Phase diagram of the Kane-Mele Hubbard model

Fakher F. Assaad (Emergent Quantum Phases in Condensed Matter, ISSP 13/6/2013)

- Model and method
- Quantum phases transitions

  Topological insulator (TI) → Antiferromagnetic Mott
  Semimetal (SM) → Antiferromagnetic Mott

- Methods to detect TIs in the presence of correlations
- Conclusions

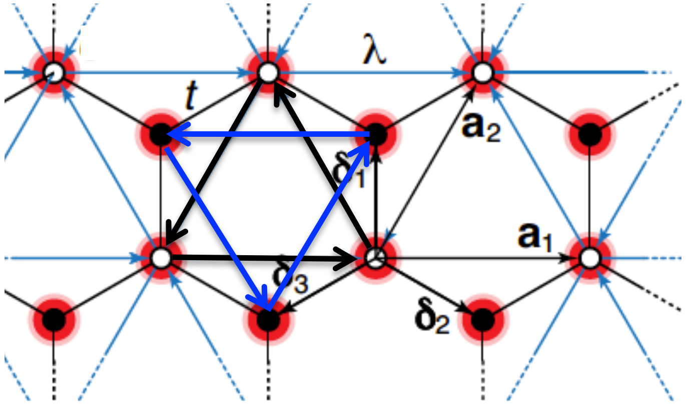
A. Muramatsu University of Stuttgart
S. Wessel RWTH Aachen
T. Lang Boston University
Z.Y. Meng Louisiana State University.

M. Hohenadler
M. Bercx
F. Goth
} University of Würzburg

I. Herbut MPIPKS-Dresden/ Simon Fraser University

Topology and correlations: Kane-Mele Hubbard model

Kane and Mele Phys. Rev. Lett. 95, 146802 (2005)



$$H_{KMU} = \sum_{\mathbf{k}} \left(a^\dagger_{\mathbf{k},\uparrow}, b^\dagger_{\mathbf{k},\uparrow}, a^\dagger_{\mathbf{k},\downarrow}, b^\dagger_{\mathbf{k},\downarrow}\right) \begin{pmatrix} H(\mathbf{k}) & 0 \\ 0 & H(-\mathbf{k}) \end{pmatrix} \begin{pmatrix} a_{\mathbf{k},\uparrow} \\ b_{\mathbf{k},\uparrow} \\ a_{\mathbf{k},\downarrow} \\ b_{\mathbf{k},\downarrow} \end{pmatrix}$$

$$+ \; U \sum_i \left(a^\dagger_{i,\uparrow} a_{i,\uparrow} - 1/2\right)\left(a^\dagger_{i,\downarrow} a_{i,\downarrow} - 1/2\right) + \left(a \leftrightarrow b\right)$$

Two copies of Haldane model

F.D.M.Haldane, PRL. 61, 2015 (1988)

$$H(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \sigma$$

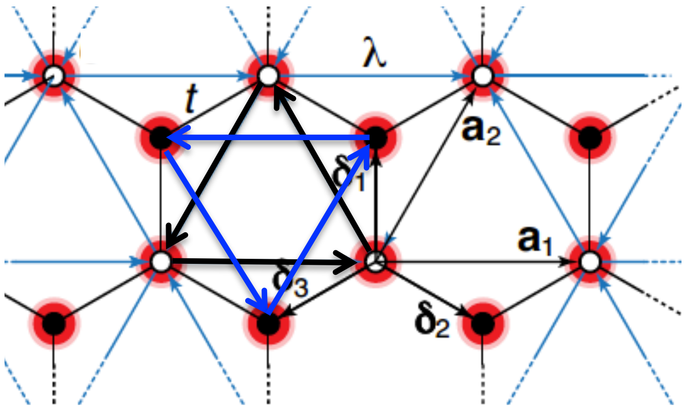
$$\mathbf{d}(\mathbf{k}) = \begin{pmatrix} -t\left[1+\cos(\mathbf{k}_1-\mathbf{k}_2)+\cos(\mathbf{k}_2)\right] \\ t\left[\sin(\mathbf{k}_1-\mathbf{k}_2)+\sin(\mathbf{k}_2)\right] \\ \lambda\left[\sin(\mathbf{k}_1)-\sin(\mathbf{k}_2)+\sin(\mathbf{k}_2-\mathbf{k}_1)\right] \end{pmatrix} \quad \rightarrow \quad C_1 = \mathrm{sign}(\lambda)$$

Symmetries

Sublattice symmetry is broken → Mass gap.
Time reversal ✓
SU(2) spin → U(1)

Topology and correlations: Kane-Mele Hubbard model

Kane and Mele Phys. Rev. Lett. 95, 146802 (2005)



$$H_{KMU} = \sum_{\mathbf{k}} \left(a^{\dagger}_{\mathbf{k},\uparrow}, b^{\dagger}_{\mathbf{k},\uparrow}, a^{\dagger}_{\mathbf{k},\downarrow}, b^{\dagger}_{\mathbf{k},\downarrow} \right) \begin{pmatrix} H(\mathbf{k}) & 0 \\ 0 & \overline{H(-\mathbf{k})} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k},\uparrow} \\ b_{\mathbf{k},\uparrow} \\ a_{\mathbf{k},\downarrow} \\ b_{\mathbf{k},\downarrow} \end{pmatrix}$$

$$+ \quad U \sum_i \left(a^{\dagger}_{i,\uparrow} a_{i,\uparrow} - 1/2 \right) \left(a^{\dagger}_{i,\downarrow} a_{i,\downarrow} - 1/2 \right) + \left(a \leftrightarrow b \right)$$

Phases:

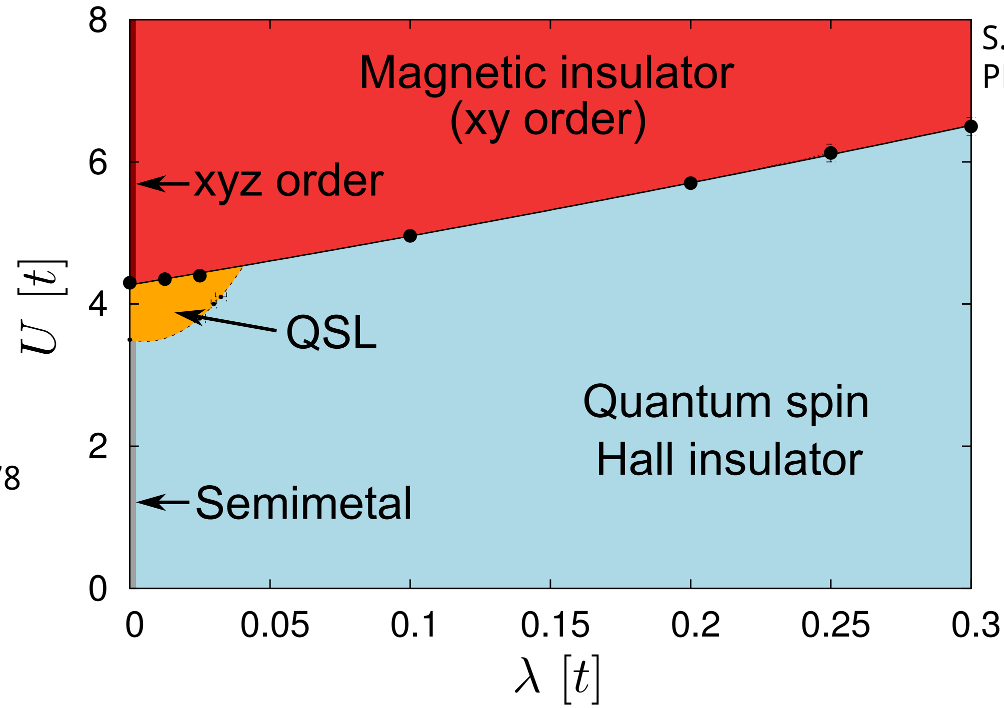
Z. Y. Meng et al.
Nature 464, 847 (2010)

S. Sorella et al.
Scientific Reports 2,
992 (2012)

F. Assaad & I. Herbut
arXiv1304.6340

B. Clark arXiv:1305.0278

Dirac fermions.



S. Rachel, K. Le Hur,
PRB 82, 075106, (2010)

M. Hohenadler, Z. Y. Meng, T. C. Lang, S. Wessel, A. Muramatsu, F. F. Assaad PRB 85 2012.

Questions.

Phases and quantum phase transitions?

TI → Magnetic Insulator

M. Hohenadler, Z. Y. Meng, T. C. Lang, S. Wessel, A. Muramatsu, FFA PRB 85 2012.

SM → Magnetic insulator

FFA, I. Herbut arXiv1304.6340

How do we detect topological states in the presence of correlations?

FFA, M. Bercx, M. Hohenadler, Phys. Rev. X 3, 011015 (2013)

How do correlations affect the helical edge state?

M. Hohenadler & FFA Phys. Rev. B 85, 081106, 2012

Magnetic impurities?

