UCDAVIS

Challenges in Simulating Quantum Systems on Classical Computers

[1.] Spatial Inhomogeneity and Lattice Size

Finite Size Scaling in Translationally Invariant Case

Antiferromagnetic Correlations in Fermion Hubbard Model

Boson Hubbard Model in a Trap

Characteristic Density

[2.] Equilibration and Parallelization

Density distribution: Fermion Hubbard Model

A Question for the Audience

[3.] The Sign Problem

It's not as bad as you think

It *is* as bad as you think

Multiband models/Hund's Rule Terms

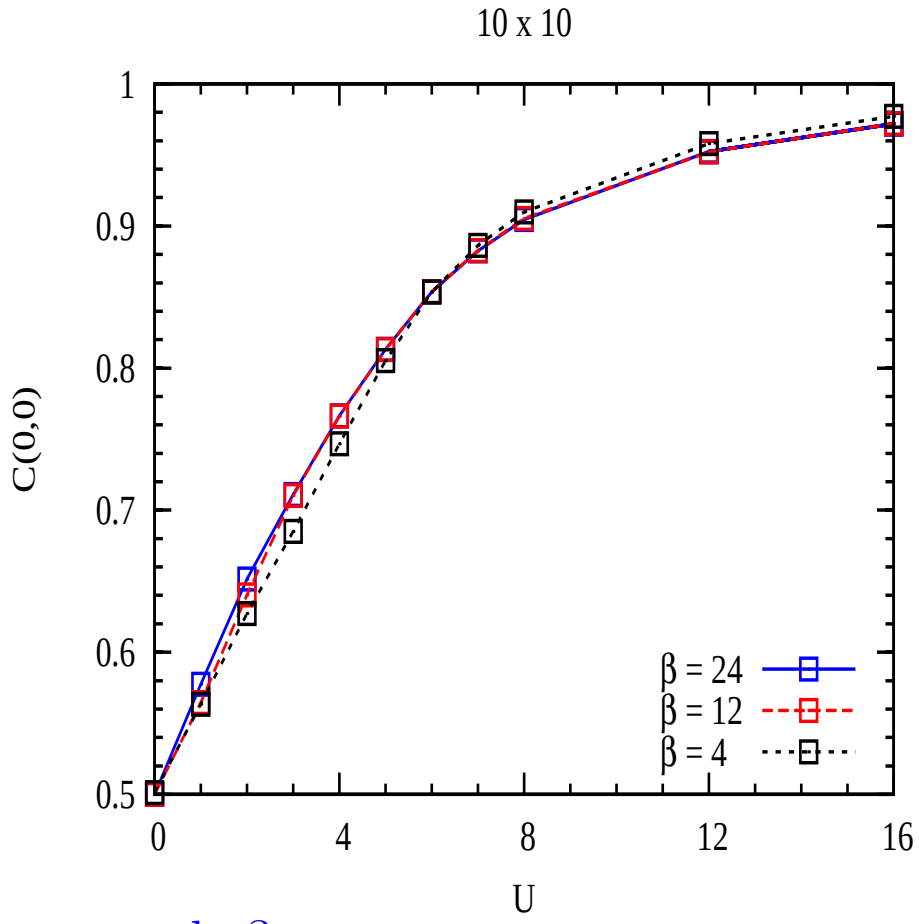
C. Varney, K. Mahmud, M. Rigol, G. Batrouni, S. Chiesa, V. Rousseau, C. Chin
I. Spielman, T. Porto, M. Jarrell, Z.J. Bai, C.R. Lee, T. Maier, E. D'Azevedo

[1.] Spatial Inhomogeneity and Lattice Size

Uniform Fermion Hubbard Model

$$H = -t \sum_{\langle \mathbf{ij} \rangle \sigma} (d^{\dagger}_{\mathbf{i}\sigma} d_{\mathbf{j}\sigma} + d^{\dagger}_{\mathbf{j}\sigma} d_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) - \mu \sum_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma}$$

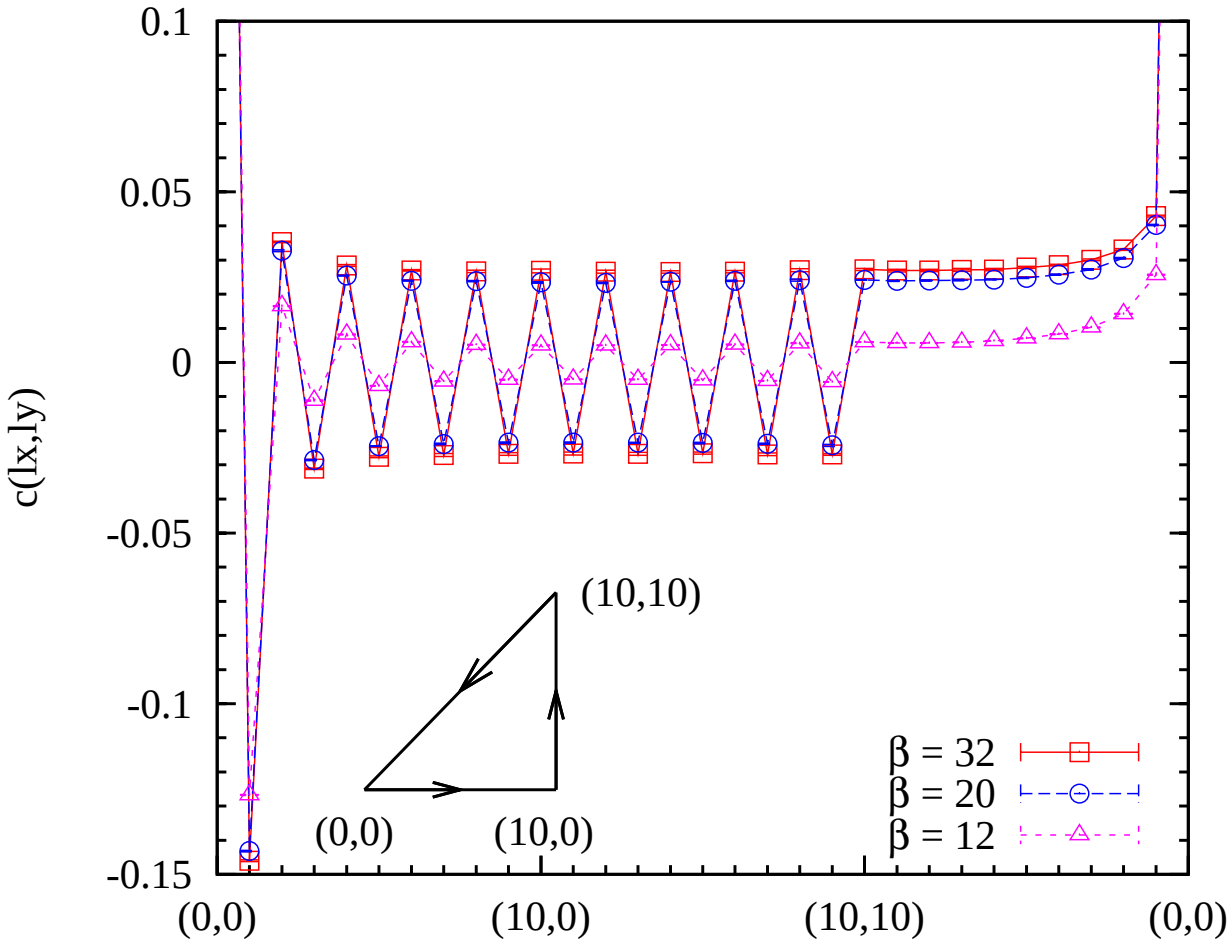
Local moments form as U increases.



