Simulations and Emulations of Fermions in Optical Lattices

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BOSONS vs FERMIONS

$^7\text{Li}$

$T = 810 \text{ nK}$

$T = 510 \text{ nK}$

$T = 240 \text{ nK}$

$^6\text{Li}$

$T/T_F = 1.0$

$T/T_F = 0.56$

$T/T_F = 0.25$

**Observation of Fermi Pressure in a Gas of Trapped Atoms**

Andrew G. Truscott, Kevin E. Strecker, William I. McAlexander,*
Guthrie B. Partridge, Randall G. Hulet†

Science 291, 2570 (2001)
What happened to the sign problem?

*Nature seems to have no difficulty reaching the ground state of bosons or fermions!*

EMULATION vs SIMULATION

Truscott et al. Science 291, 2570 (2001)
\[ t, U \ll \omega \]

\[ t \]

\[ U \]
Cold Atomic Gases in Optical Lattices → Hubbard Models

\[ H = -t \sum_{(i,j)\sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) - h \sum_i (n_{i\uparrow} - n_{i\downarrow}) \]

tunneling
interaction
chemical potential
Zeeman field
Cold Atomic Gases in Optical Lattices  

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

- tunneling
- interaction
- chemical potential
- Zeeman field

\[ \lambda \approx 1000 \text{nm} \]
\[ t \sim 10 nK \]
\[ U/t \sim 10 \]
\[ J = 4t^2/U \approx 4nK \]

\[^6\text{Li}\]
\[ |F,m_F\rangle = \left| \frac{1}{2}, \frac{-1}{2} \right\rangle = \downarrow \]
\[ |F,m_F\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \uparrow \]

\[^{40}\text{K}\]
\[ |F,m_F\rangle = \left| \frac{9}{2}, \frac{-9}{2} \right\rangle = \downarrow \]
\[ |F,m_F\rangle = \left| \frac{9}{2}, \frac{-7}{2} \right\rangle = \uparrow \]

Schneider et al. Science 322, 1520 (2008)
Jordens et al Nature 455, 204 (2008)
I. Repulsively interacting fermions in 3D optical lattices:
What are the entropy constraints required to reach the AF phase with long range order?

3D work unpublished
Determinantal QMC: Equation of state $\rho(\mu, T, U/t)$

“exact” unbiased on finite systems and finite T
Determinantal QMC: Equation of state $\rho(\mu,T,U/t)$

“exact” unbiased on finite systems and finite $T$

$$Z = \text{Tr} e^{-\beta H} = \text{Tr}[(e^{-\Delta \tau H})^L] \approx \text{Tr}[(e^{-\Delta \tau K} e^{-\Delta \tau V})^L]$$

$$\langle A \rangle = \frac{\text{Tr}[A e^{-\beta H}]}{Z}$$

$$e^{-\Delta \tau V} = e^{-\Delta \tau U \sum_i (n_{i\uparrow} - \frac{1}{2}) (n_{i\downarrow} - \frac{1}{2})} = \frac{1}{2} e^{-\frac{\Delta \tau U}{4} \sum_{S(i) = \pm 1} \Delta \tau S(i) \lambda (n_{i\uparrow} - n_{i\downarrow})}$$

$$Z = \sum_{S(i,\tau)} \text{Det}[M_{\uparrow}(S(i,\tau))] \text{Det}[M_{\downarrow}(S(i,\tau))]$$

$$\langle A \rangle = \frac{\langle A \text{sgn} \rangle}{\langle \text{sgn} \rangle}_{\text{det } M_{\downarrow}}$$

“Sign problem” at low $T \leq 0.1t$ but controlled by longer simulations
Repulsive U Hubbard model: Phase Diagram at Half Filing

\[ N_{\uparrow} = N_{\downarrow}; N_{\text{fermions}} = N_{\text{sites}}; d = 3 \]

Mott Insulator:
1. Suppression of double occupancy
2. Reduction of compressibility
3. Gap in excitation spectrum

All energies in units of t
Mott Physics and Charge Gap

Density of states at the chemical potential

Appearance of gap in low energy excitation spectrum
Gap increases with U
Repulsive U Hubbard model: Phase Diagram at Half Filing

\[ N_{\uparrow} = N_{\downarrow} ; N_{\text{fermions}} = N_{\text{sites}} ; d = 3 \]

\[ T_{\text{ch}} \sim U \]

\[ S_{\text{max}} / N k_B = \ln(4) \approx 1.4 \]
\[ S_{\text{exp}} / N k_B \approx 0.7 - 1 \]

