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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

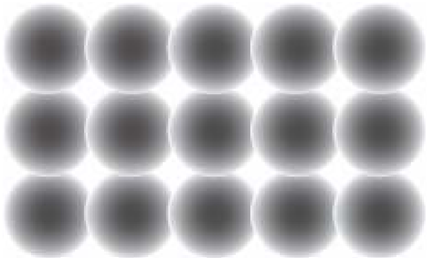
Rolf Helmes, David Rasch, Achim Rosch,
Institute for Theoretical Physics, University of Cologne
Theo Costi, Institute for Solid State Research, Research Centre Jülich

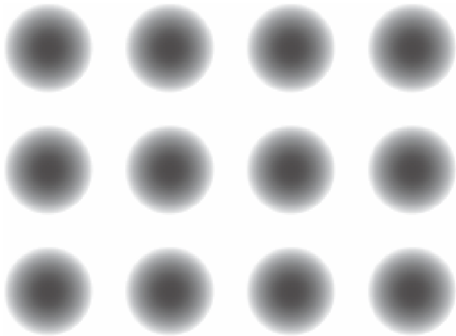
experiments: group of I. Bloch, U. Schneider

- 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:





Sir Nevill Francis Mott
1905-1996

Hubbard model

$$H = -\mathbf{t} \sum_{\langle ij \rangle, \sigma = \uparrow\downarrow} c^{\dagger}_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

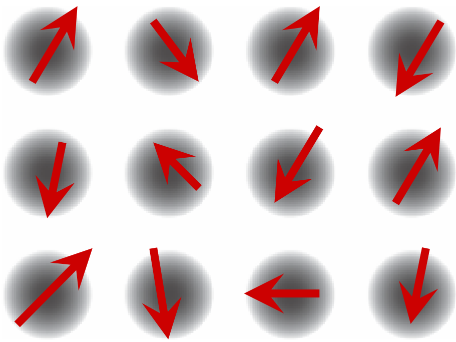
kinetic energy ⟺ **interactions**

1 electron per unit cell: **metal** for $\mathbf{U} \ll \mathbf{t}$

Mott insulator for $\mathbf{U} \gg \mathbf{t}$

Mott transition

Mott insulator: localized electrons ⇨ localized spins

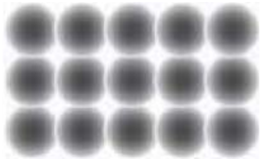


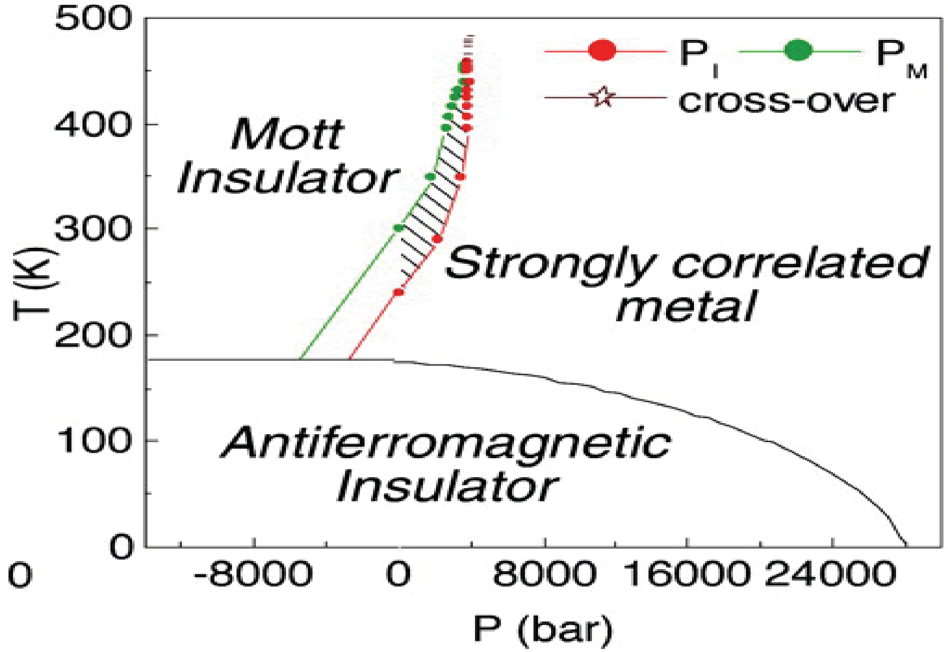
effective spins-spin coupling $J \approx \mathbf{t}^2/\mathbf{U}$

