Recent progress on the simulation of the Hubbard model by quantum Monte Carlo

Sandro Sorella
SISSA, IOM DEMOCRITOS, Trieste
Seiji Yunoki, Y. Otsuka
Riken, Kobe, Japan (K-computer)

Evora, Portugal, 11 October 2012

Outline

The phase diagram of the Hubbard model on the Honeycomb lattice

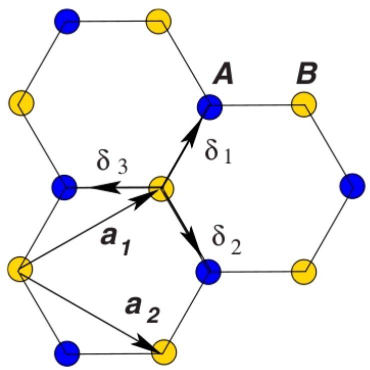
Searching for a spin liquid phase in the intermediate coupling region U/t~4 (recently proposed)

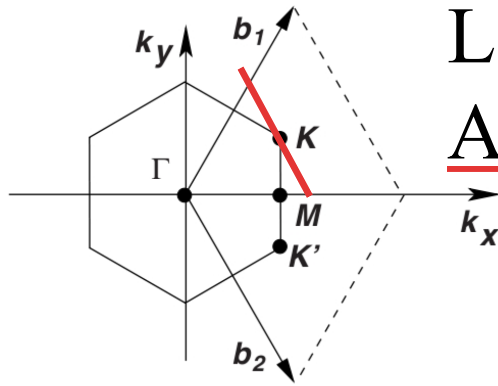
<u>Quantum Monte Carlo and Petaflop supercomputer</u>
a new possibility to understand electron correlation

How to live with the sign problem?

Recent results by massive sampling/extrapolation:
Small but non vanishing effect → Phase diagram?

Graphene

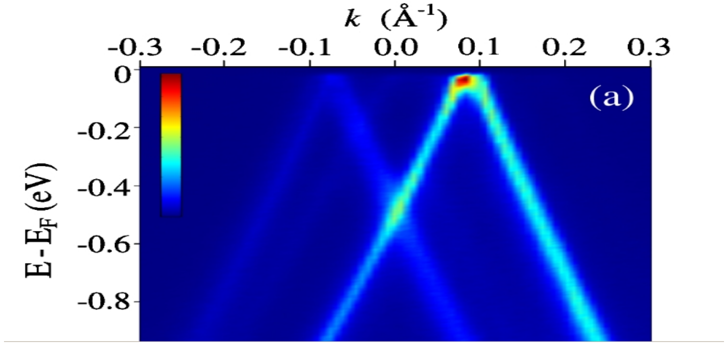




Lanzara group, PRL'10

Almost perfect Dirac spectrum:

$$E(\vec{k}+\vec{K}) = \pm v_F\,|k|$$



What happens in the Hubbard model?

$$H = \sum_{K,\sigma} E(K) c^{+}_{KA\sigma} c_{KB\sigma} + h.c. + U \sum_{R} n_{R\uparrow} n_{R\downarrow}$$

In old days (S. Sorella and E. Tosatti EPL'92) the transition was supposed to be standard HF:

(semi)metal AF-insulator

U_c/t~(223 HF) +correlation→ 4.5(5)

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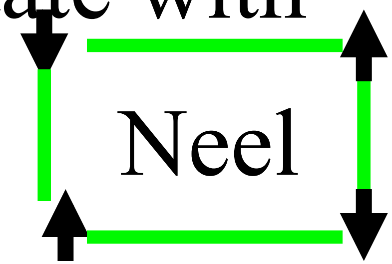
Then the spin liquid theory become popular…

A zero temperature insulating spin state with

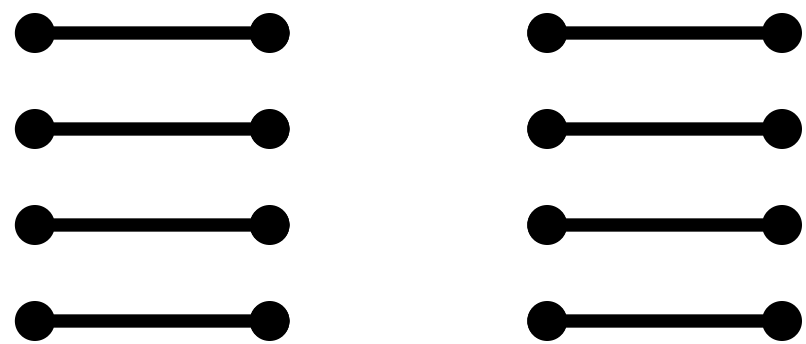


no magnetic order (classical trivial)

no broken translation symmetry (less trivial):

