# Phase diagram of the Hubbard-Honeycomb lattice.

Fakher F. Assaad (Exotic Phases of Frustrated Magnets. KITP October 08, 2012 to October 12, 2012.)

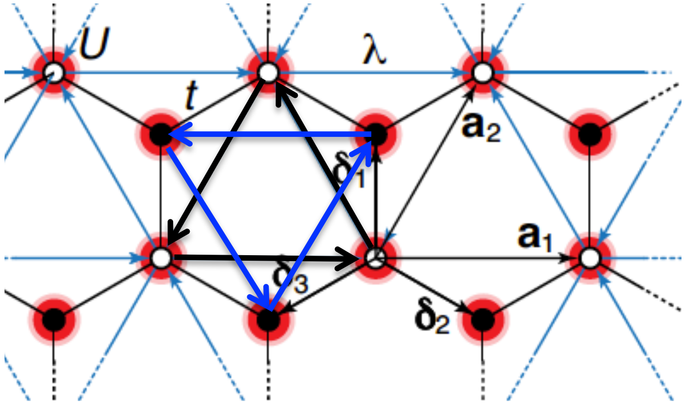
- Models and methods.
- Phase diagram of the Hubbard-Honeycomb lattice.

  → Alternative methods to compute staggered moments.

  Z.Y. Meng, T.Lang, S. Wessel, F.F. Assaad and A. Muramatsu
- Quantum spin models from $\pi$-fluxes threaded through correlated topological insulators.

  F. F. Assaad, M. Bercx and M. Hohenadler arXiv:1204.4728
- Conclusions.

<u>The half-filled Kane-Mele Hubbard Model.</u>




$$H = H_t + H_U + H_{SO}$$

$$H_t = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} c_{\mathbf{i}}^{\dagger} c_{\mathbf{j}} \,, \qquad H_U = U \sum_{\mathbf{i}} \left( c_{\mathbf{i}}^{\dagger} c_{\mathbf{i}} - 1 \right)^2$$

$$H_{SO} = i \lambda \sum_{<<\mathbf{i},\mathbf{j}>>} \upsilon_{<<\mathbf{i},\mathbf{j}>>} c_{\mathbf{i}}^{\dagger} \sigma_z c_{\mathbf{j}} \qquad \mathbf{c}_i^{\dagger} = (c_{i,\uparrow}^{\dagger}, c_{i,\downarrow}^{\dagger})$$

Left (right) turn $\upsilon_{\langle\langle i,j \rangle\rangle} = 1 \quad \left( \upsilon_{\langle\langle i,j \rangle\rangle} = -1 \right)$

<u>Hubbard</u>

SU(2) spin ✓

Sublattice symmetry ✓

Time reversal ✓

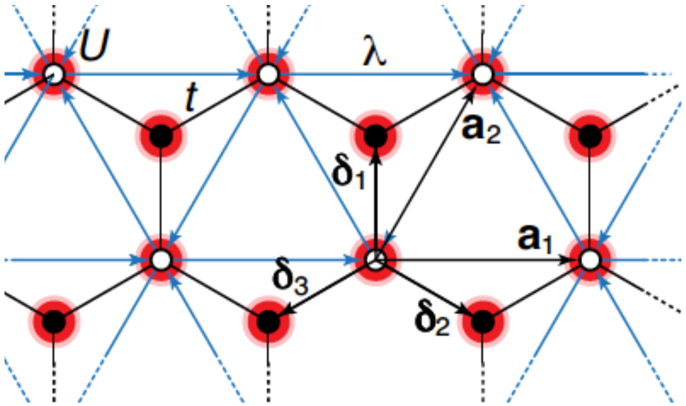
<u>Spin-Orbit</u>

SU(2) spin → U(1)

Broken sublattice symmetry → Opens a mass gap.

Time reversal ✓

## The half-filled Kane-Mele Hubbard Model.

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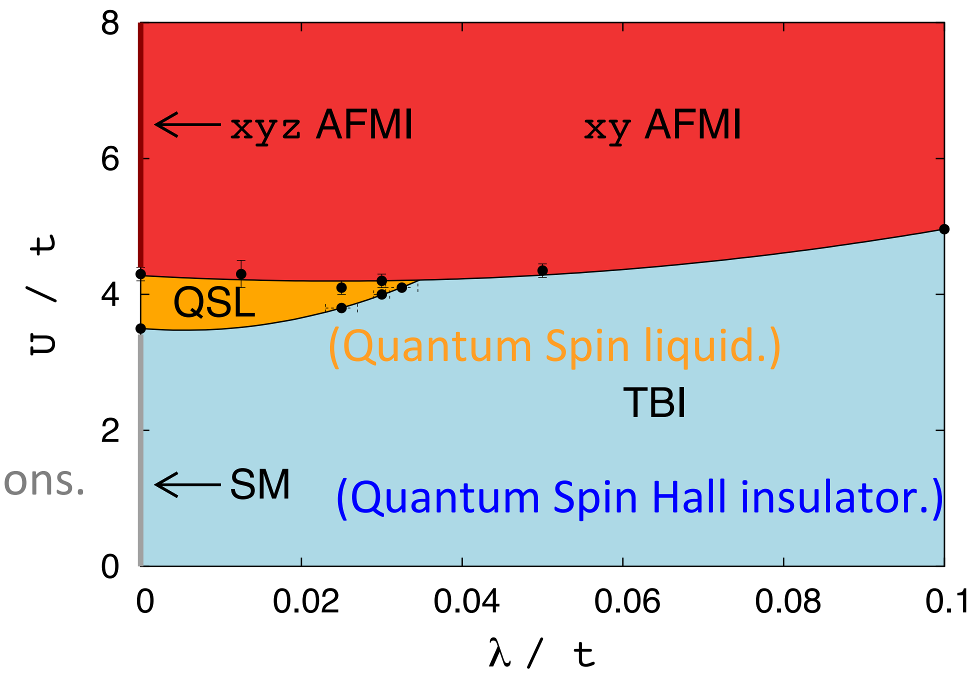
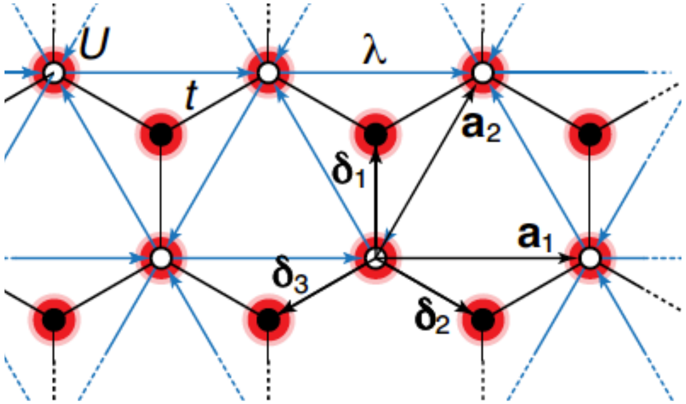
Phases:

Dirac fermions.




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

<u>The half-filled Kane-Mele Hubbard Model.</u>

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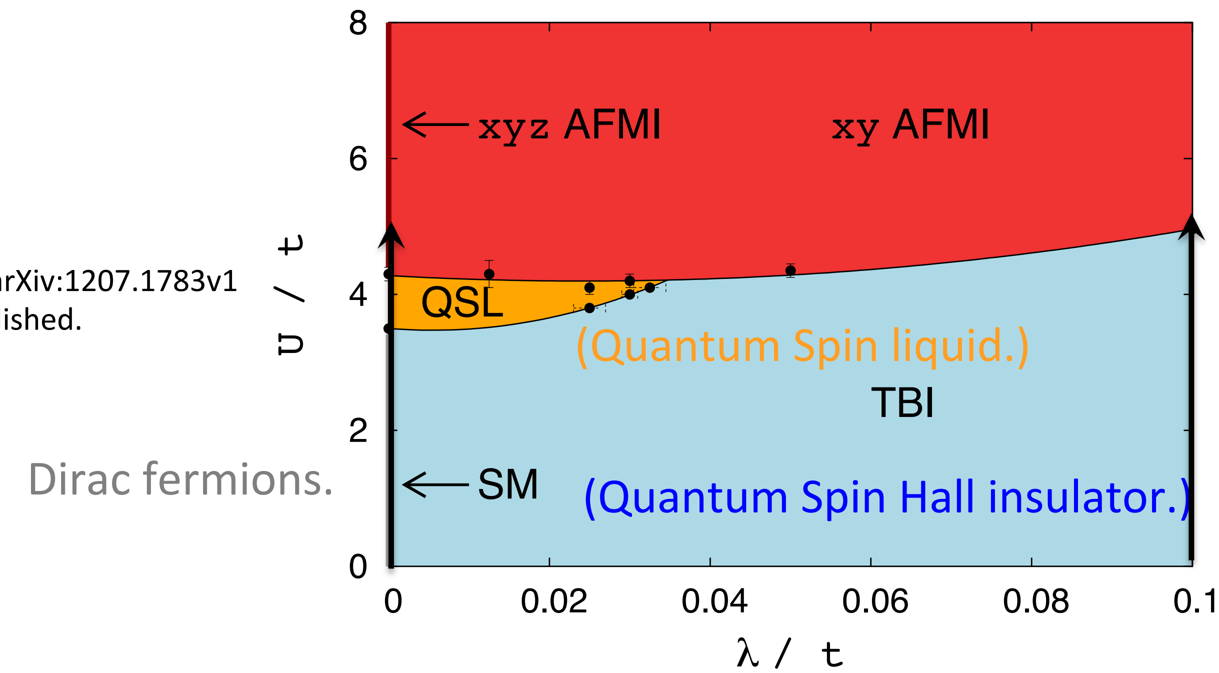
Left (right) turn $\upsilon_{\langle\langle i,j\rangle\rangle} = 1 \quad \left( \upsilon_{\langle\langle i,j\rangle\rangle} = -1 \right)$

<u>Phases:</u>

S. Sorella et al. arXiv:1207.1783v1
B. Clark, unpublished.




Quantum spin models from $\pi$- fluxes threaded through correlated topological insulators.

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

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. (GS up to 36x36 Sorella et al. arXiv:1207.1783v1)

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

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

Trotter, Hubbard-Stratonovich

MC importance sampling

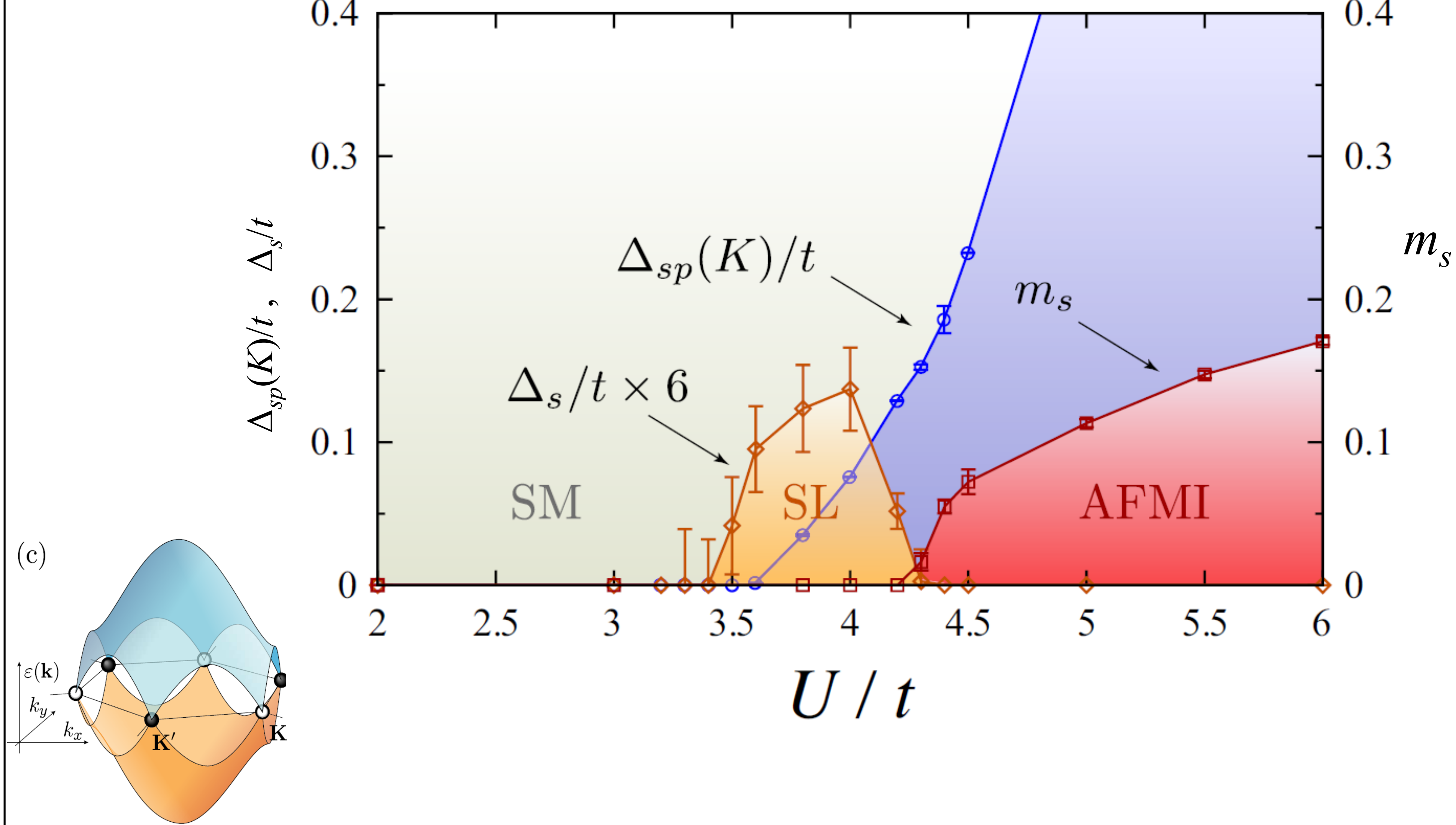
One body problem in external field.