F. Goth, D. J. Luitz, FFA arXiv:1302.0856

Phases:

Z. Y. Meng et al. Nature 464, 847 (2010)

S. Sorella et al. Scientific Reports 2, 992 (2012)

F. Assaad & I. Herbut arXiv1304.6340

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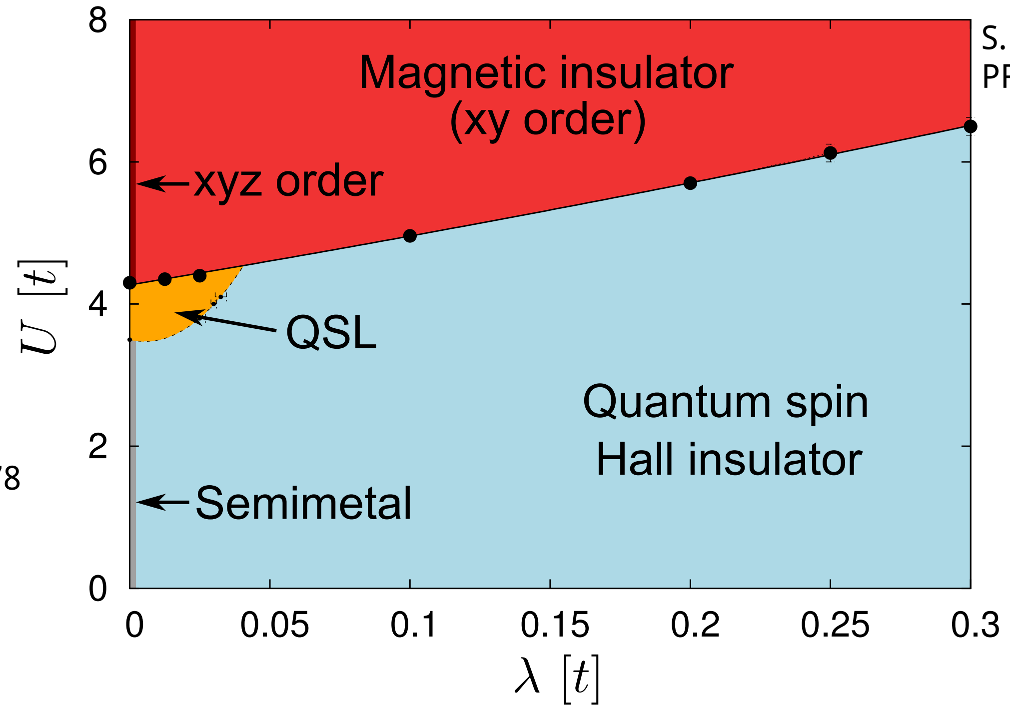

S. Rachel, K. Le Hur, PRB 82, 075106, (2010)

M. Hohenadler, Z. Y. Meng, T. C. Lang, S. Wessel, A. Muramatsu, F. F. Assaad PRB 85 2012.

Numerical method(s)

At half-band filling particle-hole symmetry allows to carry out sign free QMC simulations.

Blankenbecler, Sugar, Scalapino (BSS) auxiliary field algorithm, 1981

→ Ground state and excitations.

$$\left\langle O \right\rangle_0 = \lim_{\Theta\to\infty} \frac{\left\langle \psi_T \right| e^{-\Theta H/2} O\, e^{-\Theta H/2} \left| \psi_T \right\rangle}{\left\langle \psi_T \right| e^{-\Theta H} \left| \psi_T \right\rangle} \qquad \text{provided that} \qquad \left\langle \psi_T \middle| \psi_0 \right\rangle \neq 0$$

$$\left\langle \psi_T \right| e^{-\Theta H} \left| \psi_T \right\rangle \propto \int D\left\{\Phi(i,\tau)\right\} e^{-S\left(\left\{\Phi(i,\tau)\right\}\right)}$$

Trotter, Hubbard-Stratonovich

MC importance sampling

One body problem in external field.

$$S\left(\left\{\Phi(i,\tau)\right\}\right) = \int_0^\Theta d\tau \sum_i \frac{\Phi^2(i,\tau)}{2U} - \ln\left\langle \psi_T \right| T \exp\left(-\int_0^\Theta d\tau \;\; H_{KM} - i\sum_i \Phi(i,\tau)(c_i^\dagger c_i - 1)\right)\left| \psi_T \right\rangle$$

- The action is real! → positive weights (U(1) spin symmetry, ph and time reversal symmetry)
- CPU time: $V^3\Theta \rightarrow \Theta$ extrapolation is affordable.

M. Hohenadler, T.C. Lang and FFA PRL 106, 2011.
D. Zheng, C. Wu and G.-M. Zhang PRB 84, 2011.

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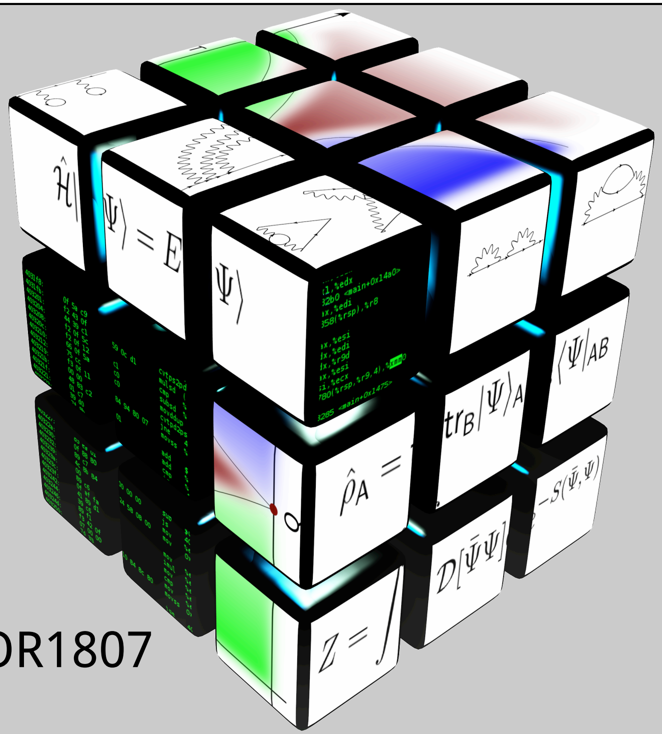


Würzburg Fall School

September 30th to October 4th (2013)

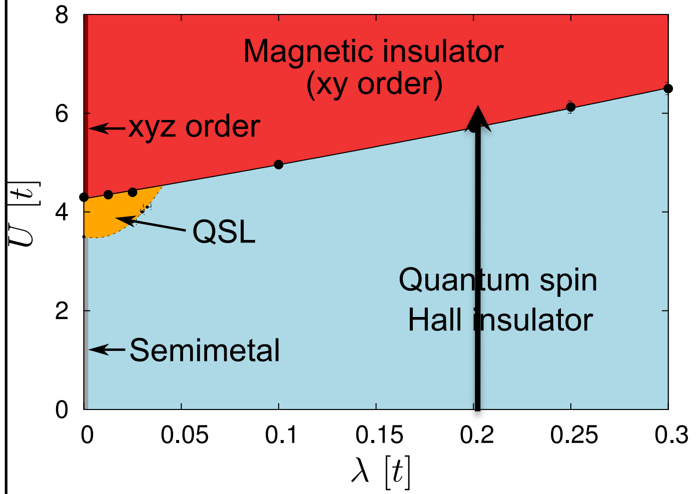
P. Corboz
M. Hohenadler
F. Heidrich-Meisner
A. Läuchli
L. Pollet
S. Trebst
M. Troyer
S. Wessel

DFG FOR1807

Advanced Computational Methods for Strongly Correlated Quantum Systems

http://for1807.physik.uni-wuerzburg.de

Effects of correlations @ λ/t=0.2 (Magnetic order disorder transition)