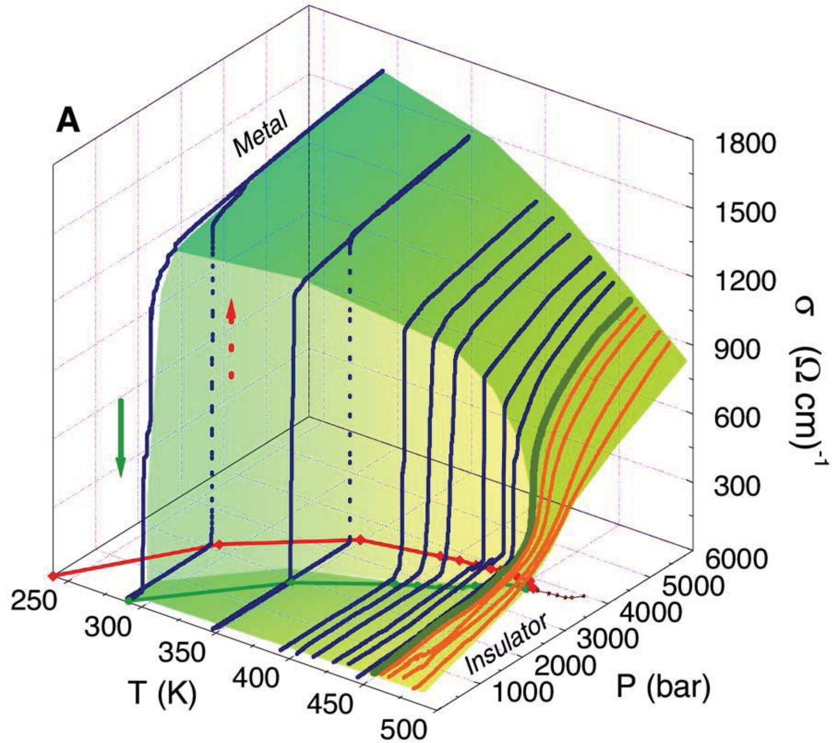
typically: antiferromagnetic order at low T

Mott transition

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





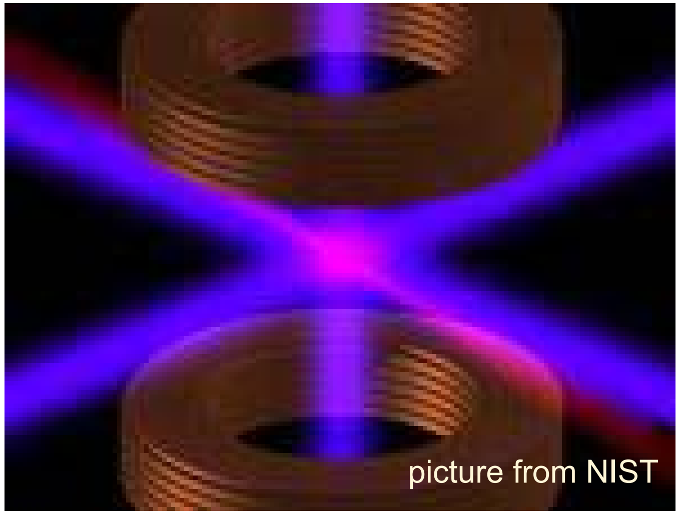


from Limelette *et al.* 03

but: **not** described by Hubbard model

orbitals, crystal fields, long-range interactions,.. (e.g. Poterayev, …,A. Lichtenstein, *et al.* 2007)

Trapped atoms in optical lattices



- trap & cool atoms
- optical lattice from standing waves of laser
  effective potential

$$\begin{aligned} V(r) &= \alpha(\omega)\langle E^2(r)\rangle \\ &\propto \cos^2(kx) + \cos^2(ky) + \cos^2(kz) \end{aligned}$$

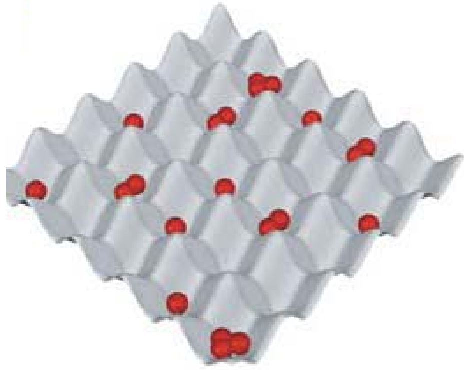
- sufficiently high laser intensity:
  - only nearest neighbor hopping
  - only local interactions
  ⇨ **perfect realization of Hubbard model**
  in external parabolic potential (Jaksch et al. 98)
- all parameters (t, U, parabolic potential) known and fully controllable !!
- bosons or fermions (or arbitrary mixtures)

Mott transition of bosons

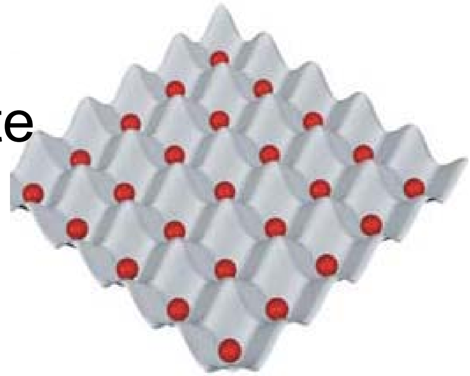
$$H = H_h + \mathbf{H}_{\rm trap}$$

$$H_h = -t \sum_{\langle ij \rangle} b_i^\dagger b_j + \mathbf{U} \sum_i n_i(n_i - 1)$$

