Recent results on the Hubbard model by quantum Monte Carlo & Petaflop computers

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Vallico, Apuan Alps, 29 August 2012

Motivations

→ The Hubbard model has been a long standing model for too many years.

→ Experiments on optical lattices can solve fundamental questions about the model (soon?)

→ Quantum Monte Carlo can exploit massive parallelism in modern supercomputers, a factor ~10000 faster than 20 years ago.

Sampling the <Sign> is the easiest task for parallelism, replicas and average!

→ More information (before optical lattices)?

Outline

From RVB insulator to High-Tc superconductivity with no electron-phonon coupling and repulsion (!)

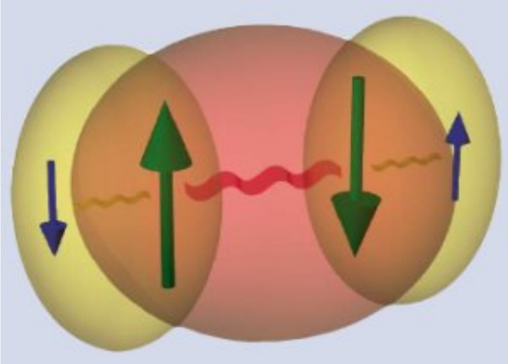
<u>Quantum Monte Carlo and Petaflop supercomputer</u>
a new possibility to understand electron correlation

The honeycomb lattice → no spin liquid phase
(contrary to previous claims)

How to survive with the sign problem?
Recent results by massive sampling/extrapolation:
Small but non vanishing effect → Phase diagram?

Resonating valence bond (RVB)

In this theory the chemical valence bond is described as a singlet pair of electrons



$$\frac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle\big)\left[\Psi_a(r)\Psi_b(r') \;+\; a\leftrightarrow b\right]$$

spin up and spin down electrons in a spin singlet state
a and *b* are nuclear indexes

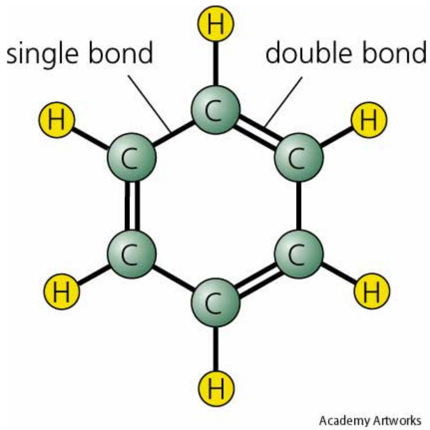
Linus Pauling

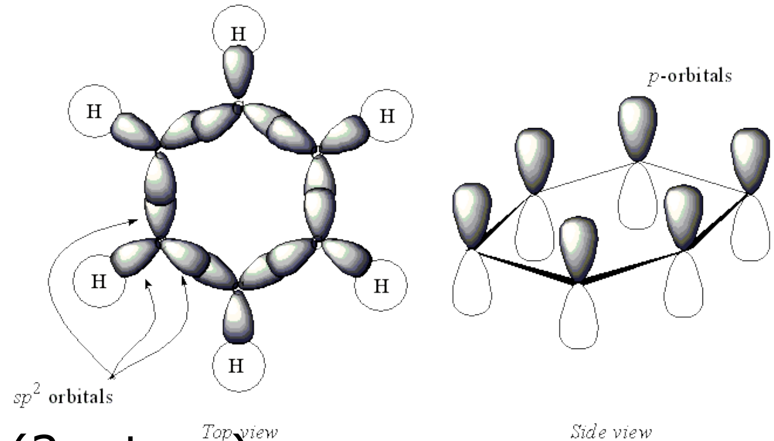
The true quantum state of a compound is a superposition or resonance of many valence bond states. The superposition usually improves the variational energy of the state.

L. Pauling, Phys. Rev. **54**, 899 (1938)

Example of RVB

Benzene C_6H_6



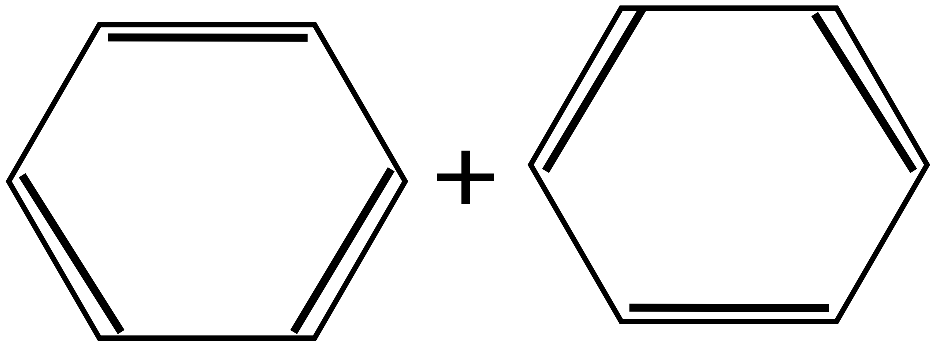


6 valence electrons in 6 sites ($2p_z$ type)
two ways to arrange nearest neighbor bonds (Kekule' states)

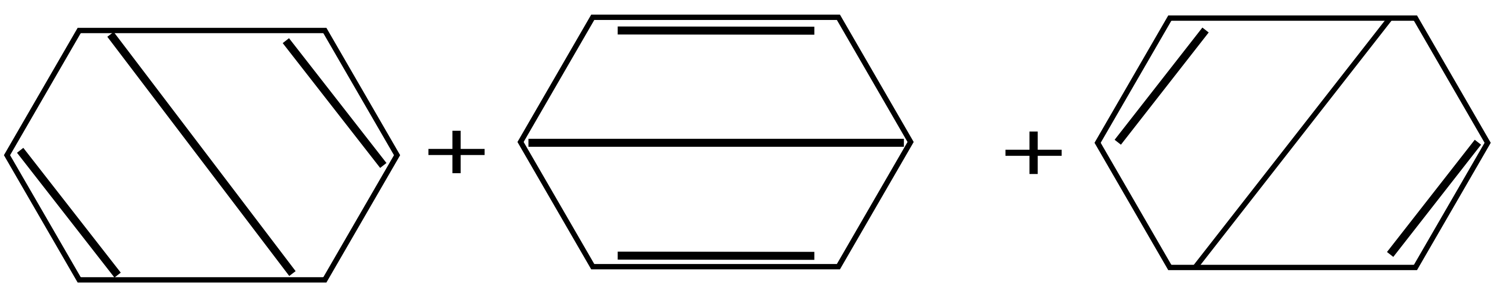
The rule: two singlet bonds cannot overlap on the same Carbon atom otherwise two electrons feel a too large Coulomb repulsion.

$$— = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)\left[\Psi_a(r)\Psi_b(r') + a \leftrightarrow b\right]$$

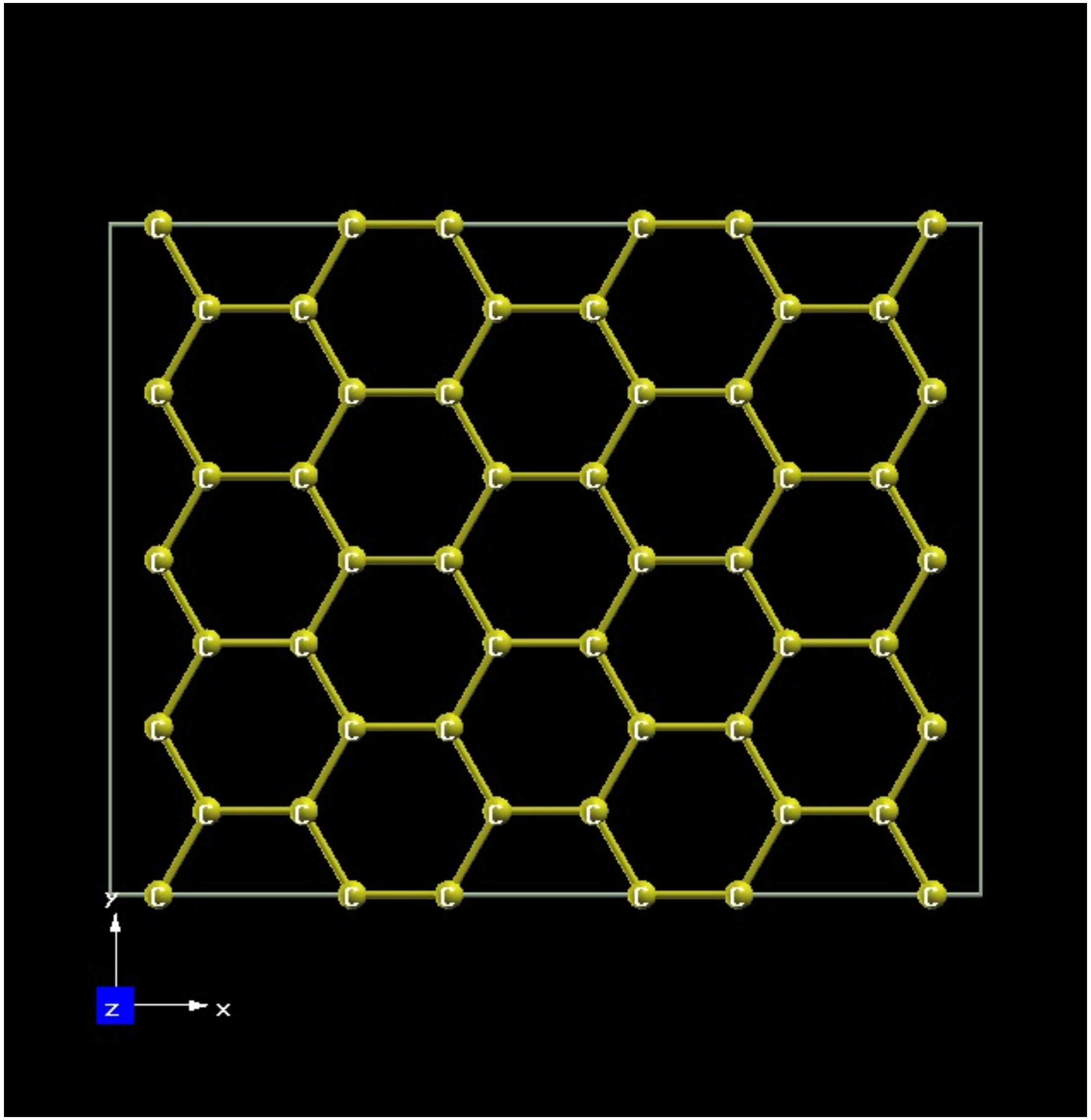
Kekule’ valence bonds



Dewar valence bond (believed less important)

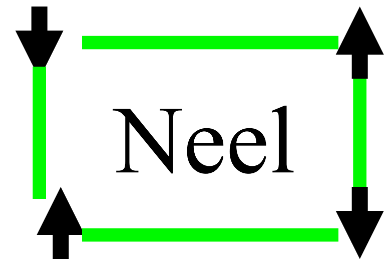


Graphene layers can be experimentally prepared



Definition of spin liquid

A spin state with

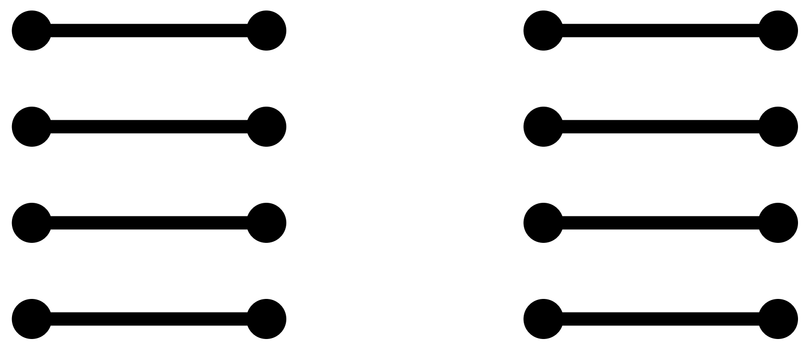


no magnetic order (classical trivial)

no broken translation symmetry (less trivial):