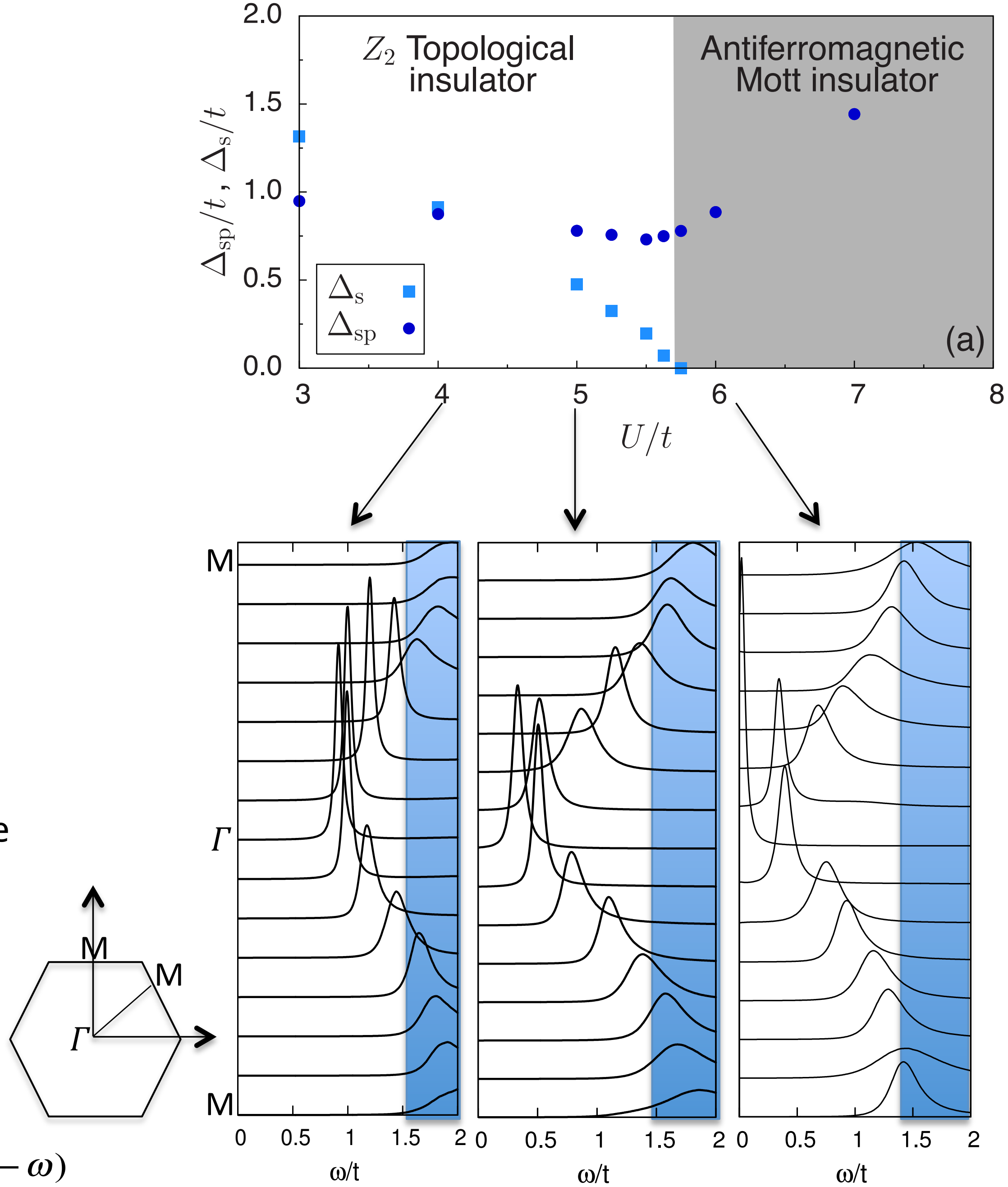
No closing of the single particle gap

Dynamical spin-spin correlations.

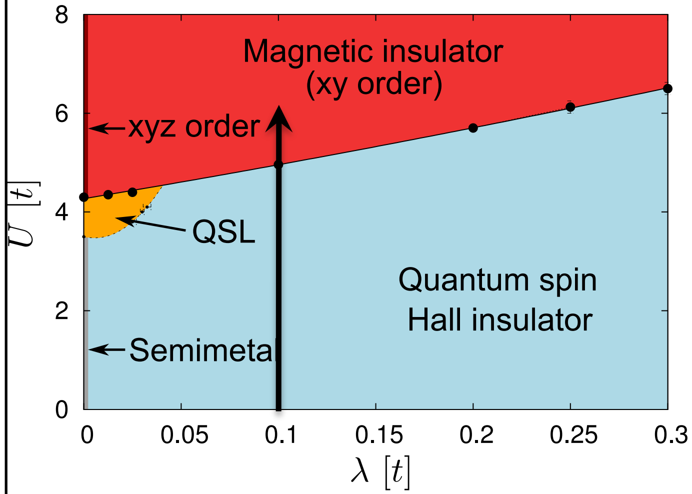
- U → U_c. Excitations of the disordered phase condense to form the order of the ordered phase.
- U(1) spin symmetry → 3D XY universality. Orientational disorder of spin.

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

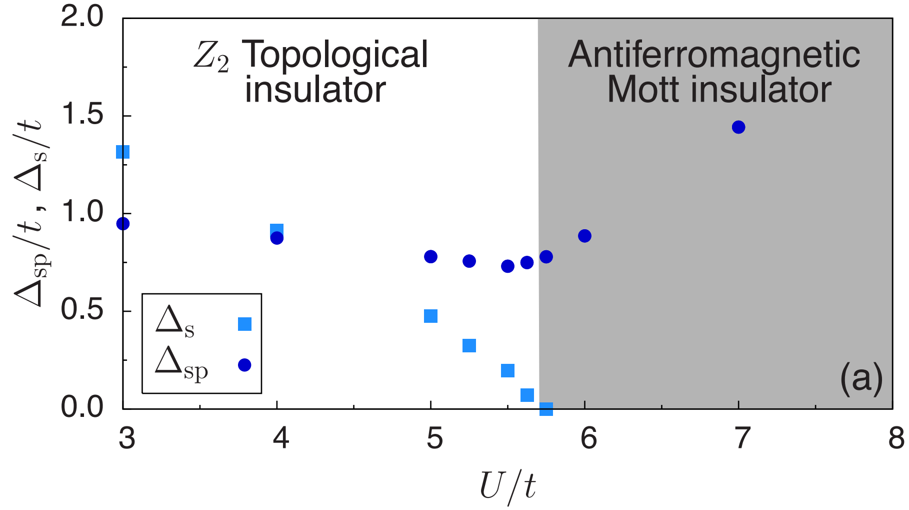
$L \rightarrow \infty,\ T = 0$



Effects of correlations @ λ/t=0.2, λ/t=0.1 (Magnetic order disorder transition)



$$L \to \infty,\ T = 0$$

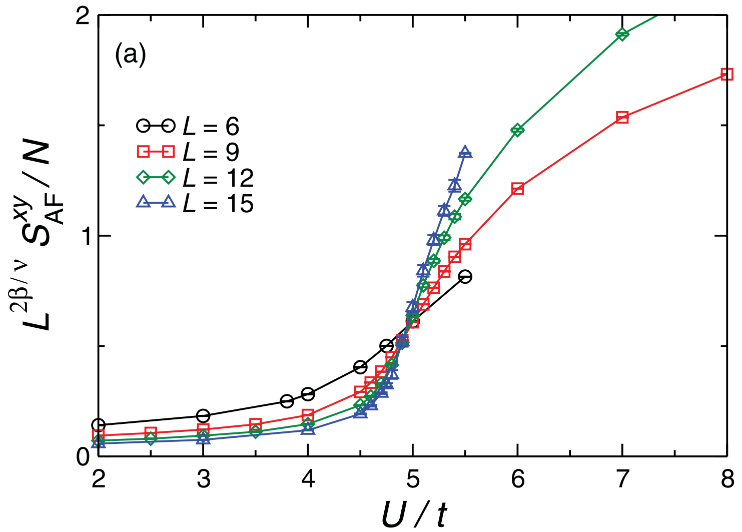


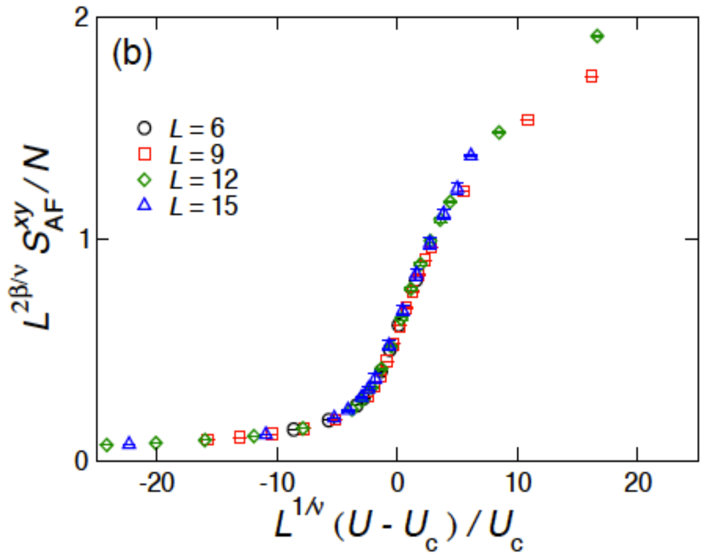
3D XY Criticality

$$S_{AF}^{xy}/N = m^2, \qquad m^2(L,U) = L^{-2\beta/\nu}\ F(\ L^{1/\nu}(U - U_c))$$

$U_c = 4.96(4),\ z = 1,\ \nu = 0.6717(1),$
$\eta = 0.0381(2),\ \beta = 0.3486(1)$

M. Campostrini, M. Hasenbusch, A. Pelissetto, and E. Vicari, Phys. Rev. B **74**, 144506 (2006).





Magnetic flux pumping

A tool to detect topological insulators in the presence of correlations.

Magnetic flux pumping:
a tool to detect Z2 topological insulators in the presence of correlations.

One spin sector *(Haldane)*

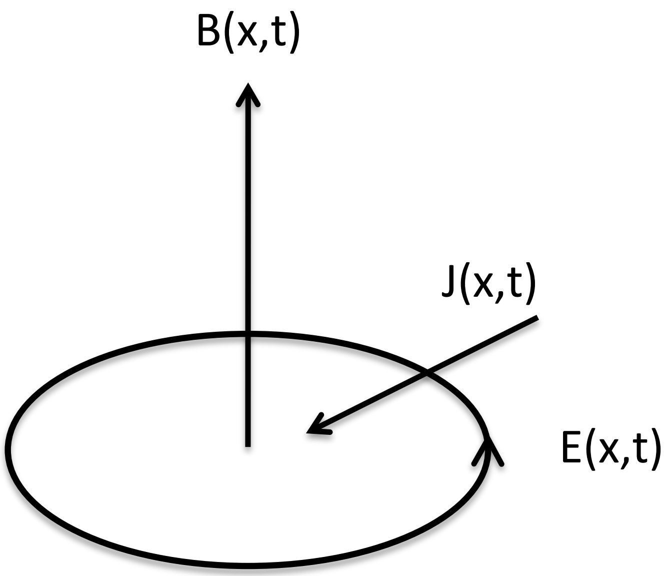
$$\mathbf{B}(\mathbf{x},t)=t\,\frac{\Phi_0}{2}\;\delta(\mathbf{x})\;\mathbf{e}_z \qquad t\in[0,1]$$

$$\mathbf{E}(\mathbf{x},t)=\frac{\Phi_0}{4\pi}\;\frac{(-y,x)}{r^2}$$

$$\sigma_{xy}=\frac{e^2}{h},\quad \sigma_{xx}=0$$

$$J(\mathbf{x},t)=\frac{e^2}{h}\;\frac{\Phi_0}{4\pi}\;\frac{(x,y)}{r^2}$$

$$\Delta Q=\frac{e}{2},\quad \left(\Delta Q=-\frac{e}{2},\;\frac{\Phi_0}{2}=-\frac{\Phi_0}{2}\right)$$



