Recent Progress in Fermion Quantum Monte Carlo Simulations

The FFLO Phase in 1D Imbalanced Fermion Systems

AntiFerromagnetic Order Parameter of 2D Half-Filled Hubbard Model

Orbitally Selective Mott Transitions

Conclusions

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I. FFLO Phase- Theoretical 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 CM systems.

Cold Atom Systems

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

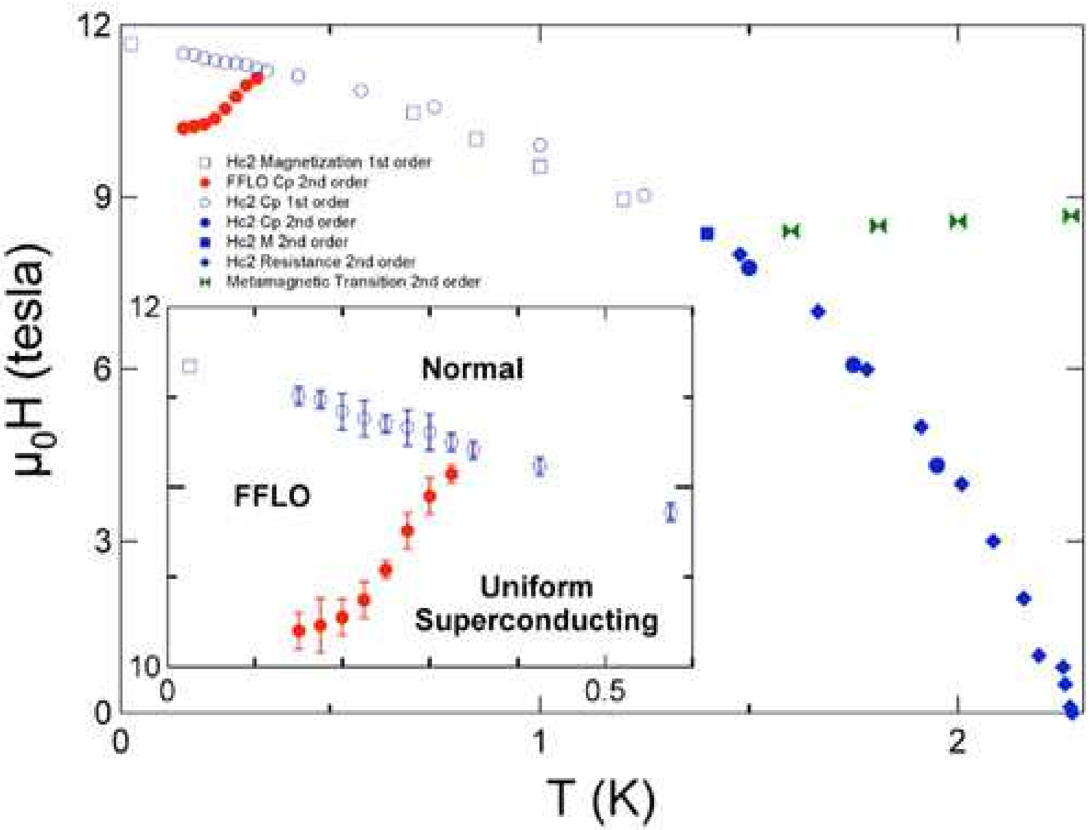
FFLO Experimental Motivation - Solid State

Forty years after its theoretical discussion, FFLO phase observed.

Heavy fermion system $CeCoIn_5$.

Requires very pure and strongly anisotropic single crystals.

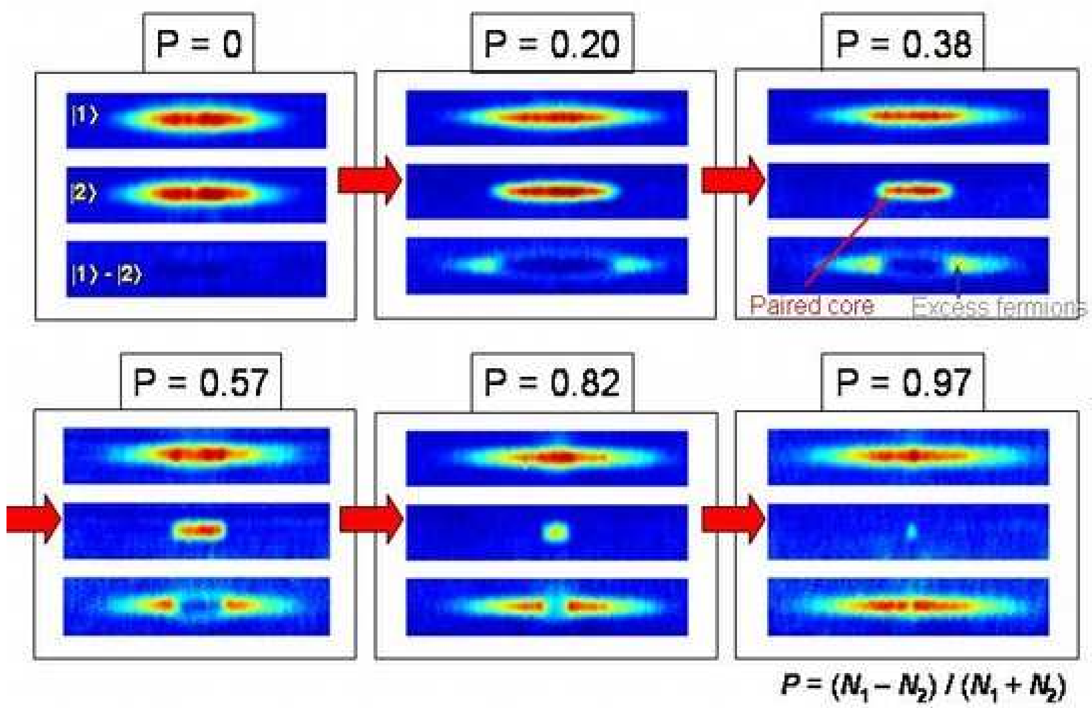
Apply large field parallel to conducting planes.



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

FFLO 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.

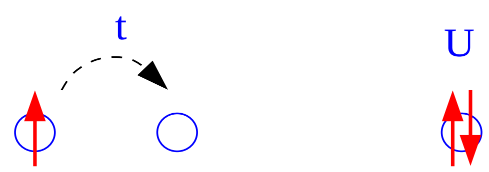


Core of system has uniform pairing ($n_1 - n_2 = 0$). Excess atoms sit at edge.
G.B. Partridge *et al.*, Science **311**, 503 (2006).
Also: M.W. Zwierlein *et al.*, Science **311**, 492 (2006); Nature **422**, 54 (2006).

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

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

Algorithm

Continuous time canonical ‘worm’ algorithm (Rombouts, Van Houcke, Pollet).

No discretization of imaginary time (no ‘Trotter’ errors).

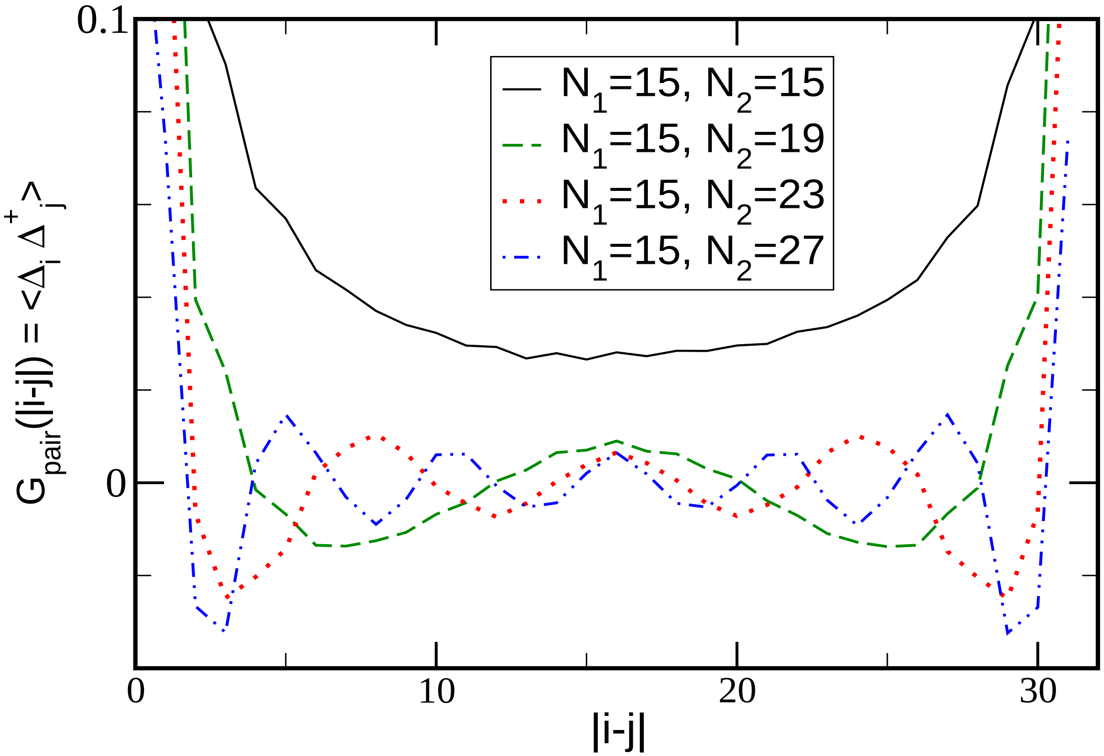
Constant particle number.

Broken world lines (‘worms’) are propagated.

- Large moves through configuration space (short correlation times).
- Can measure non-local Greens functions.

