

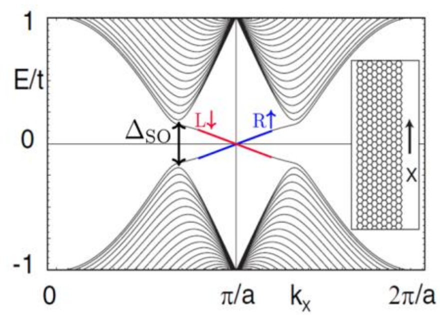
- Massless Dirac fermions with SO coupling

  Kane and Mele, Phys. Rev. Lett. (2005)
- Hubbard model on the honeycomb lattice

  Quantum spin liquid state.

  Meng, Lang, *et al.*, Nature (2010)

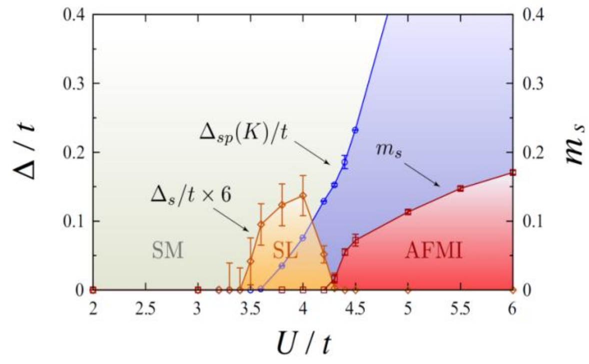




Topological / Quantum spin-Hall insulator

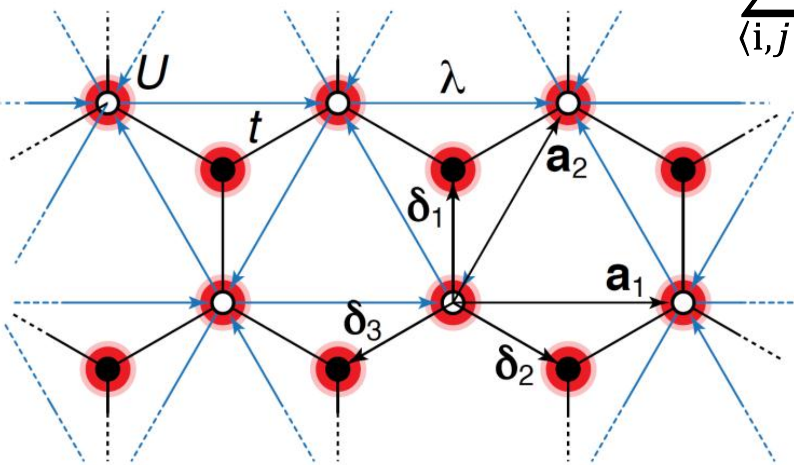
+ Interactions

Rachel and Le Hur, Phys. Rev. B (2010) (mean-field, slave rotor)
S.-L. Yu *et al.*, Phys. Rev. Lett. (2011) (VCA)
D. Zheng *et al.*, Phys. Rev. B (2011) (QMC)
W. Wu *et al.*, arXiv:1106.0943 (CDMFT)
Yamaji and Imada, Phys. Rev. B (2011) (VMC)
D.-H. Lee, Phys. Rev. Lett. (2011) (QFT)
Griset and Xu, Phys. Rev. B (2012) (QFT)
J. C. Budich et al., arXiv:1203.2928 (FDWN)



Kane-Mele-Hubbard Model

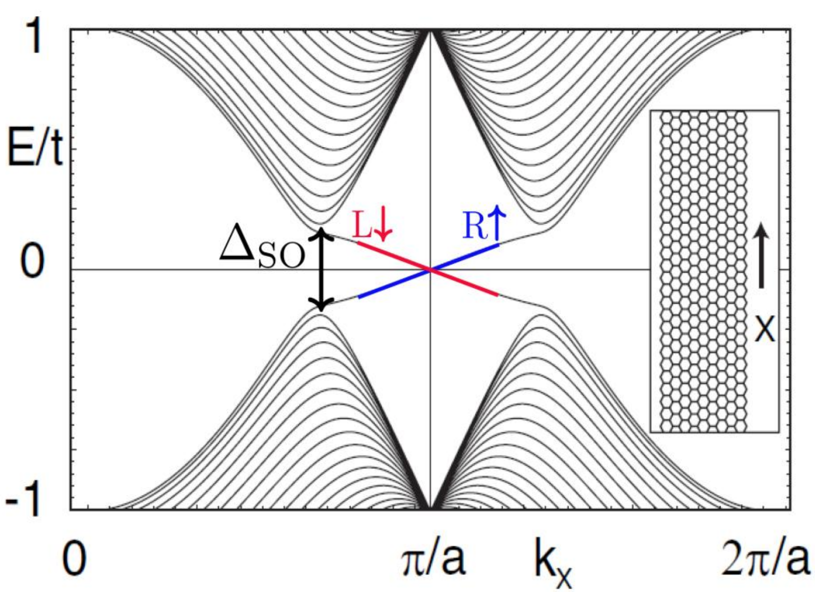
$$H = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j + i\,\lambda \sum_{\langle\langle i,j\rangle\rangle} c_i^\dagger \nu_{ij}\cdot\sigma^z c_j + \frac{U}{2}\sum_i (c_i^\dagger c_i - 1)^2$$



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

$$\nu_{ij} = \frac{\boldsymbol{\delta}_m \times \boldsymbol{\delta}_n}{|\boldsymbol{\delta}_m \times \boldsymbol{\delta}_n|}$$