A π-flux generates two mid-gap states with half an electronic charge

D. H. Lee, G-M Zhang, and T. Xiang. Phys. Rev. Lett. **99**, 196805 (2007)
Jakiv, Rebbi, Phys. Rev. D 13, 3398 (1976)
Su, Schrieffer, Heeger Phys. Rev. B 22, 2099 (1980)

Magnetic flux pumping:
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$$\mathbf{B}(\mathbf{x},t) = t\,\frac{\Phi_0}{2}\,\delta(\mathbf{x})\,\mathbf{e}_z \qquad t \in [0,1]$$

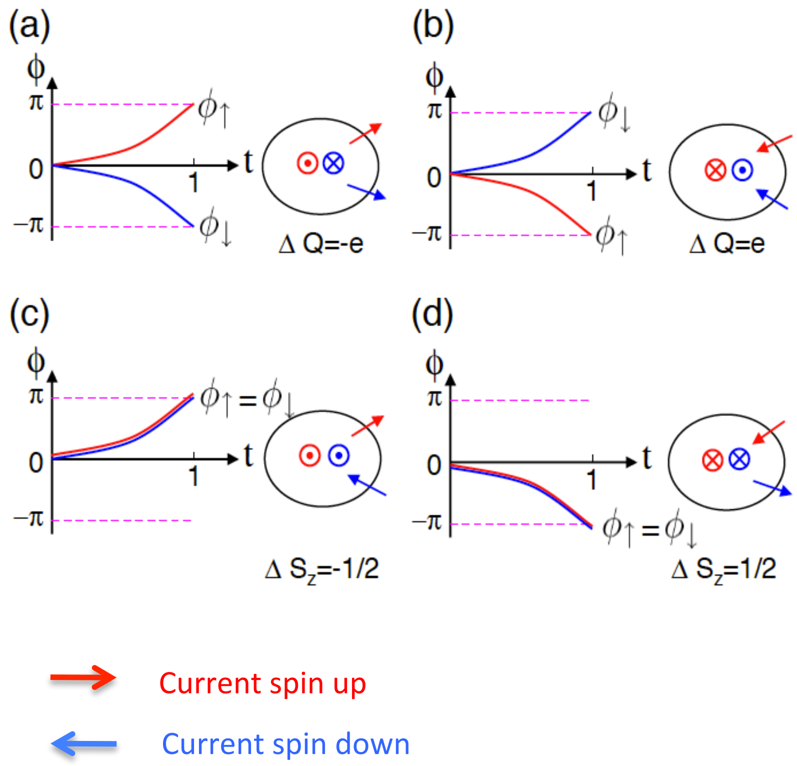
$$\mathbf{E}(\mathbf{x},t) = \frac{\Phi_0}{4\pi}\,\frac{(-y,x)}{r^2}$$

$$\sigma_{xy} = \frac{e^2}{h}, \quad \sigma_{xx} = 0$$

$$J(\mathbf{x},t) = \frac{e^2}{h}\,\frac{\Phi_0}{4\pi}\,\frac{(x,y)}{r^2}$$

$$\Delta Q = \frac{e}{2}, \quad \left(\Delta Q = -\frac{e}{2},\ \frac{\Phi_0}{2} = -\frac{\Phi_0}{2}\right)$$

Both spin sectors.



4-midgap states.

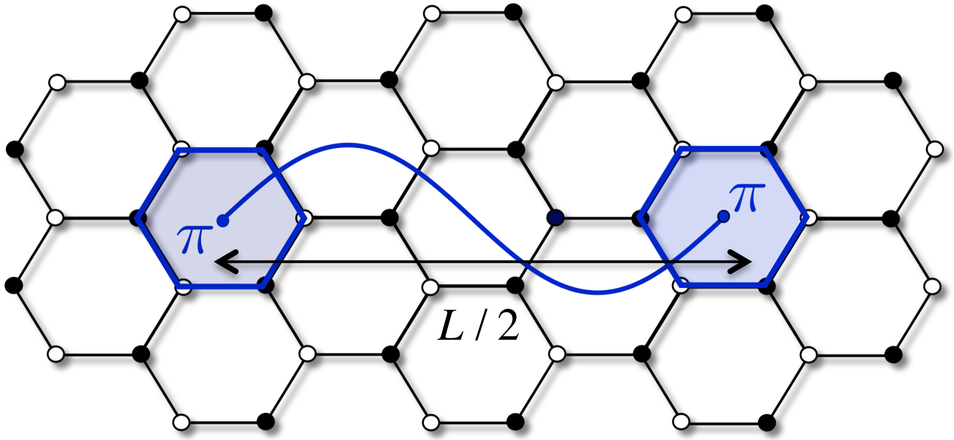
Xiao-Liang Qi and Shou-Cheng Zhang
Phys. Rev. Lett. 101, 086802 (2008)

Ying Ran, Ashvin Vishwanath, and Dung-Hai Lee
Phys. Rev. Lett. 101, 086801 (2008).

$U/t=0,\ \lambda/t=0.2$

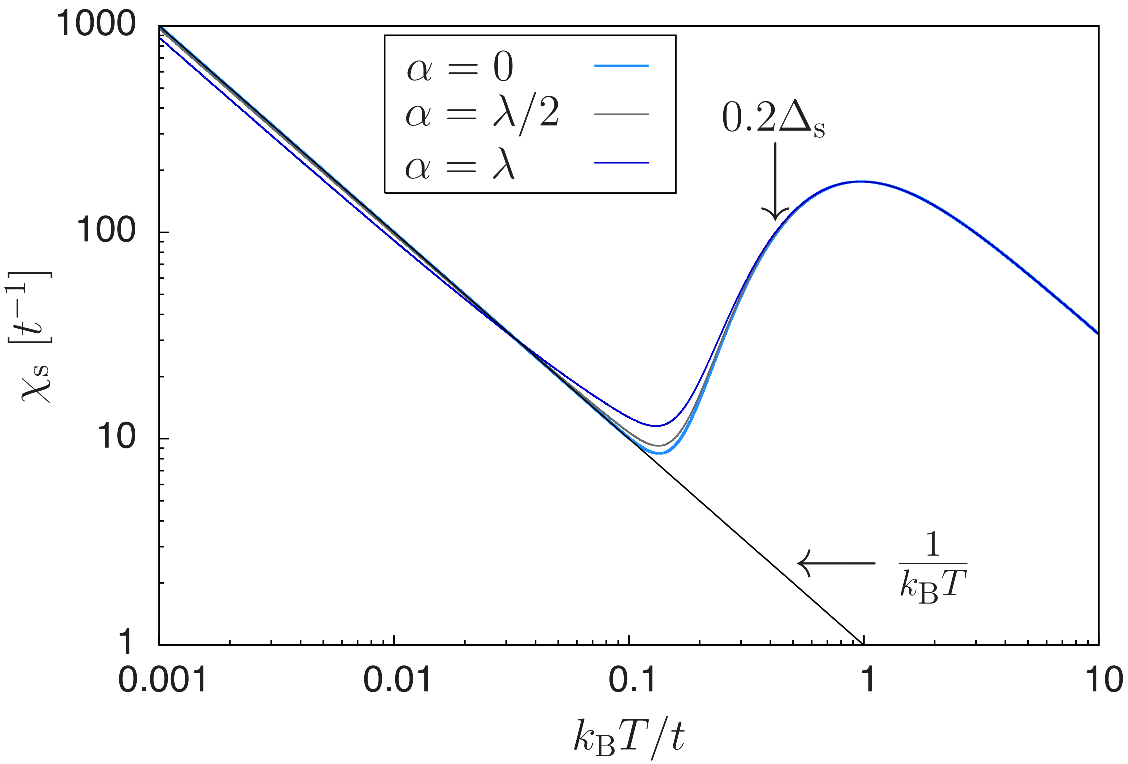
$$\chi_c = \beta\left(\left\langle \hat{N}^2 \right\rangle - \left\langle \hat{N} \right\rangle^2\right)$$

$$\chi_s = \beta\left(\left\langle M_z^2 \right\rangle - \left\langle M_z \right\rangle^2\right)$$