FFLO Results for Uniform System

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

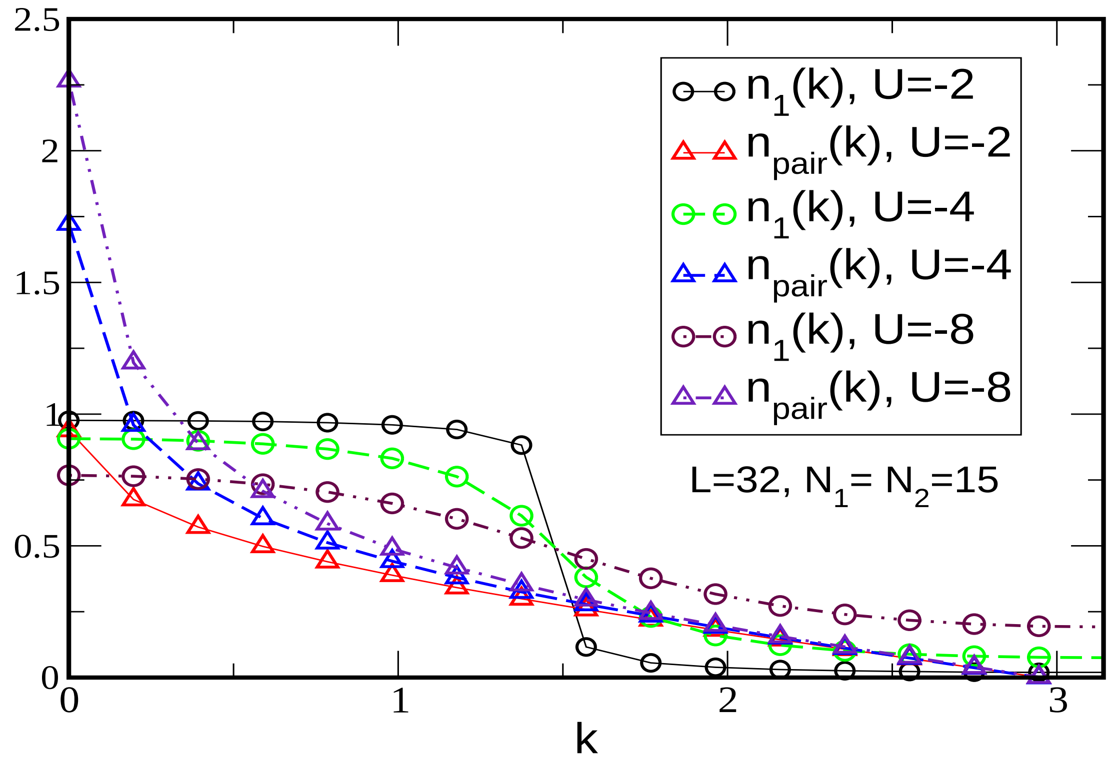


$U = -8$

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

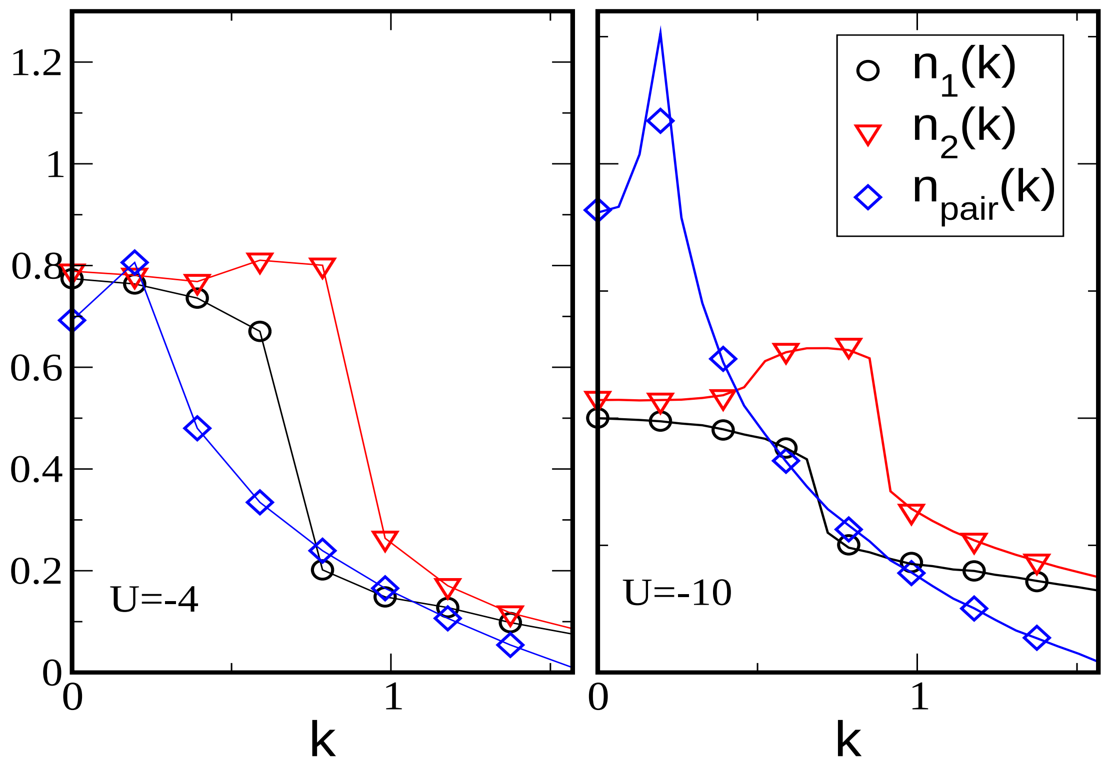
$n_{\text{pair}}(k)$ peaked at $k_{\text{majority}} - k_{\text{minority}}$ for all $|U|$.

Left panel: $U = -4$

Right panel: $U = -10$

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

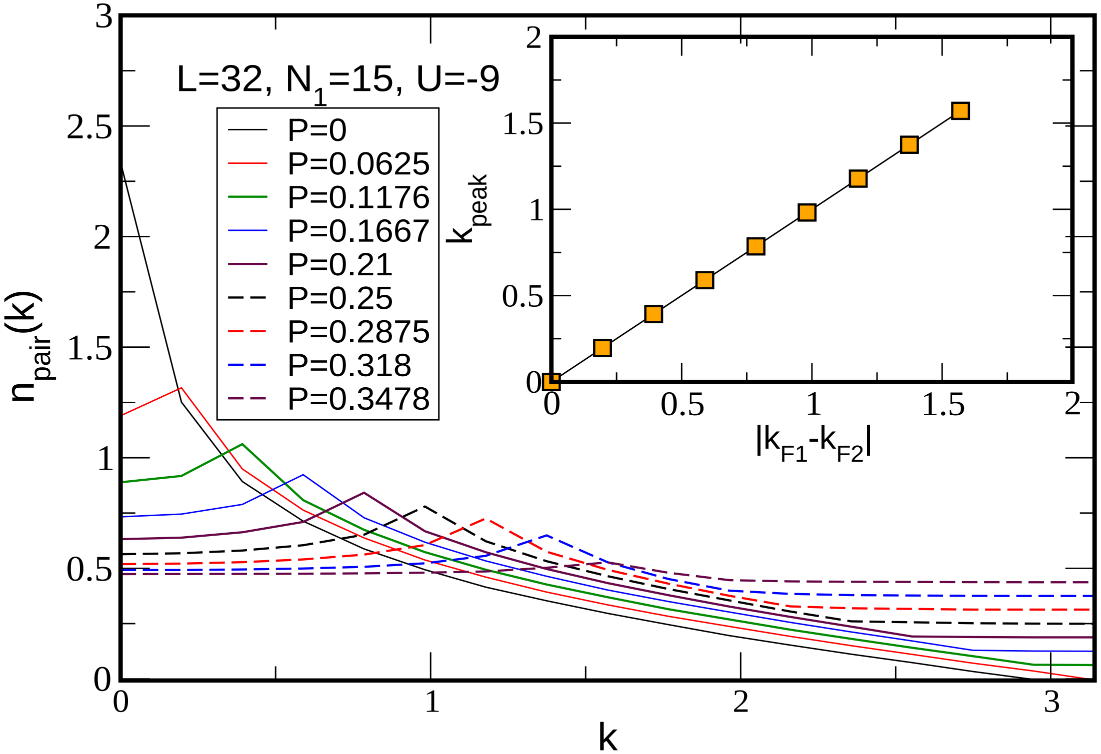
Lines: $N_1 = 21, N_2 = 27, L = 96$ sites, $\beta = 192$.



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 $k_{\mathrm{F,\,majority}} - k_{\mathrm{F,\,minority}}$.



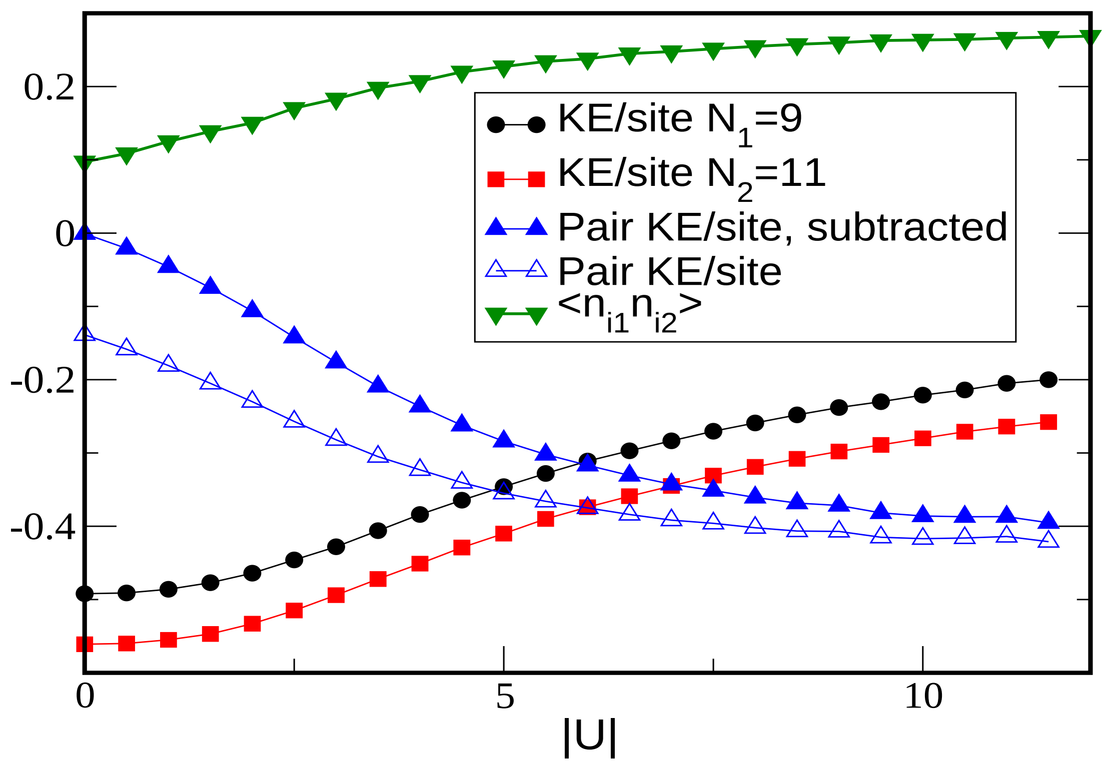
Kinetic Energy

As $|U|$ increases:

|Single particle KE| decreases

|Pair KE| increases

Hopping is increasingly "in pairs".



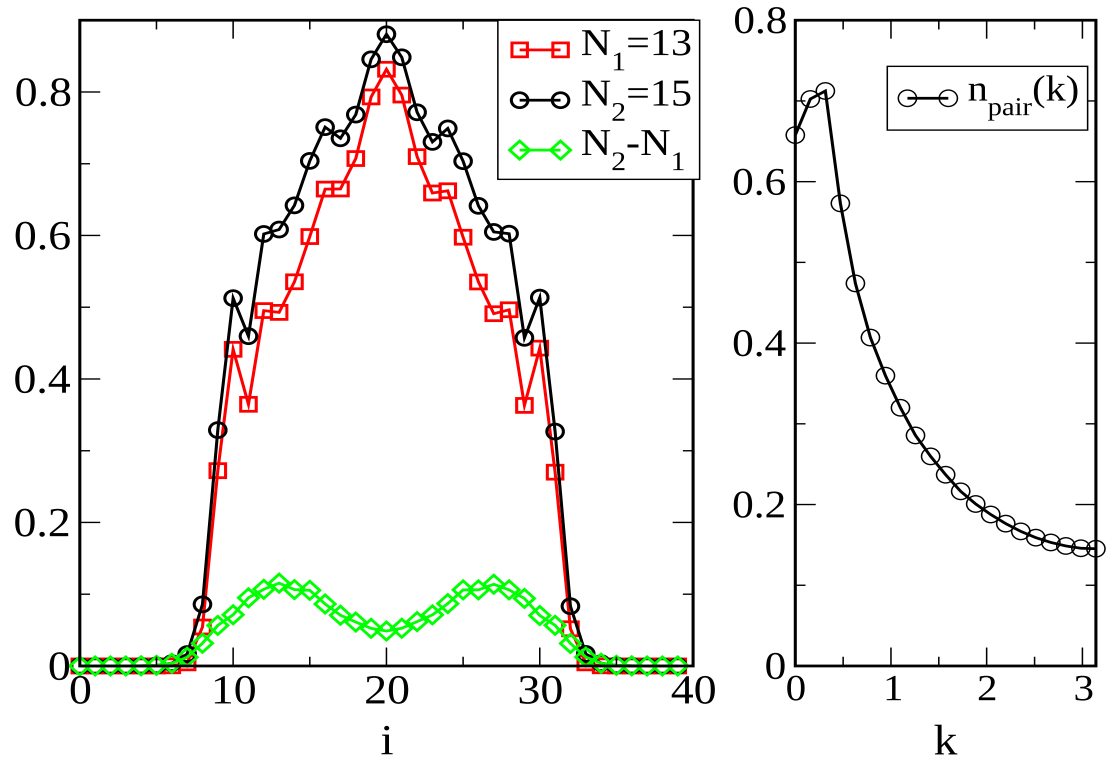
Cross-over occurs as double occupancy $\langle n_{i1} n_{i2} \rangle$ approaches saturation.