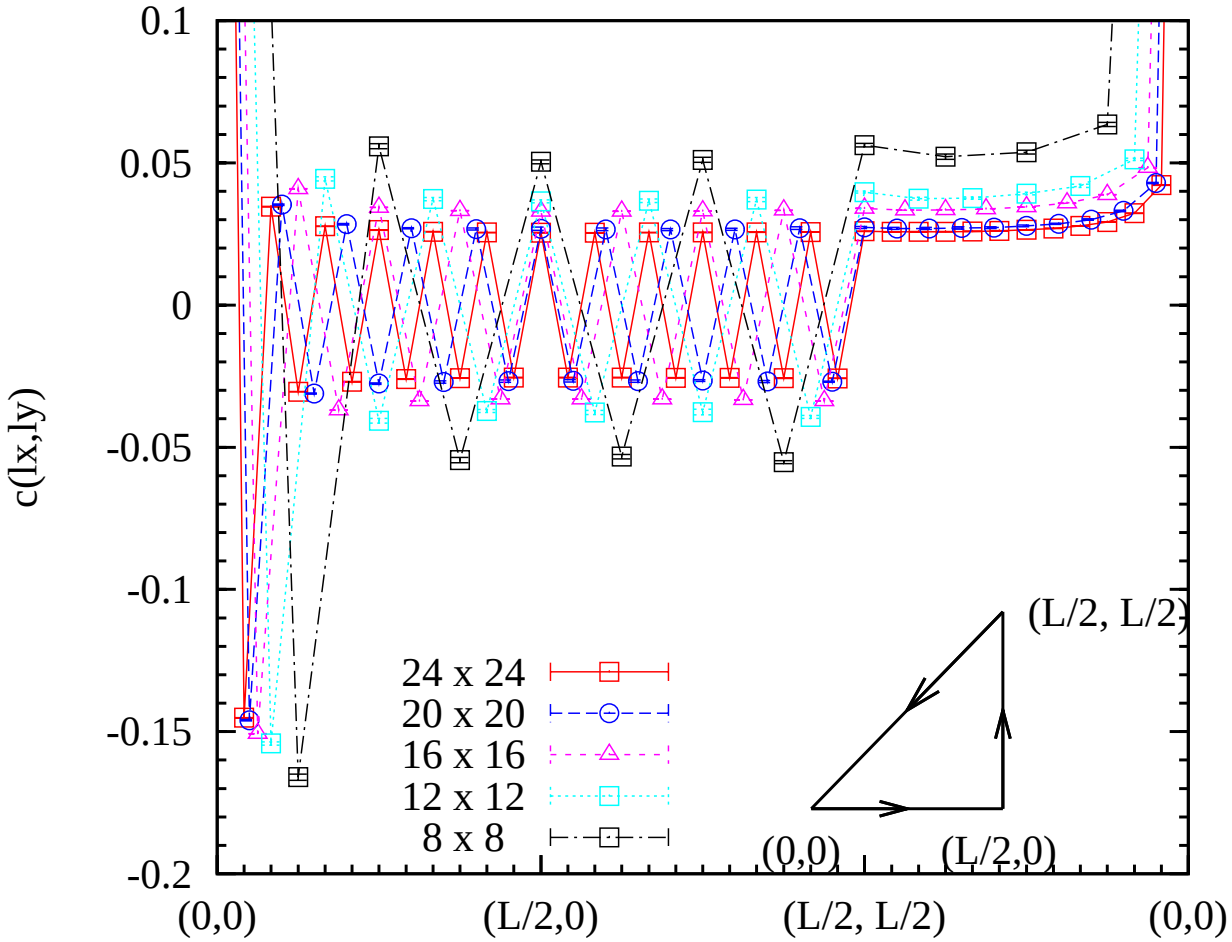
Do they exhibit long range order?

Antiferromagnetic spin correlations form at low temperature.

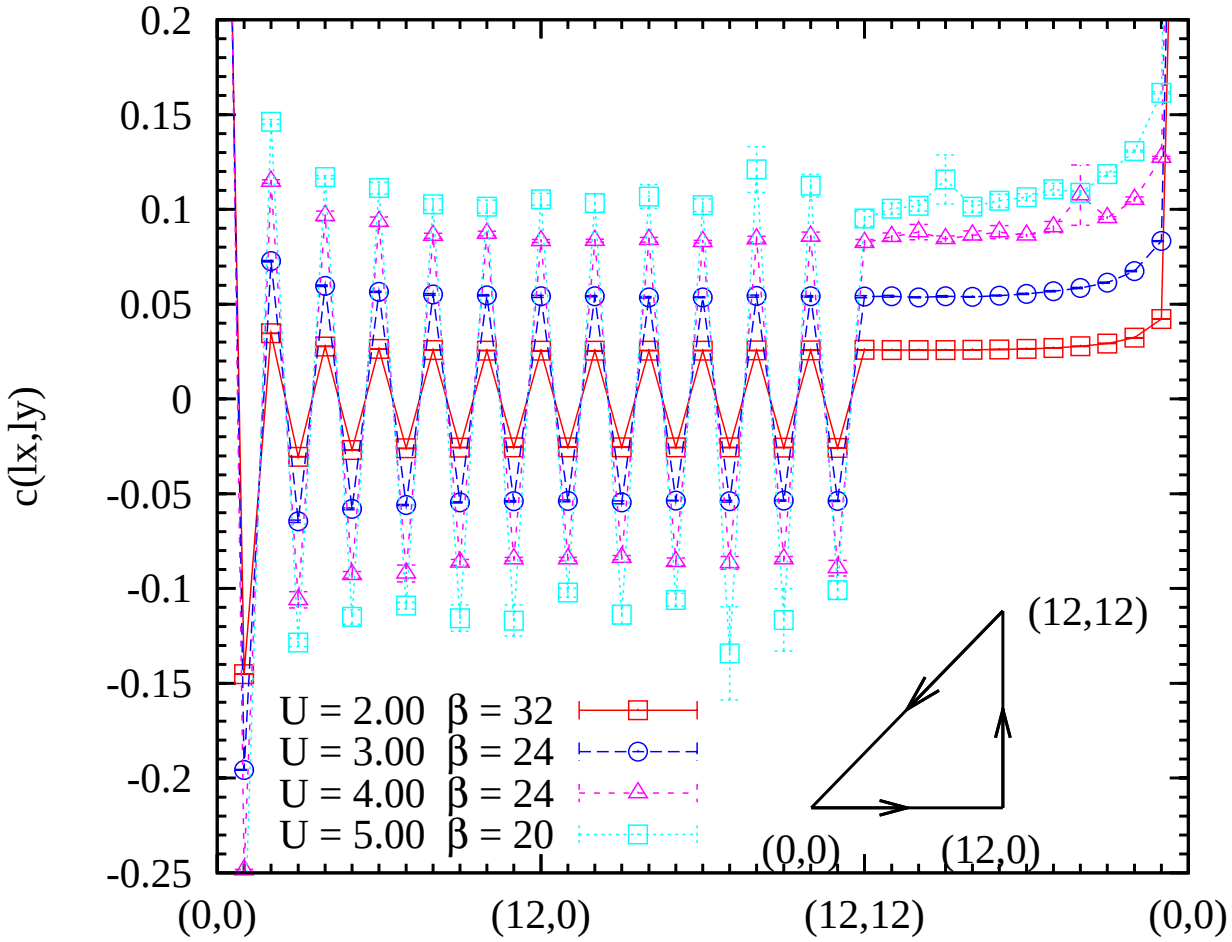
$\beta t = 20 \rightarrow T = t/20 = W/160$ (bandwidth $W = 8t$) $U = 2t$ N=20x20 lattice



Antiferromagnetic correlations are well converged for N =20x20 lattices.