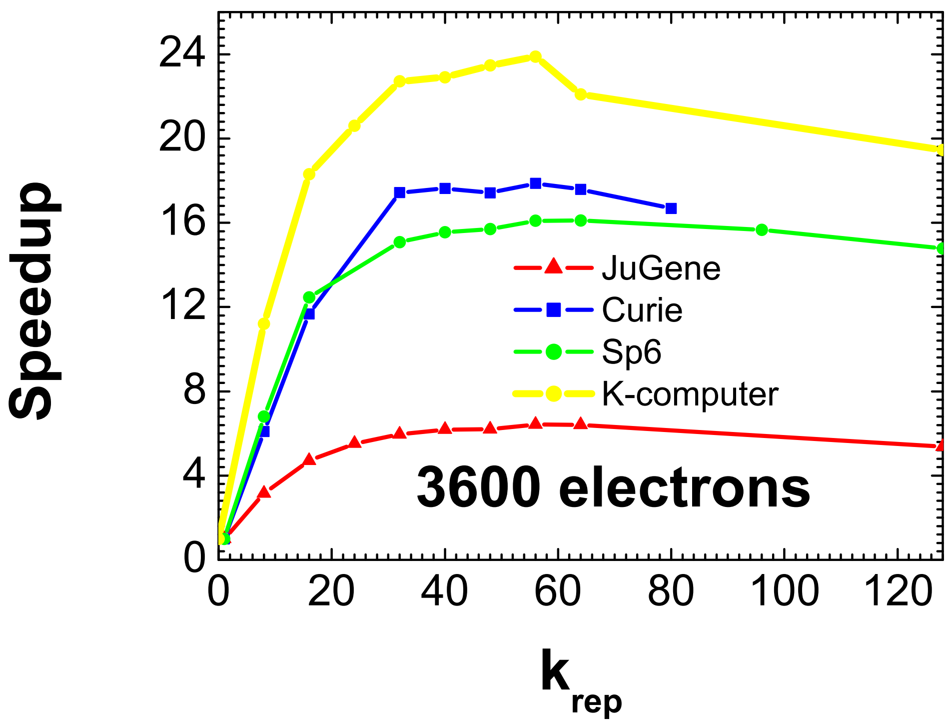
no Dimer state

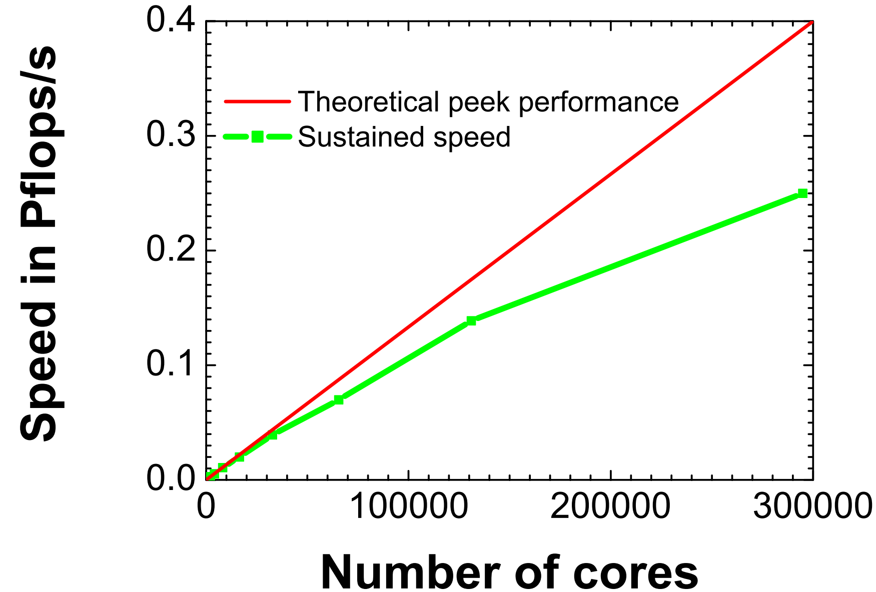
(Read,Sachdev)



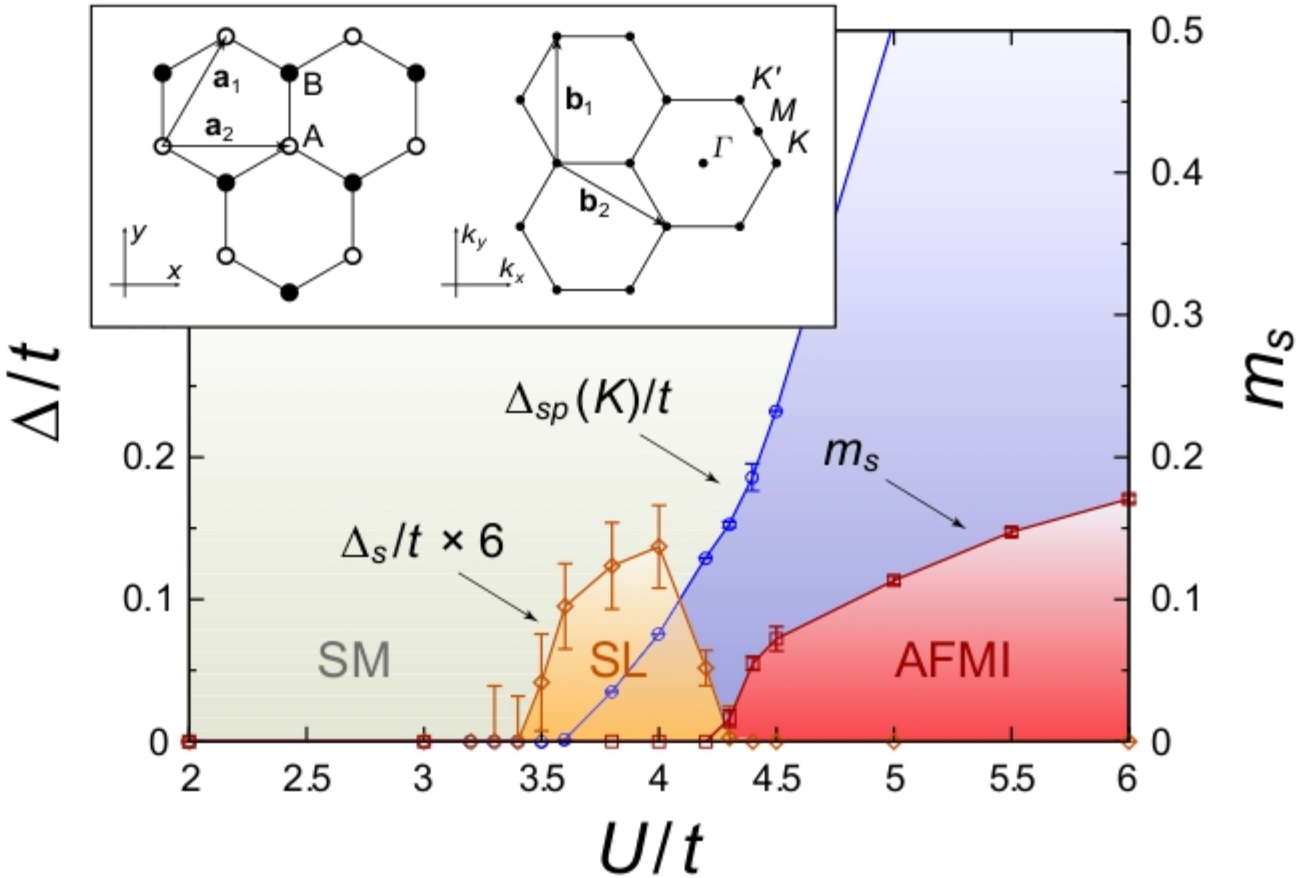
is a spin liquid

Recent development of supercomputers is based on an increased number of cores/node. But in this trend the bandwidth of the node increases much slower and the ‘’delayed updates’’ technique becomes more and more crucial. Essentially one tranforms matrix-updates (bandwidth limited) in matrix-matrix fast operations LxK_{rep}.





Recent exciting result on the Hubbard model… Muramatsu 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:

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

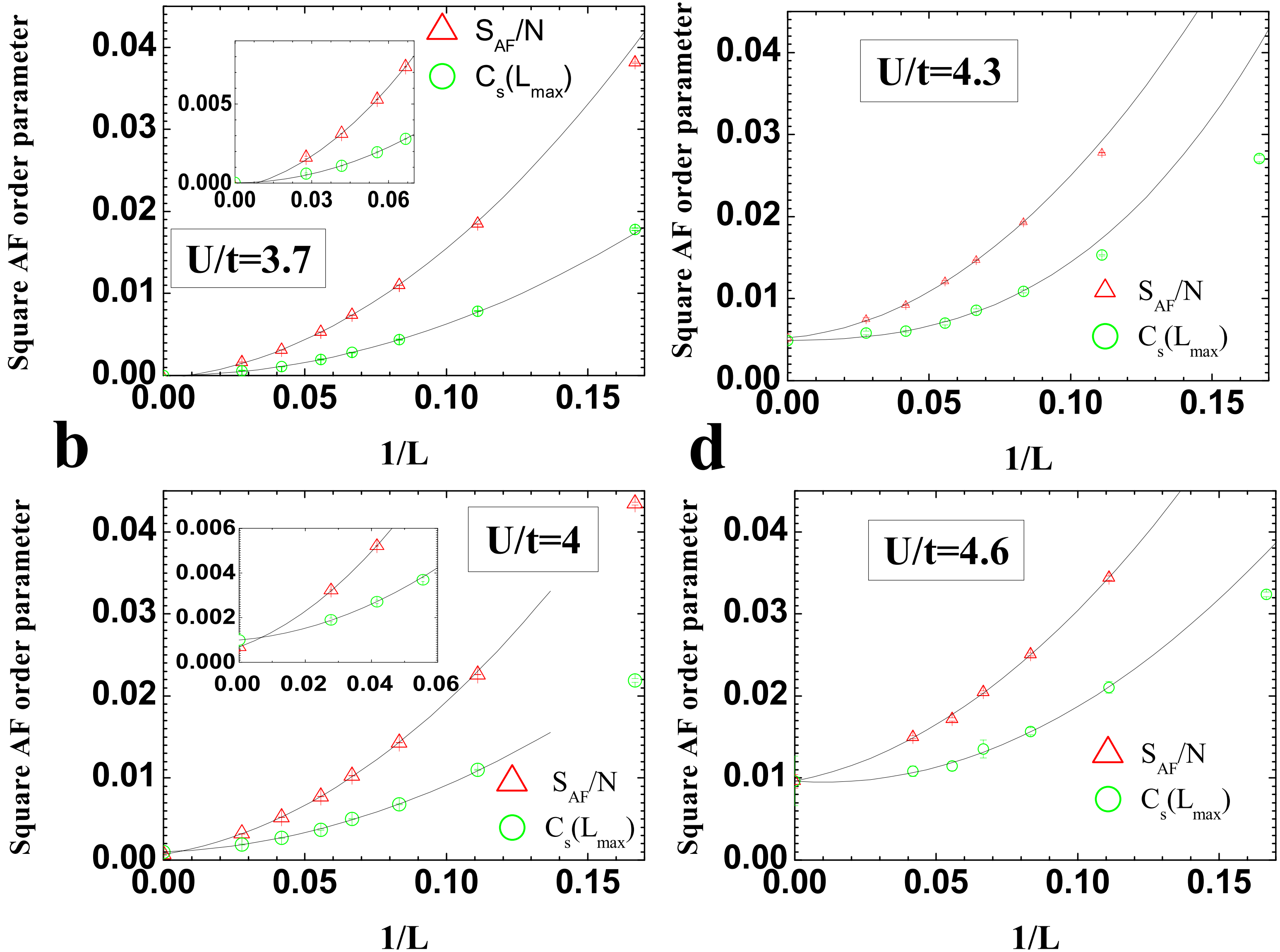
and, if $|\psi_T\rangle$ is a Slater determinant, $U_\sigma(\tau,0)|\psi_T\rangle$ can be evaluated.