FFLO Results for Trapped System

Pronounced minimum in density difference at trap center.

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

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



FFLO Conclusions

Clear evidence for FFLO phase in Imbalanced $d = 1$ Attractive Hubbard Model

Uniform System

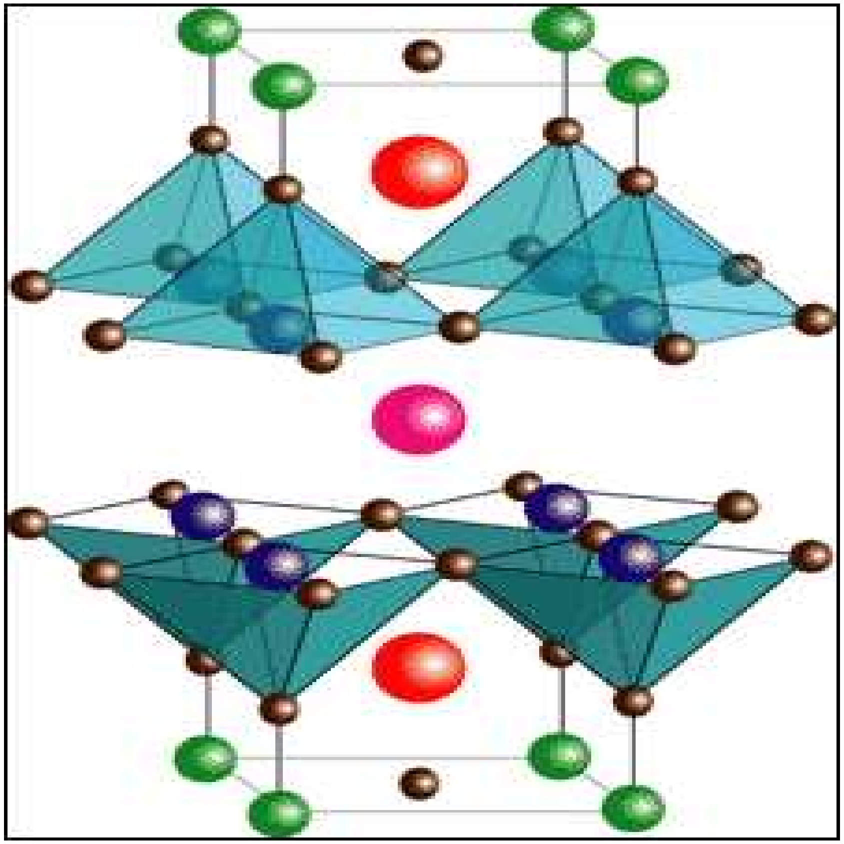
- Spatially oscillating $G_{\rm pair}(r)$
- $G_{\rm pair}(k)$ peaked at $k = k_{\rm F,majority} - k_{\rm F,minority}$
- No Clogston limit

Trapped System

- Deep minimum in local polarization at trap center.
- System retains signature of FFLO phase: $G_{\rm pair}(k)$ peaked at $k \neq 0$.

II. AntiFerromagnetic Order Parameter of 2D Half-Filled Hubbard Model

Condensed Matter Realization: CuO_2 sheets of High-Tc superconductors

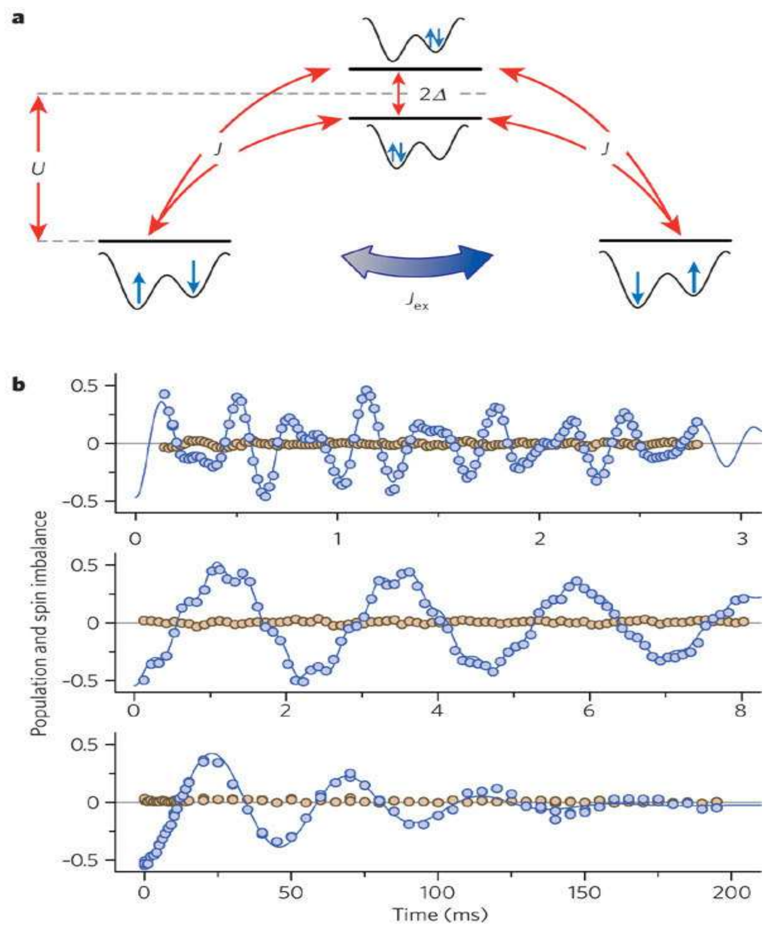


Optical Lattice Realization: In (very) early stages!

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: $J/U = 1.25,\ 0.26,\ 0.048$



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

Determinant Quantum Monte Carlo

Compute operator expectation values

$$\begin{aligned} \langle A \rangle &= Z^{-1} \text{ Tr } [A e^{-\beta H}] \\ Z &= \text{Tr } [e^{-\beta H}] \end{aligned}$$

Example: single band Hubbard Hamiltonian

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

- Inverse Temperature discretized: $\beta = L\Delta\tau$

$$Z = \text{Tr } [e^{-\beta H}] = \text{Tr } [e^{-\Delta\tau H}]^L$$

- Suzuki-Trotter Approximation

$$e^{-\Delta\tau H} \approx e^{-\Delta\tau K} e^{-\Delta\tau P}$$

Extrapolation to $\Delta\tau = 0$.

- (Discrete) Hubbard-Stratonovich Fields decouple interaction:

$$e^{-\Delta\tau U(n_{\mathbf{i}\uparrow}-\frac{1}{2})(n_{\mathbf{i}\downarrow}-\frac{1}{2})} = \frac{1}{2}e^{-\frac{U\Delta\tau}{4}}\sum_{S_{\mathbf{i}\tau}} e^{\Delta\tau\lambda S_{\mathbf{i}\tau}(n_{\mathbf{i}\uparrow}-n_{\mathbf{i}\downarrow})} = e^{-\Delta\tau\mathcal{P}_{\mathbf{i}}(\tau)}$$

where $\cosh(\Delta\tau\lambda) = e^{\frac{U\Delta\tau}{2}}$.

- Quadratic Form in fermion operators: Do trace analytically

$$\begin{aligned} Z &= \sum_{\{S_{\mathbf{i}\tau}\}} \mathrm{Tr}\,[e^{-\Delta\tau K}e^{-\Delta\tau\mathcal{P}(1)}e^{-\Delta\tau K}e^{-\Delta\tau\mathcal{P}(2)}e^{-\Delta\tau K}\ldots e^{-\Delta\tau\mathcal{P}(L)}] \\ &= \sum_{\{S_{\mathbf{i}\tau}\}} \mathrm{det}M_\uparrow(\{S_{\mathbf{i}\tau}\})\mathrm{det}M_\downarrow(\{S_{\mathbf{i}\tau}\}) \end{aligned}$$

$\dim(M_\sigma)$ is the number of spatial sites. For multi-band models

dimension is (number of spatial sites)x(number of orbitals per site).

- Sample HS field stochastically.

$$\begin{aligned} S_{\mathbf{i_0}\tau_0} &\rightarrow -S_{\mathbf{i_0}\tau_0} \\ \det M_\sigma(\{S_{\mathbf{i}\tau}\}) &\rightarrow \det M_\sigma(\{S_{\mathbf{i}\tau}\}') \end{aligned}$$

Computation of new determinant is o(N^3). Algorithm is order o($N^4 L$) since NL HS variables. Local nature of change in HS field: evaluate ratio of determinants in order N^2 ("Sherman-Morrison" formula).

Algorithm is order $N^3 L$.
$N \sim$ a hundred lattice sites/electrons
$L = \beta/\Delta\tau \sim$ a hundred imaginary time slices (low temperatures).

- Measurements

$$\langle c_{\mathbf{i}\sigma} c^\dagger_{\mathbf{j}\sigma} \rangle \leftrightarrow \langle [M_\sigma^{-1}]_{\mathbf{ij}} \rangle = \langle [G_\sigma]_{\mathbf{ij}} \rangle$$

- Sign Problem

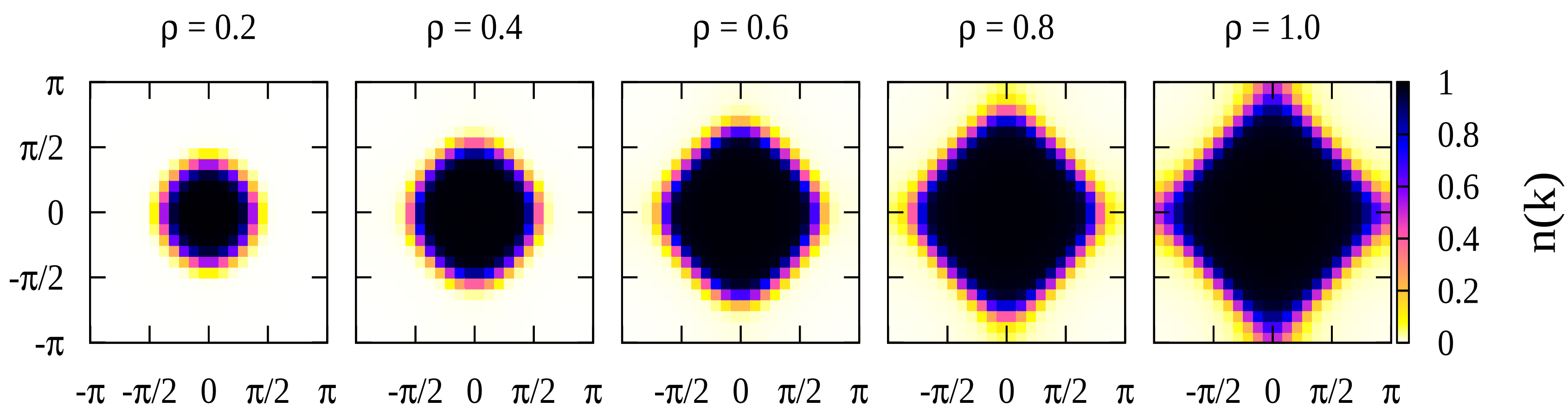
We have modernized our legacy DQMC codes