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



U=0 Kane-Mele Model

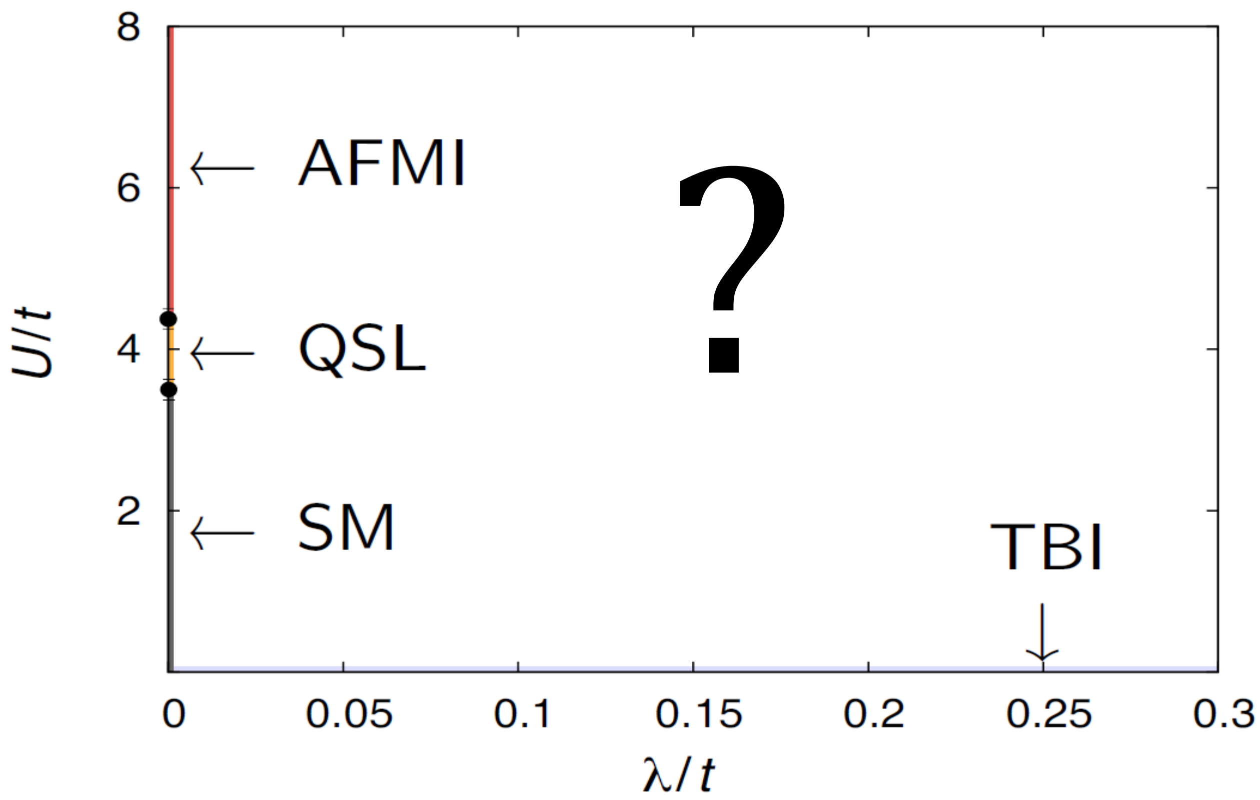
- Time reversal invariant QSH insulator
- Spin-orbital bulk gap $\Delta_{SO} = 3\sqrt{3}\lambda$
- Gapless, helical edge states (topologically protected)

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) $\Longrightarrow$ Quantum Spin Liquid (QSL) $\Longrightarrow$ Antiferromagnetic Mott Insulator (AFMI)
- Kane-Mele Model ($U = 0$) : Topological Band Insulator (TBI)



Method of choice

- Projective determinantal quantum Monte Carlo

Projective determinant quantum Monte Carlo

Blankenbecler et al., Phys. Rev. D. (1981)
Sugiyama, Koonin, Ann. Phys. (1986)
Assaad, Evertz, Lect. Notes Phys. (2008)

- Ground state expectation values

$$\langle\Psi_0|O|\Psi_0\rangle = \lim_{\Theta\to\infty} \frac{\langle\Psi_\mathrm{T}|e^{-\Theta H/2} O e^{-\Theta H/2}|\Psi_\mathrm{T}\rangle}{\langle\Psi_\mathrm{T}|e^{-\Theta H}|\Psi_\mathrm{T}\rangle}$$

with $|\Psi_\mathrm{T}\rangle = |\Psi_\mathrm{KM}\rangle$

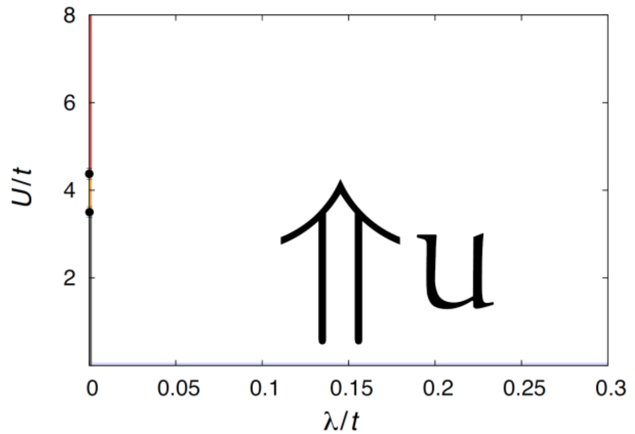
- No sign problem at half-filling, Time-reversal symmetry.

$$W = \prod_\sigma W_\sigma\,, \qquad \overline{W_\uparrow} = W_\downarrow \Rightarrow W = |W_\downarrow|^2 > 0$$

- SU(2) symmetric Hubbard-Stratonovich transformation, auxiliary field of integer spins

- System size $N = 2L^2$, with $L = 3,6,9, \ldots \ldots, 18$ to catch the nodal points. Scales as $\sim N_\tau N^3$ (N_τ imaginary time slices).

TBI to AFMI: magnetic transition



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

$\lambda > 0$: NNN transverse Ferro $J' \sim -\lambda^2/U$

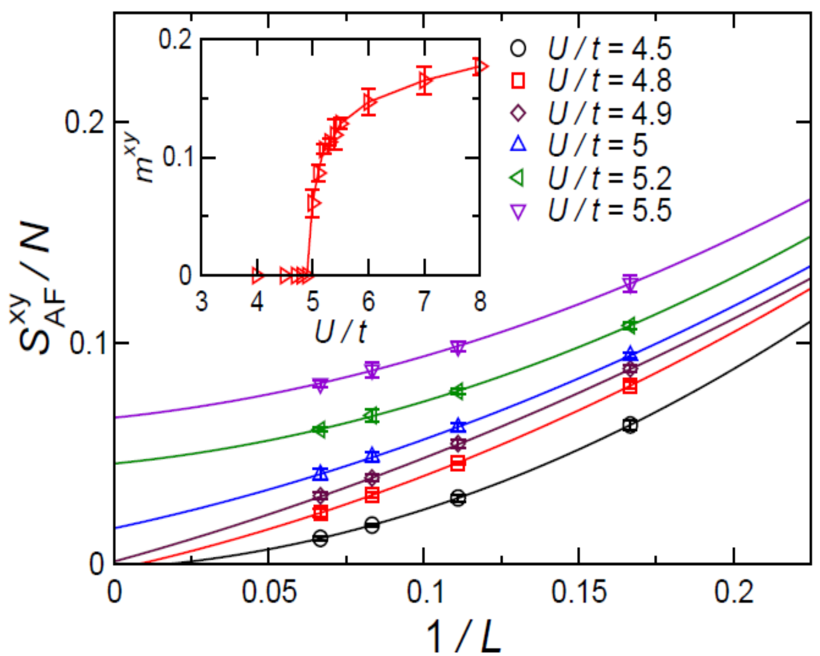
NNN longitudinal AF $J' \sim \lambda^2/U$

