Magnetic phases of the Hubbard model
some answers from quantum simulations,
the “old-fashioned” way

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Outline

• Itinerant ferromagnetism in Fermi gas – connect. w. Hubbard model
• Recent advances in quantum Monte Carlo
  ➢ Phaseless appr. controls sign/phase problem in auxiliary-field QMC
  ➢ Improves QMC accuracy, better convergence to thermodynamic limit
• Ferromagnetism in dilute Hubbard model?
• Antiferromagnetism in Hubbard models (connection with high-Tc?)
  ➢ Optical lattices: experimental simulation? Advances in QMC --> synergy
  ➢ What happens to the antiferromagnetic order upon doping?
    • prediction: incommensurate spin-density waves
Research Group:

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Some references:  (http://physics.wm.edu/~shiwei)

- Zhang & Krakauer, PRL ’03
- Al-Saidi et. al., PRB ’06; JCP ’06; JCP ’06; JCP ’07
- Suewattana et. al., PRB ’07
- Kwee et. al., PRL ’08
- Purwanto et. al., JCP ’08; JCP ’09
- Chang, Zhang & Ceperley, PRA (R) ’10
- Chang & Zhang, PRB ’08; PRL ’10

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Motivation

- What is the physical basis for ferromagnetism in metals?
- New interests: Expt aimed at emulating the Stoner Hamiltonian: hints of ferromagnetic instability observed in trapped Fermi gas

Jo et. al., Science (’09)

- At $T/T_F = 0.12$ (lowest used)
- A maximum in atom loss rate:
  \[ k_F^0 a \approx 2.5 \]
- A minimum in kinetic energy:
  \[ k_F^0 a \approx 2.2, \]
- A maximum in cloud size.

\[ \Downarrow \]

Indirect evidence of ferromagnetic ordering
Motivation

• Summary of expt: (Jo et. al., 2009)
  ✦ equal mixture of $F=1/2$ hyperfine states of Li$^6$
    ⇒ 2-component Fermi gas with short-range interaction
  ✦ $a > 0$, i.e., excited state branch (molecular bound state below)
  ✦ Transition point $ka \sim 1.9(2)$
  ✦ No observation of FM domains

• Interpretation has been debated (Ho, Zhai, ....)

• Recent MIT expt (Zwierlein et al)
Motivation

- The 3-D Hubbard model is a reasonable representation of the Stoner Hamiltonian
  itinerant electrons + local interaction

- Caveats!
  - Hubbard model: Ground state, repulsive interaction, equilibrium
    Experiment: Excited states, attractive interaction, dynamic (quench)
  - The scattering length on a lattice is bounded by lattice spacing
    (Castin 2004)
    \[
    a_{lattice} = \frac{a_s}{1 + 3.173a_s}
    \]
  - Does the model have an instability towards ferromagnetism?
    (What is the minimal model for itinerant FM in metals?)
Introduction: Hubbard model

- Simplest model combining band structure and interaction:

\[ H = K + V = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Electrons on a lattice:
- near-neighbor hopping
- on-site repulsion

Consider:
- T=0K
- \(N_{\uparrow} = N_{\downarrow}\)

Parameters:
- \(U/t > 0\) (\(t=1\))
- \(n=(0,1];\) doping \(h=1-n\)

- Optical lattice emulator?
- Extremely difficult computational problem

Size N=\(L^d\)

Filling \(n = \frac{N_{\uparrow} + N_{\downarrow}}{N}\)

Half-filling: \(n=1\)
Introduction: Hubbard model

- Simplest model combining band structure and interaction:

\[ H = K + V = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Electrons on a lattice:
- near-neighbor hopping
- on-site repulsion

Size N=L^d

Filling \( n = \frac{N_\uparrow + N_\downarrow}{N} \)

Half-filling: \( n=1 \)

Does it have a ferromagnetic instability?