- Optimized linear algebra kernals
- "Delayed Updating" (Jarrell-Maier-D'Azevedo)
- $N \sim$ five hundred lattice sites/electrons (on a small cluster of workstations)

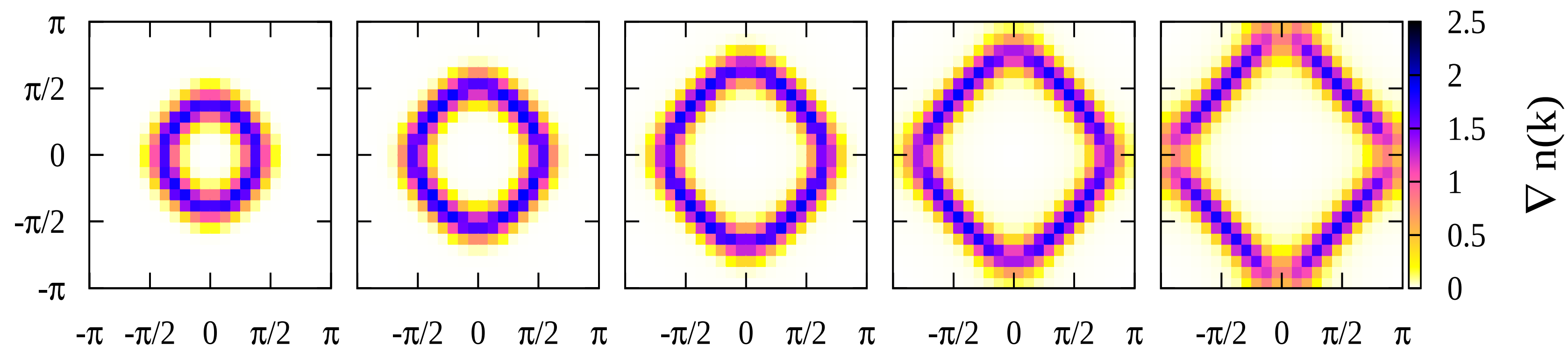
DOE SciDAC Program

Updated DQMC codes: Large lattices (N =24x24) allow for good momentum resolution.

$U = 2$ Fermi function:

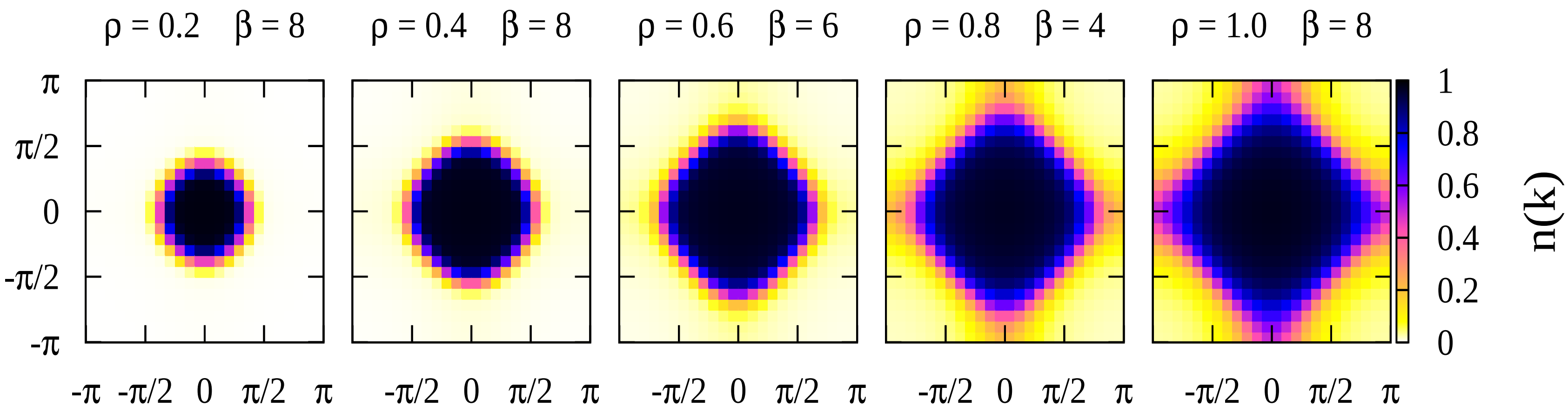


$U = 2$ Gradient of Fermi function:

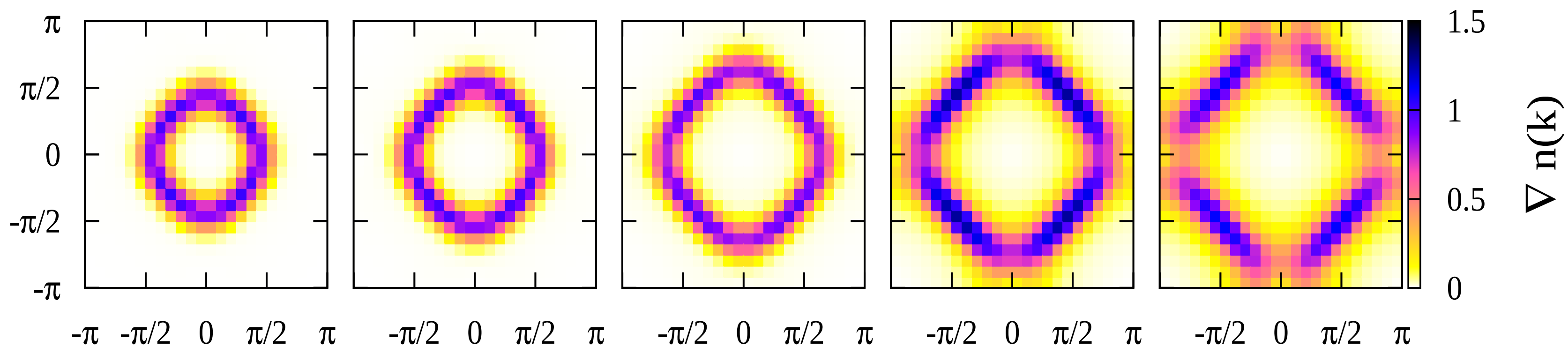


Fermi surface is smeared further by increasing interaction strength.

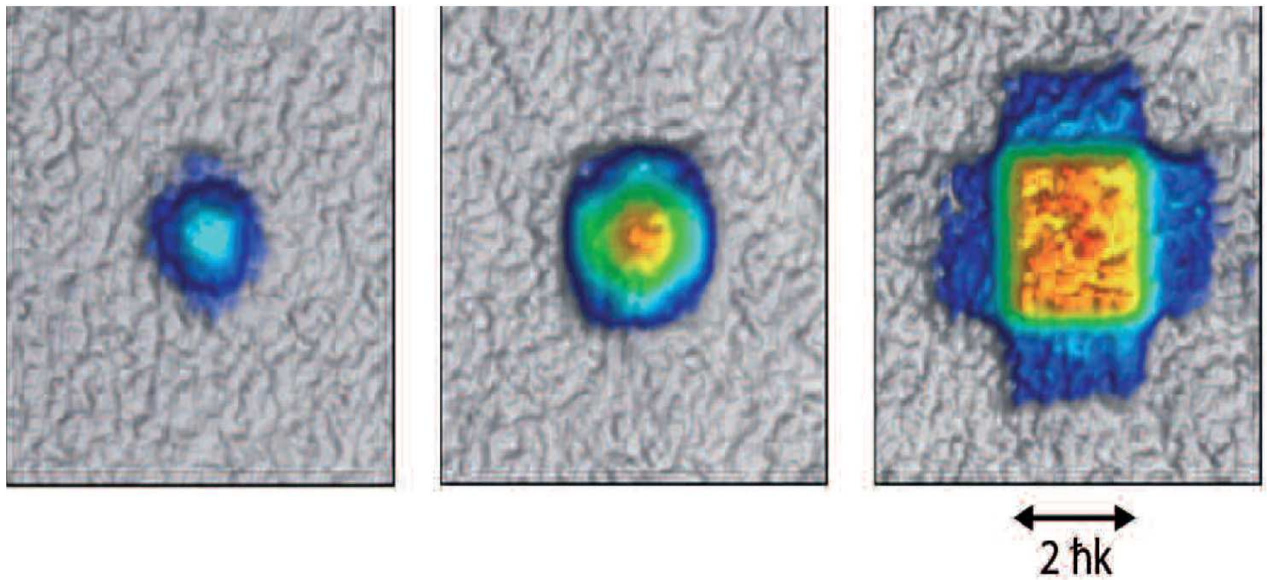
$U = 4$ Fermi function:



$U = 4$ Gradient of Fermi function:



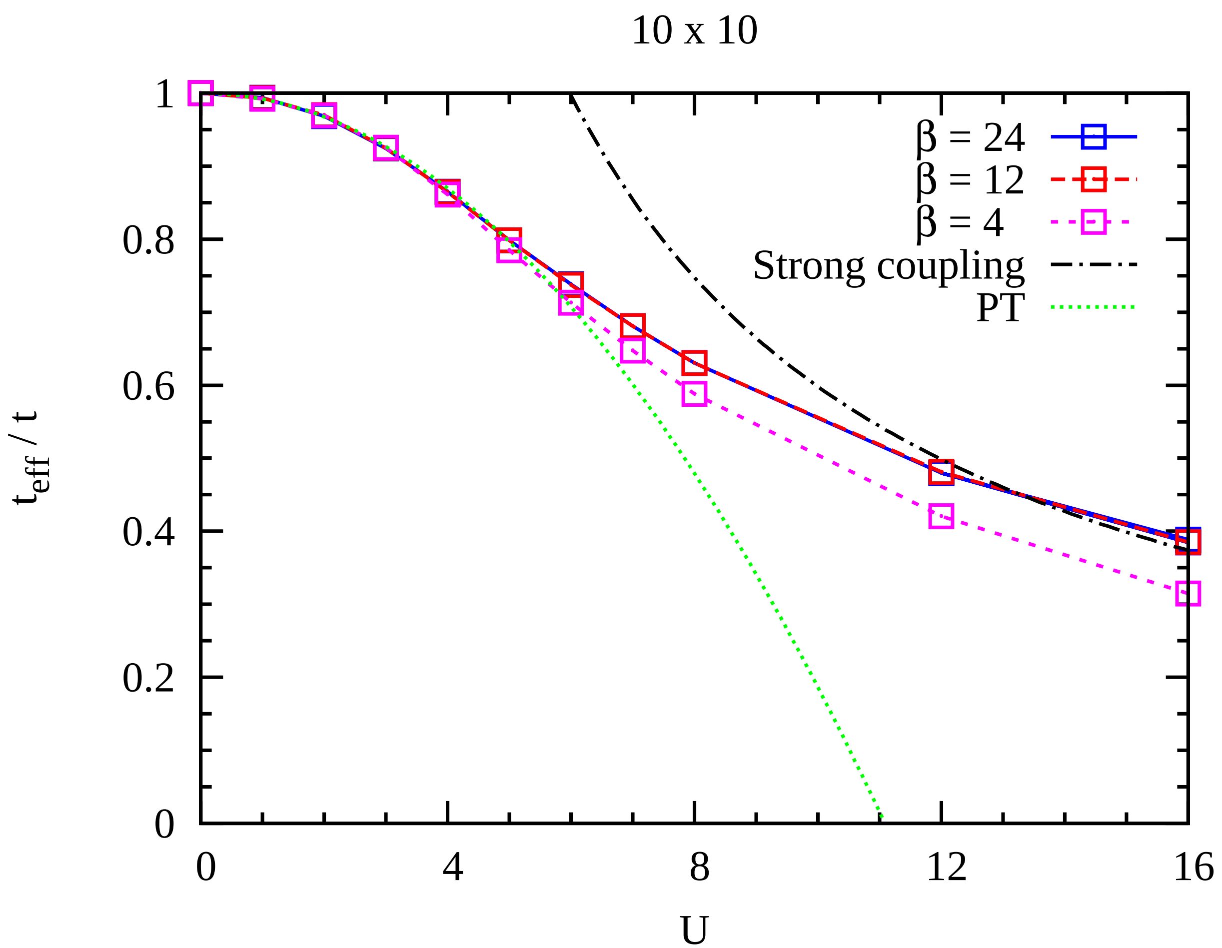
Optical Lattice Imaging of Fermi Surface