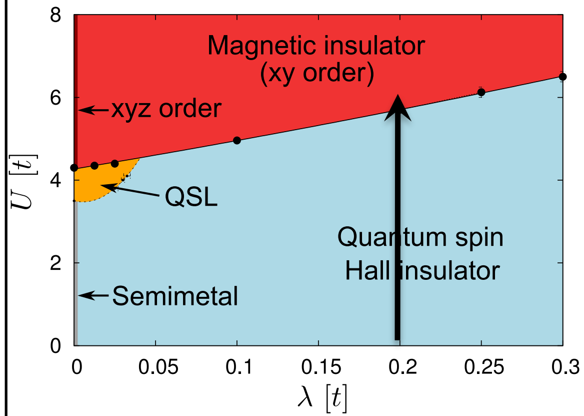


Per π-flux $\mathcal{H}=\{|\uparrow\rangle,|\downarrow\rangle,|+\rangle,|-\rangle\}$

$$\chi_s \equiv \chi_c = \frac{1}{2k_B T}$$

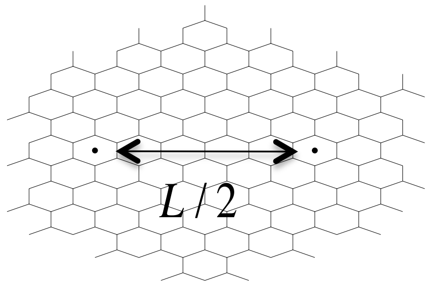


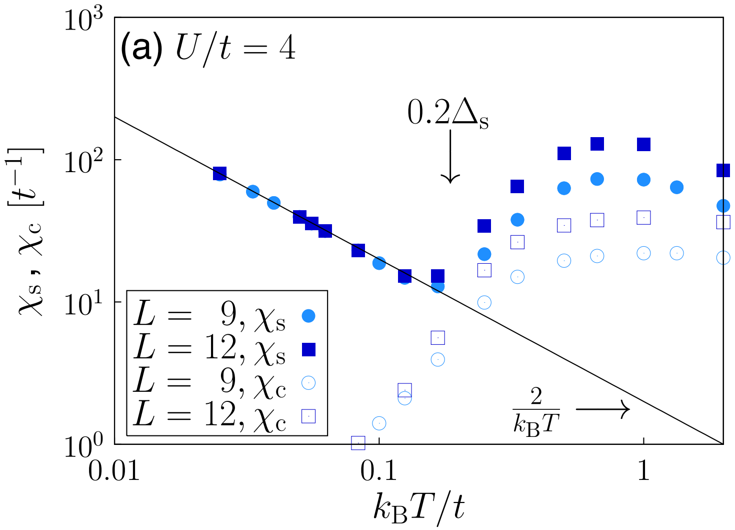
Finite values of U/t @ λ/t=0.2

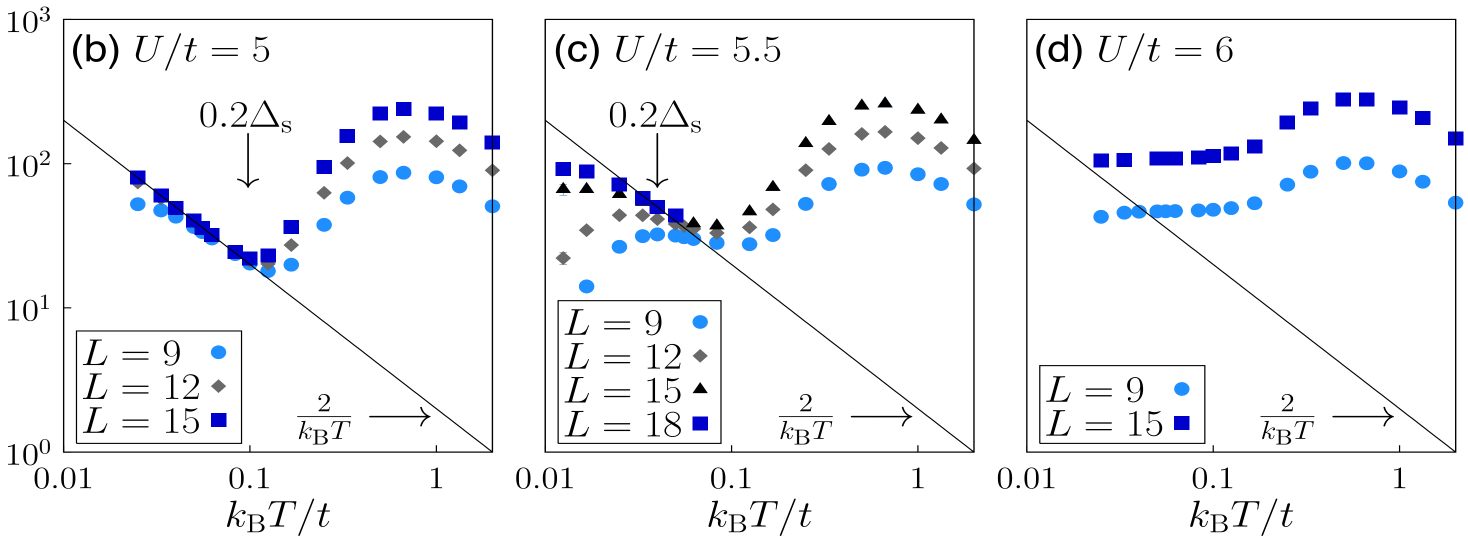


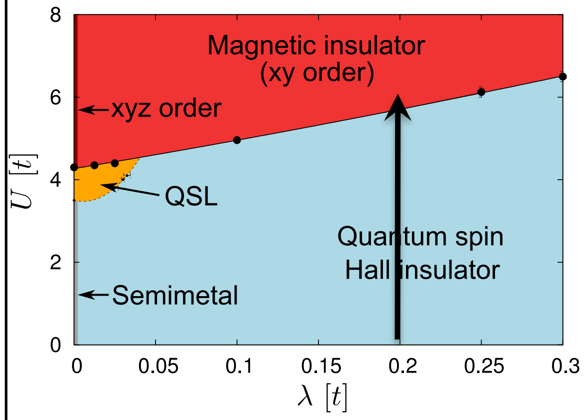
Charge is gapped out. $\chi_c = 0$

Per π-flux $\mathcal{H} = \{ |\uparrow\rangle, |\downarrow\rangle \}$ $\quad \chi_s = \frac{1}{k_B T}$



