UCDAVIS

Superconductivity in Cold Atom Systems and Quantum Simulations

The FFLO Phase in Imbalanced Fermion Systems in 1-d (Attractive Hubbard)
- Theoretical Background and Experimental Motivation
- Model and Method
- Density and Pair Correlation Functions

Trapped Fermions in Two dimensions (Repulsive Hubbard)
- Theoretical Background and Experimental Motivation
- QMC for Half-filled Uniform System
- Density, Density Fluctuation, and Spin Correlation Profiles
- d-wave Correlations

Conclusions

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Definitely qualifies as 'Further Afield' !!

(Perhaps too far afield...)

As far as one can get from room temperature superconductivity.

$T_c \approx 30\, nK$ in absolute units.

Nevertheless,

- 'Clean' realization of model Hamiltonians [?]
- High T_c in the sense of T_c/t [?]
- Inhomogeneity (Kivelson, Beasley, Mannhart, ...)

Eduardo Fradkin's Questions:

What can we learn from experiments with cold atoms? Can they be made colder than LSCO in real terms?

Will we know if the Hubbard model (in 2D) is a superconductor, say, in five years?

How can novel quantum information ideas deal with the fermion sign problem? Can they? The Grassmann Chip?

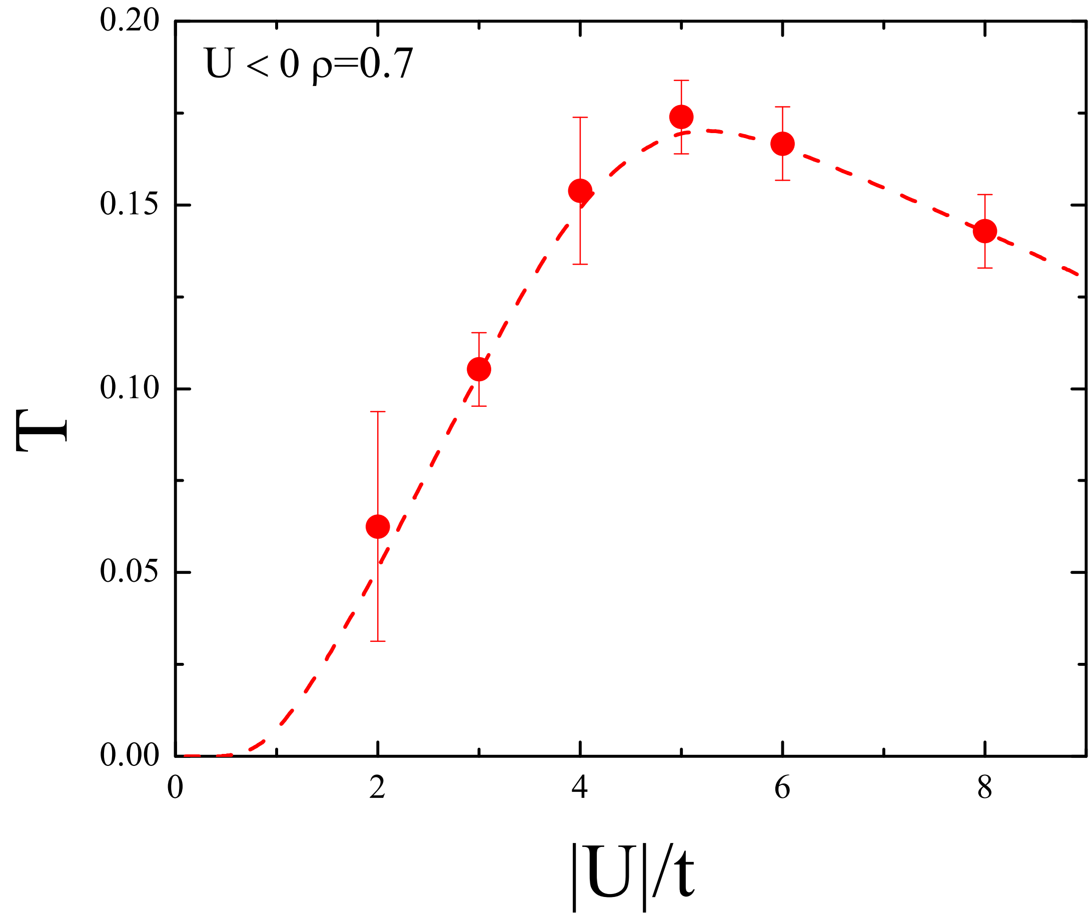
What is the future of quantum monte carlo in this context?

Prelude: Attractive Hubbard Model with no population imbalance

Quantum Monte Carlo simulations can capture BCS-BEC cross-over

$U << W$: large, weakly bound pairs with $T_c \sim te^{-ct/U}$

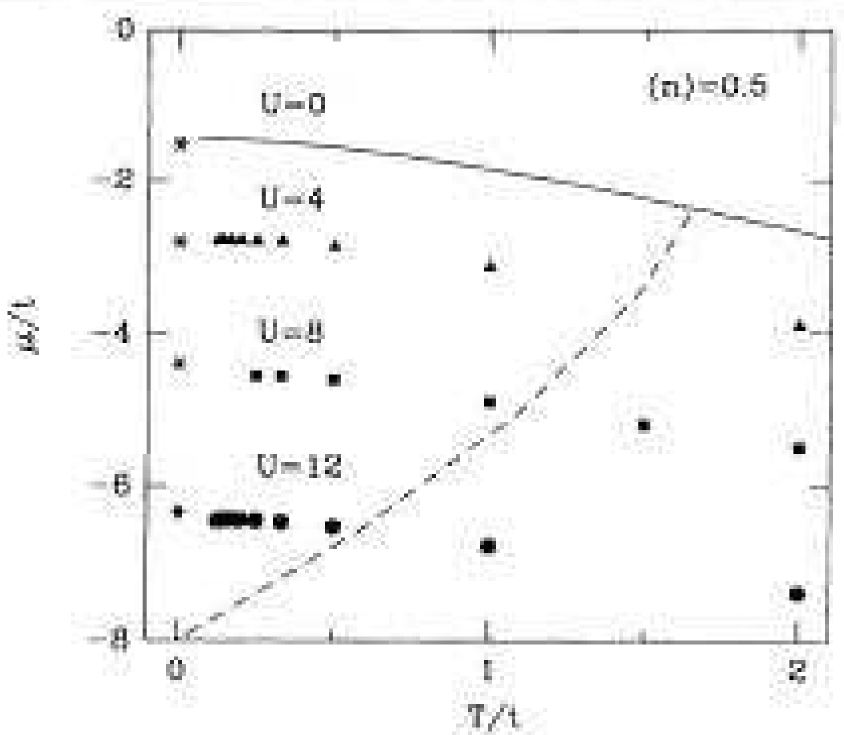
$U > W$: small tightly bound pairs with $T_c \sim t^2/U$

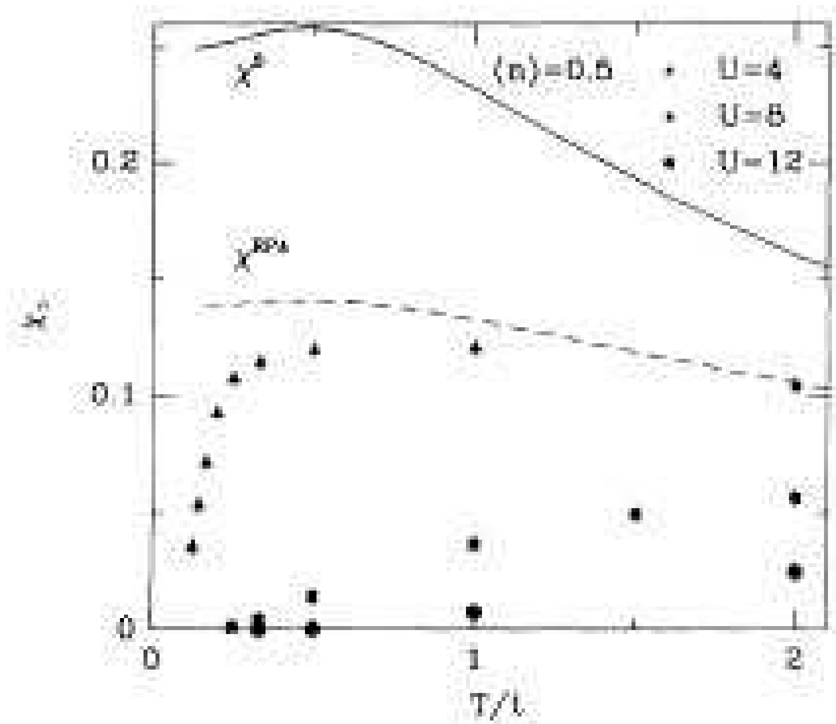


M. Randeria, N. Trivedi, A. Moreo, and RTS, PRL **69**, 2001 (1992).

T. Paiva, M. Randeria, N. Trivedi, A. Moreo, and RTS, arXiv:0906.2141.

Coexistence of bosonic (spin gap) and fermionic (Fermi surface) aspects





Left panel: $\mu(U,T)$ indicates system is degenerate. μ is much higher than T from the bottom of the band ($-4t$) including Hartree shift.

$$\mu(T,U) + 4t + \langle n \rangle U/2) > T$$

Right panel: Yet spin susceptibility χ is sharply suppressed.

Population Imbalanced Systems: Background

Usual Cooper pair: $(\, k \uparrow, \, -k \downarrow)$

What happens if $N_\uparrow \neq N_\downarrow$?

Mismatched Fermi surfaces: $k_{\mathrm{F,\,majority}} \neq k_{\mathrm{F,\,minority}}$

"Breached Pair"

- Superfluid of Cooper pairs $(\, k \uparrow, \, -k \downarrow)$ for $k < k_{\mathrm{F,\,minority}}$. coexists with normal fluid (of excess species).
- Pairs have zero momentum.
- Translationally invariant.

Fulde-Ferrell-Larkin-Ovchinnikov

- Pairs have non-zero momentum $k_{\mathrm{F,\,majority}} - k_{\mathrm{F,\,minority}}$.
- Spatially inhomogeneous.
- Hard to see in condensed matter systems.

Cold Atom Systems

- Two hyperfine states play role of spin up and down.
- One complication is role of trapping potential.