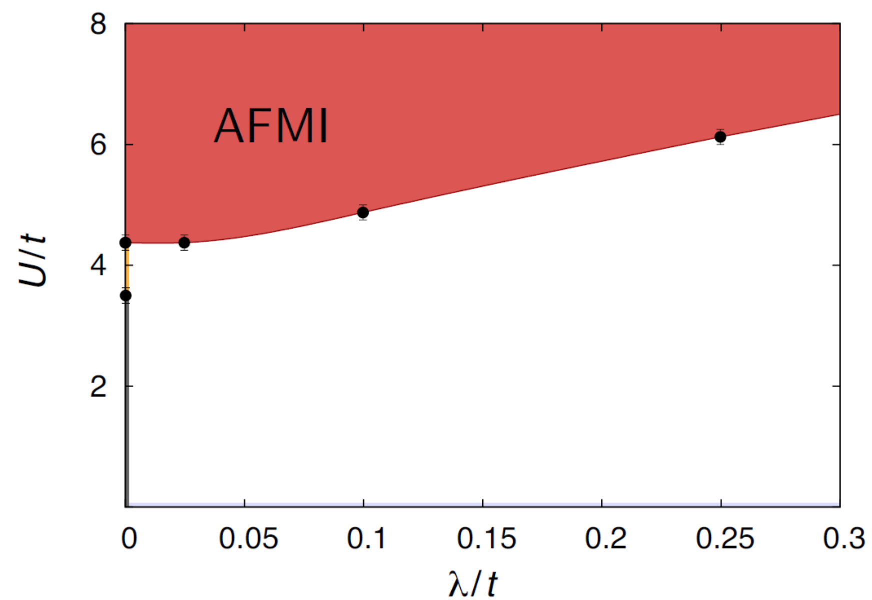
z-direction frustrated, easy-plane XY order

Magnetic structure factor:

$$S_{AF}^{xy} = \frac{1}{N}\sum_{\langle i,j\rangle}(-1)^{i+j}\langle\Psi_0|S_i^+S_j^- + S_i^-S_j^+|\Psi_0\rangle$$

Transverse magnetization: $m_{xy}^2 = S_{AF}^{xy}/N$

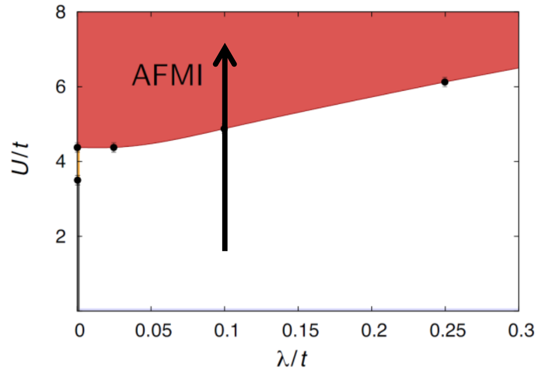


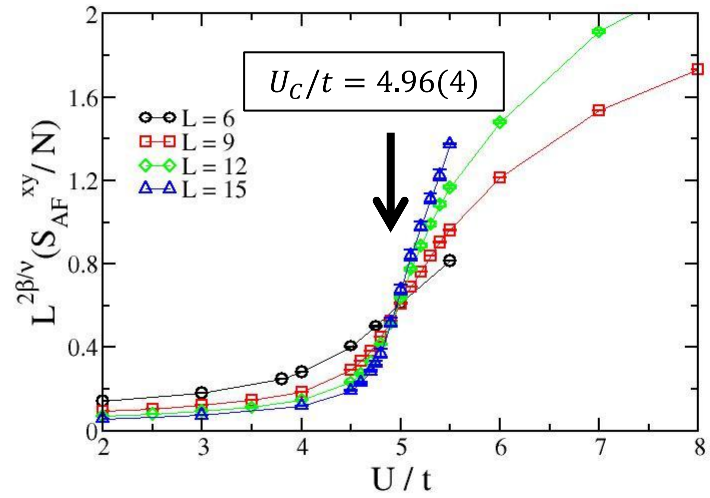


TBI to AFMI: magnetic transition

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

D.-H. Lee, PRL,107 (2011); Griset and Xu, PRB, 85 (2012)



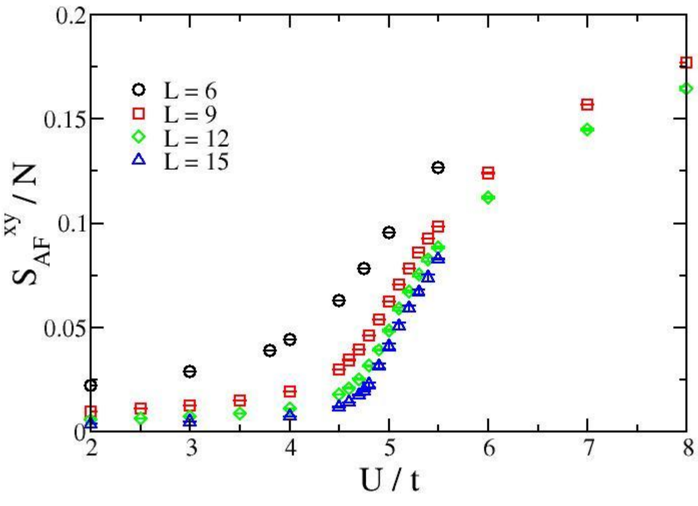


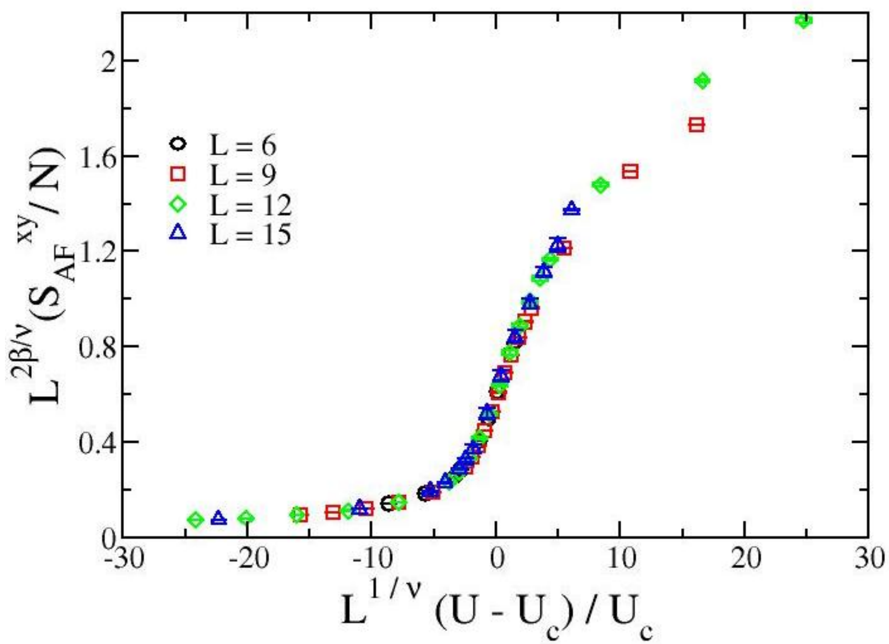
$$\frac{S_{\mathrm{AF}}^{xy}}{N} = L^{-2\beta/\nu} f_1[(U - U_{\mathrm{c}})L^{1/\nu}]$$

3D XY exponents:

$\beta = 0.3486(1)$; $\nu = 0.6717(1)$; $z = 1$

Campostrini et al., PRB 74 (2006)

