CONSTRAINED PHASE MONTE CARLO AND FINITE SIZE EFFECTS IN FERMION SIMULATIONS

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Outline

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Introduction: II
Finite Size Effects

INTRODUCTION: I

Objective

Simulate the ground-state properties of fermion lattice models in the presence of an applied magnetic field.

- The National High Magnetic Field Laboratory at Los Alamos.

Approach

Constrained-Phase Monte Carlo method (new)

- An applied magnetic field explicitly breaks time-reversal invariance which requires the ground-state wave-functions to be complex valued.
- Monte Carlo methods need to sample from a complex-valued distribution function.
  - ▷ Sign problem is replaced by a phase problem.
- The approach is extendible to quantum chemistry and nuclear shell model calculations.

Hubbard Model

- The tU Hubbard Hamiltonian

$$H = -\sum_{\langle ij \rangle,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

  ▷ $t_{ij} = t^*_{ji}$

- The negative U model means $U < 0$.

- The presence of an externally applied magnetic field means

$$t_{ij} = t \longrightarrow t \exp\Big(\frac{ie}{\hbar c}\int_i^j \mathbf{A} \cdot \mathbf{dl}\Big)$$

  where $\mathbf{A}$ is the vector potential.

With no field and at zero temperature, the two-dimensional negative U Hubbard model in the thermodynamic limit is believed to be a gapless s-wave superconductor.

- What does the Meissner effect look like in a fermion lattice model?

- How does one define a penetration depth?

- Etc.

Initial Issues

- Accuracy of the constrained-phase method.
- Behavior of the model's superconducting properties in the absence of an applied field.

Troublesome Questions

- How accurate is the BCS approximation?
- How smooth is the scaling from finite-size to the bulk?
  - ▷ At what system size do we see "true" superconducting behavior?

CONSTRAINED PHASE MONTE CARLO

Background

An applied magnetic field explicitly breaks time-reversal symmetry and requires the ground-state wavefunction necessarily to be complex valued.

Problem

Projector Monte Carlo (T=0) methods now need to sample from complex-valued "probability distributions."

- The sign problem is replaced by a phase problem.
- Propagator and wave functions are complex valued.

Solution

Instead of fixing nodes or constraining paths, one constrains phases (or fixes phases[1]).

[1] G. Ortiz, D.M. Ceperley, and R.M. Martin, Phys. Rev. Lett. **71**, 2777 (1993).

Sign Problem: CPMC method (real-valued states)

Main Features

- Projects the ground-state from some $|\Psi_T\rangle$
- Proceeds via a branched random walk in a space of Slater determinants $|\phi\rangle$
  - ▹ A type of stochastic configuration interaction method
    - ◇ The ground state

      $$|\psi_0\rangle = \sum_\phi c_\phi |\phi\rangle$$

      where $c_\phi > 0$.
    - ◇ The Monte Carlo methods samples from the distribution defined by $\{c_\phi\}$.
- Removes at any Monte Carlo step any $|\phi\rangle$ that violates

  $$\langle\Psi_T|\phi\rangle > 0$$

- Becomes exact if $|\Psi_T\rangle$ is exact

Key Characteristics

- Eliminates the exponential growth in variance due to the "sign" problem
- Produces excellent estimates of the energy
- Produces very good estimates of correlation functions

Method Summary

Generally, in a QMC method projector method, one iterates

$$|\psi'\rangle = e^{-\Delta\tau H}|\psi\rangle$$

after using a Trotter approximation (H=K+V)

$$e^{-\Delta\tau H} \approx e^{-\Delta\tau K/2} e^{-\Delta\tau V} e^{-\Delta\tau K/2} \approx e^{-\Delta\tau V/2} e^{-\Delta\tau K} e^{-\Delta\tau V/2}$$

and a Hubbard-Stratonovich transformation

$$e^{-\frac{1}{2}\mathcal{O}^2} = \frac{1}{\sqrt{2\pi}} \int dx \, e^{-\frac{1}{2}x^2} e^{ix\mathcal{O}}$$

to convert

$$e^{-\Delta\tau H} \to \int d\vec{x} \, P(\vec{x}) B(\vec{x})$$

where

$$\int d\vec{x} \, P(\vec{x}) = 1$$

and $B(\vec{x})$ is the product of exponentials of one-body operators.