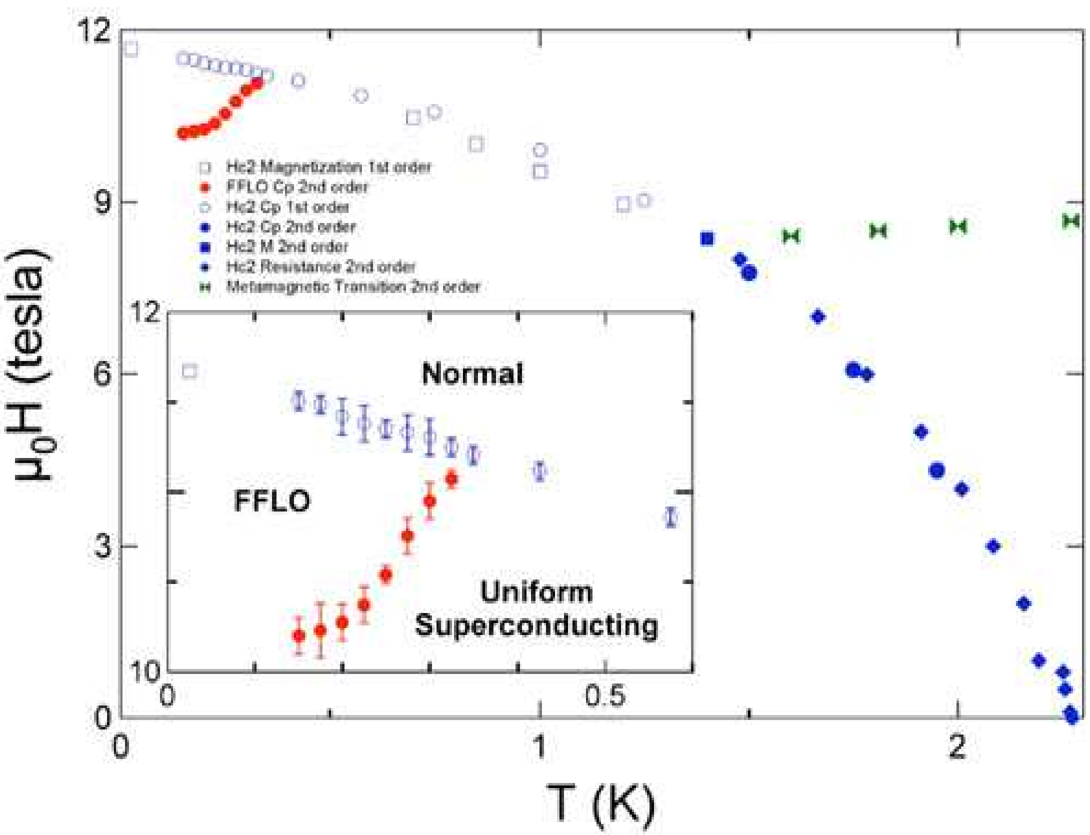
Experimental Motivation - Solid State

Forty years after its theoretical discussion, FFLO phase observed.

Heavy fermion system $CeCoIn_5$. T_c=2.3 K.

Requires very pure and strongly anisotropic single crystals.

Apply large field parallel to conducting planes.

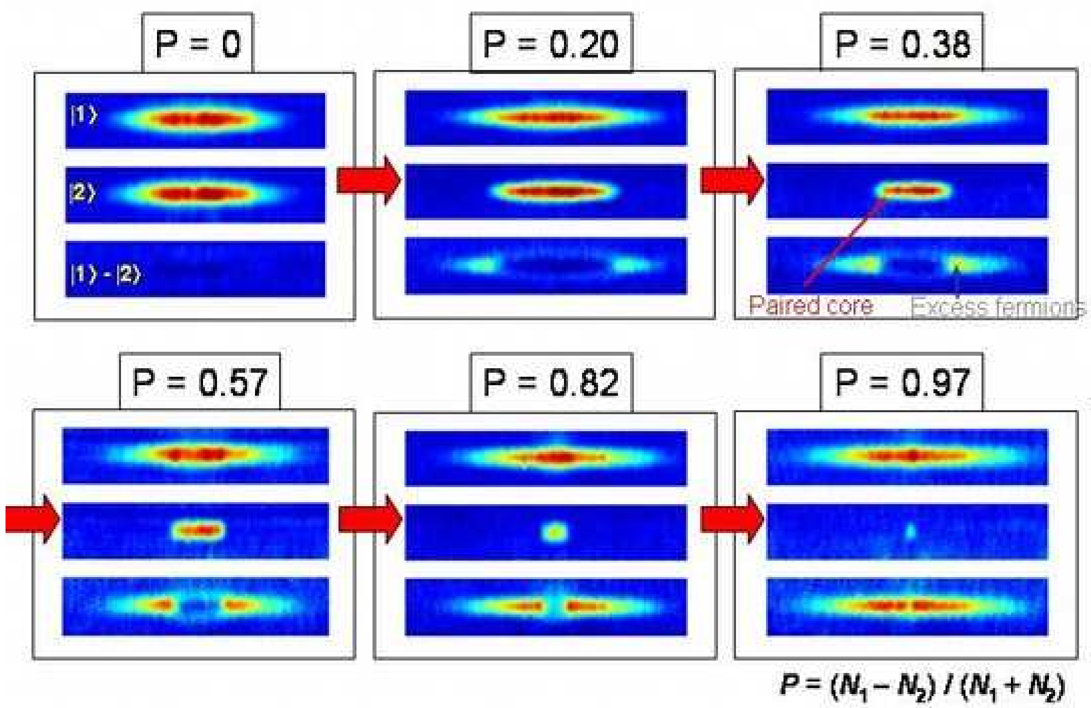


H.A. Radovan *et al.*, Nature **425**, 51 (2003).

M.R. Norman, materials dependence of FFLO in UPd_2Al_3, PRL **71**, 3391 (1993).

Experimental Motivation - Cold Atoms

Fermion ^{6}Li in hyperfine states $F = \frac{1}{2}, m_F = \pm\frac{1}{2}$.
Three dimensional, but highly elongated, traps.
Tunable interaction strength via Feschbach resonance.
Tunable relative $m_F = \pm\frac{1}{2}$ populations.

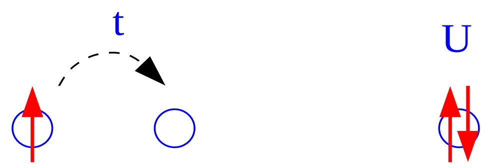


Core of system has uniform pairing $(n_1 - n_2 = 0)$. Excess atoms sit at edge.
G.B. Partridge *et al.*, Science **311**, 503 (2006).
Also: M.W. Zwierlein *et al.*, Science **311**, 492 (2006); Nature **422**, 54 (2006).

The Attractive Fermion Hubbard Hamiltonian

$$H = -t \sum_{j,\sigma} (c^\dagger_{j\sigma} c_{j+1\sigma} + c^\dagger_{j+1\sigma} c_{j\sigma}) - |U| \sum_j n_{j\uparrow} n_{j\downarrow} + V_T \sum_j j^2 (n_{j\uparrow} + n_{j\downarrow})$$

Operators $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) create (destroy) an electron of spin σ on site i.
Electron kinetic energy t; interaction energy U; Quadratic confining potential V_T.



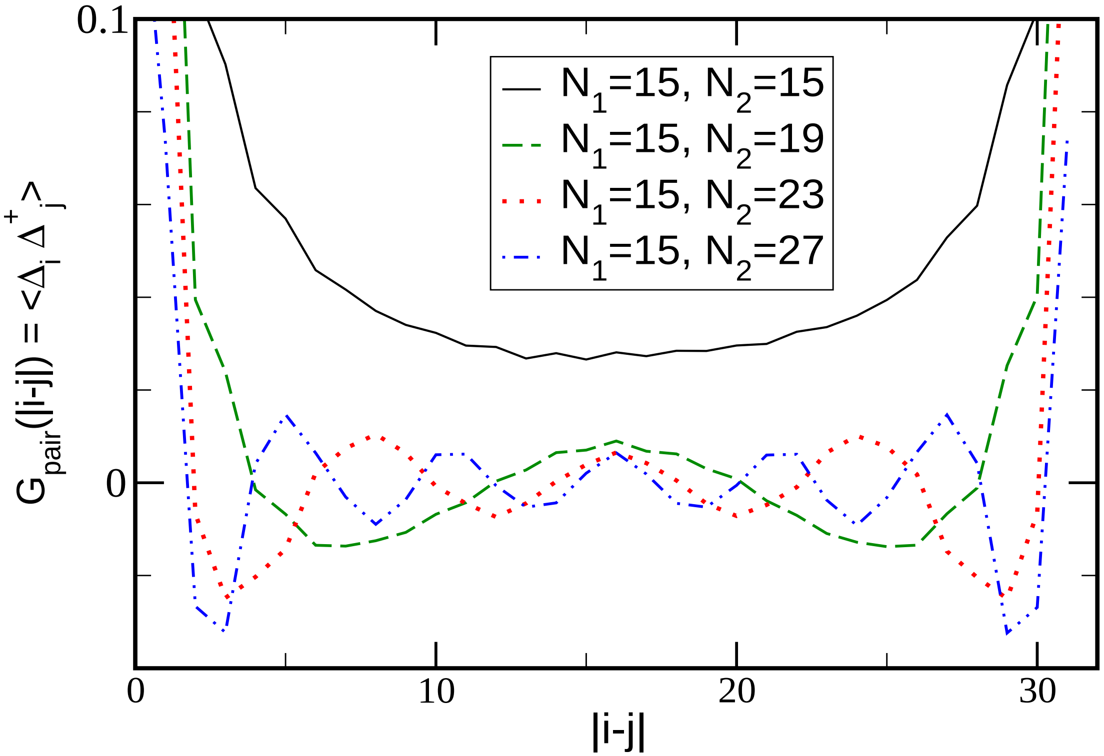
Condensed matter: Two spin species $\sigma = \uparrow, \downarrow$.
Optically Trapped Atoms: Two hyperfine states "σ" $= 1, 2$.

Observables

$$\begin{aligned} G_\sigma(l) &= \langle c^\dagger_{j+l\,\sigma} c_{j\,\sigma} \rangle && \text{Fourier transform}: n_\sigma(k) \\ G_{\rm pair}(l) &= \langle \Delta_{j+l} \Delta^\dagger_j \rangle && \text{Fourier transform}: n_{\rm pair}(k) \\ \Delta_j &= c_{j2} c_{j1} \end{aligned}$$

FFLO Results for Uniform System in One Dimension

$$\begin{aligned} G_\sigma(l) &= \langle c^\dagger_{j+l\,\sigma} c_{j\,\sigma} \rangle \qquad \text{Fourier transform} : n_\sigma(k) \\ G_{\rm pair}(l) &= \langle \Delta_{j+l} \Delta^\dagger_j \rangle \qquad \text{Fourier transform} : n_{\rm pair}(k) \\ \Delta_j &= c_{j2} c_{j1} \end{aligned}$$

