# Spin liquid phases in strongly correlated lattice models

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

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# Outline

The phase diagram of the Hubbard model on the Honeycomb lattice

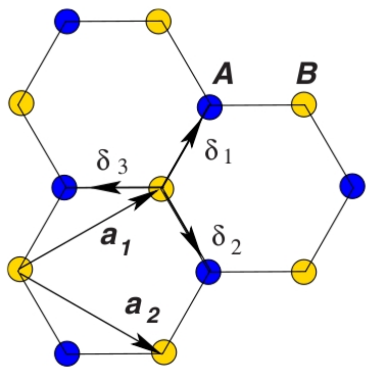
Searching for a spin liquid phase in the intermediate coupling region U/t~4 (recently proposed)

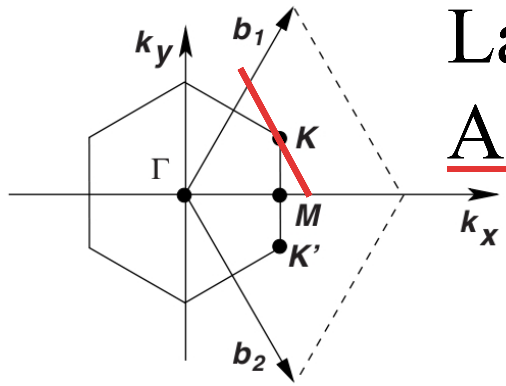
Really frustrated systems

How to live with the sign problem?

Recent results on a frustrated model:
Lanczos steps with variance extr. J1-J2 model.

# Graphene

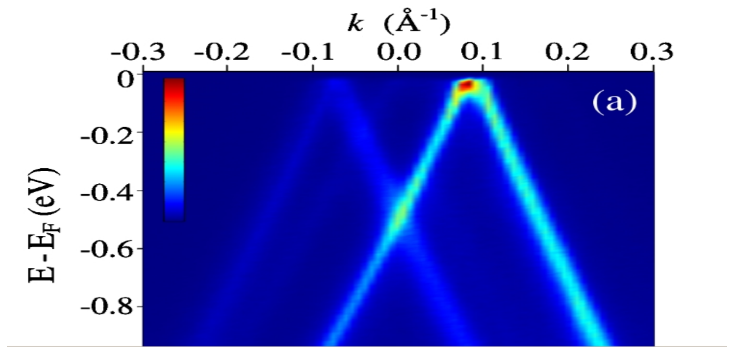



Lanzara group, PRL'10

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

$U_c/t\sim(2.23\text{ HF})$ +correlation → 4.5(5)

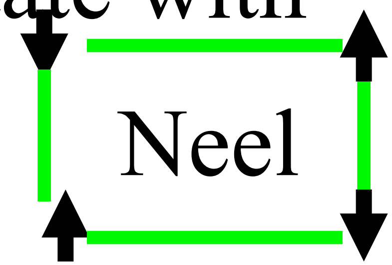
$$1/U = \int_0^\infty \frac{N(E)}{\sqrt{(Um)^2+E^2}}dE \quad \text{where } N(E)\propto E$$

and $$1/U_c = \int_0^\infty \frac{N(E)}{E}dE$$ and more importantly:

$$m \propto (U-U_c)$$ i.e. non standard

Then the spin liquid theory become popular…

A <u>zero temperature insulating</u> spin state with

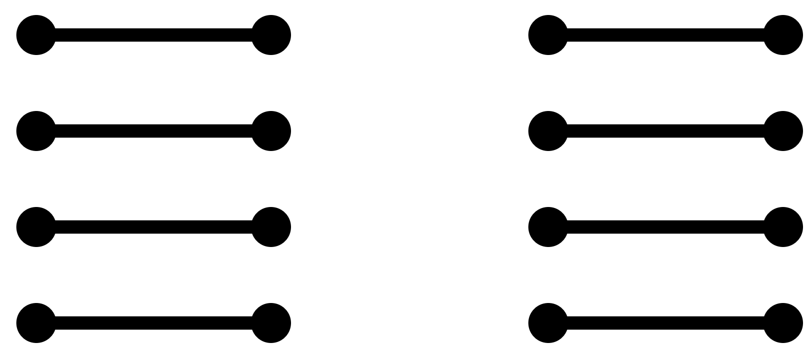



no magnetic order (classical trivial)

no broken translation symmetry (less trivial):