Increasing U enhances antiferromagnetic correlations N=24x24 lattice

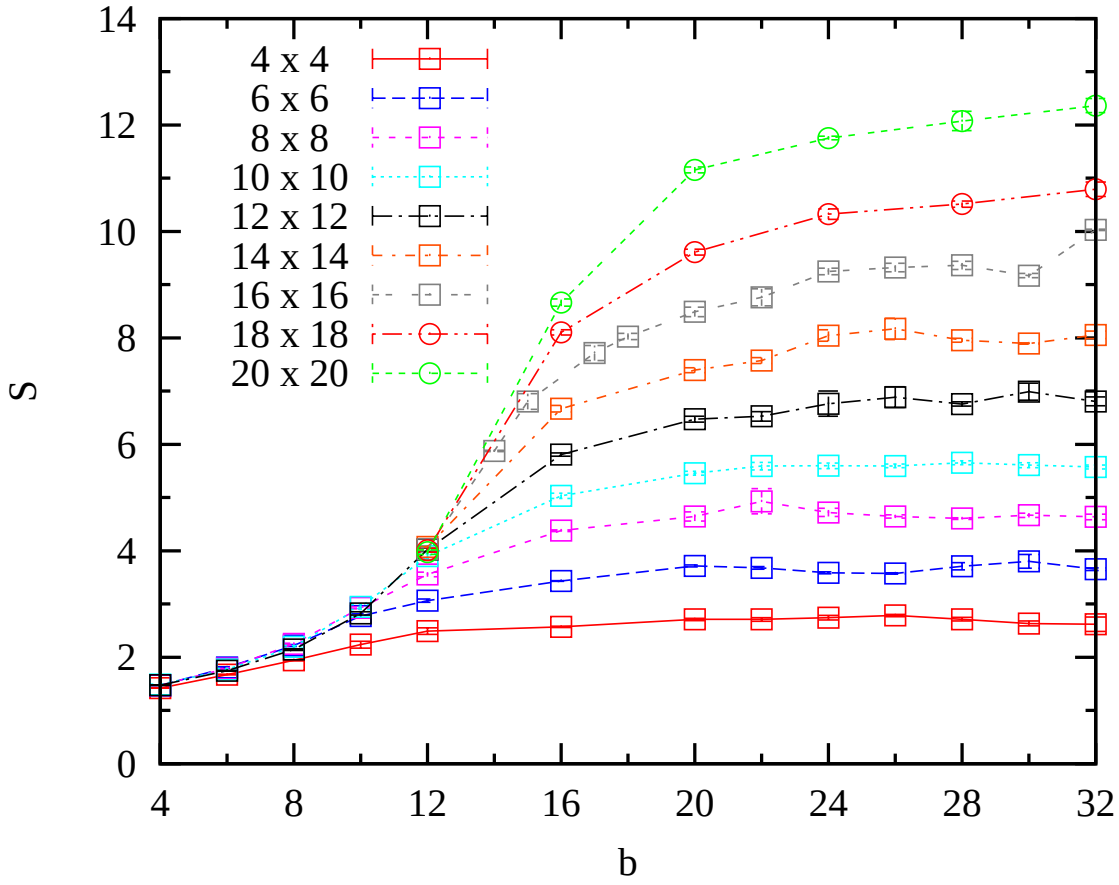


Antiferromagnetic structure factor

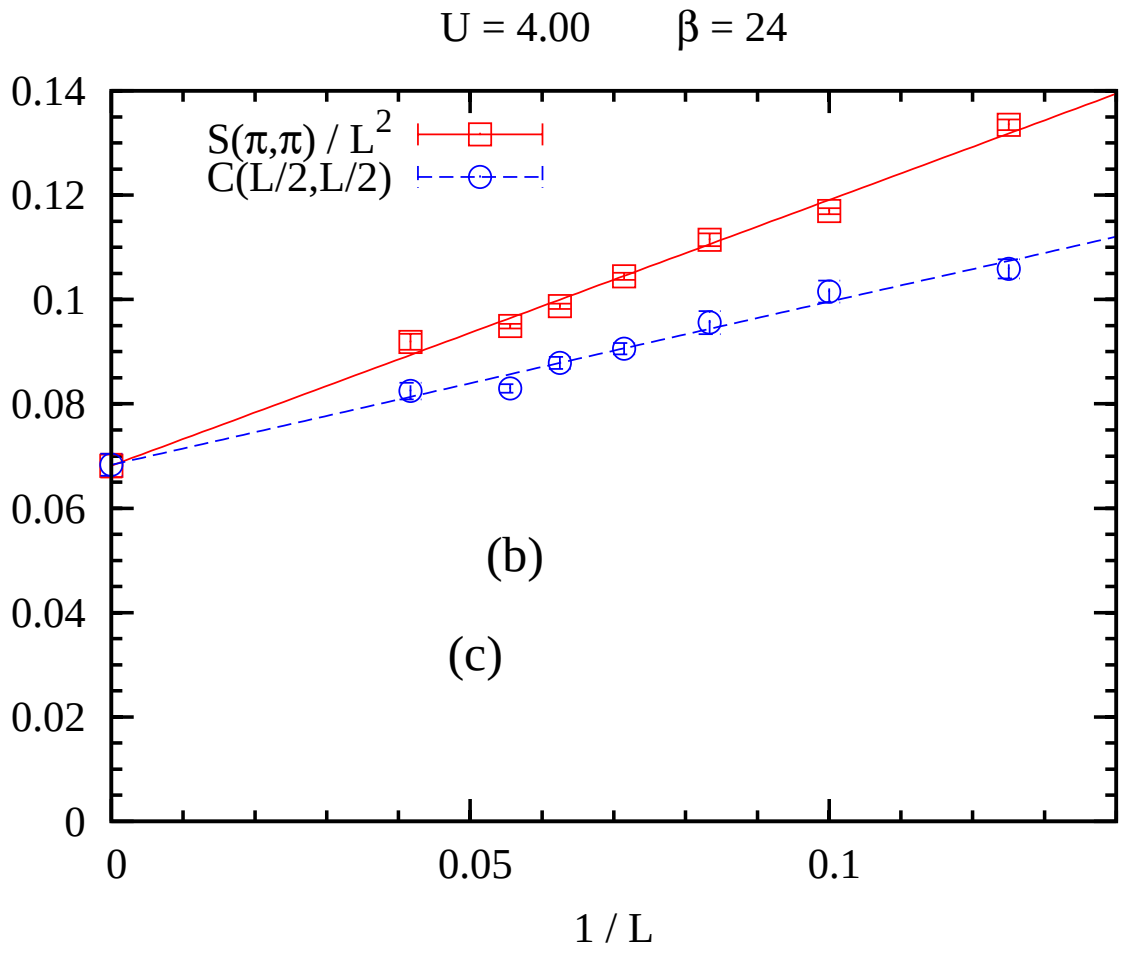
$$S(\pi,\pi) = \frac{1}{N}\sum_{ij}\langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow})\rangle$$

Reaches asymptotic ground state value as β increases. Lower T is required for larger spatial lattices. Correlation length $\xi(T)$ must exceed linear size.