$$\mathbf{H}_{\rm trap} = \sum \mathbf{V_0} r_i^2 n_i$$



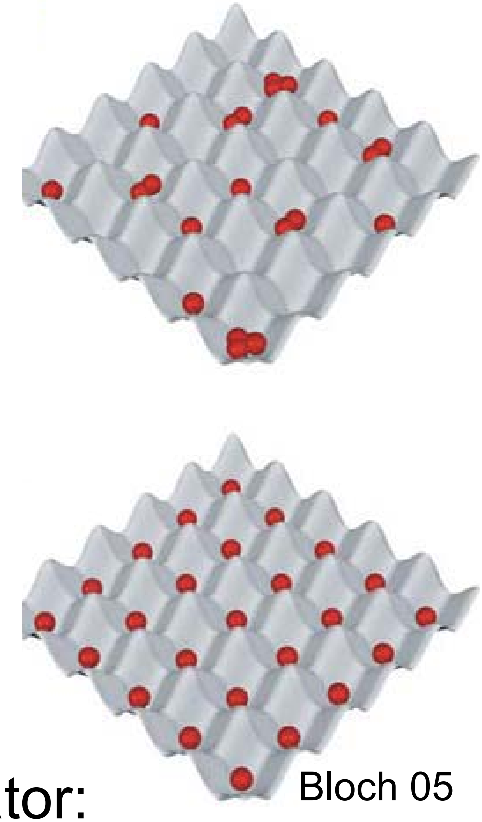
- **small *U*: *bose condensation & superfluidity***
- **large *U*:** integer number of localized atom per site
  bosonic Mott insulator
- first realization: Greiner et al. 2002

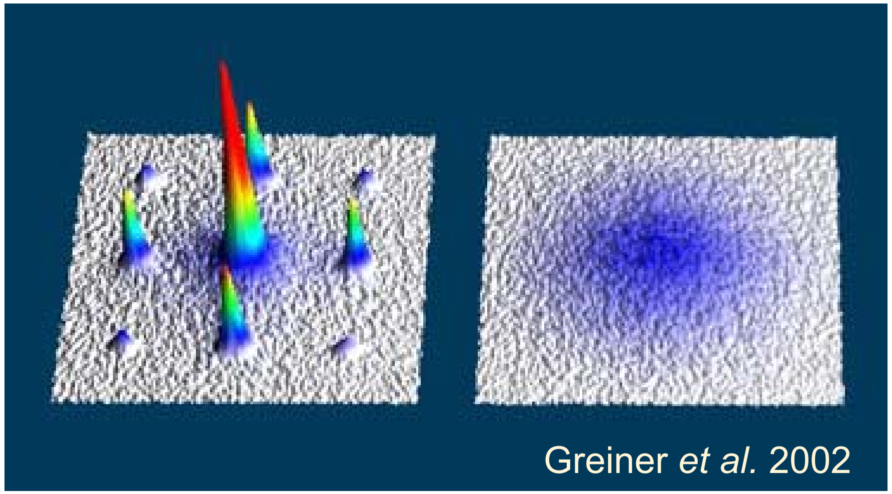


Bloch 05

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)


Bloch 05



superfluid Mott insulator

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

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**

$$\Sigma_{ij}(\omega) \approx \delta_{ij}\Sigma_i(\omega)$$

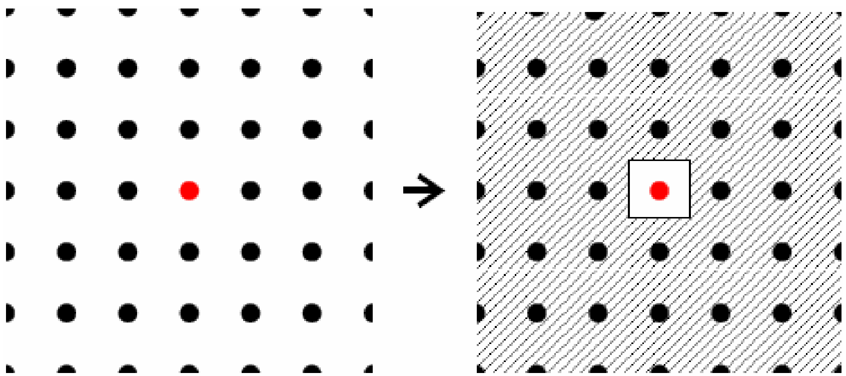
⇒ naturally generalizable to inhomogeneous systems

(Kotliar, Dobrosavljevic 97; Potthoff, Nolting 1999, Okamoto Millis 02, Freericks 04, Lee MacDonald 06)