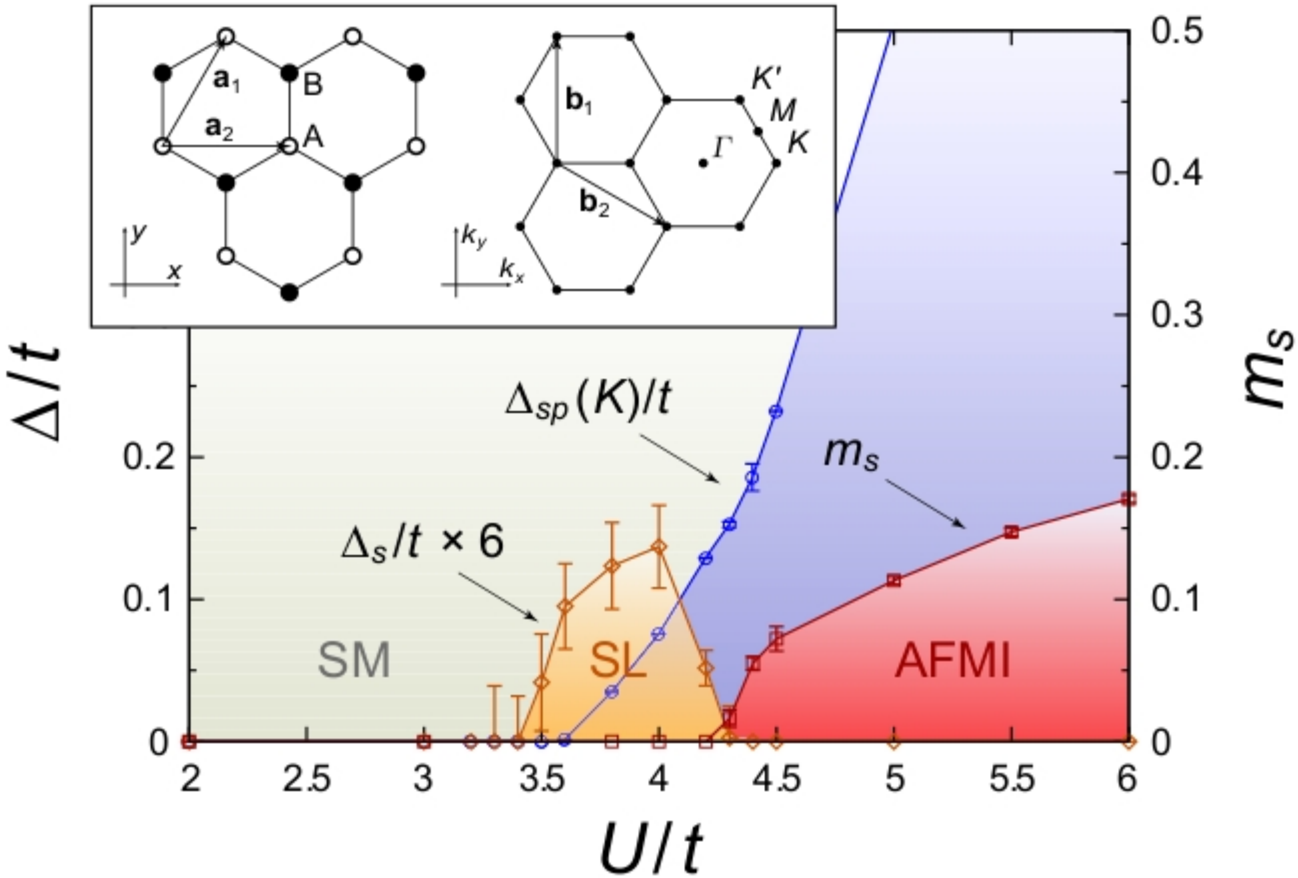
no Dimer state

(Read,Sachdev)



is a spin liquid

# Recent exciting result on the Hubbard model… Meng et al. (Muramatsu's group), Nature 2010.




No broken symmetry but a full gap at U/t~4… this is an RVB phase: a T=0 S=1/2 paramagnet

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: $W[\sigma] = \left\langle\psi_T\right|U_\sigma\ (\tau,0)\left|\psi_T\right\rangle$:

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

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

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):

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

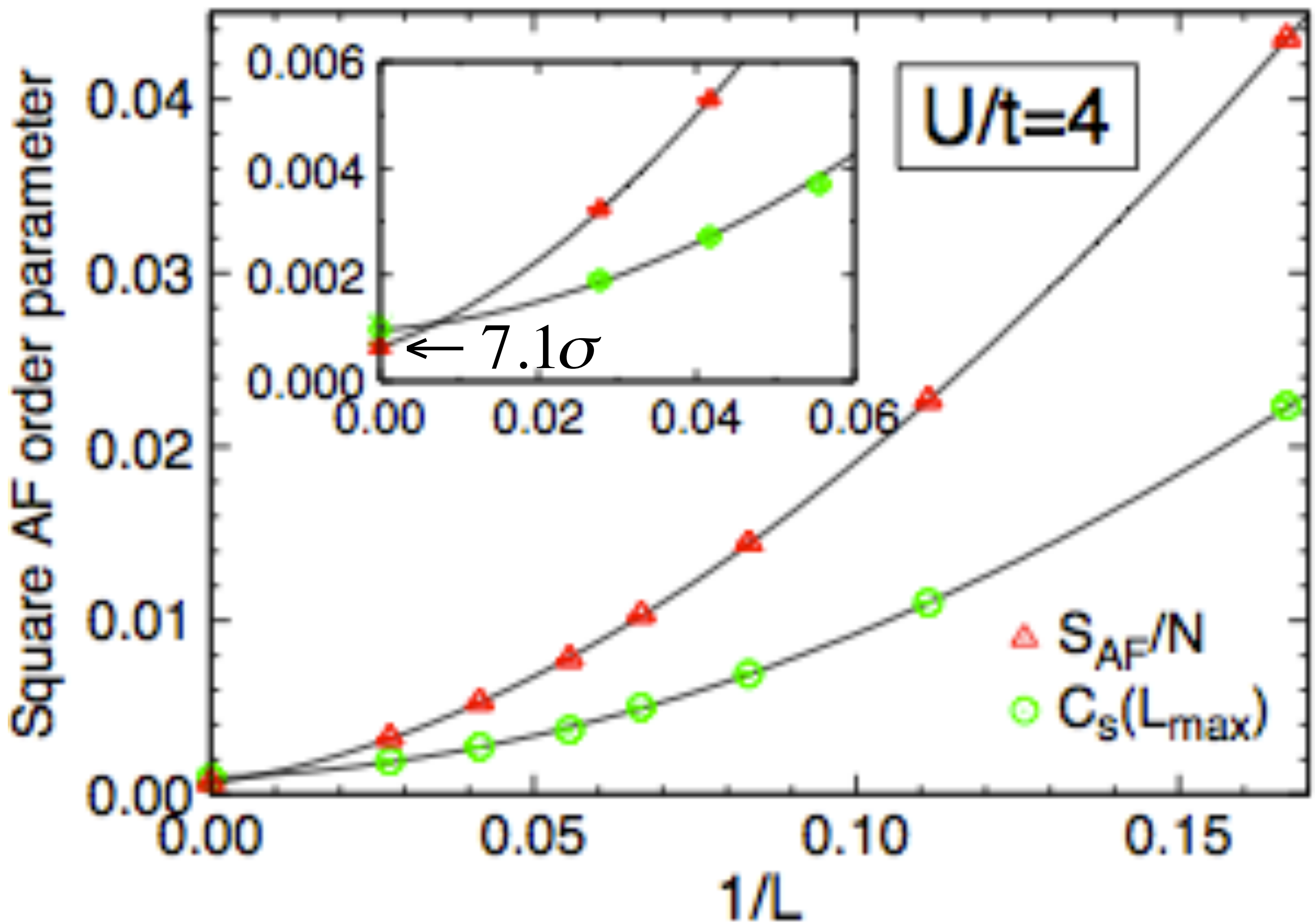
and

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

In the thermodynamic limit N→∞

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

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




Sci. Rep. 2012,2,992 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

# How to do so much larger clusters?

The basic operation in Monte Carlo is updating a 2Lx2L matrix g:

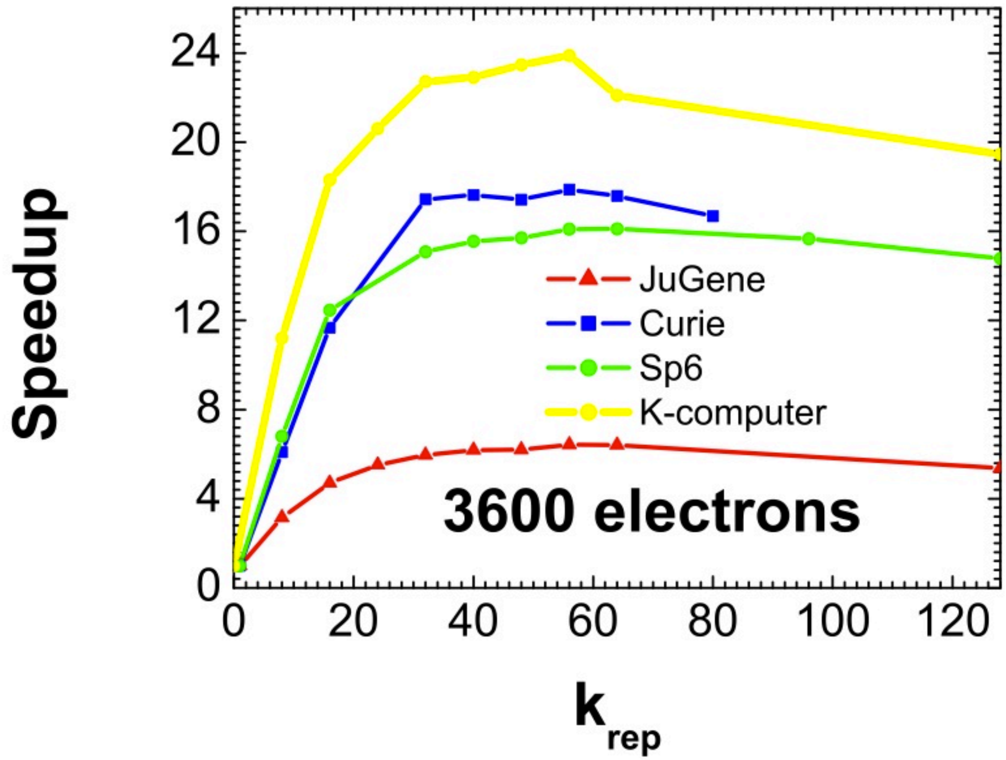
$$g_{ij}^{n+1} = g_{ij}^{n} + a_i(g^n)b_j(g^n)$$

The cost for computing both *a* and *b* given *g* is ~2L<<L$^2$

The cost for a QMC update requires only $g_{ii}$

One can "delay the updates" $k_{rep}$ times

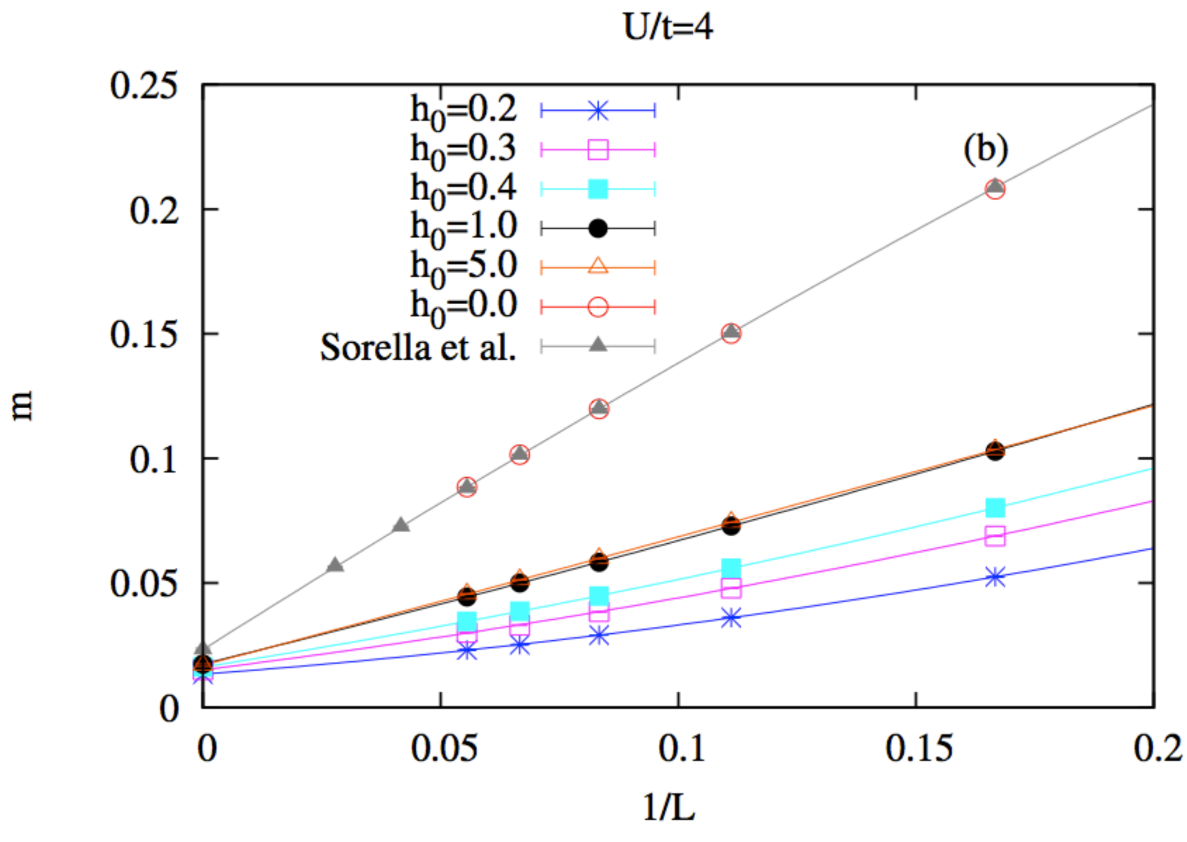
$$g_{ij}^{n+k_{rep}} = g_{ij}^{n} + \sum_{k=0}^{k_{rep}-1} a_i(g^{n+k}) b_j(g^{n+k}) = g + AB^T$$




