Correlated fermions on the honeycomb lattice

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Honeycomb-lattice
Interactions and fluctuations

Fluctuations in a honeycomb lattice

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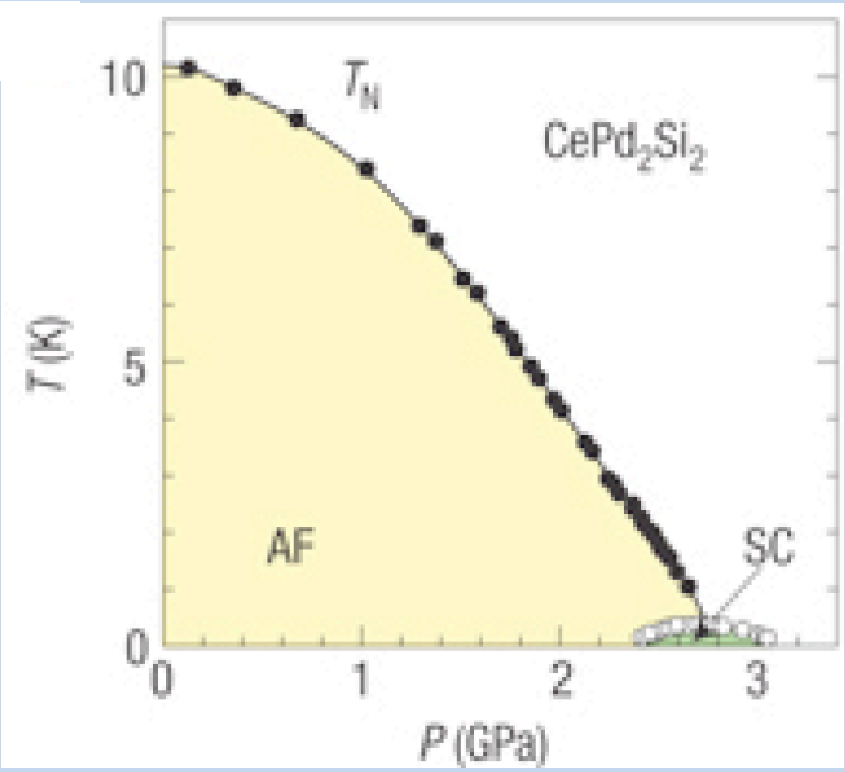

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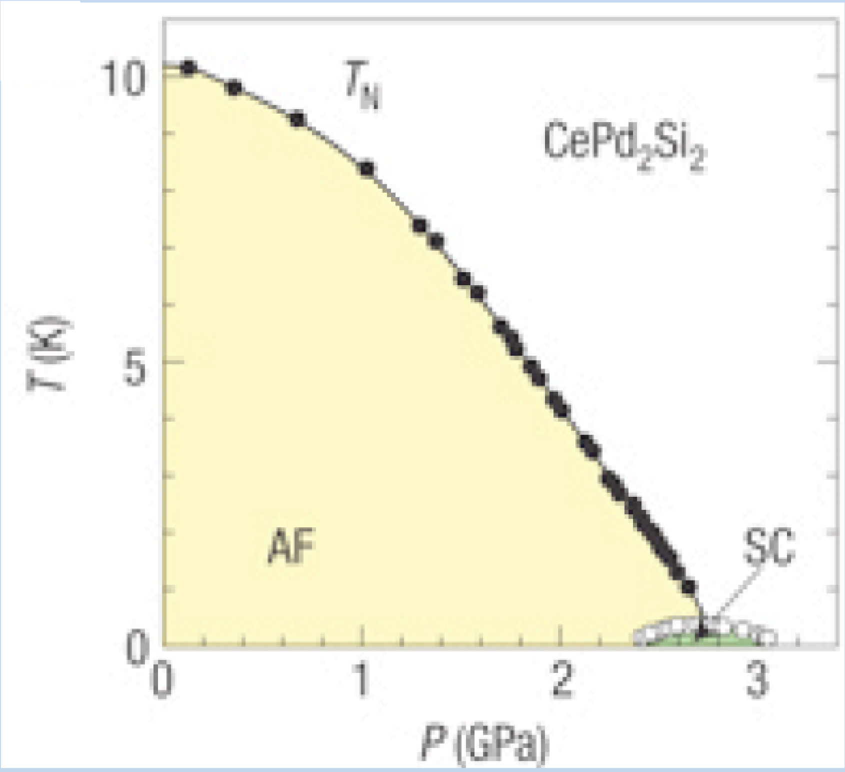
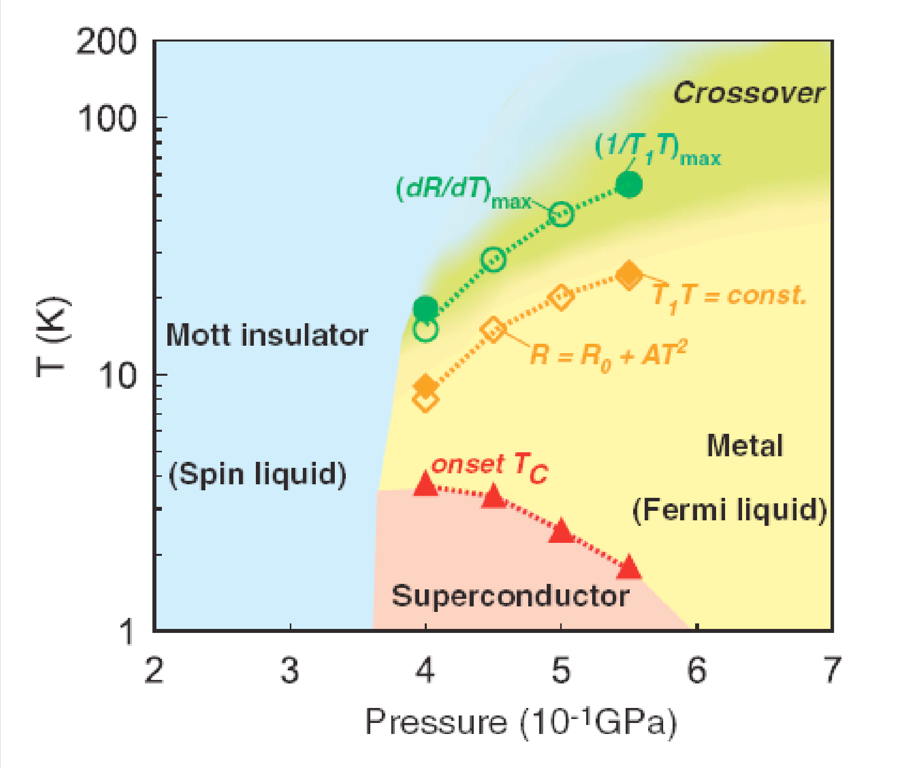


Organic superconductors



Quantum Monte Carlo simulations for the Hubbard model on the honeycomb lattice

Determinantal algorithm for T = 0

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$|\Psi_G\rangle$ **ground-state of** H

$|\Psi_T\rangle$ **trial wavefunction with** $\langle\Psi_G|\Psi_T\rangle \neq 0$

Expectation value of a physical observable in the ground-state

$$\langle\Psi_G|\hat{\mathcal{O}}|\Psi_G\rangle = \lim_{\Theta\to\infty} \frac{\langle\Psi_T|\mathrm{e}^{-\Theta H/2}\,\hat{\mathcal{O}}\,\mathrm{e}^{-\Theta H/2}|\Psi_T\rangle}{\langle\Psi_T|\mathrm{e}^{-\Theta H}|\Psi_T\rangle}$$

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In our case, choose $|\Psi_T\rangle = |\Psi_T\rangle_\uparrow \otimes |\Psi_T\rangle_\downarrow$

$|\Psi_T\rangle_\alpha$ **ground-state of the free case**

- **SU(2) invariant algorithm**

  F.F. Assaad., Phys. Rev. B **71**, 075103 (2005)