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

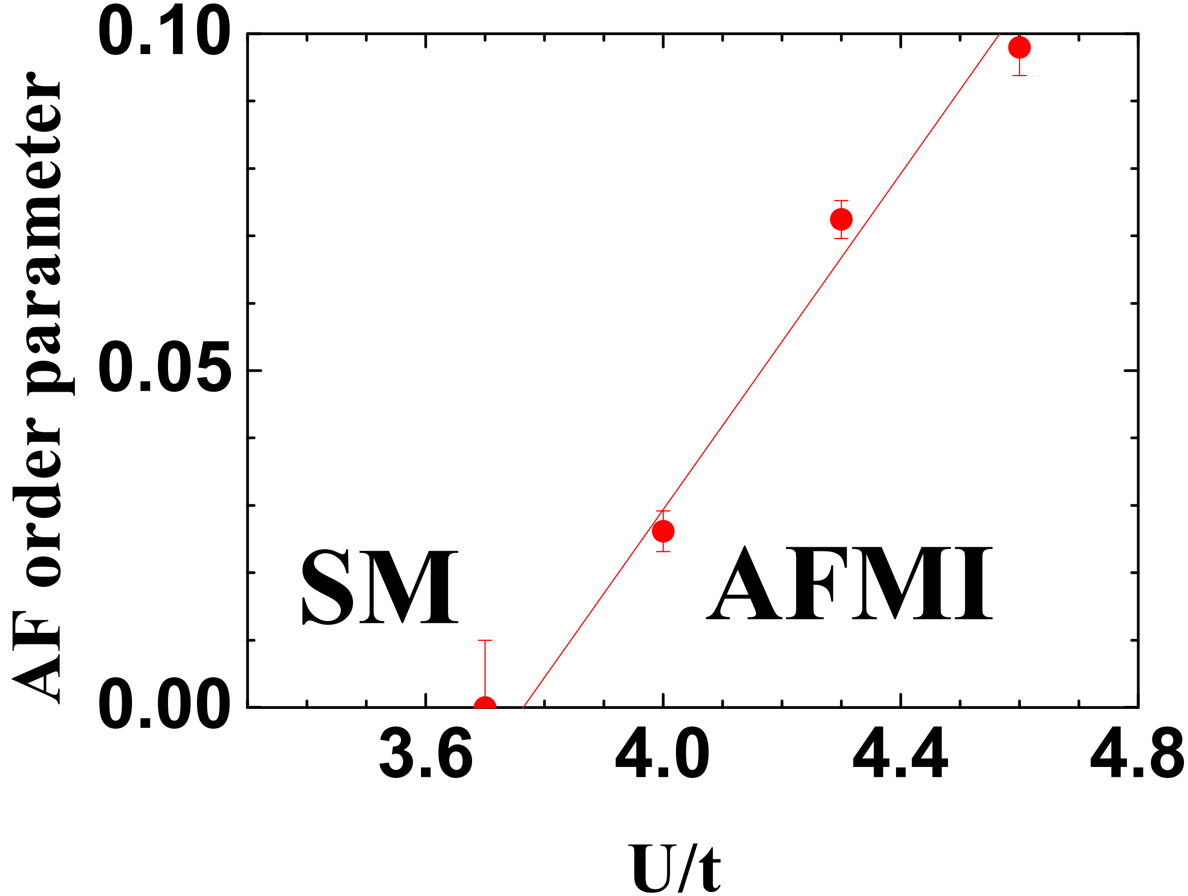
$$\langle\psi_0|O|\psi_0\rangle = \frac{\langle\psi_{\tau/2}|O|\psi_{\tau/2}\rangle}{\langle\psi_\tau|\psi_T\rangle} = \frac{\sum_{\{\sigma\}} W[\sigma]O[\sigma]}{\sum_{\{\sigma\}} W[\sigma]}$$

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

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

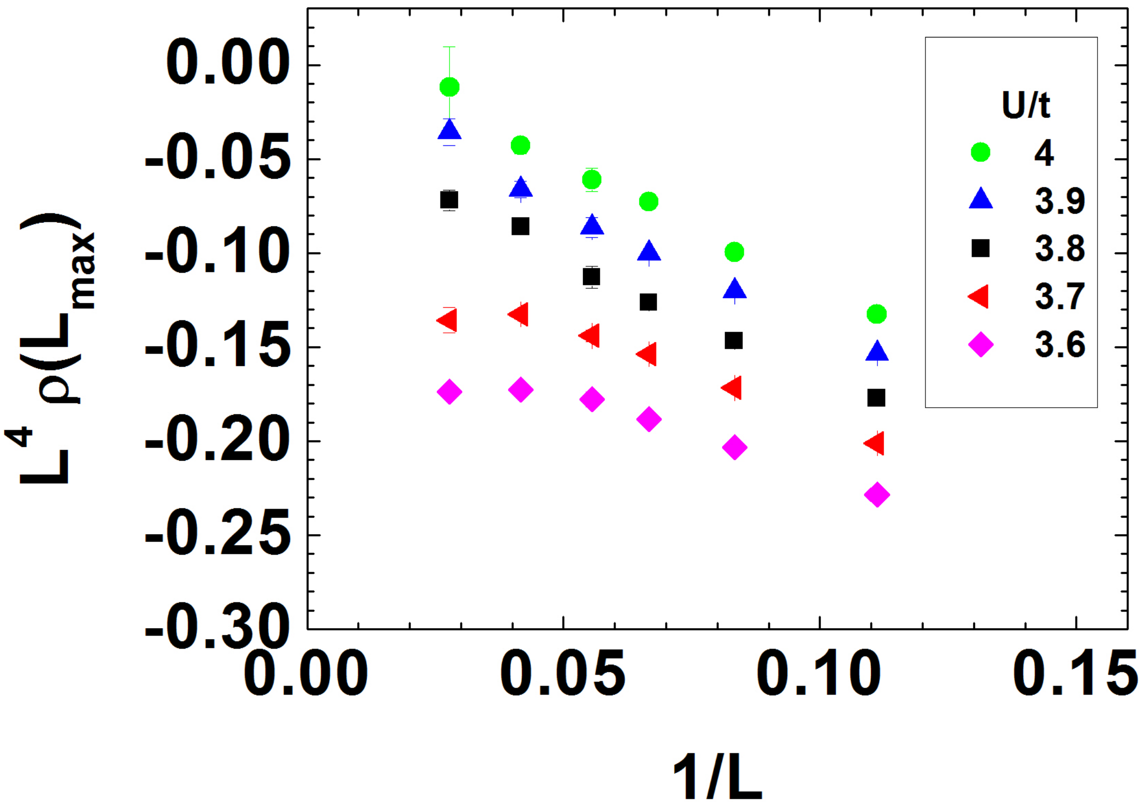


arXiv:1207:1783 S. S. , S. Yunoki, and Y. Otsukay (2012)



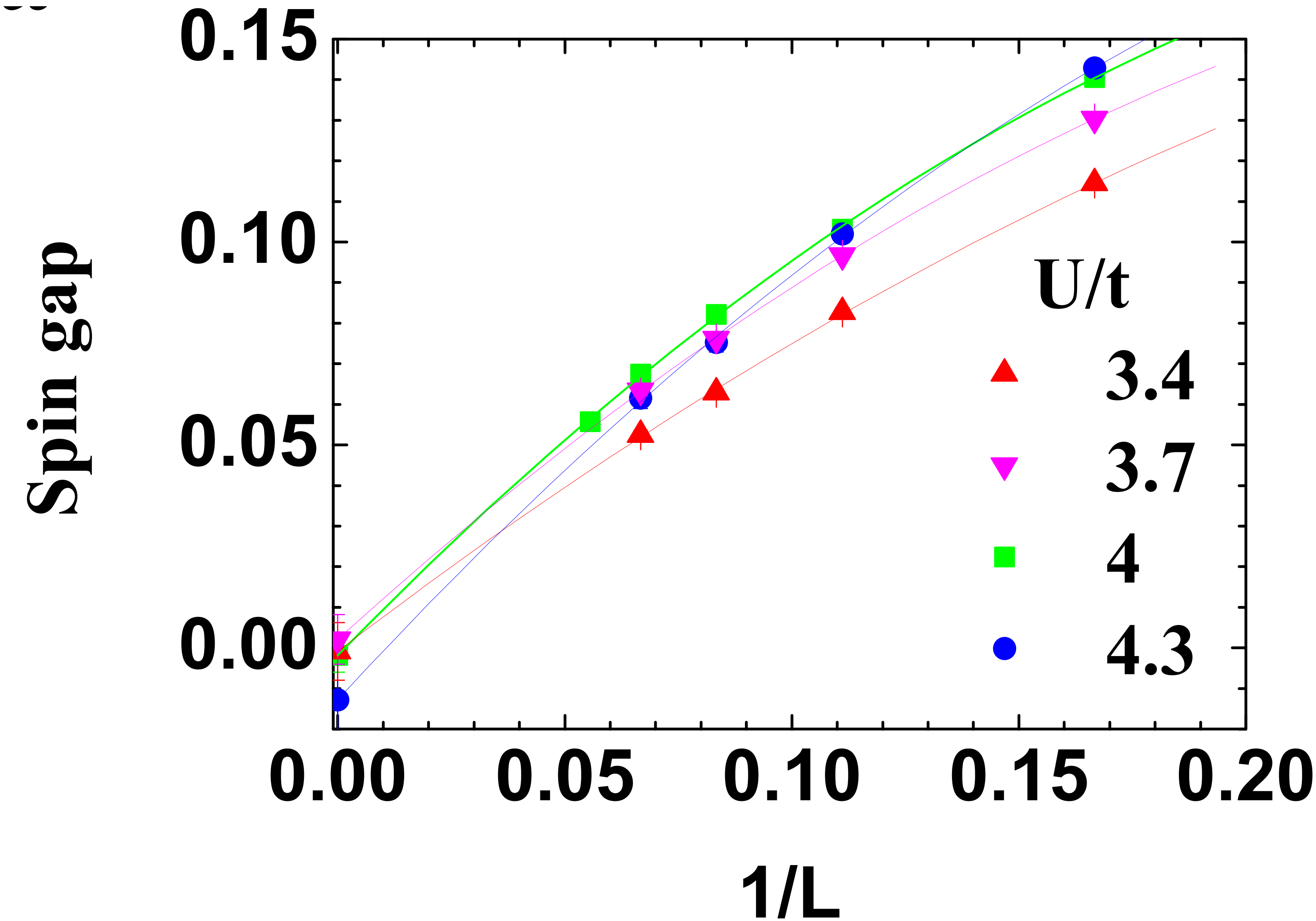
0.10
0.05
0.00
AF order parameter
SM
AFMI
3.6
4.0
4.4
4.8
U/t

The charge-charge correlation should decay as $1/r^4$ in the semimetal, as opposed to exponential in the insulator, thus by plotting $L^4\rho(L_{\max})$



We clearly see a charge transition at U/t~3.75(5) consistent with the magnetic one→ no spin liquid):

The proposed spin liquid should have a spin gap
…but no spin gap was found by direct evaluation



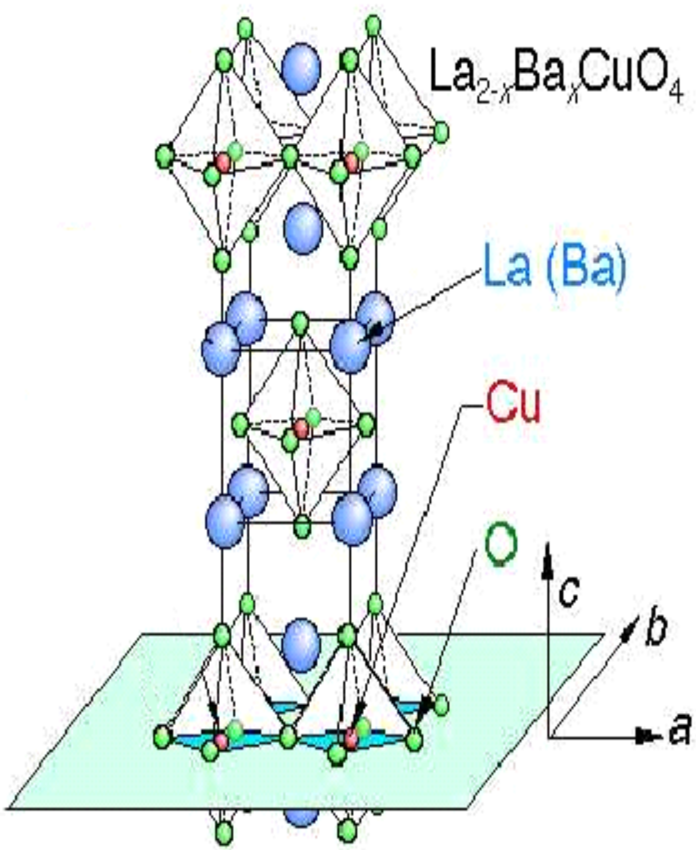
First results on a model without sign problem:

Much larger size → no spin liquid in a model with no frustration.