A speed-up of about 24 in the K-computer.

SS; F. Mancini, A. Avella, Eds.; Springer, 2013

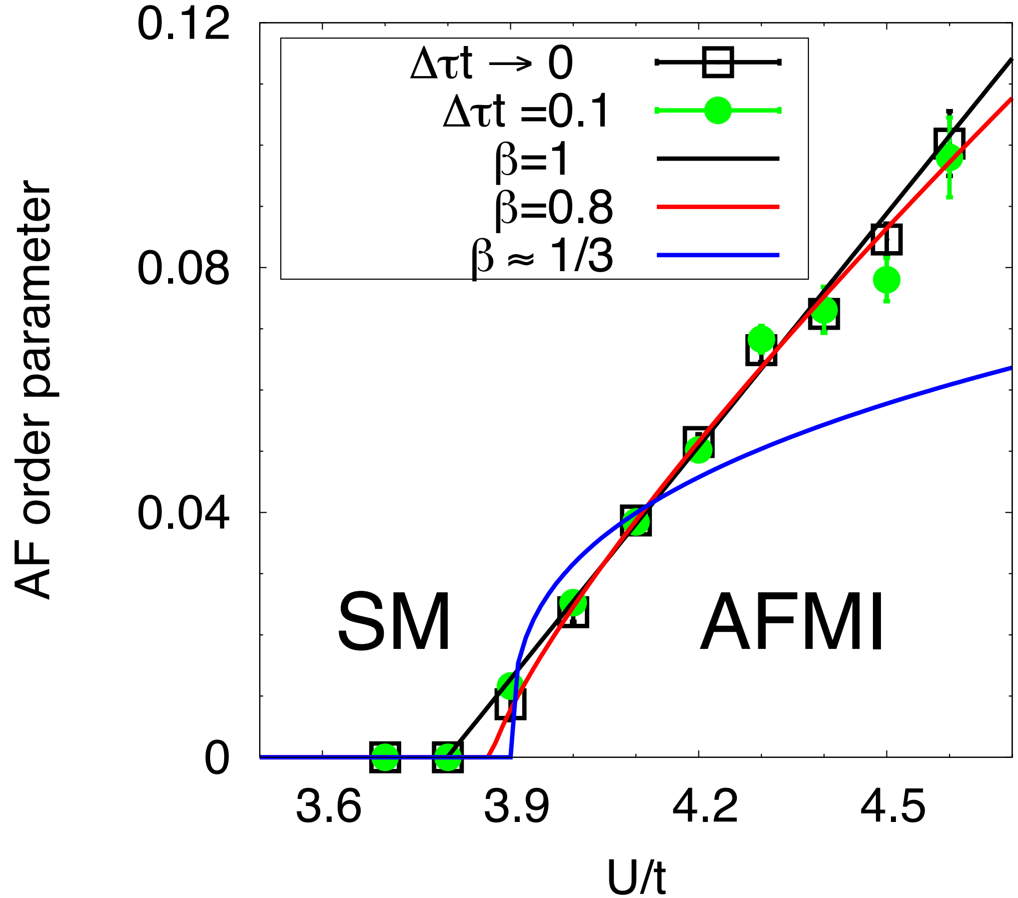
# Now also in germany agree that the spin liquid phase is no longer stable against AF order




From F. Assaad&I.F. Herbut ArXiV :1304.6340

# The AF magnetic order **m** vanishes continuously

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




The best fit gives a SM-AFMI transition at

$U_c/t$=3.869(13) β=0.80(4)

