A study of the effects of disorder in the 2D Hubbard model

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Title: A study of the effects of disorder in the 2D Hubbard model

We study the effects of disorder on long range antiferromagnetic correlations and the Mott gap in the half-filled, two dimensional, repulsive Hubbard model. We employ Hartree-Fock (HF) and Quantum Monte Carlo (QMC) techniques in our study of the bond and site disordered models. Results from mean field (HF) calculations are used to develop a qualitative picture of the physics and to guide our choice for input to the QMC methods. The basic properties of two QMC methods for correlated fermions are discussed, and the results from these different approaches are presented. This work was performed under the auspices of the U.S. Department of Energy by the University of California and Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.
A study of the effects of disorder in the 2D Hubbard model

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Introduction

- Main Goal: To study correlated Fermi systems in the presence of disorder. We will consider model systems with hopping and on-site disorder. Our focus is the destruction AFLRO and the behavior of the Mott gap in the presence of disorder.

- The single band 2D Hubbard model, it encapsulates many of the most interesting qualitative many body effects. It is also one of the simplest correlated models to work with.
  - The possibility of interacting fermions to order.
  - The appearance of insulating states in systems with partially filled bands.
  - $U < 0$, superconductivity.
  - $U > 0$, model for Metal-Insulator.
  - Boson Hubbard - a model for a supersolid.
  - 1D model is solved exactly by Bethe ansatz, an insulator for all $U > 0$, no MIT.
  - In infinite dimensions variants of the HM can be solved exactly, (Dynamical Mean Field Theory)
  - No solution for $1 < d < \infty$. Many approaches are employed for finite dimensions: MFT, QMC, RG, PT, ...

- We employ several techniques in our study:
  - Exact diagonalization of the non-interacting disordered model.
  - Restricted Hartree-Fock (rHF).
  - Unrestricted Hartree-Fock (uHF).
Hubbard Model

\[ H = - \sum_{\langle i,j \rangle, \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i (n_{i\uparrow} - 1/2) (n_{i\downarrow} - 1/2) + \sum_i (\epsilon_i - \mu) (n_{i\uparrow} + n_{i\downarrow}) \]

- \( c_{i\sigma} (c_{i\sigma}^\dagger) \), creation (annihilation) operators for fermions of spin \( \sigma \)
- \( t_{i,j} \) random hopping matrix
- \( U \), on-site repulsion
- \( \epsilon_i \) random site energy, \( \mu \) chemical potential (\( \mu = 0, 1/2 \) filling)
- We will consider systems with uniform, uncorrelated disorder:
Mean Field Treatment

Develop a qualitative picture of the 2D disordered phase diagram. A mean field decomposition of the Hubbard model,

\[ n_{i\sigma} \rightarrow \langle n_{i\sigma} \rangle + \delta n_{i\sigma}, \]

where

\[ \delta n_{i\sigma} = n_{i\sigma} - \langle n_{i\sigma} \rangle. \]

produces two independent Hamiltonians

\[
H = H_{\uparrow} + H_{\downarrow} - U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle - (U/2 + \mu) \sum_{i\sigma} n_{i\sigma} + UN/4
\]

\[
H_\sigma = - \sum_{(i,j)} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_i [U \langle n_{i\sigma} \rangle + \epsilon_i] n_{i\sigma}
\]

Two mean field treatments:

rHF: Use the ansatz \( \langle n_{i\sigma} \rangle = (n + \sigma(-1)^i m)/2 \), solve the resulting equations by exact diagonalization.

uHF: \( \langle n_{i\sigma} \rangle \) can vary in an arbitrary manner. One solve \( H \) self-consistently.

Observables:

- Staggered magnetization: \( M_s = 1/N \sum_{i=1}^N (-1)^i m_i \), where \( m_i \) is the magnetization at site \( i \).

- Local magnetization: \( M_l = 1/N \sum_{i=1}^N |m_i| \).