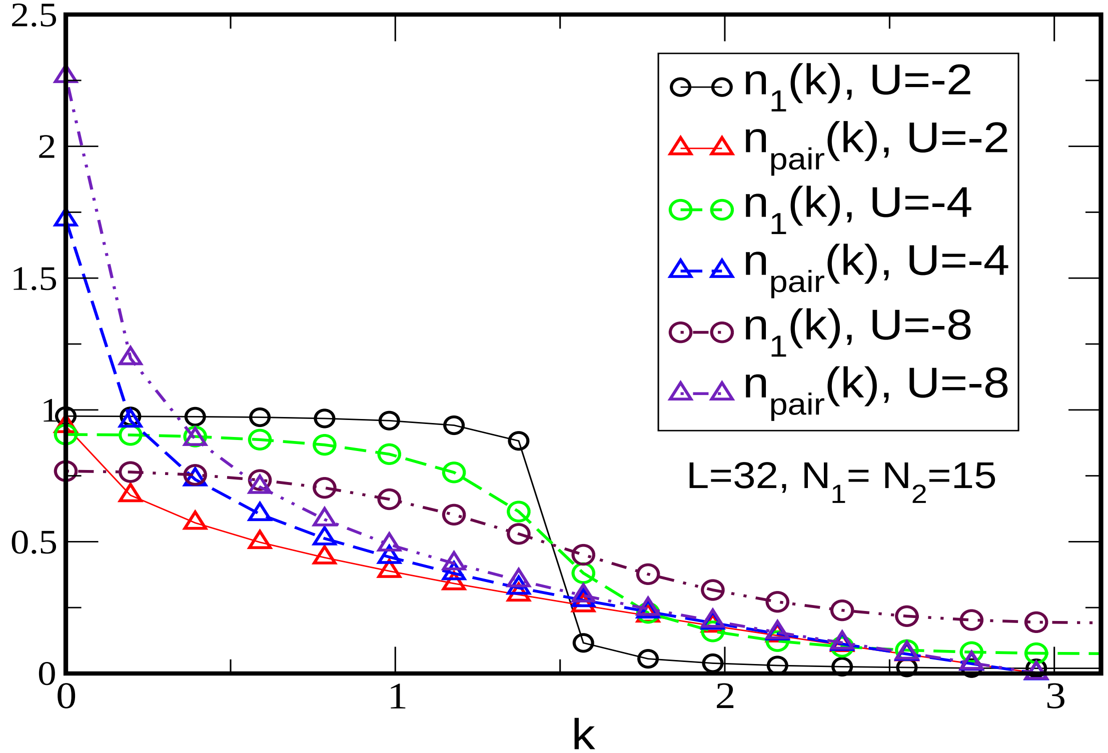


$U = -8$

$G_{\rm pair}(l)$ oscillates as $\cos(qr)$ with $q = k_{\rm majority} - k_{\rm minority}$ consistent with LO.

Begin analysis of $n_\sigma(k)$ and $n_{\rm pair}(k)$ by examining unpolarized case

- Weak coupling: $n_1(k) = n_2(k)$ is sharp.
- Strong coupling: $n_1(k) = n_2(k)$ rounded.
- $n_{\rm pair}(k)$ peaked at $k = 0$. Peak sharpens with $|U|$.



Polarized case

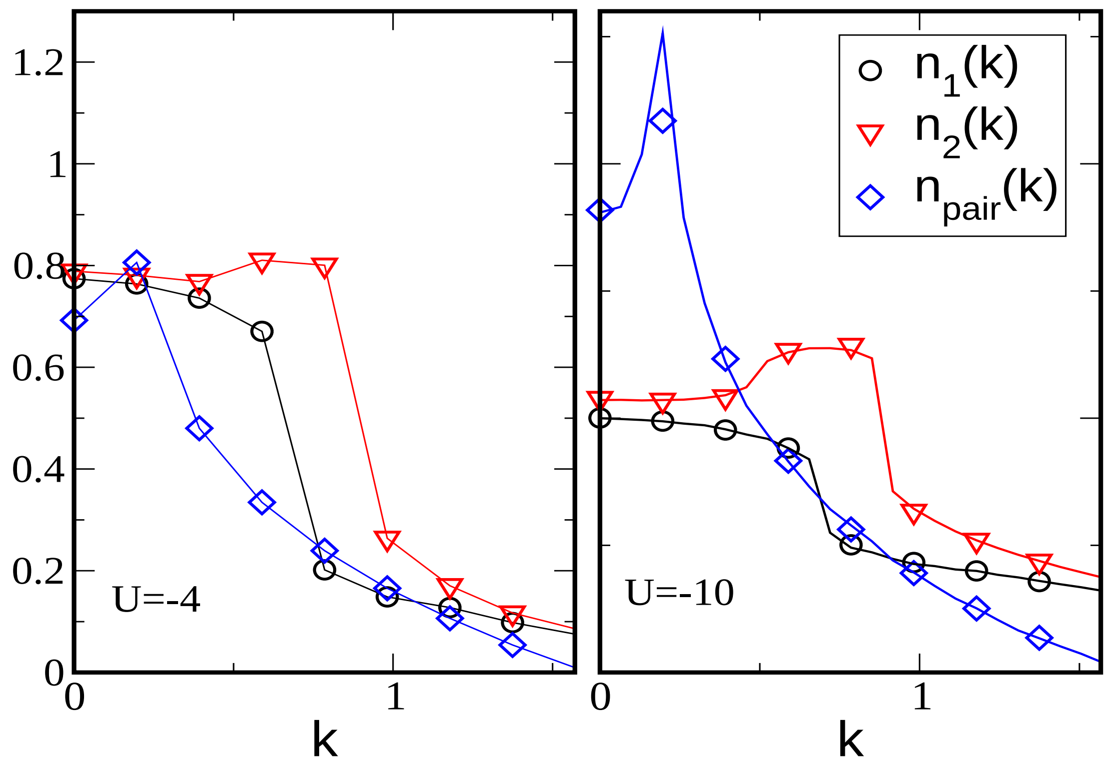
$n_{\text{pair}}(k)$ peaked at $k_{\text{majority}} - k_{\text{minority}}$ for all $|U|$.

Left panel: $U = -4$

Right panel: $U = -10$

Symbols: $N_1 = 7, N_2 = 9, L = 32$ sites, $\beta = 64$.

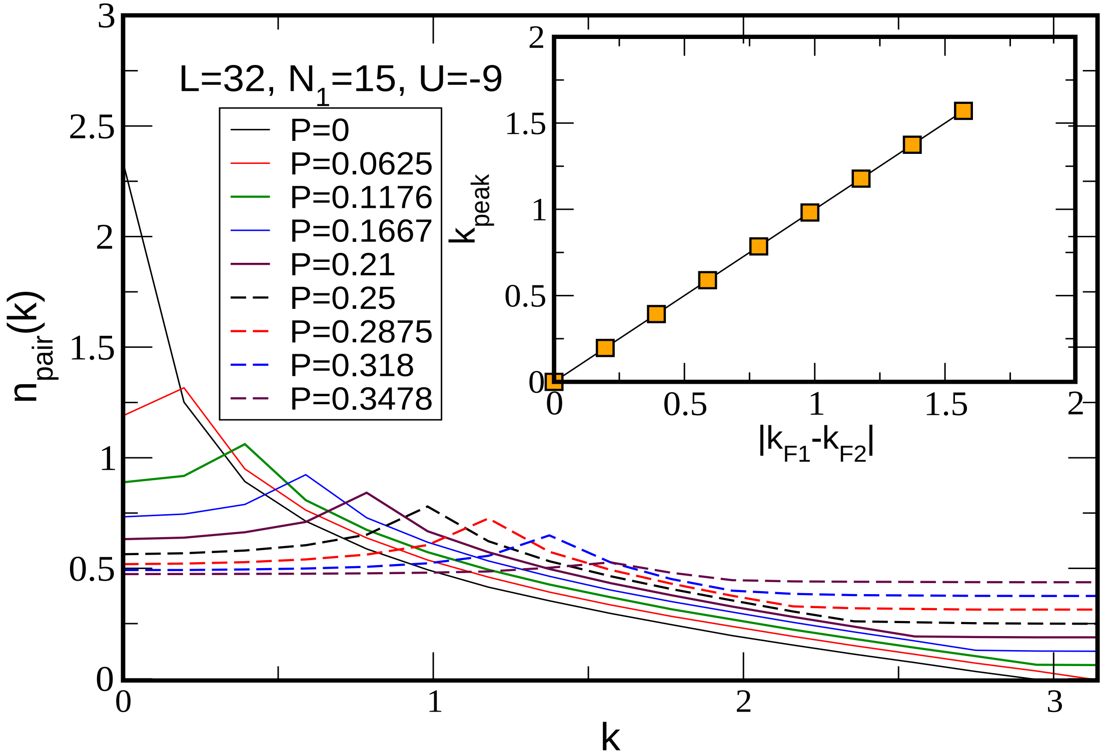
Lines: $N_1 = 21, N_2 = 27, L = 96$ sites, $\beta = 192$.



FFLO pairing no matter how large the polarization is made.

Have not seen "Clogston Limit".

Inset: Peak in $n_{\mathrm{pair}}(k)$ scales precisely as $k_{\mathrm{F,\,majority}} - k_{\mathrm{F,\,minority}}$.

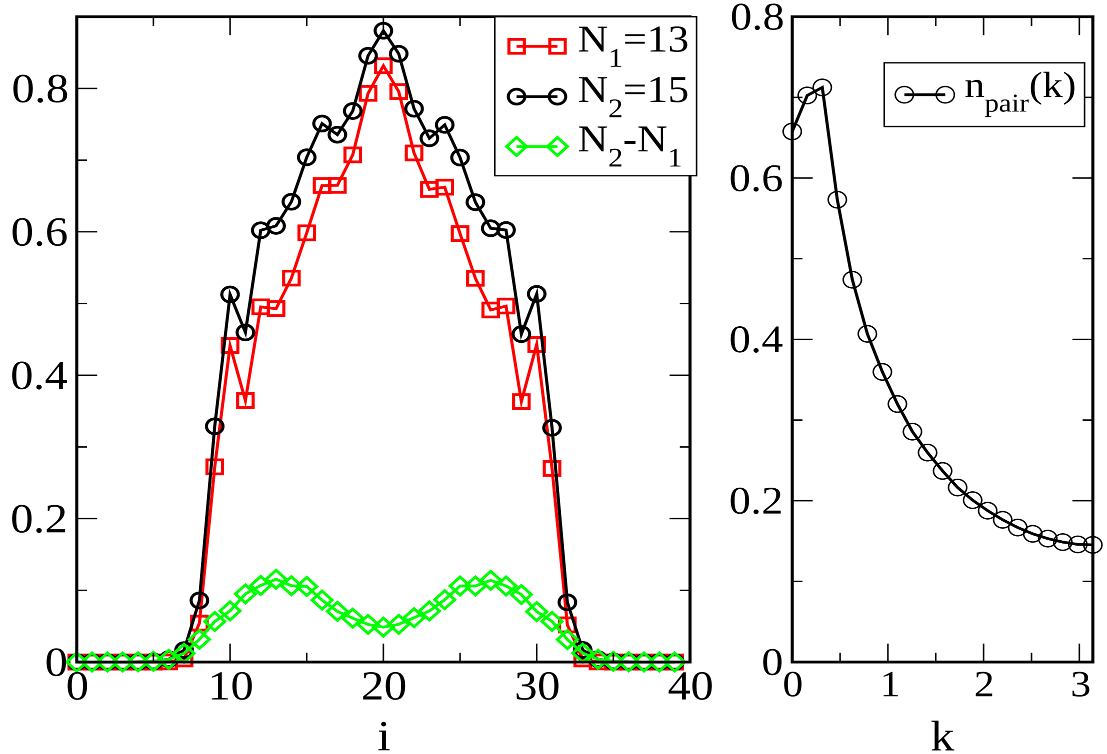


FFLO Results for Trapped System in One Dimension

Pronounced minimum in density difference at trap center.

