Miniworkshop on Strong Correlations in Materials and Atom Traps

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Fermions in optical lattices: Mott transition and tetastable superconductivity

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Mott transition in optical lattices and metastable superconductivity

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experiments: group of I. Bloch, U. Schneider

- Mott transition of trapped atoms in an optical lattice
- Dynamical mean field theory for inhomogeneous system
- Metastable s-wave superconductivity in the repulsive Hubbard model
Mott transition

Mott transition in solids:

Hubbard model

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

kinetic energy \( \iff \) interactions

1 electron per unit cell: **metal** for \( U \ll t \)

**Mott insulator** for \( U \gg t \)

Sir Nevill Francis Mott
1905-1996
Mott transition

Mott insulator: localized electrons $\rightarrow$ localized spins

Effective spins-spin coupling $J \approx t^2/U$

typically: antiferromagnetic order at low $T$
Mott transition in optical lattices and metastable superconductivity

Example \((V_{1-x}Cr_x)_2O_3\)

but: **not** described by Hubbard model orbitals, crystal fields, long-range interactions, ...
(e.g. Poterayev, ..., A. Lichtenstein, *et al.* 2007)

diagram:

- Mott Insulator
- Strongly correlated metal
- Antiferromagnetic Insulator

from Limelette *et al.* 03
Trapped atoms in optical lattices

- trap & cool atoms
- optical lattice from standing waves of laser effective potential
  \[ V(r) = \alpha(\omega)\langle E^2(r) \rangle \]
  \[ \propto \cos^2(kx) + \cos^2(ky) + \cos^2(kz) \]
- sufficiently high laser intensity:
  - only nearest neighbor hopping
  - only local interactions
  \[ \Rightarrow \text{perfect realization of Hubbard model} \]
  in external parabolic potential (Jaksch et al. 98)
- all parameters (\( t, U \), parabolic potential) known and fully controllable !!
- bosons or fermions (or arbitrary mixtures)
Mott transition of bosons

\[ H = H_h + H_{\text{trap}} \]
\[ H_h = -t \sum_{\langle ij \rangle} b_i^\dagger b_j + U \sum_i n_i(n_i - 1) \]
\[ H_{\text{trap}} = \sum V_0 r_i^2 n_i \]

- **small** \( U \): bose condensation & superfluidity
- **large** \( U \): integer number of localized atom per site
  bosonic Mott insulator
- first realization: Greiner et al. 2002
Mott transition of bosons

- detecting Mott transition?
  detect Bose condensation:
  macroscopic occupation of $k=0$
  and reciprocal lattice vectors

- method: time-of-flight picture
  switch off all potentials and take picture after time $t$
  position: $r=p/m \, t$
  direct measurement of momentum distribution $n(p)$

- Mott insulator:
  localized in real space,
  delocalized in momentum space

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Mott transition of fermions

fermionic Mott transition in optical lattices
more fun: magnetism, superconductivity, ....

• problem 1: cooling (less scattering due to Pauli principle)
• problem 2: detection

experiments in progress:
  group of T. Esslinger (ETH) arXiv:0804.4009 talk next week
  group of I. Bloch (Mainz), ....

theory for inhomogeneous system (trapping potential) needed !
Mott transition of fermions

Theory for Mott transition?

- no symmetry breaking, no obvious order parameter

Method of choice: **dynamical mean field theory (DMFT)**

Only approximation of **DMFT**: self-energy purely **local**

\[ \Sigma_{ij}(\omega) \approx \delta_{ij} \Sigma_i(\omega) \]

Naturally generalizable to inhomogeneous systems

(Kotliar, Dobrosavljevic 97; Potthoff, Nolting 1999, Okamoto Millis 02, Freericks 04, Lee MacDonald 06)
Basics of **dynamical mean field theory**:

- idea of mean field theories:
  - pick single site and mimic interactions with other sites by coupling to "mean field" (e.g. effective B-field)
- **DMFT**: use as "mean field" the coupling to non-interacting fermions
- coupling depends on frequency
- N single-impurity problems coupled by self-consistency
  N=number of inequivalent sites
Methods: dynamical mean field theory

