

# The Sign problem: overview and perspectives

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# Various promising approaches

- 1) It is an artifact of Quantum Monte Carlo. Just avoid the problem with different non-stochastic techniques, e.g. DMRG, CCSDT...
- 2) I do not want to solve the sign problem, but only reduce the prefactor of an exponentially hard problem: FCIQMC (A. Alavi), Auxiliary Fields QMC sample the sign whenever possible and use better wave functions (S. Sorella).
- 3) I want to solve the sign problem for particular problems with some “fancy trick” based on high level math. and abstraction: stochastic quantization\* (G. Aarts), Gaussian MC (P.D. Drummond), Fermion bag\* (S. Chandrasekharan), similar to Diagrammatic Monte Carlo (Prokofev-Svistunov)-e.g. no sign problem for single impurity Kondo model, Gross Neveu model...-
- 4) I accept to make some approximation because my task is to solve the problem within experimental resolution, DMC (D. M. Ceperley), CPQMC (S. Zhang) ... but still we need about 10 times more accurate methods for strongly correlated systems.

\* Methods introduced within Quantum Field Theory

# Last but not least: Just sample it

The **parallel** computer power is growing exponentially (Moore's law will not stop) with time and the statistical error is easy to reduce with several copies  $\sim 1 / \sqrt{\#\text{Processors}}$

Thus there are problems that could be solved in the near future:

The Hubbard model? The lattice QCD?

We probably have only to reduce the prefactor...

# But what is the problem?

In case the weight  $w(x)$  is not always positive one is left to sample  $|w(x)|$  which has the meaning of prob.

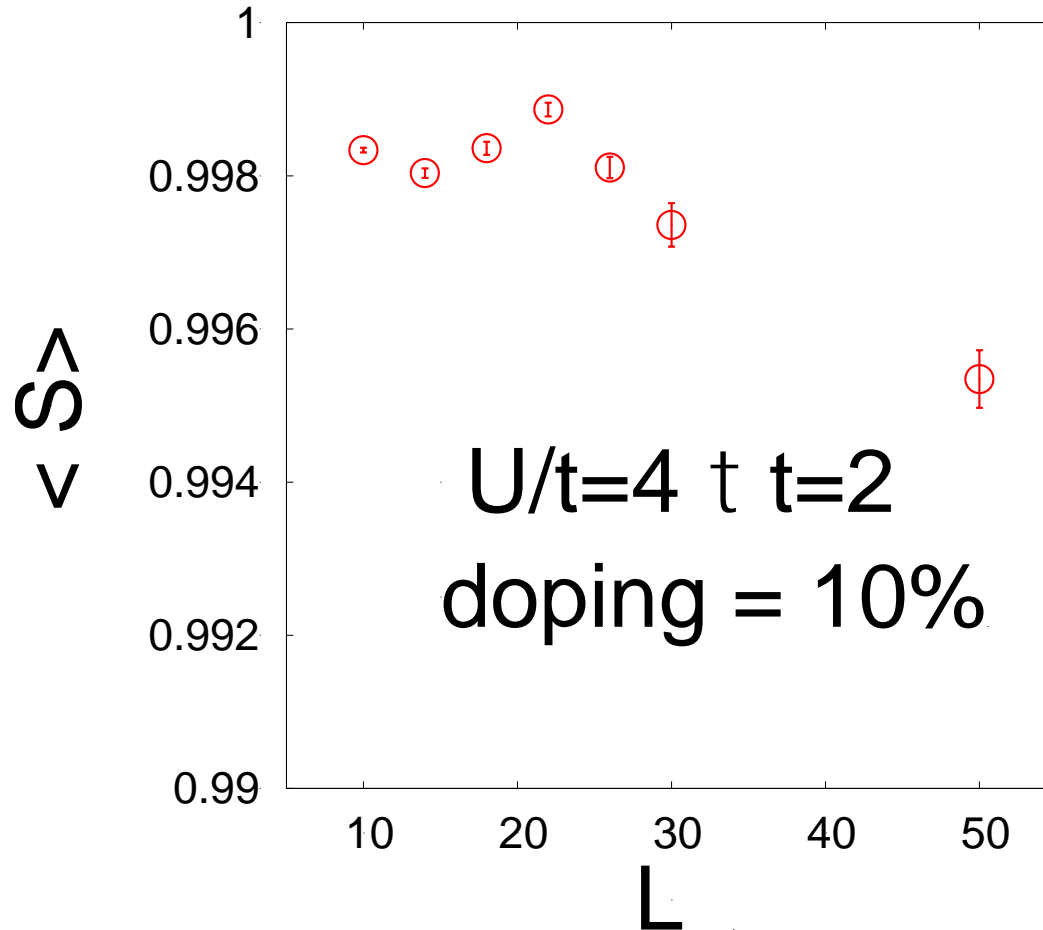
Then, in any method known, physical quantities determined only by accurate calculation of  $\langle S \rangle$  :