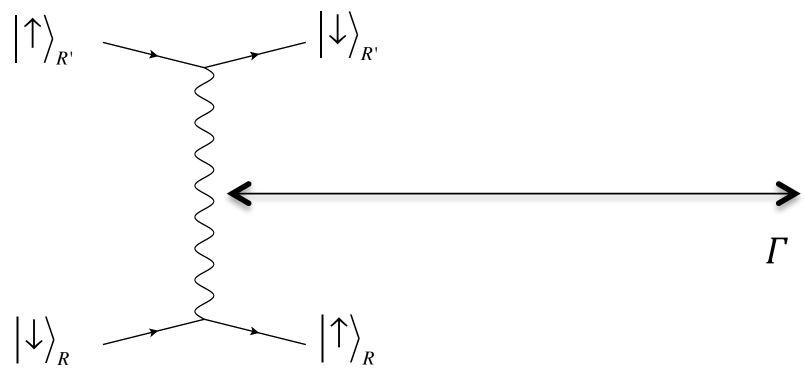


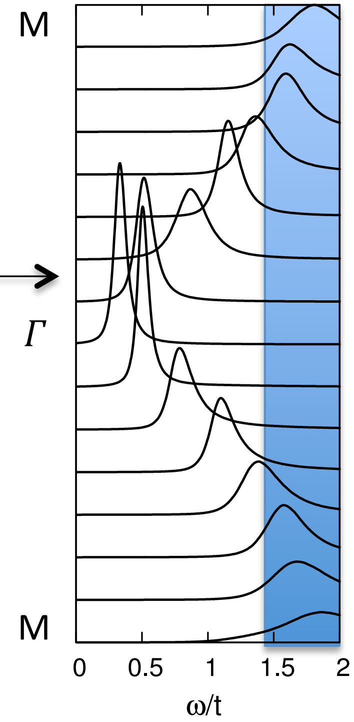


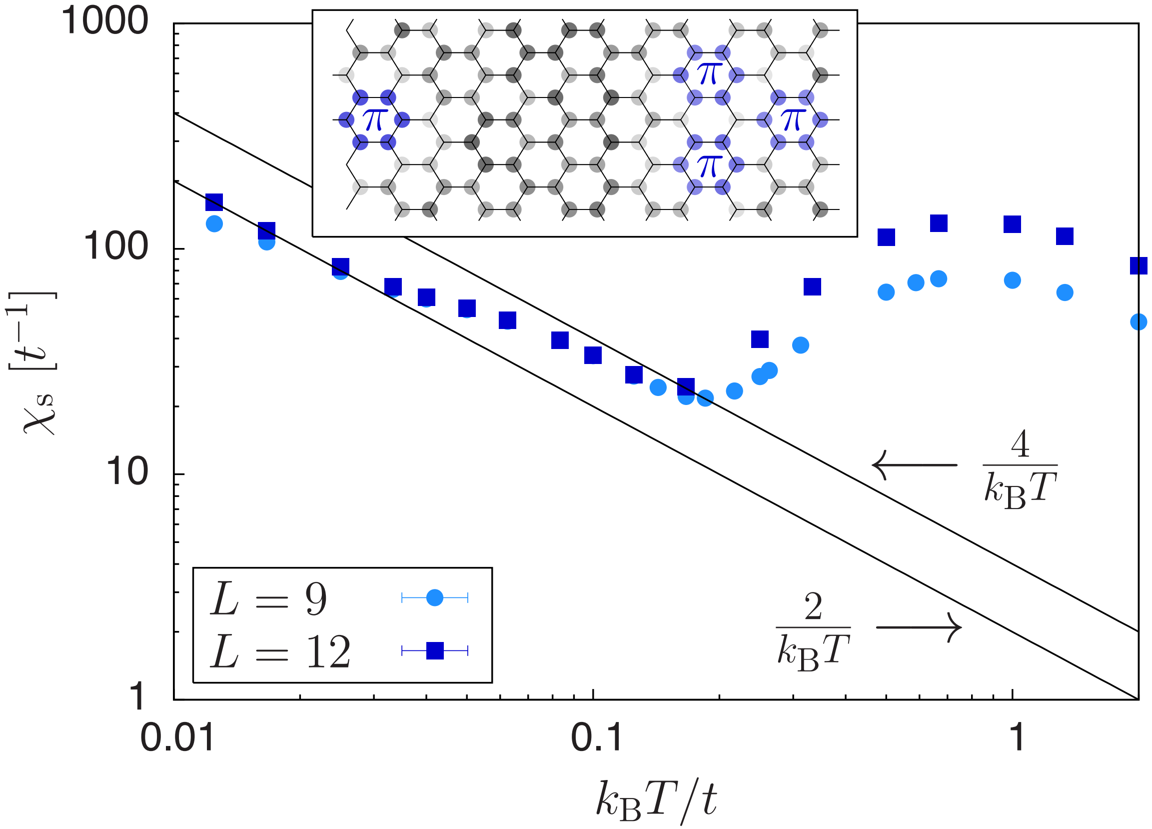


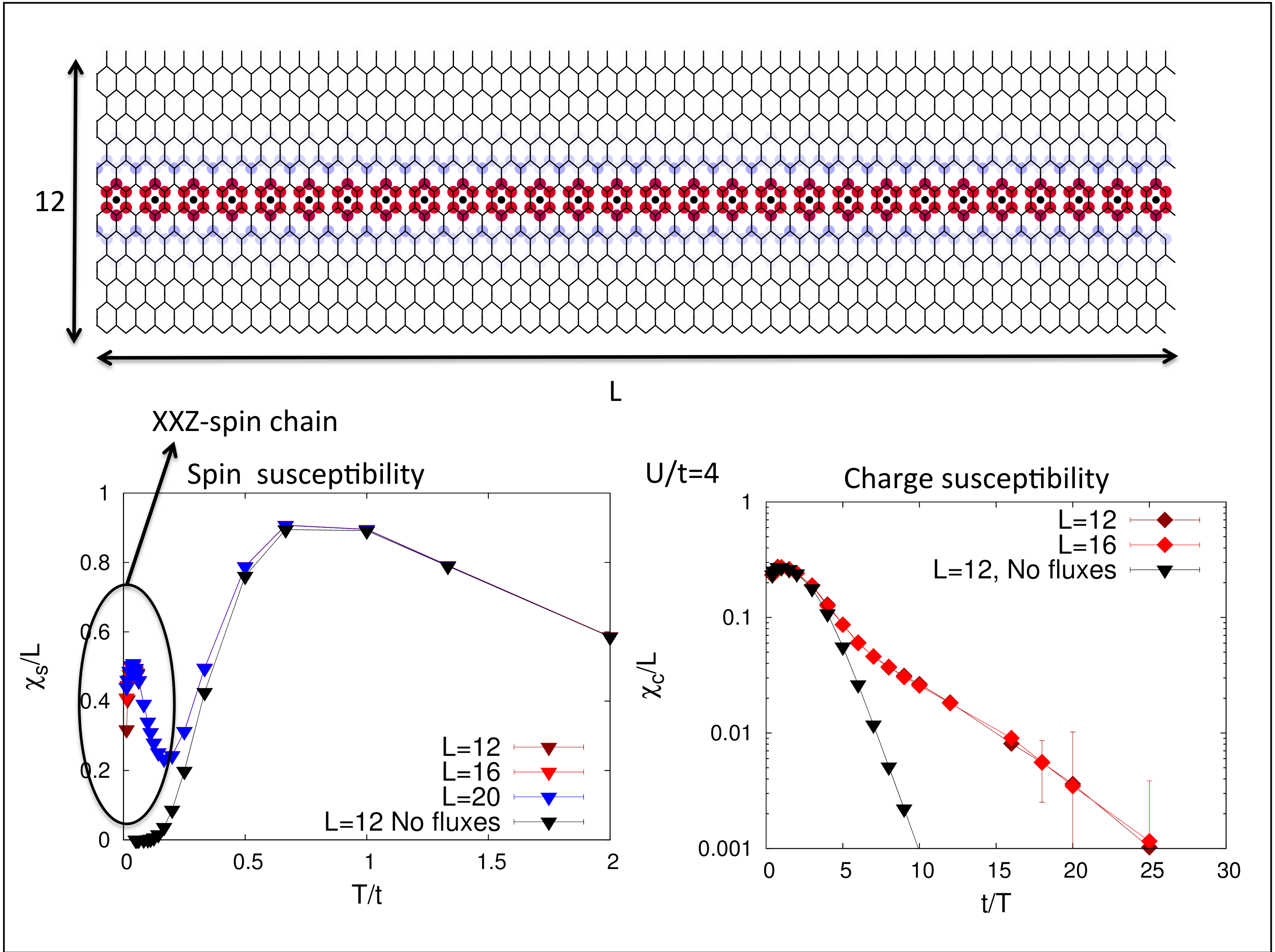
Interaction between spin fluxons.

Exchange of collective spin excitation.

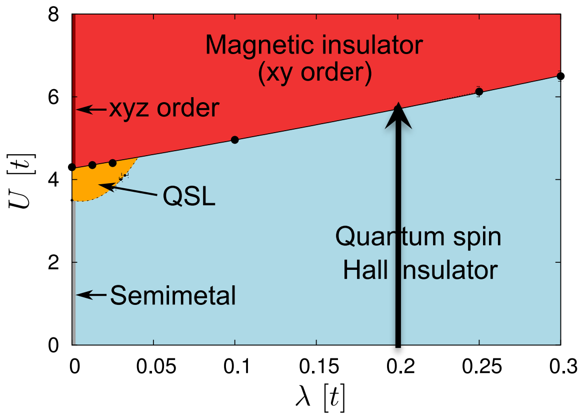







12
L
XXZ-spin chain
Spin susceptibility
U/t=4
Charge susceptibility
χ_s/L
T/t
L=12
L=16
L=20
L=12 No fluxes
χ_c/L
t/T
L=12
L=16
L=12, No fluxes

Semimetal to insulator transition

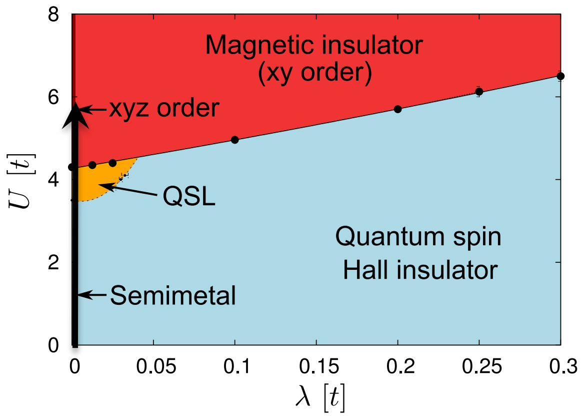


Why is it so tricky?

$$S_{AF}/N = m^2 \propto \left(U - U_c\right)^{2\beta}$$

$$\lambda = 0.2, \quad 3D\ XY, \quad \beta = 0.3486(1) \quad \rightarrow \quad S_{AF}/N = m^2 \propto \left(U - U_c\right)^{0.7}$$

Semimetal to insulator transition



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$\lambda = 0\ ?$ Gross-Neveu universality, ε-expansion around d=3, $\beta \approx 0.8$

I. Herbut, V. Juričić, O. Vafek PRB 80, 075432, (2009)

$$\rightarrow \quad S_{AF}/N \;=\; m^2 \propto (U-U_c)^{1.6}$$

→ Big lattices L=36, high precision S. Sorella, Y.Otsuka, S. Yunoki. Scientific Reports 2, 992 (2012)

Alternative

Introduce pinning fields and measure m instead of m^2

FFA & I. Herbut arXiv1304.6340

Steven R. White and A. L. Chernyshev Phys. Rev. Lett. 99, 127004

$$H = H_{tU} + h_0(n_{0,\uparrow} - n_{0,\downarrow})$$

$$m = \lim_{R\to\infty} \lim_{L\to\infty} \langle S^z(R) \rangle e^{i\mathbf{Q}\cdot\mathbf{R}}$$

$$m = \lim_{L\to\infty} \frac{1}{L^2} \sum_i e^{i\mathbf{Q}\cdot\mathbf{i}} \langle S^z(i) \rangle$$