- **Particle-hole symmetry at half-filling**

  ➡ **free of sign problem**

- **Convergence to the ground-state with** $\Theta = 40/t$

- **Systematic error below statistical fluctuations with** $\Delta\tau = 0.05/t$

- **Finite-size extrapolations to the thermodynamic limit with**

  $N = L \times L \times 2 \;, L = 3, 9, 12, 15, 18 \longrightarrow \sim 4^{648}$

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- **Metastability for large systems (local updates)**

  $N = L \times L \times 2 \;, L = 36$

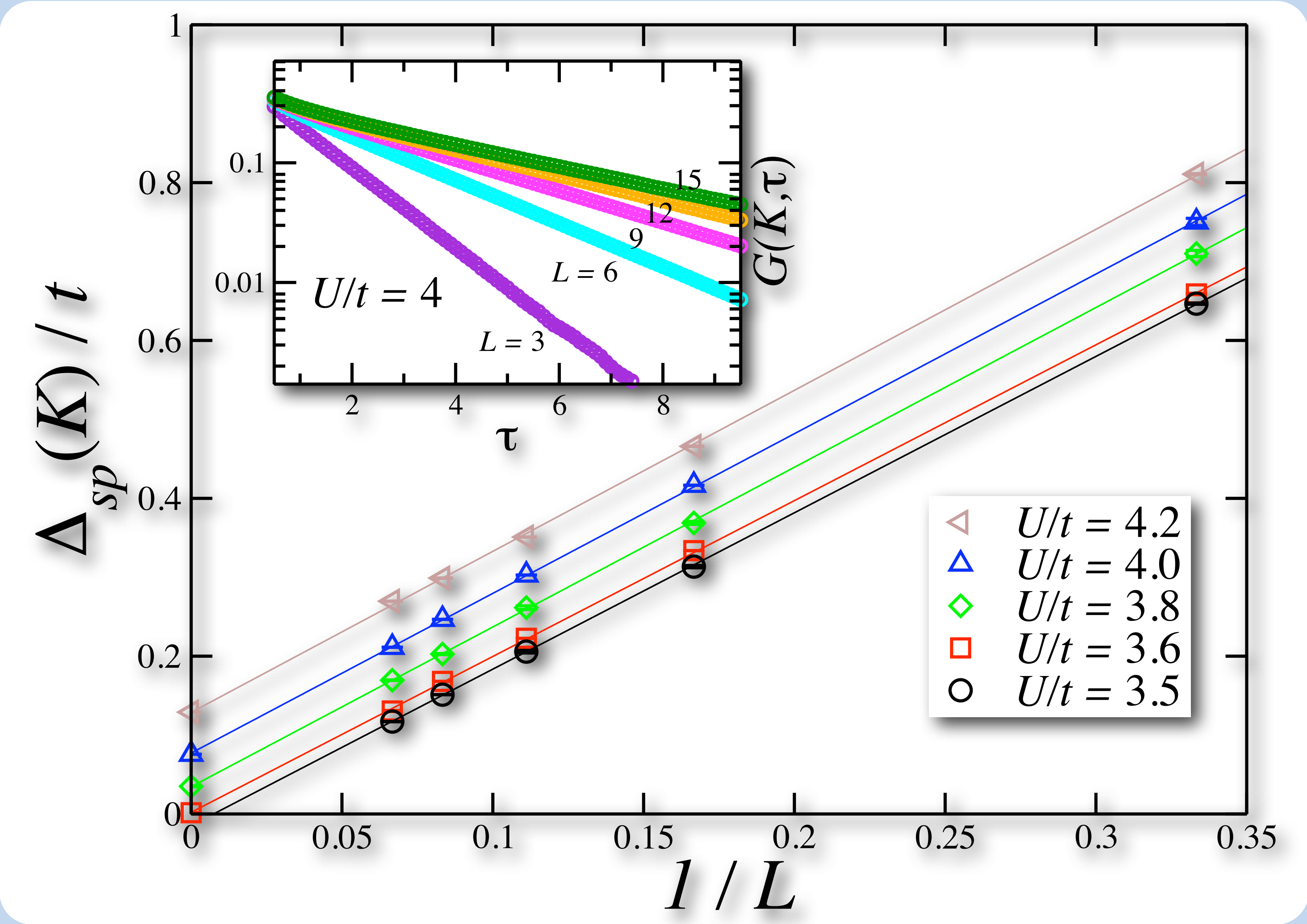
Hubbard model on the honeycomb lattice

Z.Y. Meng, T. Lang, S. Wessel, F.F. Assaad, A. M., Nature 464, 847 (2010)

Single particle excitations

One-particle propagator in imaginary time

$$G(\vec{k},\tau) = \sum_{\lambda\sigma} \langle T c_{\vec{k},\lambda,\sigma}(\tau) c^{\dagger}_{\vec{k},\lambda,\sigma}(0) \rangle = \sum_{\lambda\sigma} \langle T e^{\tau H} c_{\vec{k},\lambda,\sigma} e^{-\tau H} c^{\dagger}_{\vec{k},\lambda,\sigma} \rangle$$



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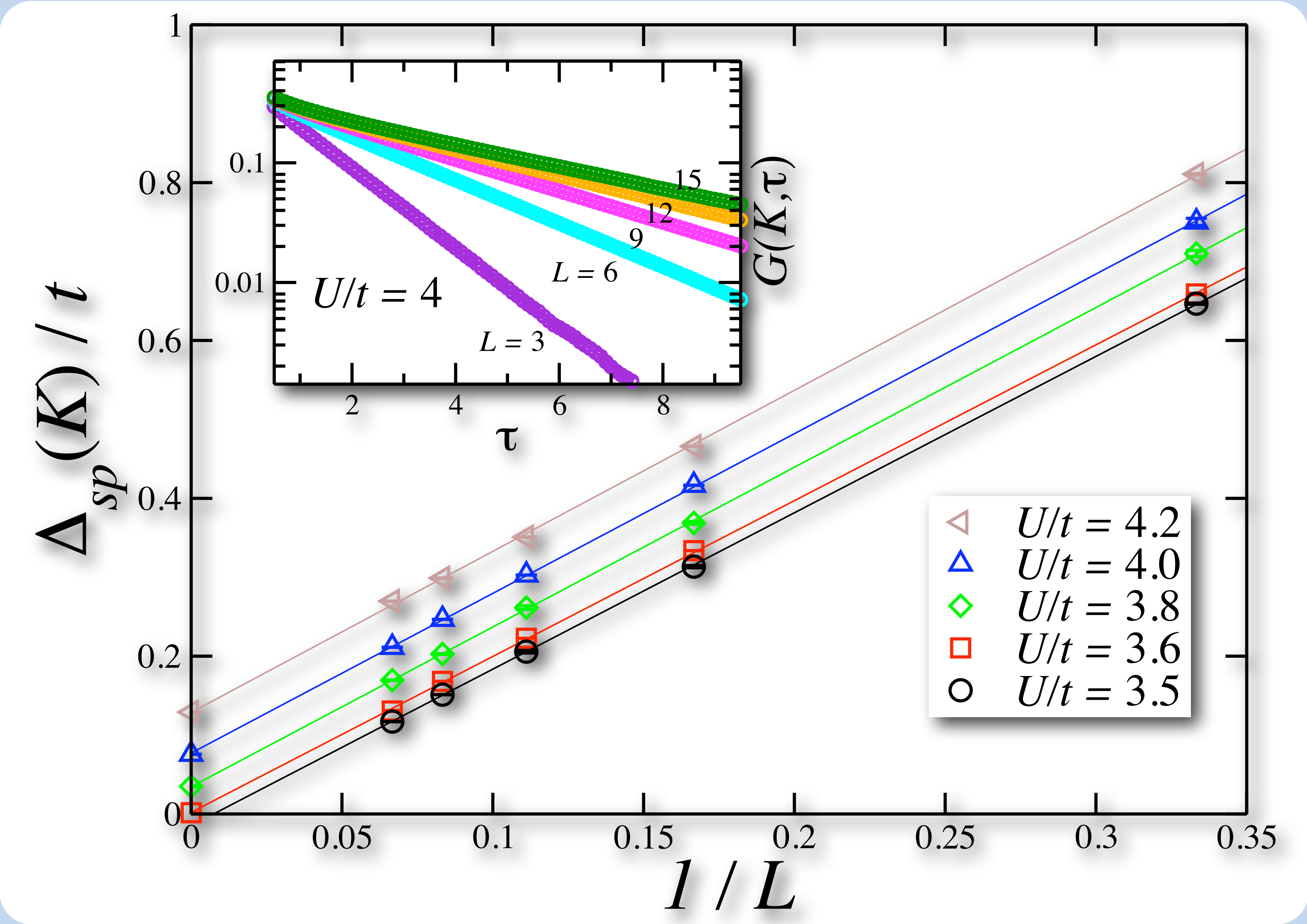

