Ab-initio simulations of ultracold atomic gases

S. Trotzky et al., Nature Physics, (November 2011)
S. Fuchs et al., arXiv:1009.2759
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- Experiments on bosons
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- Simulations of fermions
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Supercomputing: petaflop and beyond

- Supercomputing technology has broken through the petaflop-barrier and Moore’s law continues to hold.
Quantum simulators

Strongly correlated materials
interesting but little understood phenomena

Quantum simulators:
Controlled realizations of models, “simple” systems testing

Effective models:
Simple models which capture the relevant physics
Bose-Einstein condensation in cold atomic gases

- At close to zero temperatures, a macroscopic fraction of all atoms in a Bose gas occupy the same quantum state
- A diverging occupation of the zero momentum state
Optical lattices

- formed by standing waves from three pairs of laser beams

- realize quantum **lattice** models of fermions or bosons
Optical lattices and the Hubbard model

- Lasers couple to the dipole moment of the atoms
  - atoms prefer to sit at the amplitude maxima (AC Stark effect)
  - a periodic potential with periodicity half of the wave length
  - obtain a Hubbard model for the lowest band

- Tunable and controlled
  - Laser amplitude determines $U$ and $t$
  - Spatially varying couplings using optical superlattices

- Flexible
  - fermionic or bosonic atoms or mixtures are possible

- Can they be used as quantum simulators to solve the Hubbard model?
Ab-initio simulations of ultracold atomic gases

- Model all relevant details of the experiment to perform controlled *ab-initio* simulations of bosons and fermions to
  - Validate and calibrate the experiments
  - Provide reference data for thermometry
  - Test new theoretical ideas for probes and thermometry
  - Show experimentalists the next goals and milestones

- For equilibrium systems until now simulations are better than experiment even for fermions
The ab-initio microscopic model

\[ H = \int d^3r \psi^\dagger(\vec{r}) \left( -\frac{\hbar^2}{2m} \Delta + V_{\text{opt}}(\vec{r}) \right) \psi(\vec{r}) + \frac{g}{2} \int d^3r \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}) \psi(\vec{r}) \psi(\vec{r}) \]

\[ V_{\text{opt}}(r,z) = -V_0 e^{-2r^2/w^2(z)} \sin^2(kz) \]

\[ \psi(\vec{r}) = \sum_i w(\vec{r} - \vec{r}_i) b_i \]

express the bosonic field operator in terms of Wannier functions

\[ H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{h.c.}) + U \sum_i n_i (n_i - 1)/2 - \mu \sum_i n_i + V \sum_i r_i^2 n_i \]
Limitations of the Hubbard model

- Only valid in deep lattices where one band is enough
- Shallow lattices require alternative approaches
- Corrections to naïve calculations of $U$ are hard
- Equilibration is an open issue in the experiments
Bose-Hubbard model

- Use bosonic atoms for validation

\[ H = -t \sum_{\langle i,j \rangle} \left( b_i^\dagger b_j + b_j^\dagger b_i \right) + U \sum_i n_i (n_i - 1)/2 - \mu \sum_i n_i \]

Fisher et al, PRB 1989

Large \( U \): incompressible Mott-insulator at Integer filling

Quantum phase transition varying \( U/t \)

Large \( t \): superfluid BEC
The first optical lattice experiments

- Quantum phase transition as lattice depth is increased
  - measuring the momentum distribution function in time-of-flight images

Can this be made more quantitative?
Validation by Quantum Monte Carlo simulations

- Approximation-free QMC simulations
  - up to 500,000 atoms, $220 \times 220 \times 200 \approx 10$ million sites
  - a single simulation takes only 10 hours on one CPU core

- We can model all important details of the experiment
  - accurate microscopic model
  - same system size, particle numbers
  - temperature and entropy matched to experiment
  - measure quantities as observed in experiment
QMC “images” of the boson cloud

U/t = 10
U/t = 25
U/t = 50

Thursday, 21 October 2010
Image after expansion – momentum distribution

3D image

Crosssection

Thursday, 21 October 2010
Quantitative validation: the phase diagram

- Bosons in a 3D optical lattice at filling $n = 1$
- Measure suppression of $T_c$ close to the Mott insulator
- Particle number required to achieve $n = 1$ obtained from QMC
Experiments work (ideally) at constant entropy!
- Measure the momentum distribution before loading the gas into the lattice
- Get its temperature and entropy fitting to a dilute Bose gas
- Use QMC simulations to find the temperature for that entropy once loaded into an optical lattice (non-trivial simulations!)