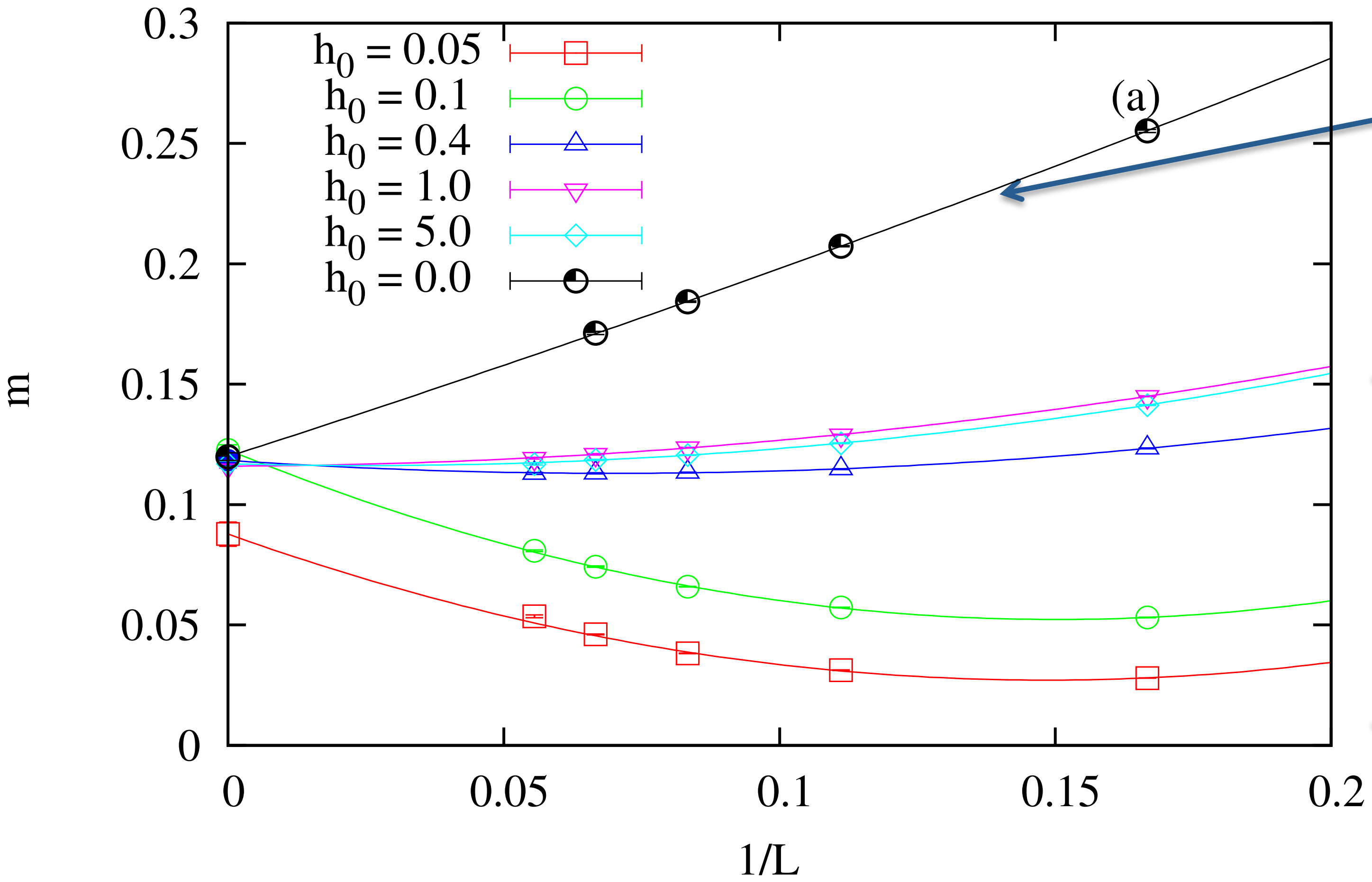
The ordered case @ U/t=5

$$H = -t\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U\sum_i (n_{i,\uparrow}-1/2)(n_{i,\downarrow}-1/2) + h_0(n_{0,\uparrow}-n_{0,\downarrow})$$

$$m = \lim_{L\to\infty} \frac{1}{L^2}\sum_i e^{i\mathbf{Q}\cdot\mathbf{i}}\langle S^z(i)\rangle$$

- Large values of projection parameter. $\Theta t = 320$
- Small values of h_0 lead to bigger finite size effects.

U/t=5



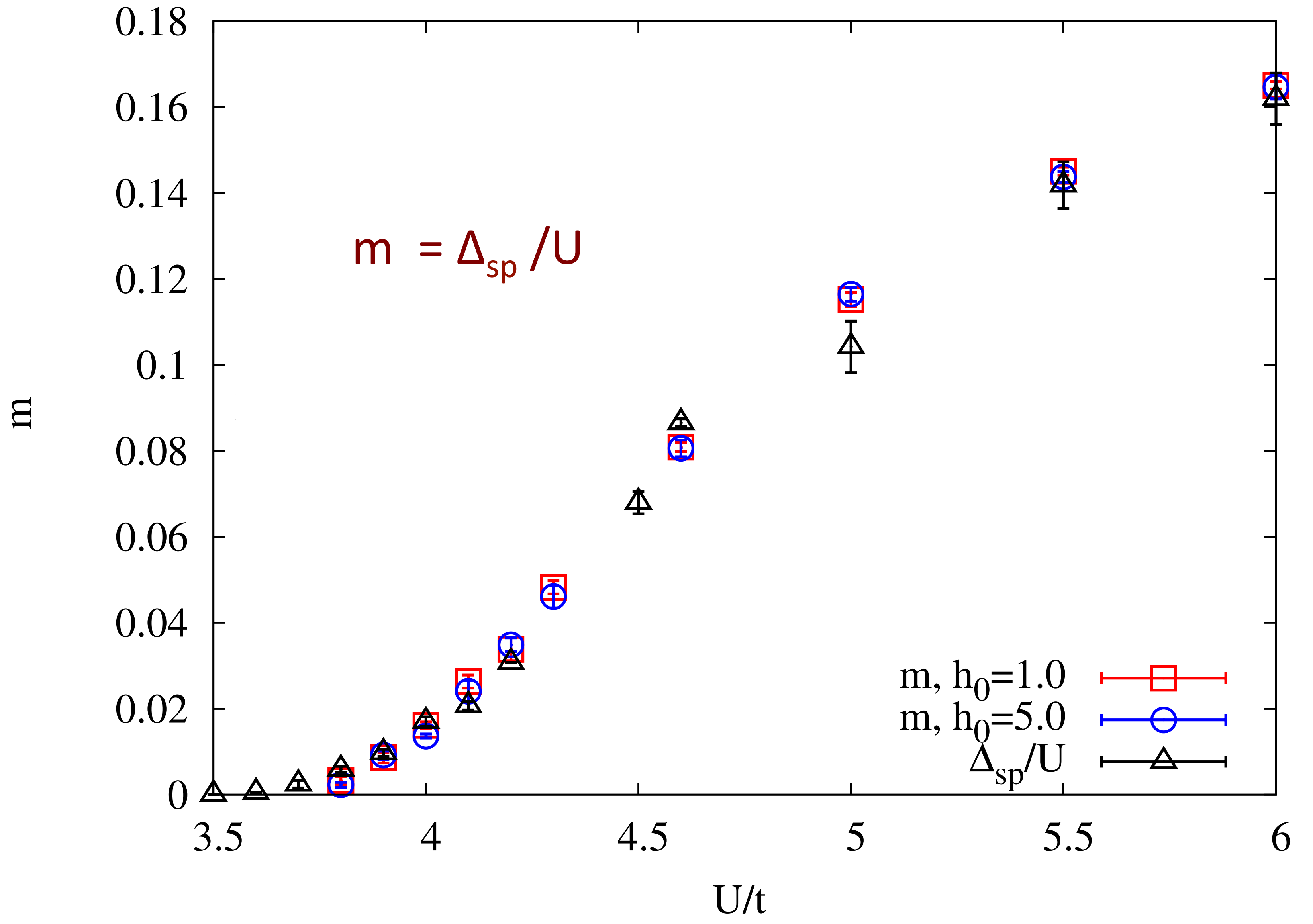
$$\sqrt{\frac{1}{L^2}\sum_{\mathbf{i}=1}^{L^2}\langle \mathbf{S}_{A,\mathbf{0}}\cdot\mathbf{S}_{A,\mathbf{i}}\rangle}$$

$@\ h_0 = 0$

$$\frac{1}{L^2}\sum_i e^{i\mathbf{Q}\cdot\mathbf{i}}\langle S^z(i)\rangle$$

$@\ h_0 = 0.05, 0.1, 1.0, 5.0$

Polynomial extrapolation of m and Δ_{sp} /U



Gross-Neveu Yukawa.

I. Herbut, V. Juričić, O. Vafek   PRB 80, 075432, (2009)

$$L_0 = \bar{\psi}(\mathbf{x},\tau)\partial_\mu \gamma_\mu \psi(\mathbf{x},\tau)$$ Dirac fermions

$$L_b = \vec{\psi}_t(\mathbf{x},\tau)\cdot\left[-\partial_\tau^2 - v^2\vec{\nabla}^2 + t\right]\vec{\psi}_t(\mathbf{x},\tau) + \lambda\left(\vec{\psi}_t(\mathbf{x},\tau)\bullet\vec{\psi}_t(\mathbf{x},\tau)\right)^2$$ Order parameter

$$L_y = g\ \vec{\psi}_t(\mathbf{x},\tau)\cdot\bar{\psi}\,\vec{\sigma}\,\psi$$ Yukawa coupling

$$\boxed{\Delta_{sp} \propto g\left|\left\langle \vec{\psi}_t \right\rangle\right|}$$