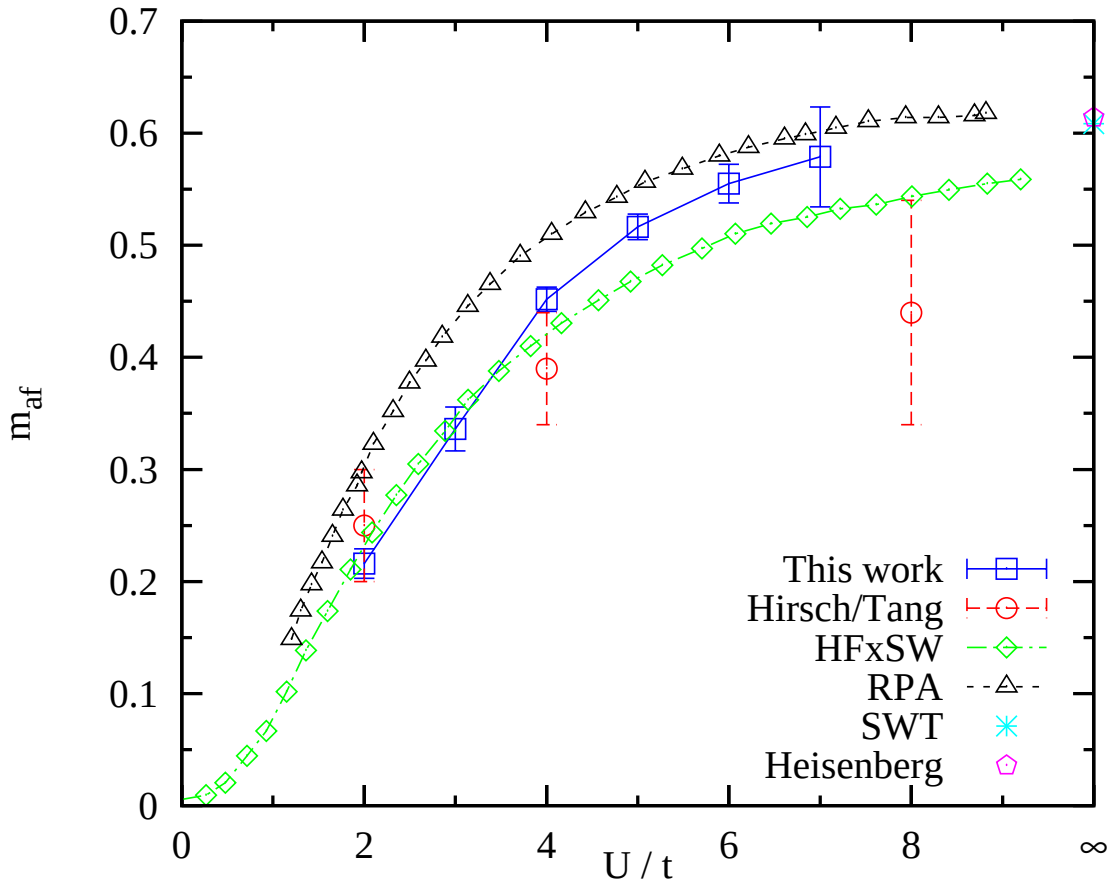
- In ordered phase $S(\pi,\pi)$ grows with N.



Finite size scaling of AF structure factor



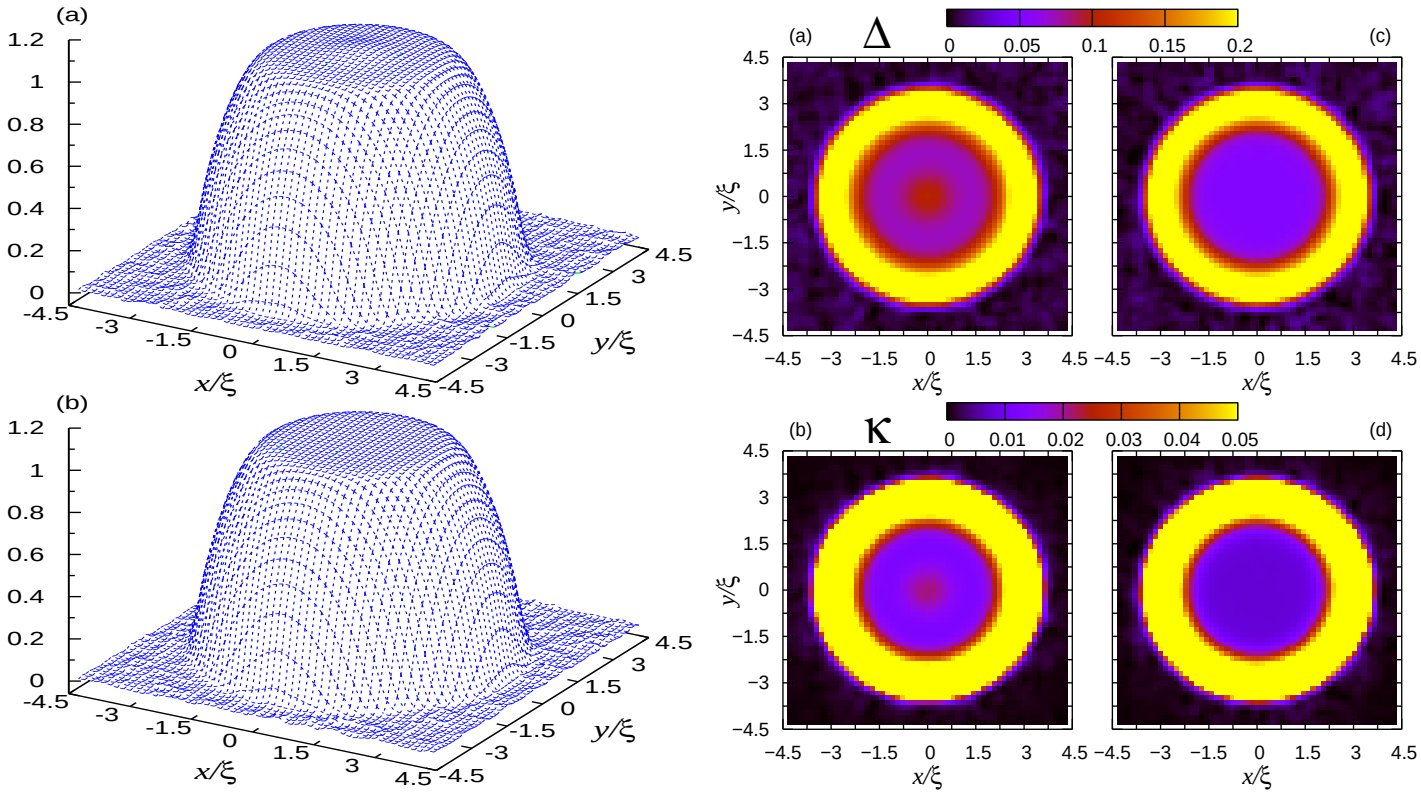
U dependence of AF order parameter



Useful for benchmarking optical lattice emulations.

Many systems of great interest which are not spatially uniform

Two dimensional Bose Hubbard Hamiltonian with confining potential.
QMC density, number fluctuation, and compressibility profiles:



Top: $U/J = 17.5$ Bottom: $U/J = 18.5$ Uniform: $(U/J)_c = 16.7$
$N_b = 1200$, $V_{\rm trap}/J = 0.025$.