$$\langle S \rangle = \langle \langle \text{Sgn}(w(x)) \rangle \rangle_{|w(x)|} \mu \exp[-\mu \text{Volume} \cdot t]$$

where  $t$  = Inverse temp. or projection time

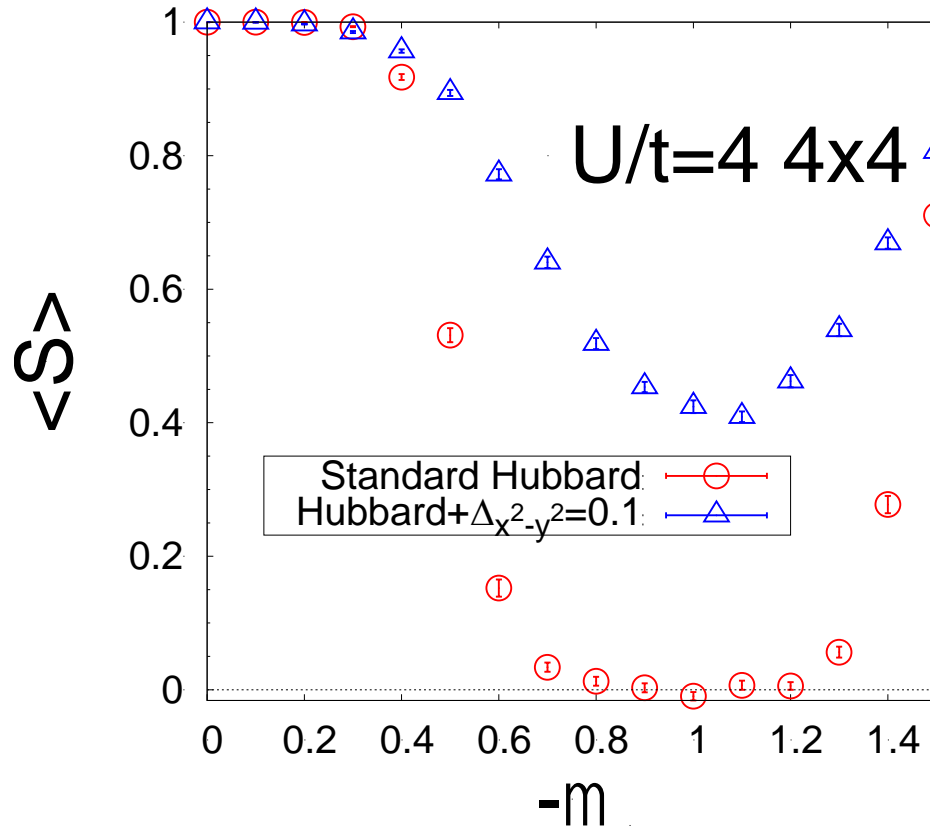
Thus CPU  $\mu \exp(\mu \text{Volume} \cdot t)$

Sometimes is not a problem:  
take the Hubbard model on  $L \times L$  clusters



Auxiliary fields QMC has an amazing stability in  $L$   
for small projection times (high temperatures)

It is also possible we are not studying the “right” model



By adding a small perturbation sign becomes “good”

# Why we should hope

We want to solve the ground state of a many body system far from phase transitions:

The Hilbert space is exponential  $\exp(\sim L)$ , but the low energy spacing is  $\sim 1/L^z$   $z = \text{dyn. critical exp.}$

For instance lowest excitation in antiferromagnet:

$$e_{k_{\min}} \sim c/L \quad (z = 1), \quad c \text{ is the spin-wave velocity}$$

The problem is much simpler even compared to a classical minimization problem (e.g. travelling salesman, spin glass)

# Take for instance the Sherrington-Kirkpatrick model

$$H = -\sum_{ij} J_{ij} s_i^z s_j^z \quad J_{ij} = \pm 1$$

This problem is **hard** just because there is an exponentially large number of minima at low energy. By quantizing it we obtain that it remains hard with (M. Troyer) or without sign problem (a small field //x) because the QMC will show up sign problem or an exponentially large correlation time  $\sim 1/\text{Gap}$