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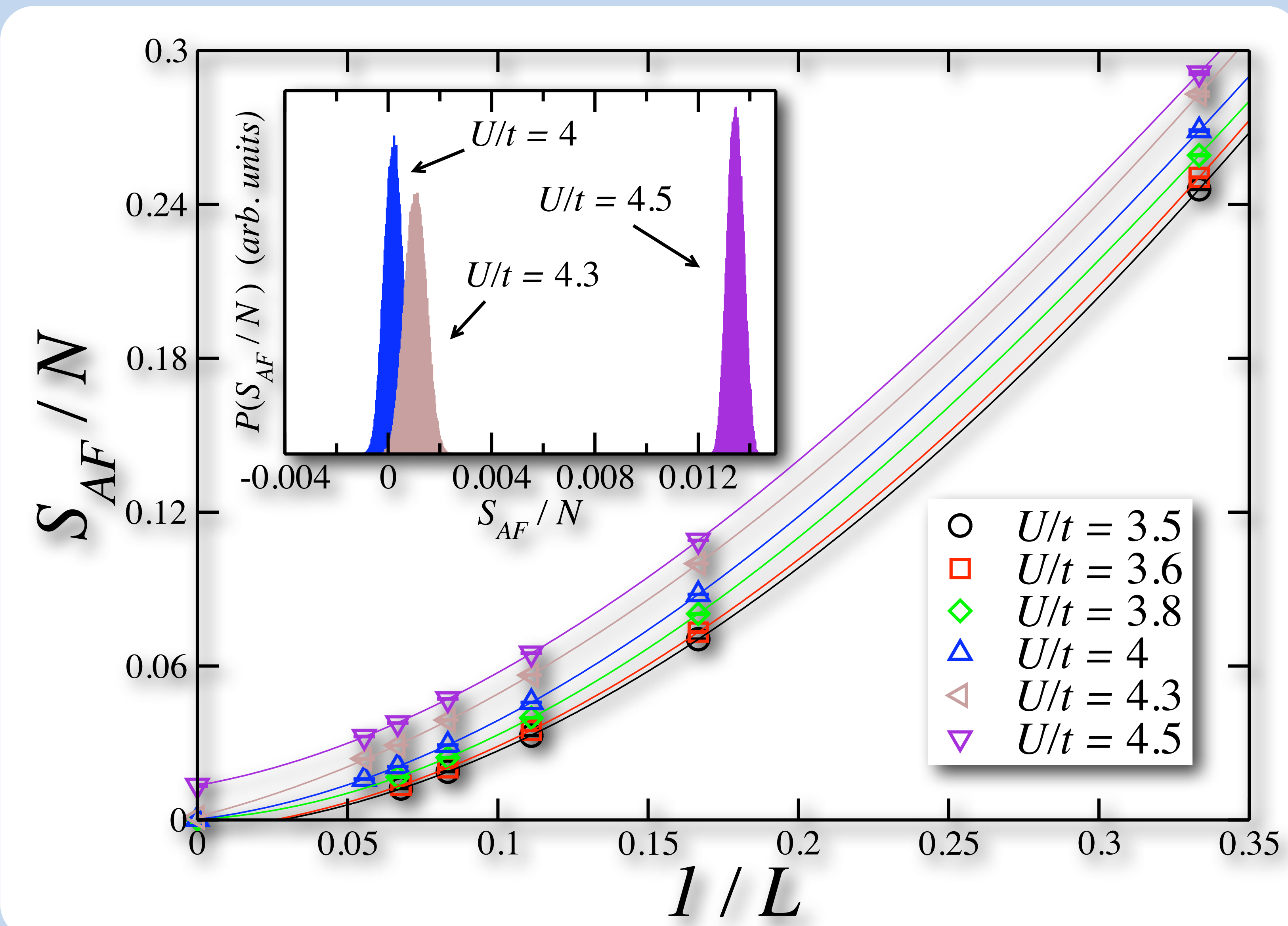
- **Metal-insulator transition**

Antiferromagnetism

Antiferromagnetic structure factor

$$S_{AF} = \frac{1}{N} \left\langle \left[\sum_{\vec{x}} \left(\vec{S}_{\vec{x}A} - \vec{S}_{\vec{x}B} \right) \right]^2 \right\rangle$$



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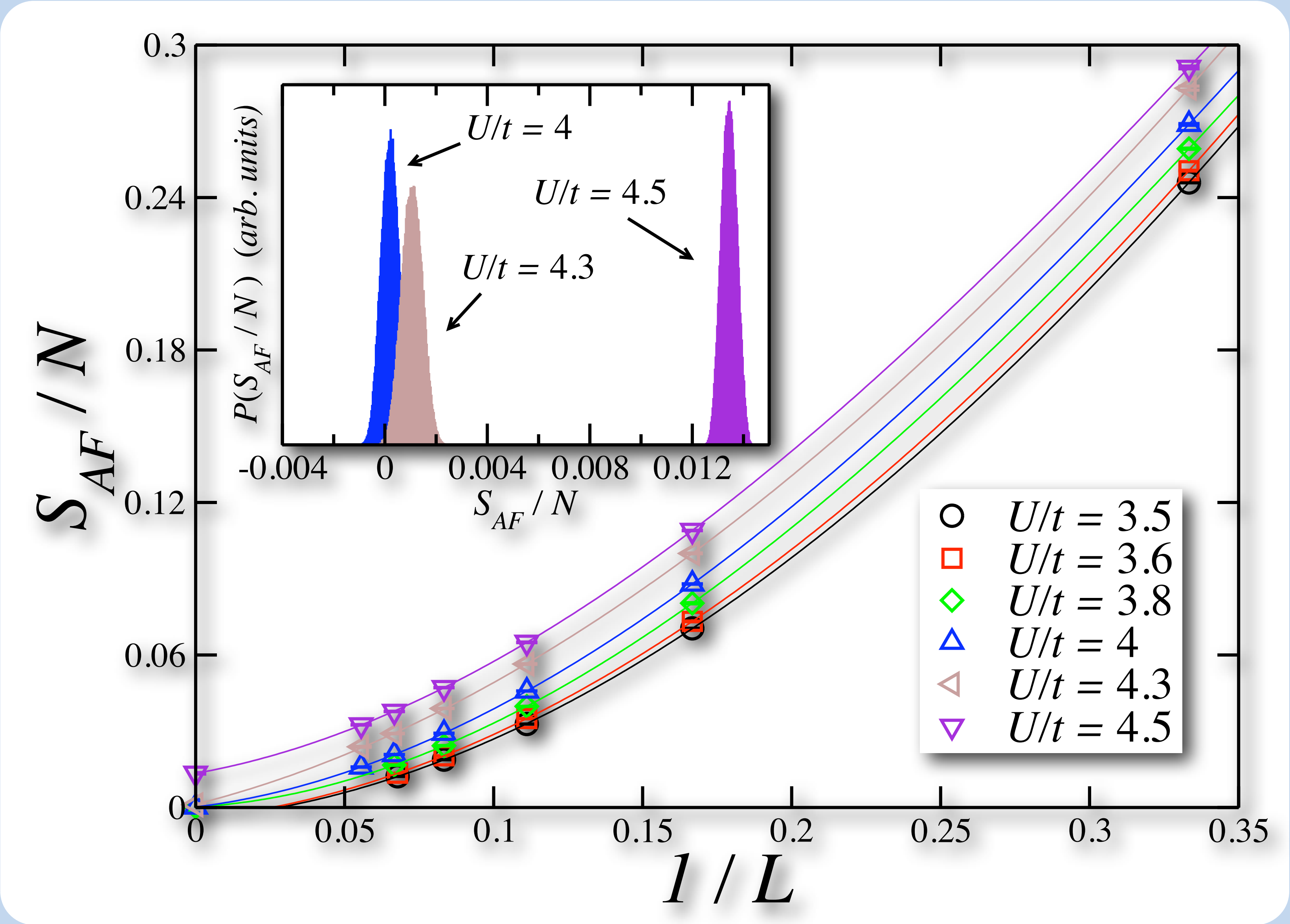