- Neither \( K \) nor \( V \) term favors FM alone
- **Academic** case: Nagaoka-Thouless:
  1 hole, \( U=\infty \), bipartite: yes
**Mean-field theory**

- **Stoner's criterion** \( U \cdot N(\epsilon_F) > 1 \)

- For different densities:
  - \( n = 0.25 \)
  - \( n = 0.0625 \)

\[
H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]
Mean-field theory

- **Stoner’s criterion** \( U \cdot N(\epsilon_F) > 1 \)

- The ground state is antiferromagnetic at half-filling \( n = 1 \)

- Phase diagram has large domain of ferromagnetism

How does correlation modify this?
Constrained path auxiliary field QMC

To obtain ground state, use projection in imaginary-time:

\[ |\Psi^{(n+1)}\rangle = e^{-\tau \hat{H}} |\Psi^{(n)}\rangle \xrightarrow{n\to\infty} |\Psi_0\rangle \]

\( \tau: \) cnst, small \quad |\Psi^{(0)}\rangle: \) arbitrary initial state

Hamiltonian:

\[ \hat{H} = \hat{H}_1 + \hat{H}_2 = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Hubbard–Stratonovich transformation

\[ e^{-\tau \hat{H}} \rightarrow e^{-\tau \hat{H}_1} \int e^{-x^2/2} e^{x\sqrt{\tau} \hat{v}} \, dx \quad \hat{v}: \) one-body

interacting system \rightarrow \sum (non-interacting system in auxiliary fields)

E.g., trick by Hirsch:
Toy system: Hubbard model

Illustration of how AFQMC works:

- Formalism similar to LGT
- But sign problem severe in most problems of interest
- Reformulated into open-ended random walks
The sign problem

E.g., in Hubbard:

- $e^{-\tau \hat{H}} \rightarrow$ paths in Slater determinant space

- Suppose $|\Psi_0\rangle$ is known; consider “hyper-node” line

- If path reaches hyper-node

  $\langle \Psi_0|\phi\rangle = 0$
  
  $\Rightarrow \langle \Psi_0|e^{-n\tau \hat{H}}|\phi\rangle = 0$

  then its descendent paths collectively contribute 0

- MC signal is exponentially small compared to noise

  In special cases (1/2 filling, or $U<0$), symmetry keeps paths to one side

  $\rightarrow$ no sign problem
How to control the sign problem?

- Constrained path appr.

\[ \langle \Psi_0 | \phi \rangle = 0 \]

keep only paths that never reach the node

require \[ \langle \Psi_T | \phi \rangle > 0 \]

Trial wave function used to make detection

- Phaseless approximation

Zhang & Krakauer, ’03; Chang & Zhang, ’08

general interaction: complex HS --> phase problem

twisted boundary condition: removes shell effects --> complex w.f.
Benchmark

- Sampling 1000 random TABCs
  
  3x3: Largest relative error:
  
  ~ 0.2% for U/t = 4
  ~ 1.0% for U/t = 8
  
  dilute 4x4 at n=0.25
  ~ 0.2% for U/t = 16
  ~ 0.6% for U/t = 30

- Summary: CPMC + TABCs
  - controls sign problem
  - many benchmarks (including ab initio electronic structure)
  - Most accurate many-body method available at intermediate interactions for large systems (2- & 3-D)

Equation of state for 3x3 Hub

\[
\text{Relative error} \% = \frac{e_{QMC}(n) - e_{Exact}(n)}{|e_{Exact}(n)|}
\]

Chang & SZ, PRB ’08
Ferromagnetism in 3D dilute Hubbard model?

Energy results:

- $n = 0.25$
- $n = 0.0625$

Essentially no finite size effects in the QMC data

- No FM transition was found: $0 < n < 0.5$
- Partially polarized state is unlikely to be stable
Individual energy components

- Interaction creates excitations beyond the Fermi surface, increasing the kinetic energy.
- At large U, the interaction energy is lowered by correlation: reduced double occupancy.
Correlation effects

Pair-correlation function:

- Enhanced ferromag. corr, but short-range, weaker than in FM phase
- Consistent with a paramagnetic Fermi liquid
Comment & connection to other calculations

- **Expt:**
  - Transition point $k a \sim 1.9(2)$
  - Quench of excited state (dynamics?)