$n_{\rm pair}(k)$ peaked at nonzero k. (System remains FFLO.)

$k_{\rm peak}$ consistent with value of local polarization at trap center.

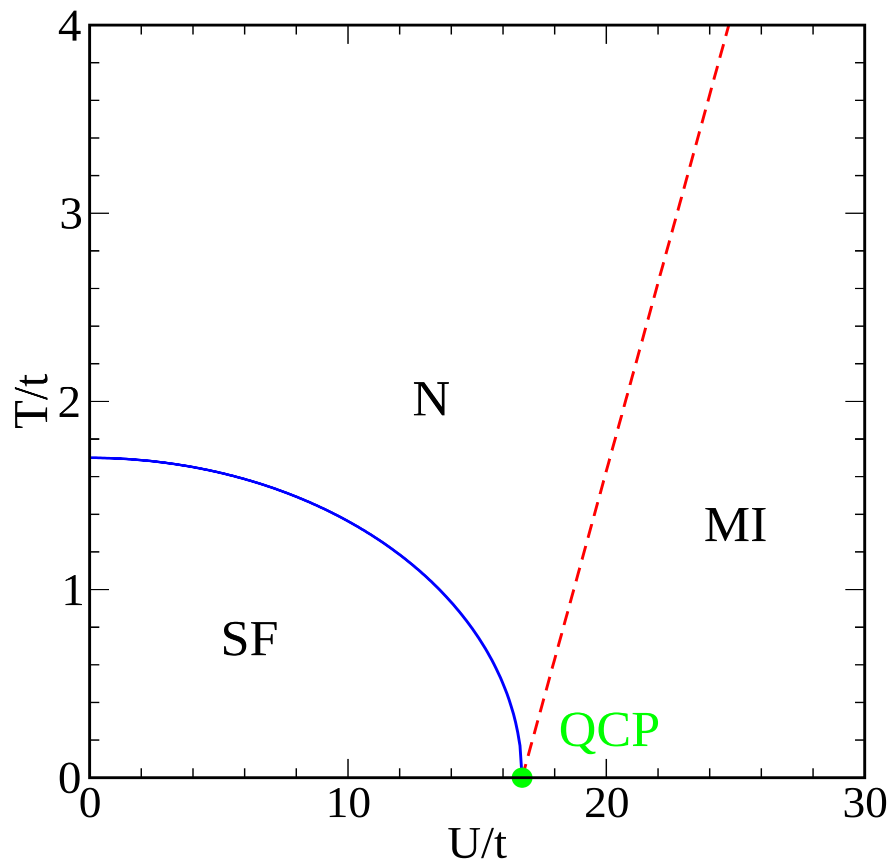


Interlude: Two Dimensional Boson Hubbard Model

M.P.A. Fisher *etal.*

Integer filling: Superfluid to Mott Insulator transition with increasing U/t

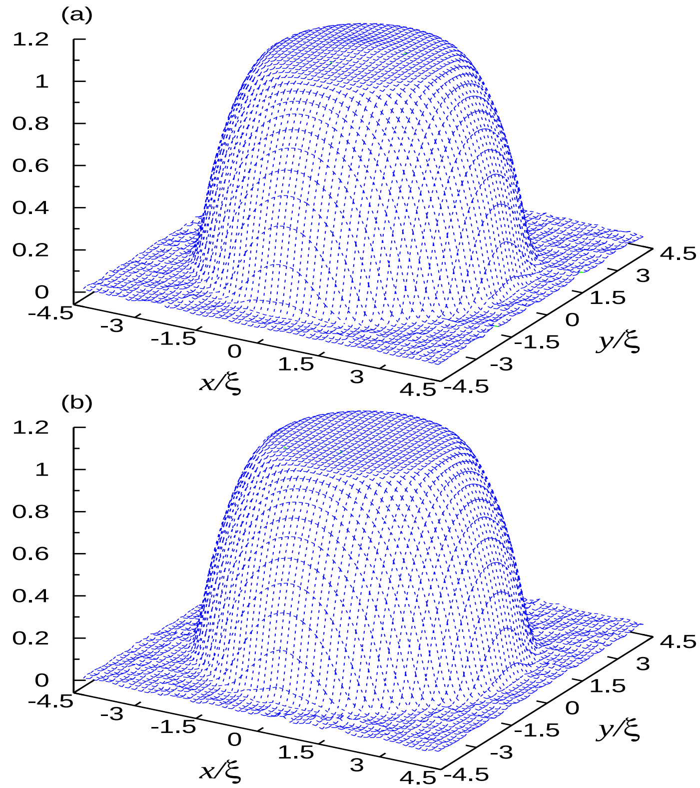
Phase diagram of uniform system in $d = 2$ and $\rho = 1$:

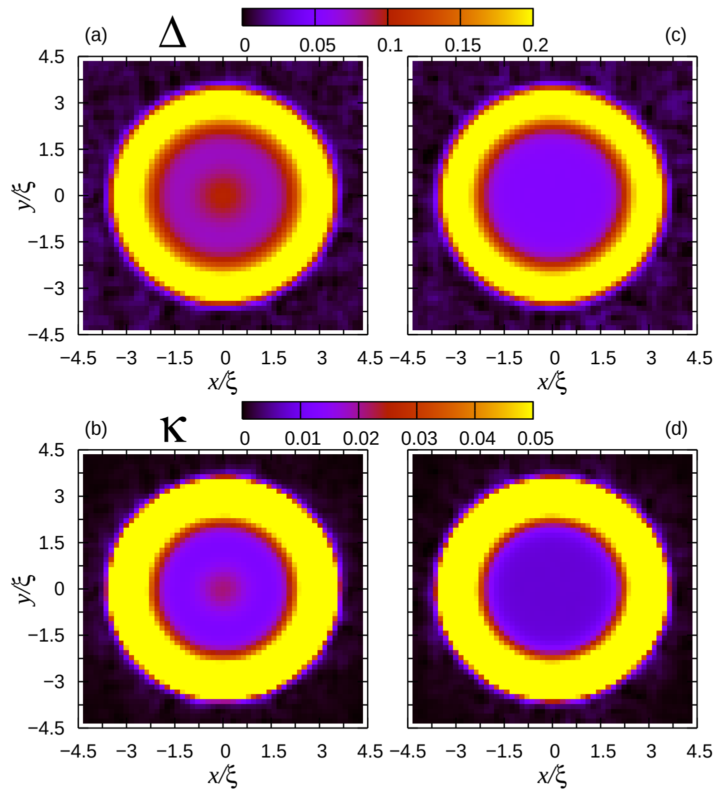


At zero temperature, $(U/t)_c = 16.74$ [Prokof'ev *etal*]

Explore effect of a confining potential in a model where simulations have no difficulties.

QMC density, number fluctuation, and compressibility profiles:





$\text{Top: } U/t = 17.5 \quad \text{Bottom: } U/t = 18.5 \quad \text{Uniform: } (U/t)_c = 16.7$

$N_b = 1200, \;\; V_{\text{trap}}/t = 0.025.$

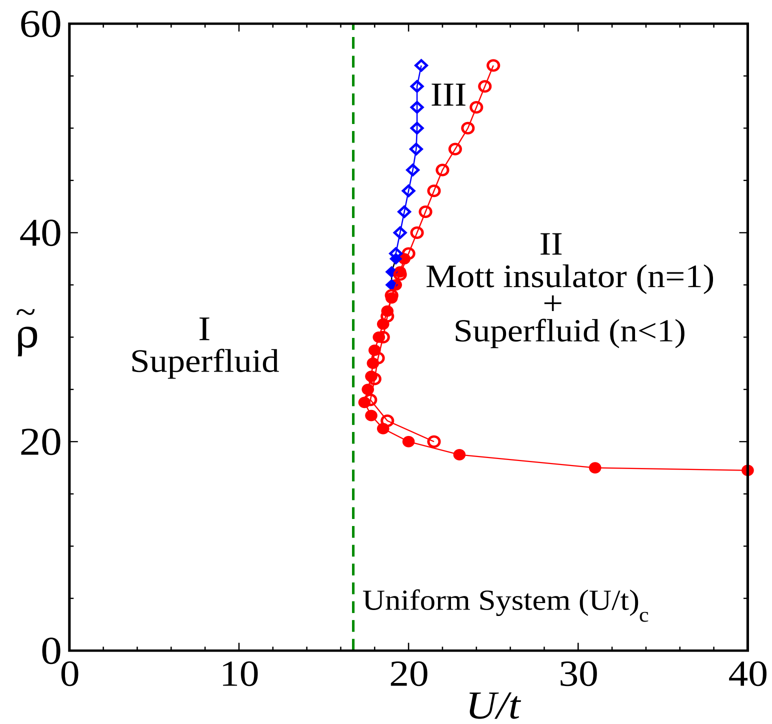
Despite extra energy scale (confining V), no more parameters than homogeneous case!

Curvature V_{trap} provides length scale $\xi = \sqrt{\frac{t}{V_{\text{trap}}}}$

Plays same role as linear lattice size

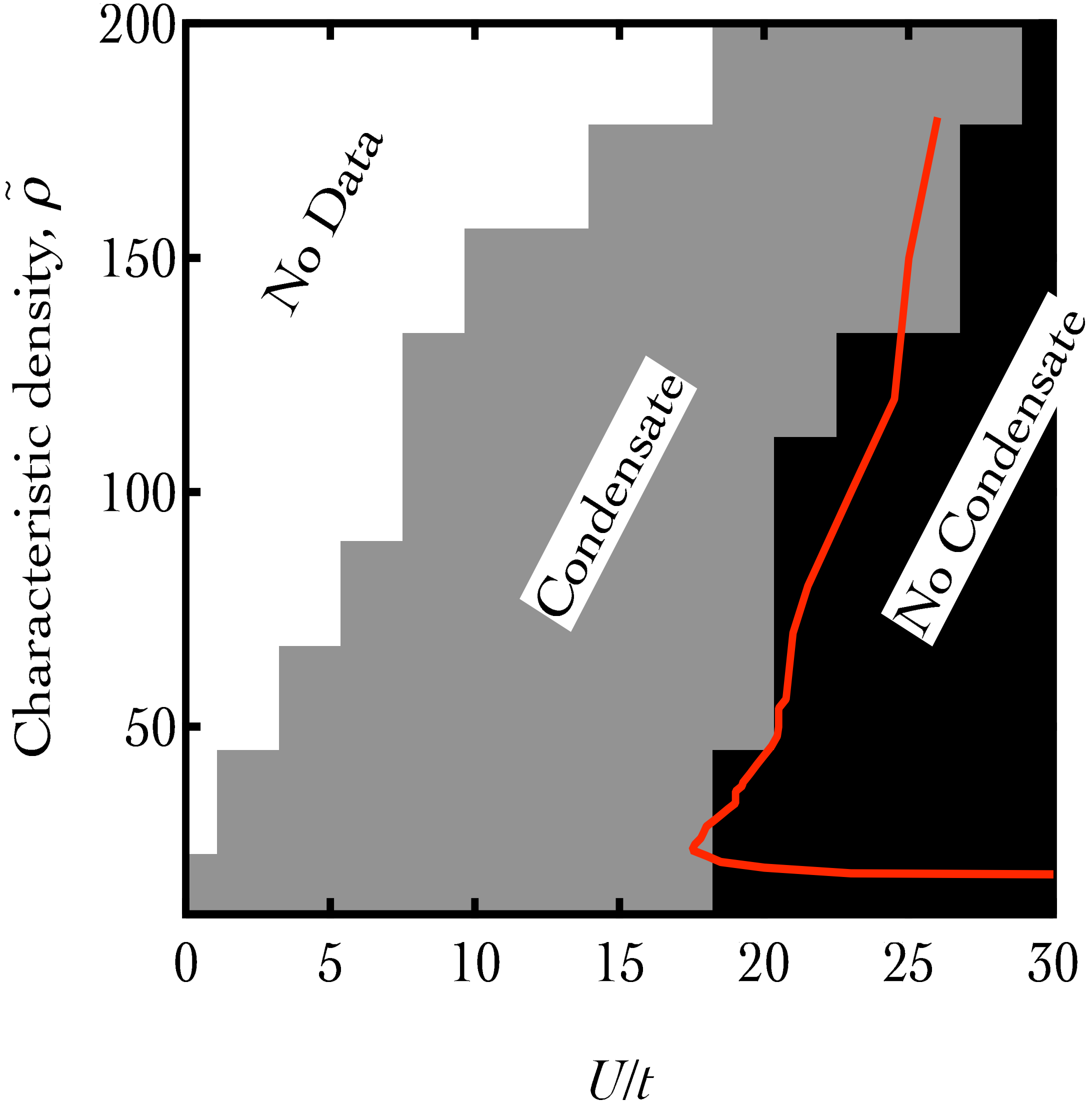
"Characteristic Density" $\tilde{\rho} = N_b/\xi^d$