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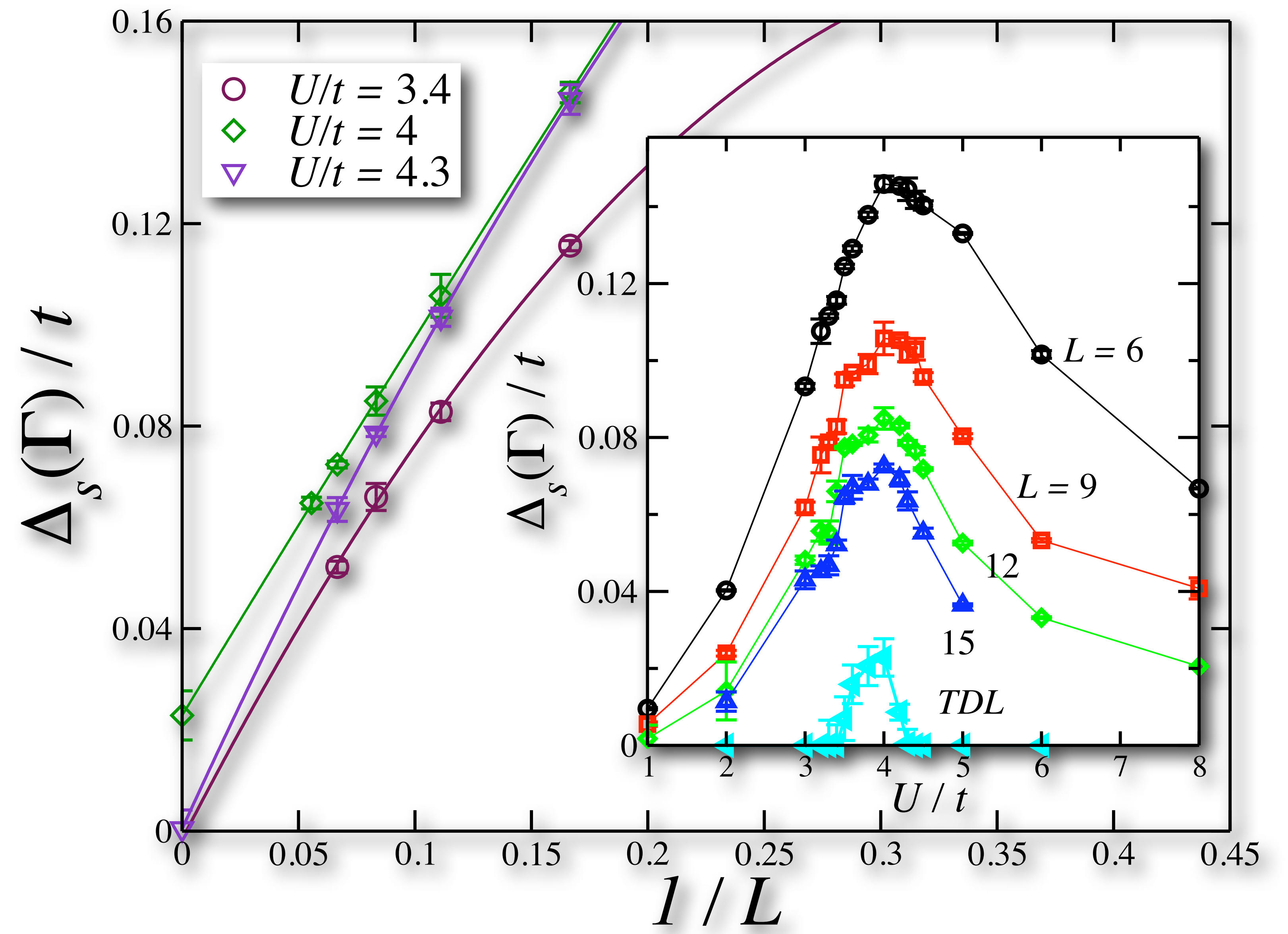
- **Paramag.-AF transition**

Magnetic excitations

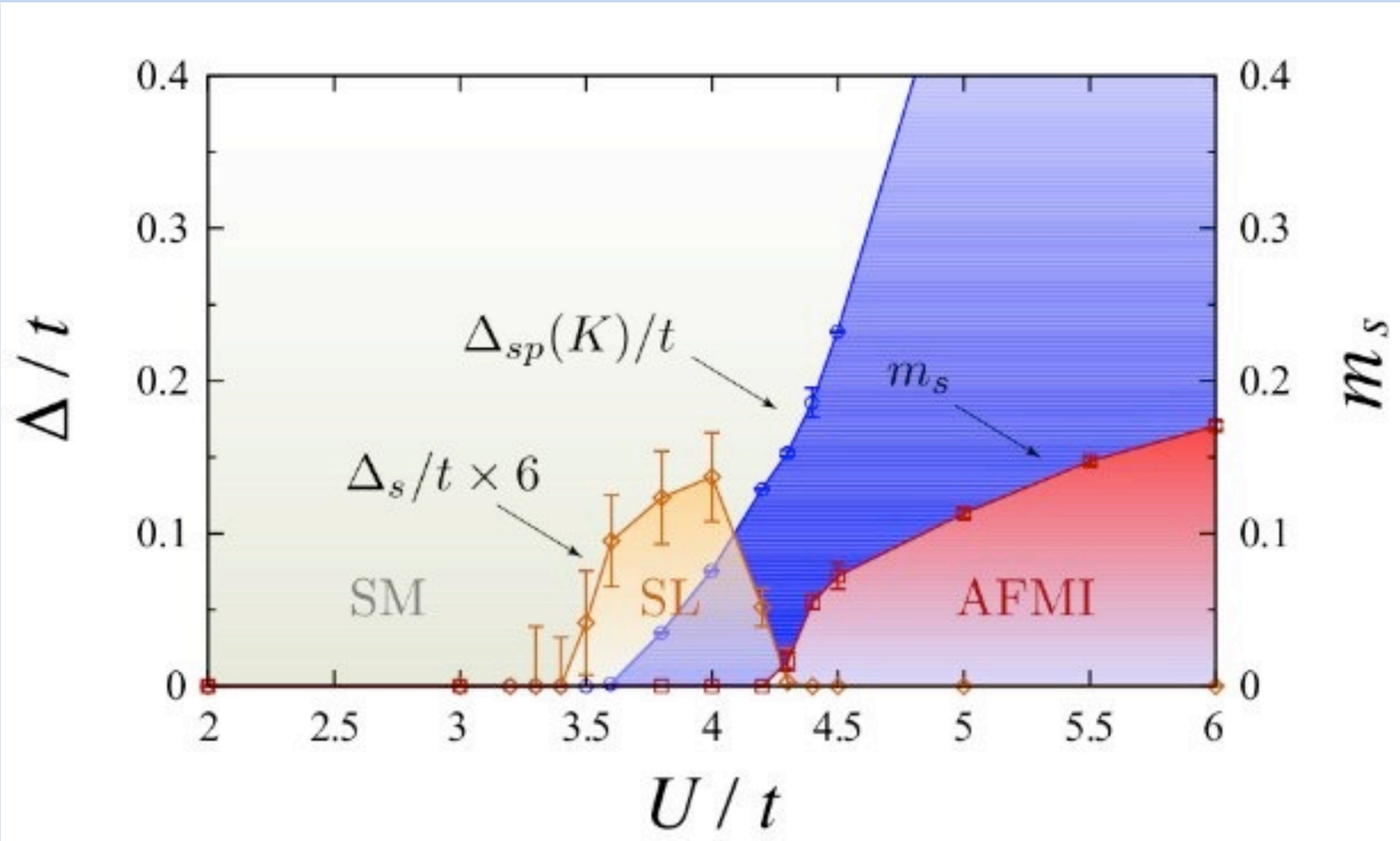
Spin-spin correlation function in imaginary time

$$S_s(\vec{k},\tau) = \Big\langle \Big[\vec{S}_{\vec{k}A}(\tau) - \vec{S}_{\vec{k}B}(\tau)\Big] \cdot \Big[\vec{S}_{\vec{k}A}(0) - \vec{S}_{\vec{k}B}(0)\Big] \Big\rangle$$