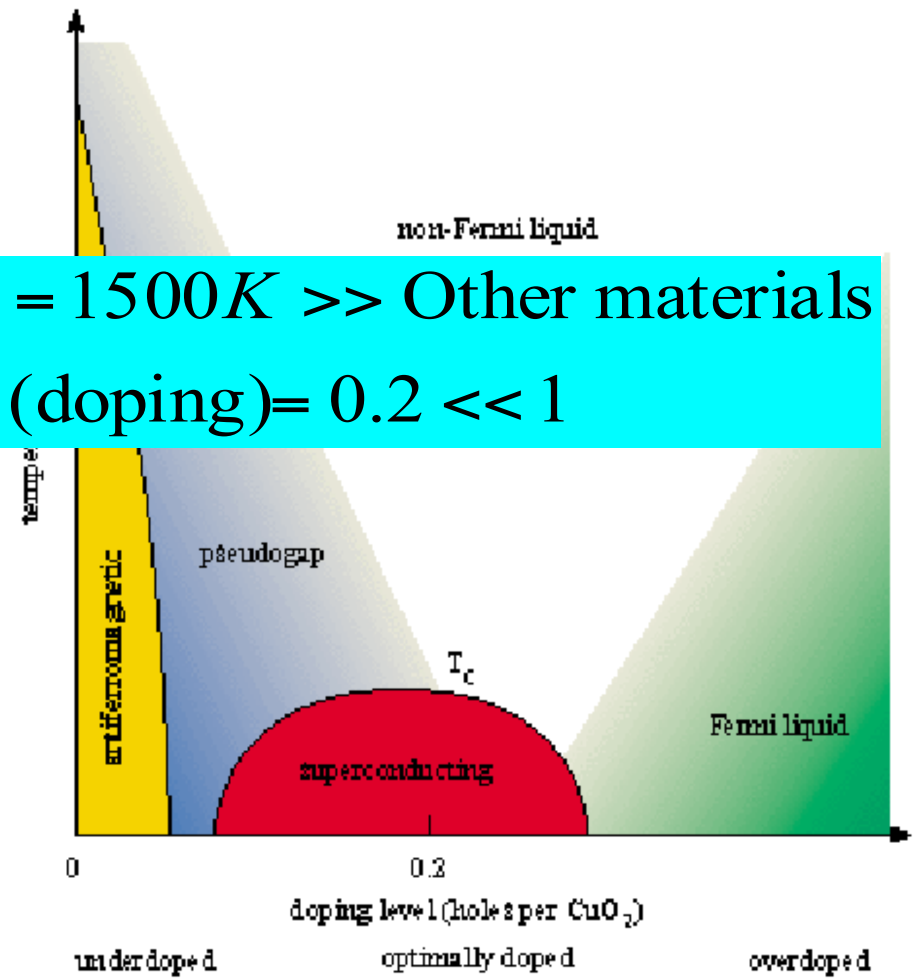
As a consequence of the Murphy's law
''No interesting results can be obtained with a fermionic model without sign problem….''
but this is under debate. There are exceptions, but have to be also tested on much larger sizes and lower temperatures.

Cuprates

quasi-2D structure



Phase diagram: temperature vs. doping

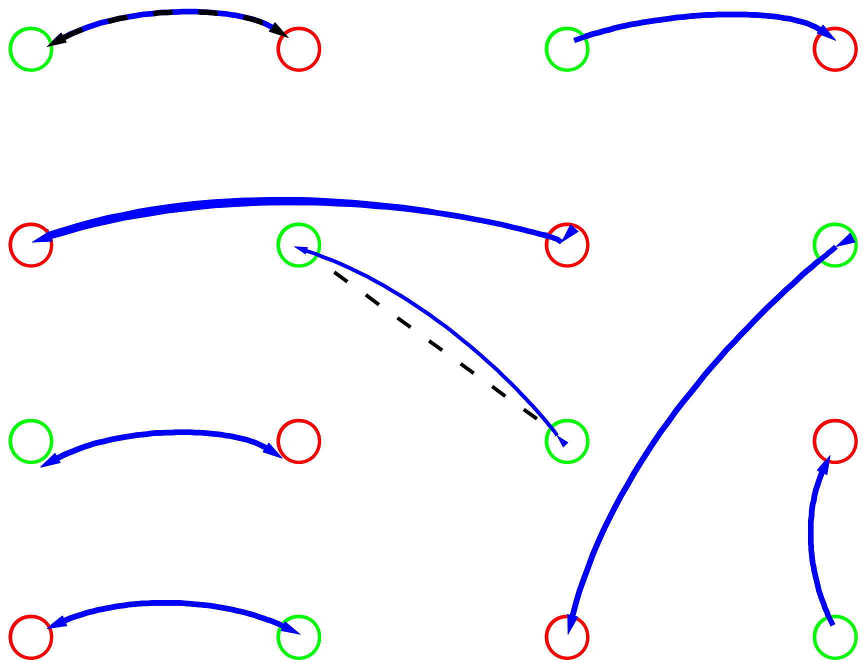


$J = 1500K$ >> Other materials

δ (doping)= 0.2 << 1

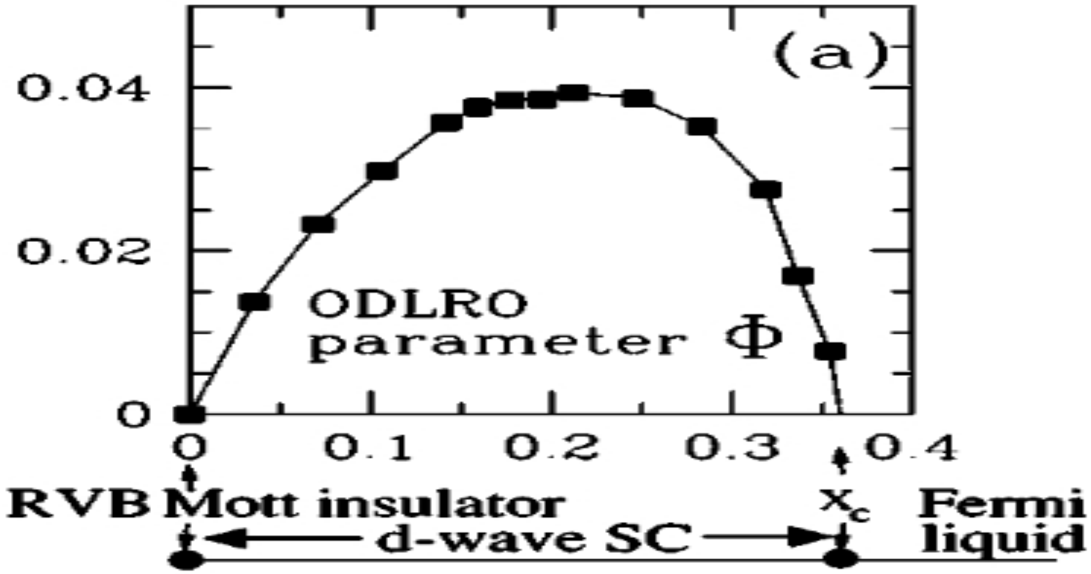
From RVB to superconductivity

$$\left[N(\#\text{particles}), \theta(\text{phase coherence})\right] = -i$$



The presence of holes (empty sites) allows charge (super-) current and <u>superconductivity</u>

RVB→ the actual order parameter ~ x (doping)



$$\Phi = \left\langle \left(c^{+} c^{+} \right)_{d-wave} \right\rangle \neq 0 \ \text{ only for } x > 0$$

This is the most important feature of an RVB superconductor

Is there superconductivity in the square lattice Hubbard U>0?
At half-filling (as in the honeycomb) it is magnetic (not RVB)

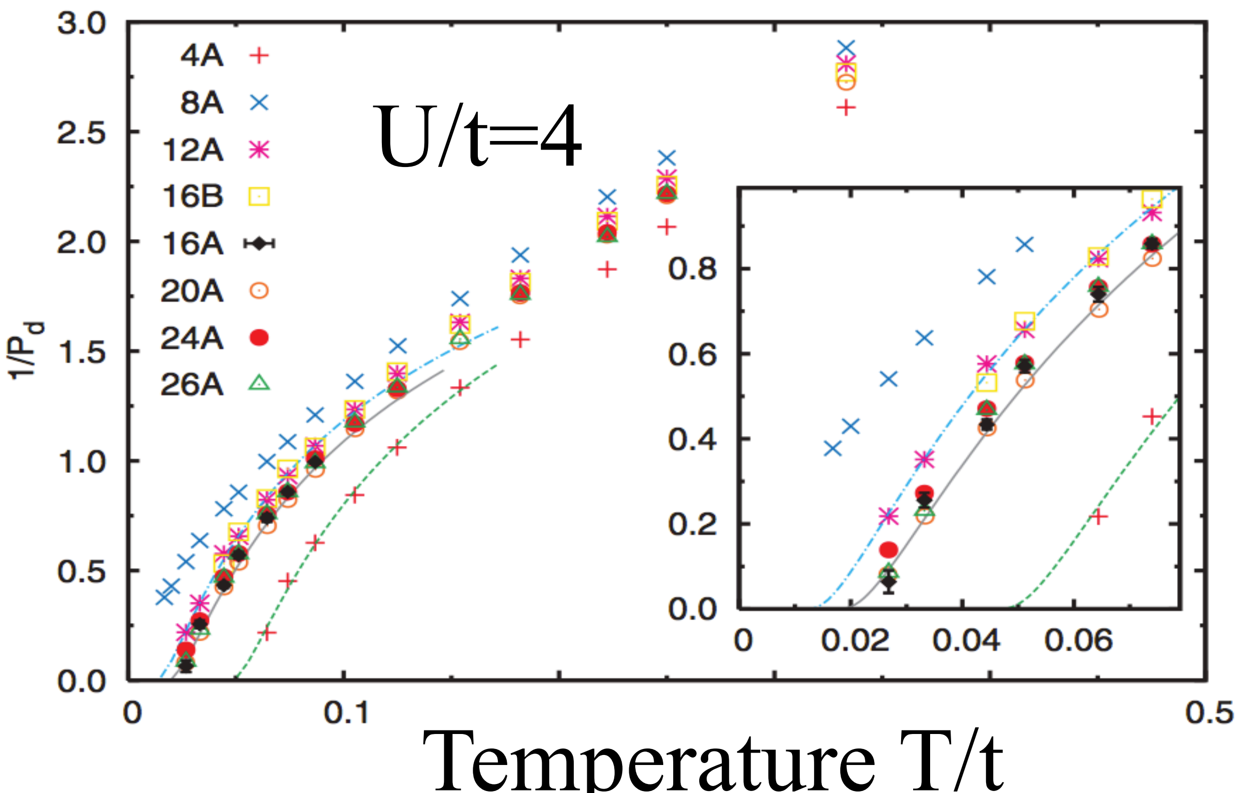


FIG. 3 (color). Inverse d-wave pair-field susceptibility as a function of temperature for different cluster sizes at 10% doping. The continuous lines represent fits to the function $P_d = A\exp[2B/(T-T_c)^{0.5}]$ for data with different values of z_d. Inset: magnified view of the low-temperature region.