Can meaningfully compare systems with different V_{trap}.



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

Experimental Comparison; Ian Spielman, Trey Porto (NIST Gaithersburg)



Approx 2000 ^{87}Rb atoms per 2D layer; $T = 33$ nK

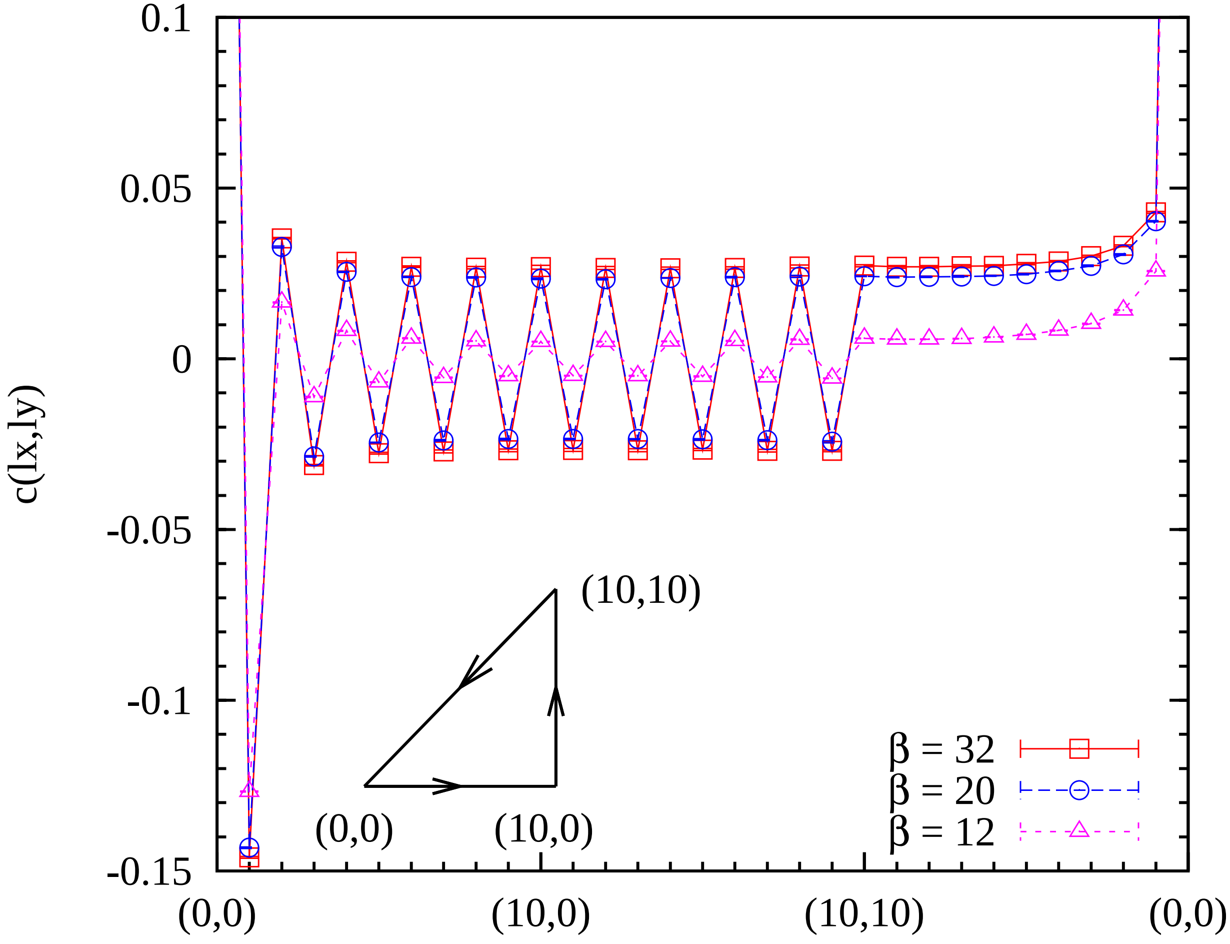
Fermions in Two Dimensions

Review of QMC capabilities for uniform system at half-filling.

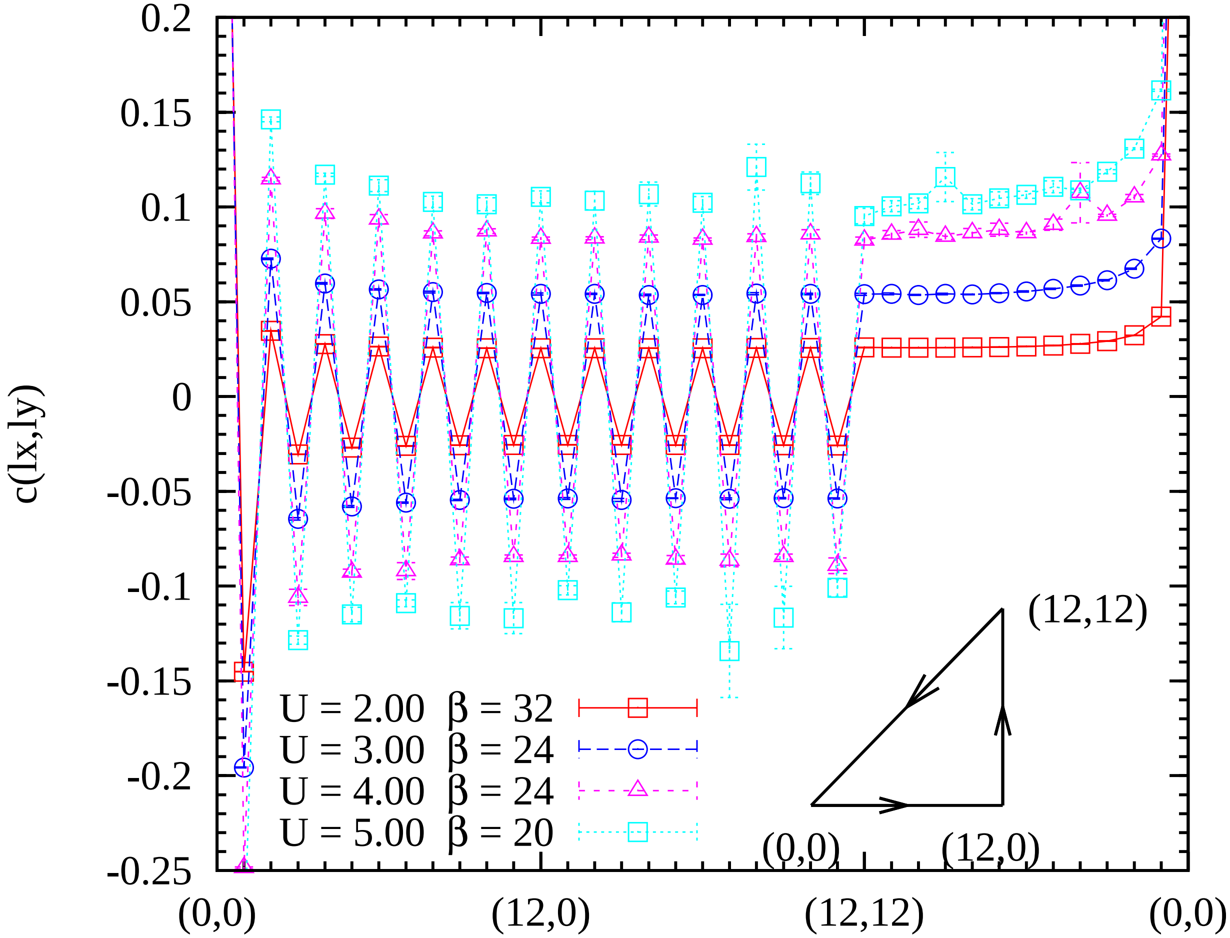
Bottom line: Can do 500-1000 fermions on desktop computers.

Antiferromagnetic spin correlations at low temperature.