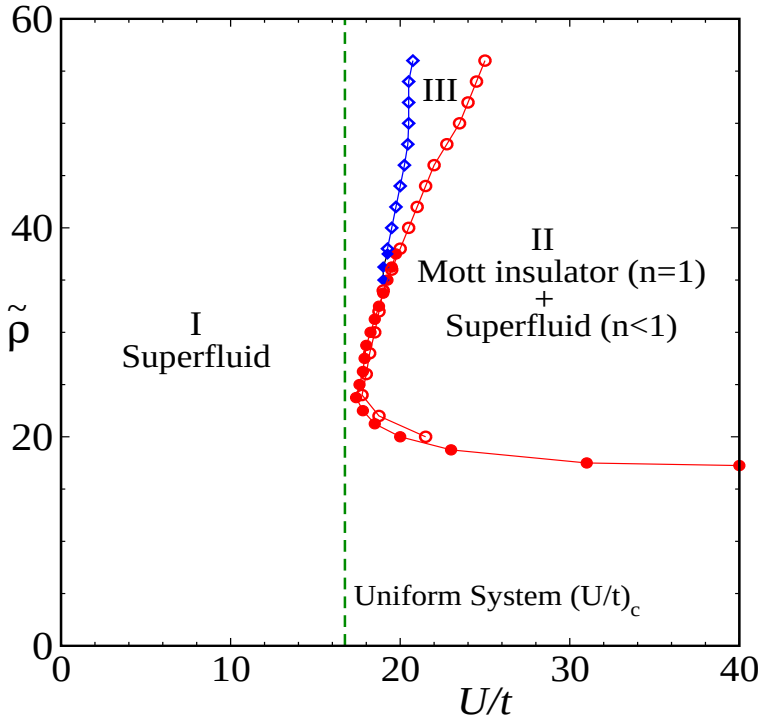
Despite extra energy scale (confining V), no more parameters than homogeneous case!

Curvature $V_{\rm trap}$ provides length scale $\xi = \sqrt{\frac{J}{V_{\rm trap}}}$

Plays same role as linear lattice size

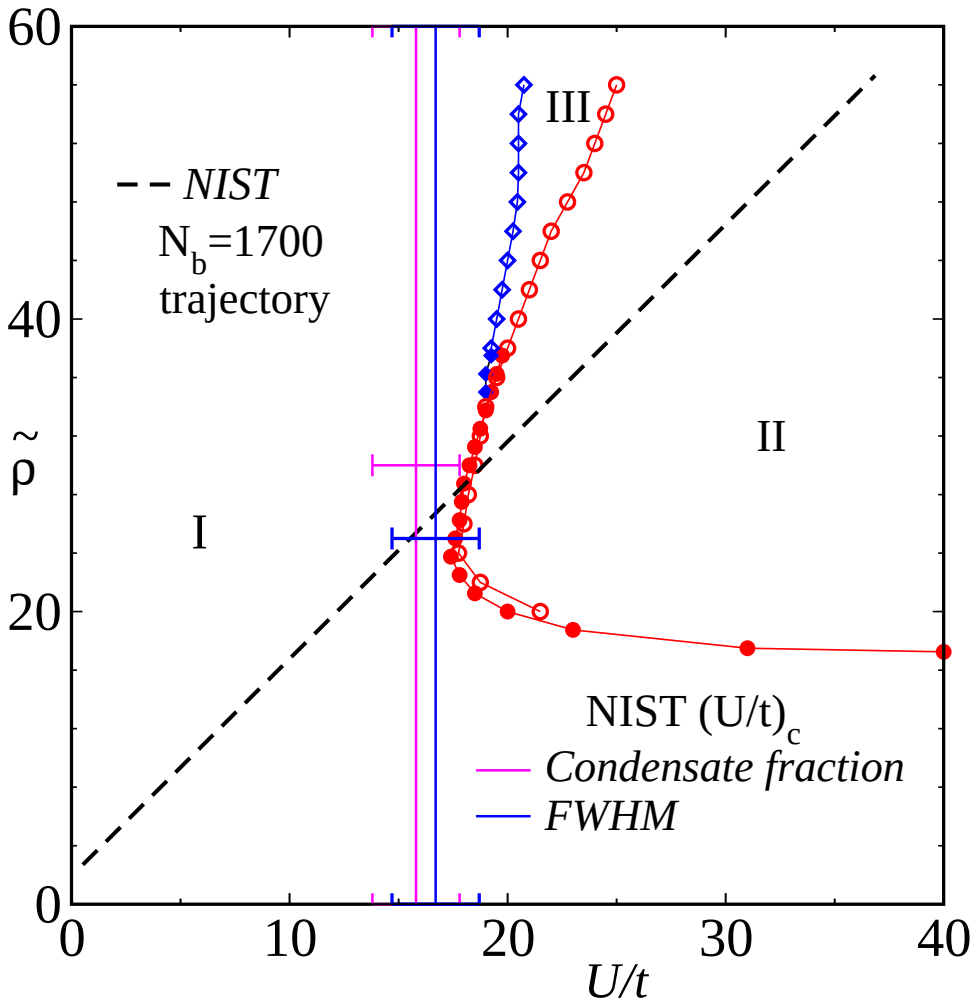
"Characteristic Density" $\tilde{\rho} = N_b/\xi^d$

Can meaningfully compare systems with different $V_{\rm trap}$.

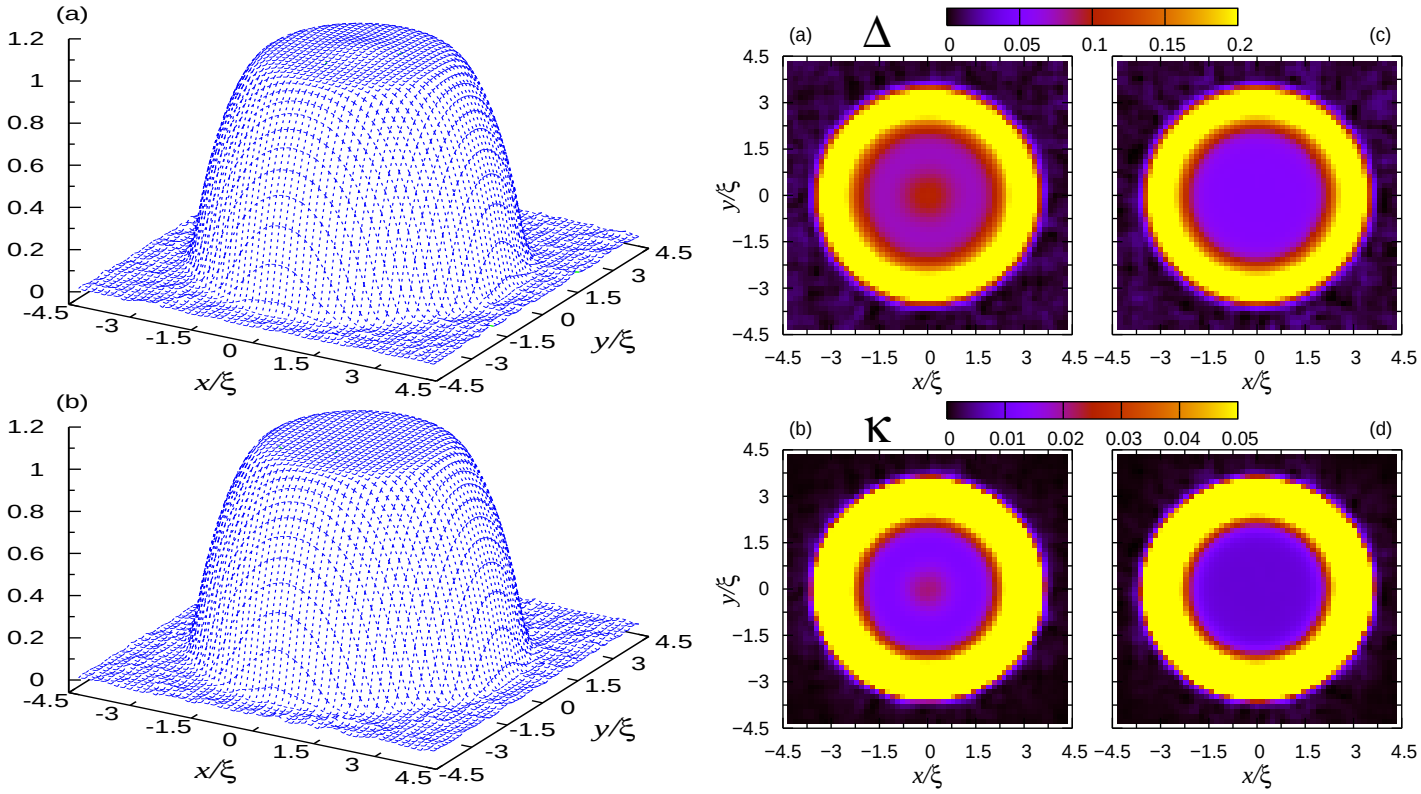


M. Rigol, G.G. Batrouni, V.G. Rousseau, and RTS, Phys. Rev. **A79**, 053605 (2009).

Initial Experimental Comparison (NIST)