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

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

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

Phase diagram of the Hubbard Honeycomb lattice

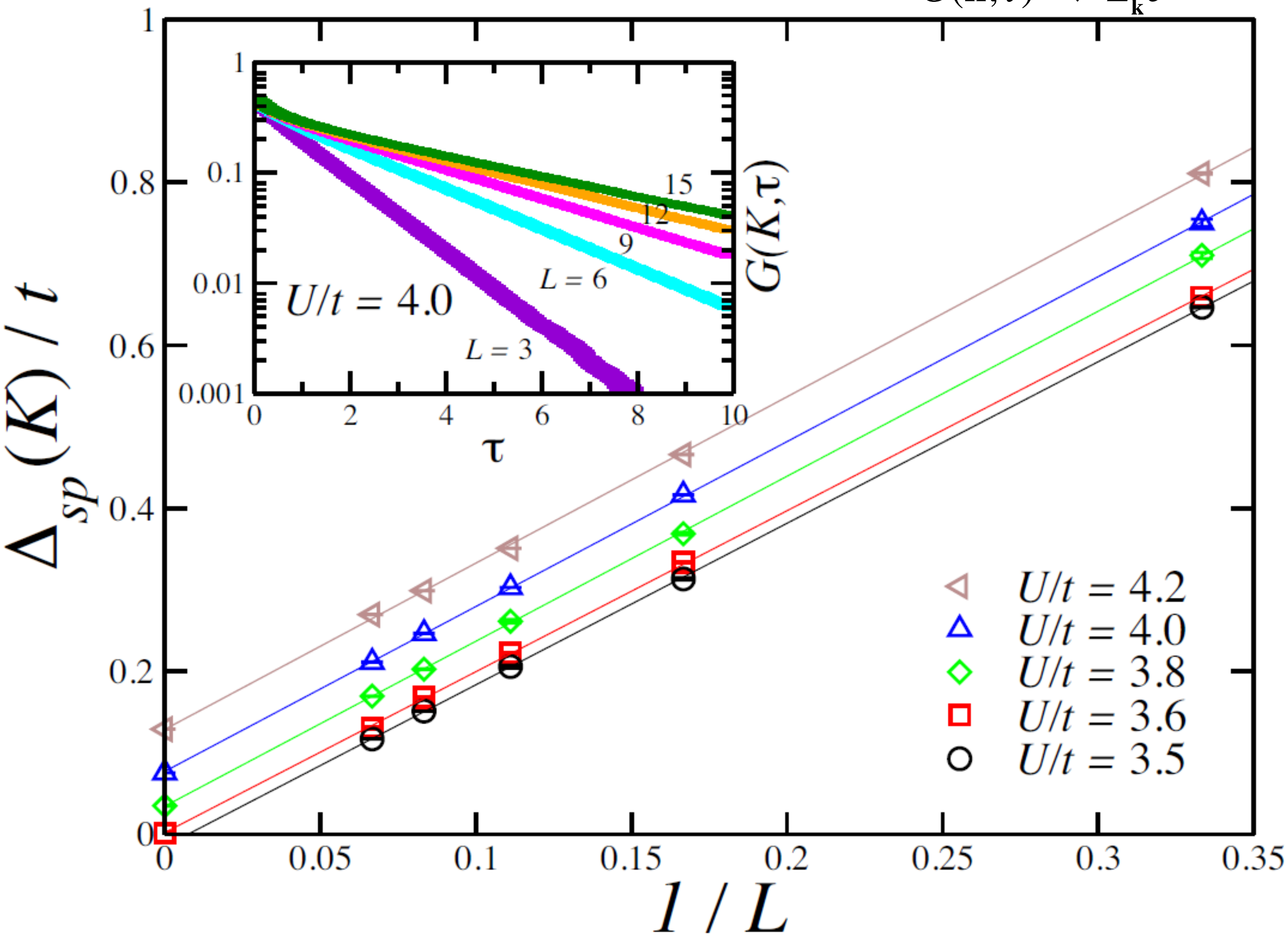


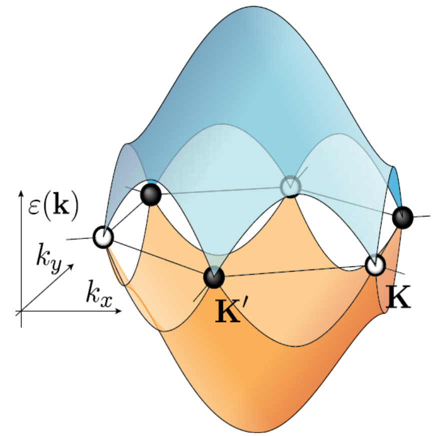

Z.Y. Meng, T.Lang, S. Wessel, F.F. Assaad and A. Muramatsu (Nature 2010).

Single-Particle Gap

$$G(\vec{k},\tau) = \frac{1}{2}\sum_{a}\langle c^{\dagger}_{\vec{k}a\uparrow}(\tau)c_{\vec{k}a\uparrow}(0)\rangle$$

$$G(\vec{\mathbf{k}},\tau) \rightarrow Z_{\vec{\mathbf{k}}}e^{-\Delta_{sp}(\vec{\mathbf{k}})\tau}$$



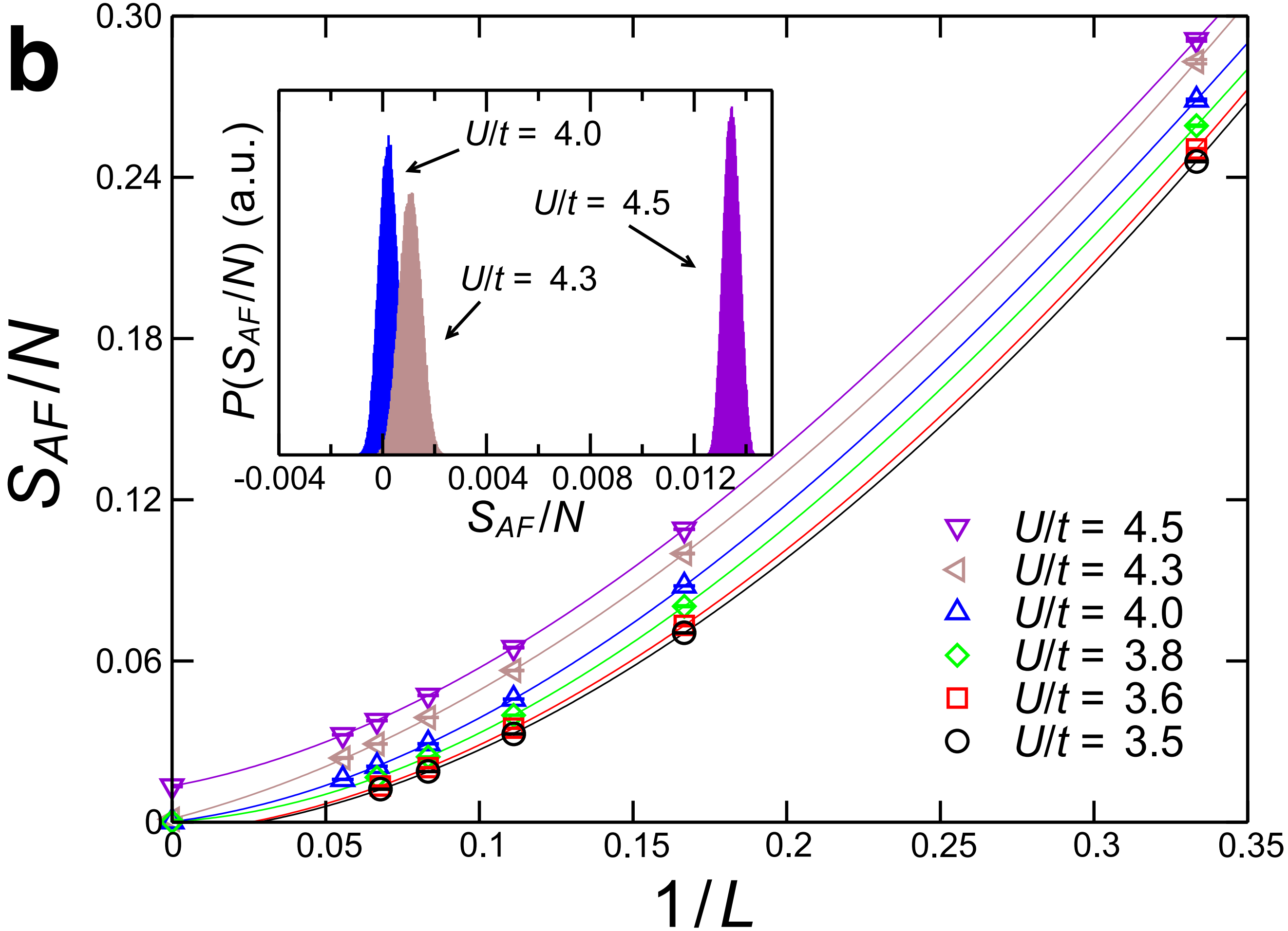



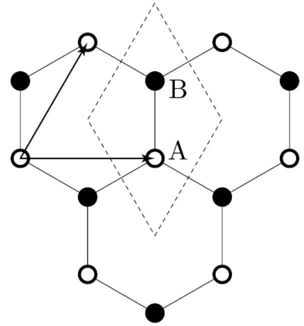

Single particle gap opens beyond

$U/t > 3.6$

# Antiferromagnetic Order

$$S_{AF} = \left\langle \sum_{\mathbf{i}} (-1)^{\mathbf{i}} \mathbf{S}_{\mathbf{i}} \bullet \mathbf{S}_{\mathbf{0}} \right\rangle$$




Antiferromagnetic order beyond

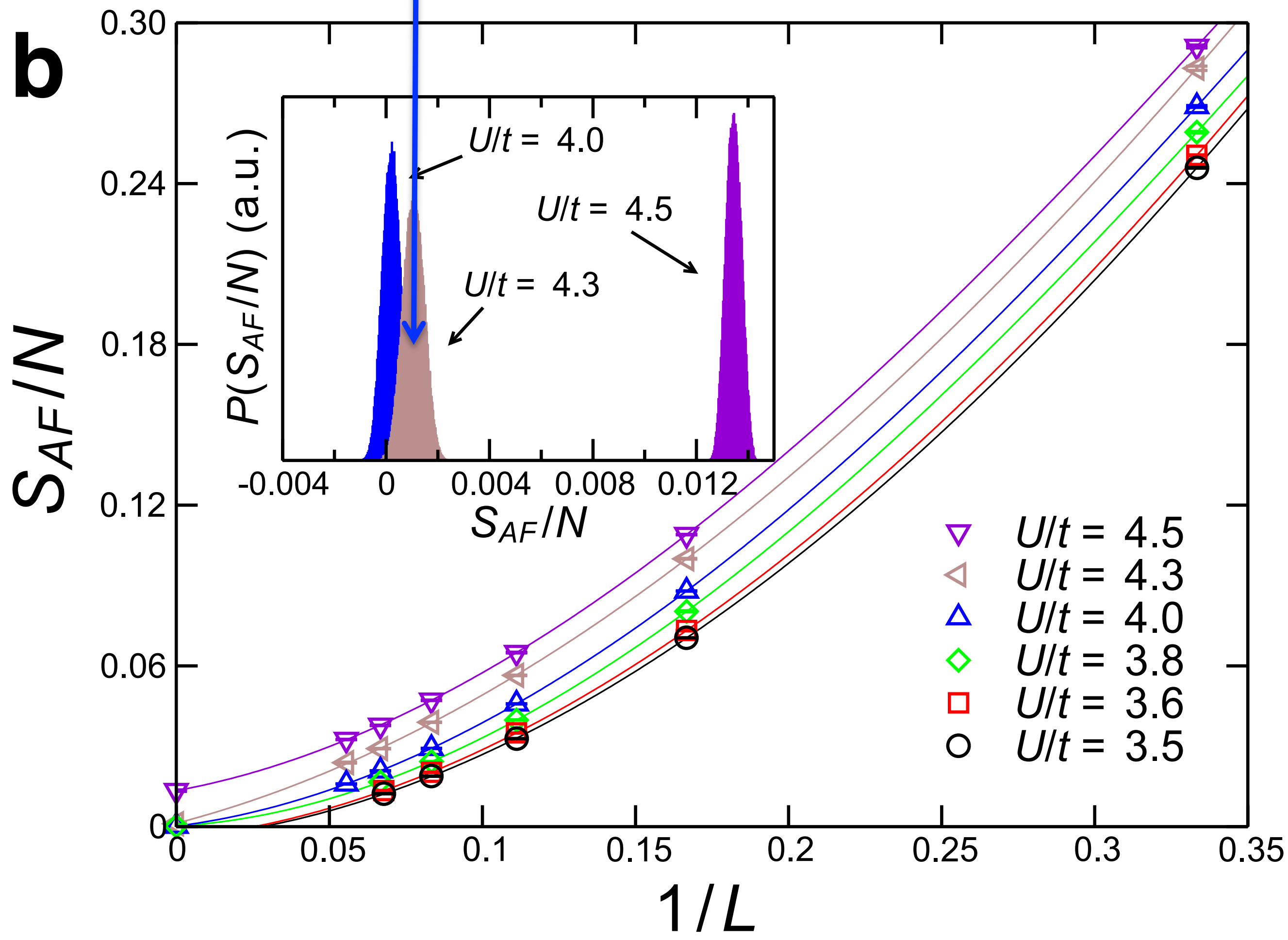
$U/t > 4.3$

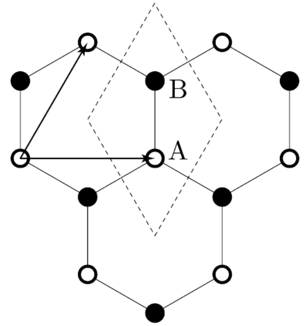
# Antiferromagnetic Order

Sorella et al.