- Compressibility: \( \kappa = \frac{1}{N} \partial \langle n \rangle / \partial \epsilon = \frac{\beta}{N} (\langle N^2 \rangle - \langle N \rangle^2) \)

- Inverse participation ratio: \( R^{-1} = 1/N \sum_{n,i} |\psi_i^n|^4 \), where the sum is over all states \( n \) and sites \( i \).
rHF Results

Phase-diagram for on-site disorder

A near linear relationship between $V_c$ and $U$.

rHF equations:

$$H = H_\uparrow + H_\downarrow - \mu \sum_{i,\sigma} n_{i\sigma} + (Un/2 - U/2) \sum_{i,\sigma} n_{i\sigma} + UN(m^2 - n^2)/4$$

$$H_\sigma = -\sum_{i,j} t_{i,j}(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_i (\epsilon_i + \delta(-1)^iUm/2)n_{i\sigma}$$

Solve $H_\uparrow$ and $H_\downarrow$ by ED.
uHF Results

Procedure:

\[ H = H_{\uparrow} + H_{\downarrow} - U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \]

\[ H_{\sigma} = - \sum_{\langle ij \rangle} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_i [U \langle n_{i\bar{\sigma}} \rangle + \epsilon_i] n_{i\sigma} \]

1. Choose a disorder realization, \( t_{i,j} \) or \( \epsilon_i \).
2. Choose an initial mean occupation, \( \langle n_{i\sigma} \rangle \).
3. Diagonalize the two Hamiltonians, \( H_{\uparrow} \) and \( H_{\downarrow} \).
4. Form a new mean occupation distribution, \( \langle n_{i\sigma} \rangle \).
5. Substitute the new \( \langle n_{i\sigma} \rangle \) into the Hamiltonian.
6. Iterate steps 3-5 to self-consistency.
7. Measure observables.
8. Repeat steps 2-7 with a different initial condition. Test for convergence of physical quantities.
9. Repeat steps 1-8 for a different disorder realization.

Results:

- The same three phases are observed for the two types of disorder.
- The system always remains an insulator.
uHF Results

Hopping Disorder ($N = 36, 64, 100$)

$M_l = M_s$ always, no spin glass
$R^{-1} \neq 0$, always an insulator

On–Site Disorder ($N = 36, 64, 100, 144$)

AFMI
$M_s \neq 0$
$\kappa = 0$

AFAI
$M_s \neq 0$
$\kappa \neq 0$

PMAI
$M_s = 0$
$\kappa \neq 0$

Note: At $U = 4$, disorder does not destroy AFLRO.
uHF Results

Evolution of the staggered magnetization and compressibility with on-site disorder

Disorder destroys magnetic order for $U = 2$ but not for $U = 4$

$12 \times 12$ lattice
CPQMC Results

The CPQMC algorithm:

- $|\Psi^{(n+1)}\rangle = \exp^{-\Delta \tau H} |\Psi^{(n)}\rangle$
- $|\Psi^{(n)}\rangle = \sum_k c_k^{(n)} |\phi_k^{(n)}\rangle$, Slater determinant basis.
- $|\Psi_T\rangle$, trial wave function.
- $\langle \Psi_T | \phi_k^{(n)} \rangle \neq 0$, constraint.
- The method ($T = 0$) allows for investigations of the Hubbard model in regions where there is a sign problem. This is an issue for the case of on-site disorder.
- In our calculations, $|\Psi_T\rangle$ is a disorder unrestricted Hartree–Fock state with $U = 0.5$.

Hopping Disorder

Spin Wave Theory:  
Huse PRB 37,2380(1988)  
$S(\pi, \pi)/N = M^2/3 + O(L^{-1})$

Critical disorder  
$V_c \approx 2.1$

Compare to DQMC result,  
Ulmke et al. PRB 55,4149(1997)  
$V_c \approx 1.6$
CPQMC Results

On-site Disorder

Critical Disorder:

\[ V_c < 0.4 \]

No DQMC or analytic data available for comparison.
CPQMC Results

Correlations

![Graphs showing correlations for different values of \( V \).]

- \( V_L = 0.0 \)
- \( V_L = 0.8 \)
- \( V_L = 1.2 \)
- \( V_L = 1.8 \)
- \( V_L = 2.0 \)
Summary

- In the mean field limit, unrestricted Hartree–Fock, the disordered Hubbard model is an insulator. At appreciable interaction strengths, disorder does not destroy AFLRO. These results hold for hopping and on-site disorder.

- Monte Carlo simulations at $U = 4$ show a loss of AFLRO with increased disorder.

- Preliminary results from CPQMC yield $V_c \approx 2.1$ for the case of hopping disorder. This result is in reasonable agreement with that obtained via DQMC, $V_c \approx 1.6$.

- Preliminary results for on-site disorder indicate that the $V_c \leq 0.4$. The enhanced ability to form on-site pairs rapidly destroys AFLRO.

Future Plans

- Need to study the effect of the trial wave function on our results; the extrapolated values for staggered magnetization are high.

- Complete work on the critical disorder at $U = 4$.

- Study the effect of the interaction strength $U$ on the half-filled model.

- Map out the ground state phase diagram as a function of $V$ and $U$. 