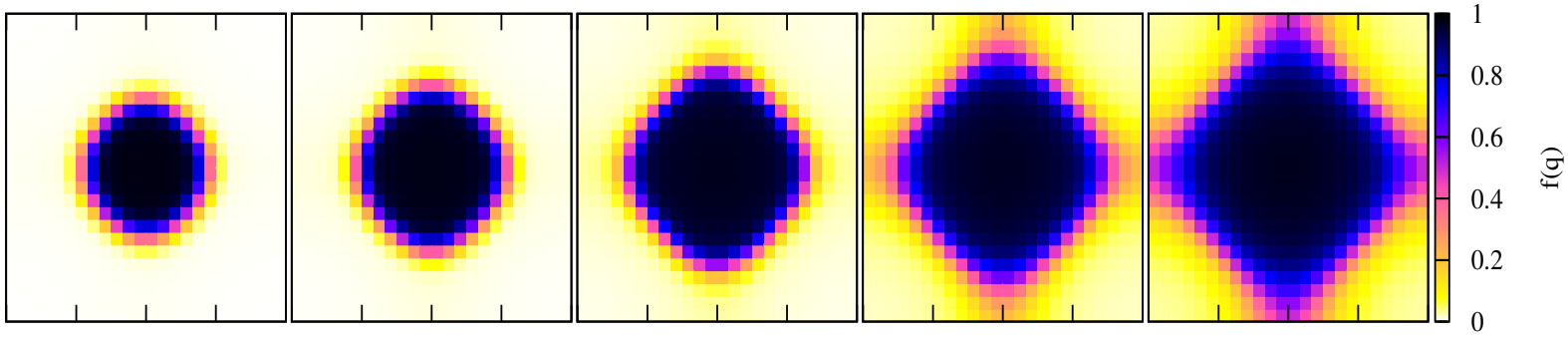
This is a success story (can define analog of phase diagram), but...
There is a significant problem with lattice sizes.
Wide enough to capture different regions (superfluid/Mott) ??
Phase transitions, critical exponents, in presence of inhomogeneity ??



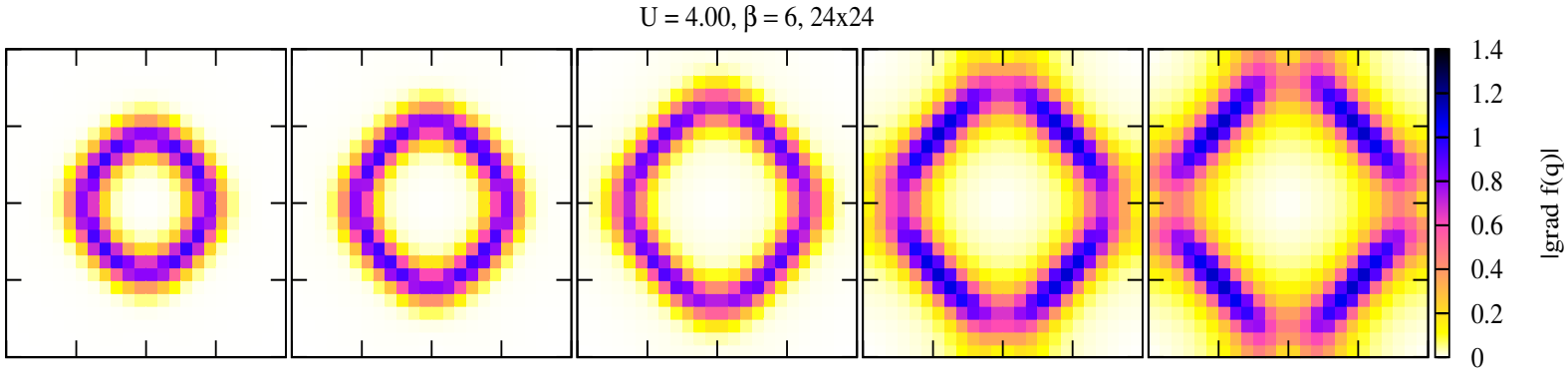
[2.] Equilibration and Parallelization

Return to fermion Hubbard model.
Large lattices now allow good momentum resolution.

$U = 4$ Fermi function: N=24x24, $\beta = 8$; $\rho = 0.23, 0.41, 0.61, 0.79, 1.00.$



$U = 4$ Gradient of Fermi function:



These results on small cluster (10 nodes). Not parallelized.

Algorithm scales at N^3.

Order of magnitude larger N (72x72 lattices) on parallel machine.

Use 'trivial' strategy of parallelizing the monte carlo averaging.

What about equilibration?

A question for the audience:

Start off many simulations with different initial configurations on a parallel machine.

Every few sweeps compare the weights.

Copy (large weight)/eliminate (small weight) configurations.

(It is known how to do this in a way that satisfies detailed balance.)

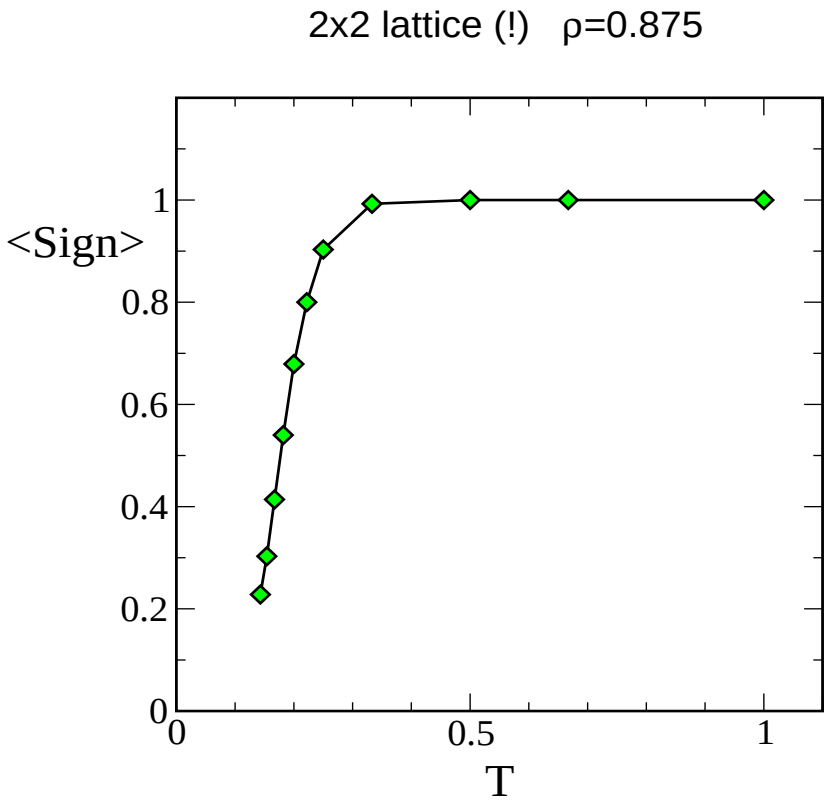
Continue simulation (copied configuration with different seeds).