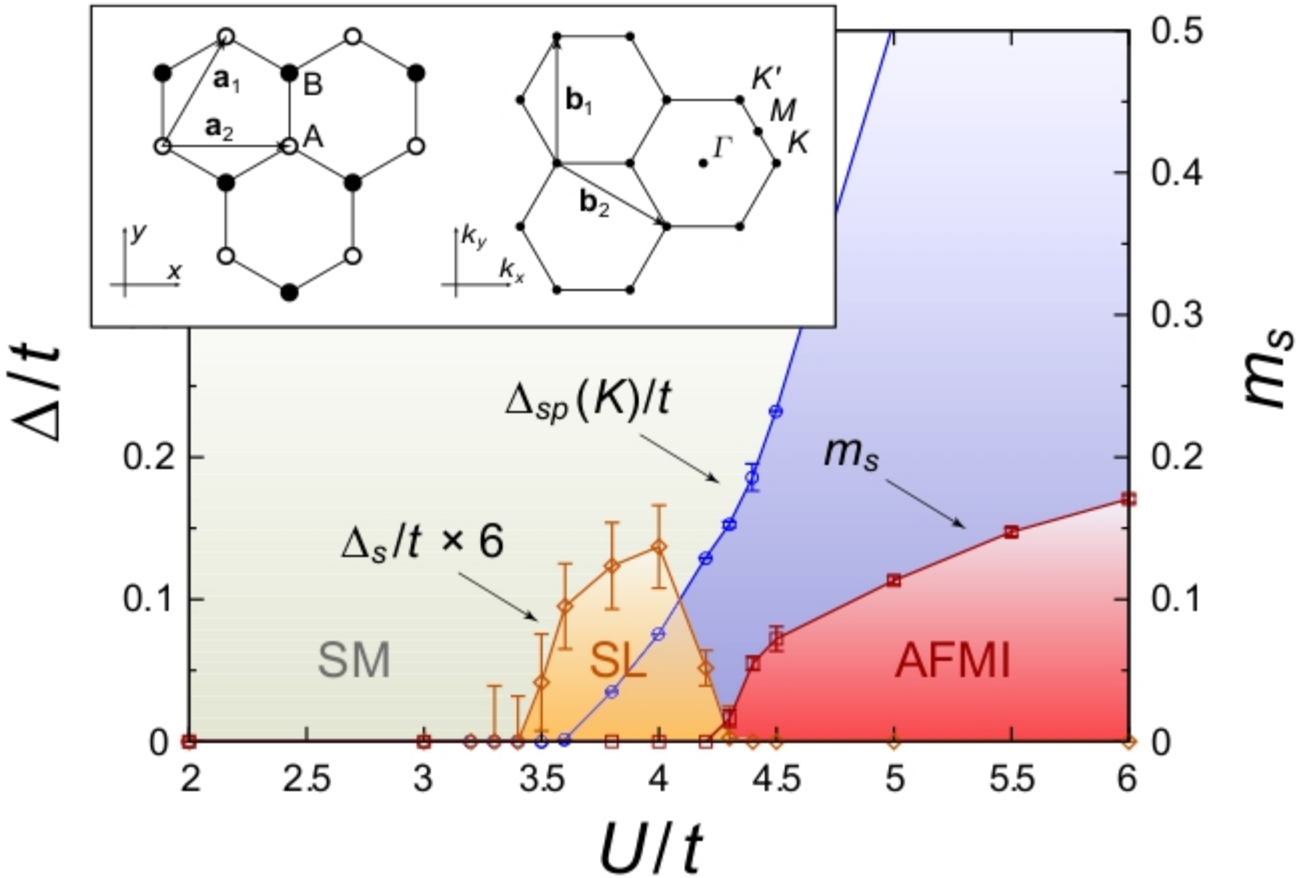
no Dimer state

(Read,Sachdev)



is a spin liquid

Recent exciting result on the Hubbard model…
Meng et al. (our organizer group), Nature 2010.



No broken symmetry but a full gap at U/t~4…
this is an RVB phase…

The auxiliary field technique based on the Hubbard-Stratonovich (Hirsch) transformation provides a big reduction of the sign problem as:

The discrete HST (Hirsch '85):

$$\exp[g(n_{\uparrow} - n_{\downarrow})^2] = \frac{1}{2}\sum_{\sigma=\pm 1}\exp[\lambda\sigma(n_{\uparrow} - n_{\downarrow})]$$

$$\cosh(\lambda) = \exp(g/2)$$

With this transformation the true propagator is a superposition of ‘’easy” one-body propagators:

$$\left|\psi_\tau\right\rangle = \exp(-H\tau)\left|\psi_T\right\rangle = \sum_{\{\sigma\}} U_\sigma(\tau,0)\left|\psi_T\right\rangle$$

and, if $\left|\psi_T\right\rangle$ is a Slater determinant, $U_\sigma(\tau,0)\left|\psi_T\right\rangle$ can be evaluated.