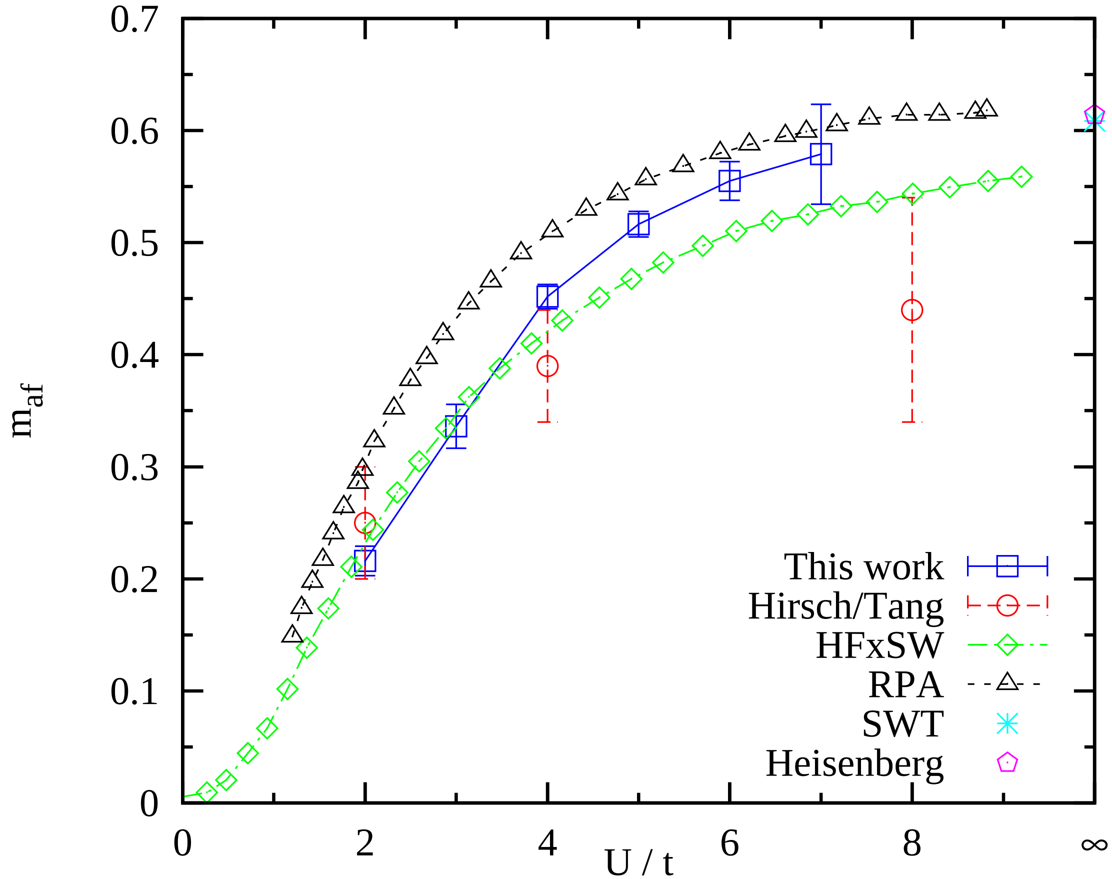
$\beta t = 20 \rightarrow T = t/20 = W/160$ (bandwidth $W = 8t$) $U = 2t$ N=20x20 lattice



Increasing U enhances antiferromagnetic correlations (N=24x24 lattice)



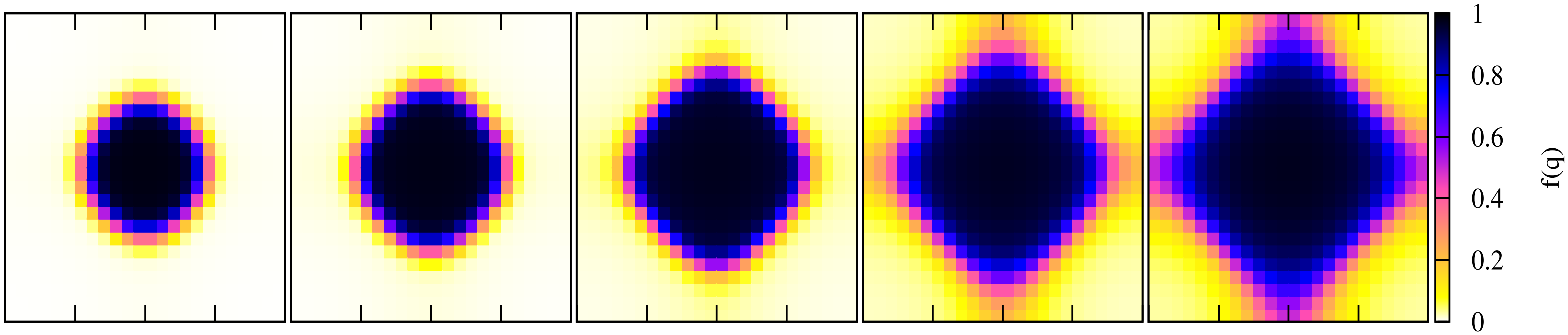
U dependence of AF order parameter



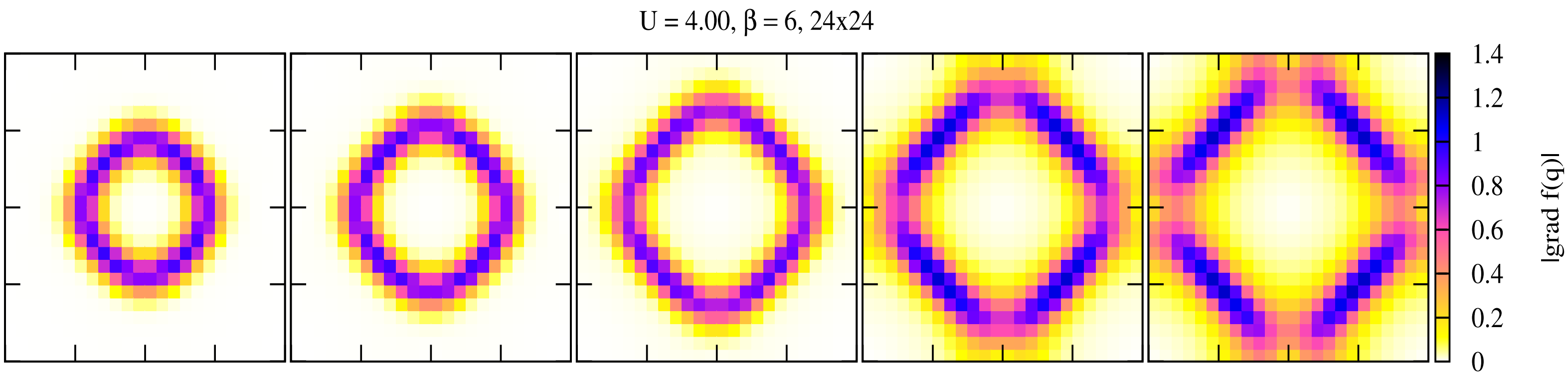
Useful for benchmarking optical lattice emulations.

Large lattices now allow good momentum resolution of Fermi surface.

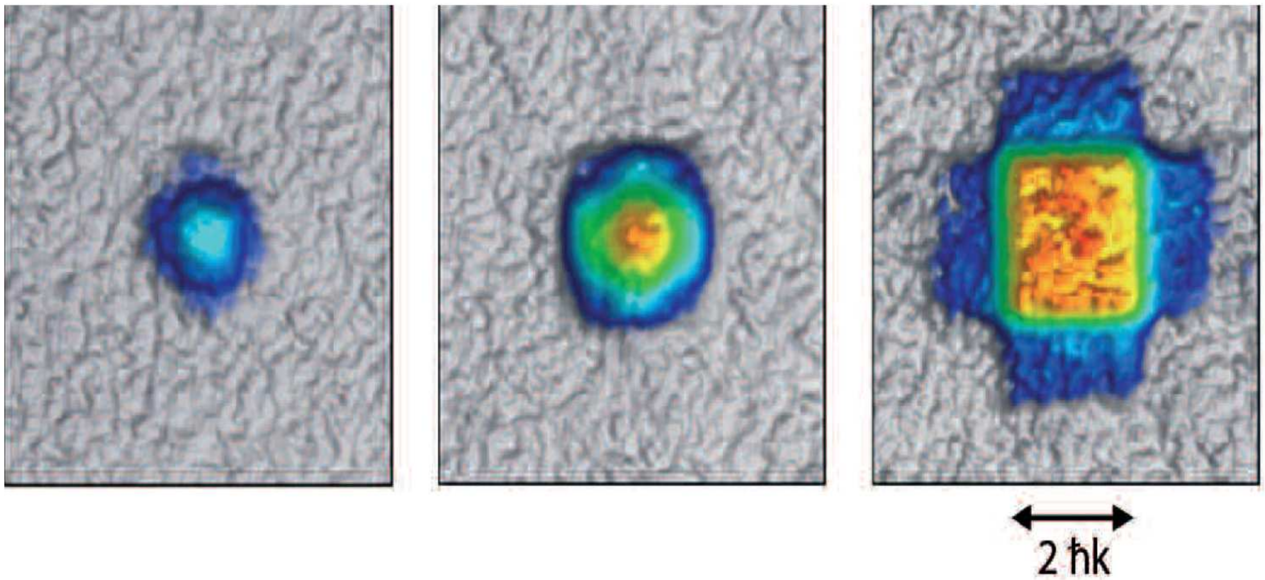
$U = 4$ Fermi function: N=24x24, $\beta = 8$; $\rho = 0.23, 0.41, 0.61, 0.79, 1.00.$



$U = 4$ Gradient of Fermi function:



Optical Lattice Imaging of Fermi Surface Possible:



Noninteracting Fermionic ^{40}K atoms in 3d cubic lattice.

Increase particle number (left to right).

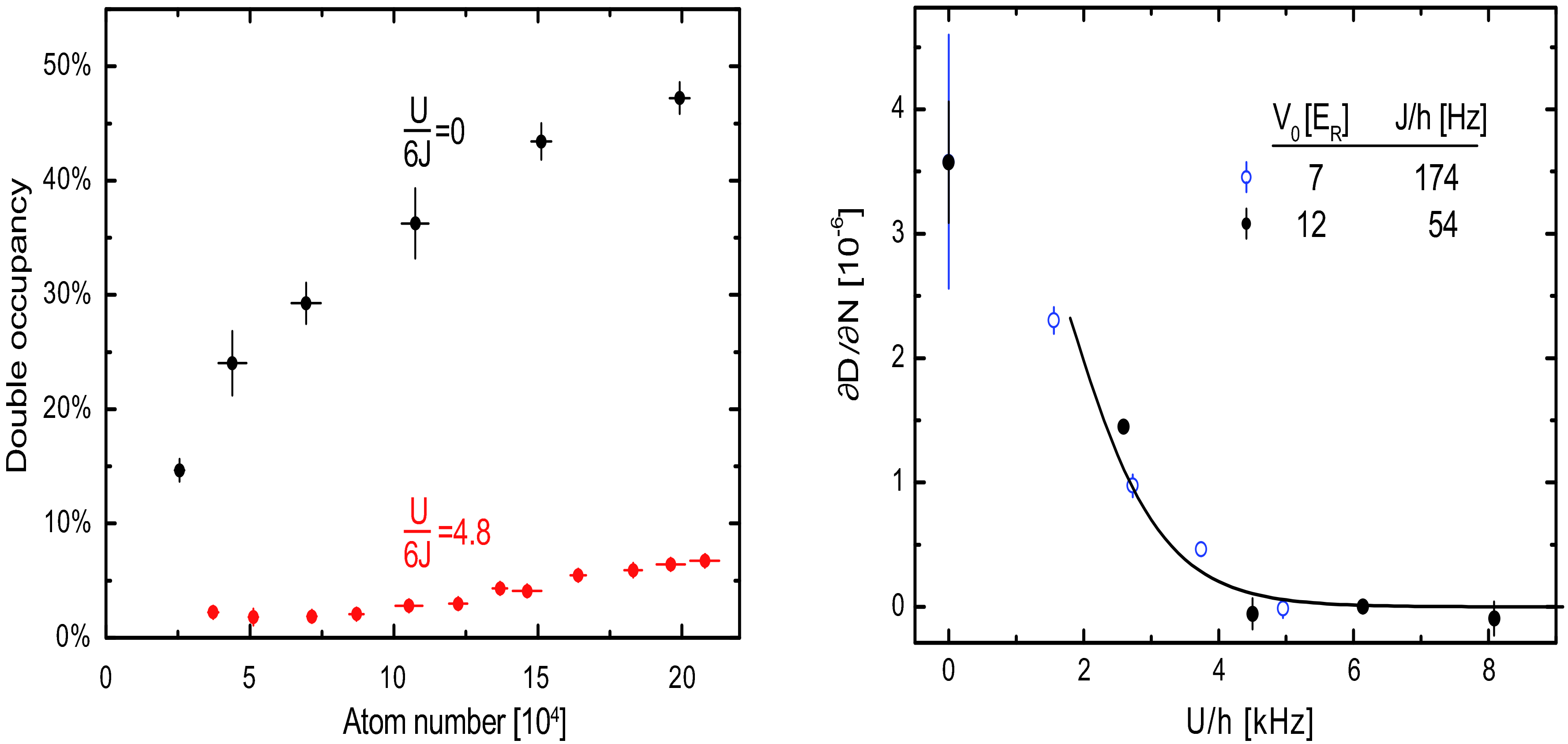
Ultimately completely fill first Brillouin zone: momentum range $(\,0, \hbar\, 2\pi/a\,)$.