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

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

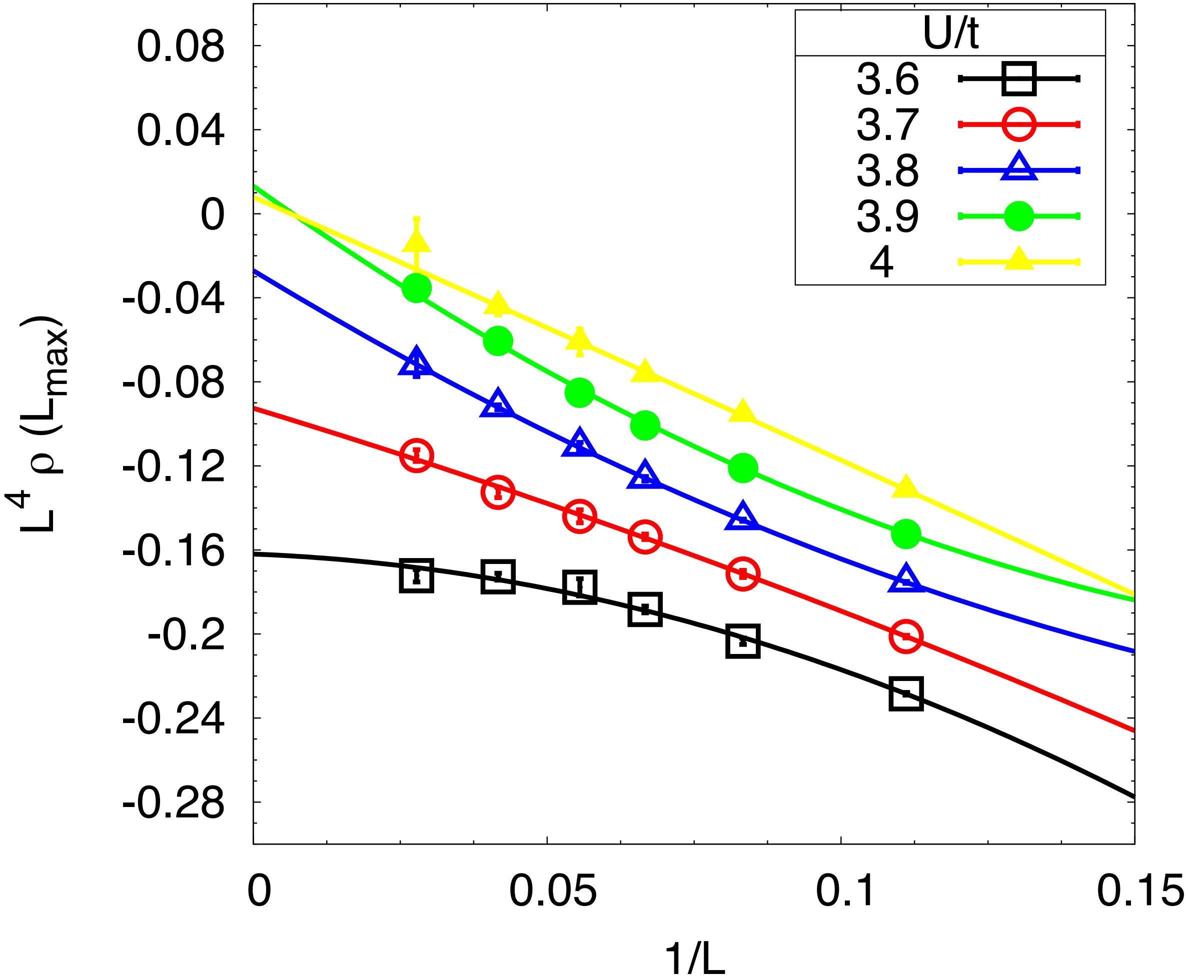
Due to commensurate Friedel oscillation

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

in the semimetallic region U < 3.9

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

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




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

# New phase diagram with large scale simulations

(semi)metal ?? AF-insulator

3.2 $U_c \sim 3.87$ 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 true only for S=1/2 SU(2) models so far

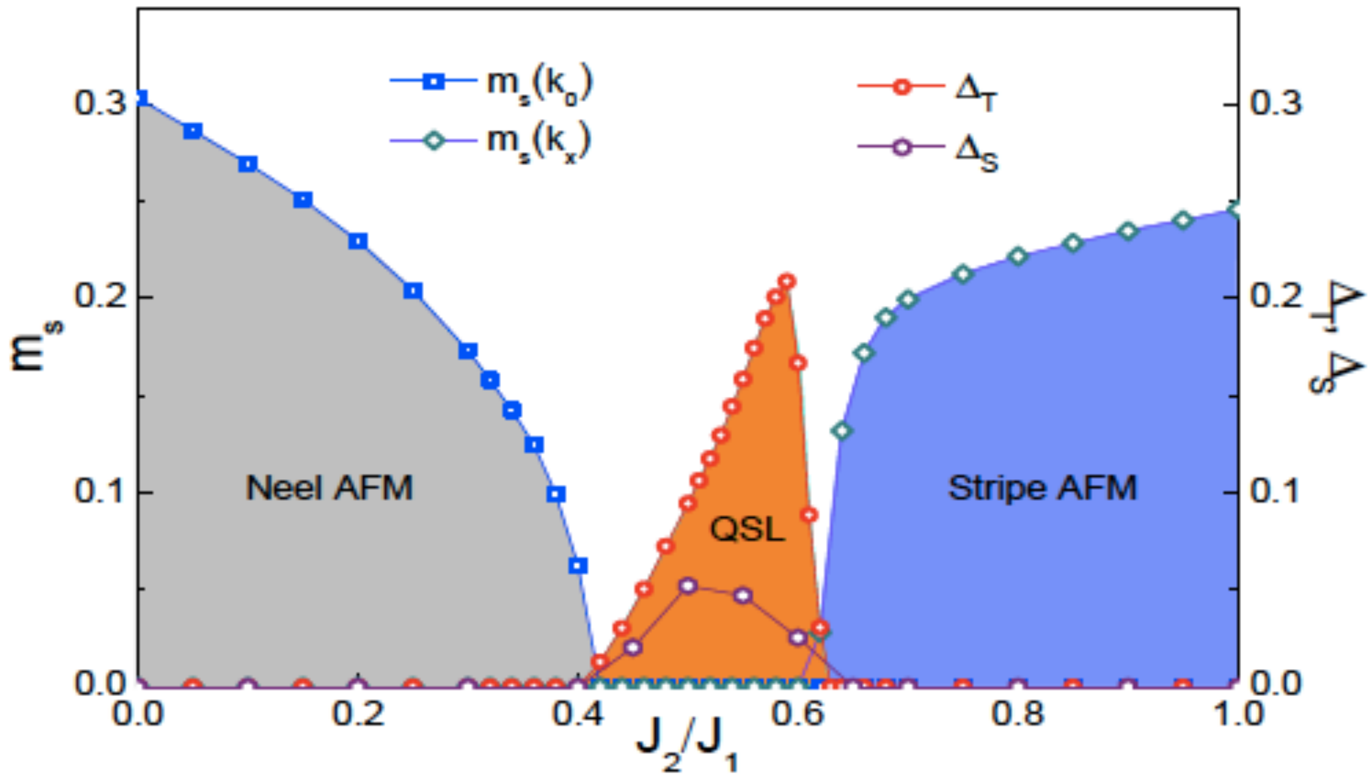
The transition is clearly continuous and we found a critical exponent $\delta = \sim 0.8 \gg 1/3$ (standard ?)