We can compute any correlation function O with standard MC with weight: $W[\sigma] = \left\langle\psi_T\right|U_\sigma\ (\tau,0)\left|\psi_T\right\rangle$:

$$\left\langle\psi_0\right|O\left|\psi_0\right\rangle = \frac{\left\langle\psi_{\tau/2}\right|O\left|\psi_{\tau/2}\right\rangle}{\left\langle\psi_\tau\middle|\psi_T\right\rangle} = \frac{\sum_{\{\sigma\}} W[\sigma]O[\sigma]}{\sum_{\{\sigma\}} W[\sigma]}$$

$$O[\sigma] = \frac{\left\langle\psi_T\right|U_\sigma(\tau,\frac{\tau}{2})OU_\sigma(\frac{\tau}{2},0)\left|\psi_T\right\rangle}{\left\langle\psi_T\right|U_\sigma(\tau,0)\left|\psi_T\right\rangle}$$

In order to establish a finite order parameter **m** we compute the following quantities in a finite cluster LxL=N/2 (N=#sites, i.e. 2 sites/unit cell):

$$S_{AF}/N = \left\langle \vec{m}^2 \right\rangle \text{ where } \vec{m} = 1/N\left[\sum_A \vec{S}_A - \sum_B \vec{S}_B\right]$$

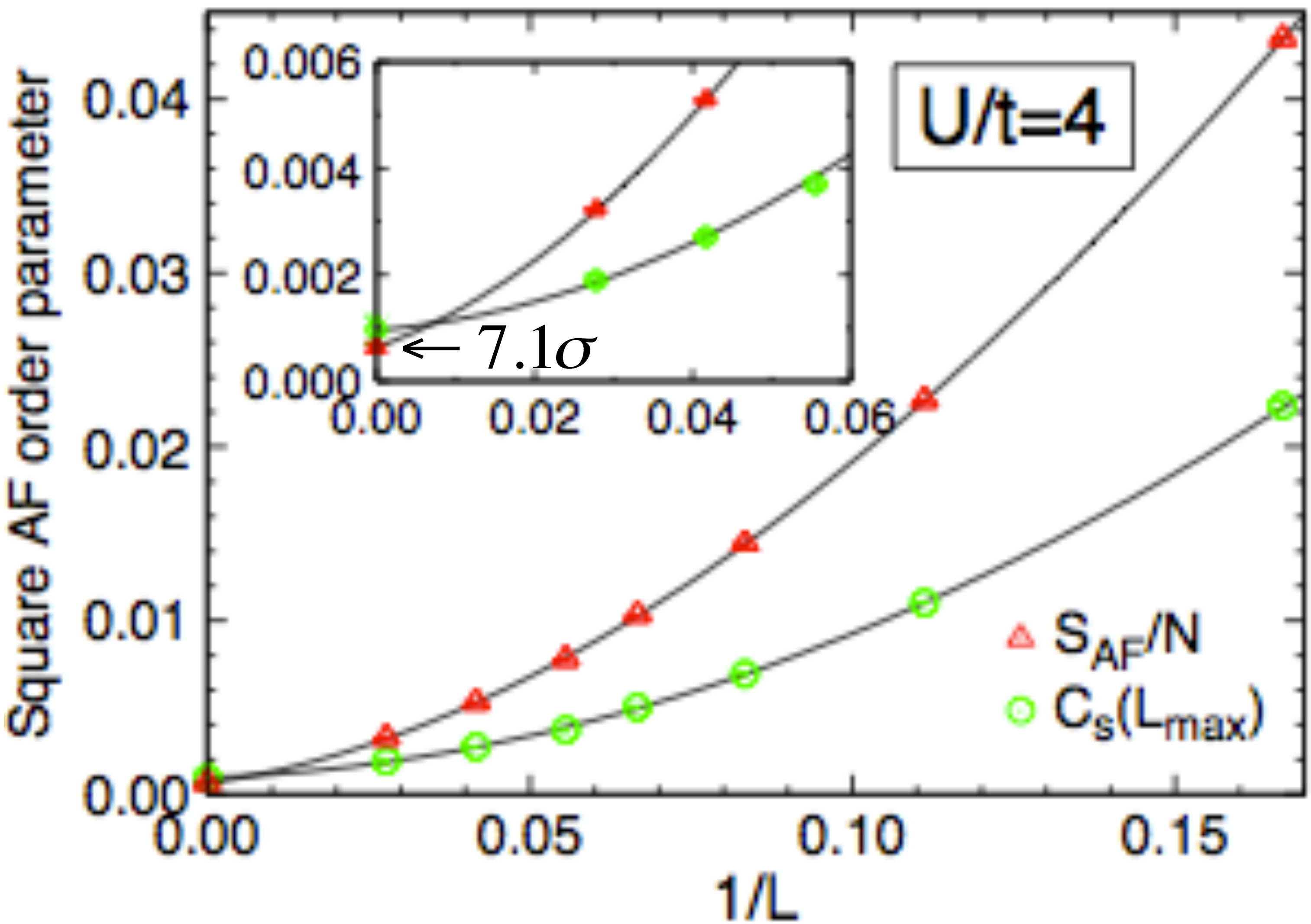
and

$$C(L_{\max}) = \left\langle \vec{S}_R \bullet \vec{S}_{R'} \right\rangle \text{ at the maximum distance}$$

In the thermodynamic limit N→∞

$C(L_{max}) = S_{AF}/N = m^2$

Finite size scaling up to 2592 sites (previous 648)!



arXiv:1207:1783 S. S. , S. Yunoki, and Y. Otsukay (2012)