Methods: dynamical mean field theory

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

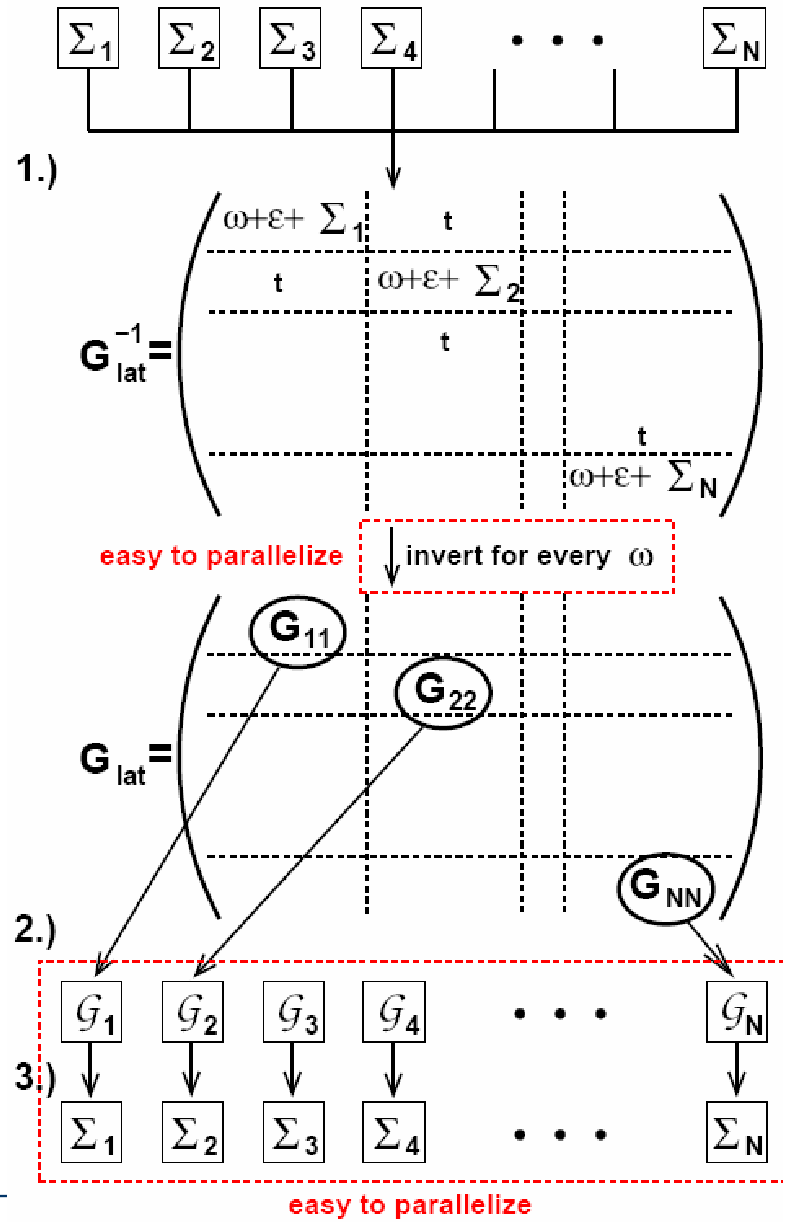
dynamical mean field theory for inhomogeneous systems

+ 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)

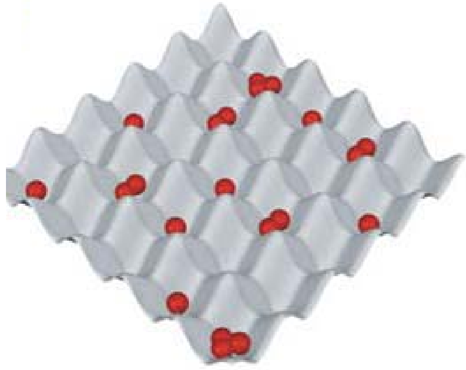
Methods: dynamical mean field theory

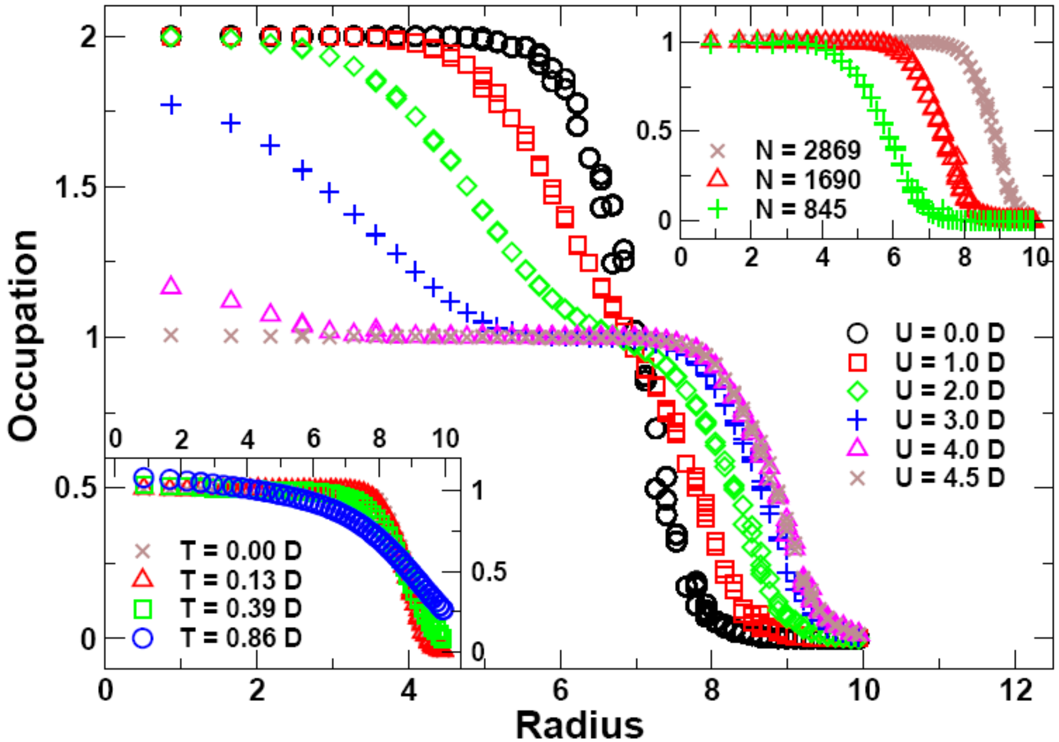
- difficult: obtain self-energy of interacting impurity model
- here:
  numerical renormalization group (**NRG**)
  (R. Helmes and T. Costi)
- computationally expensive but easy to parallelize