In the CPMC method, one iterates

$$|\phi'\rangle = \int d\vec{x} \, P(\vec{x}) O(\vec{x}) B(\vec{x}) |\phi\rangle$$

where the constraining operator

$$O(\vec{x}) = \begin{cases} 1, & \text{if} \quad \langle\psi_T|\phi\rangle \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

Phase Problem: CϕMC method (complex-valued states)

As before one iterates

$$|\phi'\rangle = \int d\vec{x}\, P(\vec{x}) O(\vec{x}) B(\vec{x}) |\phi\rangle$$

but now

$$O(\vec{x}) = \frac{1}{2}\left[1 + \frac{\langle\psi_T|\phi\rangle^*}{\langle\psi_T|\phi\rangle}\right] = \frac{1}{2}\left[1 + e^{-2i\theta}\right]$$

Consequences

- If $|\psi_T\rangle = |\psi_0\rangle$, then the method is exact.
- If there is no phase problem, then the method is exact.
- Imaginary-time "Schrödinger's" equation becomes

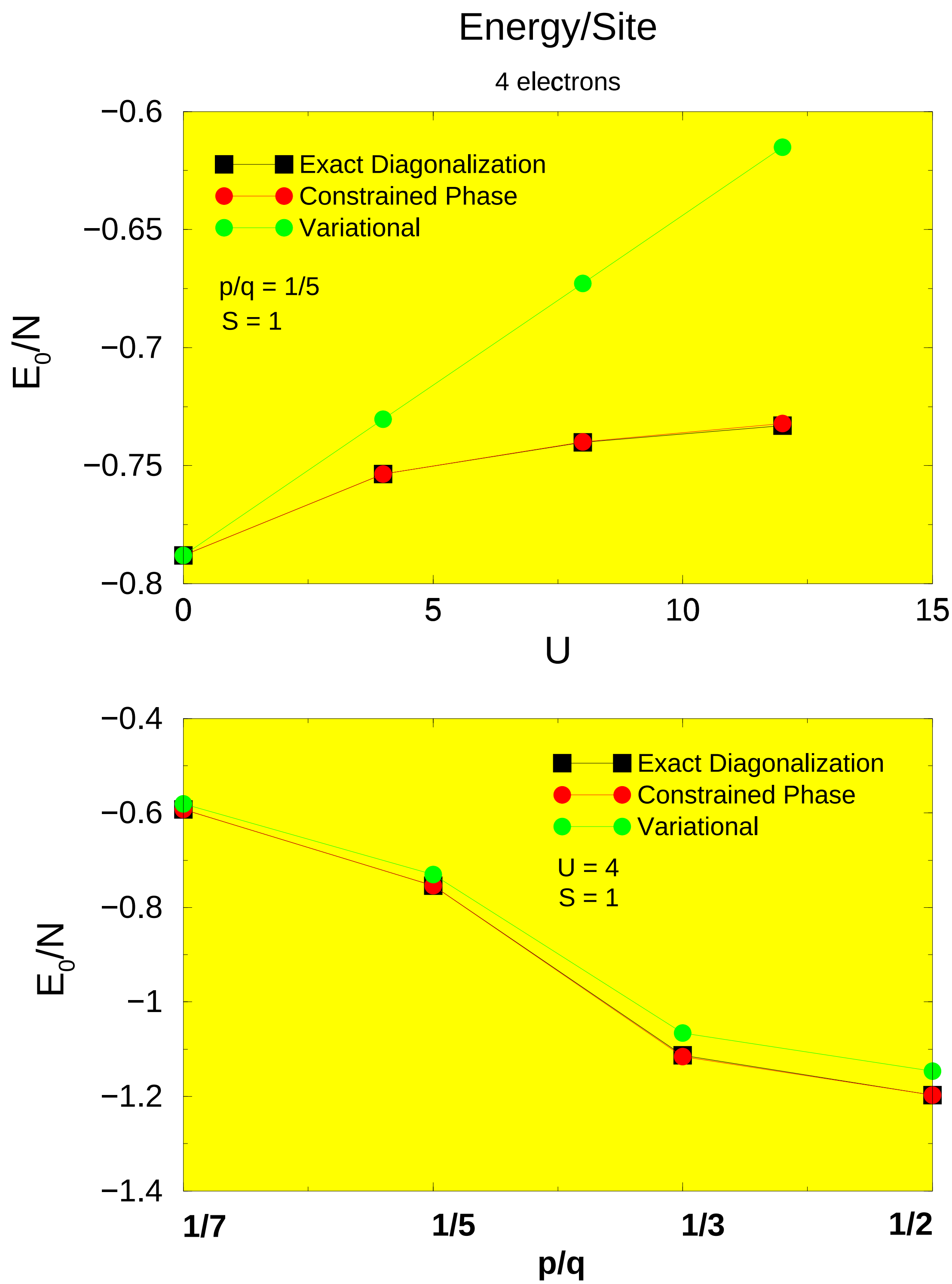
  $$\frac{\partial|\psi_c\rangle}{\partial\tau} = -H_{\text{eff}}|\psi_c\rangle$$