Stability of the fit (unit x 10^4) U/t=4

Type of fit	S_{AF}/N	#σ
Cubic all	6.4(9)	7.1
Cubic no L=6	8.2(20)	4.8
Cubic no L=36	5.5(12)	4.3
Quadratic L>6	1.92(53)	3.6
L>9	4.67(97)	4.8
L>12	8.2(14)	5.8

The fit is not perfect but S_{AF}/N is non zero

Accelerating the convergence in imaginary time

We have the freedom for large τ to use a different Left and right wave function:

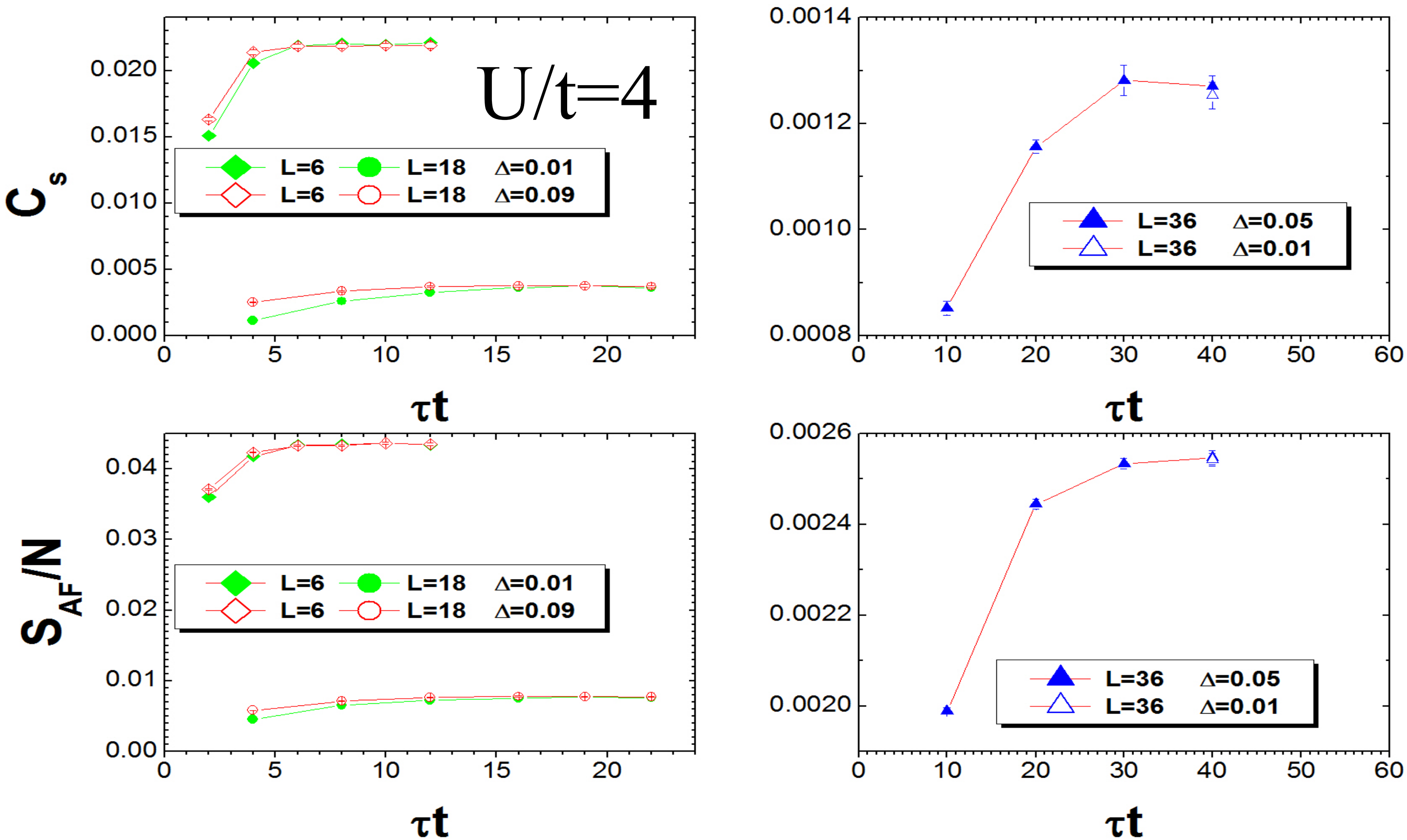
$$\langle O \rangle = \frac{\langle \psi_L | \exp(-H\tau/2) O \exp(-H\tau/2) | \psi_R \rangle}{\langle \psi_L | \exp(-H\tau) | \psi_R \rangle} + O(\exp(-\text{Gap}\ \tau))$$

where Gap is the lowest gap non orthogonal to both to ψ_L and ψ_R

For all fully symmetric operators the convergence is faster if we use an AF wf for ψ_L and a perfect singlet (but broken rotation) for ψ_R

Convergence by imaginary time projection & Dependence on the initial trial wf:

Even close to the critical point U_c ,m grows vs τ



For technical reason we have to use a small Δ:

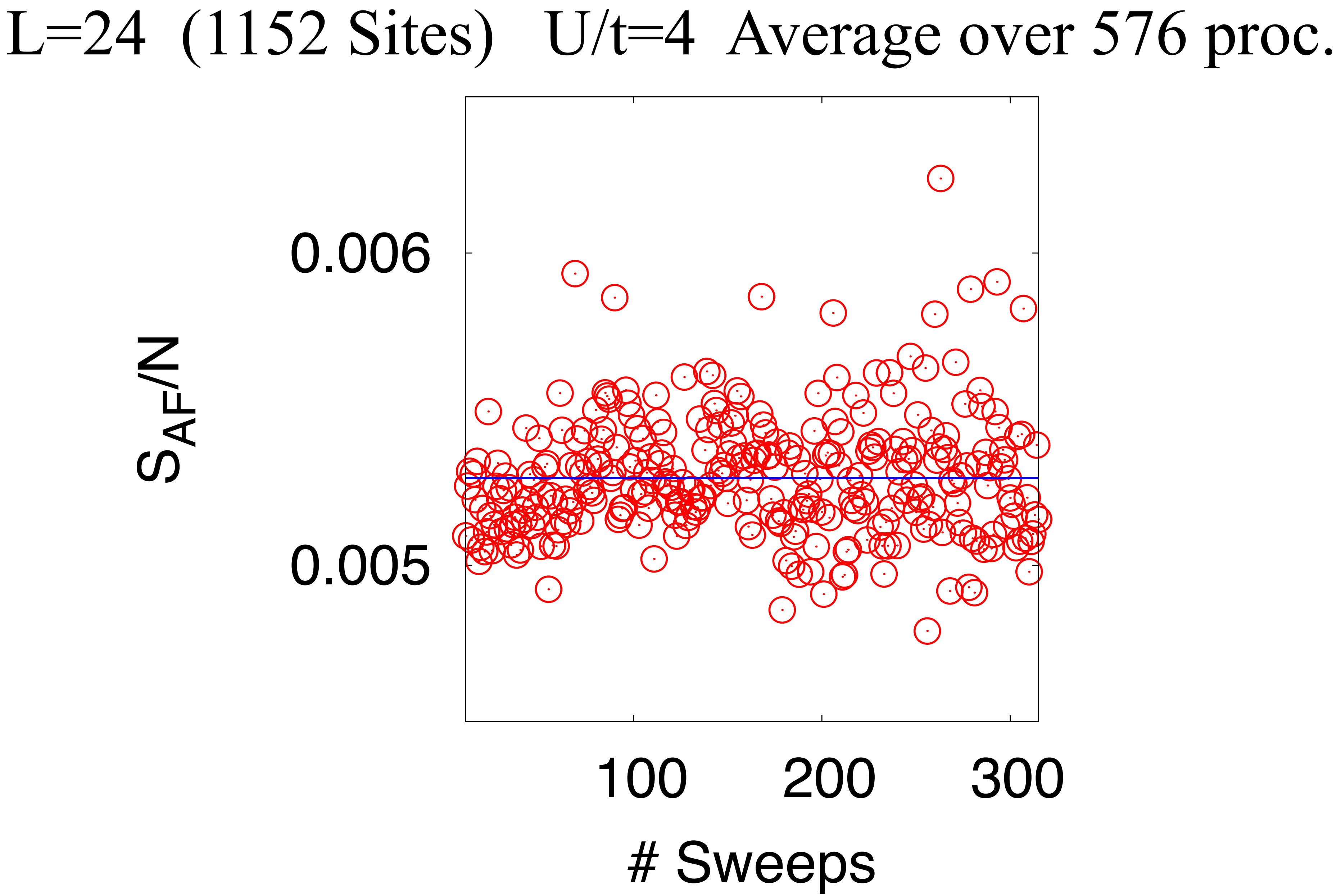
$$H_{\psi_L} = H_{FREE} + \Delta\left(\sum_A S_A^x - \sum_B S_B^x\right)$$

$$W(\sigma) = \langle \psi_L | U_\sigma(\tau,0) | \psi_R \rangle \geq\sim \left(\frac{\Delta}{t}\right)^{N/2} > 0$$