U/t=4: Extrapolated value is 0.0012 +/- 0.0002

$$S_{AF} = \left\langle \sum_{\mathbf{i}} (-1)^{\mathbf{i}} \mathbf{S}_{\mathbf{i}} \bullet \mathbf{S}_{\mathbf{0}} \right\rangle$$

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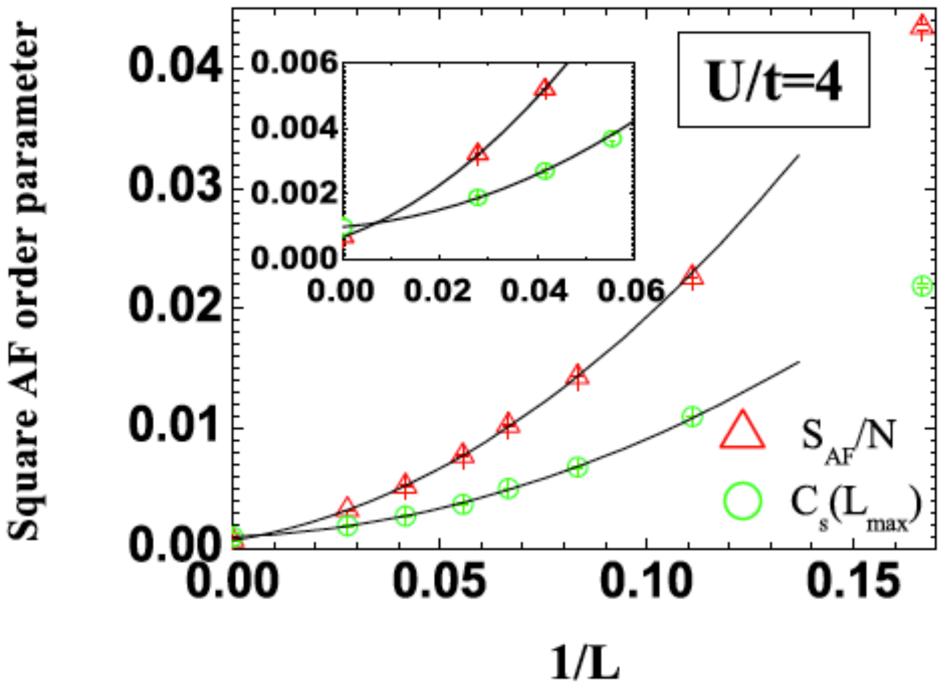
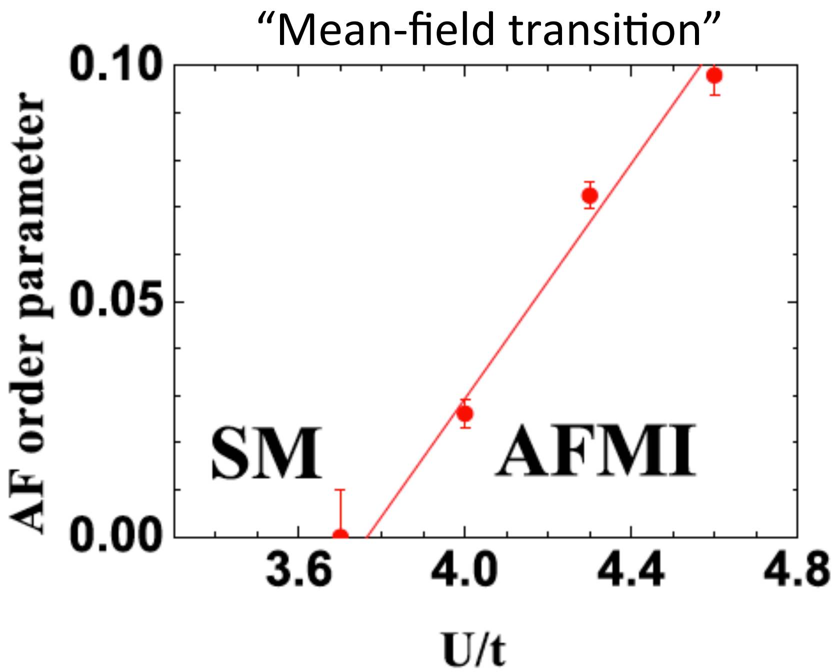
Sorella et al.




Sorella: Mean-field. $m \propto (U_c - U)$

Herbut: $\varepsilon = 3 - d$ expansion $m \propto (U_c - U)^{0.88}$ Herbut, Juričić, Vafek PRB **80**, 075432 (2009)

Difficulty of pinning down small staggered moment is related to the fact that we are measuring the square of the order parameter!

# Phase diagram of the Hubbard-Honeycomb model.

→ Methods to detect magnetically ordered states with small staggered moments.

Calculate the staggered by introducing a pinning field.

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

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

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

$$H = H_{tU} + \sum_q h(q) S^z(q)$$

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

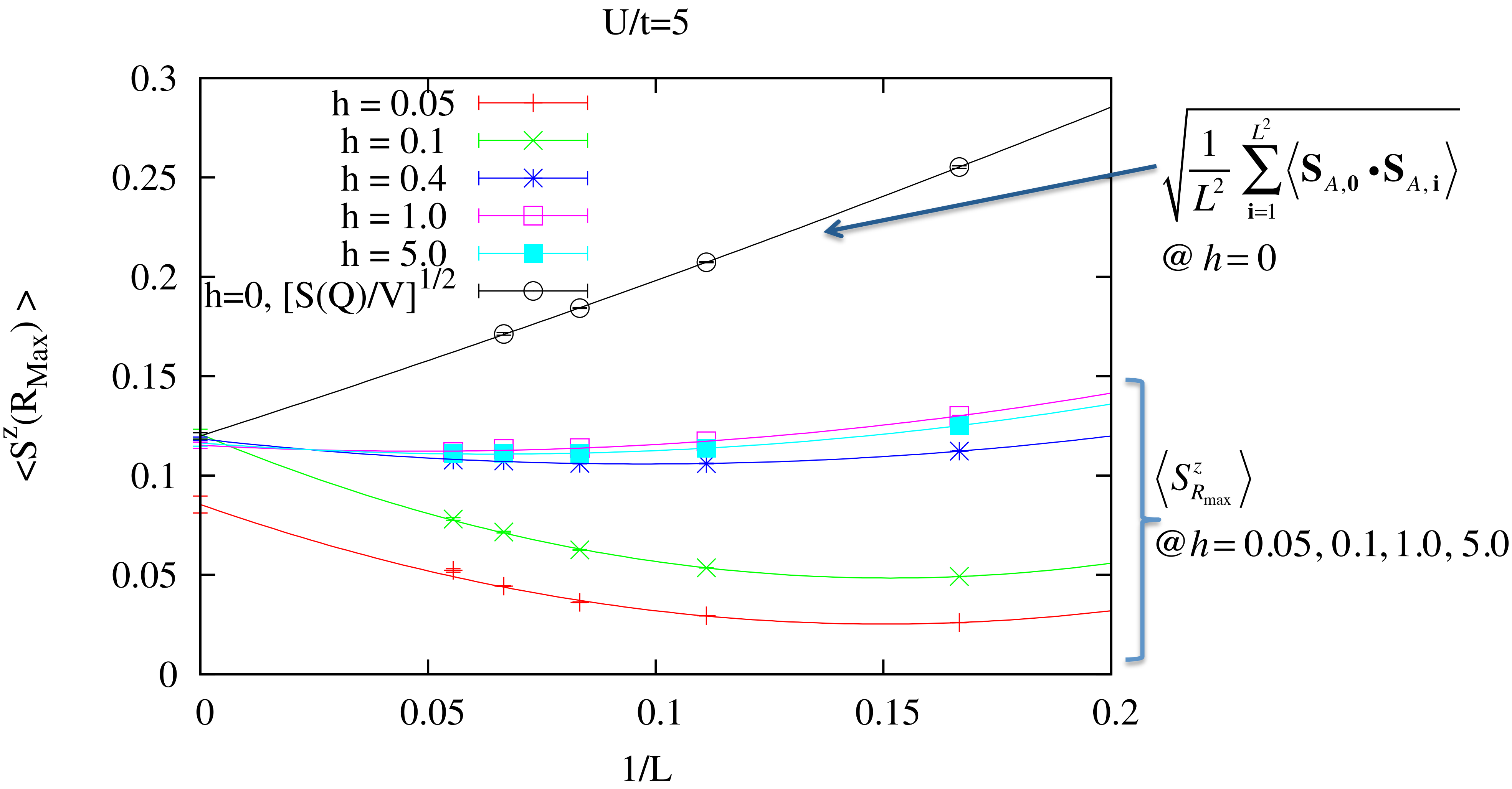
$$h(q) = 2h/L^2 \qquad S^z(q) = \sum_{\mathbf{i}} e^{i\,\mathbf{q}\cdot\mathbf{i}} S^z(\mathbf{i})$$