  where H_{eff} is a non-Hermitian operator.
- Mixed estimator

  $$\text{Re}\left\{\frac{\langle\psi_T|H|\psi_c\rangle}{\langle\psi_T|\psi_c\rangle}\right\} = \frac{\langle\psi_T|H_{\text{eff}}|\psi_c\rangle}{\langle\psi_T|\psi_c\rangle} = E_{\text{eff}}$$

- Unresolved

  $$E_{\text{eff}} \quad \geq \quad E_0 = \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}$$


Energy/Site
4 electrons
Exact Diagonalization
Constrained Phase
Variational
p/q = 1/5
S = 1
E_0/N
U
−0.6
−0.65
−0.7
−0.75
−0.8
0
5
10
15
Exact Diagonalization
Constrained Phase
Variational
U = 4
S = 1
E_0/N
−0.4
−0.6
−0.8
−1
−1.2
−1.4
1/7
1/5
1/3
1/2
p/q

INTRODUCTION: II

Condensed-Matter Physics

- Of secondary interest — energy
- Of primary interest — correlation functions

Broken Symmetry in Many-Body Ground States

- Broken symmetry means the many-body ground state has lower symmetry than the Hamiltonian H
- Broken symmetry implies long-range order (LRO).

Long-Range Order
If $\mathcal{O}_{\mathbf{q}}$ is the Fourier transform of some local order parameter $\mathcal{O}(i)$ and h is the symmetry breaking field, then LRO exists

- if $H_h = H - h\mathcal{O}_{\mathbf{q}}$ and

$$\lim_{h \to 0^+} \lim_{N \to \infty} N^{-1} \langle \mathcal{O}_{\mathbf{q}}(h, N) \rangle_{H_h} \neq 0$$