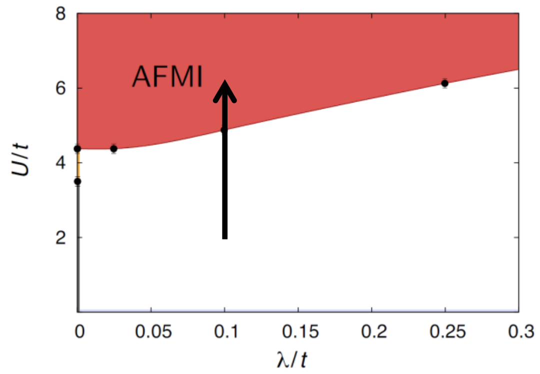




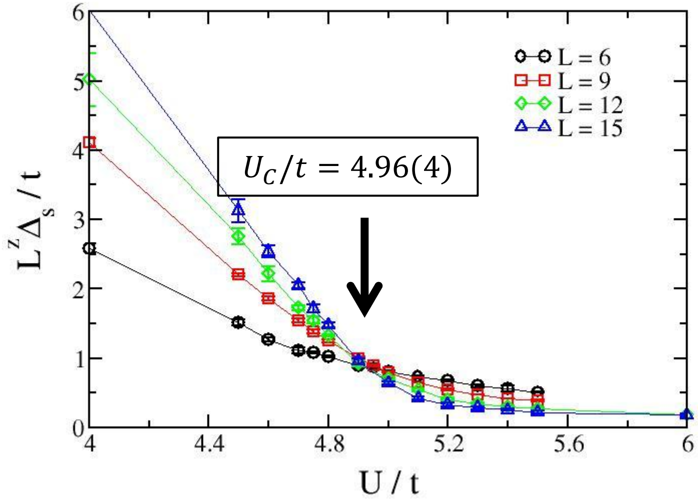
TBI to AFMI: magnetic transition

U(1) symmetry is spontaneously broken, condensation of magnetic excitations

D.-H. Lee, PRL, 107 (2011); Griset and Xu, PRB, 85 (2012)



$$\Delta_s/t = L^{-z} f_2[(U - U_c)L^{1/\nu}]$$



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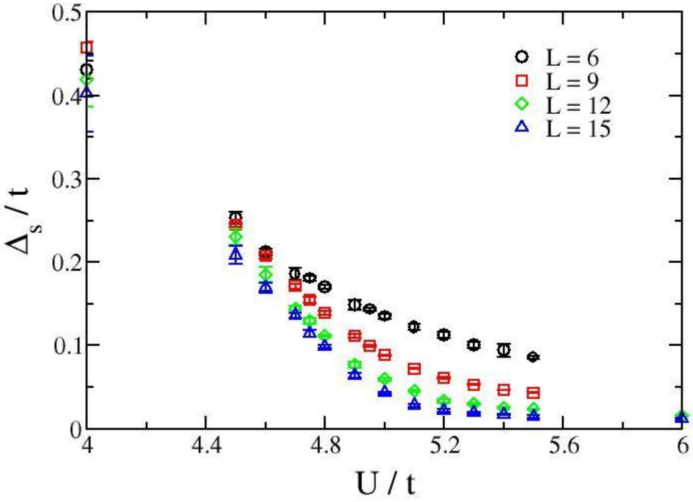
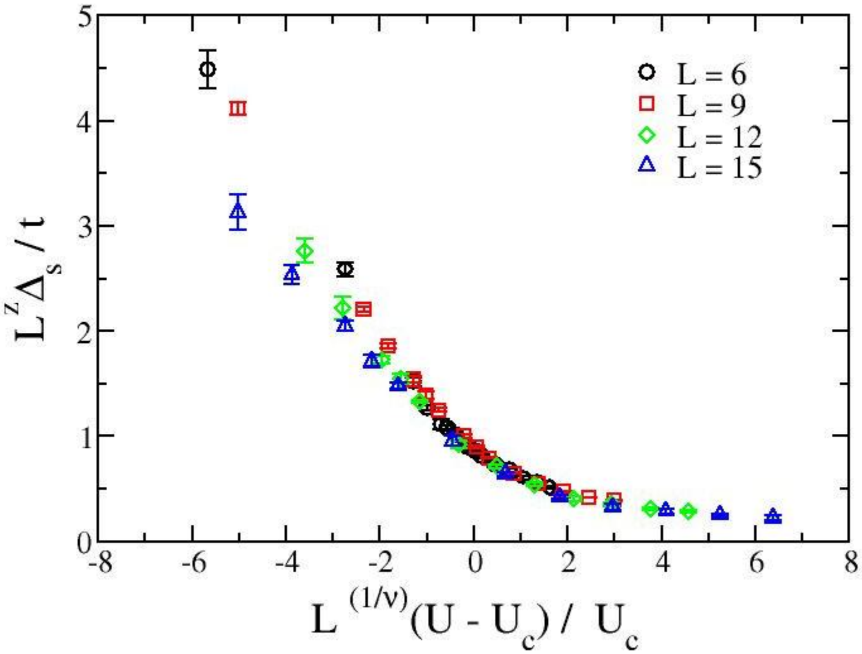
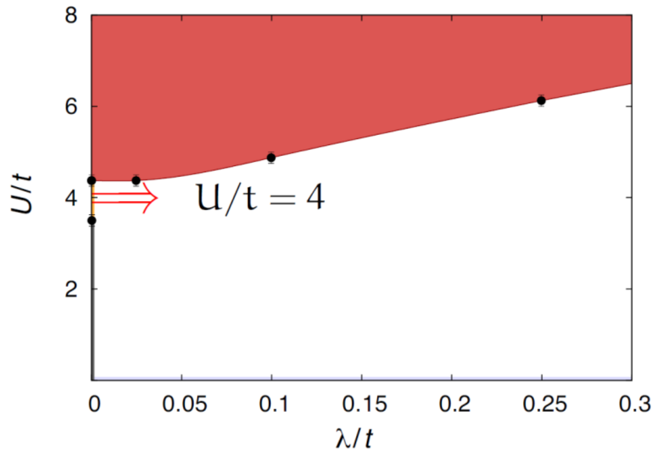
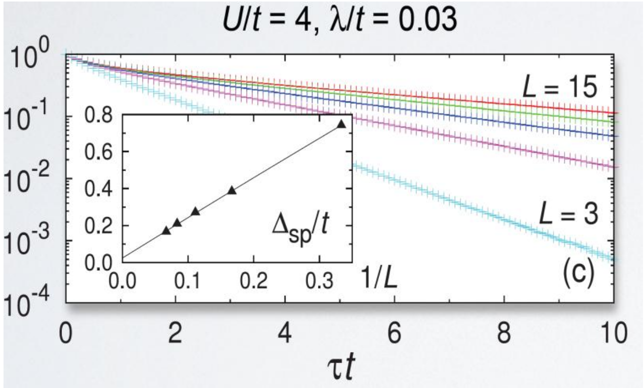




What happens to QSL at $\lambda > 0$?