# Entanglement entropy argument

$$S_{vN} = -\text{Tr}_A r \ln(r) \propto \text{Area}(A)$$

For a random generic state  $S_{vN} \propto \text{Vol}(A)$   
so much more complicated and probably hard

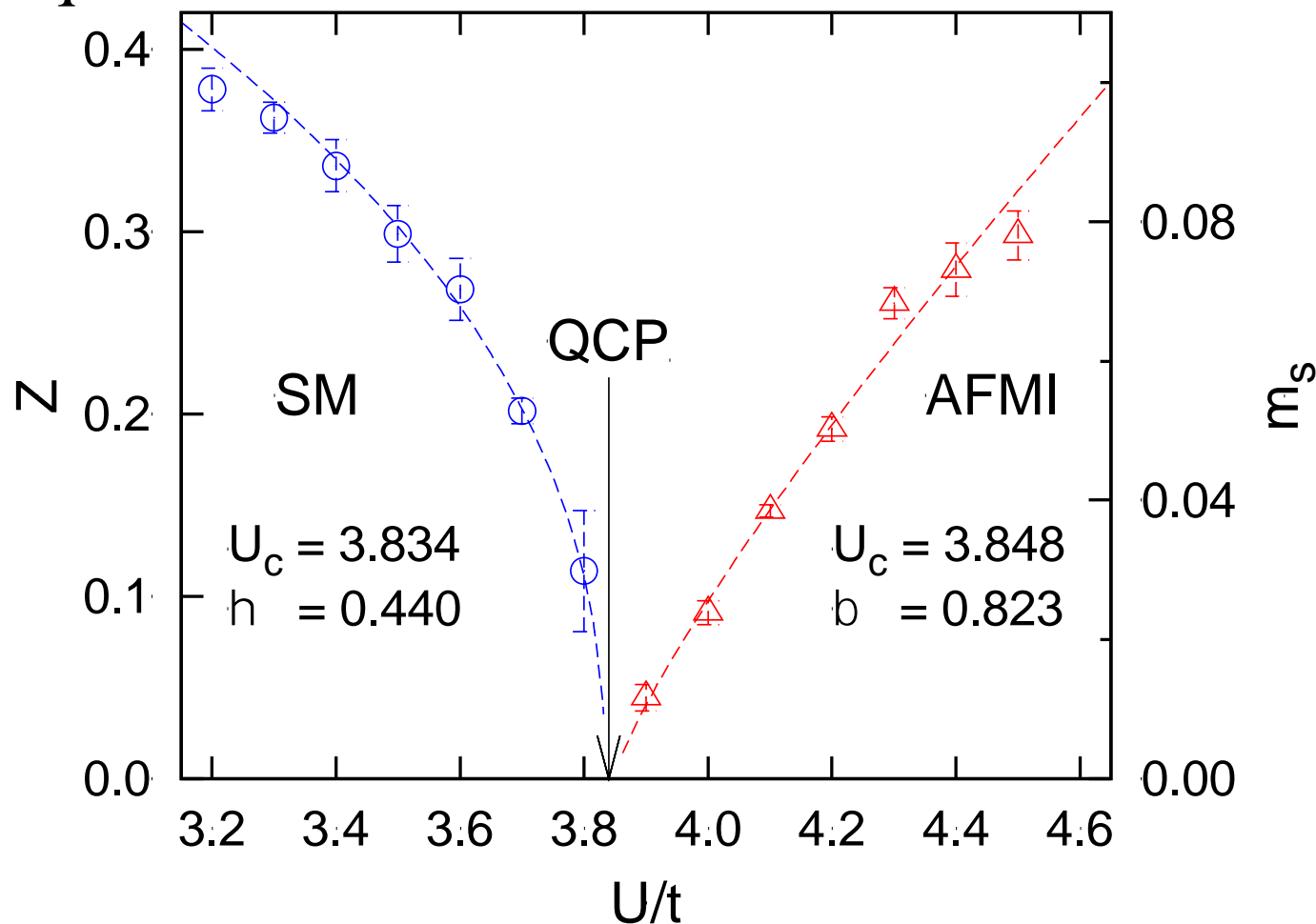
The main recent idea is to build systematically convergent wave functions with area law satisfied

→ Then the problem becomes a classical minimization problem

→ No sign problem but maybe hard (?)

# SemiMetal-Insulator Transition in a fermionic model

The half-filled Hubbard model in the honeycomb lattice  
equivalent to the Gorss-Neveu model  $N=2$



A beautiful phase transition occurs seen after careful finite size scaling with up to  $\sim 2600$  sites (Y. Otsuka, SS and S. Yunoki, in preparation)