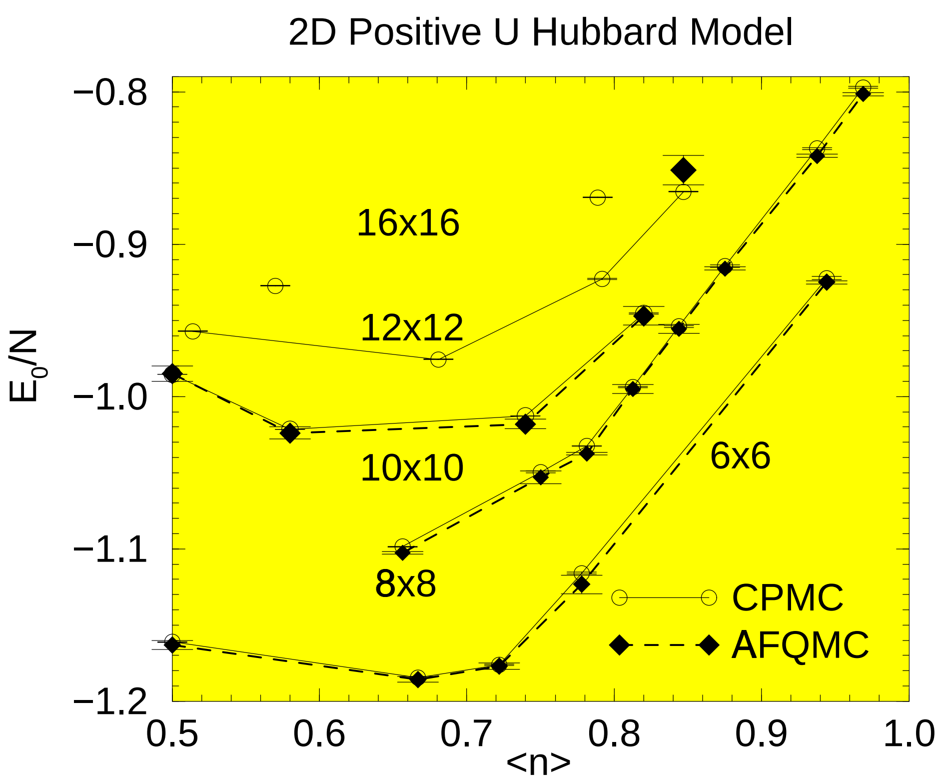
- or else if

$$\lim_{|i-j| \to \infty} \lim_{N \to \infty} \langle \mathcal{O}(i) \mathcal{O}^\dagger(j) \rangle_H \neq 0$$

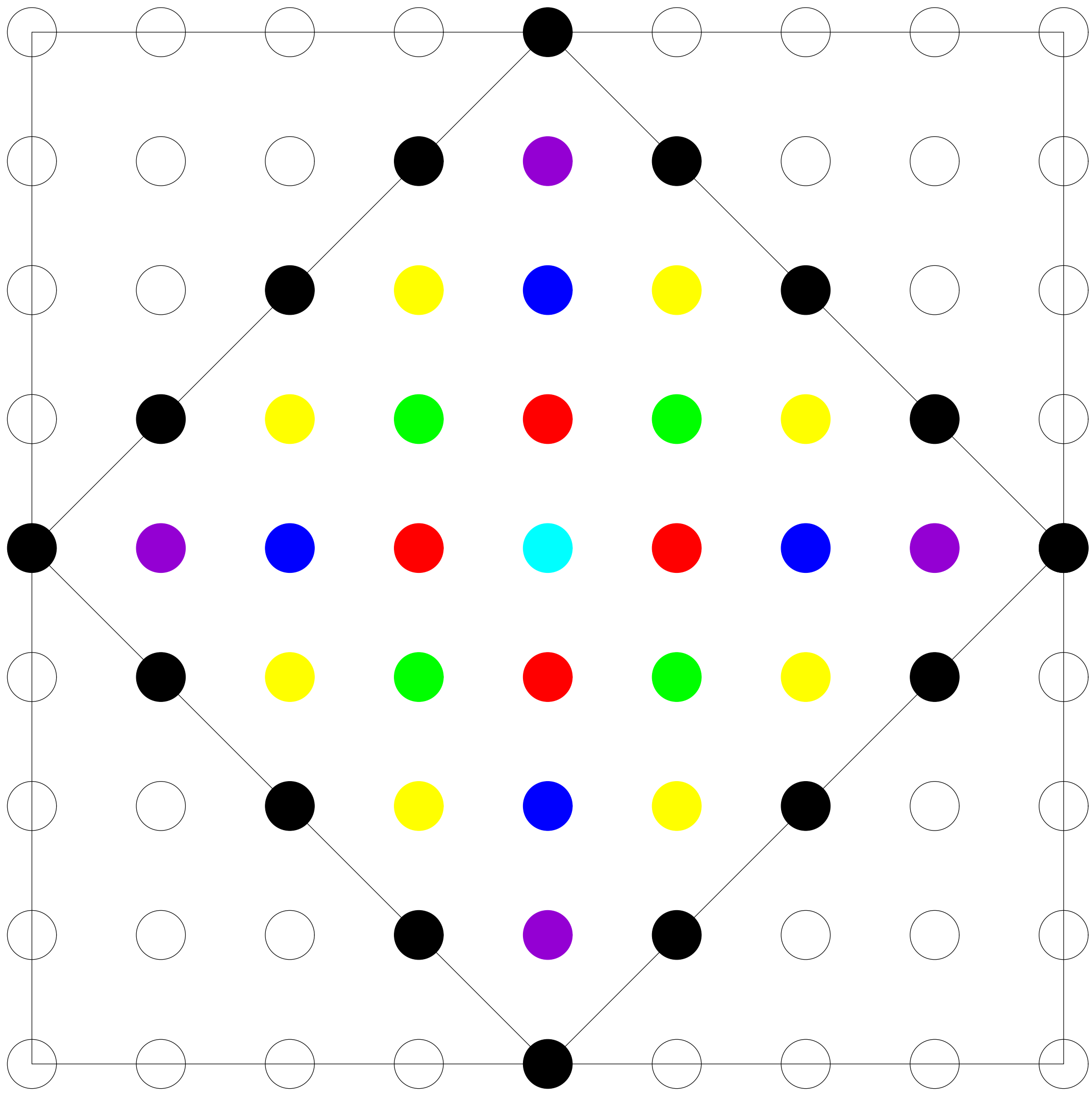
When a continuous symmetry is broken, LRO can exist only at $T = 0$ if $d < 3$.