- dynamical mean field theory for inhomogeneous systems
- single particle physics and strong interactions
- works in strongly inelastic regime (not-so-cold atoms)
- heavily used for correlated electron systems (LDA+DMFT)
- heterostructure, nanostructures of strongly correlated systems “oxide electronics”

- critical fluctuations not captured in mean-field theory
- magnetism treated only on mean field level (or ignored)
Methods: dynamical mean field theory

- difficult: obtain self-energy of interacting impurity model
- here: numerical renormalization group (NRG) (R. Helmes and T. Costi)
- computationally expensive but easy to parallelize
Mott transition of trapped atoms in optical lattices

\[ H = H_h + H_{\text{trap}} \]

\[ H_h = -t \sum_{\langle ij \rangle, \sigma = \uparrow \downarrow} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

\[ H_{\text{trap}} = \sum V_0 R_i^2 n_i \]

~3000 atoms in cubic trap increasing $U$:
- atoms pushed out of center of trap
- plateaus formed for $U \gtrsim U_c$

How can Mott transition be detected?
Problem: Cooling of Fermions
Effects of large $T$?
What determines $T$?
Mott transition of trapped atoms in optical lattices

Time-of-flight experiment: switch off confining potential + optical lattice picture of expanding cloud = measurement of momentum distribution (projected on $k_x, k_y$ plane)

flat momentum distribution $\rightarrow$ localized in space $\rightarrow$ band or Mott insulator
Mott transition of trapped atoms in optical lattices

What happens at interface of metal and Mott insulator?

How does the metallic state penetrate into Mott insulator?

relevant for heterostructures, nanostructures,…

Kondo proximity effect
digression: Metal/Mott insulator interface

- most simple inhomogeneous situation: metal / Mott insulator interface
- How does metal penetrate into Mott insulator? How well insulating is a Mott insulator?
- Mott insulator: localized spins at surface: metal penetrates Mott insulator by Kondo effect \( \implies \) “Kondo proximity effect”
- proximity effect close to quantum critical point \( U \sim U_c \)
- ignore charge reconstruction (particle-hole symm.) and magnetism, vary only \( U \) across interface
Kondo effect

\[ H = H_{\text{kin}} + \mathbf{J} \vec{S} \cdot \sum_{\alpha\beta} c_0^\dagger \vec{\sigma}_{\alpha\beta} c_0 \beta \]

- resonant spin-flip scattering
- effective $\mathbf{J}$ grows logarithmically towards low energies
- spin is ‘absorbed’ in Fermi surface (confinement)
digression: Metal/Mott insulator interface

metal / quantum-critical Mott insulator interface

\[ U = U_c \]

\[ T = 1.14 \times 10^{-5} \text{ D} \]

Kondo effect

at \( T = 10^{-5} \text{ D} \): metal penetrates only 5 sites into Mott insulator only tiny (mean-field) critical regime
digression: Metal/Mott insulator interface

good metal / bad metal interface \( T = 0, \ U \lesssim U_c \)

![Graph showing quasiparticle weight scaling](image)

scaling of quasiparticle weight \( Z \) close to QCP:

\[
Z(U, T, x) \approx \frac{0.01}{x^2} f \left( \frac{x}{|U - U_c|^{1/2}}, \frac{T}{|U - U_c|} \right)
\]

- \( x \): distance from interface, \( f(0,0) = 1 \)
- mean field exponents: \( \nu = \frac{1}{2}, \ z = 2, \text{small prefactor!} \)
digression: Metal/Mott insulator interface

metal / Mott insulator interface

\[ T = 0, \quad U \gtrsim U_c \]

\[ 0.01/x^2 \text{ for } x < \xi \]

\[ \text{exponential decay for } x > \xi \]

numerical problems for extremely small \( Z \)
digression: Kondo proximity effect

main result of quantitative analysis:

- Kondo proximity effect (penetration of metal into Mott insulator) practically nonexistent

- prefactors ridiculously small: \( Z_x \sim \frac{0.01}{x^2} \)

- washed out by finite T or magnetism
back to trapped atoms:

problem 1: cooling of Fermions
problem 2: detection of Mott transition
Mott transition of trapped atoms in optical lattices

- detecting Mott insulator: look for incompressible state
- measure radius of cloud varying confining potential (I. Bloch)
- important: fixed entropy $S$
- surprising: Mott plateau even visible for $\frac{S}{N} \gtrsim 2 \ln 2$, $T_{\text{initial}} \gtrsim 0.15 \epsilon_F$
- impossible for homogeneous system ($S < \ln 2$ for $T < U$)

Calculation: DMFT using Thomas Fermi approx.

Mott transition in optical lattices and metastable superconductivity Trieste 08
Mott transition of trapped atoms in optical lattices

- Evolution of temperature upon **adiabatically** compressing trap
  - strong heating but also cooling by spin-entropy of Mott insulator
    (Pomeranchuk 1950, Werner et al. 95, Koetsier et al. 07 homogeneous system)
  - present experiments: entropy/particle >> ln(2)
    Mott insulator visible only because of configurational entropy of diluted metallic belt

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Image: Diagram showing the relationship between temperature and entropy in the context of Mott transition.
Mott transition of trapped atoms in optical lattices

- preliminary experimental results: U. Schneider, I. Bloch et al. (2008)
- about $10^5$ $^{40}$K atoms in optical lattice, initial $T \sim 0.15 \ E_F$

preliminary experimental figure removed
- soon to be published
Metastable superconductivity

- Up to now: well known Mott physics in unusual context
- More fun: new **metastable** states of matter in Hubbard model for $U \gg t$

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

Lifetime of doubly occupied site for $U \gg t$?
Get rid of huge energy $U$: Create $O(U/t)$ excitations with energy $t$

**lifetime exponentially large**

\[ t_d \sim \exp(c(n)U/t) \]

Formal argument:
construct unitary transformation to remove all
processes changing number of doubly occupied sites
to arbitrarily high order in $t/U$
(Schrieffer Wolff transformation)

**experiment:** Winkler *et al.* (2006)
Metastable superconductivity

Include again trapping potential \( H_{\text{trap}} = \sum V_0 r_i^2 n_i \)

large \( V_0 \) \( \rightarrow \) band insulator

reduce \( V_0 \) \( \mathbf{slowly} \) compared to \( 1/t \) or \( U/t^2 \)

but \( \mathbf{fast} \) compared to \( \frac{1}{t} \exp[cU/t] \)

Bose condensation of diluted doubly occupied sites

\( \mathbf{s-wave superconductivity} \) in strongly repulsive Hubbard model!
Metastable superconductivity

possible alternative: **phase separation**! needed: **controlled** calculation.

Simple case: only doubly occupied and empty sites:

\[
H_{\text{eff}} = \frac{2t^2}{U} \sum_{\langle ij \rangle} (1 - n_{i\uparrow})(1 - n_{i\downarrow})n_{j\uparrow}n_{j\downarrow} + \frac{2t^2}{U} \sum_{\langle ij \rangle} c_{i\uparrow}c_{i\downarrow}c_{j\downarrow}c_{j\uparrow}
\]

Trick: rewrite as spin Hamiltonian:

\[
H_{\text{eff}} = -\frac{2t^2}{U} \sum_{\langle ij \rangle} S_i \cdot S_j
\]

ferromagnetic Heisenberg model
SU(2)-charge symmetry of \( m=0 \) Hubbard model

exact groundstates:
magnetization in +z direction: band insulator
magnetization in –z direction: no particles
magnetization in x/y direction: s-wave superconductivity with momentum \( p,p,p \),
\( (h–\text{paring}, \text{C.N. Yang 1989}) \)

uniform system with \( m=0 \): phase separation and superconductivity degenerate
Metastable superconductivity