From T. Maier et al. PRL ’05 U/t=4 Cluster DMFT

A very controversial results (see e.g. our VMC).
Older paper by S. Zhang et al. PRL'97 by CPQMC

$\Delta_{i,j} = c_{i\uparrow} c_{i\downarrow} + c_{j\uparrow} c_{i\downarrow}$ destroys a singlet bond.

ODLRO if , for $|i - j| \to \infty$:

$$\left\langle \psi_0 \middle| \Delta^+_{i,i+x} \Delta_{j,j+x(y)} \middle| \psi_0 \right\rangle = +(-\text{ d-wave}) P_d^2 > 0$$

$|\psi_0\rangle$ is estimated by projection techniques:

$$|\psi_0\rangle = \exp(-H\tau)|\psi_T\rangle \text{ for } \tau \to \infty$$

with constraned path approximation (CPQMC)

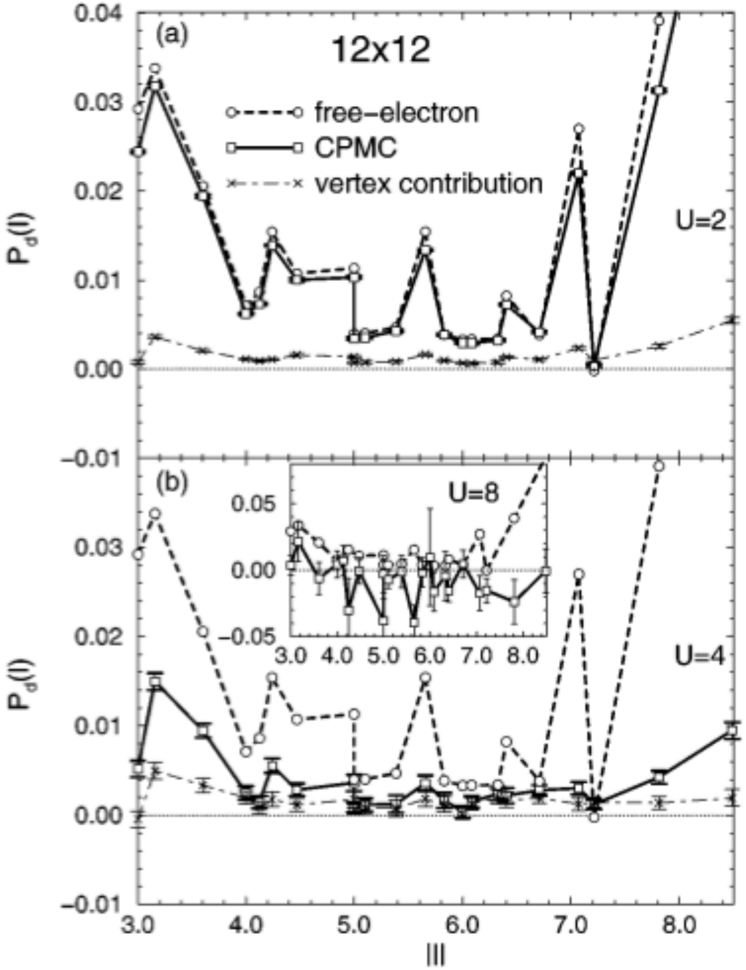


FIG. 2. Long-range behavior of the $d_{x^2-y^2}$ pairing correlation function versus distance for 0.85 filled 12×12 lattice at $U = 2$, 4, and 8. This behavior is shown for the free-electron and CPMC calculations. Also shown is the vertex contribution.

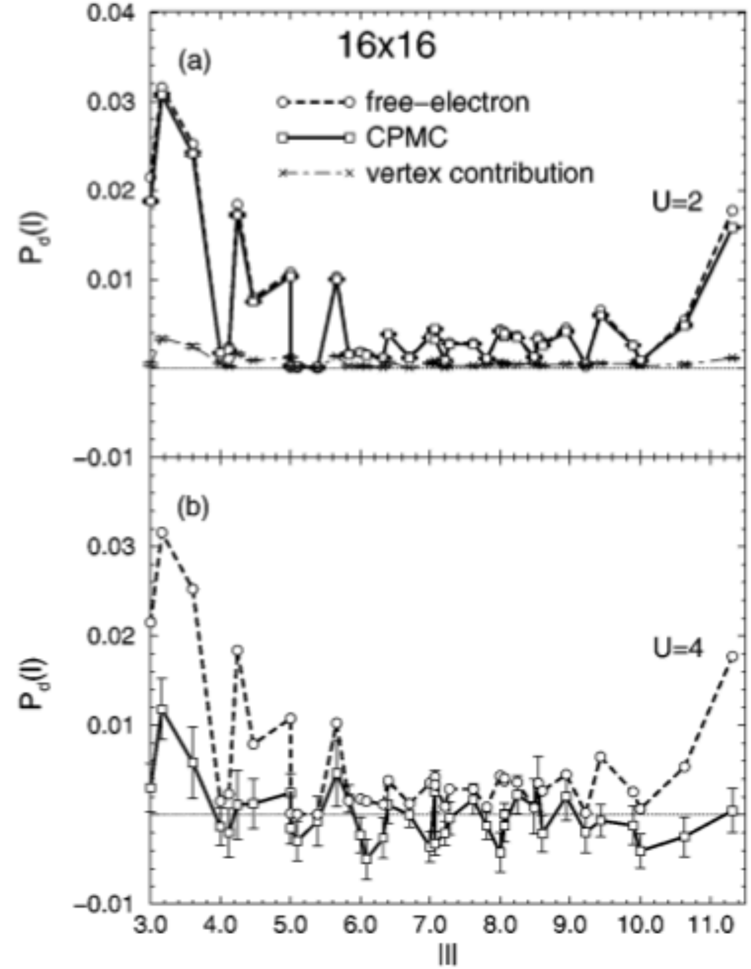


FIG. 3. Long-range behavior of the $d_{x^2-y^2}$ pairing correlation function versus distance for a 0.85 filled 16×16 lattice at $U = 2$ and 4. This behavior is shown for the free-electron and CPMC calculations. Also shown is the vertex contribution.

Note the huge scale of the pairing !!!!

For a lattice model we use here the Gutzwiller wf

$$\psi_{RVB} = \exp(-g\sum_i n_{i\uparrow}n_{i\downarrow})\ \exp\sum_{i,j} f_{i,j}\ \underbrace{(c^+_{i,\uparrow}c^+_{j,\downarrow} + c^+_{j,\uparrow}c^+_{i,\downarrow})}_{\text{Singlet bond}}\ \left|0\right\rangle$$

where f is determined by one parameter $\Delta^{BCS}_{x^2-y^2}$

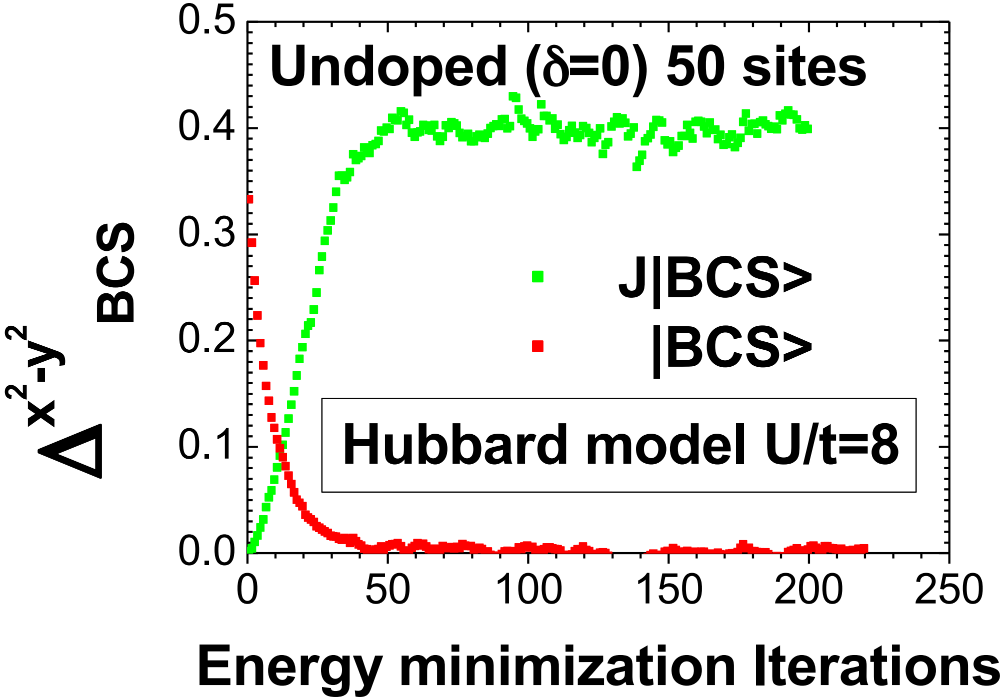
$$H_{BCS} = \sum_{k,\sigma} \varepsilon_k c^+_{k,\sigma} c_{k,\sigma} + \Delta^{BCS}_{x^2-y^2} \sum_k (\cos k_x - \cos k_y) c^+_{k\uparrow} c^+_{-k\downarrow} + h.c.$$

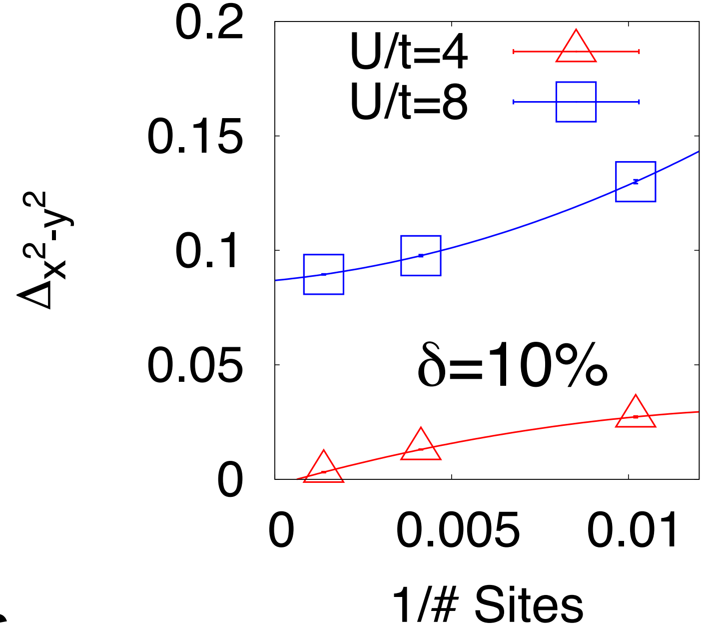
and $\varepsilon_k = -2t(\cos k_x + \cos k_y) - \mu$, i.e. $f_k = \Delta_k \Big/ \varepsilon_k + \sqrt{\varepsilon_k^2 + \Delta_k^2}$

Use of Quantum Monte Carlo mandatory:
Gutzwiller approximation too poor in general,
e.g. Mott transition in cubic lattices…etc.

Why we have to optimize J(=g) and $\Delta^{BCS}_{x^2-y^2}$?