$k_L = 2\pi/\lambda_L = \pi/a$ (lattice constant $a = \lambda/2$).

First BZ momentum range $2\hbar k_L$.

M. Kohl *etal.* Phys. Rev. Lett. **94**, 080403 (2005).

Observing the Mott transition



Weakly coupled phase: adding particles increases double occupancy.

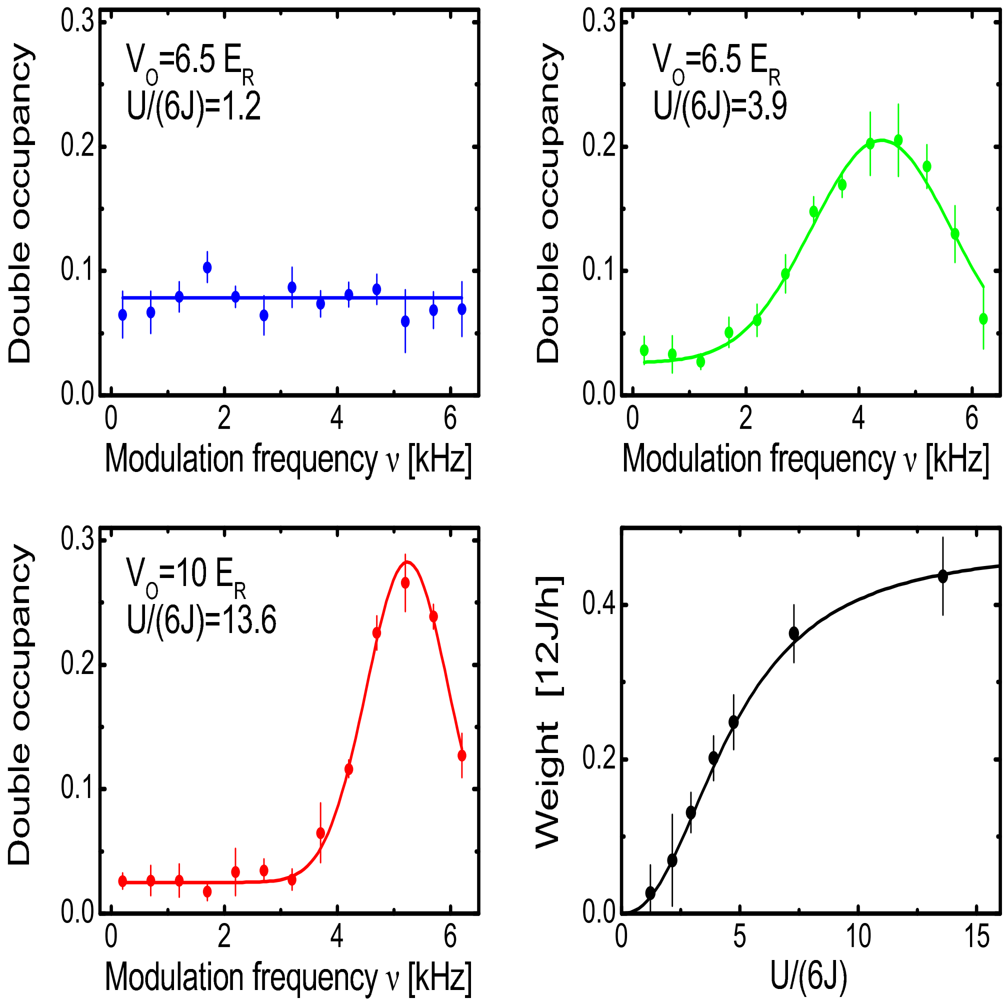
Mott phase: double occupancy doesn't increase as density increased.

Added particles go to empty trap periphery, not already singly occupied central sites.

[Useful conversion factor: 1 KHz ≈ 50 nK.]

R. Jördens *etal*, Nature **455**, 204 (2008).

Modulate the lattice depth and look for response of D.



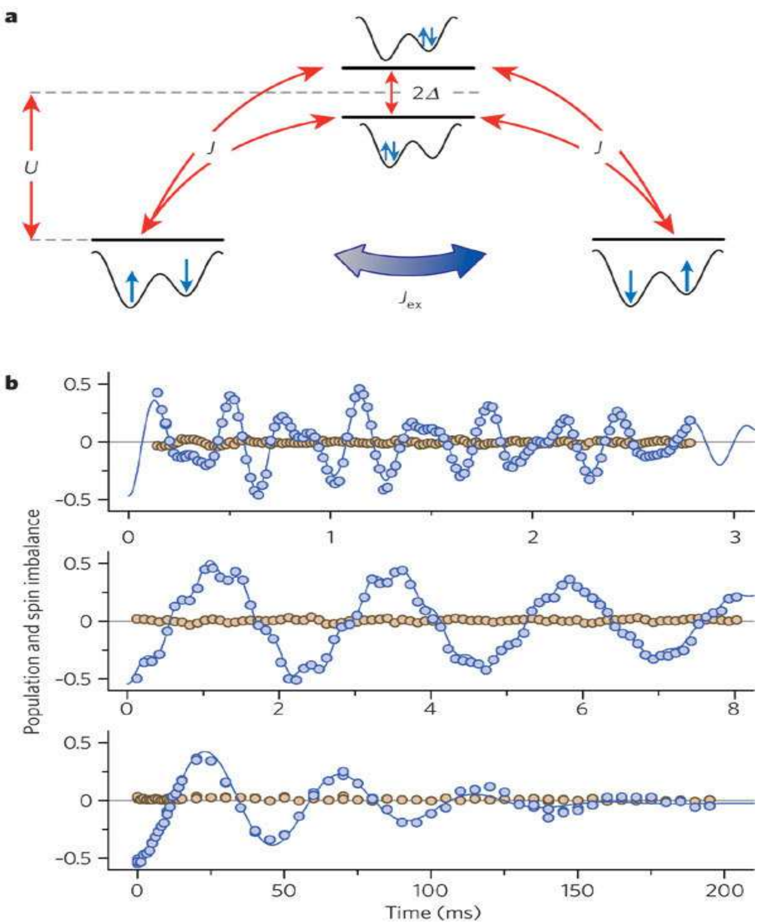
- Primary diagnostic of Mott transition at this point is double occupancy.
- Temperature $T \approx 0.1U$ (not too low).

Optical lattice realization of antiferromagnetism in early stages.

Observation and control of superexchange interactions in two site system.

$$J = 2t^2/(U+\Delta) + 2t^2/(U-\Delta)$$

Oscillations in magnetization; Top to bottom: $J/U = 1.25,\ 0.26,\ 0.048$



^{87}Rb atoms (spin-1 bosons)

Can tune Δ and t/U

Blue circles: $S_z(t) = \langle n_\uparrow(t) - n_\downarrow(t)\rangle$

Grey circles: $n(t) = \langle n_\uparrow(t) + n_\downarrow(t)\rangle$

Model: Two site (spinful) Bose-Hubbard

Diagonalize and compute time evolution.

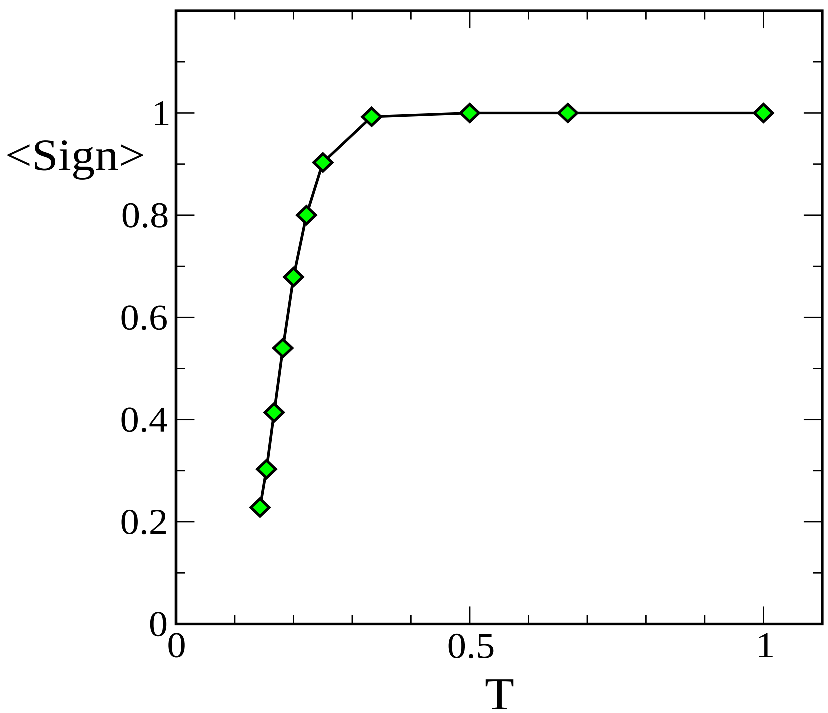
S. Trotzky *et.al.* (Demler), condmat:0712.1853; I. Bloch, Nature **453**, 1016 (2008).

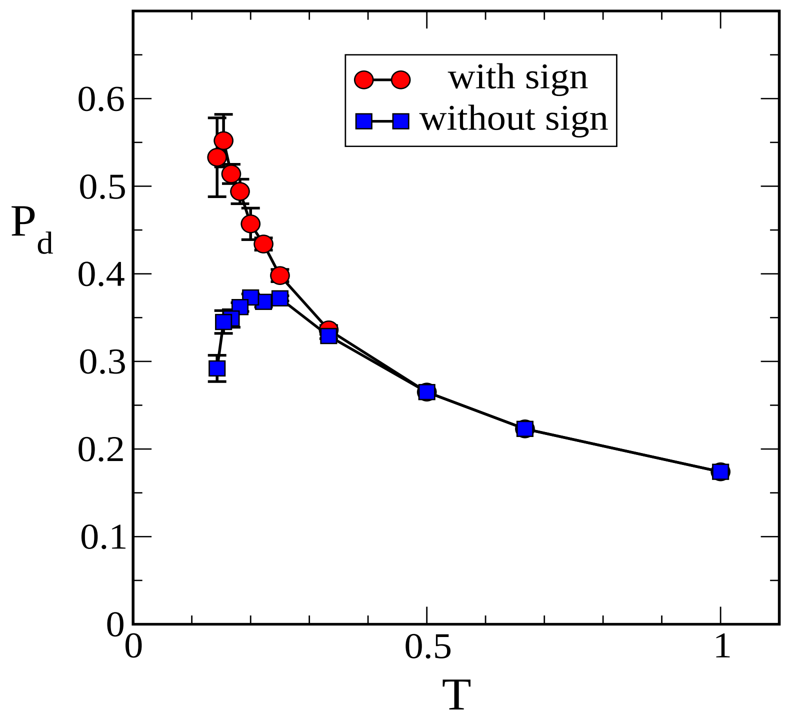
Trapped System in Two Dimensions: Must confront sign problem

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!)