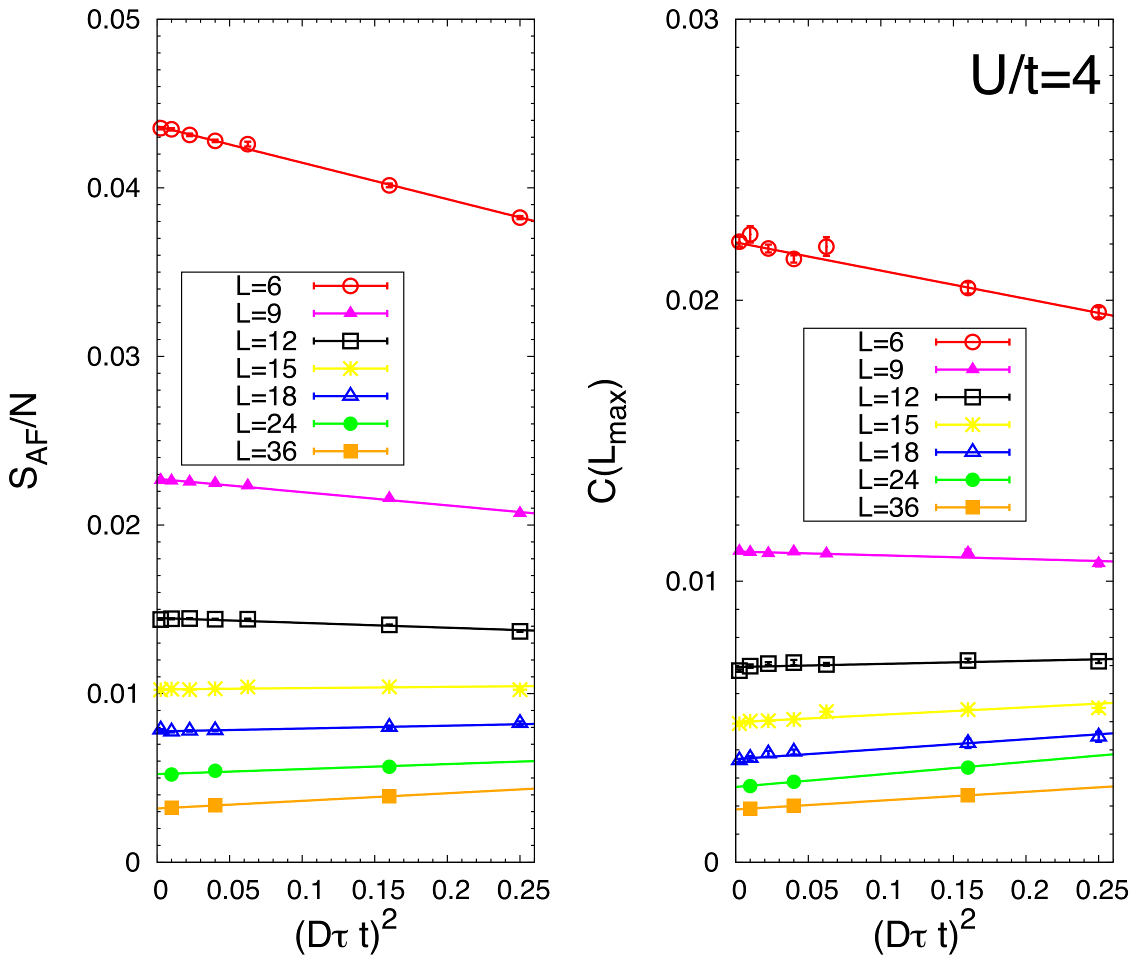
For the proof ask me privately if interested

Thus our weight is <u>strictly</u> positive that guarantees

$$O[\sigma] = \frac{\langle \psi_L | U_\sigma(\tau,\frac{\tau}{2}) O U_\sigma(\frac{\tau}{2},0) | \psi_R \rangle}{\langle \psi_L | U_\sigma(\tau,0) | \psi_R \rangle} \sim \frac{1}{W(\sigma)}$$ has finite variance


L=24 (1152 Sites) U/t=4 Average over 576 proc.
0.006
0.005
S_{AF}/N
100
200
300
Sweeps

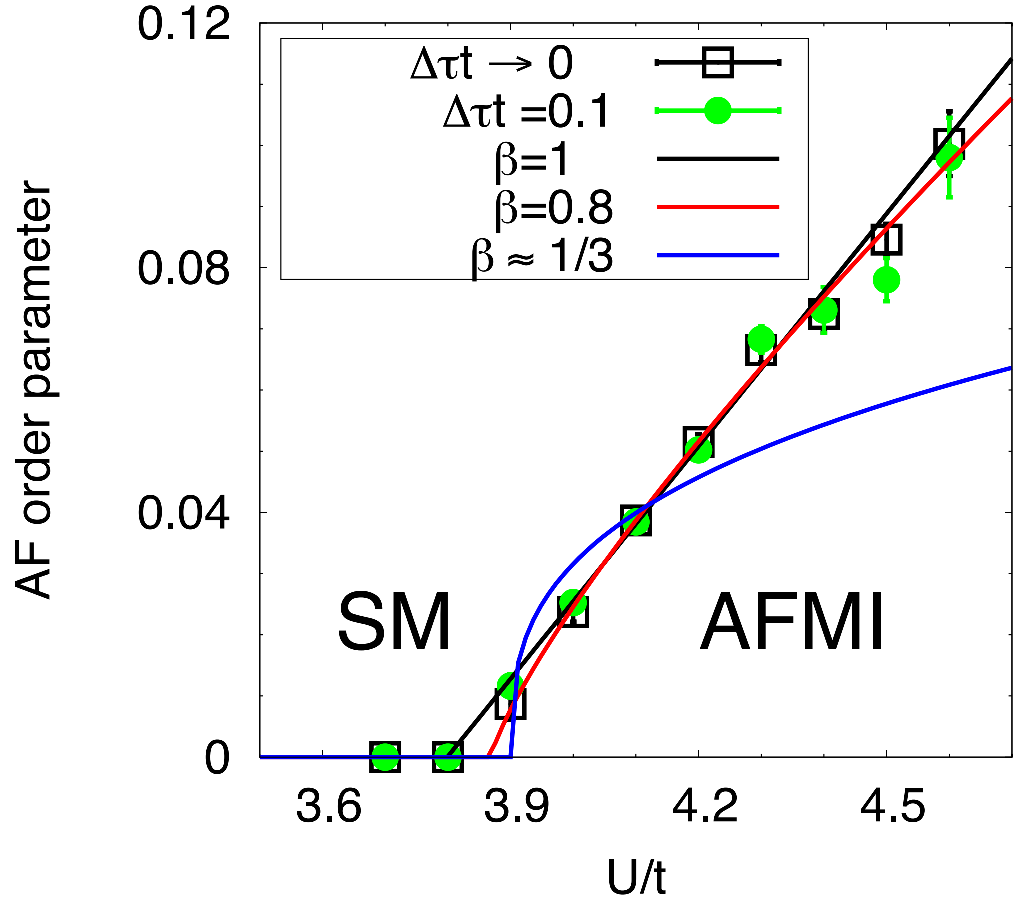
iii) The error due to Trotter is negligible for Δτt=0.1