Hubbard Model: $H = -t \sum_{<ij>,\sigma} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_i^\uparrow n_i^\downarrow$





In mean field (BCS) no way to have BCS>0 for U>0

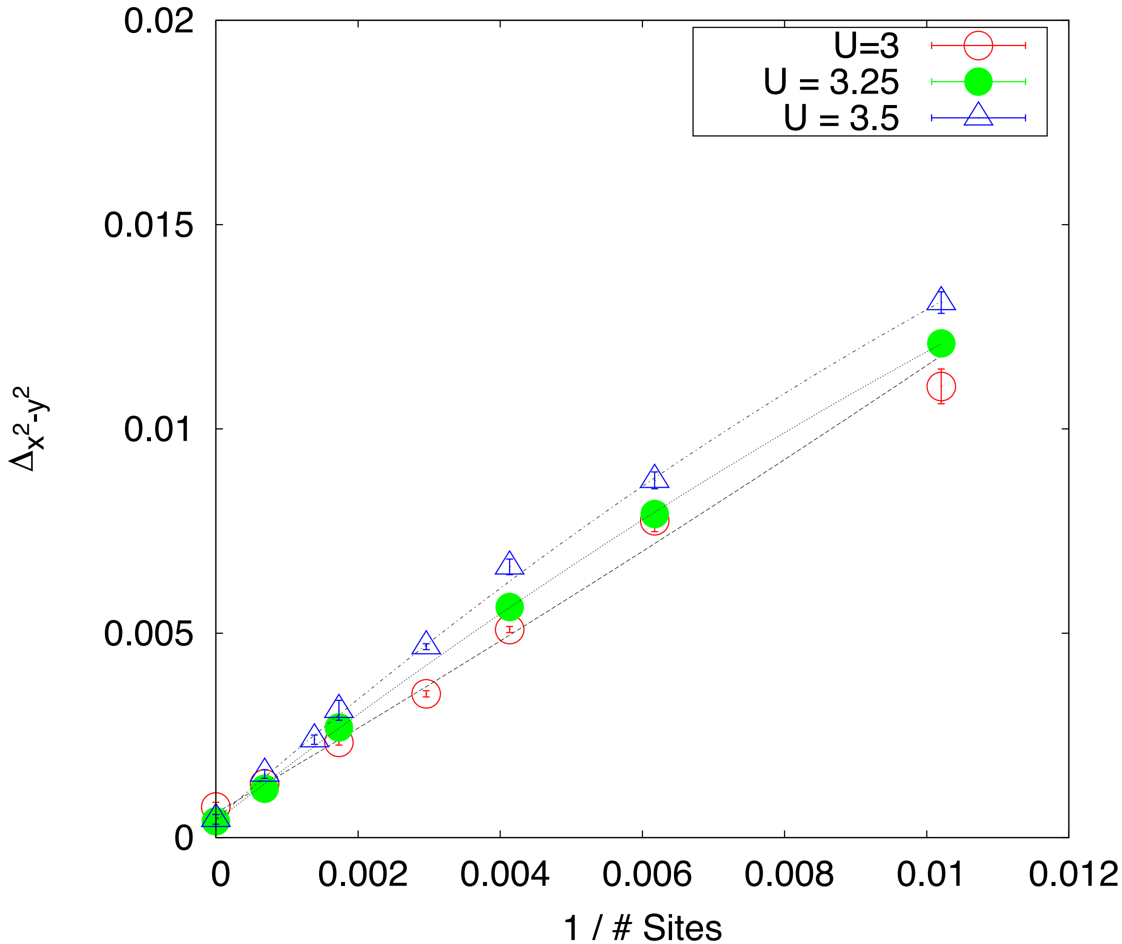
Theorem Lieb '90

Qualitative new features appear if J and BCS are optimized toghether: RVB insulator or supercond.

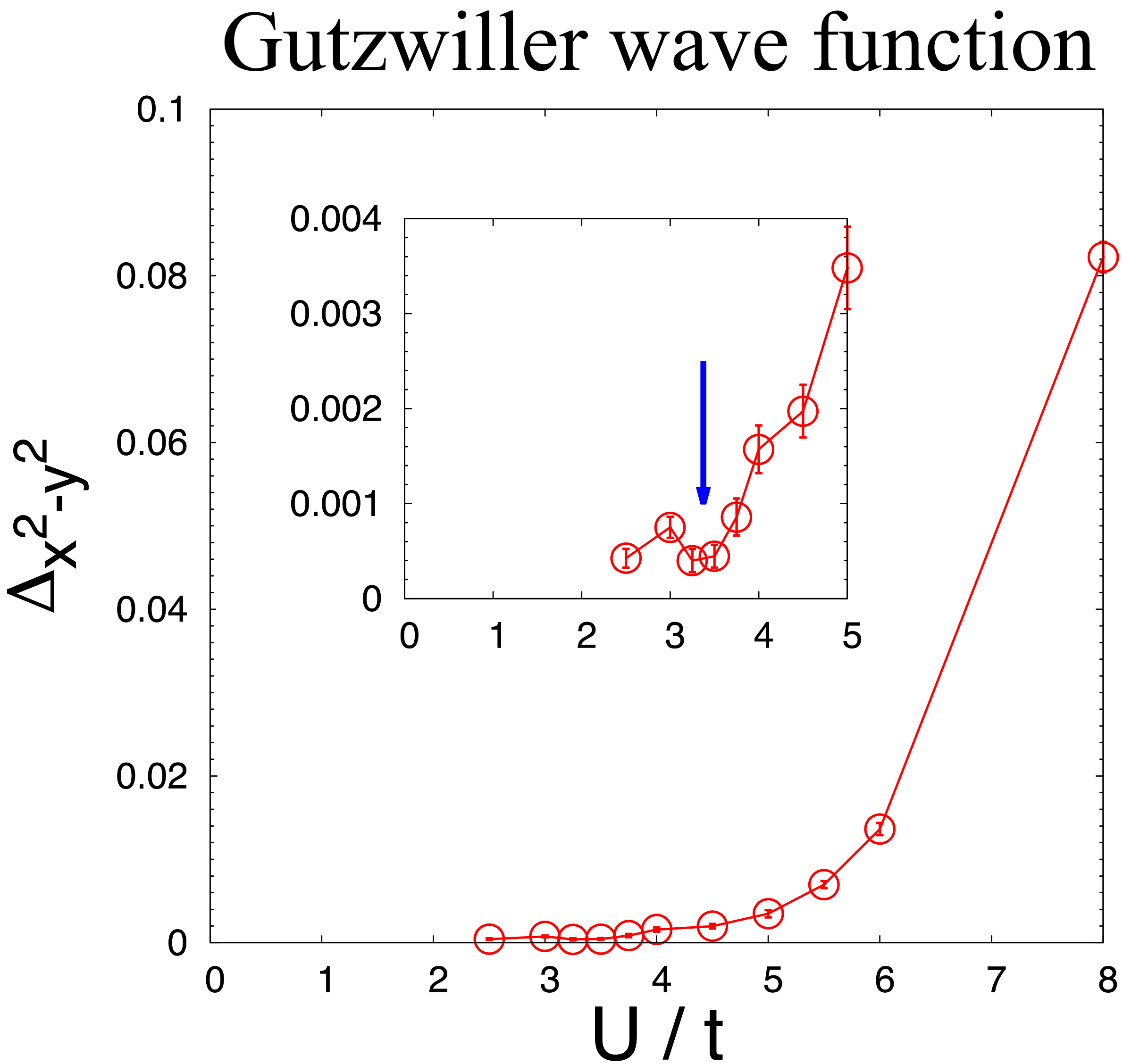
There are ''huge'' finite size effects and

$$\Delta^{BCS}_{x^2-y^2} \sim 0.01 \div 0.001 \ \text{ for \#Sites } \to \infty$$

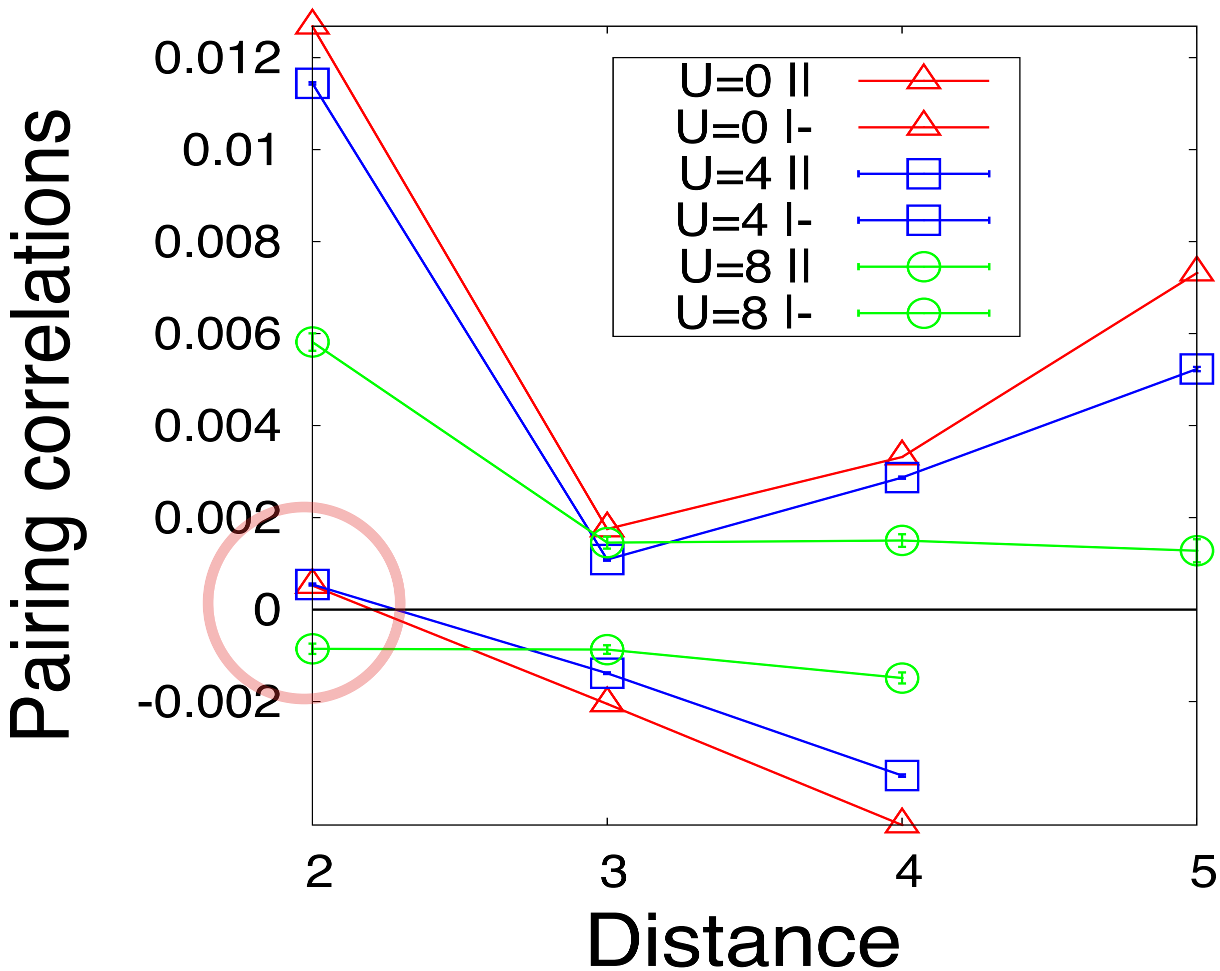
$$P_d^2 \sim (\Delta^{BCS}_{x^2-y^2})^2 \sim 10^{-4} \div 10^{-6} \ \text{ almost unmeasurable by QMC}$$