Spin-gap phase between the semimetal and the AF Mott-insulator
$(3.5 < U/t < 4.3)$

Phase diagram of the Hubbard model on the honeycomb lattice



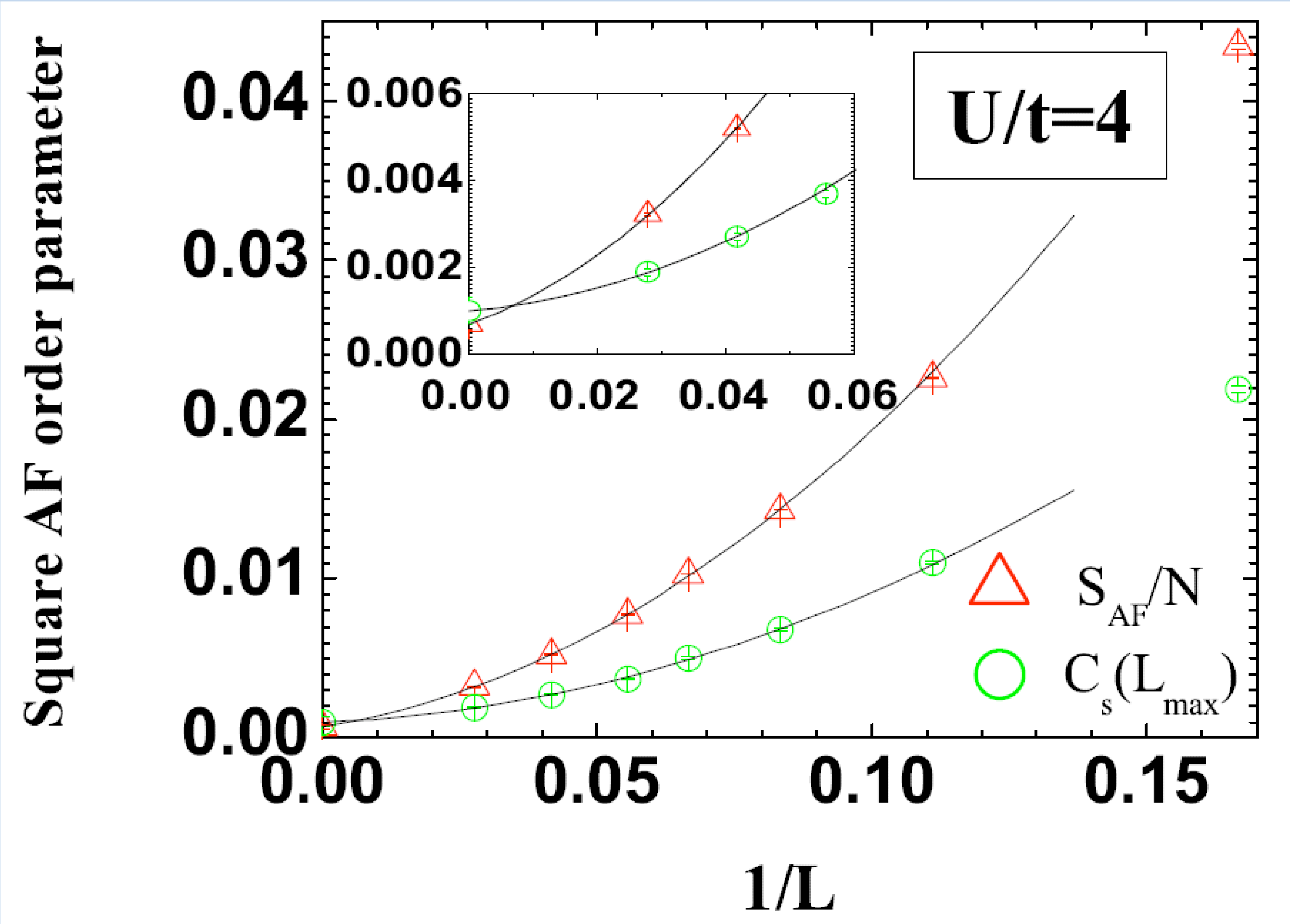
Controversy: no spin liquid

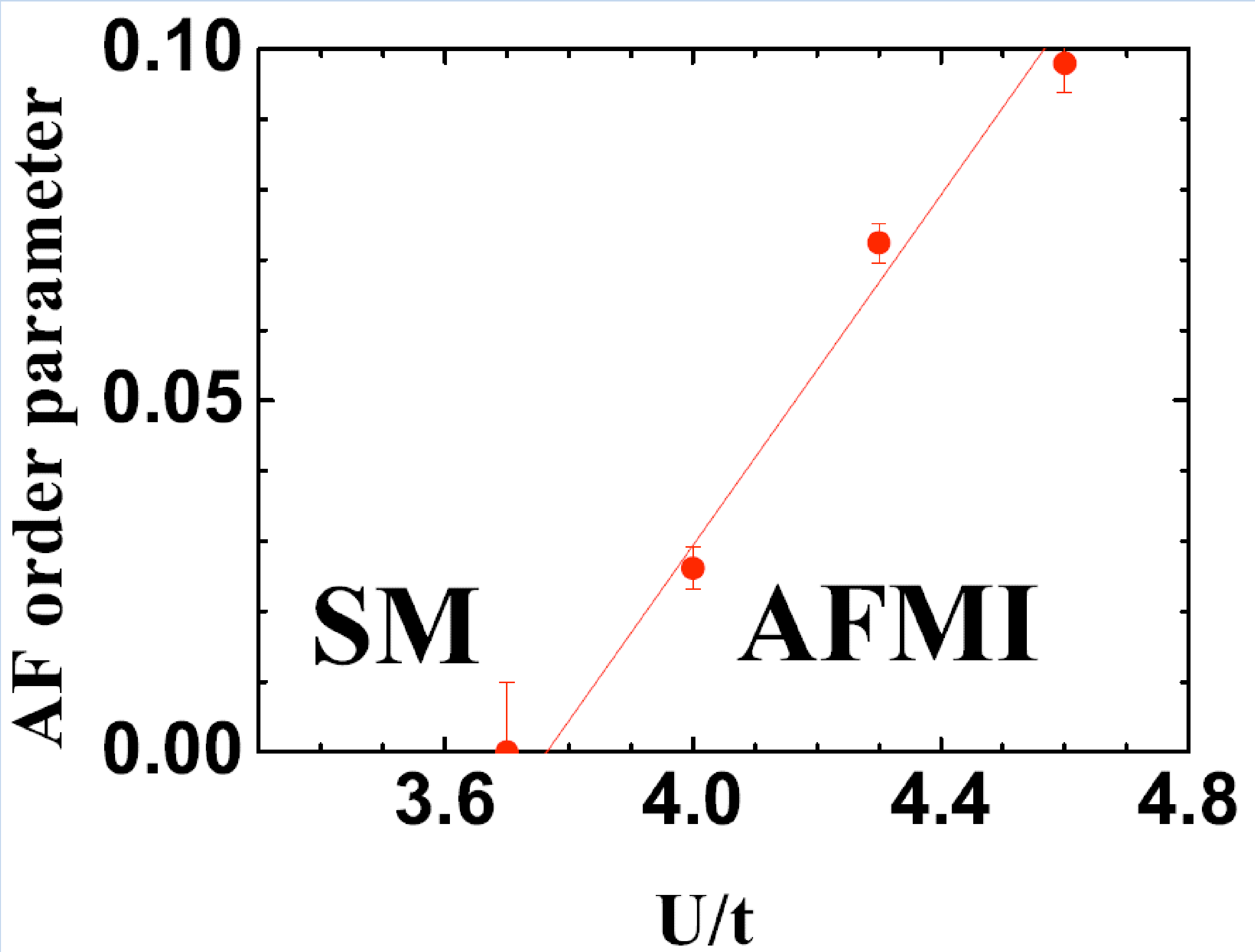
S. Sorella, Y. Otsuka, S. Yunoki, arXiv:1207.1783

$$\langle\hat{\mathcal{O}}\rangle = \frac{\langle\Psi_L|\mathrm{e}^{-\theta H/2}\hat{\mathcal{O}}\mathrm{e}^{-\theta H/2}|\Psi_R\rangle}{\langle\Psi_L|\mathrm{e}^{-\theta H}|\Psi_R\rangle}$$