with trapping and chemical potential:

\[ H_{\text{eff}} = -\frac{2t^2}{U} \sum_{\langle ij \rangle} S_i \cdot S_j + \sum_i (V_0 r_i^2 - \mu) S_i^z \]

fixed by initial state: number of doubly occupied size \( \sum (2S_i^z + 1) \)

variational solution in the 3d scaling limit: superconductivity

\[ V_0 \approx 20J/N^{4/3} \]
Metastable superconductivity

\[ \alpha = V_0 N_d^{4/3} \frac{U}{t^2} \]

large \( \alpha \): condensation only at domain wall
small \( \alpha \): superfluid fraction 100%
Metastable superconductivity

ferromagnet: quadratic dispersion of Goldstone modes

no superfluid ~ BEC of non-interacting bosons

tiny particle hole symmetry breaking terms either induce repulsive or attractive forces can affect phase diagram drastically

uniform system
In thermodyn. Limit

t' > 0 in optical lattices

for \( t' > t \), \( t/(12U) \)
superfluid phase with finite stiffness stable

\[
E_{\text{eff}}[\hat{n}] \approx \int \frac{2t^2}{U} (\nabla \hat{n})^2 + V_0 r_i^2 \hat{n}^z - \frac{t'^2}{2U} \hat{n}^2_z - 6 \frac{t^2t'}{U^2} \hat{n}^3_z
\]
conclusions

- implementation of DMFT+NRG for inhomogeneous systems: domains and domains walls, heterostructures, disorder effects, trapped atoms …
- How does metal penetrate into a quantum critical Mott insulator? Almost not! Prefactors small
- fermionic Mott transition of cold atoms: soon to be “discovered”
- High precision test of DMFT by experiments?
- metastable s-wave superconductivity stabilized by local repulsion

R. Helmes, T. Costi, A. Rosch, PRL 100, 056403 (2008)
A. Rosch, D. Rasch, B. Binz, 2008
Repulsively bound atom pairs in an optical lattice

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(Dated: 8 May 2006)

lifetime 700 ms probably restricted by scattering from lattice photons
Ginzburg-Landau style description

- close to $U_c$: only quasiparticle weight $Z$ relevant?
  - guess ‘Ginzburg Landau theory’ formulated with $Z$ only:
    (Zhang, Rosenberg, Kotliar 93; Potthoff, Nolting 99; Bulla, Potthoff 00)

$$Z'_x = \frac{3}{22} (Z_{x-1} + \frac{16}{3} Z_x + Z_{x+1})$$

- gradient term from 2nd moment of lattice Green’s function, Potthoff, Nolting 99

$$Z_x = Z'_x - \alpha \frac{U - U_c}{U_c} Z'_x - \beta Z'_x^2$$

- mass and interaction term

- reproduces DMFT exponents, 2 free parameters determined from
  $$Z = \frac{\alpha}{\beta} \frac{U - U_c}{U_c}, \quad Z_x = \frac{9\beta}{11x^2}$$ for $U = U_c$

- asymptotics analytically solvable, e.g.
  $$\xi = \sqrt{\frac{3}{22\alpha} \left( \frac{U - U_c}{U_c} \right)^{1/2}} \approx 0.09 \left( \frac{U - U_c}{U_c} \right)^{1/2}$$

- Does it fit in scaling regime? Probably not (non-trivial $\omega$ dependence not captured)
include both singly and doubly occupied sites:

assisted hopping of doubly occupied sites (bosonic field \(d\)):

\[
H = -t \sum_{\langle ij \rangle} \tilde{f}^\dagger_{i\sigma} \tilde{f}_{j\sigma} + d^\dagger_i \tilde{f}_{i\sigma} \tilde{f}_{j\sigma}^\dagger d_j + \text{constraint} + O\left(\frac{t^2}{U}\right)
\]

- \(T_c \sim t\) instead of \(t^2/U\)
- same SU(2) charge symmetry
- superconducting but with gapless Fermi surface
- use Gutzwiller