Mott transition of trapped atoms in optical lattices

$$H = H_h + \mathbf{H}_{\text{trap}}$$
$$H_h = -t \sum_{\langle ij\rangle,\sigma=\uparrow\downarrow} c^\dagger_{i\sigma} c_{i\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$$
$$\mathbf{H}_{\text{trap}} = \sum \mathbf{V_0} R_i^2 n_i$$



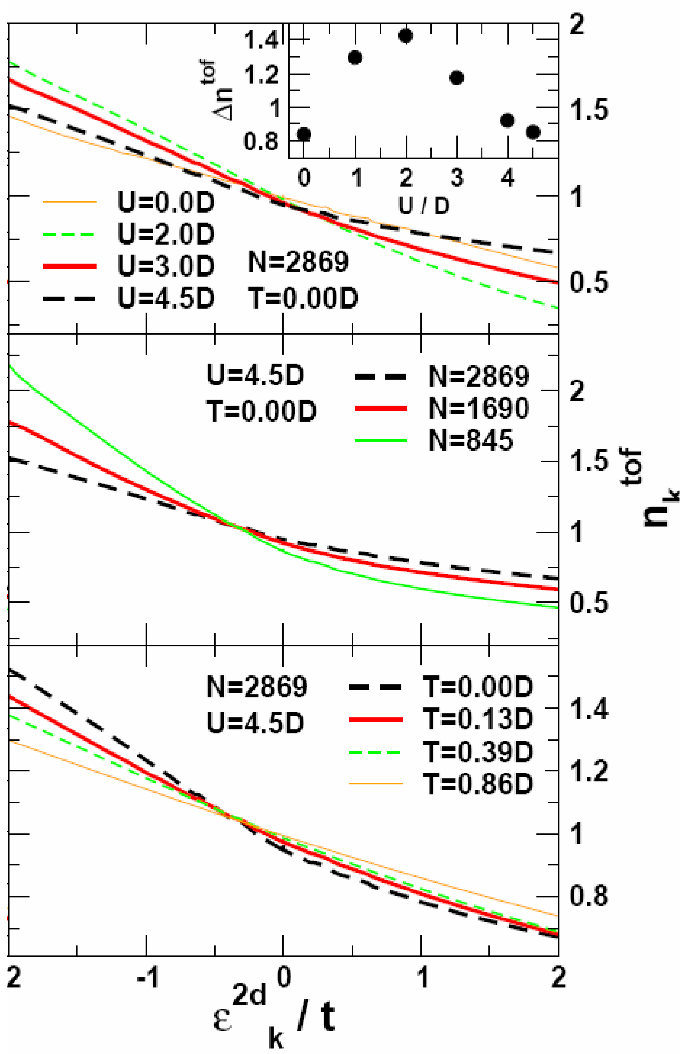


~3000 atoms in cubic trap increasing **U**:

- atoms pushed out of center of trap
- plateaus formed for $\mathbf{U} \gtrsim \mathbf{U_c}$

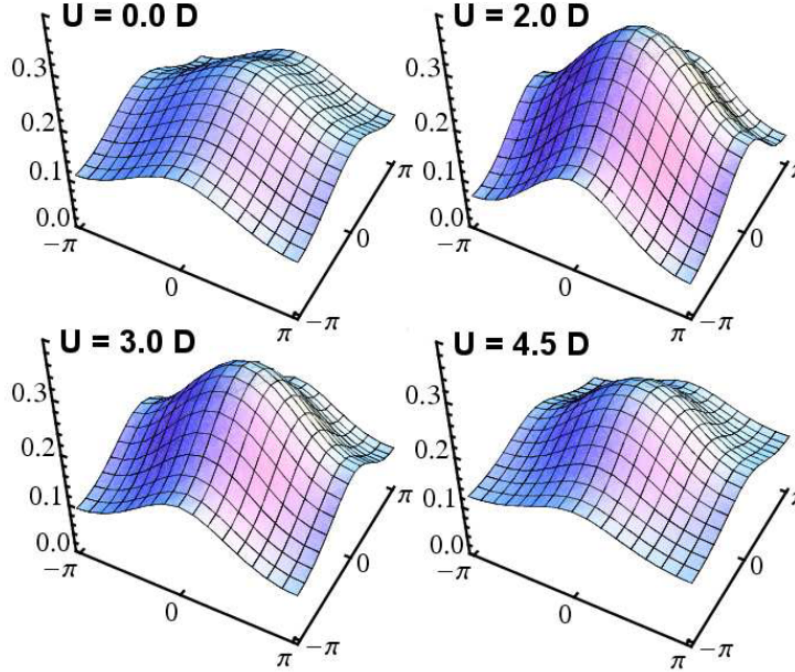
How can Mott transition be detected?
Problem: Cooling of Fermions
Effects of large T?
What determines T?