Use QMC simulations for thermometry
Accurately model time of flight (TOF) images

CCD camera

pixel size: 4.4 micron
further broadening by optical elements

faster atoms fly farther
records the momentum distribution

TOF duration = 15 ms
Time-of-flight images: momentum distribution?

\[ \hat{\Psi}(r, t) = \sum_{\nu} w_{\nu}(r, t) \hat{a}_{\nu} \]

contribution from all sites

\[ w_{\nu}(r, t) = \langle r | e^{-i \frac{\hat{p}^2 t}{2m\hbar}} | w_{\nu}(t) \rangle \]

ballistic expansion

\[ w_{\nu}(r, t) = \int \frac{d^3 k}{(2\pi)^3} e^{-i \frac{\hbar k^2 t}{2m} + i k \cdot (r - r_{\nu})} \tilde{w}(k) \]

\[ \tilde{w}(k) \sim e^{-\frac{a_0^2 k^2}{2}} \]

Gaussian approximation for Wannier function

\[ n(r, t) = \sum_{\mu, \nu} w_{\mu}^*(r, t) w_{\nu}(r, t) \langle \hat{a}_{\mu}^\dagger \hat{a}_{\nu} \rangle \]

density matrix from QMC

Intensity
Time of flight (TOF) images

Do we really measure $n(k)$ in experiment? [F. Gerbier et al, PRL (2008)]

$$n(r, t) \sim e^{-i \frac{K(r_\mu - r_\nu)}{1 + \delta^2}} e^{-i \frac{m(r_\nu^2 - r_\mu^2)}{2\hbar t (1 + \delta^2)}} e^{-i \frac{\delta K(r_\mu + r_\nu)}{1 + \delta^2}} e^{-i \frac{m\delta(r_\mu^2 + r_\nu^2)}{2\hbar t (1 + \delta^2)}} \langle \hat{a}_\mu^\dagger \hat{a}_\nu \rangle.$$ 

$a_0$: width of the initial Gaussian Wannier function

$$K = \frac{mr}{\hbar t}, \quad \text{“quasi-momentum”}$$

$$\delta = \frac{ma_0^2}{\hbar t} = 2 \frac{m\lambda^2}{8\hbar t} \left( \frac{a_0}{\lambda/2} \right)^2 \approx 5.10^{-4}$$

$$K_y = \frac{r y m}{\hbar t} + gmt$$

taking gravity semi-classically into account
Finite time of flight broadens the peaks

finite time of flight cuts off spatial correlations
broadens peaks

F. Gerbier et al, accepted in PRL
Validation of experiment by QMC: small $U/t$

$$V_0 = 8E_r, \quad U/J = 8.11, \quad T_c = 26.5\text{nK}$$

- **Experiment**
  - 13.6 nK
  - 18.8 nK
  - 26.5 nK
  - 30.7 nK
  - 43.6 nK

- **QMC**
  - 11.9 nK
  - 19.1 nK
  - 26.5 nK
  - 31.8 nK
  - 47.7 nK

- **OD vs $x_{TOF} (2hk)$**
  - Red dashed line: Exp.
  - Black line: QMC
Validation of experiment by QMC: large $U/t$

\[ V_0 = 11.75E_r, \quad U/J = 27.5, \quad T_c = 5.31 \text{nK} \]
Non-adiabaticity: heating from lattice laser

Entropy determined by comparing TOF images to QMC simulations
Severe limitation on accessible temperatures in experiments

Phase diagram obtained by the quantum simulation

- Mott; $U/t = 29.34(2)$
- fit: Mott; $U/t = 28.5 +/- 1.0$
- $T_c / J$ vs $U / J$

Normal phase region
Testing new theoretical ideas

Thermometry
Thermometry from fluctuation-dissipation theorem

- Proposal of Qi Zhou and T.-L. Ho

\[ -\frac{k_B T}{M \omega^2 r} \frac{\partial \langle \hat{n}(r) \rangle}{\partial r} = \langle \hat{n}(r) \hat{N} \rangle - \langle \hat{n}(r) \rangle \langle \hat{N} \rangle \]