To study LRO by QMC, one needs to simulate systems of successively increasing size.

Shell Behavior



8x8 Brillouin Zone



FINITE-SIZE EFFECTS

Characteristic of finite-sized fermions systems are shell effects. These are seem in numerical simulations.

Numerical Evidence

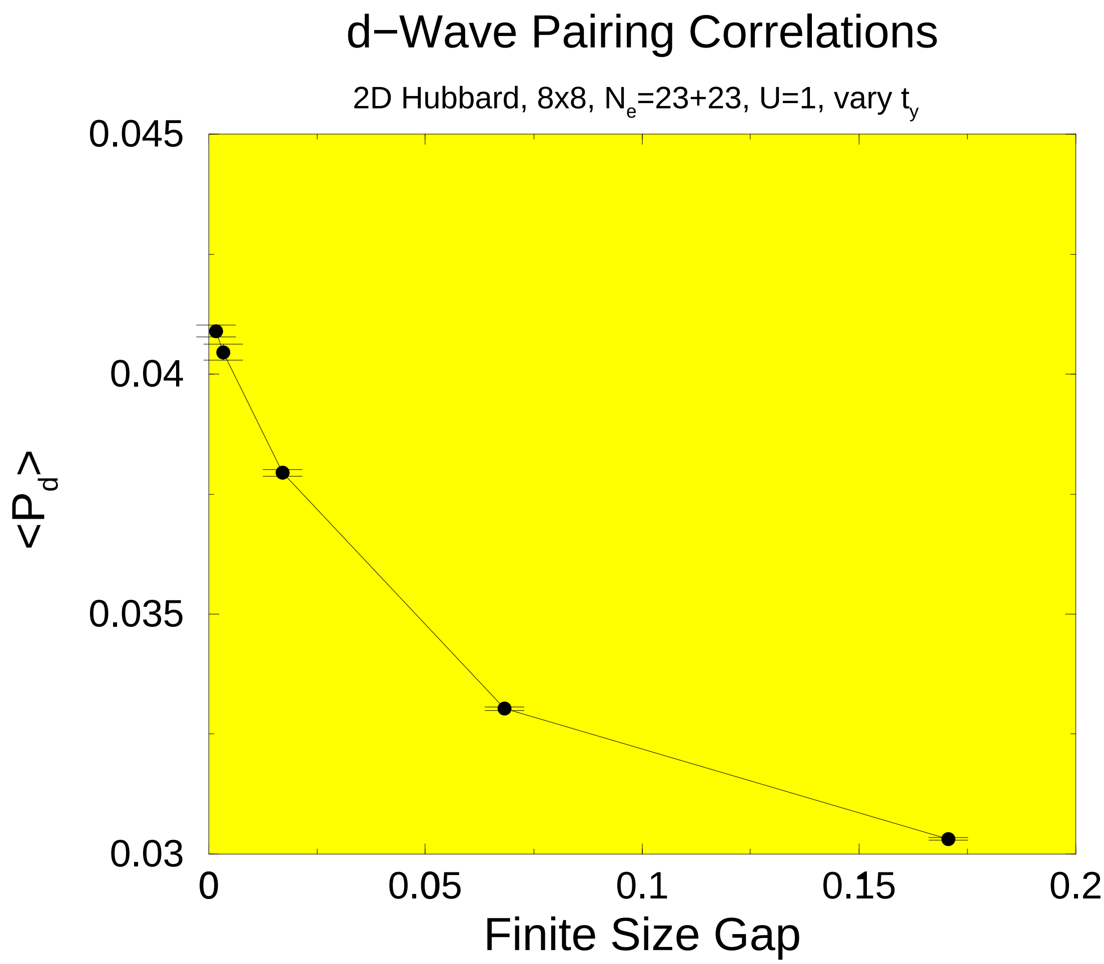
- Quantum Monte Carlo: CPMC and/or AFQMC
  - ▷ tU Hubbard model
  - ▷ $tt'U$ Hubbard Model
  - ▷ periodic Anderson model (a 2 band Hubbard model)
  - ▷ cuprate model (a 3 band Hubbard model)
- Exact Diagonalization
  - ▷ tU Hubbard model
  - ▷ $tt'U$ Hubbard Model
  - ▷ tJ model (strong-coupling approximation to tU Hubbard model)

Also seen in continuum models, e.g., the electron gas!

Fact
Quantum Monte Carlo and especially exact diagonalization are limited to relatively small system sizes.

Issues

- Absence of monotonic size dependence for some properties
- Presence of improper signatures for LRO
- Absence of proper signatures for LRO


d−Wave Pairing Correlations
2D Hubbard, 8x8, N_e=23+23, U=1, vary t_y
0.045
0.04
0.035
0.03
<P_d>
0
0.05
0.1
0.15
0.2
Finite Size Gap