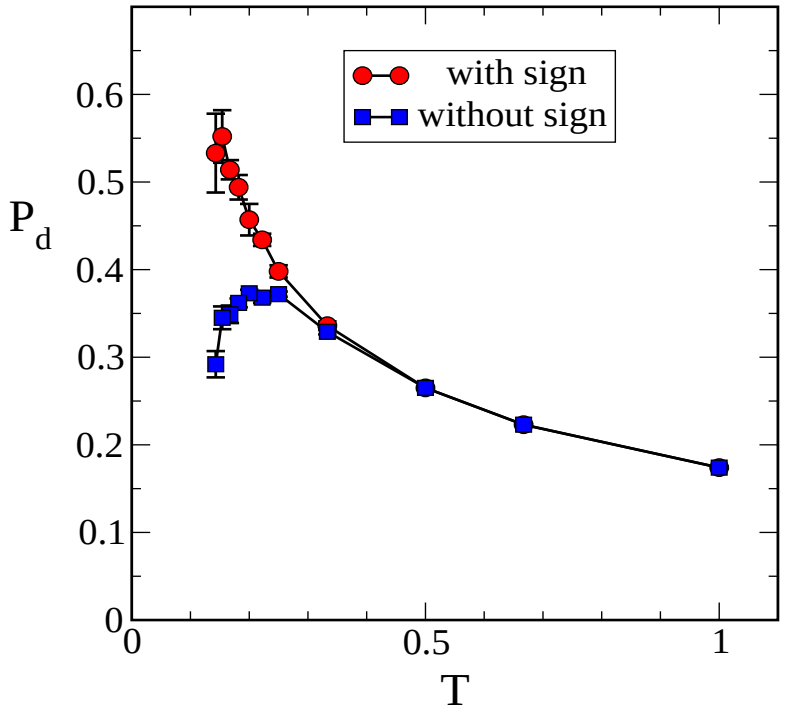
What is known about equilibration time?

[3.] The Sign Problem

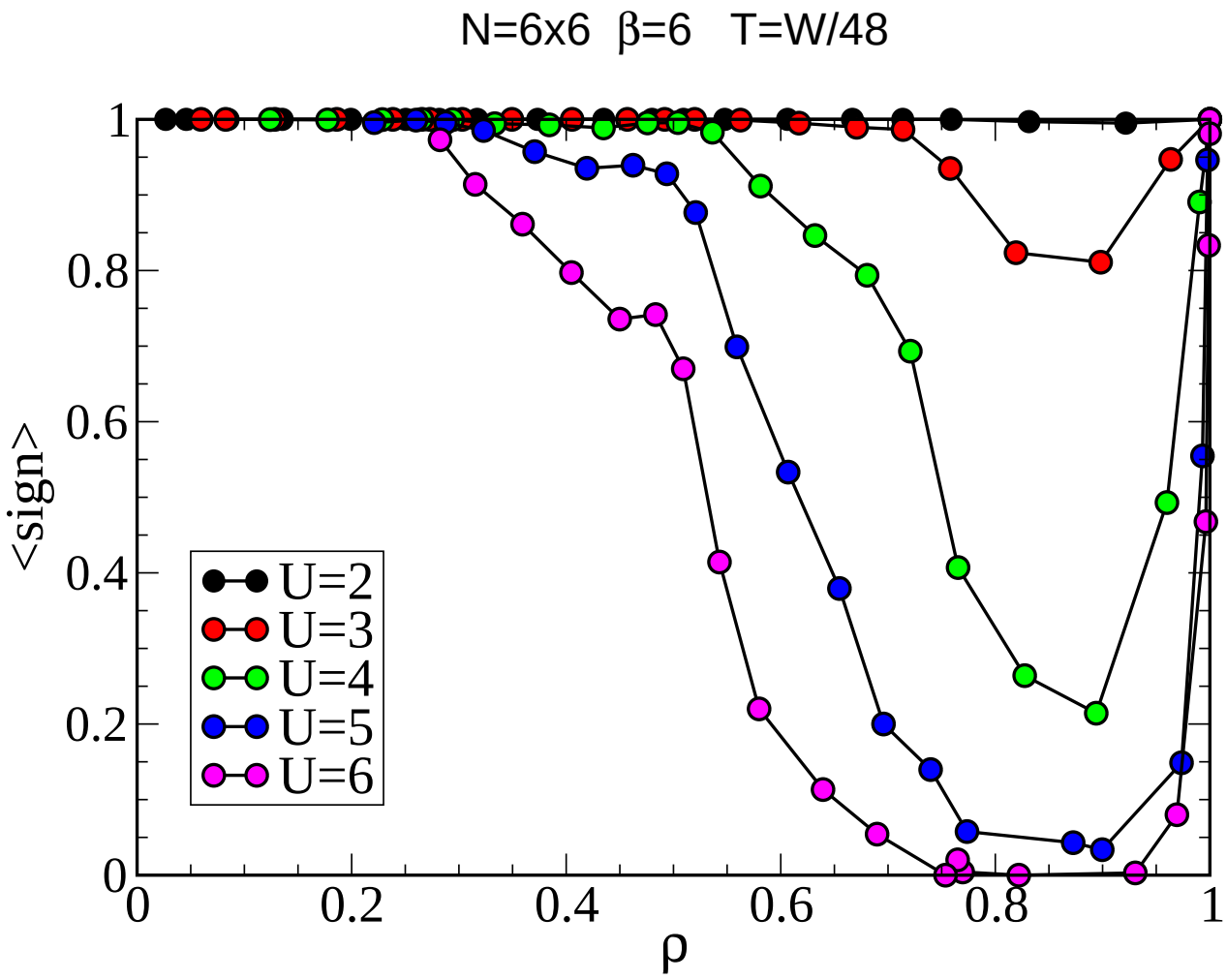
Cuprates caused focus on $\rho = 0.875$ (optimal doping for highest T_c).
In fermion Hubbard model, sign problem is worst there!
Kills you even on the smallest lattices (N=2x2!)

It is essential to include the sign.