Mott transition of trapped atoms in optical lattices



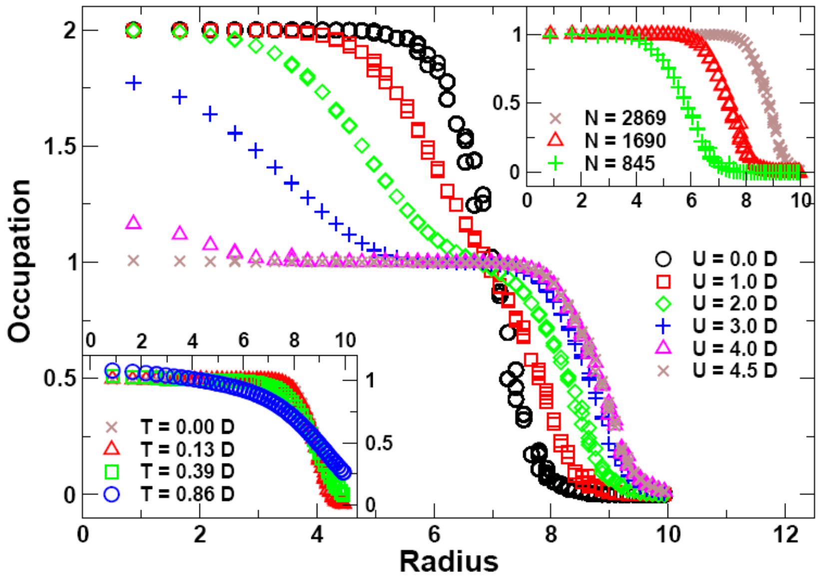
Time-of-flight experiment: switch off confining potential + optical lattice

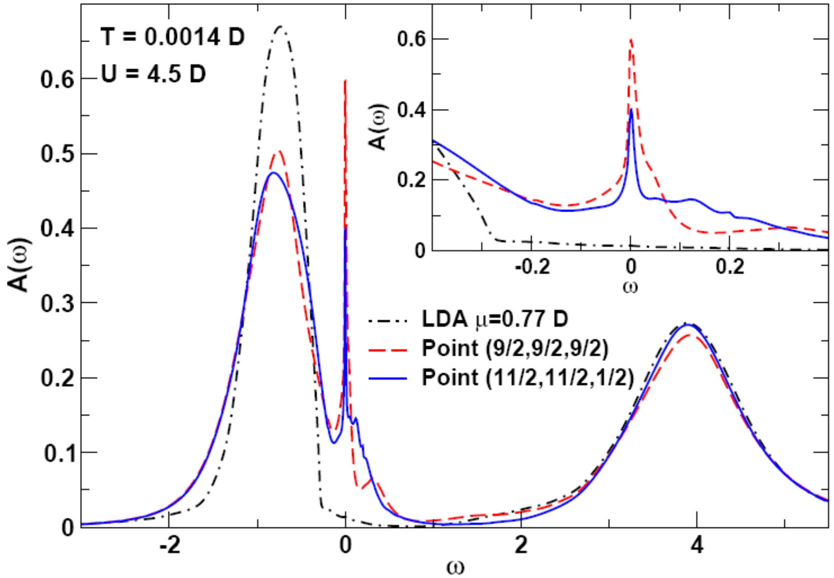
picture of expanding cloud = measurement of momentum distribution (projected on k_x,k_y plane)



flat momentum distribution ⇨ localized in space ⇨ band or Mott insulator

Mott transition of trapped atoms in optical lattices





What happens at interface of metal and Mott insulator?

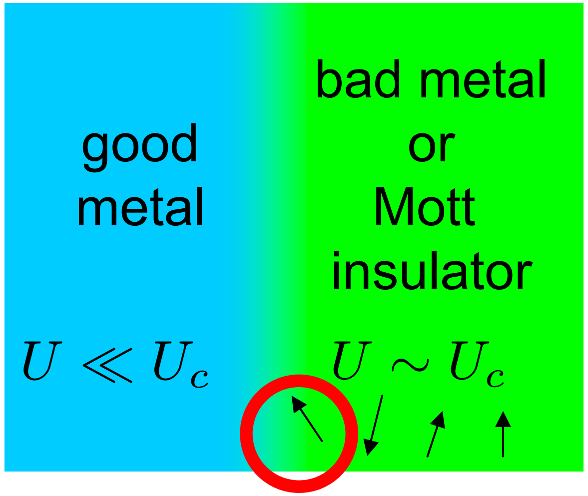
How does the metallic state penetrate into Mott insulator?