- No local order parameter in the QSL, nor TBI
- Single particle gap Δ_{sp}, Spin gap Δ_s

$$G(\mathbf{K},\tau) = \frac{1}{2}\sum_{a=A,B}\langle\Psi_0|c^\dagger_{a,\sigma}(\mathbf{K},\tau)c_{a,\sigma}(\mathbf{K},0)|\Psi_0\rangle \propto \exp(-\tau\Delta_{sp})$$

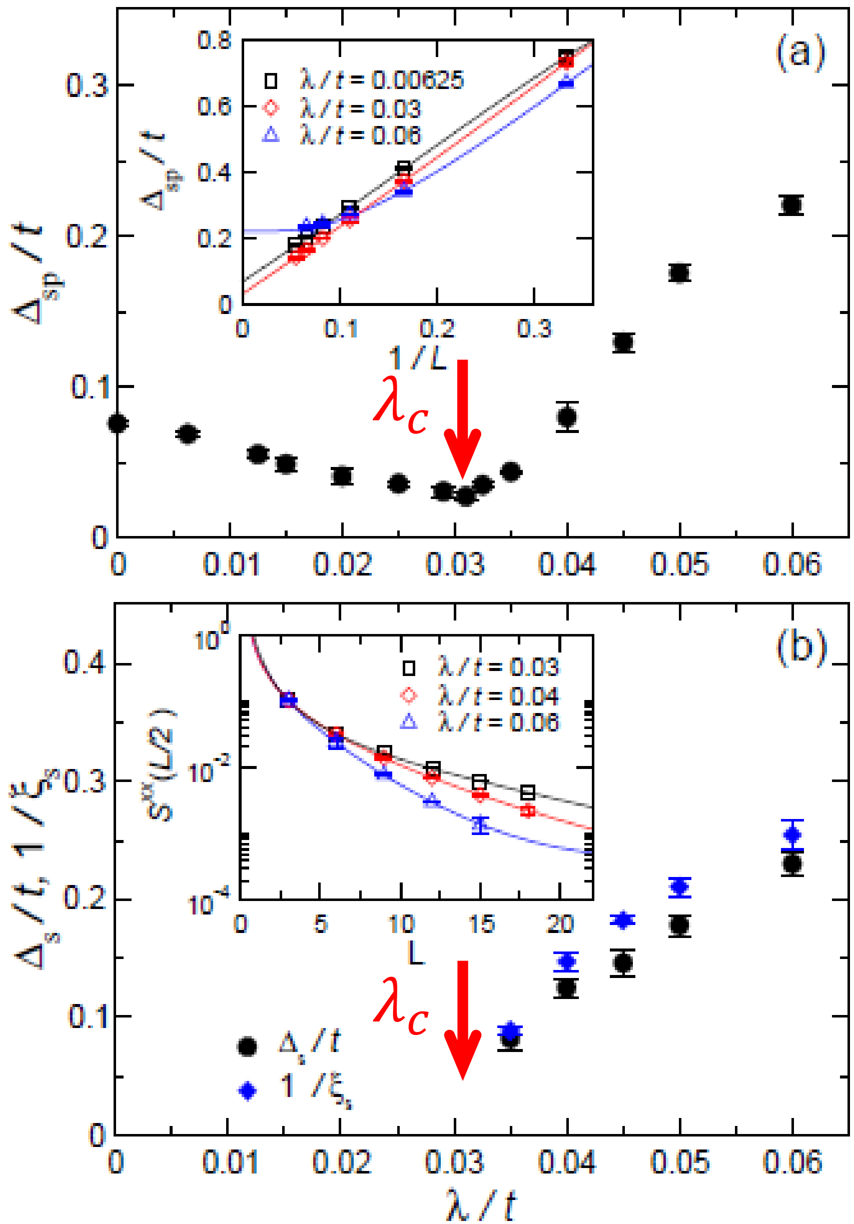
$$S^{xy}(\mathbf{\Gamma},\tau) = \frac{1}{2}\sum_{a=A,B}\langle\Psi_0|S^+_a(\mathbf{\Gamma},\tau)S^-_a(\mathbf{\Gamma},0) + S^-_a(\mathbf{\Gamma},\tau)S^+_a(\mathbf{\Gamma},0)|\Psi_0\rangle \propto \exp(-\tau\Delta_S)$$

$$\Delta_{sp/s}(L)/t = a + e^{-\frac{L}{\xi_{sp/s}}}(b/L + c/L^2)$$

- Spin-spin correlation length ξ_s

$$\langle S^x_r S^x_0\rangle = e^{-\frac{r}{\xi_s}}(a/r + b/r^2)$$

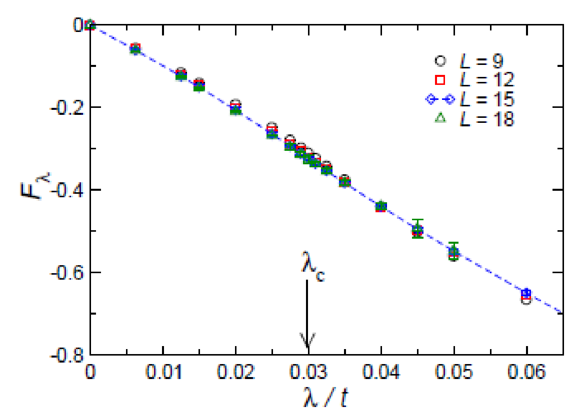
QSL to TBI transition at U/t = 4



- QSL – TBI transition at $\lambda_C \approx 0.03t$
- Fully gapped QSL at small λ
- QSL & TBI are not adiabatically connected
- Severe finite size effect close to λ_C

Free energy derivative:

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

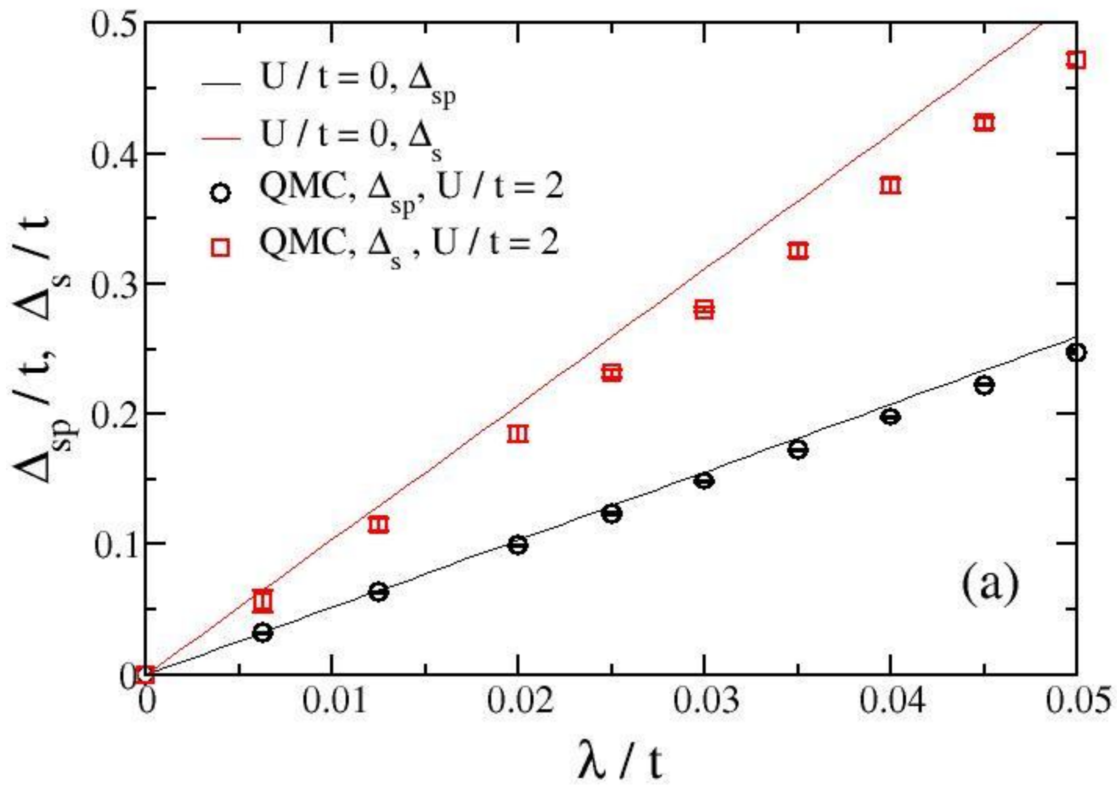


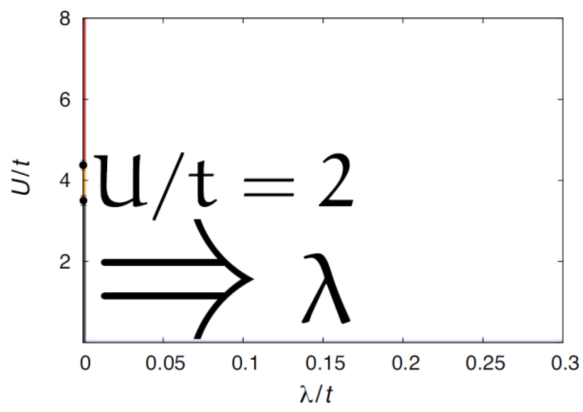
Transition appears to be continuous.
Predicted to be 1^{st} order

Griset and Xu, PRB, 85 (2012)

Effect of Spin-Orbit coupling on semi-metal

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

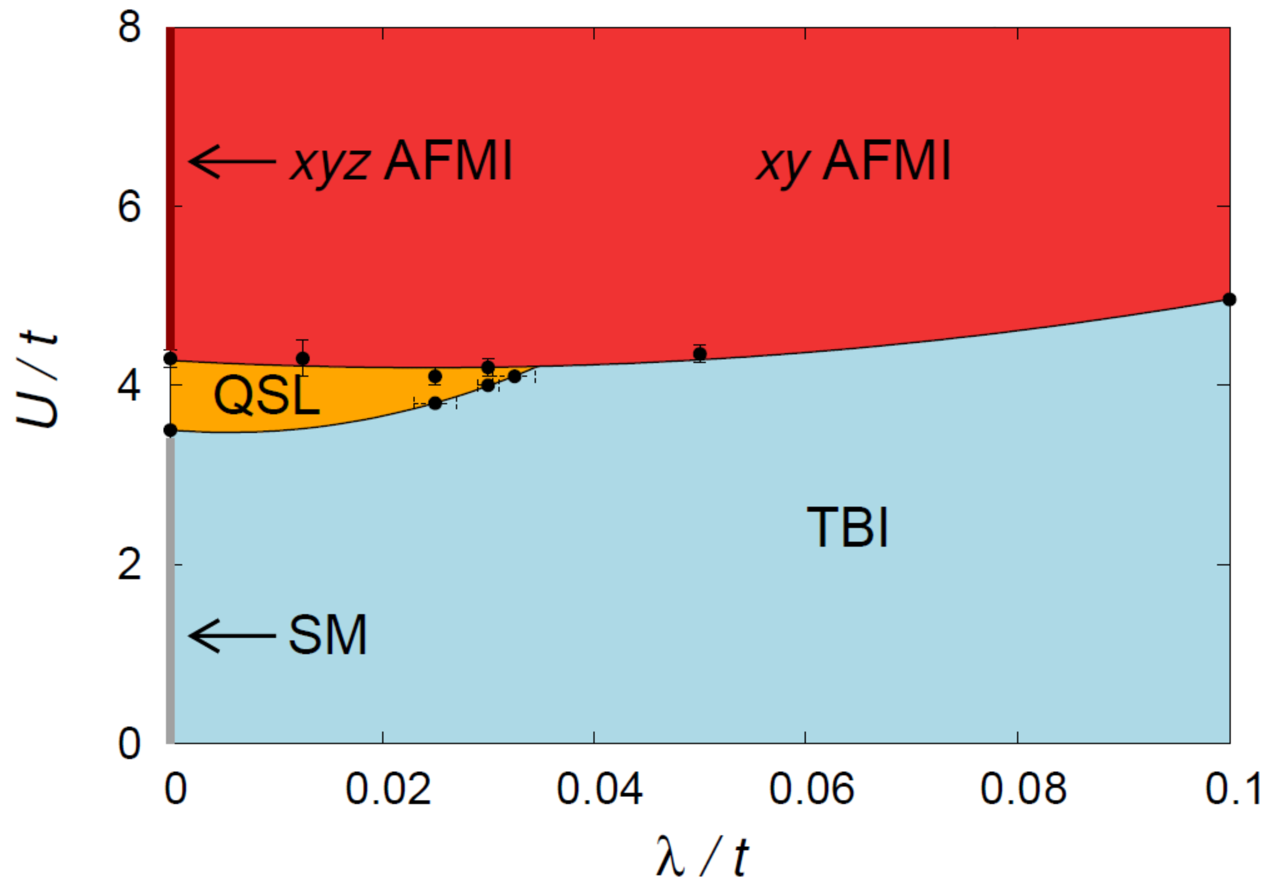




- Agree with U/t = 0 results: $\Delta_{sp} = 3\sqrt{3}\lambda,\ \Delta_s = 2\Delta_{sp}$ Kane and Mele, Phys. Rev. Lett. (2005)
- SM to TBI transition at $\lambda = 0^+$
- TBI at small U is adiabatically connected to the ground state of Kane-Mele model

Phase diagram of Kane-Mele-Hubbard Model

5 different phases



Benchmark recent works:

Rachel and Le Hur, Phys. Rev. B (2010) (mean-field, slave rotor)
S.-L. Yu *et al.*, Phys. Rev. Lett. (2011) (VCA)
D. Zheng *et al.*, Phys. Rev. B (2011) (QMC)
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Griset and Xu, Phys. Rev. B (2012) (QFT)
J. C. Budich et al., arXiv:1203.2928 (FDWN)