Perfect linearity with $(\Delta\tau t)^2 \rightarrow 0$, easy to remove.

The AF magnetic order **m** vanishes continuously

$m \propto (U - U_c)^{\beta}$ with β<1 (e.g. β~1/3 for QCP)



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

This does not exclude the spin liquid for U/t<~3.9

We study the density-density correlation $\rho(r)$

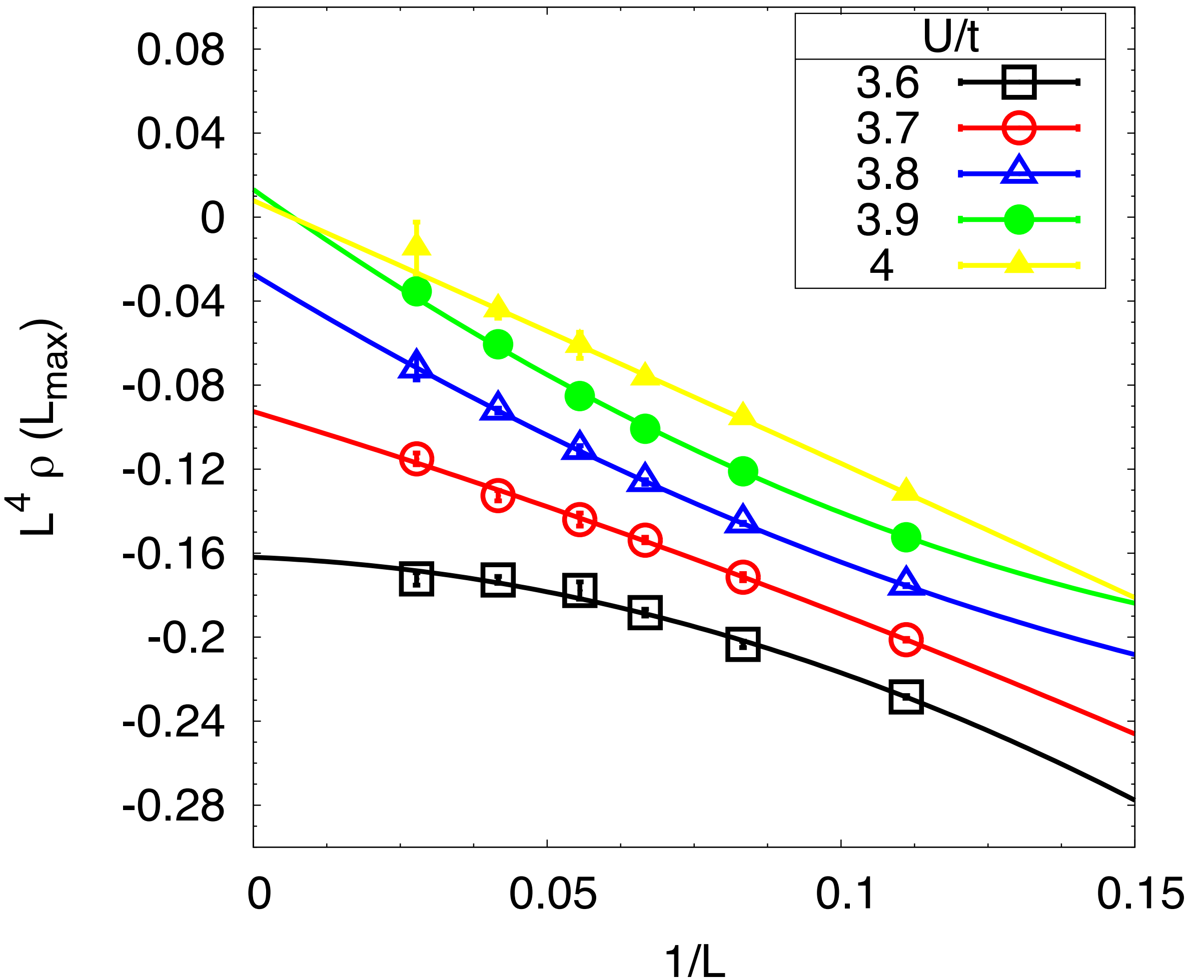
Due to commensurate Friedel oscillation

$$\rho(r) \sim \exp(2k_F r) / r^4$$

in the semimetallic region U < 3.9

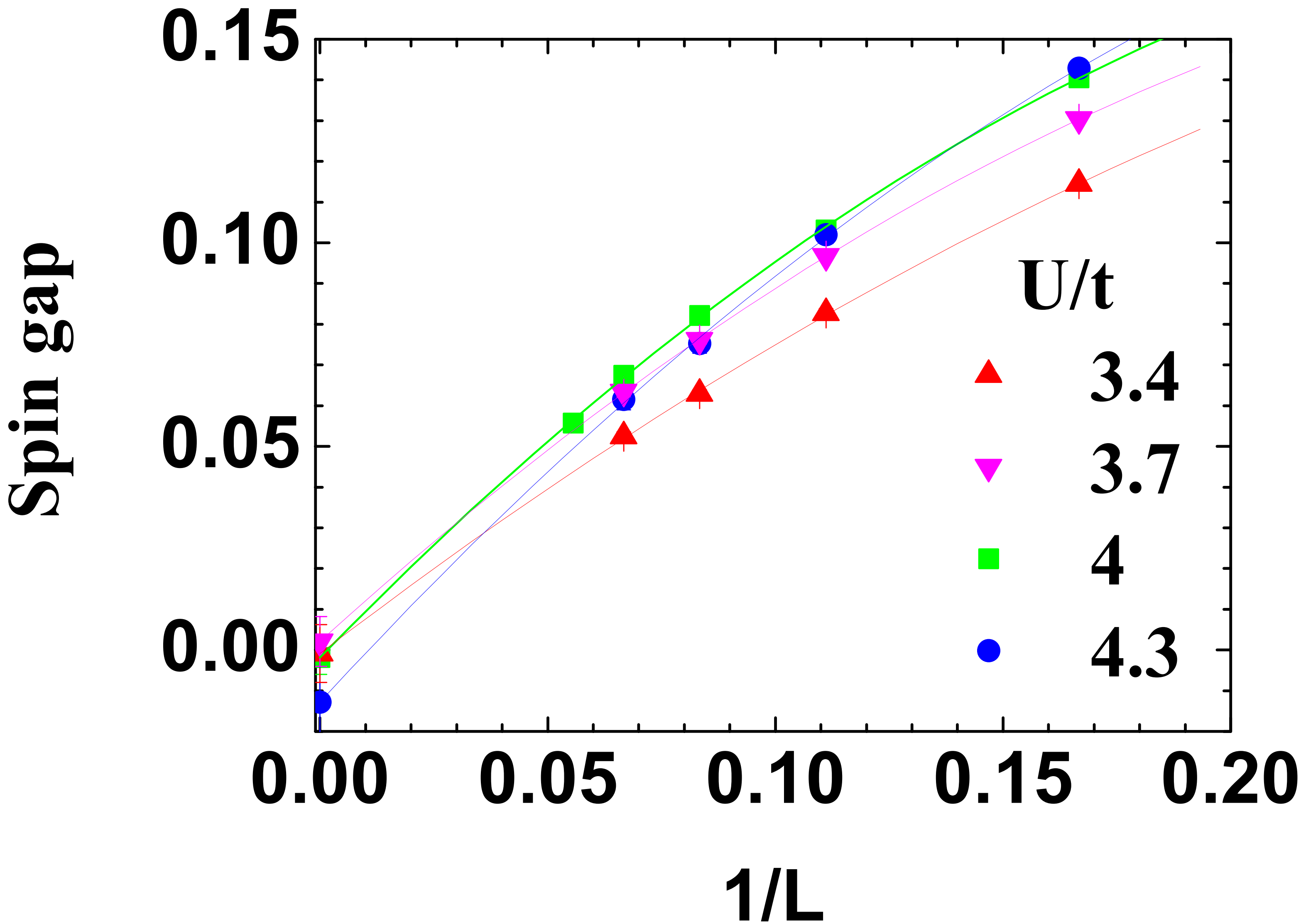
If we plot r^4 x Exponential → 0 in the insulator.

The critical point is $U_c \mid L^4 \rho(r = L_{max}) \rightarrow 0$ for $L \rightarrow \infty$



We clearly see that U_c is between 3.8 and 3.9 with this definition, now exactly consistent with **m**.

No spin gap was found by direct evaluation



New phase diagram with large scale simulations

(semi)metal ?? AF-insulator

3.2 $U_c \sim 3.85$ 4.6

U/t

Previous results with 648 Sites:

SM Spin Liquid AFI

3.4 4.3

U/t

First results on a model without sign problem:
Much larger size → spin liquid unlikely
or almost gapless in an very small region.
Certainly at the critical point we have a gapless SL.

As a consequence of the Murphy's law
''No interesting results can be obtained with a fermionic model without sign problem….''
but this is not completely true...

The transition is clearly continuous and we found a critical exponent $\delta = \sim 0.8 \gg 1/3$ (standard ?)
or consistent with 3-d expansion 0.88

The first continuous metal-insulator transition model.

Several questions still open and can be solved exactly.