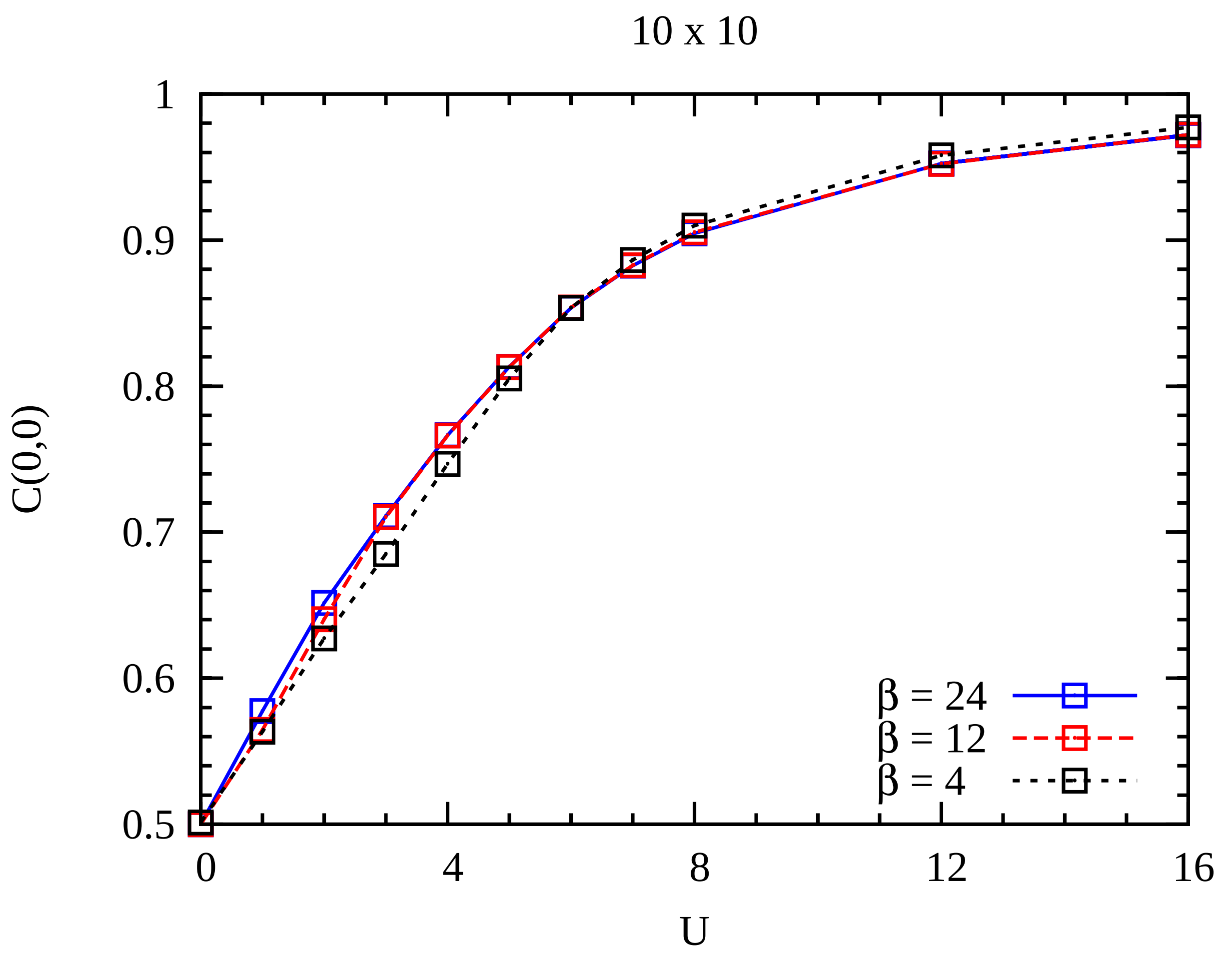
M. Kohl *etal.* Phys. Rev. Lett. **94**, 080403 (2005).
Fermionic ^{40}K atoms

Interactions reduce the effective hopping/kinetic energy

$$\frac{t_{\rm eff}}{t} = \frac{\langle c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{i\sigma} c_{j\sigma}\rangle}{\langle c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{i\sigma} c_{j\sigma}\rangle_{U=0}} \ .$$

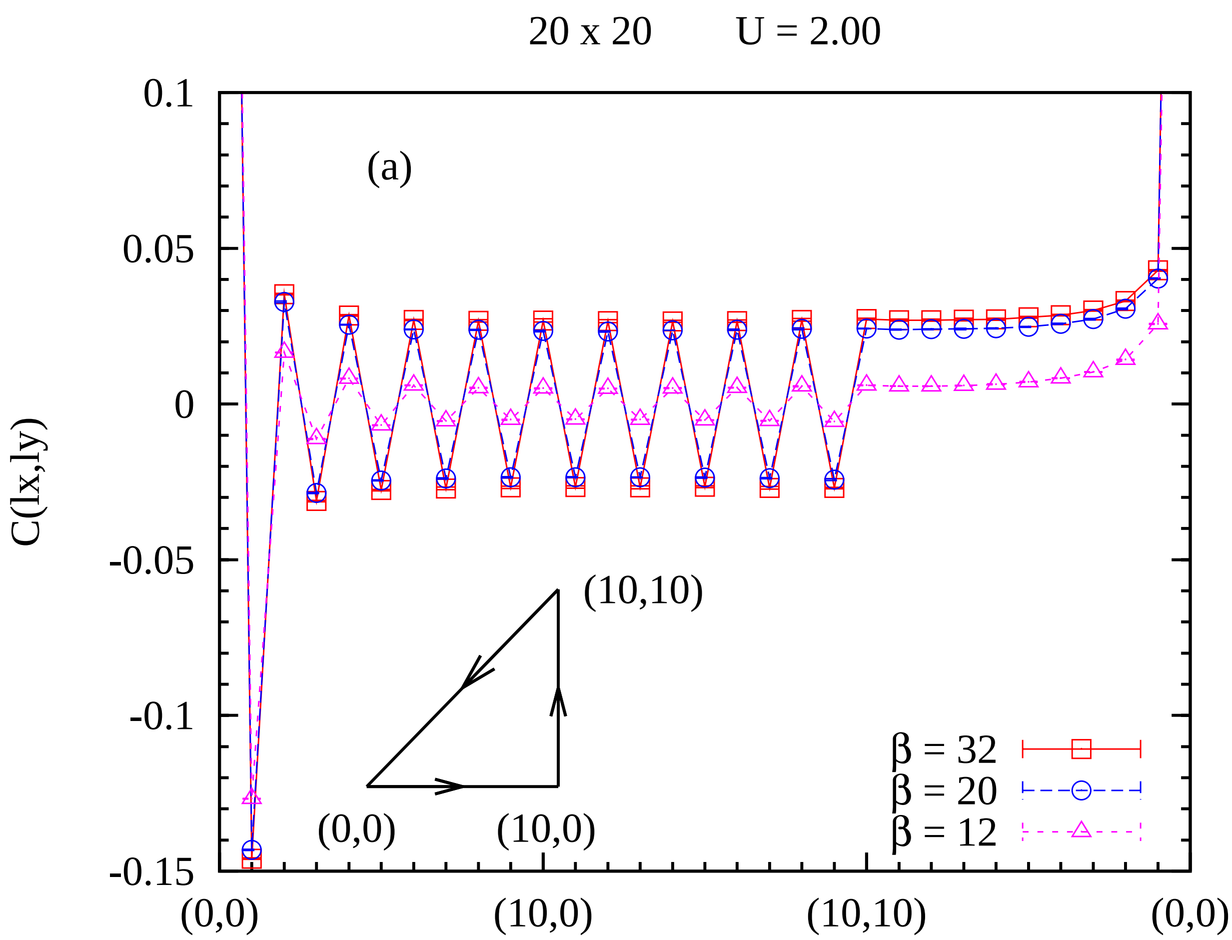


Local moments form as U increases.

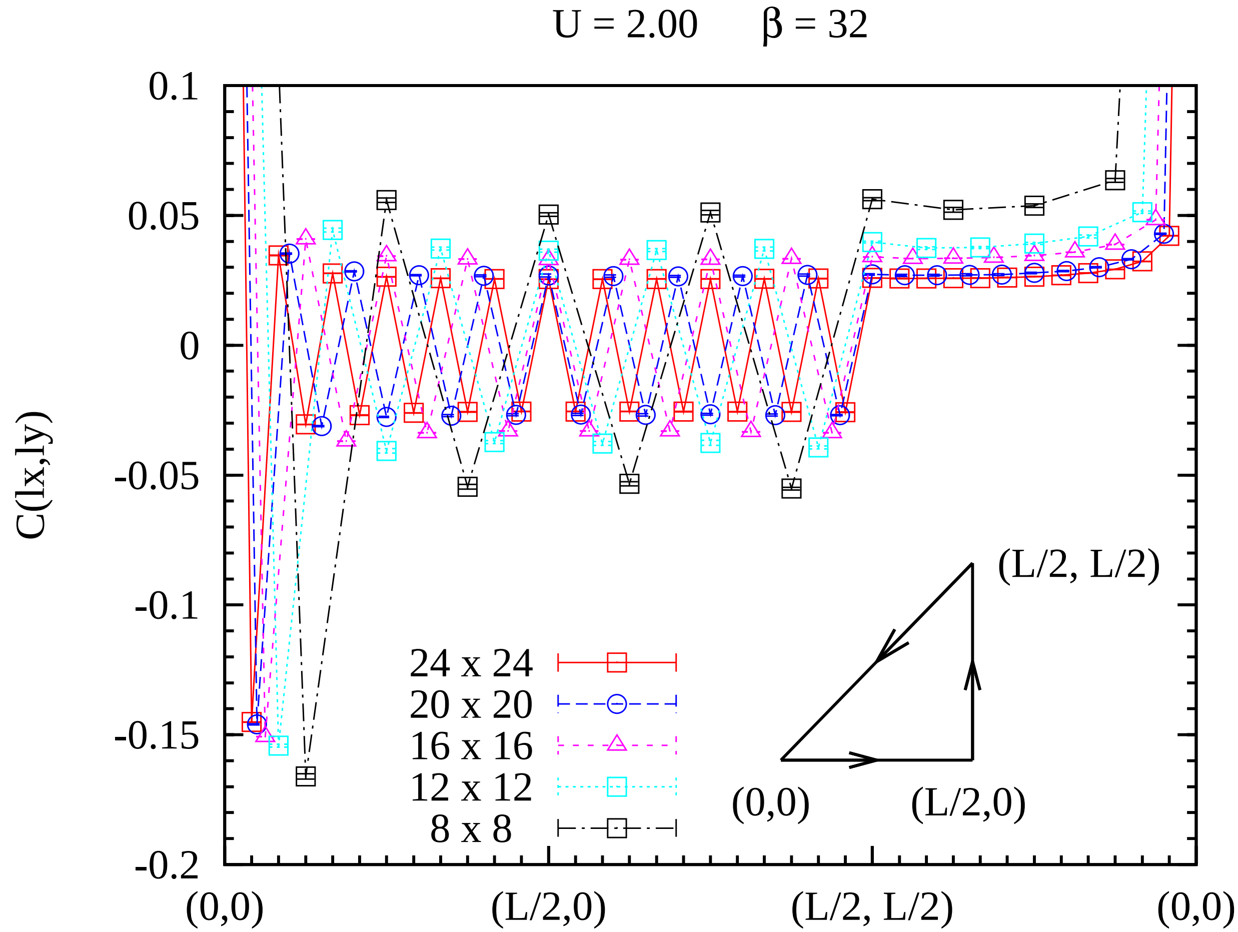


Antiferromagnetic spin correlations form at low temperature.