The pairing is almost unmeasurable for U<~5t



50 Sites (tilted square) 8 holes (big sign problem!)

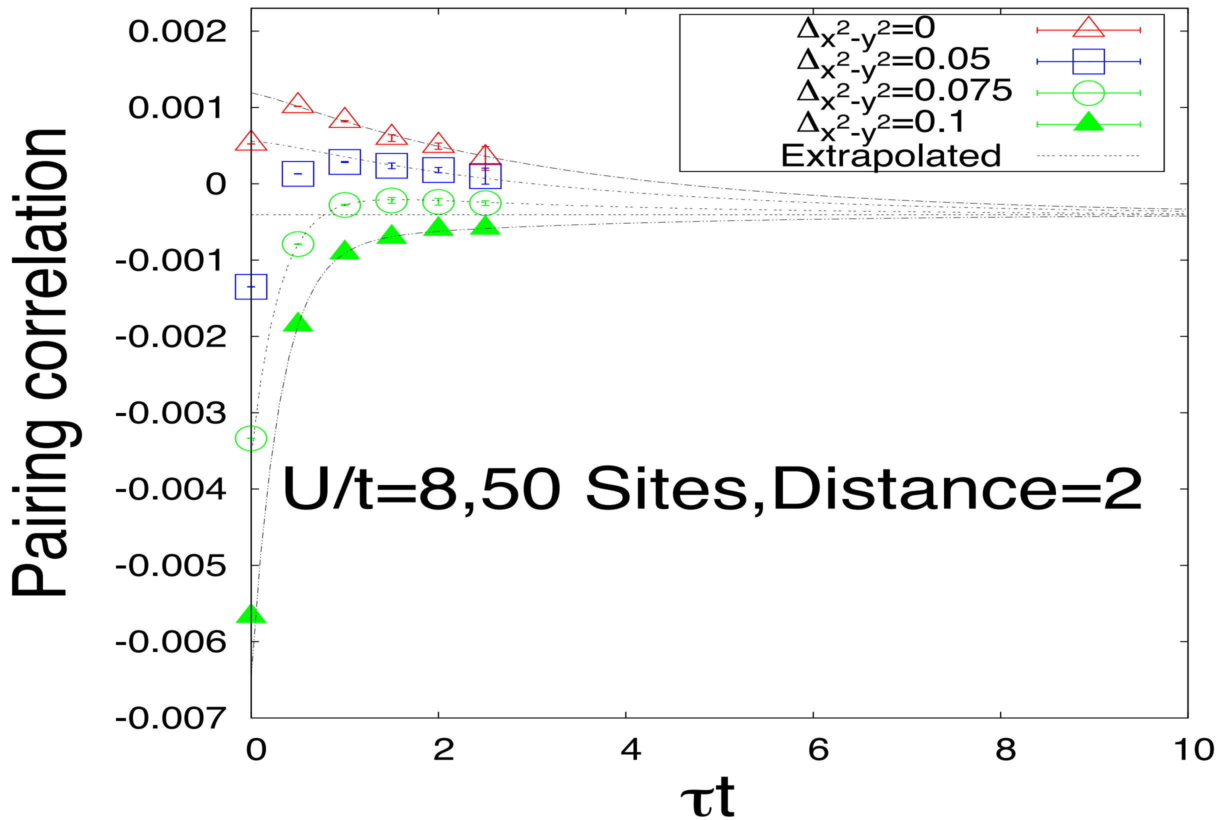


$\leftarrow \langle \psi_0 | \Delta^+_{i,i+x} \Delta_{j,j+x} | \psi_0 \rangle$

$\leftarrow \langle \psi_0 | \Delta^+_{i,i+x} \Delta_{j,j+y} | \psi_0 \rangle$

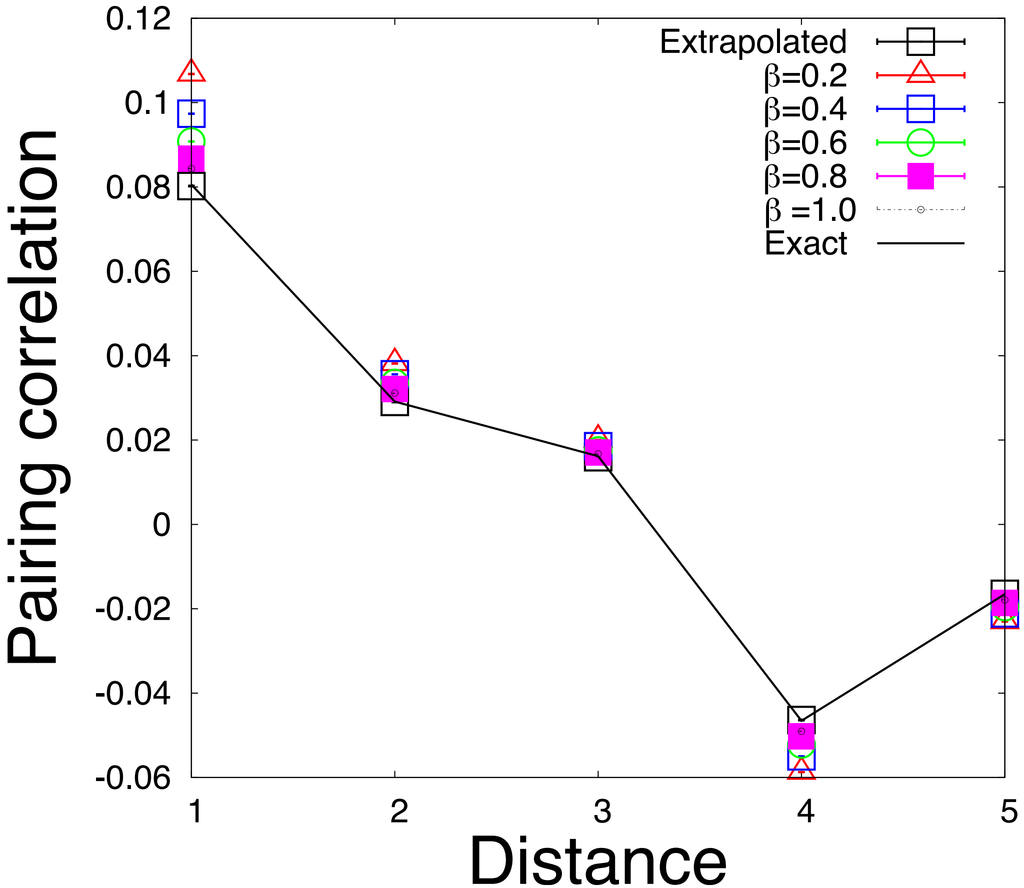
Converged computations can be done by sampling Sign ~0.01 and by extrapolation (see later).

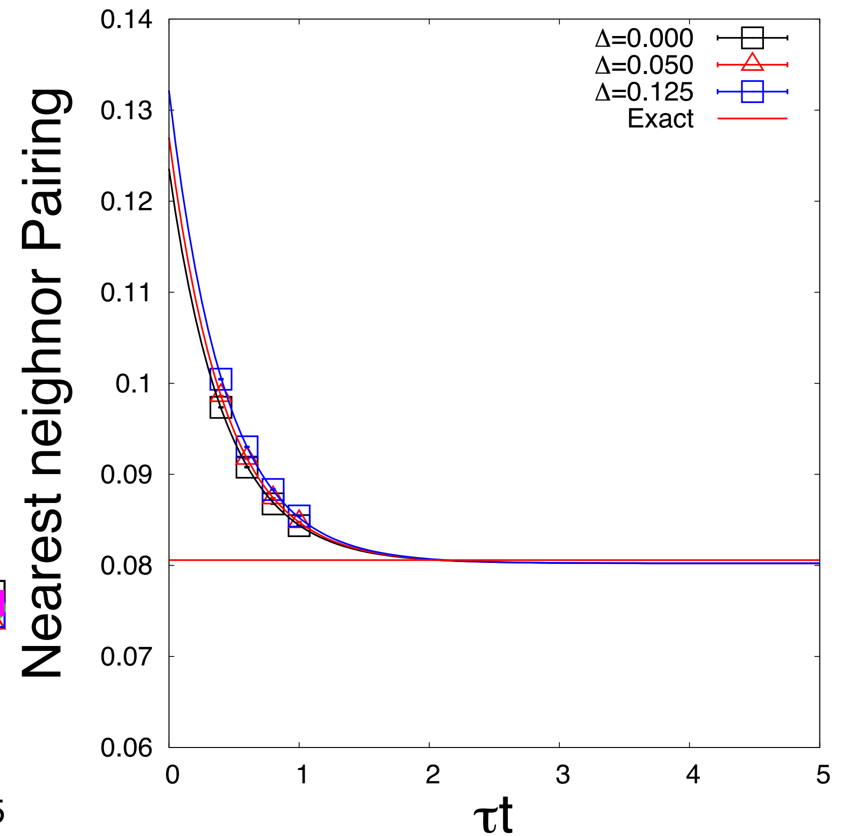
e.g. for the smallest U=0 pairing we start with
Several different trial functions with different $\Delta^{BCS}_{x^2-y^2}$



We use that all wf's for $\tau \rightarrow \infty$ converge
to the same value. Notice also non monotonic…

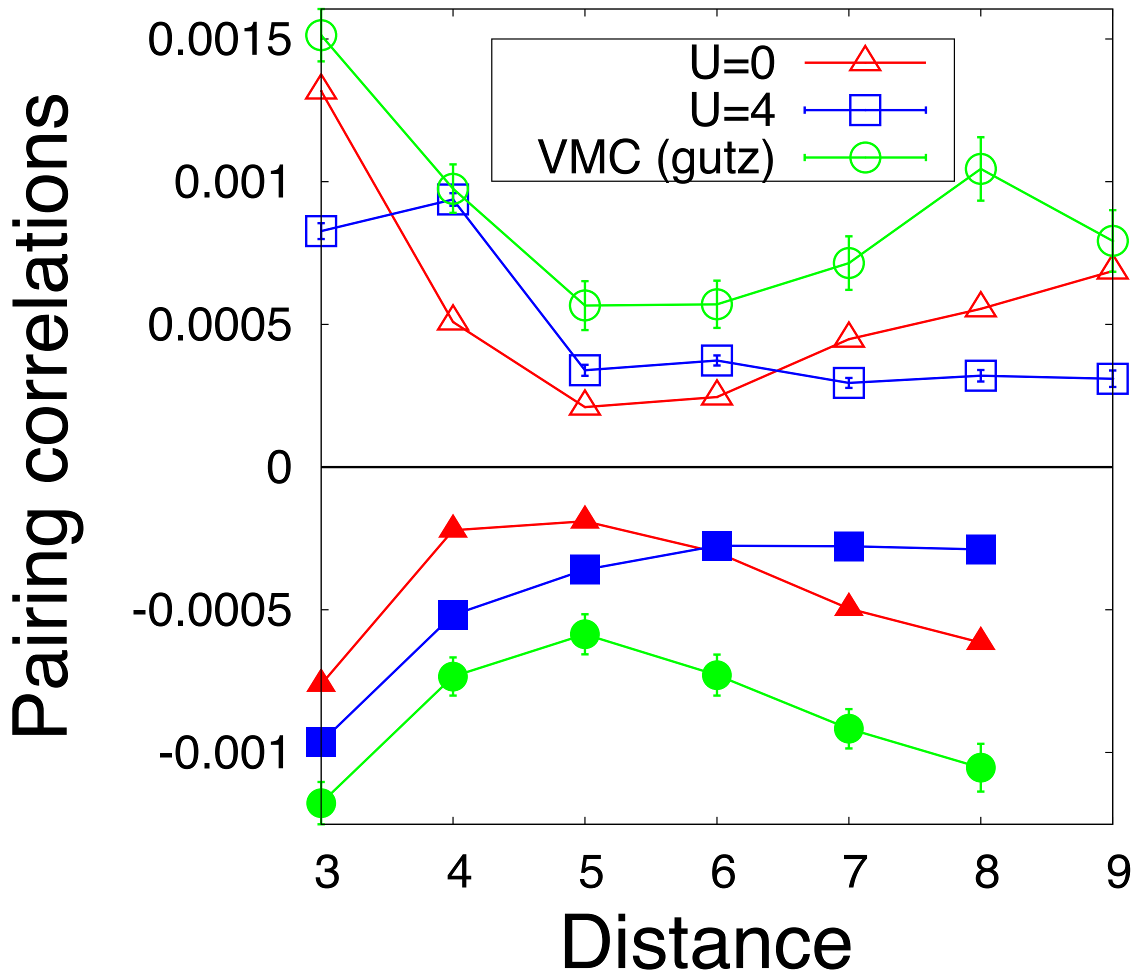
Test on an 18 sites where exact results known