- **Other calculations/theory:**
  - Mean-field in continuum gives $k a \sim 1.5$; fluctuation correction: $k a \sim 1$
  - Diffusion Monte Carlo: $k a = 0.8-0.9$
    - Conduit et al, ‘09; Pilati et al, ‘10; Chang et al. ‘09
  
  - **However,** all used “hard-sphere” potential (scattering length appr.) to remove molecular states. This over-estimates trends for FM and can cause errors
    - see Zhou, Ceperley, **SZ:** arXiv/1103.3534
No ferromagnetism is found in the dilute 3-D Hubbard model up to $U \sim 30t$, with density up to $n=0.5$.

Energy is lowered by creating correlation holes (cf. Wigner, electron gas).

Caveats:

- ground state; repulsive contact int.; equilibrium (calc) vs. excited state; attractive int. ($a>0$); dynamic (expt)

- scattering length in our model (repulsive 3D Hubbard) is bounded by latt. spacing
Magnetic properties at larger density?

- Half-filling: antiferromagnetic (AF) order
  (Furukawa & Imada 1991; Tang & Hirsch 1983; White et al, 1989; ....)
- Model for high-Tc? Must understand magnetism and its fluctuations first!

Calculate AF correlation:

\[ C(r) = \frac{1}{L \times L} \sum_{r'} \langle S_r \cdot S_{r+r} \rangle \]

What happens to the AF order with doping?
Note even the HF answer has not been unambiguous

Xu, Chang, Walter, SZ, 2011

How does correlation modify this?
Equation of state in 2D

- Free-electron trial w.f.
- Use 20 ~ 300 random twist angles
- Data of different lattice sizes has good agreement at $n < 0.9$
- “Unstable” region is found on 8x8, 12x12, 16x16

frustrated long wavelength mode ?

phase separation ?
Spin-spin correlation

- Use rectangular lattices to probe correlation length $L > 16$
- Up to $8\times128$ supercell (dimension of CI space: $10^{600}$ !)
- Detect spatial structures using correlation functions

$$C(r) = \frac{1}{N_s} \sum_{r'} \langle S_r \cdot S_{r+r'} \rangle$$

- Periodic boundary condition is used when calculating $C(r)$
- The observed structure emerges from a free electron trial state

"staggered": $(-1)^y C(x,y)$

$8\times32$

$n = 0.9375$
Equation of state, again

- TABC removes one-body shell effects, but not two-body finite-size effects:

- Instability is from frustration of SDW due to finite size
- At \( n = 0.9375 \), need \( L \sim 32 \) to detect SDW state

(Previous calculations: \( L_y \sim 12 \), with large shell effects)
Wavelength versus doping

Doping $h = (1-n)$ dependence

- Wavelength decreases with doping; as does the amplitude
- SDW terminates at finite doping (~0.15), enters paramagnetic state
- Wavelength appears $\propto 1/h$

Chang & SZ, PRL 104, 116402 (2010)
Dependence on U

- At $U/t=4$, charge is uniform:
  - No peak in charge struc. factor
  - holes fluid-like (de-localized)

- At $U/t=8-12$, CDW develops:
  - Peak in structure factor
  - Clumps of density=1, separated by dips (SDW nodes)
  - Consistent with DMRG results at large $U/t$ (White et al, ‘03, ‘05)
  - holes Wigner-like (localized)
Magnetic phases in repulsive Hubbard model using CPMC + TABCs

- Accurate QMC results
- No ferromagnetism in 3D up to n~0.5; paramagnetic Fermi liquid?
- Near half-filling, in 2D, at low to intermediate U/t:
  - AF spin density wave (SDW) with long wavelength modulation
  - Wavelength decreases with doping (infinity at half-filling)
  - SDW amplitude decreases with doping, vanishes at n~0.85(5)
  - Charge-charge correlation almost uniform

- LO state in spin-imbalanced attractive optical lattice?