## The ordered case U/t=5.

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

$$m = \lim_{R\to\infty} \langle S^z(R) \rangle$$

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



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

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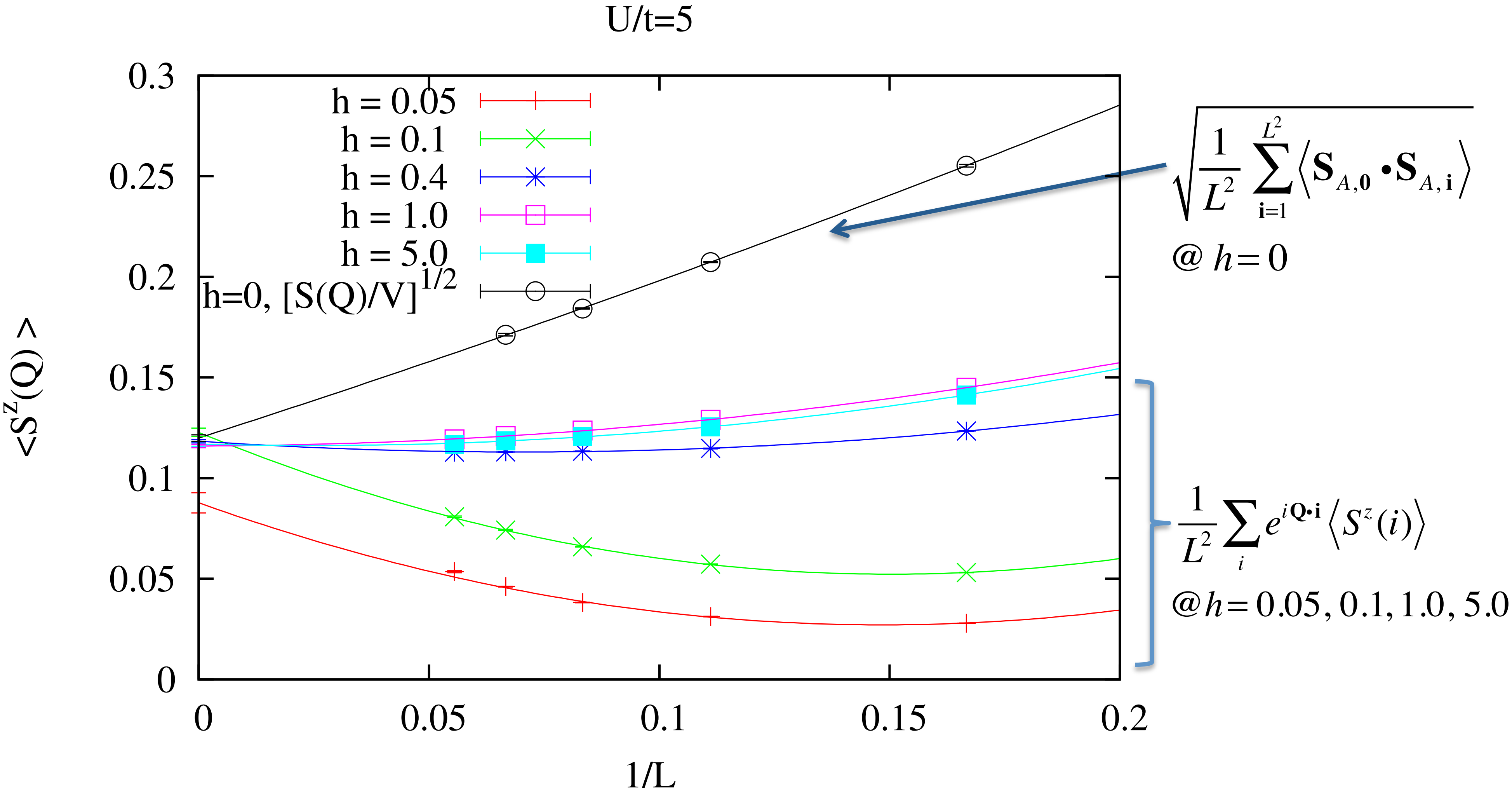
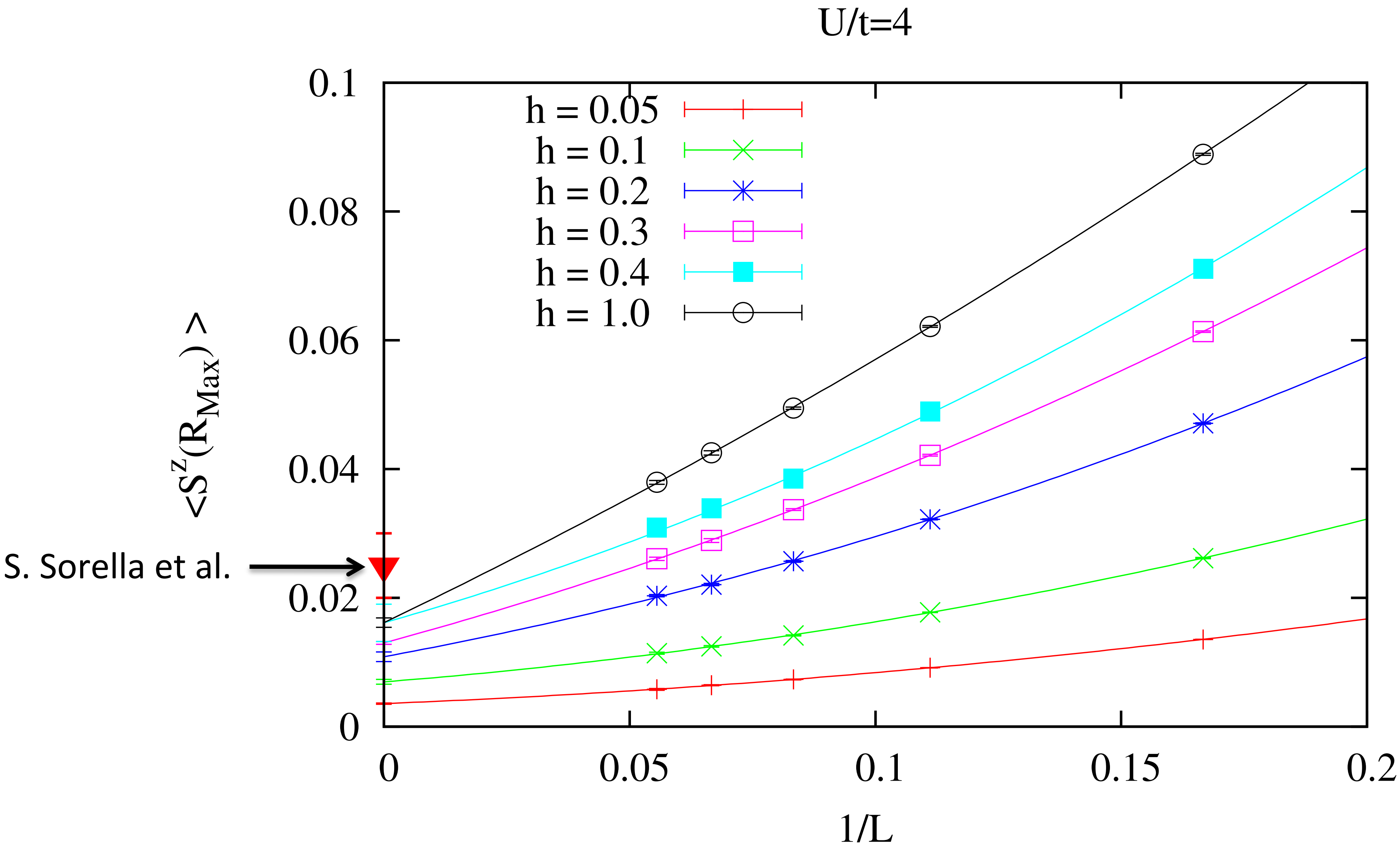
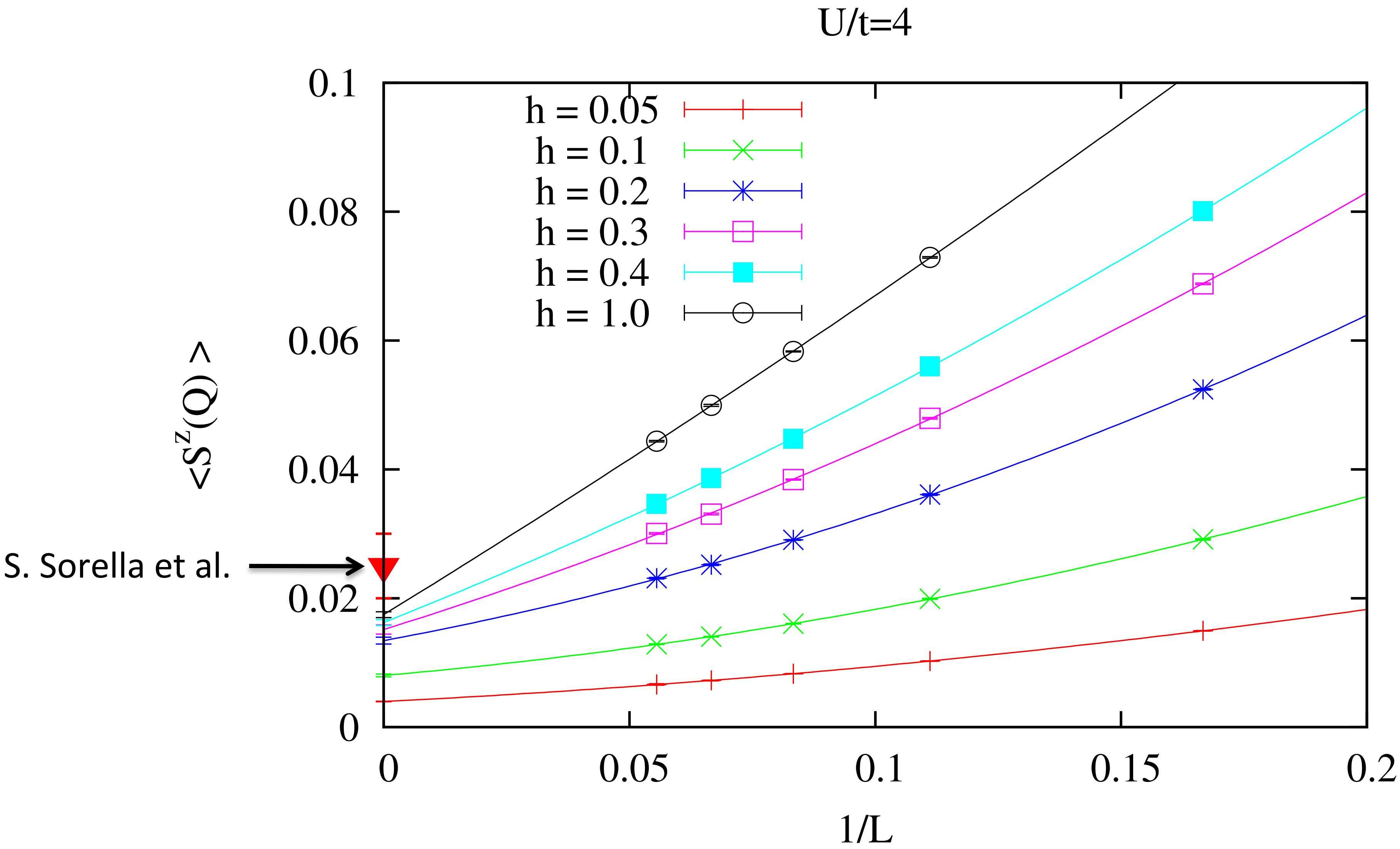


U/t=4.




Consider large values of h so as to minimize size effects?

U/t=4.

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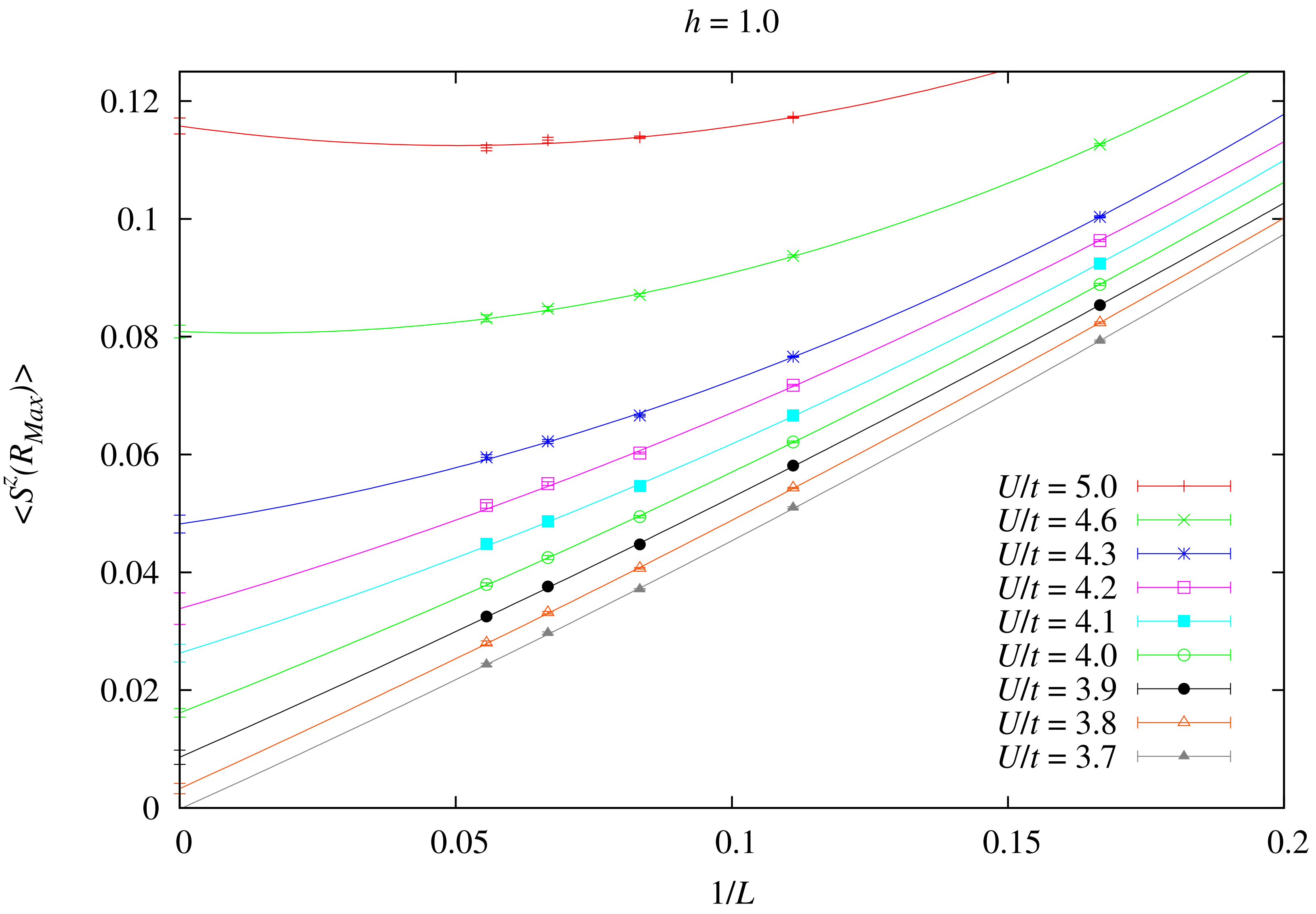
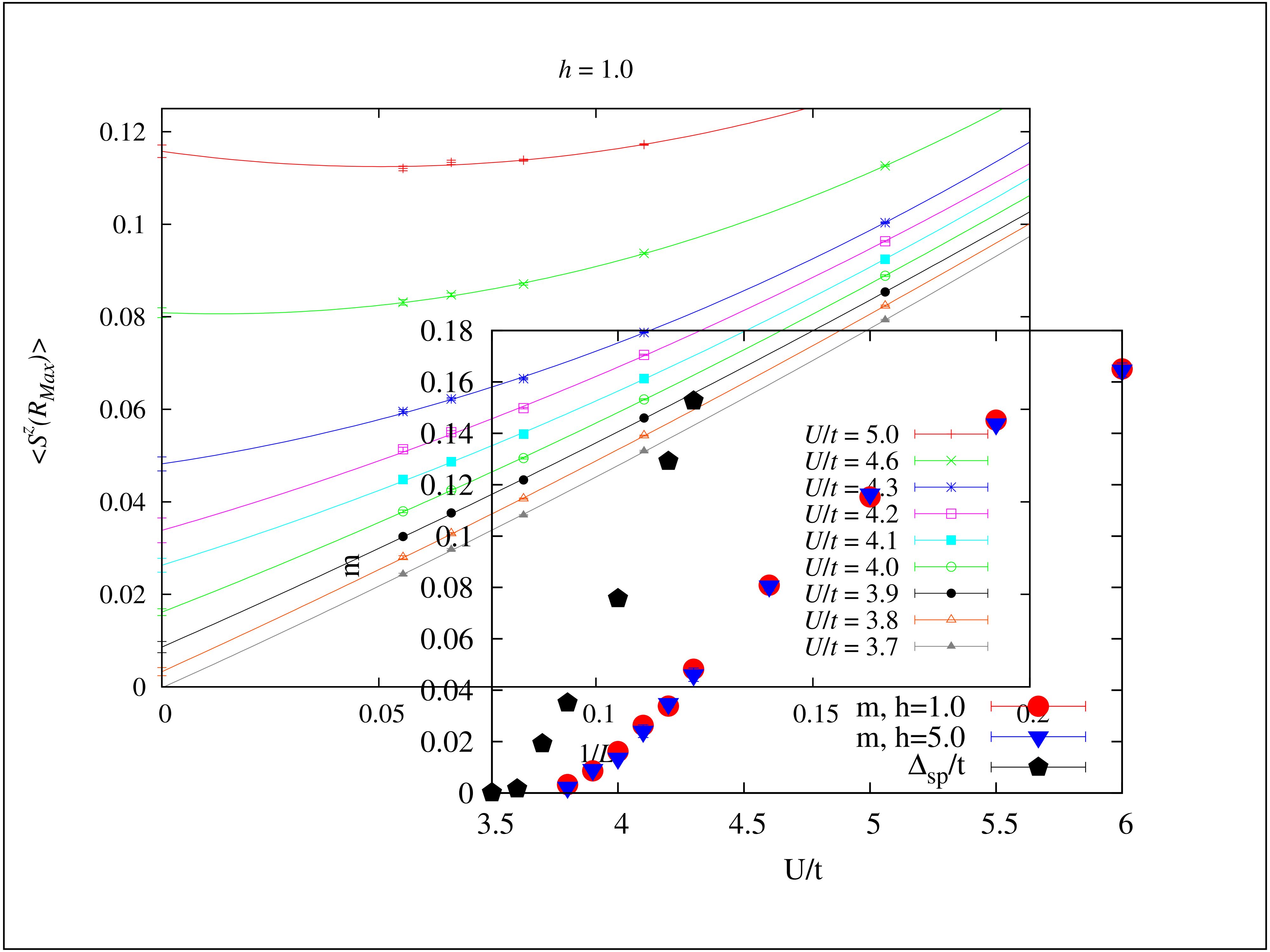
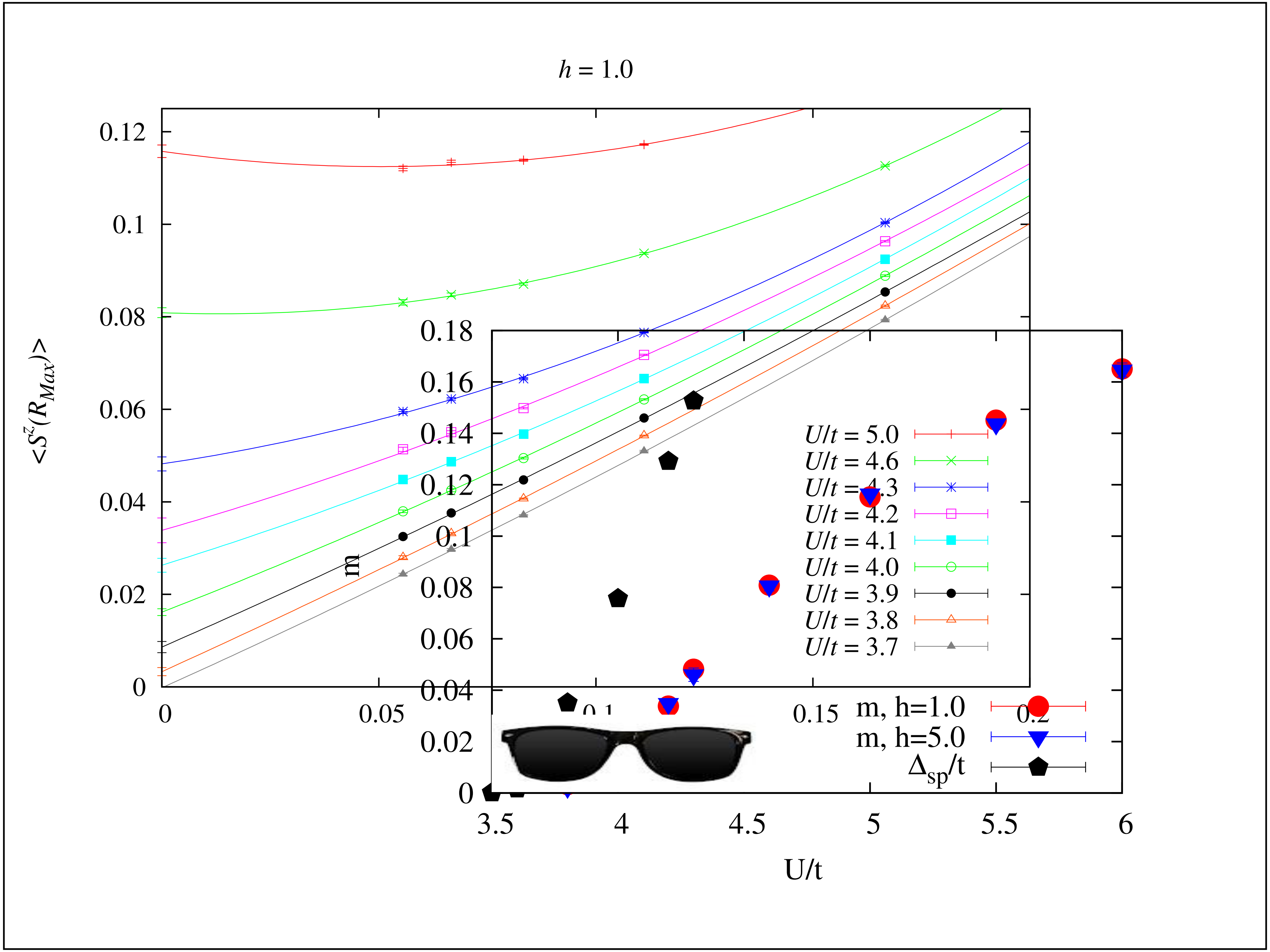