The first continuous metal-insulator transition model.

S.Sorella Y. Otsuka and S. Yunoki, Sci. Rep. 2012,2,992

# $J_1 - J_2$

The $J_1 - J_2$ Heisenberg Model $H = \sum_{\langle ij \rangle} J_1 \vec{S}_i \bullet \vec{S}_j + \sum_{\langle\langle ij \rangle\rangle} J_2 \vec{S}_i \bullet \vec{S}_j, (J_1, J_2 > 0)$




DMRG results show gapped Z2 QSL

H.-C. Jiang *et al.* PRB 86, 024424 (2012)

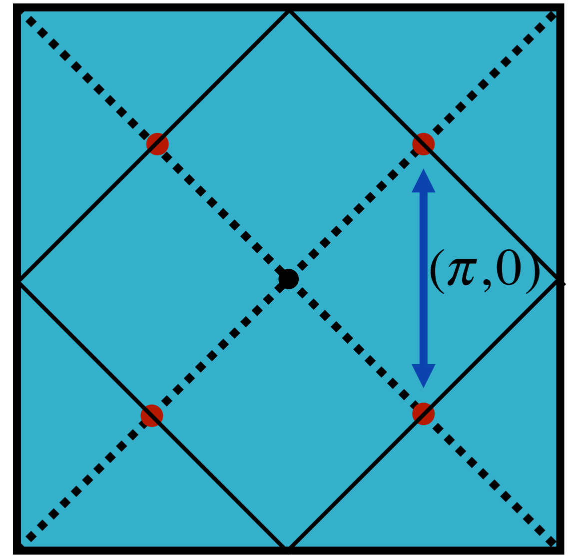
- ground state S=0

projected fermionic RVB state

$$|\Psi_V\rangle = P_{Gutz.}|\psi_{MF}\rangle$$

hopping + pairing → $\Delta_{x^2-y^2} + \Delta_{xy}$

Z2 spin liquid




- S=1 $(\pi,0)$ excitation

$$|\Psi_{S=0}\rangle \xrightarrow{\text{two spinons, } (\pi,0)} |\Psi_{S=1,(\pi,0)}\rangle$$

- A genuine fingerprint is a gapless mode at (π,0)
  N.B. a gapless antiferromagnet has a gap at (π,0)

## variance extrapolation

To improve the variational wave function:

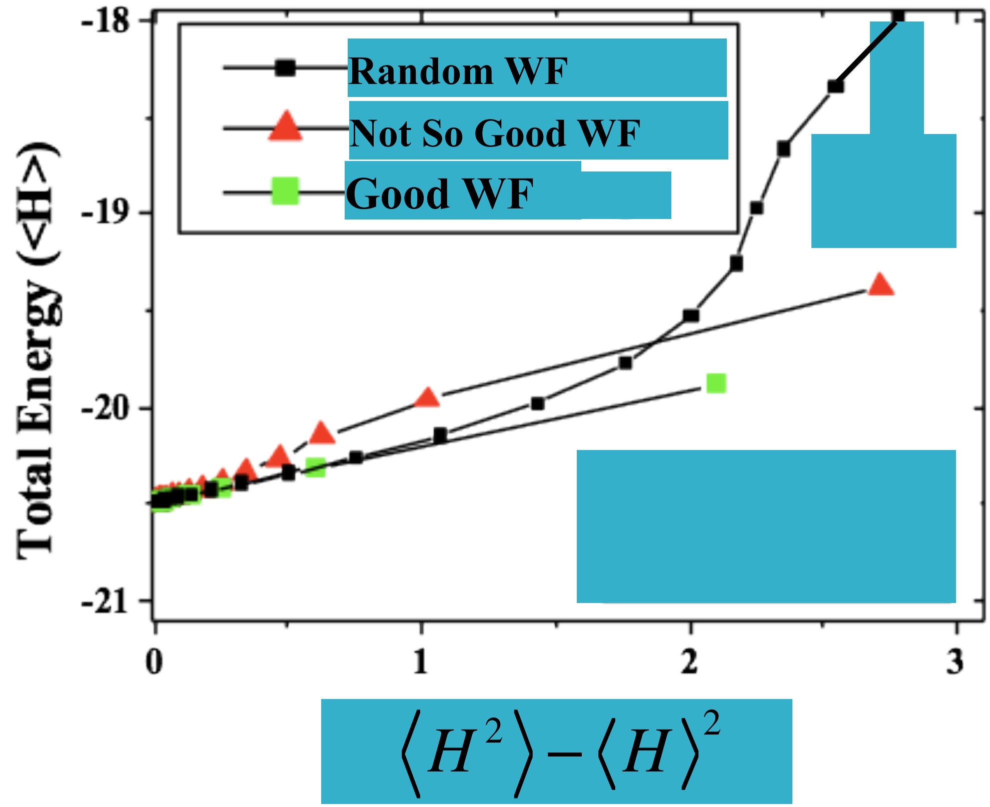
# Lanczos steps

$$|\Psi_p\rangle = \left(1 + \sum_{k=1}^{p} \alpha_k H^k\right)|\Psi_v\rangle$$

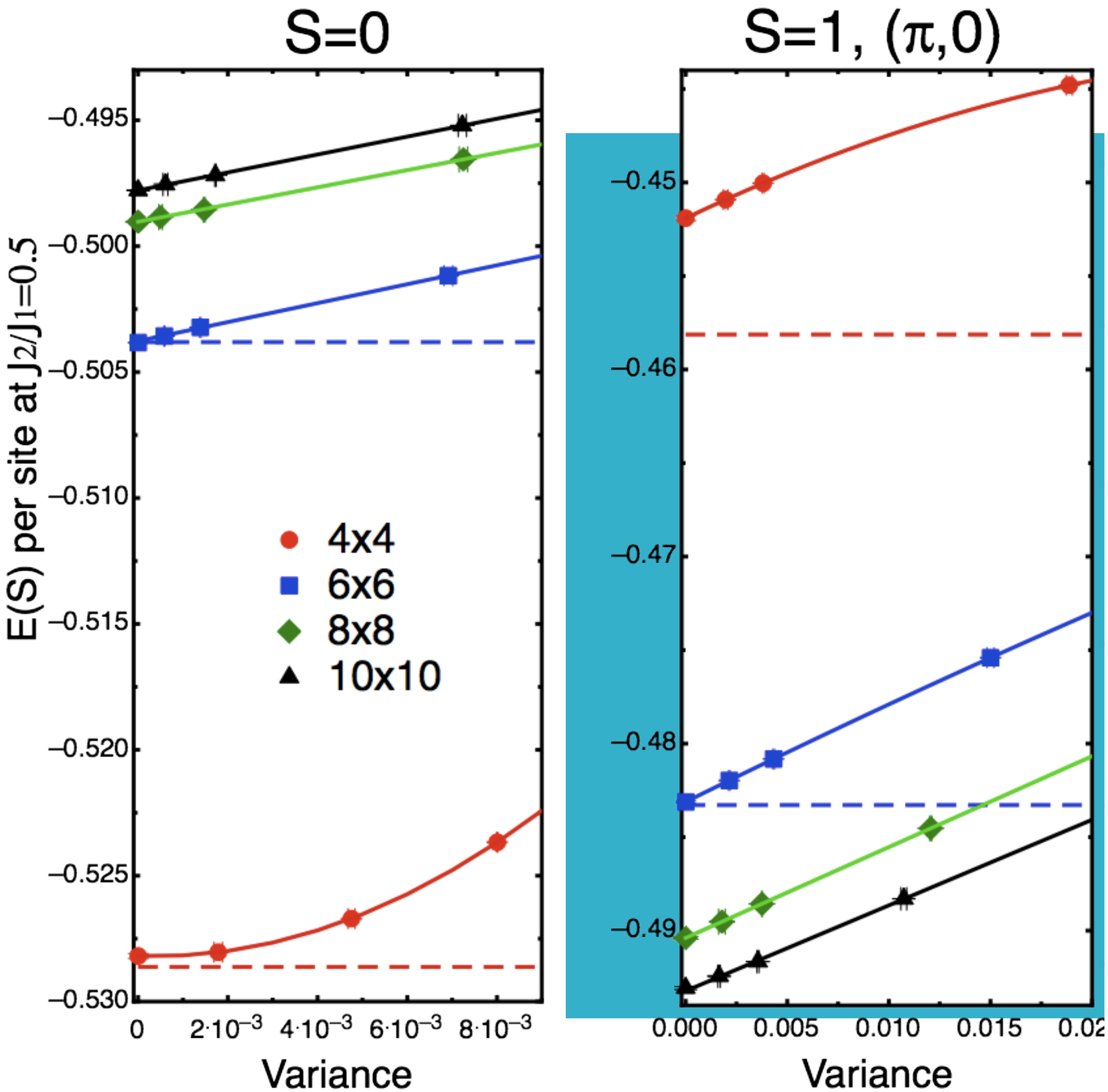
$$p = 0,1,2$$

With QMC scaling $L^{p+2}$

S.S. PRB '01




Effect of different WF

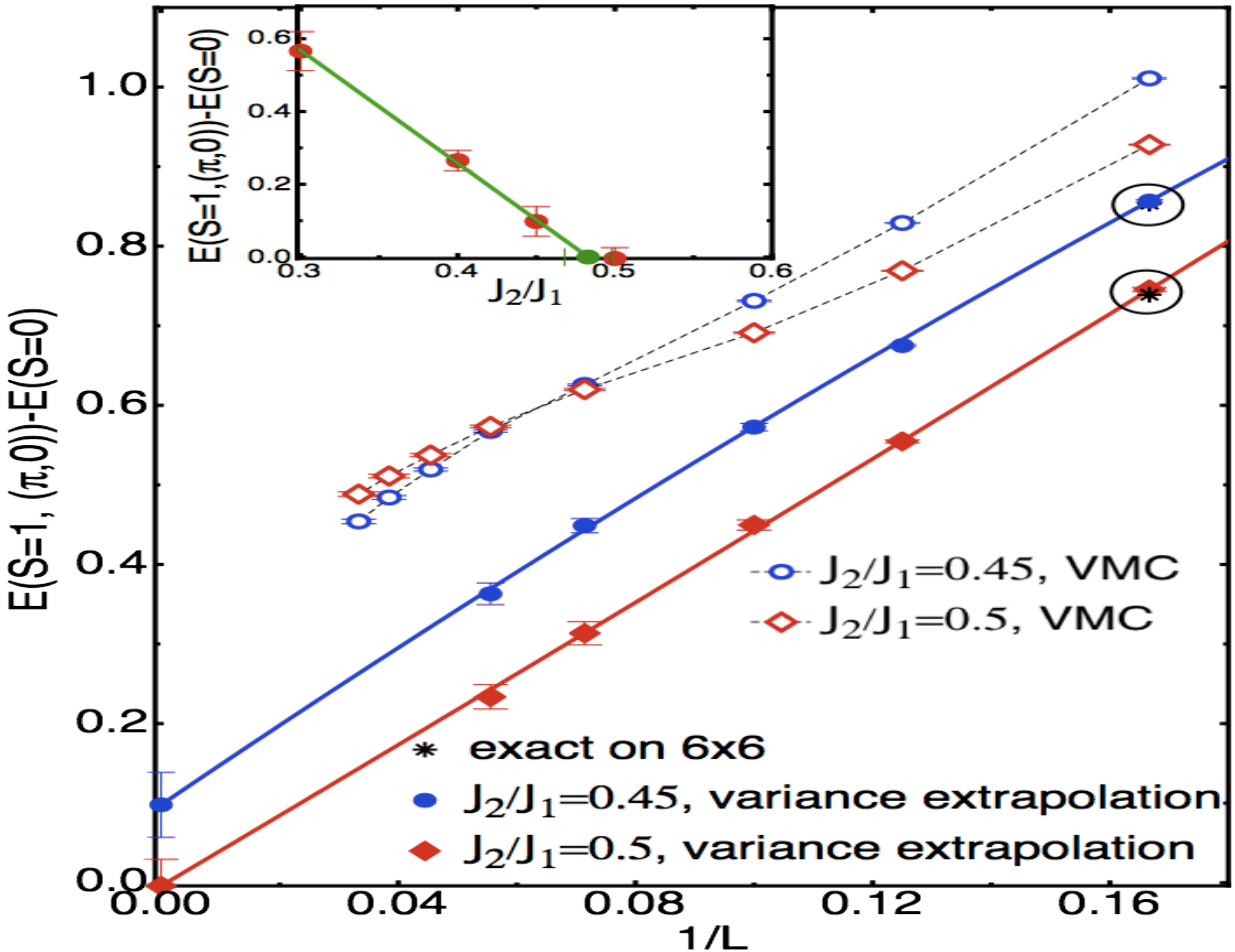



Perfect linearity is obtained for large sizes and exact on 6x6

The wf. seems more accurate for larger clusters!!

# A new (measurable) effect: zero spin-gap at (π,0)

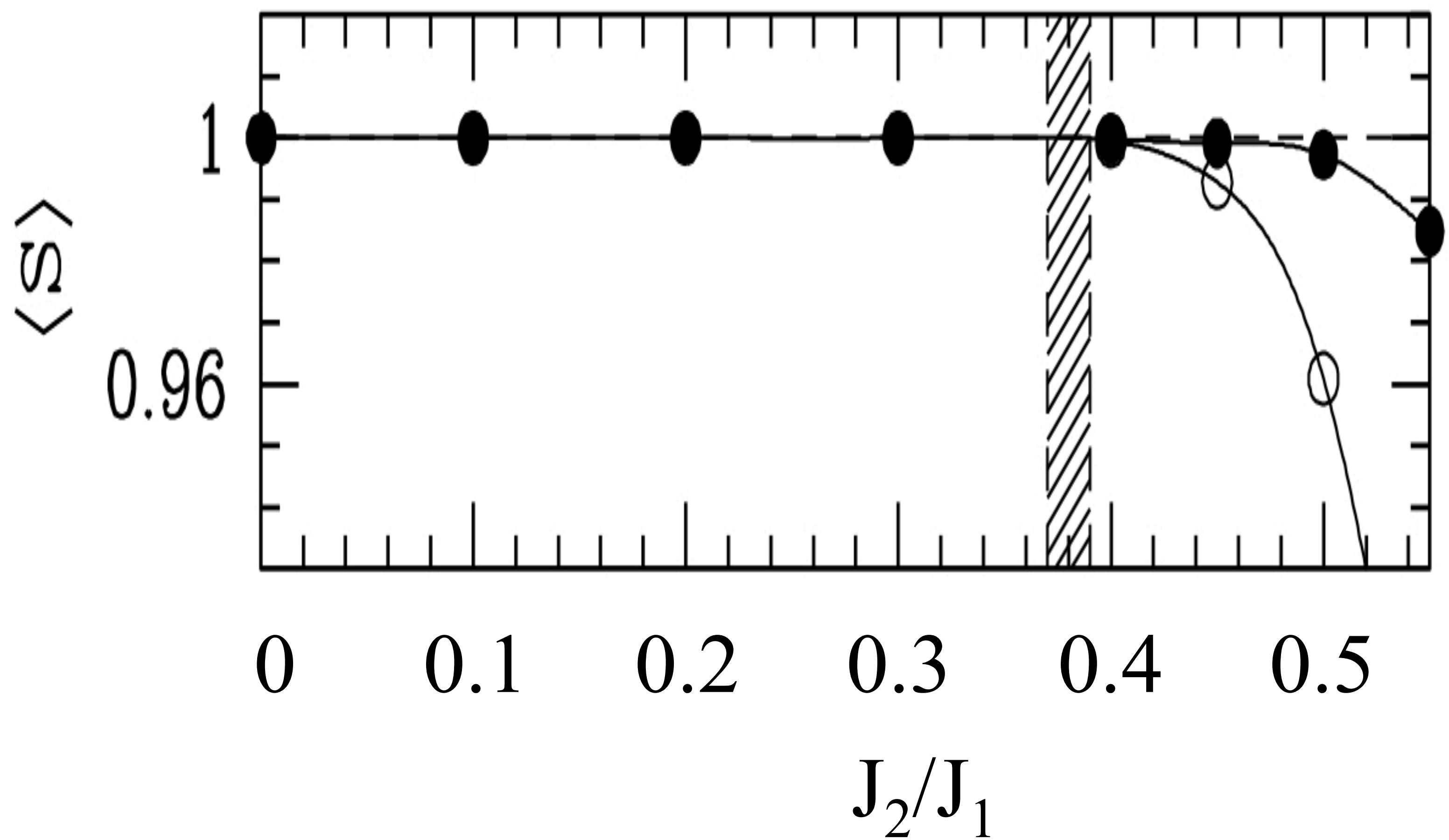
W. Hu F. Becca and S.S. **arXiv:1304.2630**



In an antiferromagnet the sign of the ground state wave function is given by a simple rule (Marshall):

$$\text{Sign} = (-1)^{\#\text{ spin up in one sublattice}}$$

The average sign relative to the Marshall sign (6x6).



We are temped to make the following simple conclusion:

**When there is no sign problem it is hard to stabilize a spin liquid.**

Spin ½ systems are equivalent to bosonic systems and they cannot avoid Bose condensation at T=0 without being protected by the sign, the key ingredient that distinguishes a “classical” from a quantum wave function.

This is indeed a quite precise statement…

Given a wave function $\psi(x)$ define:

$$\psi_S(x) = Sign\left[\psi(x)\right]$$

In any trivial classical state

$$\psi_S^{A+B}(x) = \psi_S^A(x) \times \psi_S^B(x)$$

For instance Marshall sign $(-1)^{\text{Number of spin up in one sublattice}}$

This means that a spin liquid is possible only when the sign is entangled and protects from trivial boson condensation.