All energies in units of \( t \)
Repulsive U Hubbard model: Phase Diagram at Half Filling

\[ N_{\uparrow} = N_{\downarrow}; N_{\text{fermions}} = N_{\text{sites}}; d = 3 \]

Note: Isoentropic curve is also an isothermal curve
As U is increases T remains rather constant

\[ S_{\text{max}} / Nk_B = \ln(4) \approx 1.4 \]
\[ S_{\text{exp}} / Nk_B \approx 0.7 - 1 \]
$N_\uparrow = N_\downarrow ; N_{\text{fermions}} = N_{\text{sites}} ; d = 3$

3D Repulsive U Hubbard model: QMC Phase Diagram

$T_{\text{ch}} \sim U$

$T_{\text{Neel}} \sim J = 4t^2 / U$

Double occupancy suppressed Local Moments form

Local moments order antiferromagnetically

Band Antiferromagnetism

Heisenberg model for local moments

Staudt, Dzierzawa and Muramatsu EPJ B17, 411 (2000)
3D Hubbard Model at half filling: Isoentropic Curves (QMC)

Critical Entropy vs U

\[ S_{AF, Quantum} / Nk_B \approx 0.3 \]

Target entropy to see AF LRO in 3D Hubbard Model

\[ S_{exp} / Nk_B \approx 0.7 - 1 \]
QMC vs DMFT: No significant adiabatic cooling from QMC

**QMC (“exact”)**
Adiabatic cooling not significant

**Dynamical Mean Field Theory:**
Werner, Parcollet, Georges, Hassan, PRL 95, 056401 (2005)

DMFT misses important singlet correlations even above $T_{\text{Neel}}$
Trap
Determinantal QMC for homogeneous system to calculate equation of state $\rho(\mu,T,U/t)$

Particle-hole symmetry $\rho(-\mu) = 2 - \rho(\mu)$
3D Hubbard Quantum Simulations with a Trap

\[ H = -t \sum_{(i,j)\sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma}) + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) - \mu \sum_i n_i \]

- Determinantal QMC for homogeneous system to calculate equation of state \( \rho(\mu,T,U/t) \)
  
- Local density approximation to include the inhomogeneous distribution in trap
  
\[ \mu(r) = \mu - \alpha \frac{r^2}{d^2} \]

\[ N = \int dr^3 \rho(r) = \frac{4\sqrt{2}\pi}{(m\omega^2)^{3/2}} \int_{-\infty}^{\mu_0} d\mu \sqrt{\mu_0 - \mu} \rho(\mu) \]

\[ \left. \frac{\partial \rho}{\partial T} \right|_{\mu} = \left. \frac{\partial s}{\partial \mu} \right|_{T} \]

\[ s(\mu) = \int_{-\infty}^{\mu} d\mu \left. \frac{\partial \rho}{\partial T} \right|_{\mu} \]

\[ \nu = [20 - 120] Hz \Rightarrow \alpha = [0.0006 - 0.021] t \]
Inhomogeneous Distribution of Phases in a Trap

\[ U = 8 \quad N = 4 \times 10^6 \quad S/N_{k_B} = 0.65 \]

\[ \nu = [20 - 120] Hz \Rightarrow \alpha = [0.0006 - 0.021] t \]
Compressibility suppressed in BI and MI

\[ U = 8 \ N = 4 \times 10^6 \]
\[ S/Nk_B = 0.65 \]
Entropy Distribution in Trap

BI: entropy $\sim 0$
MI: low but finite entropy
because of spin waves
Metal: entropy sinks

$U=8 \ N=4 \times 10^6$
$S/Nk_B=0.65$
Even when the total entropy per site is above the critical entropy to see the AF phase in a homogeneous system, in a trap the entropy in the center can drop below $s_c \sim 0.3k_B$. 