By extrapolating consistently up to τt=1 with 3wf’s

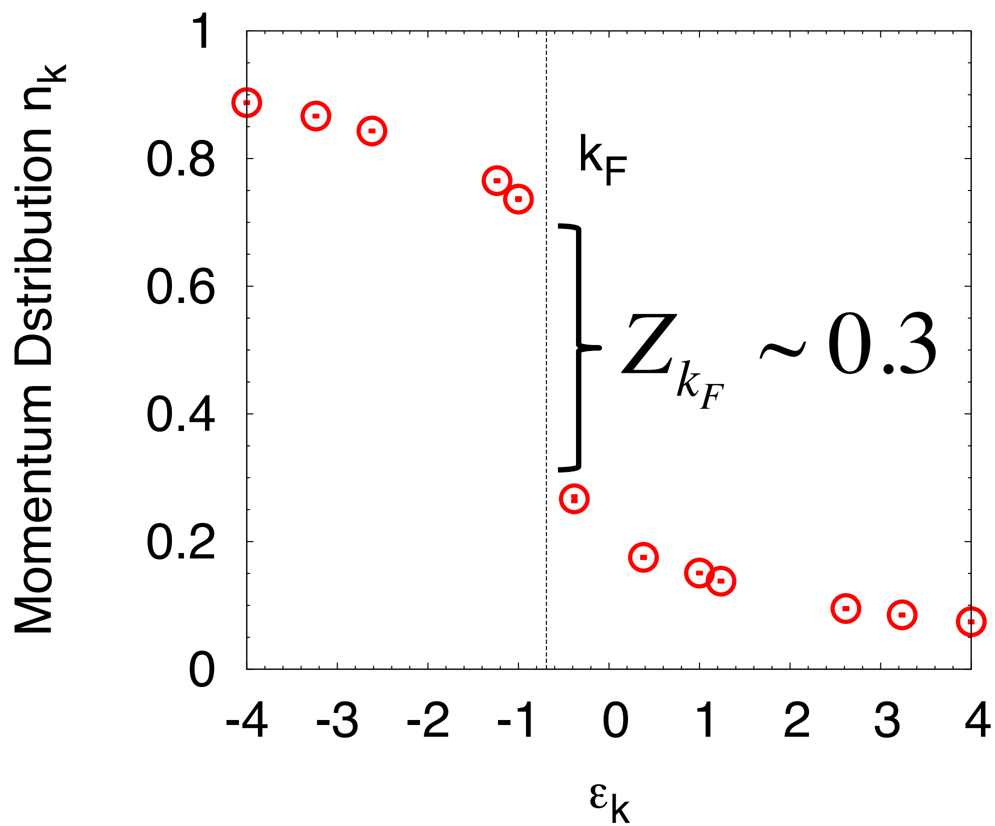
The right scale is different and caught by the GW



In general the ‘’right” pairing are much smaller than U=0 but much flatter (see blue), showing short coherence.

Why much smaller?

Correlation (U) makes a strong renormalization of the quasiparticle weight: $c^{+}_{k_F} \rightarrow Z_{k_F} \tilde{c}^{+}_{k_F}$ with $Z_{k_F} << 1$



The pairing correlations contains 4 c's→ Z_K^4 ~1/100

$$\left|\psi_{\tau/2}\right\rangle = \exp(-H\tau/2)\left|\psi_T\right\rangle = \sum_i a_i \exp(-E_i\tau/2)\left|\psi_i\right\rangle$$

$$\text{where } a_i = \left\langle\psi_T\middle|\psi_i\right\rangle \text{ and } \quad H\left|\psi_i\right\rangle = E_i\left|\psi_i\right\rangle$$

$$\frac{\left\langle\psi_{\tau/2}\middle|O\middle|\psi_{\tau/2}\right\rangle}{\left\langle\psi_\tau\middle|\psi_T\right\rangle} = \frac{\sum_{i,j} a_i a_j \left\langle\psi_i\middle|O\middle|\psi_j\right\rangle \exp[-(E_i + E_j)\tau/2]}{\sum_i a_i^2 \exp(-E_i\tau)}$$

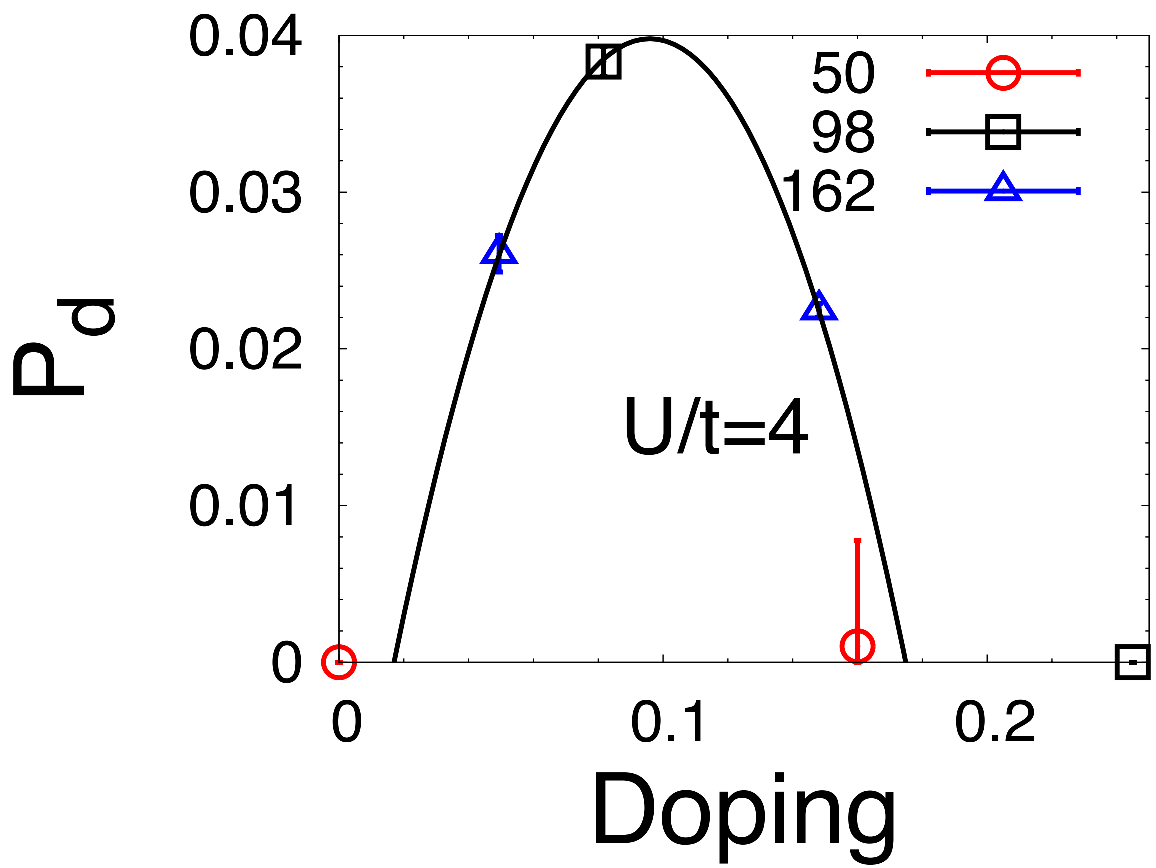
$$\sim \left\langle\psi_0\middle|O\middle|\psi_0\right\rangle + \sum_i b_i(O,\psi_T)\exp(-\Delta_i) \qquad \Delta_i = |E_i - E_0|$$

By using two Δ and two ''b'' for each O and ψ_T

→ stable fits for estimating accurately $\left\langle\psi_0\middle|O\middle|\psi_0\right\rangle$

We have considered several closed shell fillings Studying the evolution for U>0 of the pairing correlation, the smallest one for U=0.

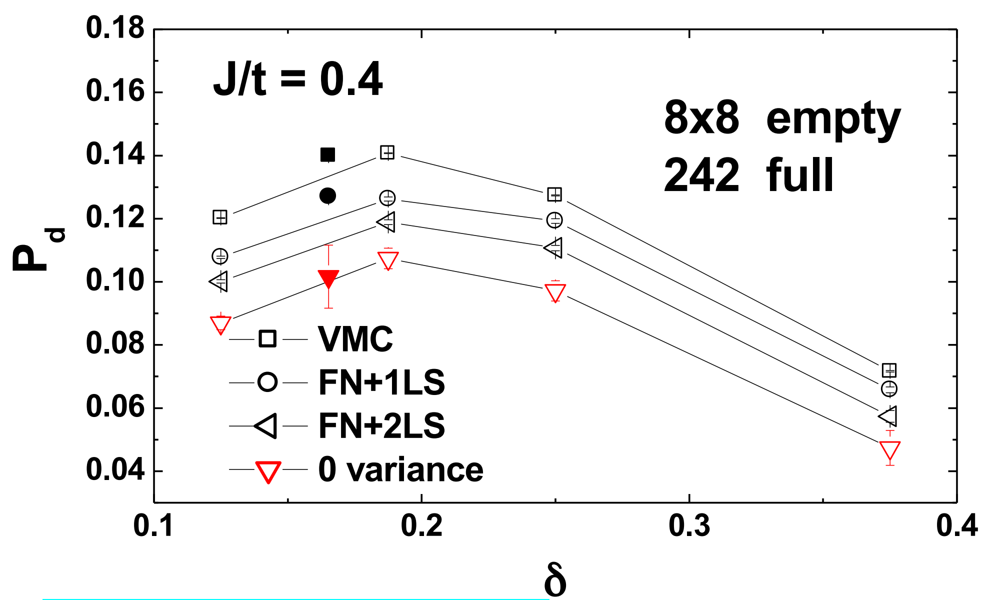
P_d can be estimated by subtracting the ''small'' U=0 contribution (vertex correction).



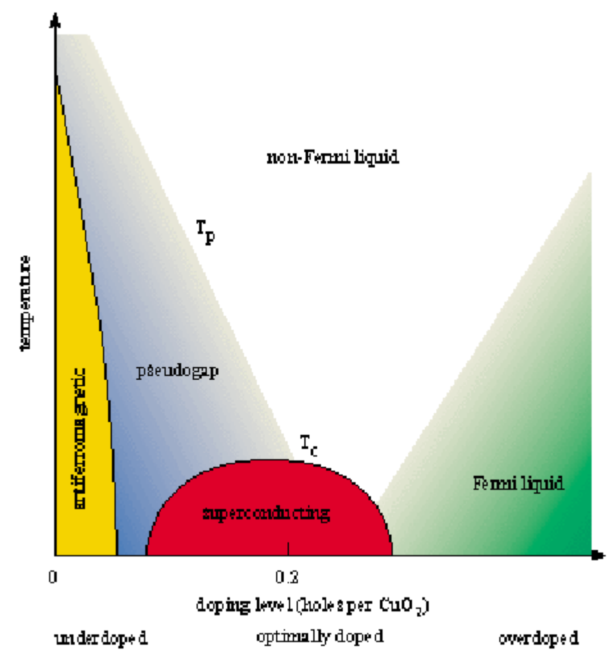
Superconductivity from strong correlation t-J model

$$P_d = 2\sqrt{\left|\langle \psi_0 | \Delta^{+}_{i,j} \, \Delta_{k,l} | \psi_0 \rangle\right|}$$

at the largest distance



S. Sorella et al. PRL ‘02



P_d is an order of magnitude larger than Hubbard!

Conclusions

No spin liquid phase in the Honeycomb lattice.
No spin liquid without sign problem?

Gutwiller wavefunction predicts d-wave pairing in the U>0 Hubbard model, but is indeed very small for U~<4t (if not zero at all).

By sampling the sign reasonably converged /extrapolated ground state properties can be obtained in closed shell #Sites ~100.

Good evidence of d-wave pairing, phase diagram possible by assuming small size effects in vertex cor