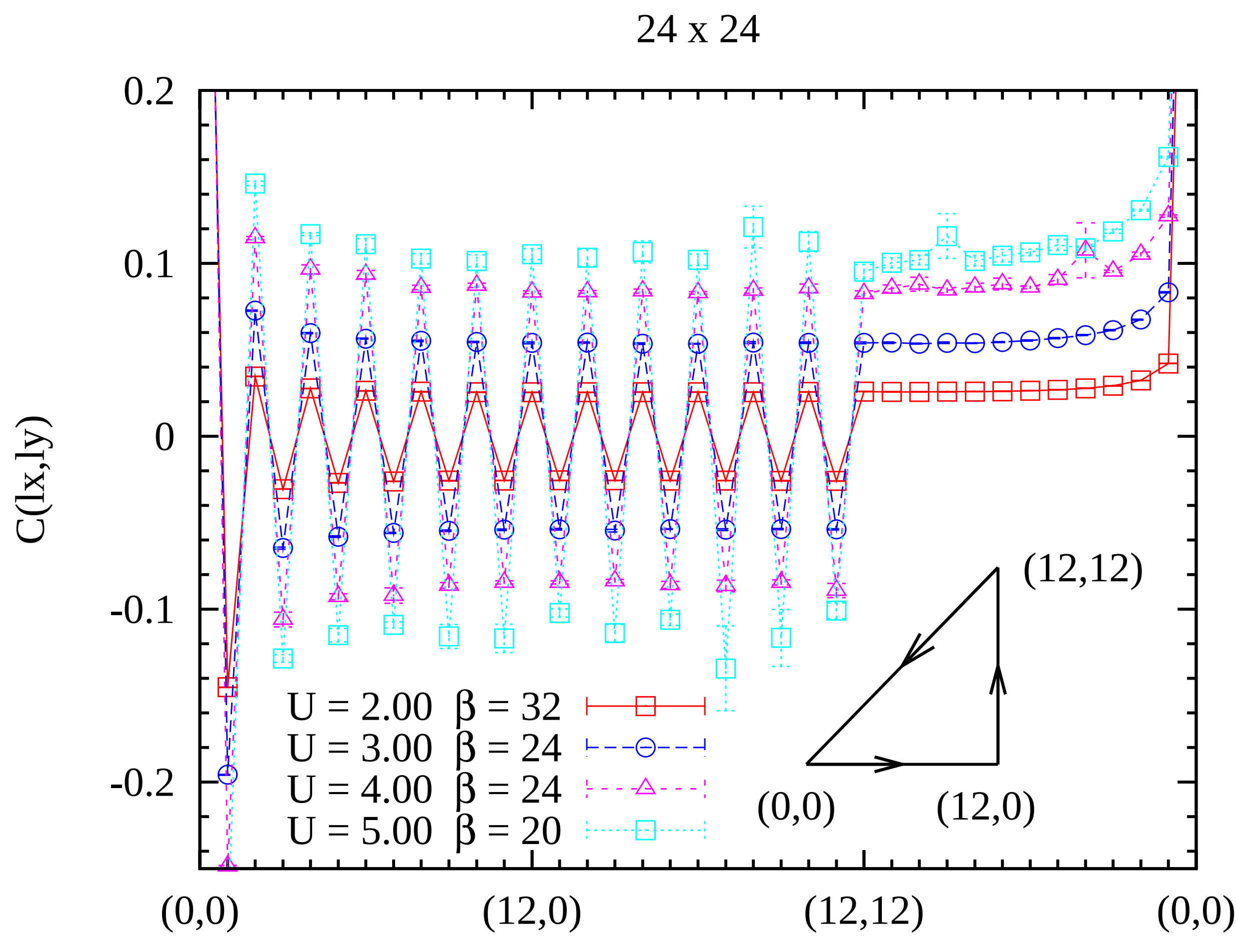
$\beta t = 20 \to T = t/20 = W/160$ (bandwidth $W = 8t$)



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



Increasing U enhances antiferromagnetic correlations

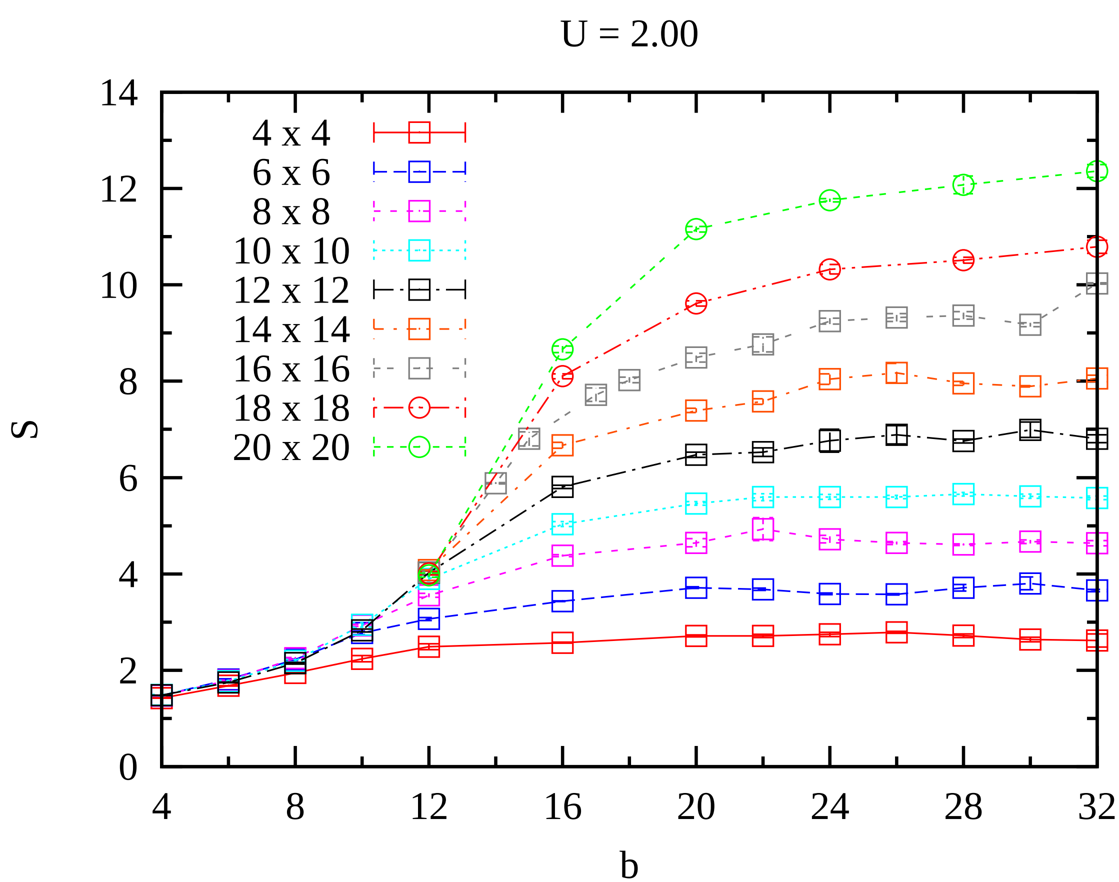


Antiferromagnetic structure factor

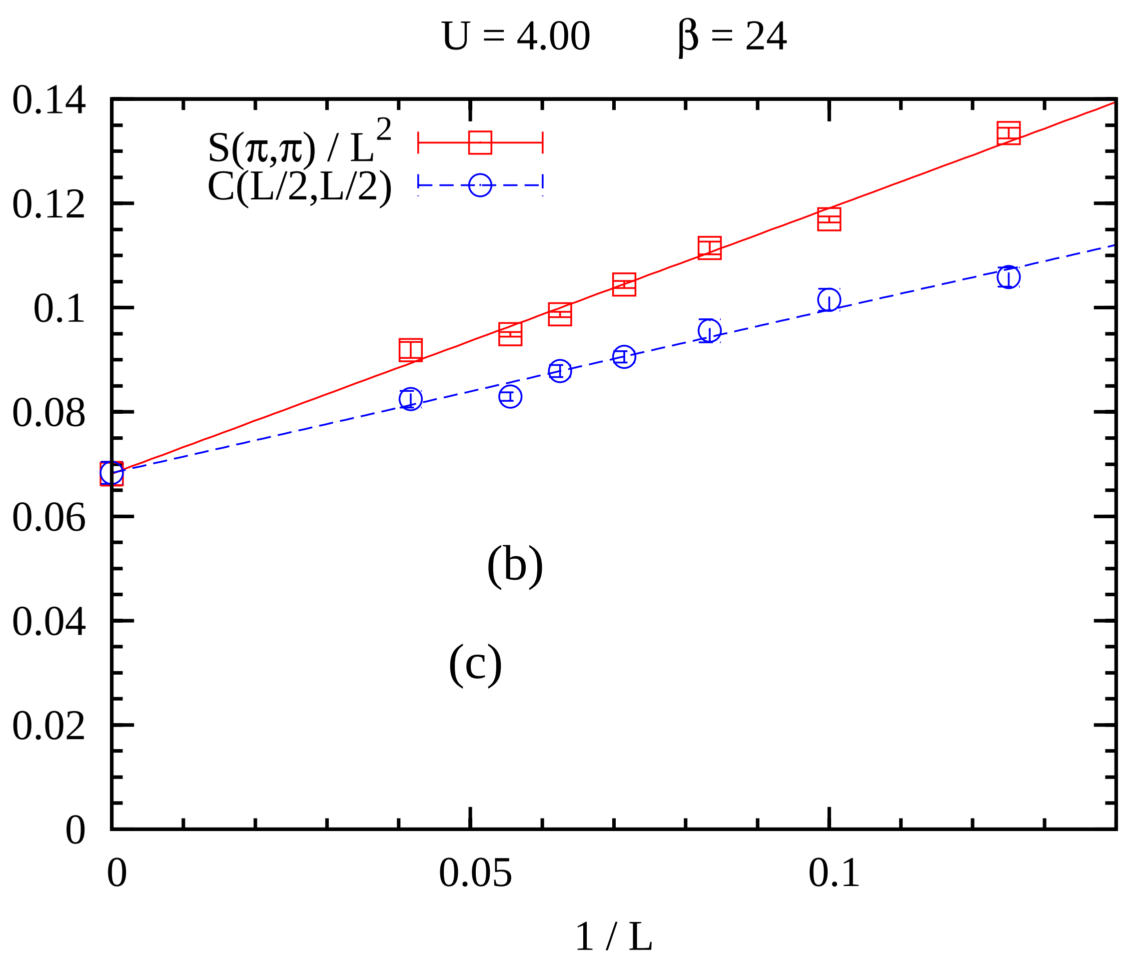
$$S(\pi,\pi) = \frac{1}{N} \sum_{ij} \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle$$