Entropy Distribution in Trap
BI: entropy $\sim 0$
MI: low but finite entropy
because of spin waves
Metal: entropy sinks

$U=8$ $N=4 \times 10^6$
$S/Nk_B=0.65$
Nearest neighbor spin-spin correlation function
Grows as the trap opens up and tracks the Mott region
Lower entropy is not always a good thing!

\begin{align*}
U &= 8 \\
N &= 4 \times 10^6 \\
S/Nk_B &= 0.3
\end{align*}
Lower entropy is not always a good thing!

If $S$ is very low the system generates a large BI region in center

MI away from center which may be harder to find
Many other ideas for cooling...
Using a bosonic sympathetic species
[T.L. Ho and Q. Zhou, PNAS, 106, 6916 (2009)]
Using dimpled potentials [Ho & Zhou, arXiv:0911.5506]

Our proposal of “decompression cooling” here is really simple
To just judiciously utilize the trap to redistribute entropy
And most importantly the numbers work out
Unequal fermion populations with attractive interactions:

Does the FFLO phase
(Superfluid phase with modulating order parameter) exist?
What are the observable signatures of such a phase?
3D Attractive Hubbard model with $N_\uparrow \neq N_\downarrow$ (BdG)
Y.-L. Loh and NT PRL 104, 165302 (2010);

1D Spectral functions: Role of fluctuations (QMC)
K. Bouadim, Y.-L Loh, R. Rousseau, NT (unpublished)
At unitarity the FFLO phase disappears.

Large region of LO in a lattice

Phase separated region replaced by LO
Interactions further enhance the LO region

\[ P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = \frac{m}{n} \]

\[ n = \frac{N_\uparrow + N_\downarrow}{N_{\text{sites}}} \]
3D Attractive Hubbard phase diagram for imbalanced gases

BdG-HF calculations in 3D

LO enhanced due to nesting in lattice and Hartree corrections

→ Size of LO region comparable to BCS!!

“continuum” results

Also: Koponen-Paaninen-Martikainen-Törmä PRL 99, 120403, 2007 studied $\Delta \sim \exp i q \cdot r$

We find that $\Delta \sim \cos q \cdot r$ (or more complicated patterns) have significantly lower energy
Large LO phase in trap center: cannot be missed in lattice!

\[ \mu(r) = \mu(0) - \alpha r^2 \]

80% of atoms in LO phase at trap center!

\[ P = 0.37 \quad U = -6t \]

BdG + LDA with trap
LO phase and Domain Walls

Domain Walls

$\Delta$

$m$

$x$

Microscale
Phase separation

Order parameter changes sign
Excess fermions piled up in the regions where the order parameter crosses zero
Domain Walls and Andreev Bound States

Bound state energies within gap
Bound state wavefunctions localized in vicinity of domain wall

\[ H = \begin{pmatrix} K & \Delta \\ \Delta^* & -K \end{pmatrix} \]
Spectroscopic Signatures of Andreev Bound States

Usual coherence peaks in a superfluid

Andreev bound states (ABS) within gap

Increase gap using $U$ to better separate ABS

$N_{\uparrow}(E)$

$N_{\downarrow}(E)$

Usual coherence peaks in a superfluid
Spectroscopic Signatures of Andreev Bound States

Density of states for 1D LO: BdG
Determinantal QMC + Maximum Entropy methods for analytic continuation

Note: compared to BdG the Andreev “bound” states are not so well defined and merge with continuum

See also DMRG: Feiguin and Huse PRB 79, 100507 (2009)
Next: Coupled chains to stabilize LO state

\( L = 80 \)
\( U = -4t \)
\( N_+ = 24 \)
\( N_\downarrow = 16 \)
I. Repulsively interacting fermions in optical lattices:

In a homogeneous system must go below $S/Nk_B \approx 0.3$ to see an AF phase

In a trap can start with high entropy e.g. $S/Nk_B \approx 0.7$

Decompress
Entropy redistributed over a larger region
Can achieve low temperatures to see AF / Mott

*In fact starting with very low entropy may be detrimental!*

II. Attractive fermions in optical lattices:

LO phase enhanced by lattice effects; low dimensions
Control fluctuations using coupling between ladders
Spectroscopic signatures within gap and pair momentum enhancement at $q_{LO}$
Explore “Pseudogap” Region in All Hubbard models

We understand the phases...

Explore the intermediate temperature scale where the incoherent degrees of freedom organize themselves into a coherent phase

\[ T_c < T < T^* \]
end