

High Precision QMC Study of the 2D Fermion Hubbard Model

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Outline

Introduction

Motivation

Model and Method

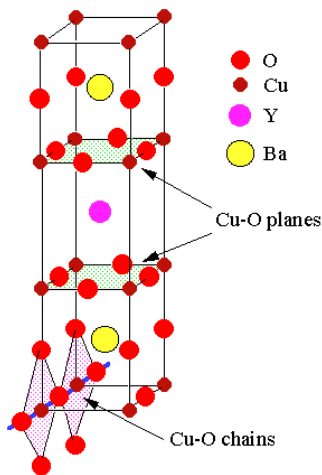
Results

Single Particle Properties

Magnetic Correlations

Summary

Motivation

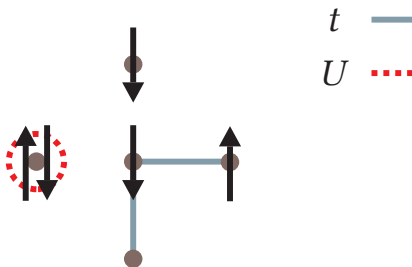


- ▶ Ultracold fermionic atoms
 - ▶ Precise comparison of theoretical and experimental phase diagrams
- ▶ Long range antiferromagnetic order
 - ▶ Weak coupling: Instability in fermi surface
 - ▶ Strong coupling: Suppression of electron mobility

Hubbard Hamiltonian

$$H = -t \sum_{\langle \mathbf{i}\mathbf{j} \rangle \sigma} (c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + \text{h.c.})$$

$$+ U \sum_{\mathbf{i}} \left(n_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \left(n_{\mathbf{i}\downarrow} - \frac{1}{2} \right) - \mu \sum_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma}$$



QUEST

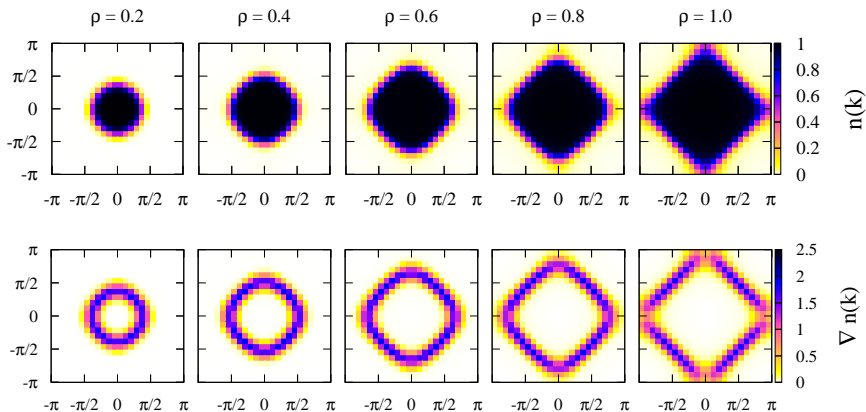
Determinant Quantum Monte Carlo:

- ▶ QUantum Electron Simulation Toolbox (QUEST)
 - ▶ Global moves
 - ▶ Delayed updating
 - ▶ Blas / Lapack
 - ▶ General lattice geometries
 - ▶ Up to 500 sites on a modest cluster