Negative U Hubbard Model with No Field

BCS Approximation

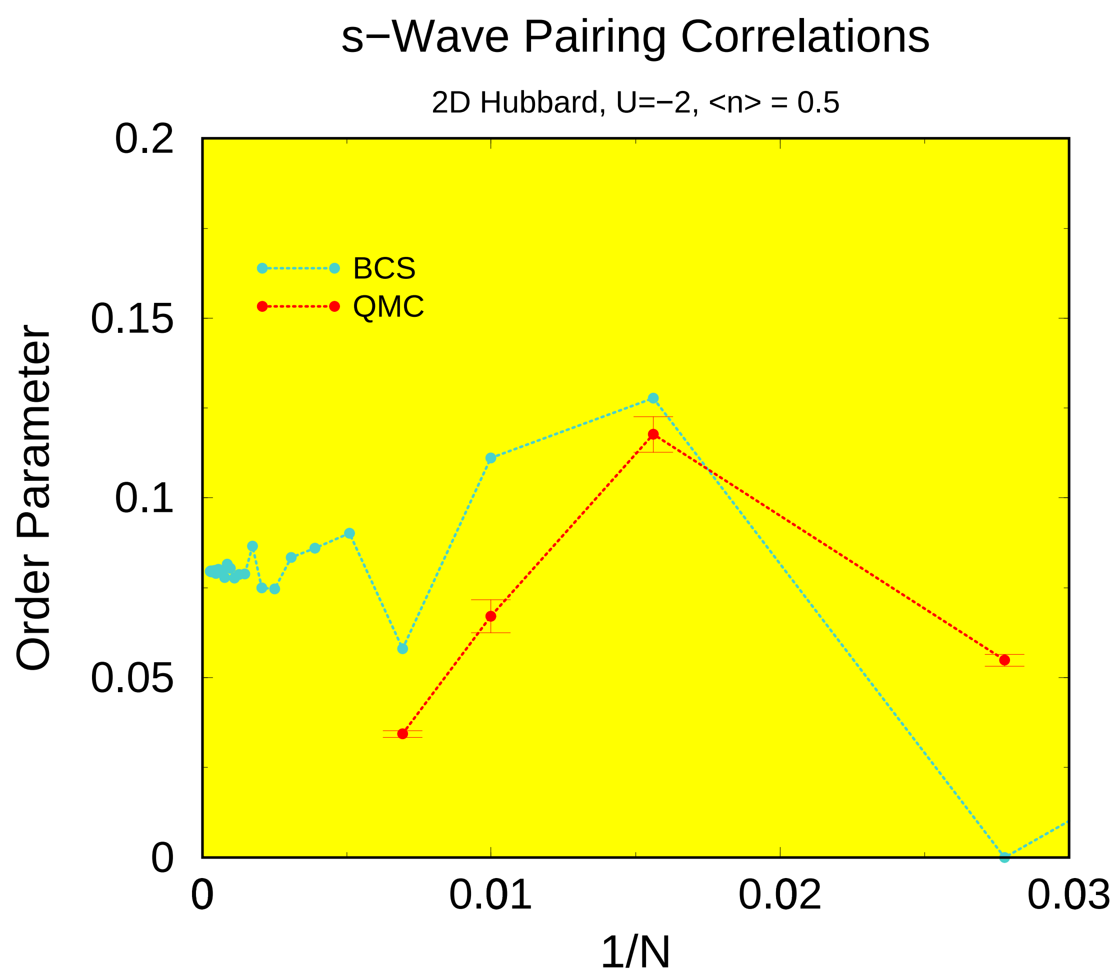
- quantitatively useful at weak and strong coupling and at dilute electron densities
- overestimates the magnitude of the order parameter
  - ▷ On site, s-wave order parameter: $\Delta_s(i) = c_{i\uparrow}c_{i\downarrow}$
- shows significant finite-size effects
- always shows ODLRO

QMC Results

- obtained with no sign problem
- establish BCS approximation estimates energies reasonably
- restrict the utility of the BCS approximation at $\langle n \rangle = 1/4$ to $-1.0 \leq U \leq 0.0$
- have yet established ODLRO; i.e.,

$$\lim_{|i-j|\to\infty} \lim_{N\to\infty} P_s(|i-j|) = \text{ positive constant}$$

  where $P_s(|i-j|) \equiv \langle \Delta_s(i)\Delta_s^\dagger(j) \rangle$
  - ▷ significant finite-size effects
    - ◇ $4m \times 4m/(4m+2) \times (4m+2)$ effects?


s−Wave Pairing Correlations
2D Hubbard, U=−2, <n> = 0.5
BCS
QMC
Order Parameter
1/N
0
0.05
0.1
0.15
0.2
0
0.01
0.02
0.03

SUMMARY

The Constrained Phase method appears promising.

- presently being benchmarked for larger sizes against DMRG predictions

From comparisons with exact QMC results, the physics of the 2D negative U Hubbard model is in general only qualitatively described by the BCS wavefunction.

In general this physics shows

- significant finite-size effects

which are inhibiting seeing ODLRO.[2]

> Exhibition of superconducting properties requires the spacing in the energy levels near the “Fermi surface” to be smaller than the superconducting energy gap (Anderson, 1959).

[2]cf. Scalettar, et al. PRL 62, 1407 (1989).