$|\Psi_L\rangle$: **Slater determinant with antiferromagnetic oder parameter**

$|\Psi_R\rangle$: **Slater determinant with definite spin S**

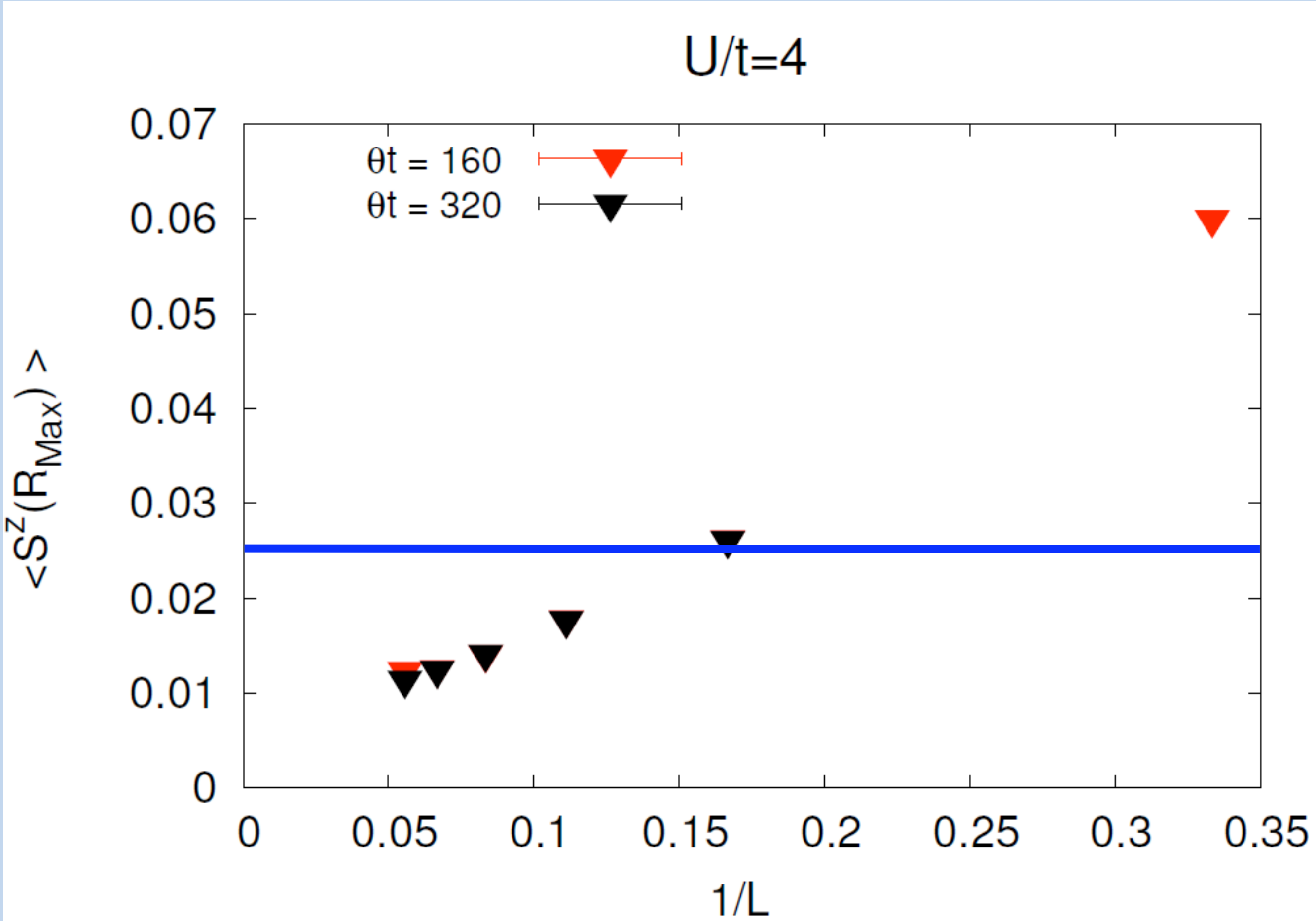




Controversy: overestimation of AF order

Local magnetic field and magnetization on the most distant point

$$h_0 = 0.1t$$



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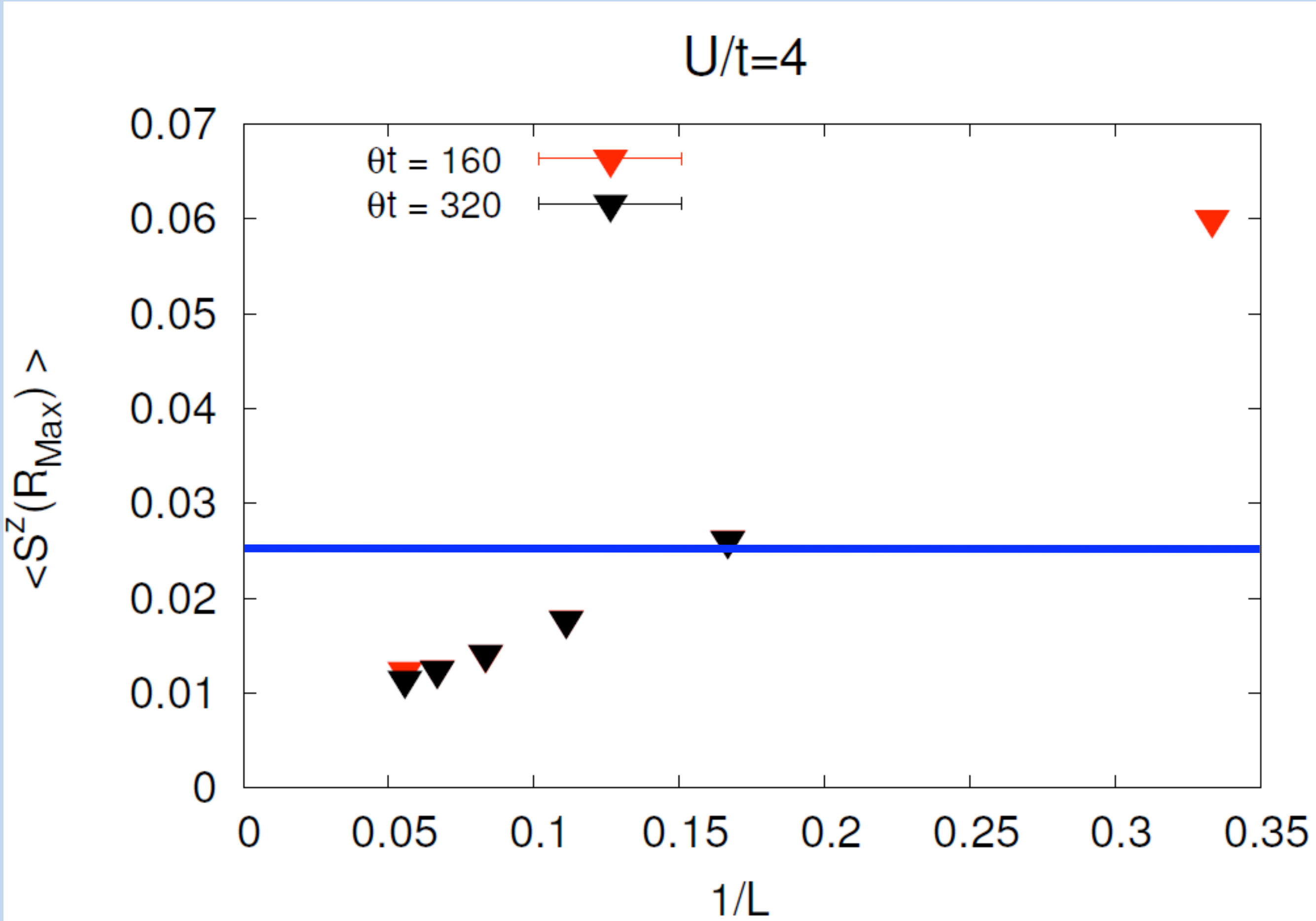