<http://www.cs.ucdavis.edu/~bai/QUEST/>

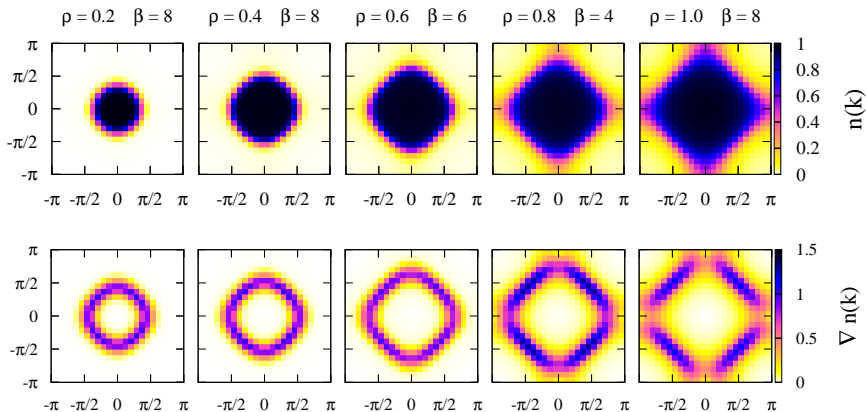
Green's Function

$$U = 2, \beta = 8$$

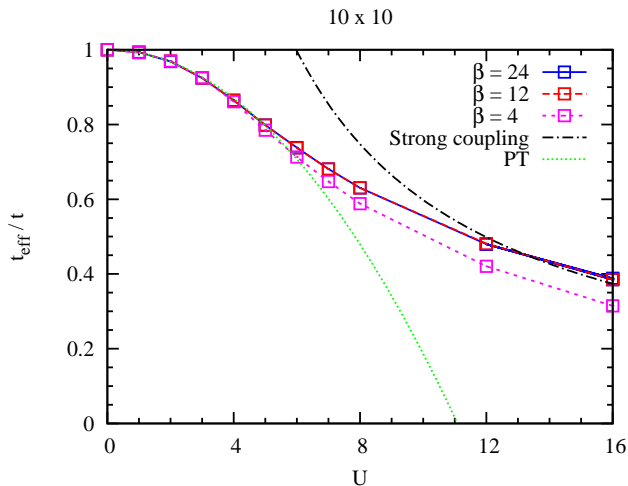


Green's Function

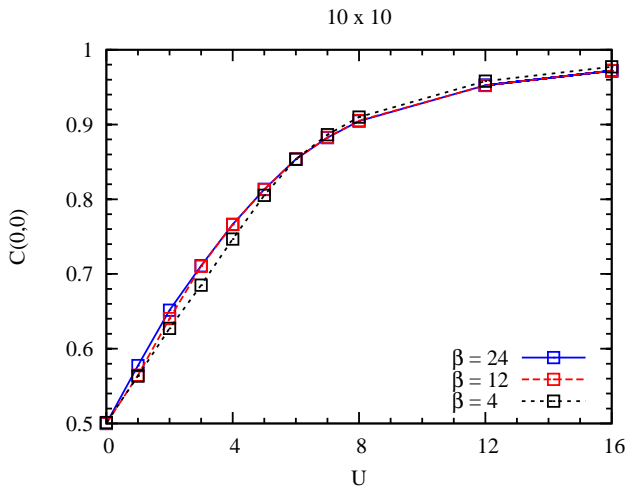
$$U = 4$$



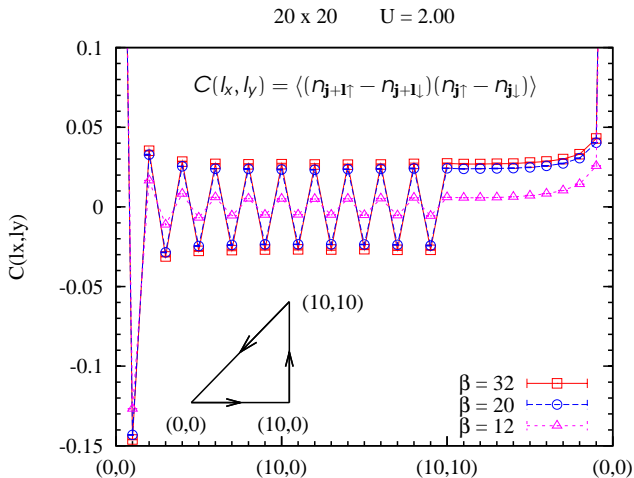
Kinetic energy



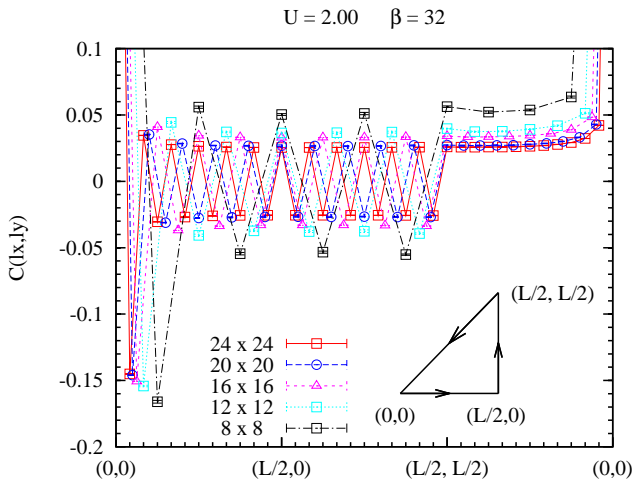
Local Moment



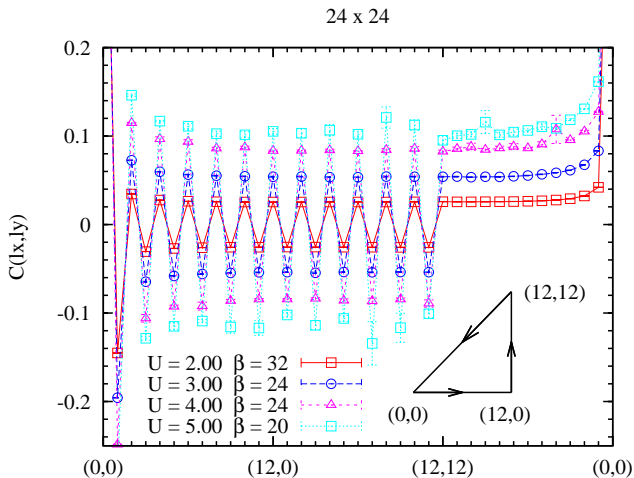
Spin Correlations



Spin Correlations

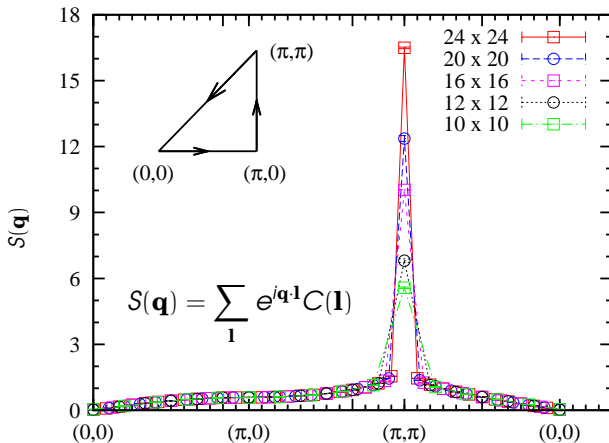


Spin Correlations

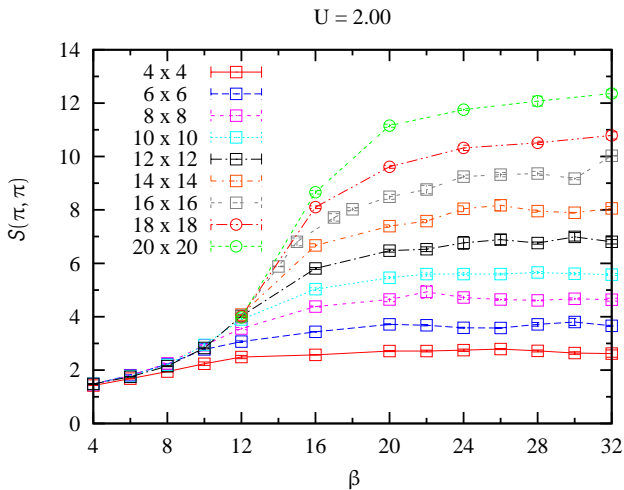


Structure factor

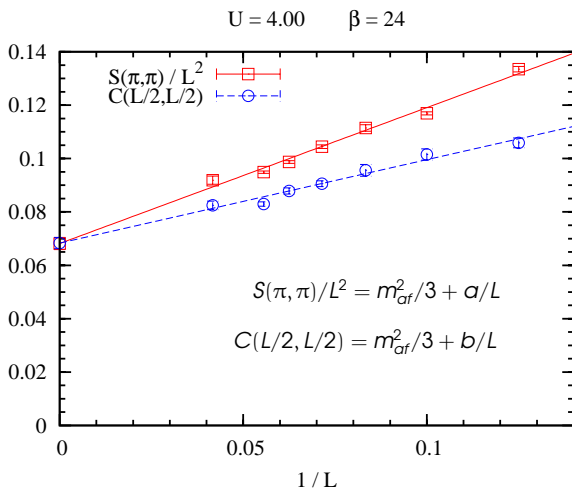