h = 1.0
<S^z(R_Max)>
1/L
0
0.02
0.04
0.06
0.08
0.1
0.12
0
0.05
0.1
0.15
0.2
U/t = 5.0
U/t = 4.6
U/t = 4.3
U/t = 4.2
U/t = 4.1
U/t = 4.0
U/t = 3.9
U/t = 3.8
U/t = 3.7



h = 1.0
<S^z(R_Max)>
1/L
U/t = 5.0
U/t = 4.6
U/t = 4.3
U/t = 4.2
U/t = 4.1
U/t = 4.0
U/t = 3.9
U/t = 3.8
U/t = 3.7
m
U/t
m, h=1.0
m, h=5.0
Δsp/t



h = 1.0
<S^z(R_Max)>
0.12
0.1
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U/t = 5.0
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U/t = 4.0
U/t = 3.9
U/t = 3.8
U/t = 3.7
m
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
3.5
4
4.5
5
5.5
6
U/t
m, h=1.0
m, h=5.0
Δsp/t

Open questions.

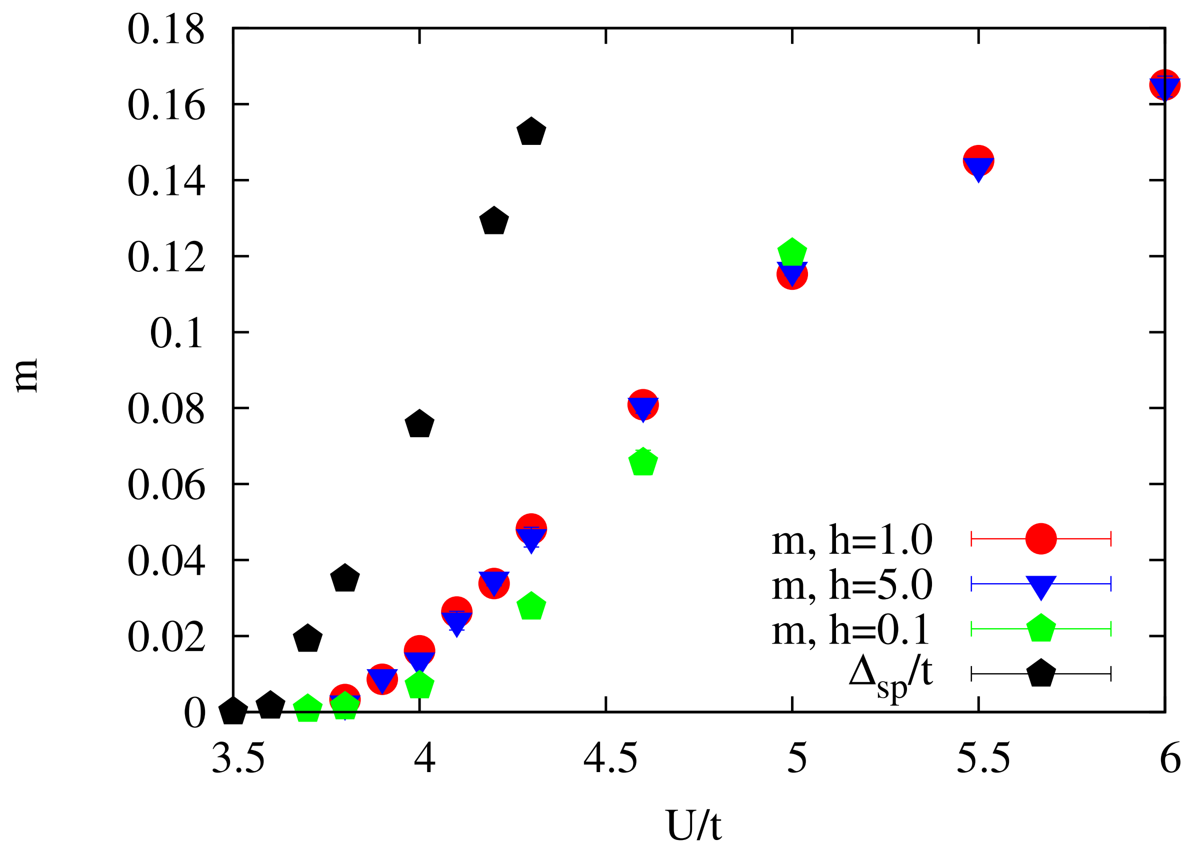
Magnetic field dependence ?

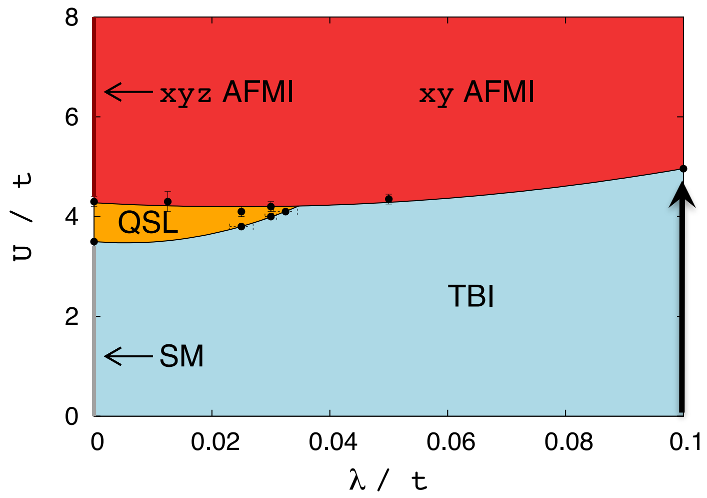
Pinning field on more than a single site ?

Other models? $\pi$-flux model.

→ Combine this method with large scale simulations.

Simple and very stable quantity to measure.






Quantum spin models from $\pi$-fluxes threaded

through correlated topological insulators.

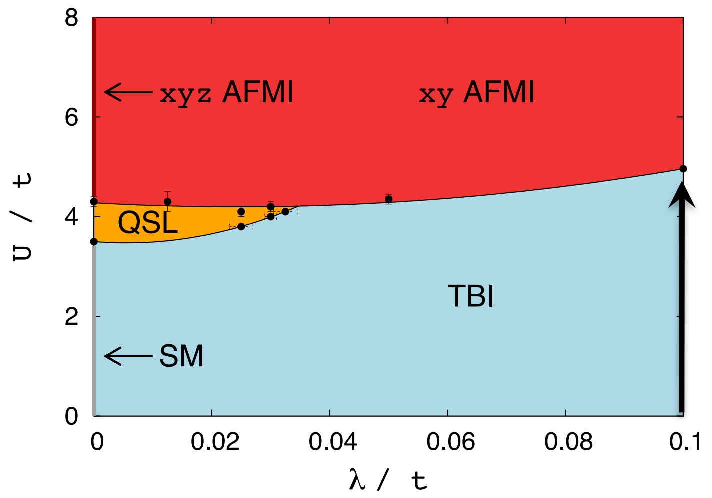
Motivation.

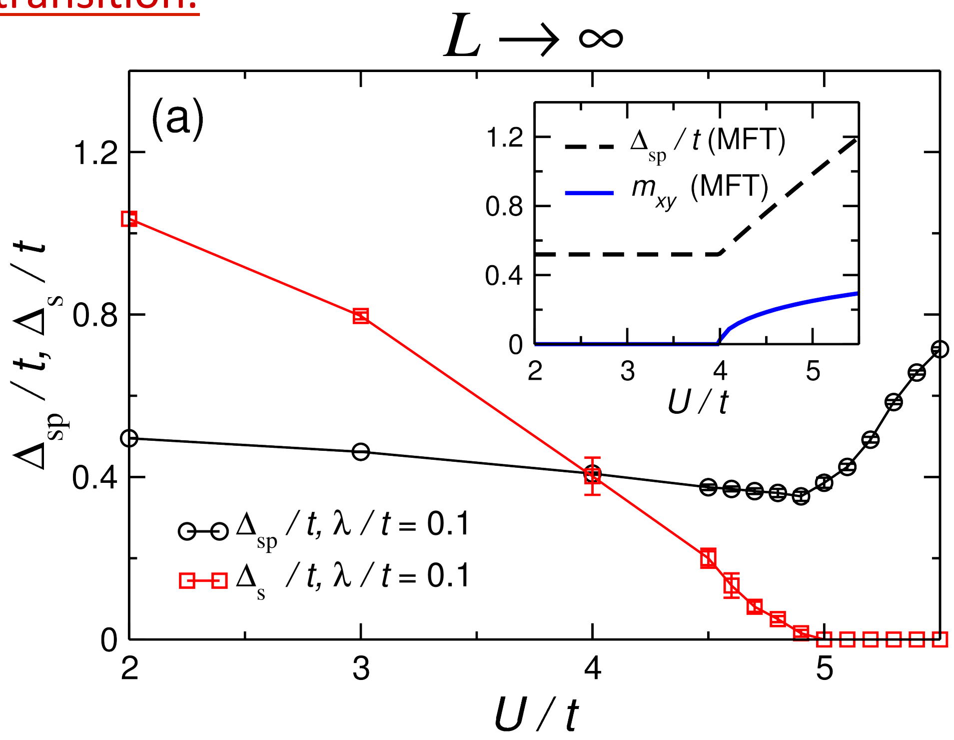
- Method to detect topological insulators in the presence of correlations.
- Toolbox for building quantum spin systems.