- Beautiful smooth data from QMC corresponding to averages of 1000s of measurements, but still noisy thermometry
Thermometry from fluctuation-dissipation theorem

\[- \frac{k_B T}{M \omega^2 r} \frac{\partial \langle \hat{n}(r) \rangle}{\partial r} = \langle \hat{n}(r) \hat{N} \rangle - \langle \hat{n}(r) \rangle \langle \hat{N} \rangle\]

  - restrict correlation measurement to a small window of size $\xi$
  - needs only about 20 measurements for 10% accuracy
  - total particle number fluctuating by less than 3%

\[j = 2\]

$N_{\xi}(r)$

$R_{\xi}(\rho)$

True temperature $\xi = 3$

Thursday, 21 October 2010
Fermions
The fermion sign problem in QMC

- Quantum systems mussed first be mapped to classical systems
  
  \[ Z = \text{Tr} e^{-\beta H} = \sum_{i} p_i \]

- There is a “sign problem” if two fermions exchange: \( p_i < 0 \)
  
  - cannot sample using negative weights
  
  - “ignoring” sign in sampling gives exponentially growing errors
Simulating fermions

- There is no “black box” solution for all fermion problems
  - We need to think hard and find good approximate methods
  - The good news: we’ll not be out of business until quantum simulators come online

- We can still simulate fermions in experimentally relevant regimes:
  - High-temperature expansions: valid down to \( T \approx t \)
  - Dynamical mean field theory approximation and cluster extensions
  - Diagrammatic QMC methods
Determining the temperature for fermions

- Fit to high-temperature series expansions to measurements of double occupancy gives temperature and entropy


\[ \rho = N / N_0 \]

\[ N_0 = \left(12t / m\omega^2a^2\right)^{3/2} \approx 7400 \]
Reaching the Néel state

- At large $U/t$ a Mott-insulating phase has been reached in the center but the temperature is still too high to see the Néel state
- How low do we have to cool?
- Which entropy per particle $S/N$ do we need at the Néel temperature?
Dynamical mean field theory

- Lattice model

\[ H_{latt} = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} \]

- Quantum impurity model

\[ H_{imp} = U n_{\uparrow} n_{\downarrow} - \sum_{k,\sigma} (t_k c_{\sigma}^\dagger a_{k,\sigma}^{bath} + h.c.) + H_{bath} \]
Cluster versions of DMFT: DCA

- DMFT: momentum independent self energy
- Cluster DMFT methods: approximate momentum-dependence of the self-energy

\[
\Sigma(p, \omega) = \sum_a \phi_a(p) \Sigma_a(\omega)
\]

- Dynamical cluster approximation (DCA): ``tiling’’ of the Brillouin zone

- Becomes exact upon extrapolation in cluster size
Extrapolation of DCA results

- Reliable extrapolation of DCA
  - Large clusters are needed since there is structure in momentum space!

S. Fuchs et al., arXiv:1009.2759
E. Gull et al., arXiv:1010.3690
DCA results

- Full thermodynamic data available for $U/t \leq 12$, $T \geq T_N$
  - energy
  - entropy
  - density
  - free energy
  - double occupancy
  - nearest neighbor spin correlation

- Numerical data included in auxiliary material of arXiv:1009.2759

- Can be used for validation and thermometry of fermionic experiments down to lower temperature
Entropy in a trap

- Homogeneous system: \( s_N \approx 0.41(3) \)
- Trap captures entropy in metallic shell: \( s_N \approx 0.65(6) \) is sufficient!
- It will be a bit easier to reach the Néel state in a trap!
Spin correlation thermometry

- The nearest neighbor spin correlation is very sensitive to temperature close to TN and an ideal thermometer.
Summary: ab-initio simulation of experiments

- We can perform controlled *ab-initio* simulations of current optical lattice experiments
  - validation of quantum simulators (Bose Hubbard model)
  - thermometry (fermions and bosons)

- We can test proposals, e.g. thermometry schemes
- Look forward to the next milestones: Néel state in 3D fermions
What have we learned for experiments?

- Quantum simulations using cold atoms work
- Transition temperatures can be determined
- Big challenges are ahead
  - Better calibration of atom numbers, lattice depths
  - Substantial heating is a problem for further cooling