relevant for heterostructures, nanostructures,…

Kondo proximity effect

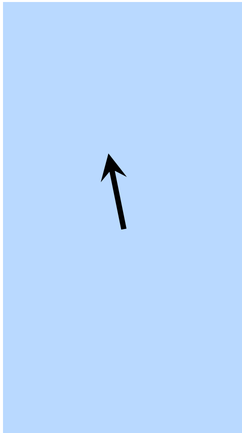
digression: Metal/Mott insulator interface

- 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** ⇨ **"Kondo proximity effect"**
- proximity effect close to **quantum critical point** $\mathbf{U \sim U_c}$
- ignore charge reconstruction (particle-hole symm.) and magnetism, vary only **U** across interface



Kondo effect

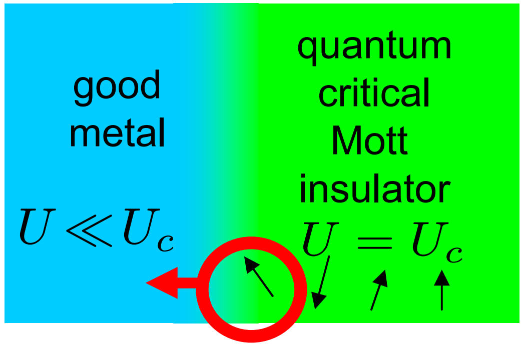
$$H = H_{\text{kin}} + \mathbf{J}\vec{S} \cdot \sum_{\alpha\beta} c^{\dagger}_{0\alpha} \vec{\sigma}_{\alpha\beta} c_{0\beta}$$

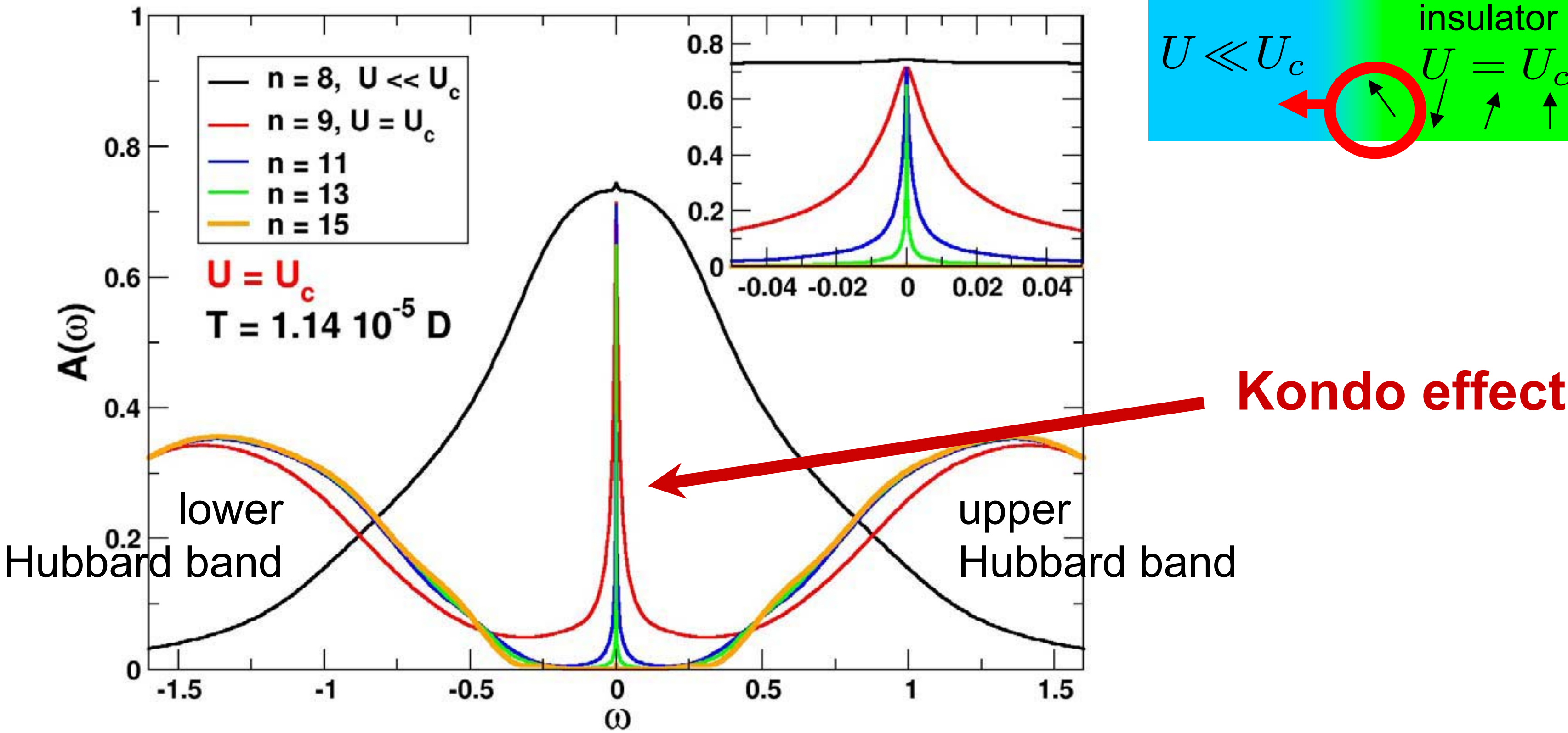


- resonant spin-flip scattering 
- effective **J** grows logarithmically towards low energies
- spin is 'absorbed' in Fermi surface (confinement)