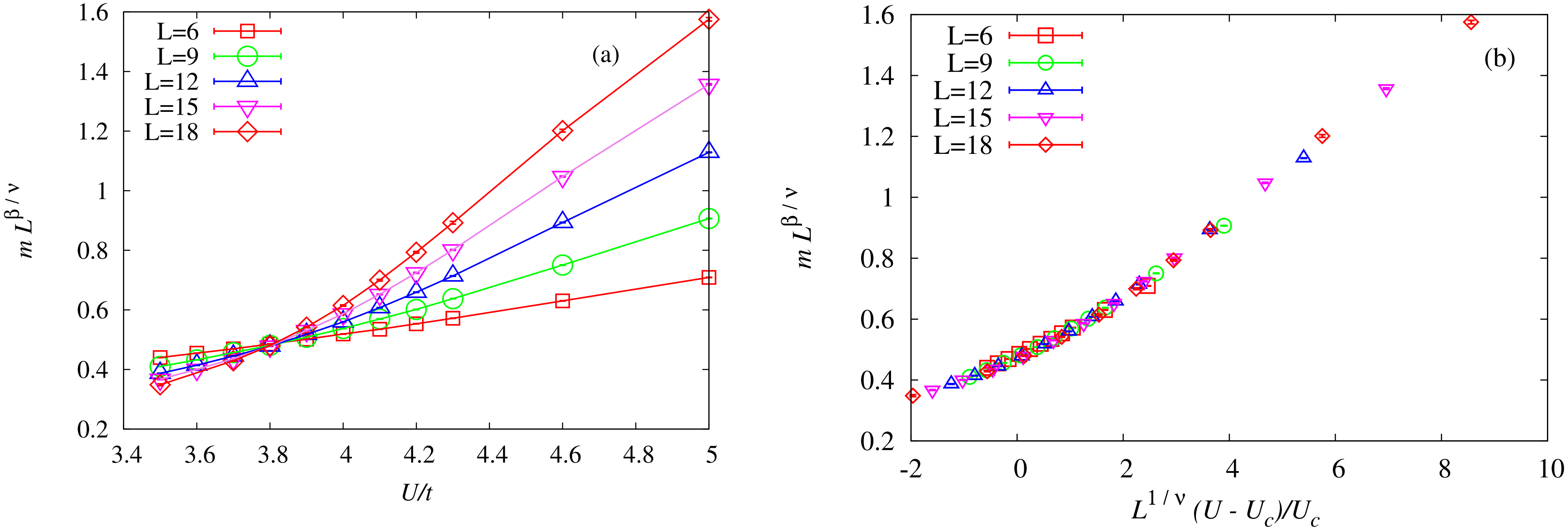
Upper critical dimension d=3 → ε-expansion

$$\boxed{\begin{aligned} \frac{\beta}{\nu} &= 1 - \frac{\varepsilon}{10} + O\left(\varepsilon^2\right) \\ \nu &= \frac{1}{2} + \frac{21}{55}\varepsilon + O\left(\varepsilon^2\right) \end{aligned}}$$

$$\frac{\beta}{\nu} = 1 - \frac{1}{10} + O\left(1^2\right)$$

$$\nu = \frac{1}{2} + \frac{21}{55}1 + O\left(1^2\right)$$

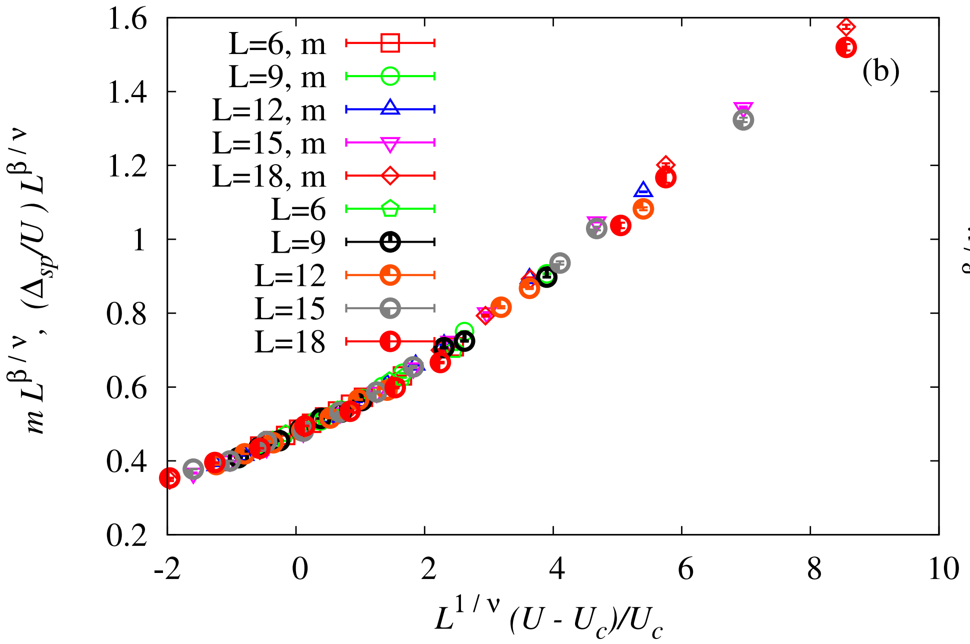
$$m(L,U) = L^{-\beta/\nu} \;\; F(\; L^{1/\nu}(U - U_c))$$

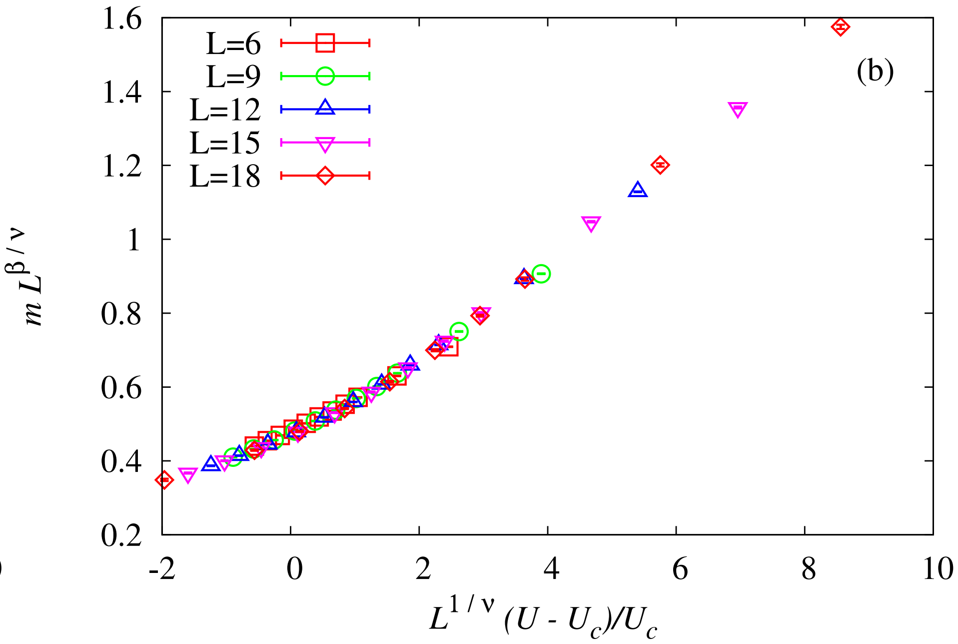


$$\boxed{\begin{aligned}\frac{\beta}{\nu} &= 1-\frac{1}{10}+O\left(1^{2}\right)\\ \nu &= \frac{1}{2}+\frac{21}{55}1+O\left(1^{2}\right)\end{aligned}}$$

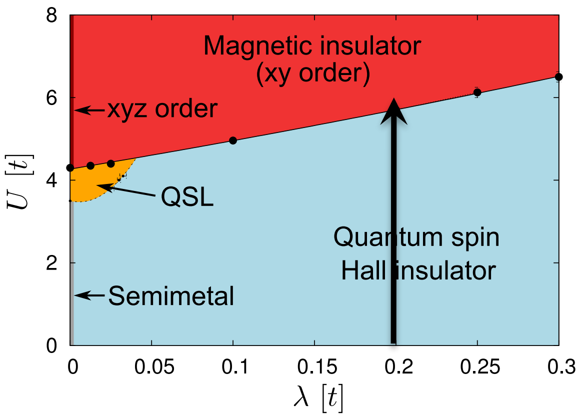
$$m(L,U) = L^{-\beta/\nu}\ F(\,L^{1/\nu}(U-U_c))$$

$$\Delta_{sp}(L,U)/U \;=\; L^{-\beta/\nu}\ \tilde{F}(\,L^{1/\nu}(U-U_c))$$



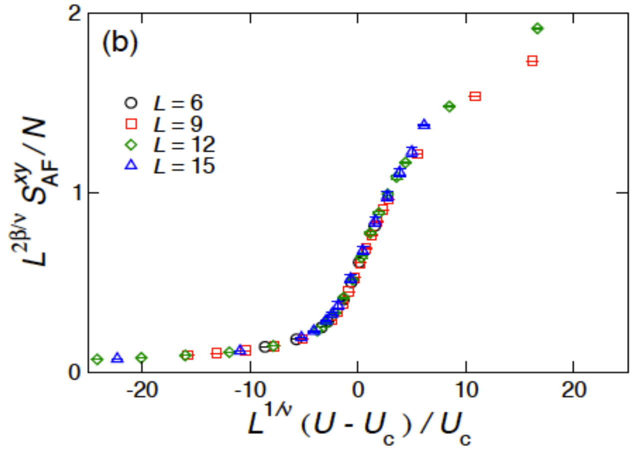


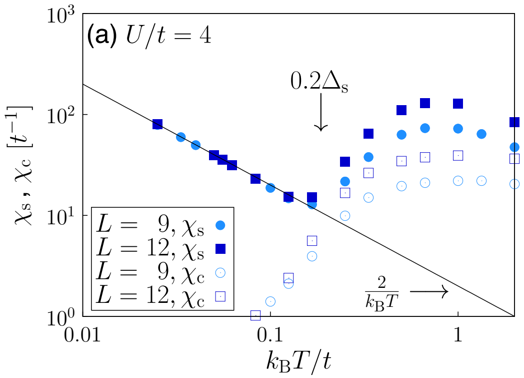
Summary



3D XY Criticality.

$$U_c = 4.96(4),\ z = 1,\ \nu = 0.6717(1),$$
$$\eta = 0.0381(2),\ \beta = 0.3486(1)$$





π-fluxes are a good tool detect correlated topological insulators.

Gross-Neveu criticality.