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

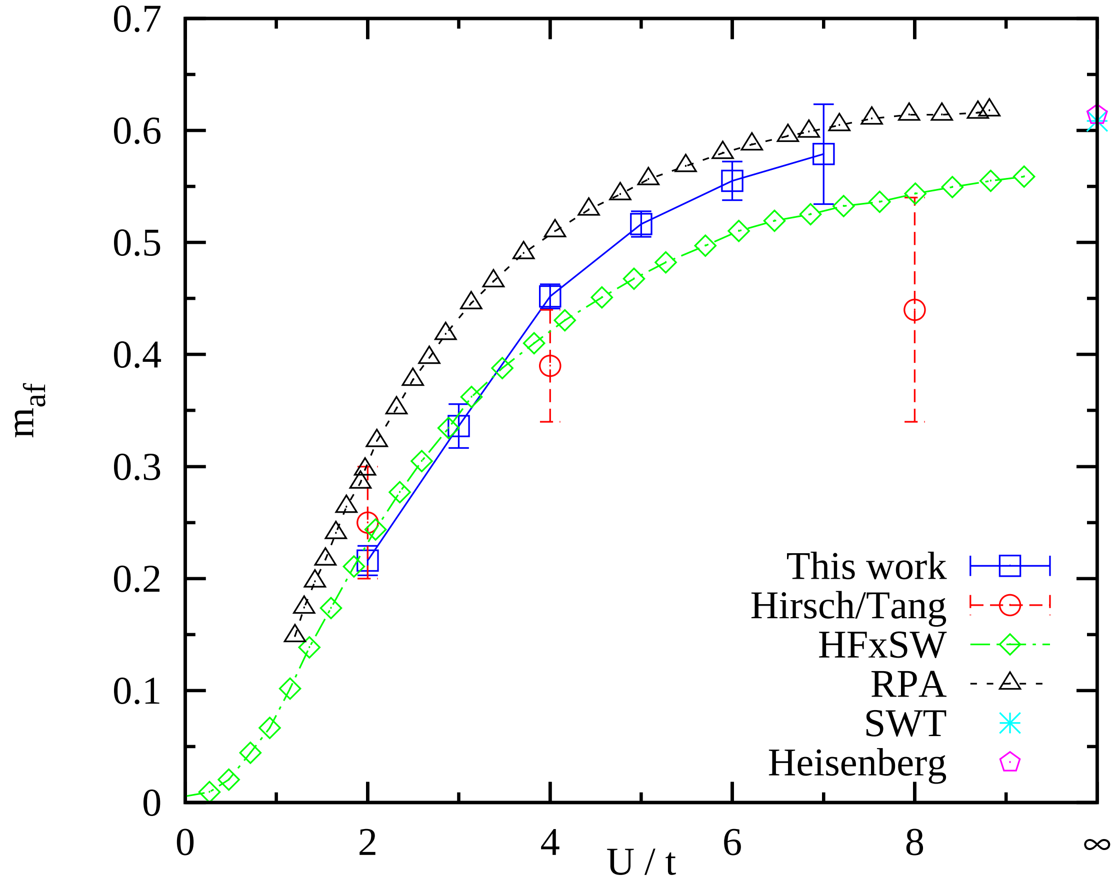
- In ordered phase $S(\pi,\pi)$ grows with N.



Finite size scaling of AF structure factor



U dependence of AF order parameter



Possible use for benchmarking optical lattice emulations

III. Orbitally selective Mott Transitions

Multiple bands with different degree of electronic correlation, e.g.

- One band with $U > U^c_{\mathrm{Mott}}$
- Another with $U > U^c_{\mathrm{Mott}}$

What happens with interband hybridization or interactions?

$$
\begin{aligned}
H &= -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \\
&+ \sum_i \left[J_z S^z_i (n_{i\uparrow} - n_{i\downarrow}) + J_\perp (S^+_i c^\dagger_{i\downarrow} c_{i\uparrow} + S^-_i c^\dagger_{i\uparrow} c_{i\downarrow}) \right] \\
&+ U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})
\end{aligned}
$$

Itinerant band (adjustable U) and a fully localized orbital (spin-$\frac{1}{2}$ degrees of freedom)

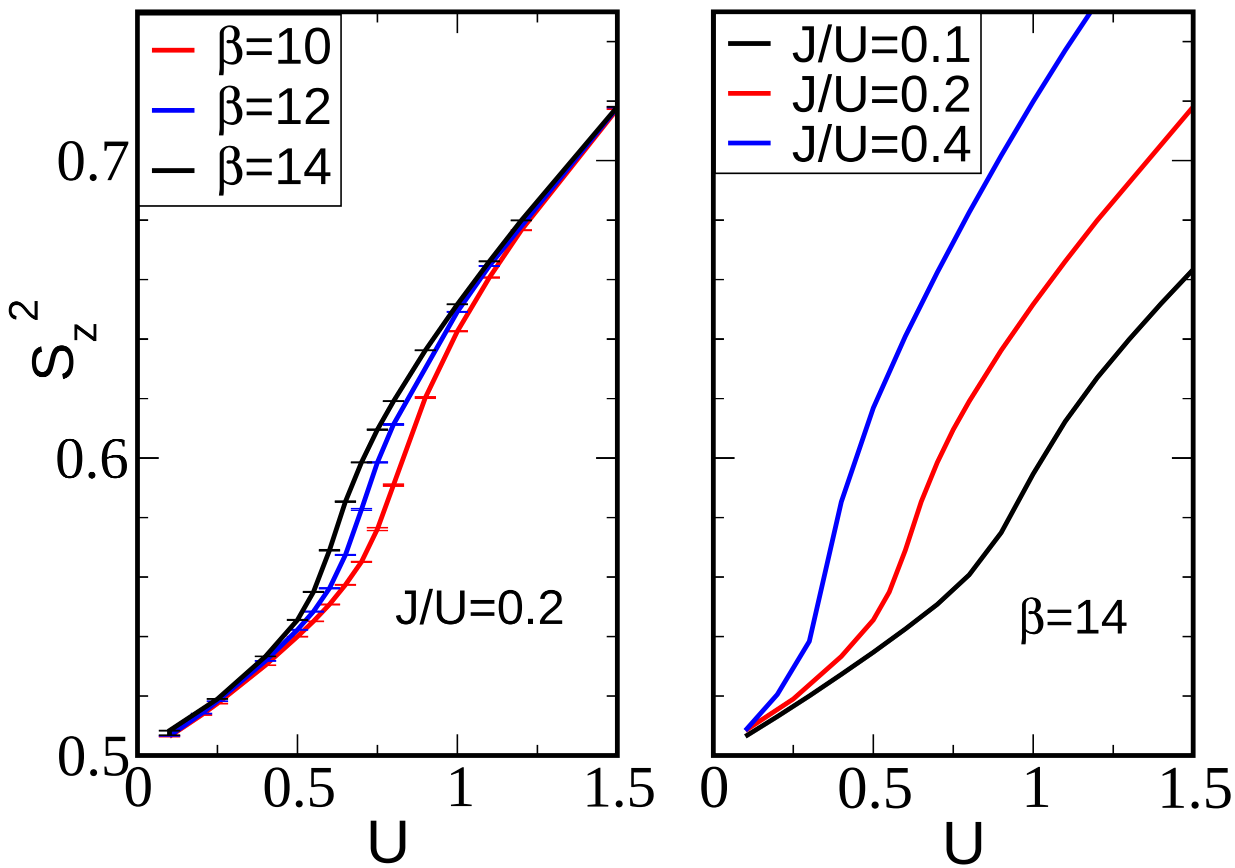
OSMT: Is band metallic or localized?

Local Moment

DMFT (Costi) shows first order OSMT at U_c

Signaled by discontinuous jump in $\langle S_z^2 \rangle$

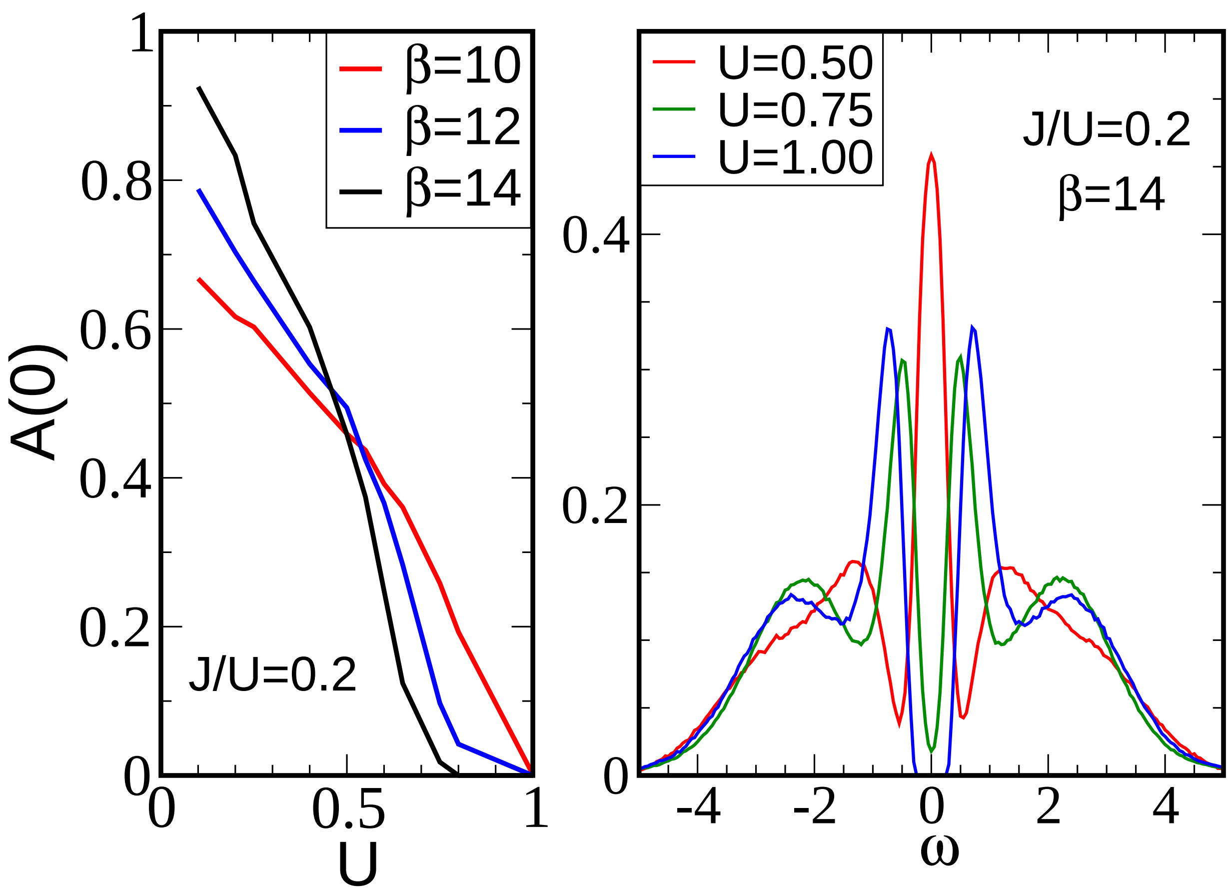
DQMC Results:



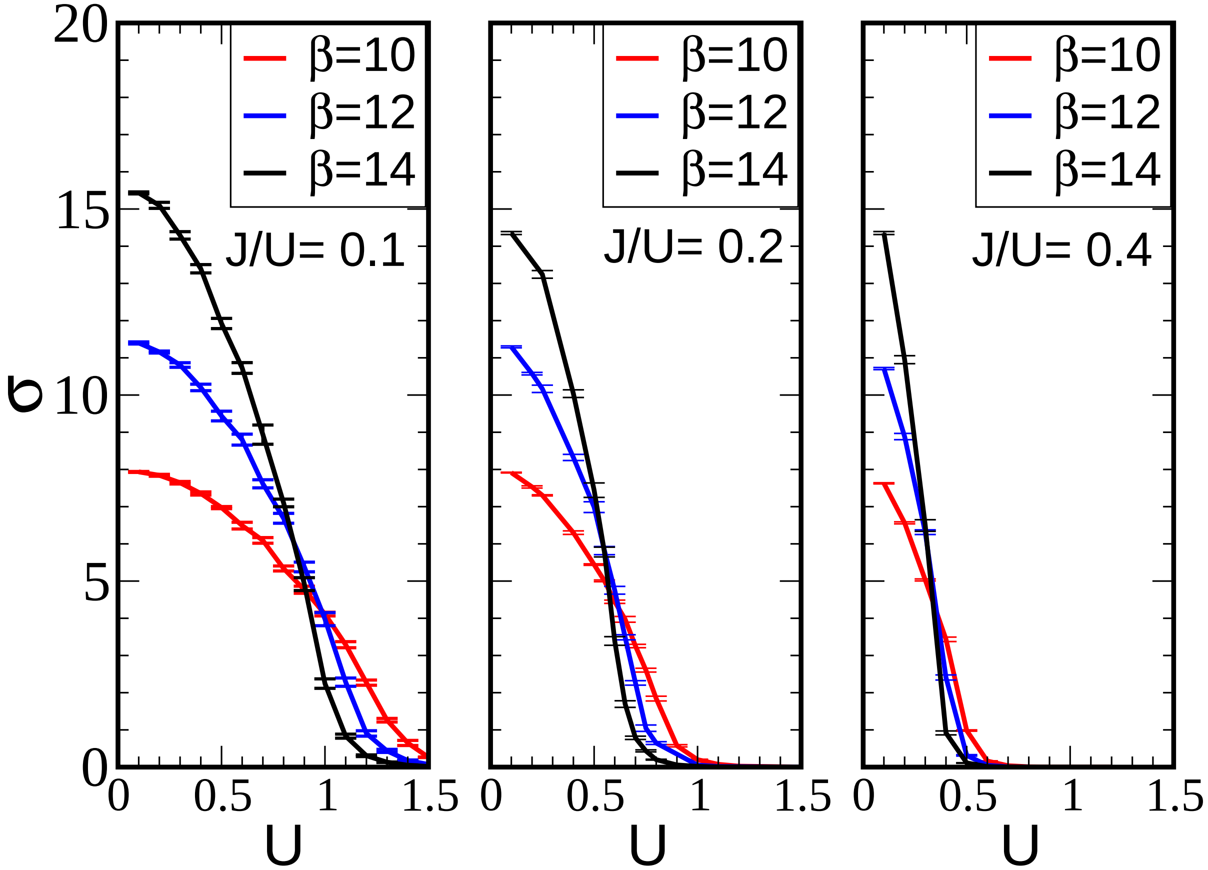
Spectral Function

In same range of U values

- Temperature dependence of $A(\omega = 0)$ changes sign
- Gap opens in $A(\omega)$

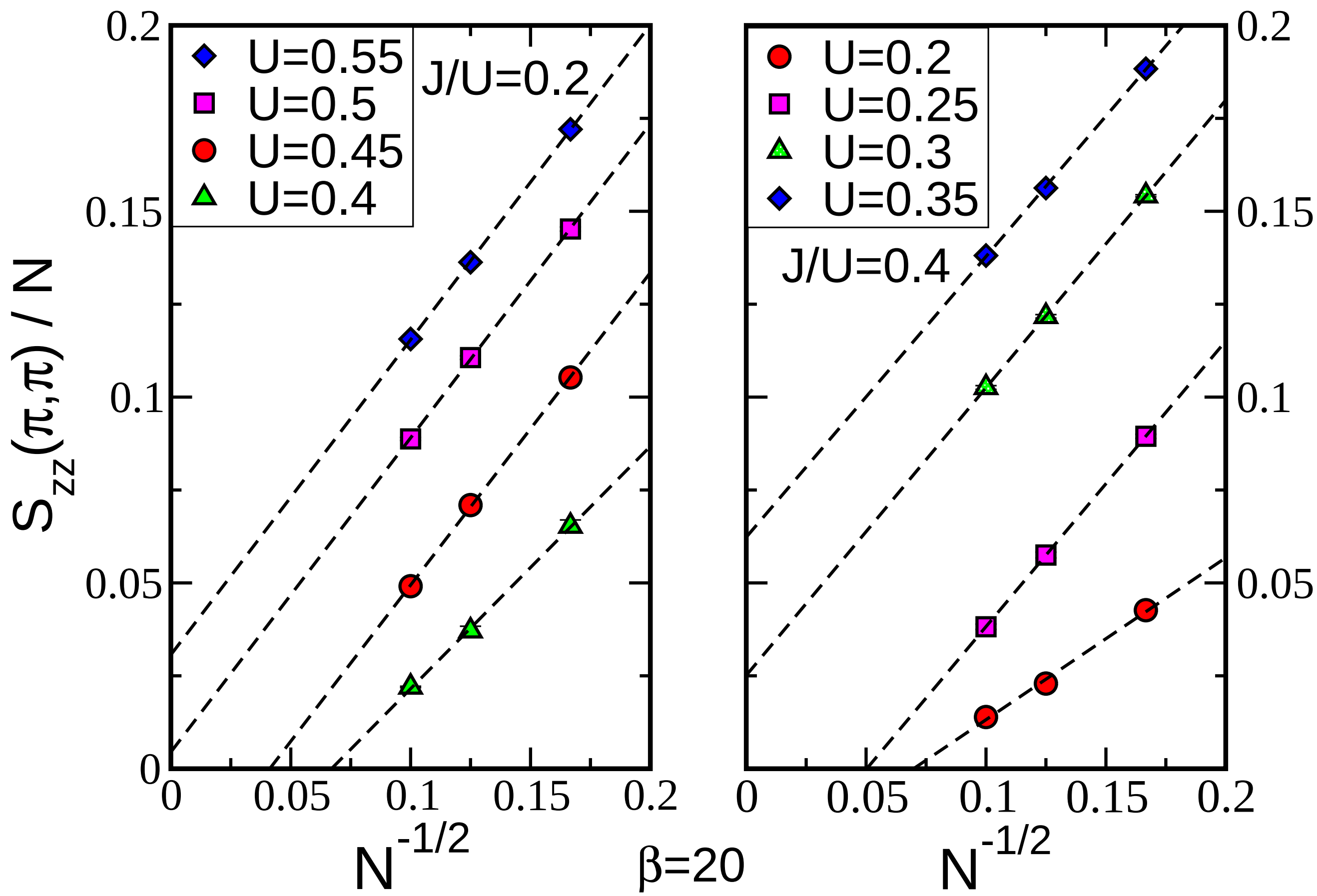


Change in sign of $d\sigma(T)/dT$ provides additional signal of MIT.



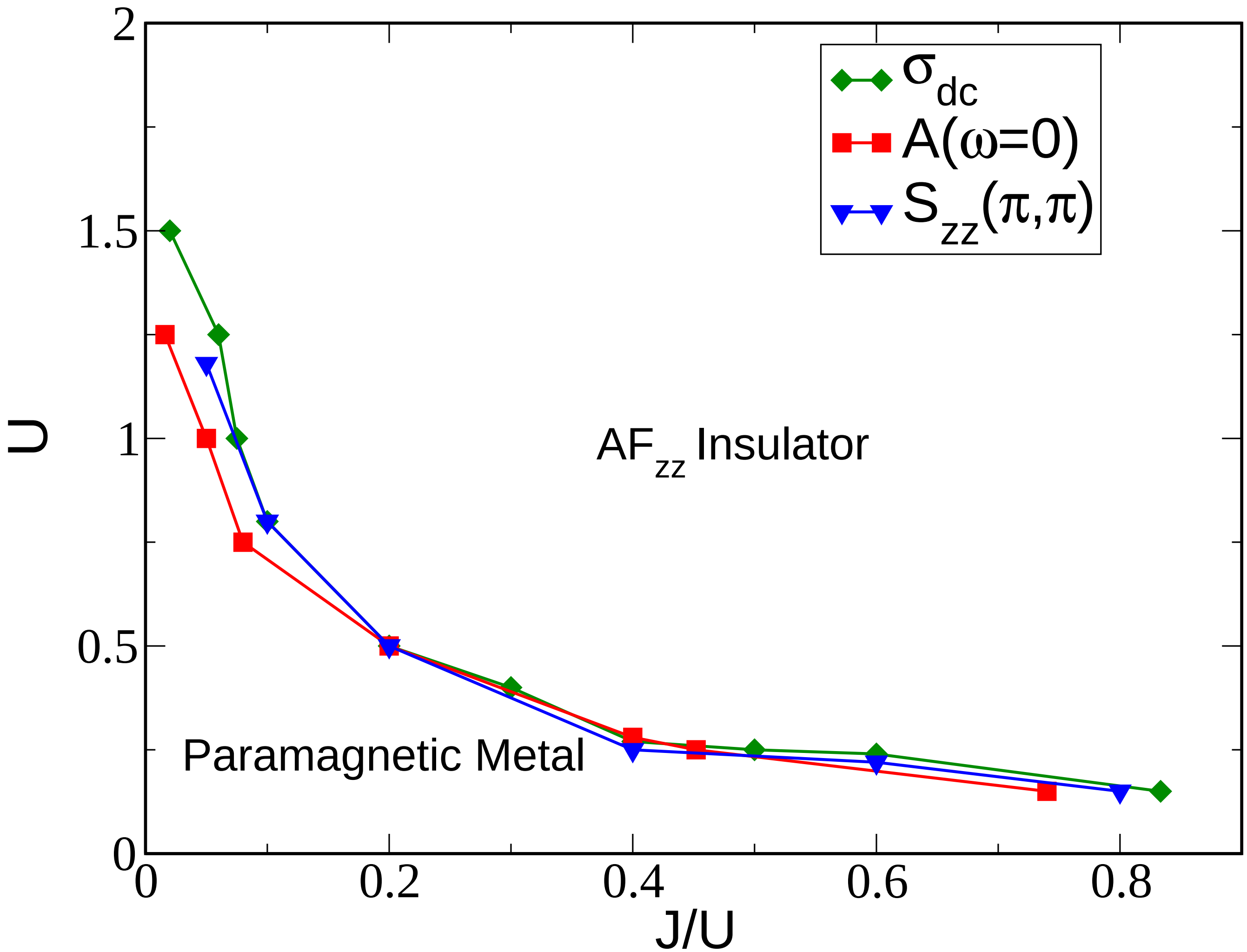
Scaling of AF Order Parameter

Change in transport at OSMT accompanied by a paramagnet-antiferromagnet transition.



Phase Diagram

Different measurements provide numerically consistent picture of OSMT



CONCLUSIONS

- Observe FFLO Phase in Spin Polarized Attractive Hubbard Hamiltonian
- Large lattice ($N \sim 24x24$) of half-filled Repulsive Hubbard Hamiltonian
  $\longrightarrow$ Antiferromagnetic Order Parameter $\langle m^2_{\rm af}(U) \rangle$
- Observation of OSMT in Two Orbital Repulsive Hubbard Hamiltonian

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