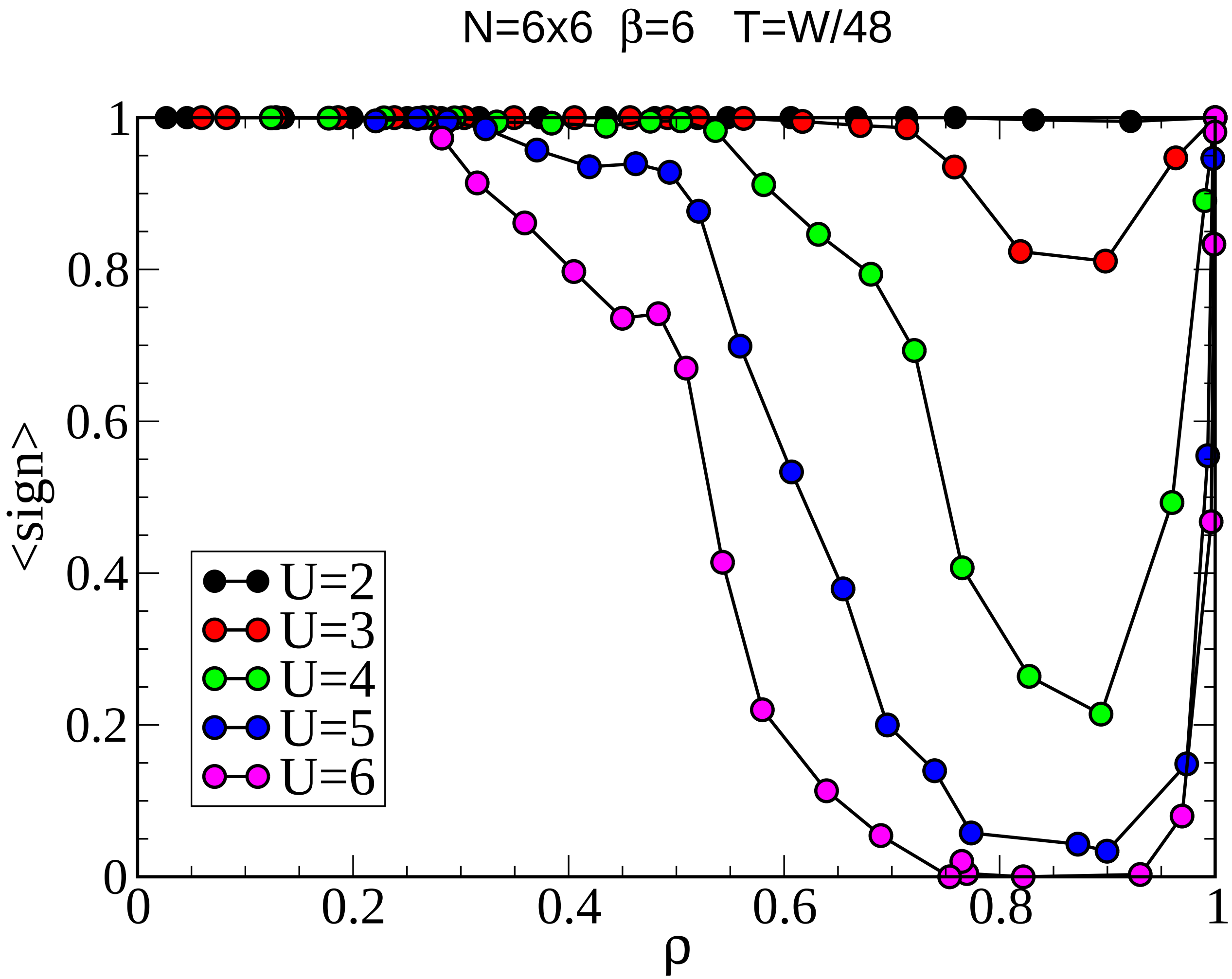
It is essential to include the sign.

2x2 lattice (!) ρ=0.875





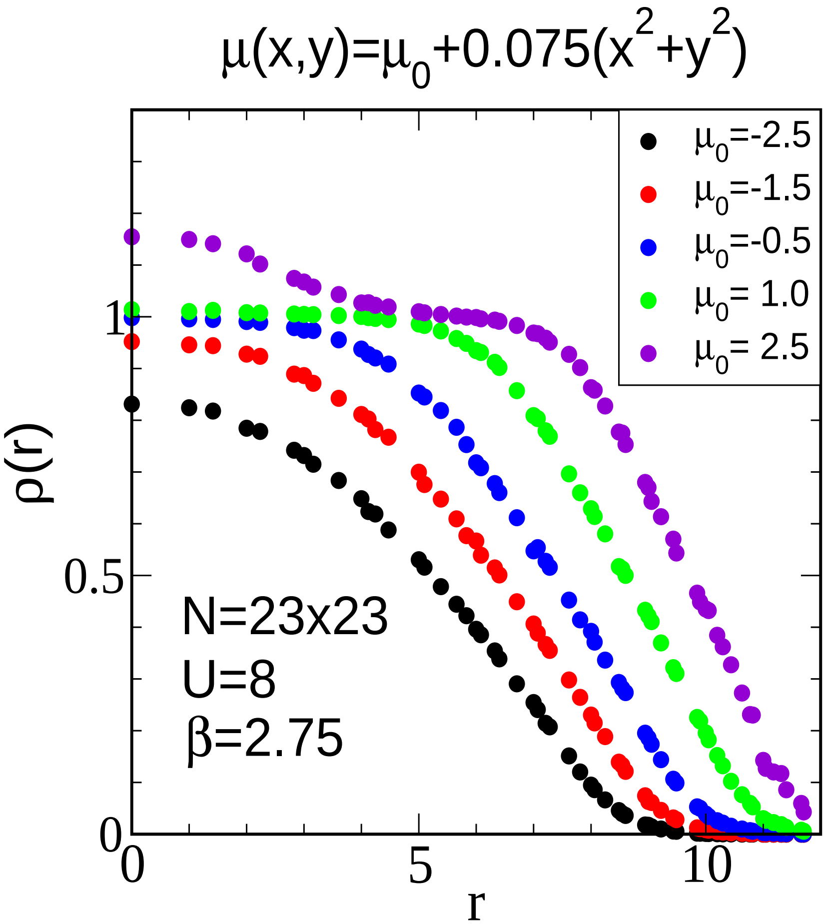
Sign problem at other fillings

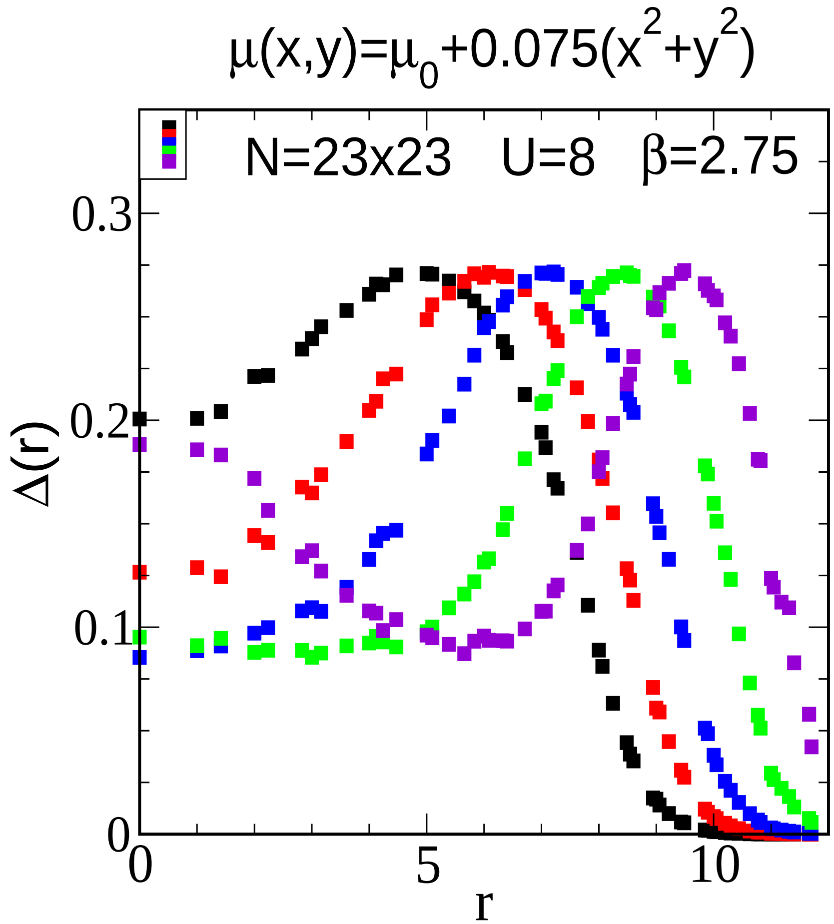


Good quality momentum distribution $n(k)$, N=24x24 lattices, different ρ.

What happens to sign problem for inhomogeneous $\rho(x)$???

First attempts at simulating trapped Fermi systems (N=23x23)





Can see Mott region $\rho(x) = 1$ forming in trap center.

Significantly reduced density fluctuations $\Delta(x) = \langle \rho(x)^2 \rangle - \langle \rho(x) \rangle^2$.

Spatially resolved antiferromagnetic correlations coming soon.

Conclusions - Eduardo's Questions Answered?

What can we learn from experiments with cold atoms? Can they be made colder than LSCO in real terms?

Present experimental status: struggling to get $T \approx J$.

Will we know if the Hubbard model (in 2D) is a superconductor, say, in five years?

From QMC? (See Jarrell-Scalapino.)

From experiments on cold atoms? Requires much lower T.

Intrinsically inhomogeneous (trapping potential).

How can novel quantum information ideas deal with the fermion sign problem? Can they? The Grassmann Chip?

No.

What is the future of Quantum Monte Carlo in this context?

QMC: $T_{\rm min} \approx t/4 = W/32$. Will certainly help cold atom community: $T_{\rm min} \approx t$.

Possible frontier: Layers of strongly correlated materials (Mannhart).

- Arbitrarily low T if layers half filled, even with very different U/t.
- Can (perhaps) go to low T if doping is in weakly correlated layer.