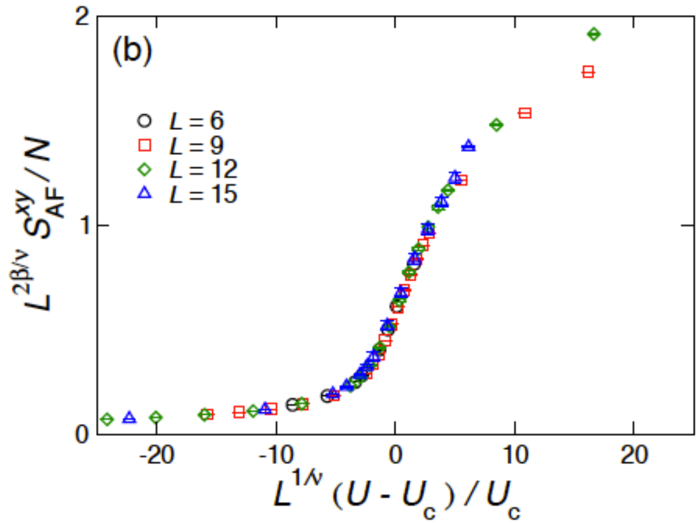
F. F. Assaad, M. Bercx and M. Hohenadler arXiv:1204.4728

# (2+1)D XY transition.



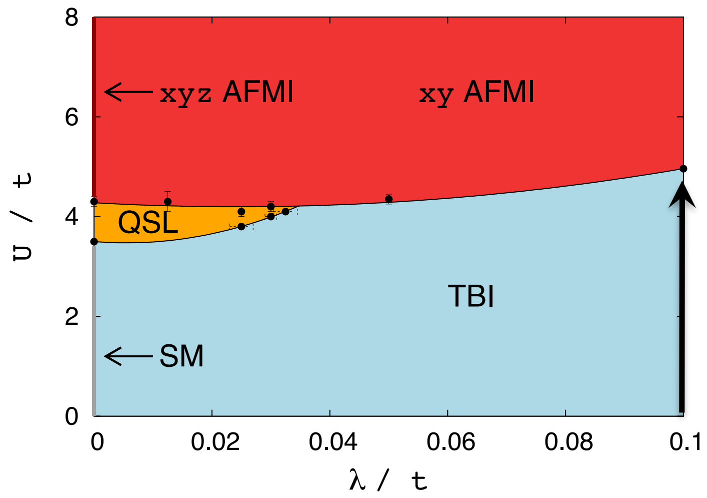



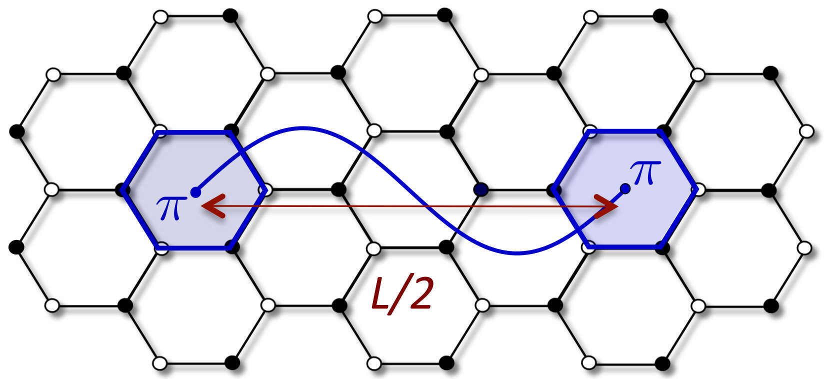

$$U_c = 4.96(4),\ z = 1,\ \nu = 0.6717(1),$$
$$\eta = 0.0381(2),\ \beta = 0.3486(1)$$




- $U > U_c$ Magnetic order in XY-plane. S. Rachel, K. Le Hur, PRB (2010).
- $U \to U_c$ spin excitations condense to from order in the ordered phase.
- No closing of the single particle gap.
- Criticality: orientation disordering of spin → 3D XY.

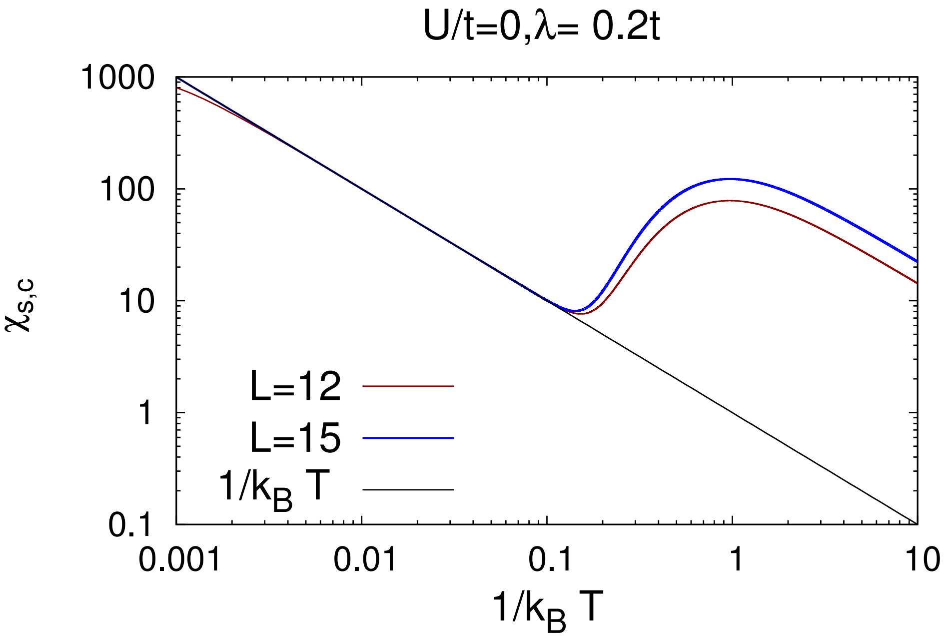
# Fluxes @ U/t=0.



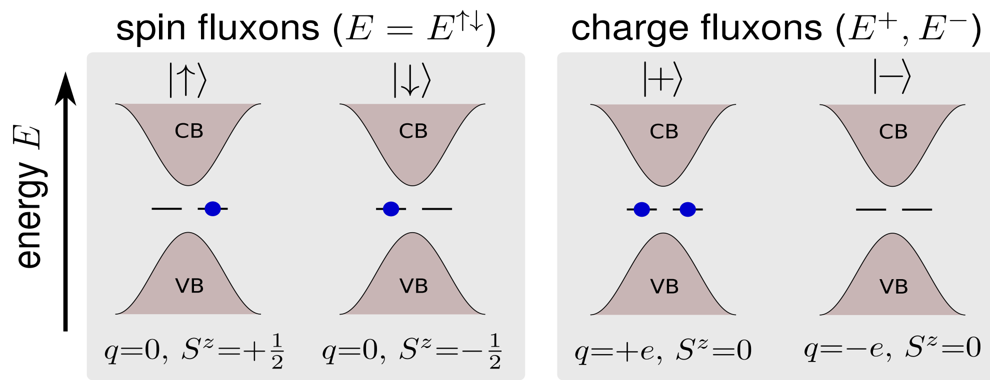




$$\chi_c = \beta\left(\left\langle \hat{N}^2 \right\rangle - \left\langle \hat{N} \right\rangle^2\right), \ \chi_s = \beta\left(\left\langle M_z^2 \right\rangle - \left\langle M_z \right\rangle^2\right)$$

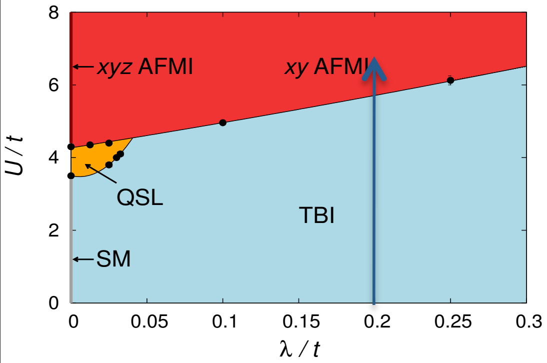
$$\chi_s \equiv \chi_c = \frac{1}{2k_B T}$$ Per $\pi$-flux




Four mid-gap states per $\pi$-flux.




Qi and Zhang , Phys. Rev. Lett. 101, 086802,(2008).
Ran, Vishwanat and Lee, Phys. Rev. Lett. 101 086801 (2008).