$U = 2.00$ $\beta t = 32$



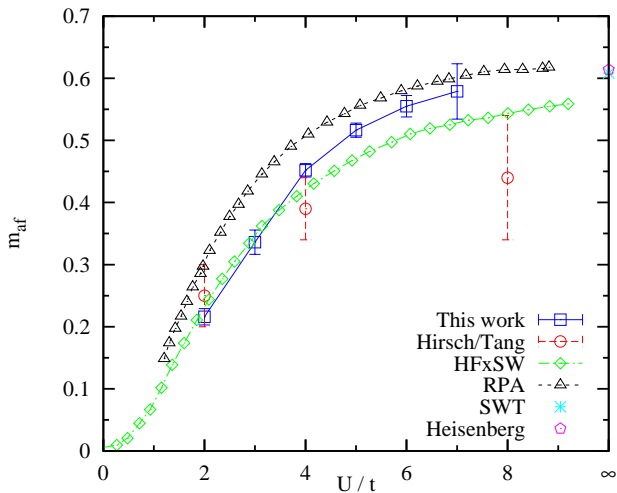
Structure factor



Structure factor



Order Parameter



¹PRL 62, 591 (1989); ²PRB 31, 4403 (1985); ³PRB 72, 115114(2005);

⁴PRB 39, 11663 (1989); ⁵PRB 56, 11678 (1997)

Summary

- ▶ Order parameter as a function of interaction strength, $m_{\text{af}}(U)$.
- ▶ DQMC connects the weak and strong coupling regimes.
- ▶ QUEST significantly improves capacity to simulate interacting fermion systems.

QUEST can be accessed at:

<http://www.cs.ucdavis.edu/~bai/QUEST/>

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