Thank you for your attention

Acknowledgement

NSF

LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

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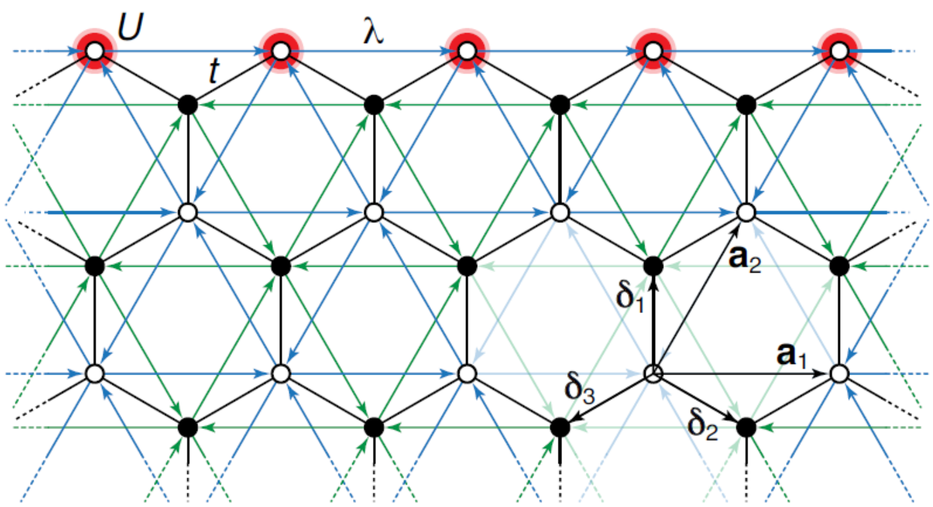
Correlation Effect on the Helical Edge States

- TBI at U/t > 0 adiabatically connected to U = 0.
- Edge state exponentially localized.

Kane and Mele, Phys. Rev. Lett. (2005)



Effective model

- Semi-infinite ribbon, p.b.c. in $\boldsymbol{a}_1$ direction
- *U* only on the zigzag edge sites
- Integrate out bulk to obtain effect model

One dimensional action:

$$S = -\sum_{r,r',\sigma} \iint_0^\beta d\tau d\tau' c^\dagger_{r,\sigma}(\tau) G^{-1}_{0,\sigma}(r-r',\tau-\tau') c_{r',\sigma}(\tau') + U \sum_r \int_0^\beta d\tau \left[n_{r,\uparrow}(\tau) - \frac{1}{2}\right]\left[n_{r,\downarrow}(\tau) - \frac{1}{2}\right]$$

$G_{0,\sigma}(r,\tau)$: Green function of the Kane-Mele model, non-interacting bulk

Weak coupling expansion Continuous-Time Monte Carlo

Dynamical correlation functions

Single-particle spectral function

$$A_\sigma(q,\omega) = -\frac{1}{\pi}\mathrm{Im}G_\sigma(q,\omega) \qquad [A_\uparrow(q,\omega) = A_\downarrow(-q,\omega)]$$

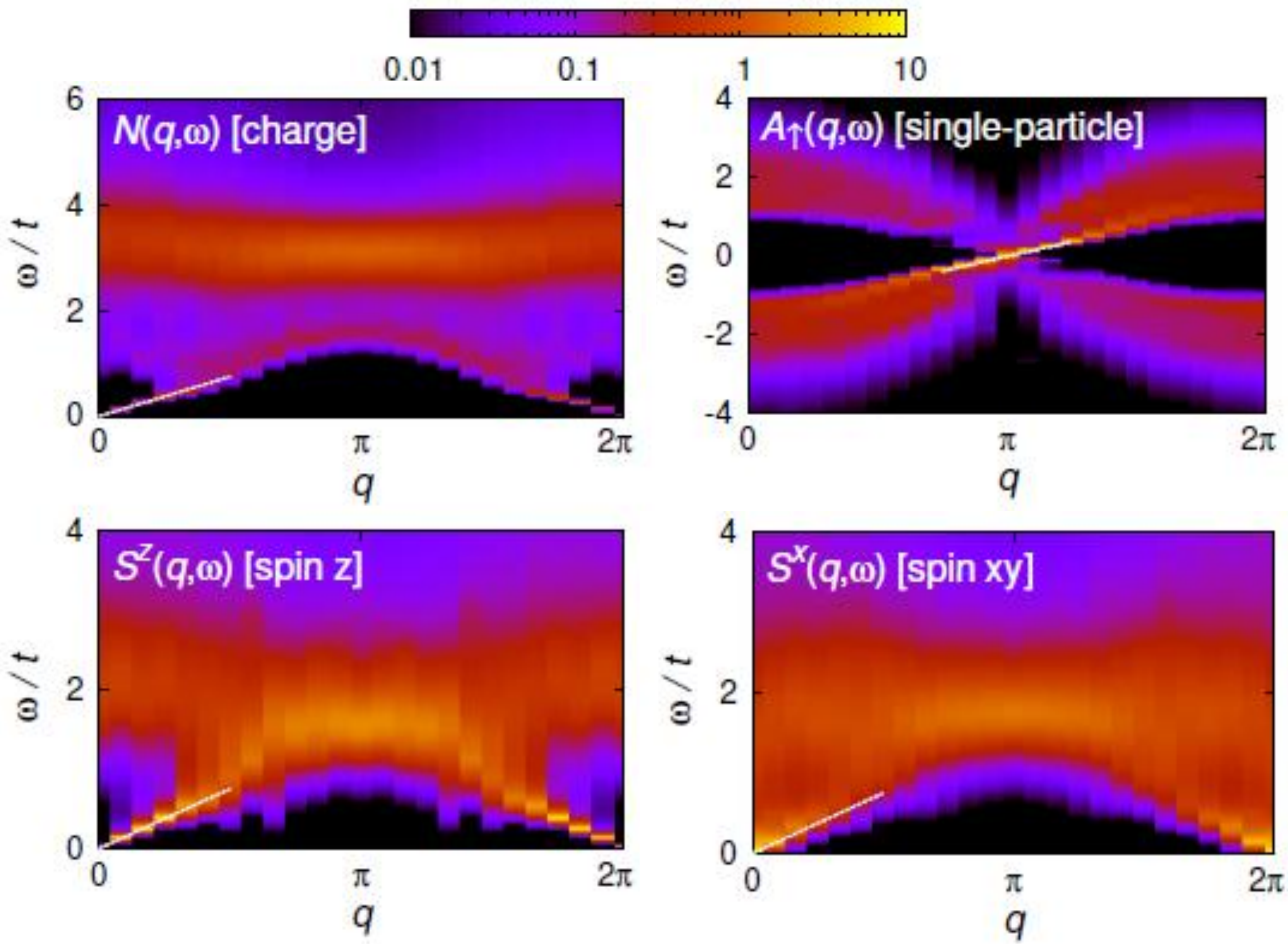
Dynamic charge structure factor

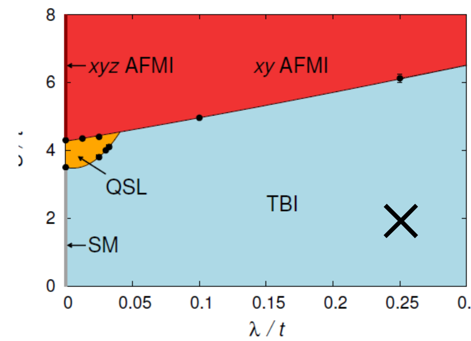
$$N(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_n}|\langle m|N(q)|n\rangle|^2\delta(E_m - E_0 - \omega)$$