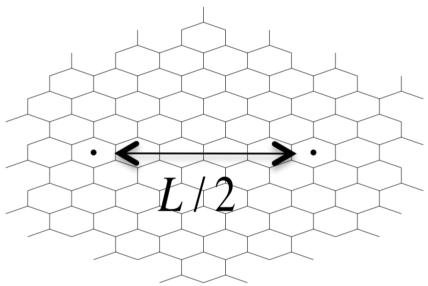


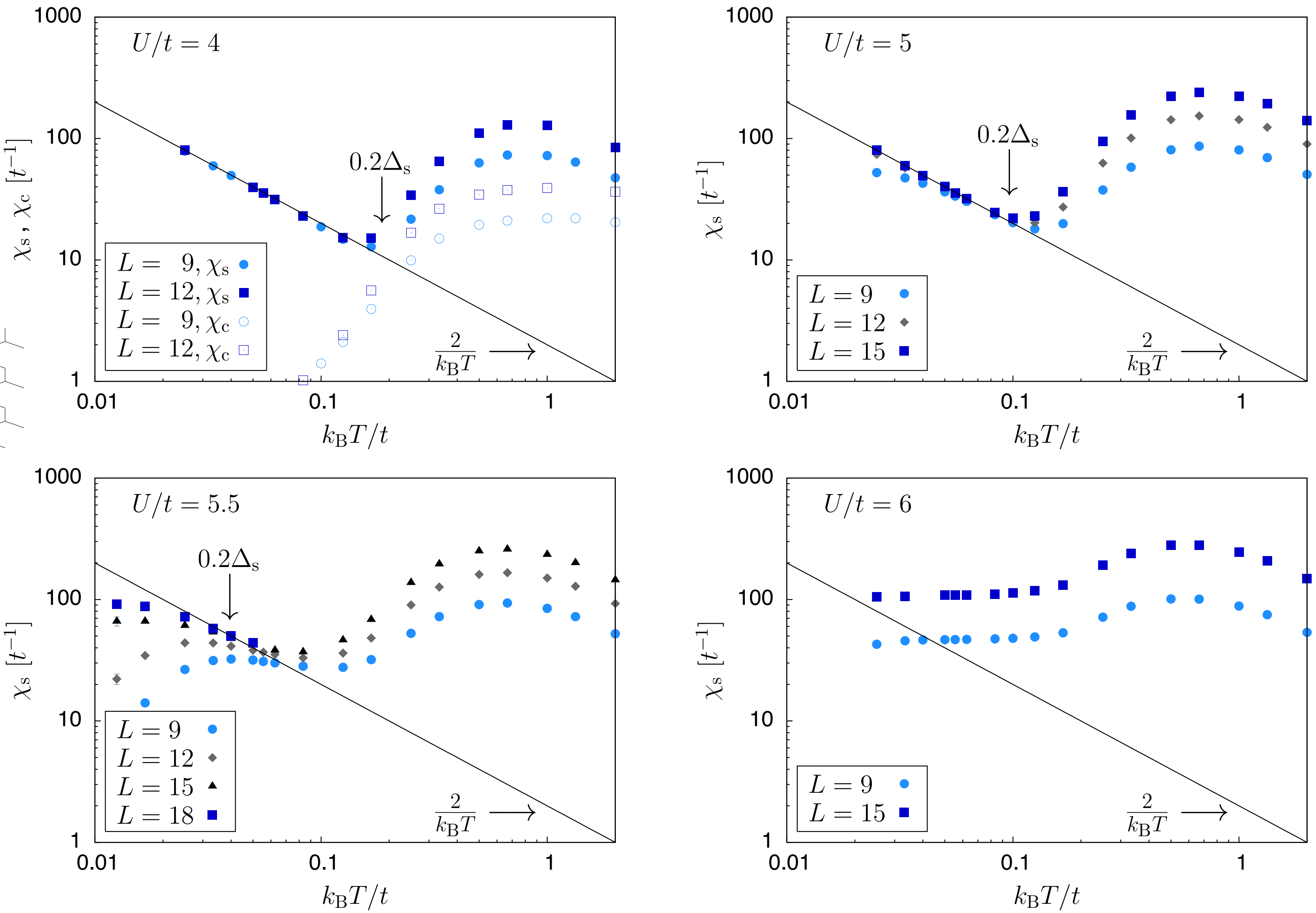

## Finite values of U/t.

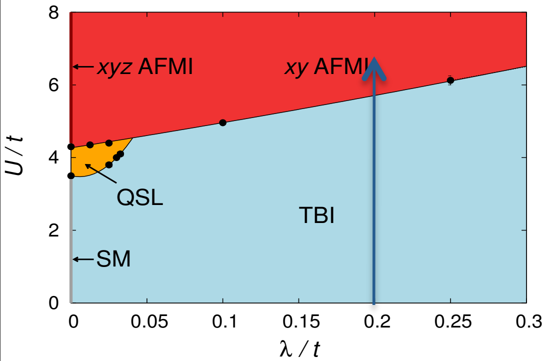
Charge is gapped out. $\chi_c = 0$

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

λ/t=0.2

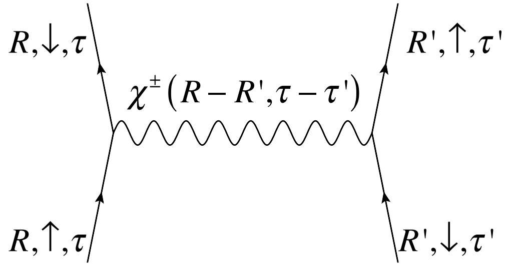




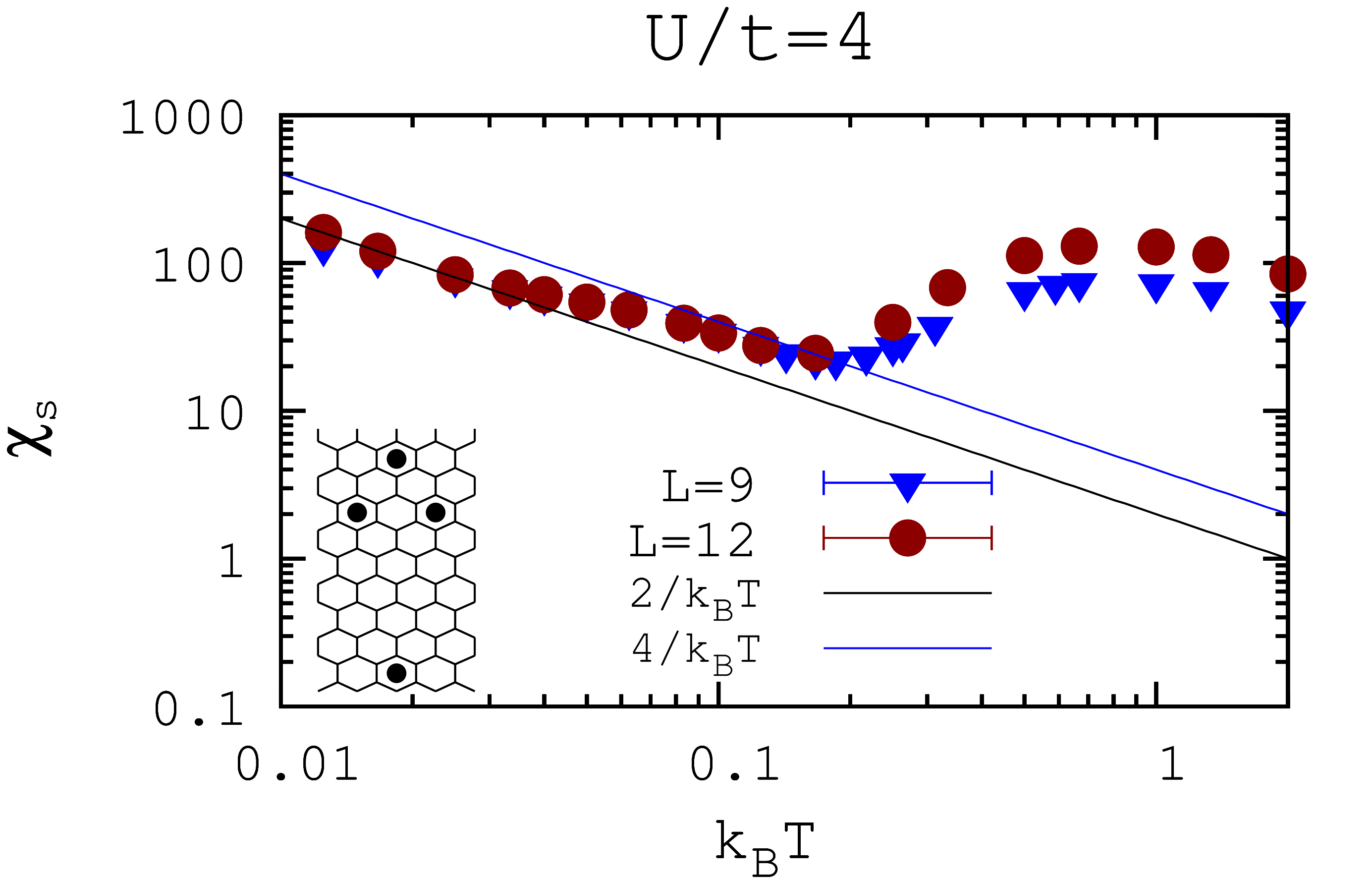

## Interaction between spin-fluxon:

Exchange of a transverse collective spin excitation.

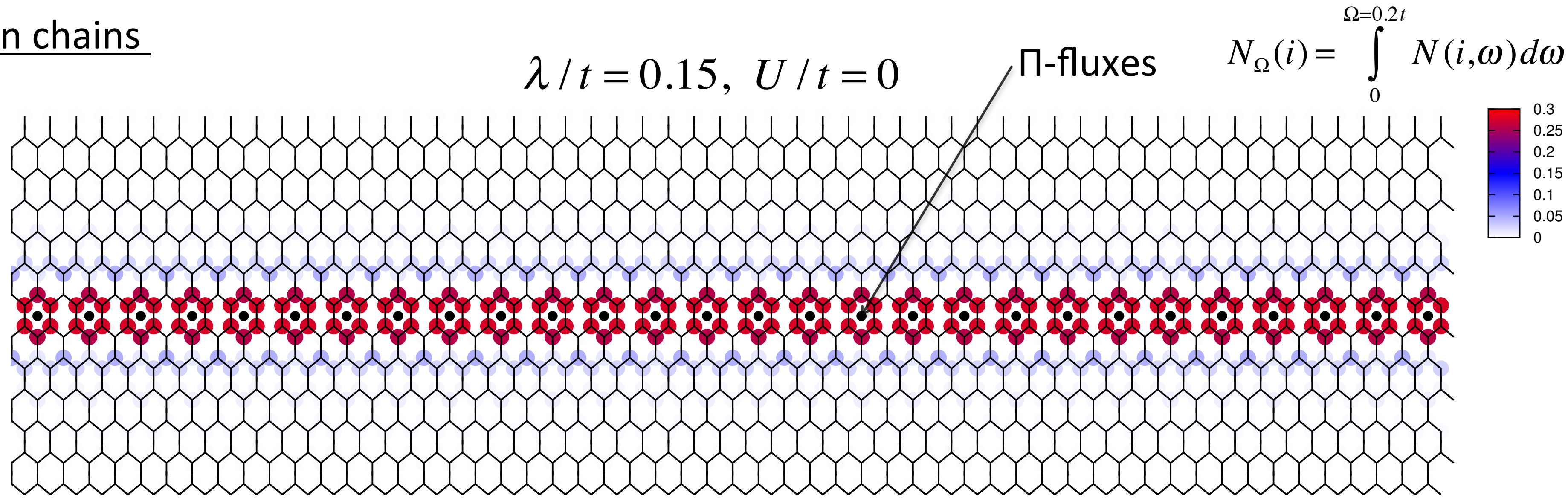



$$\chi^{\pm}(q,i\Omega_m) = \frac{1}{\omega(q)-i\Omega_m} + \frac{1}{\omega(q)+i\Omega_m}$$

$$\omega(q) = \sqrt{v^2\left[1-\cos(q-Q_0)\right]+\Delta_s^2}$$



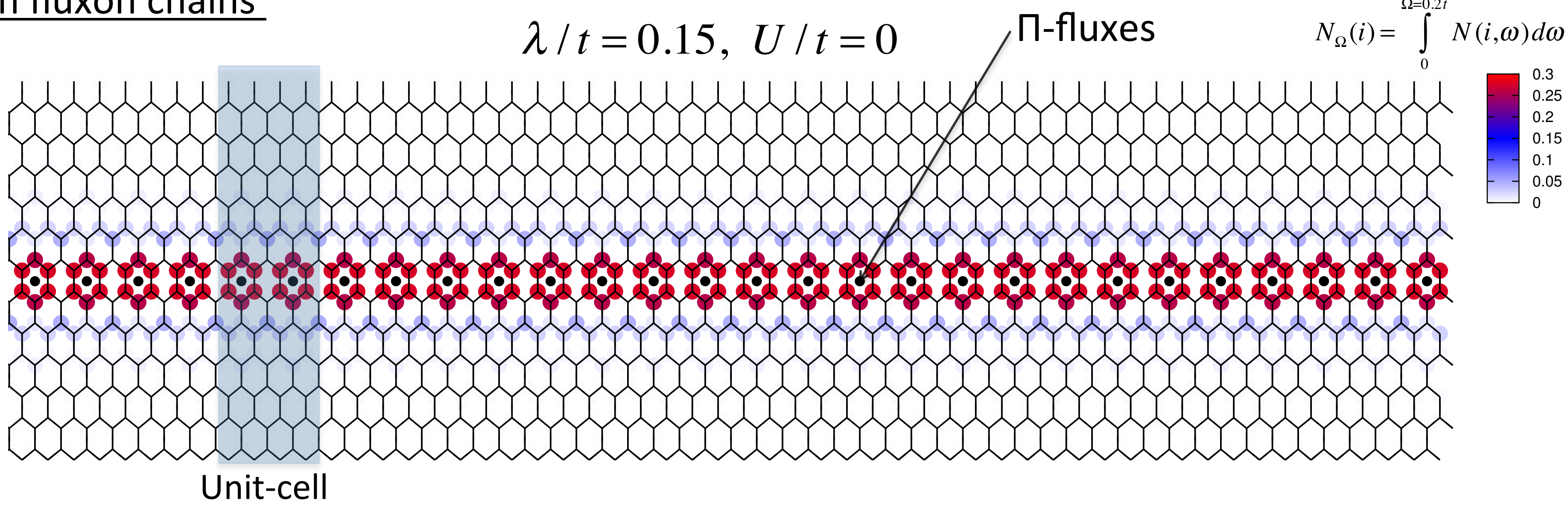
Spin chains

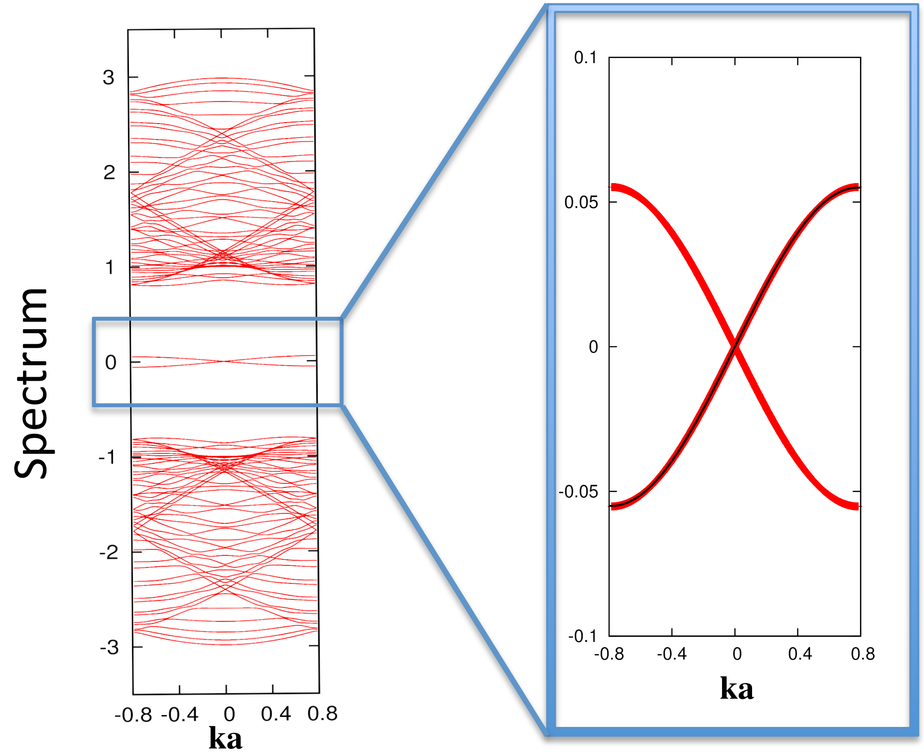

$\lambda / t = 0.15,\ U / t = 0$
Π-fluxes
$N_{\Omega}(i) = \int_{0}^{\Omega=0.2t} N(i,\omega)\,d\omega$
0.3
0.25
0.2
0.15
0.1
0.05
0