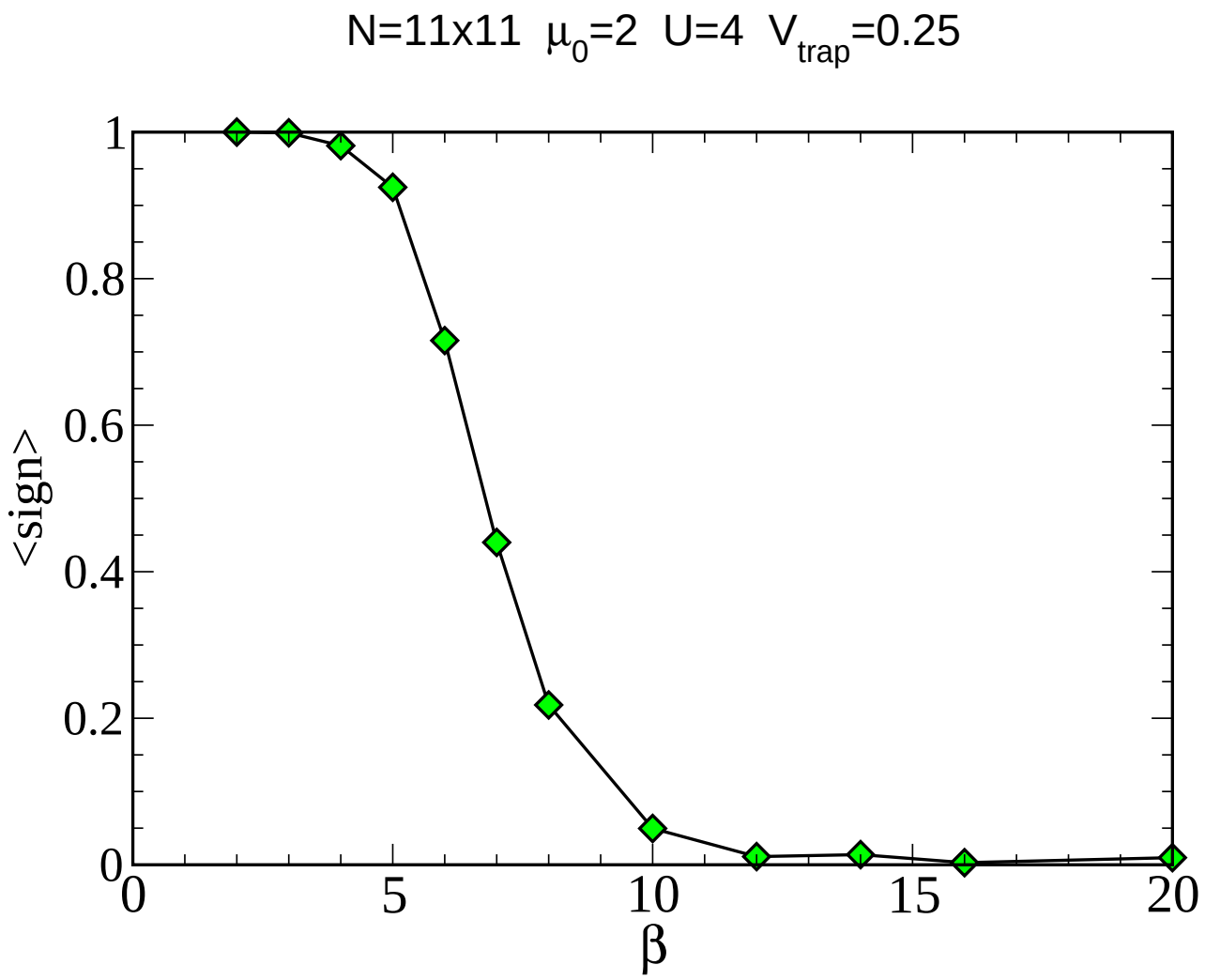


Sign problem at other fillings.



Good quality data for momentum distribution $n(k)$, N=24x24 lattices, different ρ.

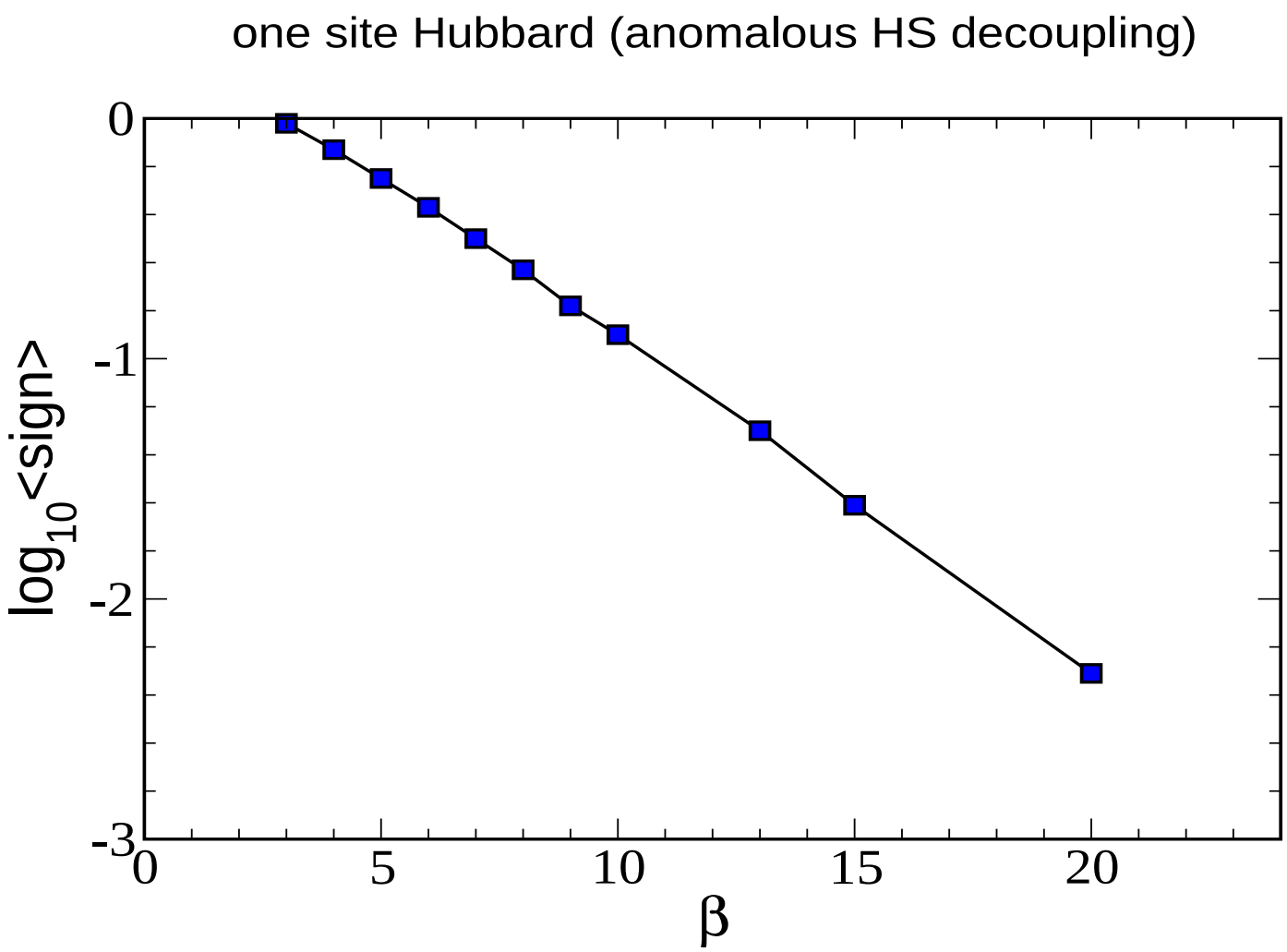
Given the sensitivity of the sign to density, a very interesting question is what it will be like for inhomogeneous systems.



Single band model away from 'optimal' doping might be okay.

But, sign problem quickly escalates with multiple bands/Hund's rule terms.

$$U\, n_{i\uparrow} n_{i\downarrow} = U\, c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} \rightarrow \lambda\, h_i \left(c^{\dagger}_{i\uparrow} c_{i\downarrow} - c^{\dagger}_{i\downarrow} c_{i\uparrow} \right)$$



CHALLENGES

- Increase system sizes to accomodate 'reasonably sized' regions of different character.
- Parallelize equilibration to take advantage of 'embarassingly parallel' nature of MC.
- Sign problem, especially multiple orbitals and associated interactions.

Collaborators:
G.G. Batrouni (INLN)
M. Rigol (Georgetown)
C. Chin (Chicago)
I. Spielman, T. Porto (NIST)
M. Jarrell, V.G. Rousseau (LSU)
K. Mahmud, Z.J. Bai, S. Chiesa, C.N. Varney, R.T. Scalettar (UC Davis)
C.R. Lee (NTHU Taiwan)
T. Maier, E. D'Azevedo (ORNL)

Funding:
ARO Award W911NF0710576 with funds from the DARPA OLE Program
DOE SciDAC Program DOE-DE-FC0206ER25793