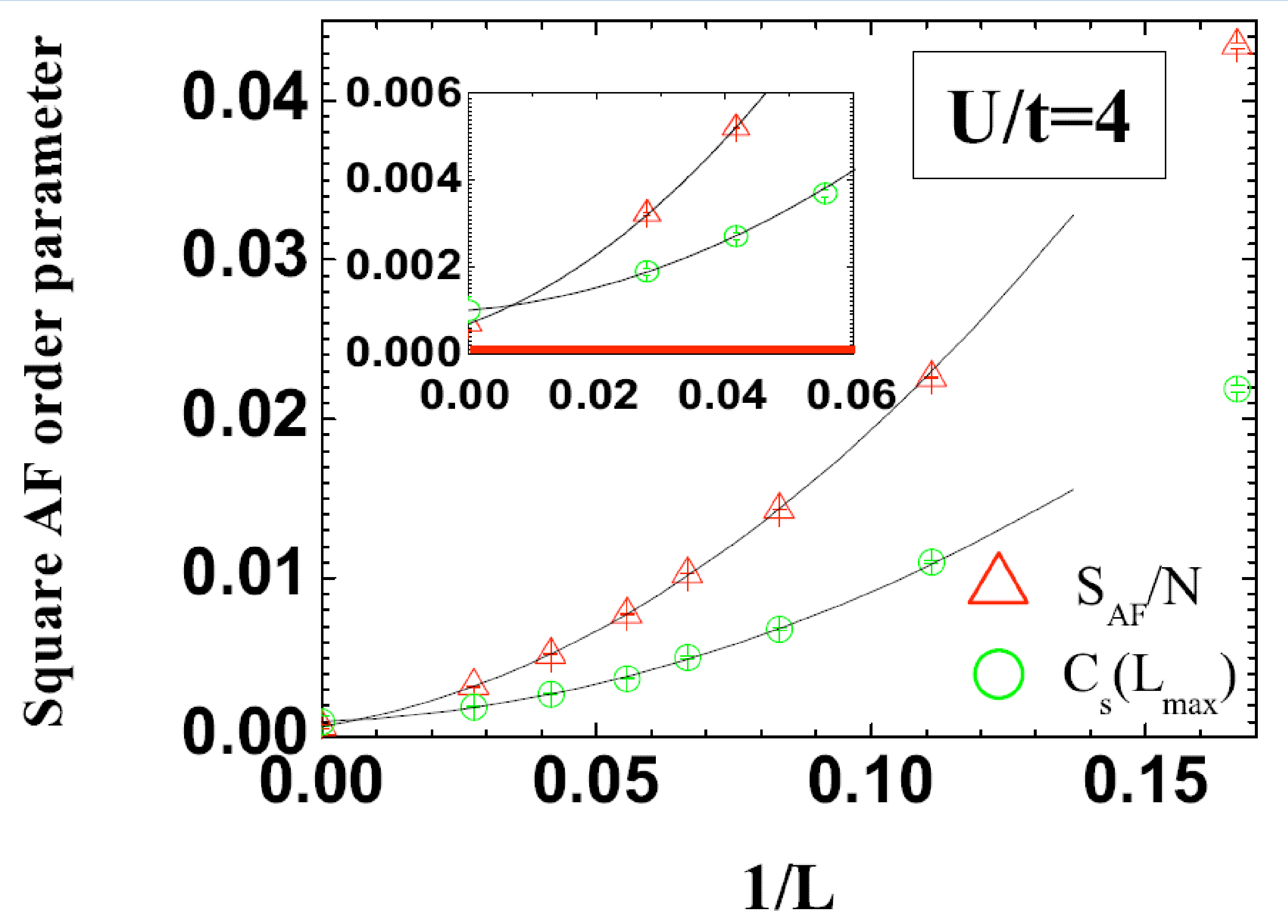

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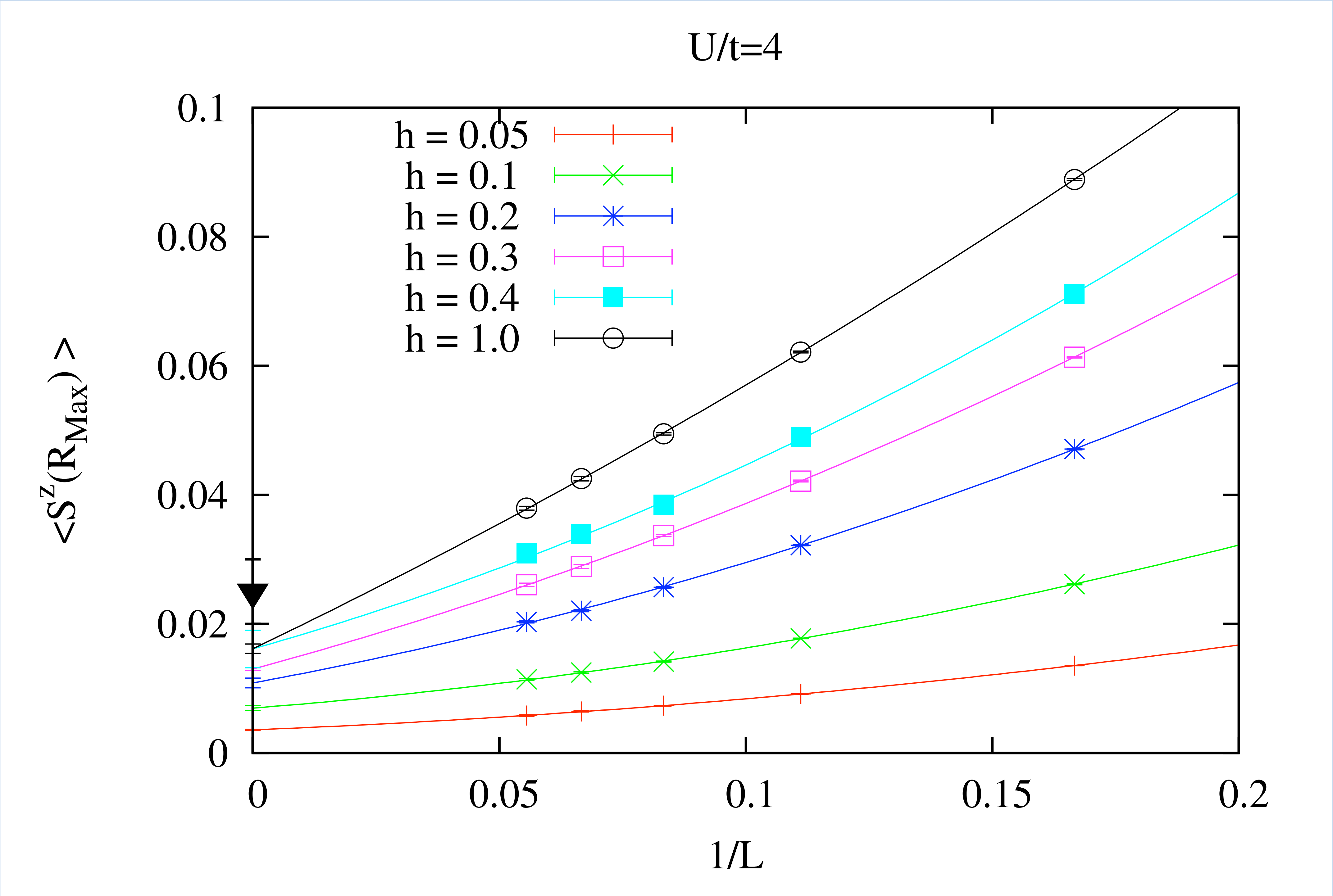
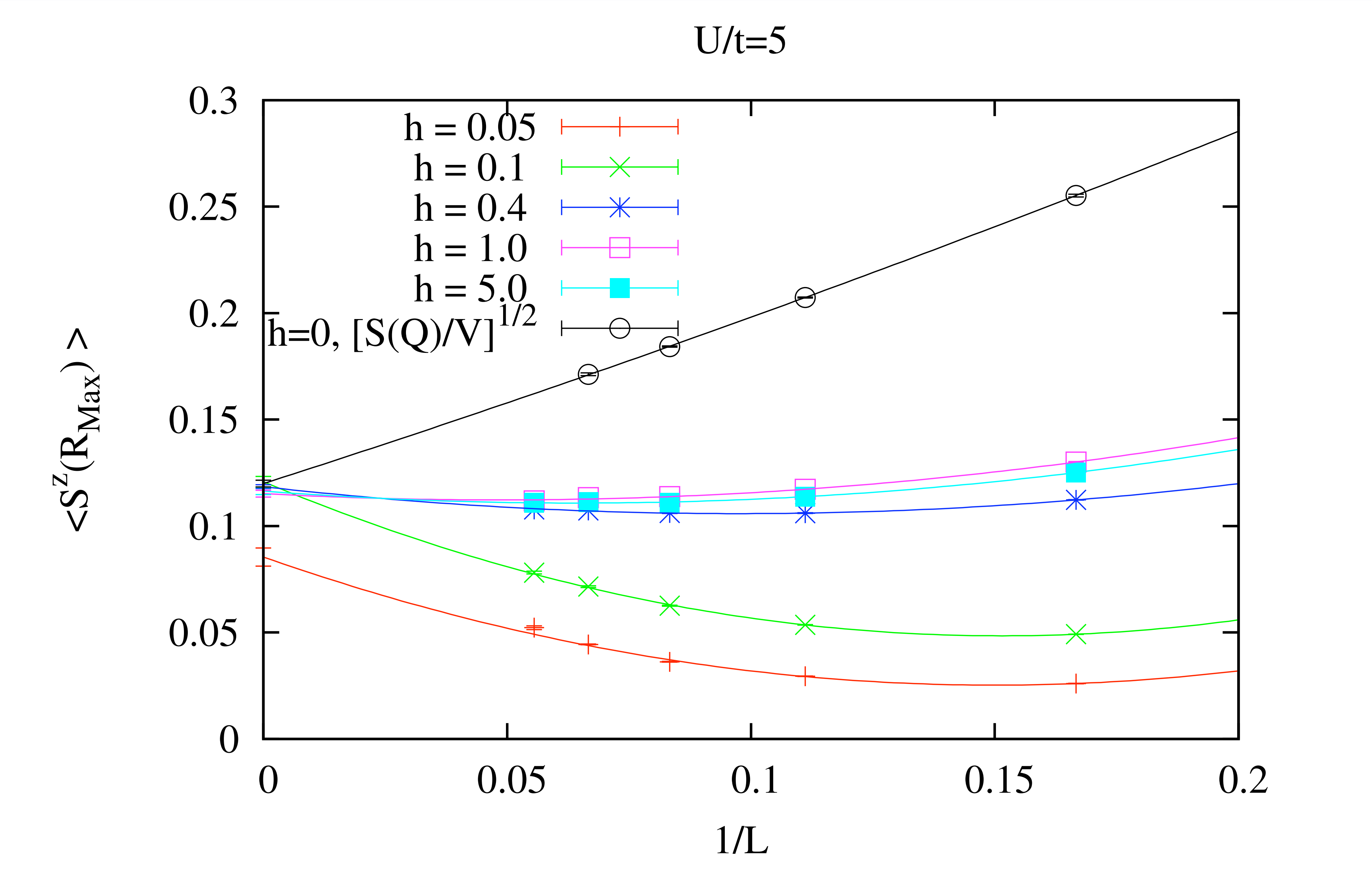


Controversy: estimation of AF order

Local magnetic field and magnetization on the most distant point

$$h_0 = 5.0t$$