## Spin fluxon chains

$$\lambda / t = 0.15,\ \ U / t = 0$$

$$N_{\Omega}(i) = \int_{0}^{\Omega=0.2t} N(i,\omega)\, d\omega$$

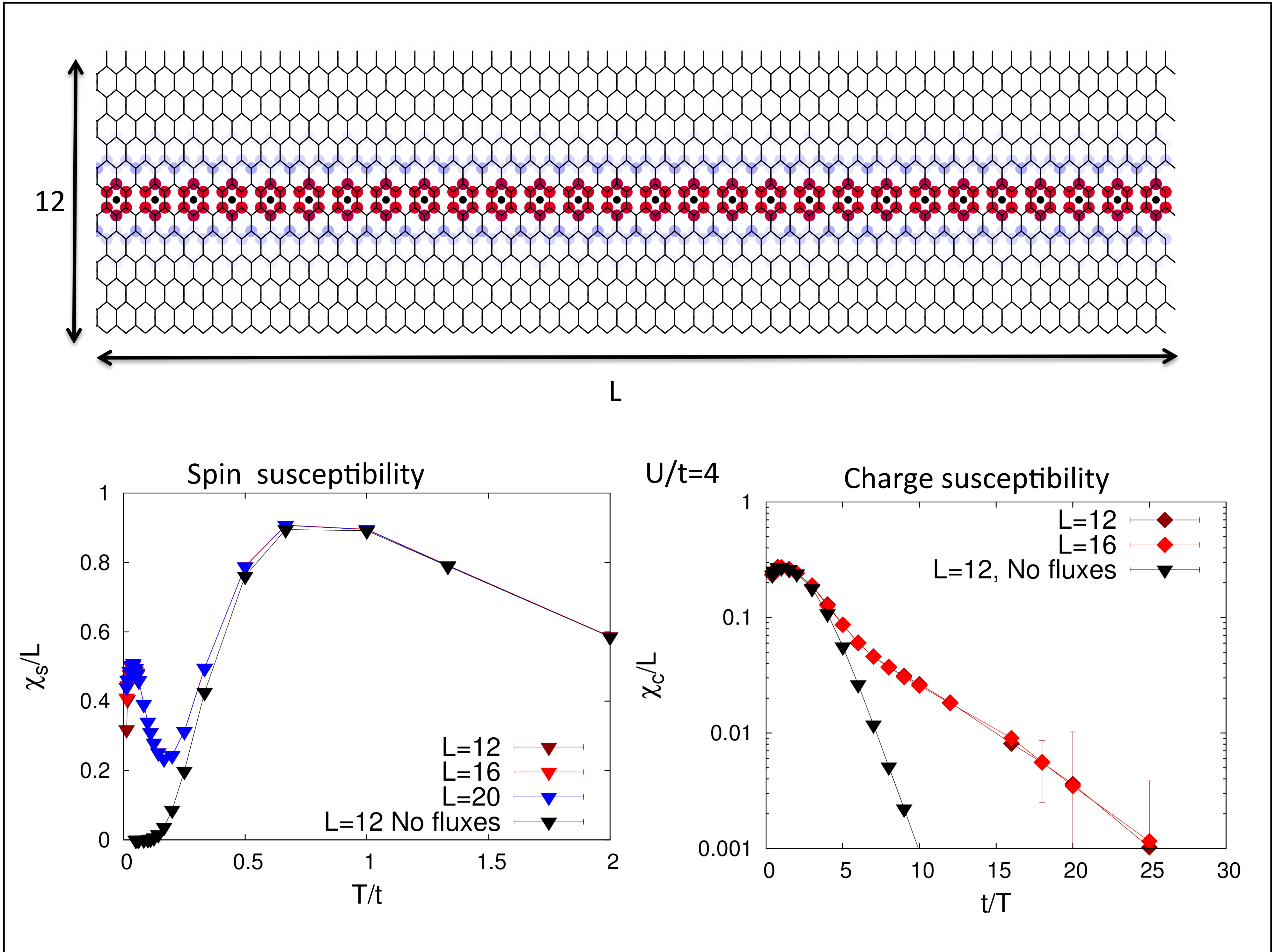



$$\varepsilon(k) = \pm 2t \left|\sin(2\mathbf{ka})\right|$$

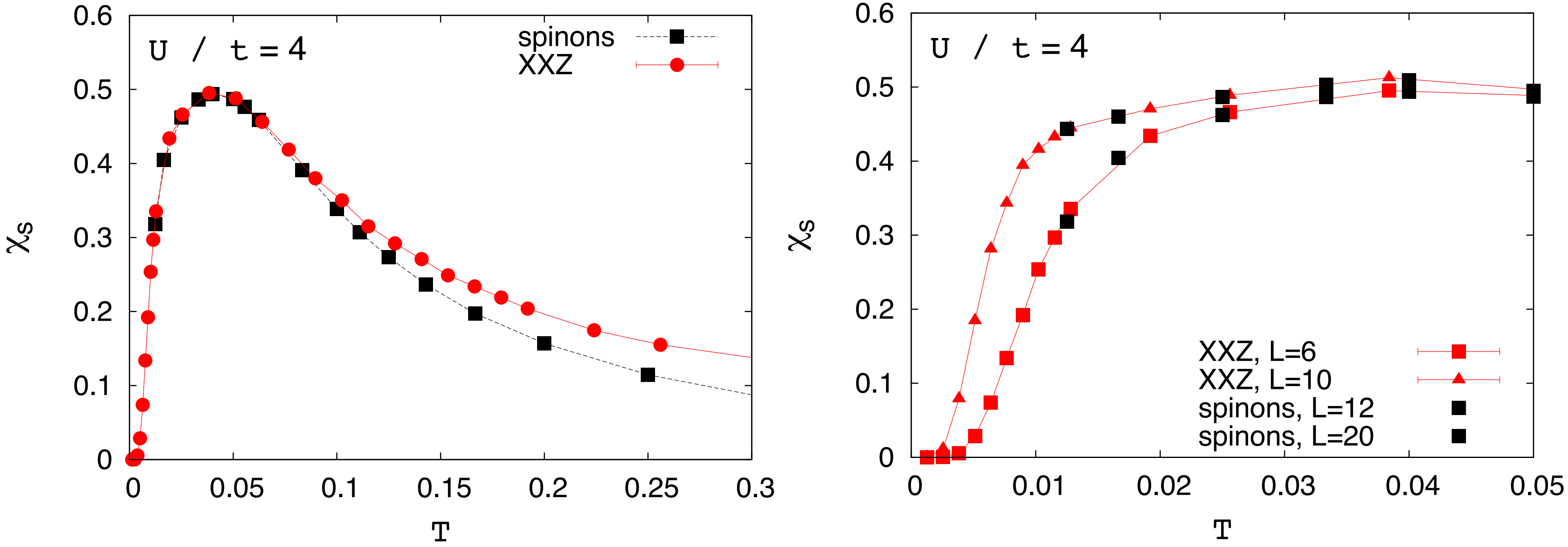
$$H = -t \sum_{\mathbf{R},\sigma} \left[ a^{\dagger}_{\mathbf{R},\sigma} b_{\mathbf{R},\sigma} - b^{\dagger}_{\mathbf{R},\sigma} a_{\mathbf{R}+4\mathbf{a},\sigma} + h.c. \right].$$

Finite values of U/t → C0S1



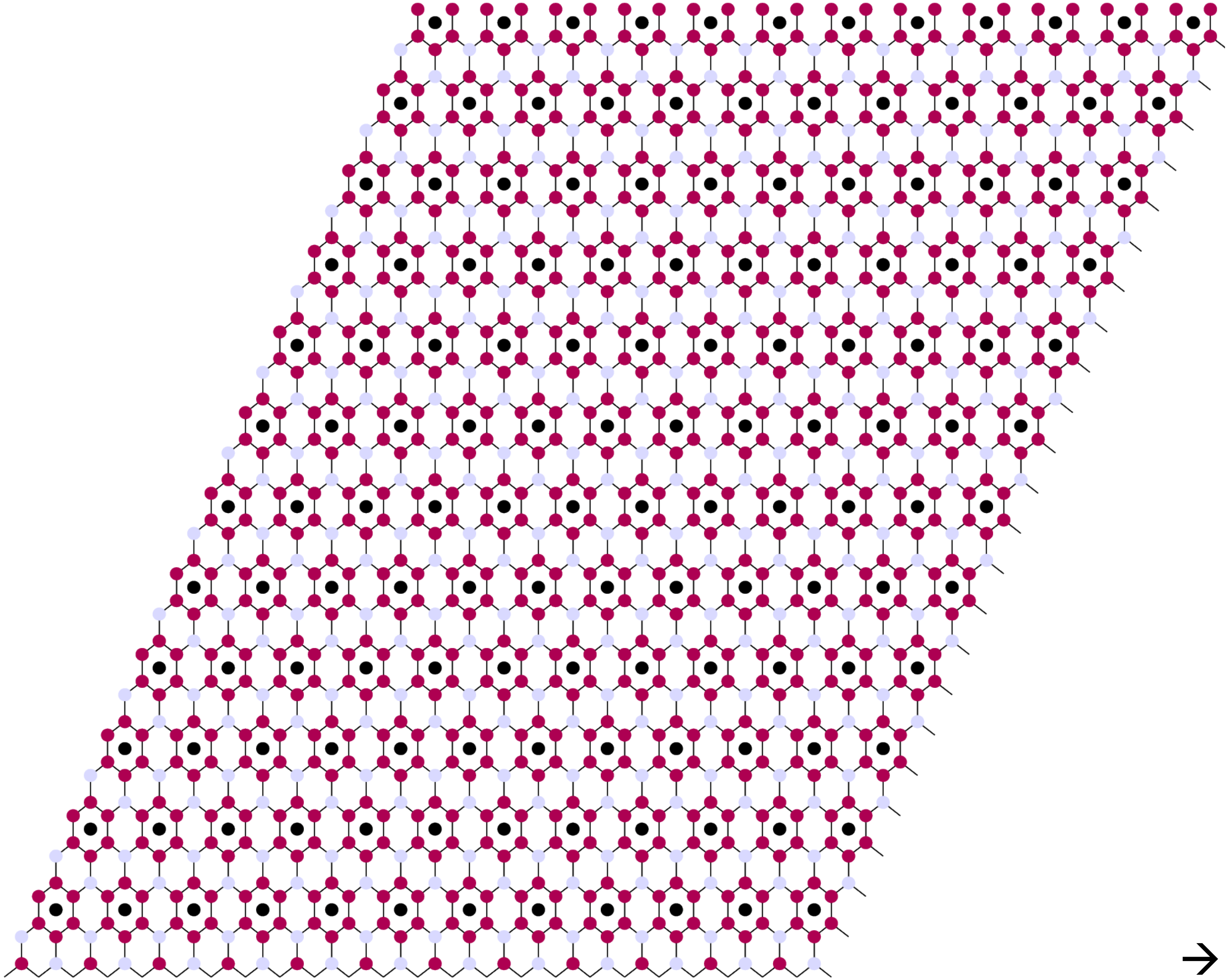
12
L
Spin susceptibility
U/t=4
Charge susceptibility
$\chi_s/L$
T/t
L=12
L=16
L=20
L=12 No fluxes
0
0.2
0.4
0.6
0.8
1
0.5
1.5
2
$\chi_c/L$
t/T
L=12
L=16
L=12, No fluxes
0.001
0.01
0.1
5
10
15
20
25
30

Spin-susceptibility of the spin-fluxon chain.




Fit: XXZ model. $J_{zz} / J_{xx} = 0.1$, $J_{zz} < 0$

Triangular lattice of fluxons….

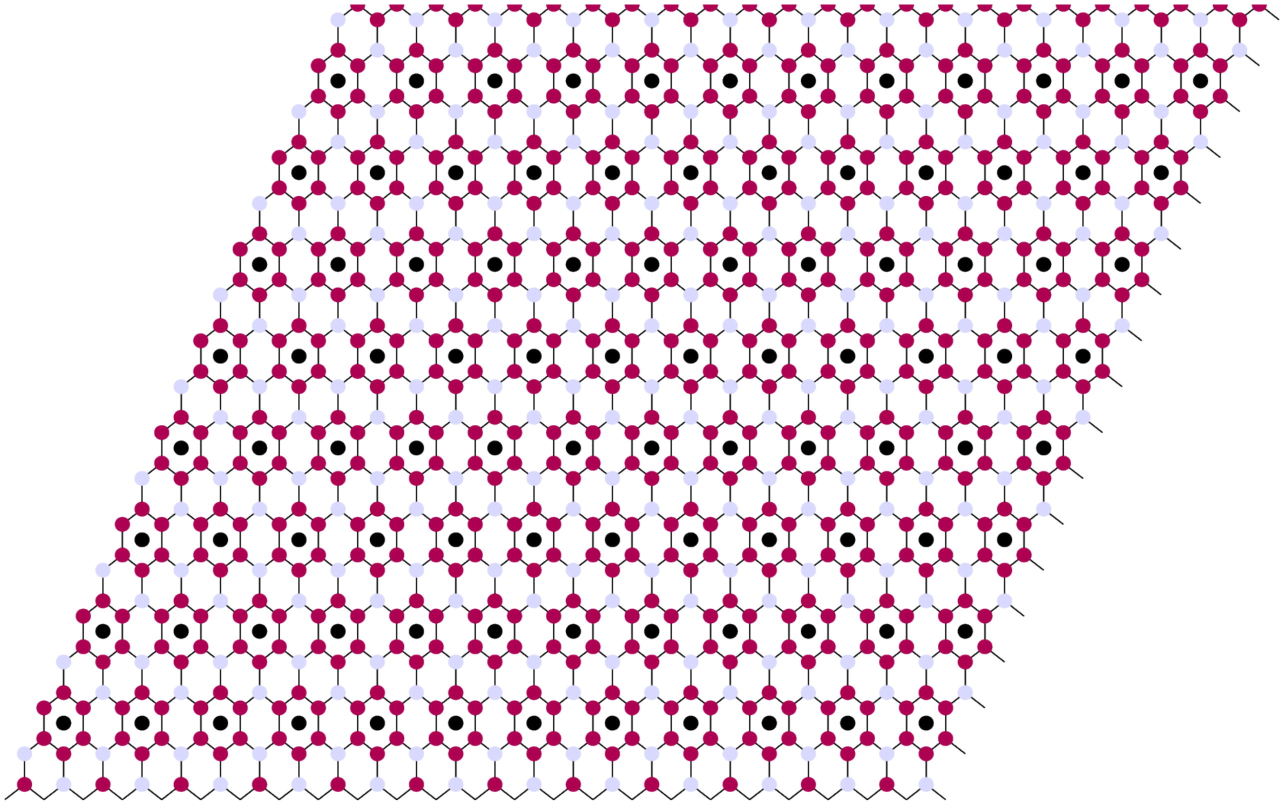


→

Conclusions:

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

The offer the vision  of engineering non-trivial quantum spin system.



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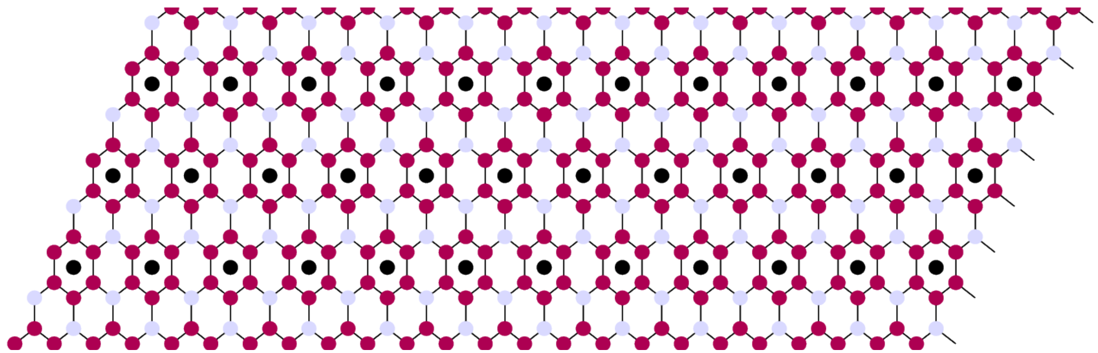

Pinning fields.

Allows determination of  magnetic order with unprecedented accuracy.