Dynamic spin structure factor

$$S^\alpha(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_n}|\langle m|S^\alpha(q)|n\rangle|^2\delta(E_m - E_0 - \omega)$$

Edge dynamics at weak interaction

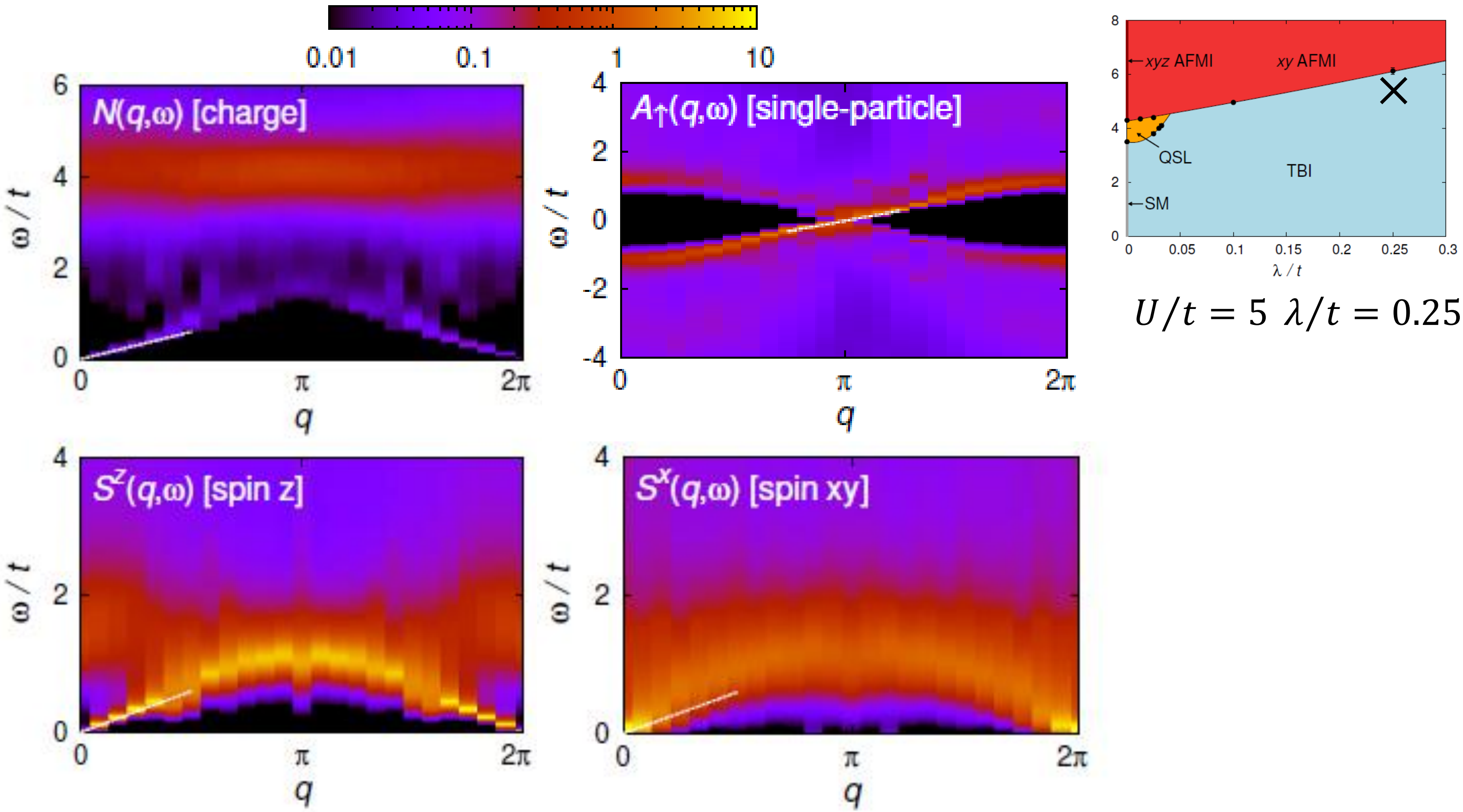




$U/t = 2, \lambda/t = 0.25$

- $A_{\uparrow}(q,\omega)$: gapless, helical edge state similar with U=0
- $N(q,\omega)$ and $S^z(q,\omega)$ conserve S^z, excitations within L and R movers
- Excitation continuum in S^x due to spin flips, mixing of L and R movers

Large U/t suppress charge transport

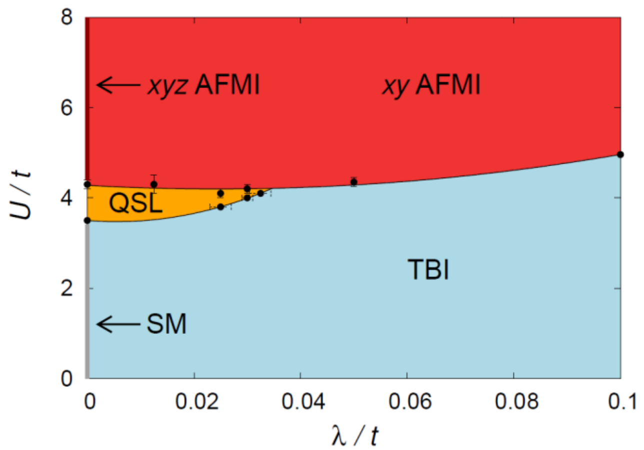


$U/t = 5 \;\; \lambda/t = 0.25$

- Velocity renormalized with U/t – helical Luttinger liquid C. Wu et al., Phys. Rev. Lett. (2006)
- **Strong suppression of charge excitations, reduction of Drude weight by order of magnitude**
- Strong transverse spin correlations, piling up spectral weight at $q \to 0$

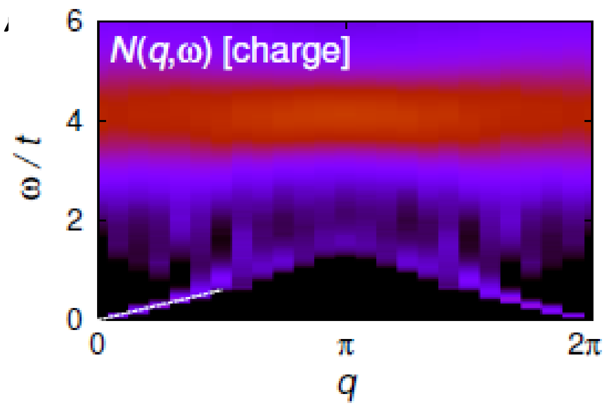
Summary and Outlook

- Ground state phase diagram of the Kane-Mele-Hubbard model from QMC



- Quantum phase transitions:
  TBI – AFMI, QSL – TBI,
  SM—TBI, QSL—AFMI

- Correlation effect on the helical edge state, strong suppression of charge transport



- Detail study of the TBI—QSL, QSL—AFMI transitions

- Direction measurement of the topological number