Controversy: estimation of AF order

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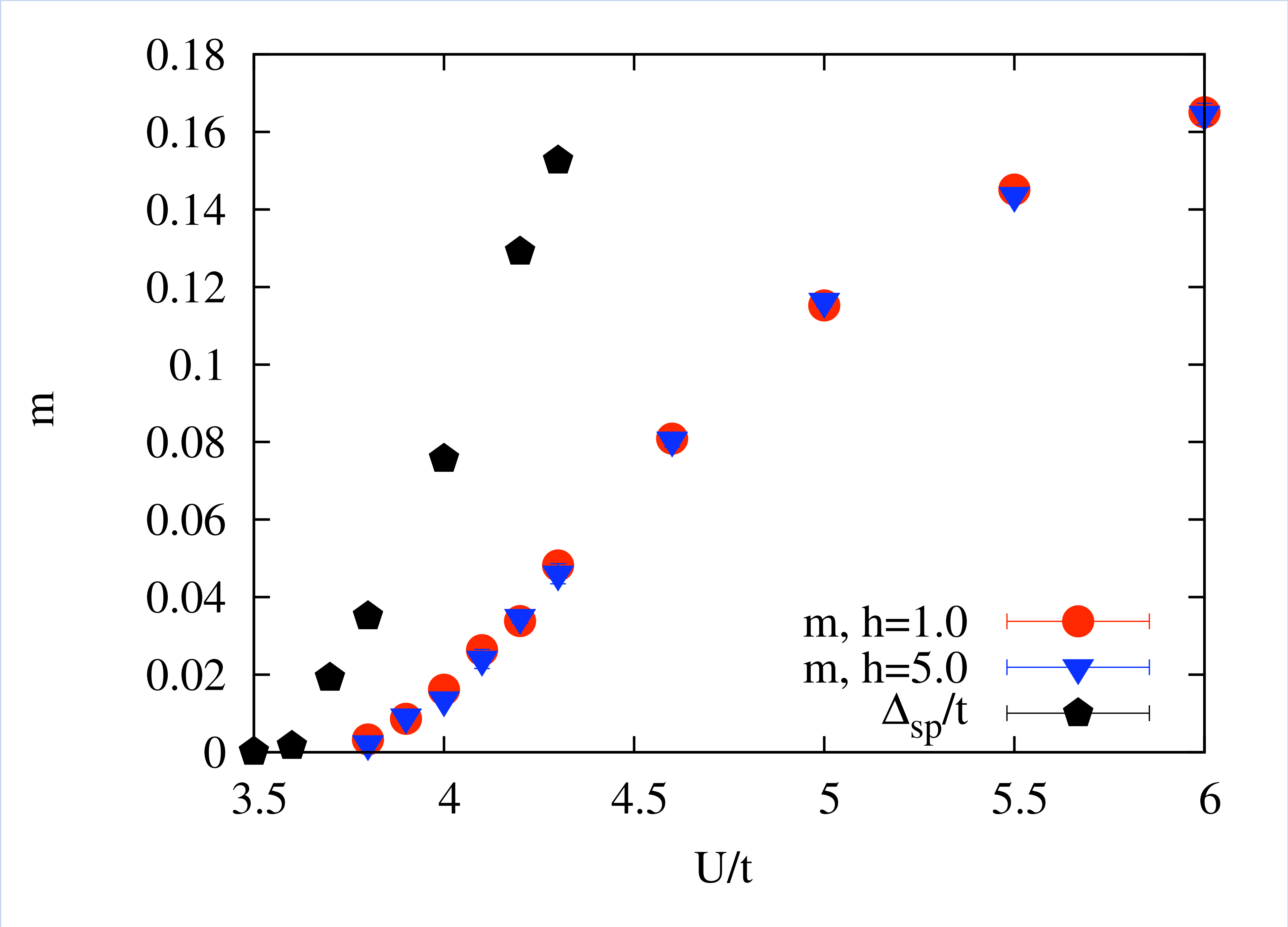

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- Fidelity susceptibility being presently calculated

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