digression: Metal/Mott insulator interface

metal / quantum-critical Mott insulator interface



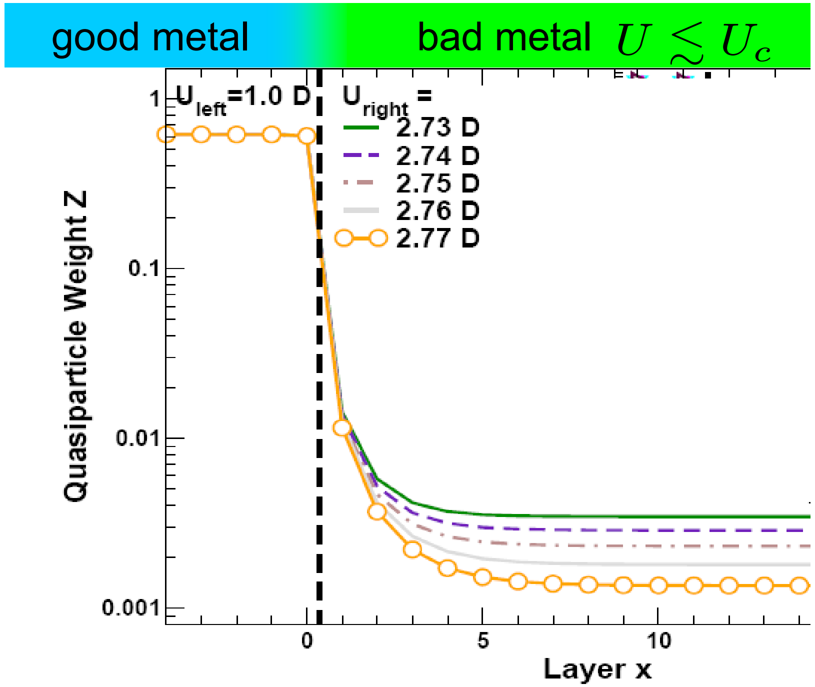


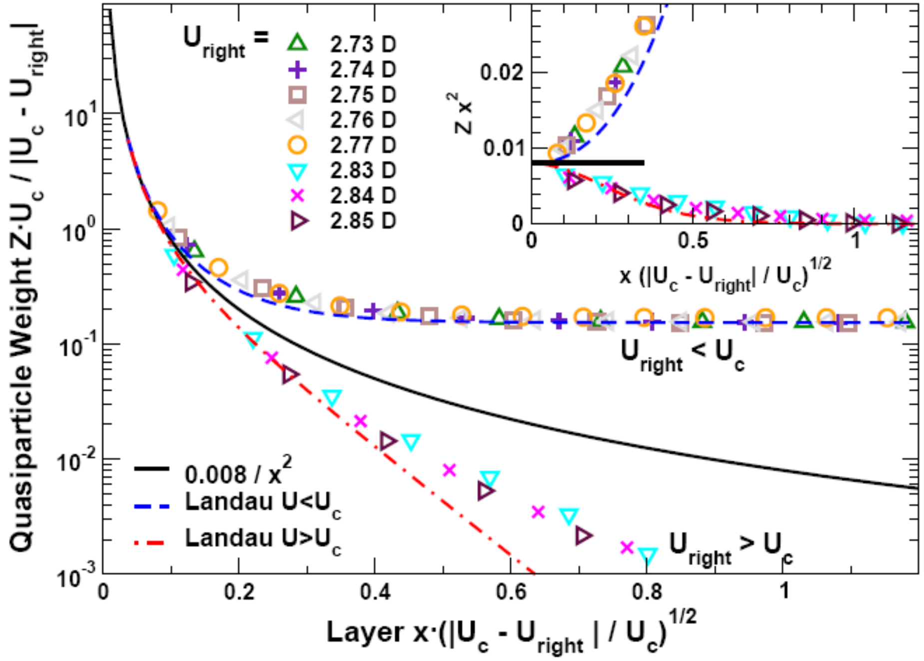
at T = 10^{-5} D: metal penetrates only 5 sites into Mott insulator

only **tiny** (mean-field) critical regime

digression: Metal/Mott insulator interface

good metal / bad metal interface $T = 0, \quad \mathbf{U} \lesssim \mathbf{U_c}$





scaling of quasiparticle weight **Z** close to QCP:

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

x: distance from interface, f(0,0)=1

mean field exponents: ν = ½, **z** = 2, **small** prefactor!

digression: Metal/Mott insulator interface

metal / Mott insulator interface

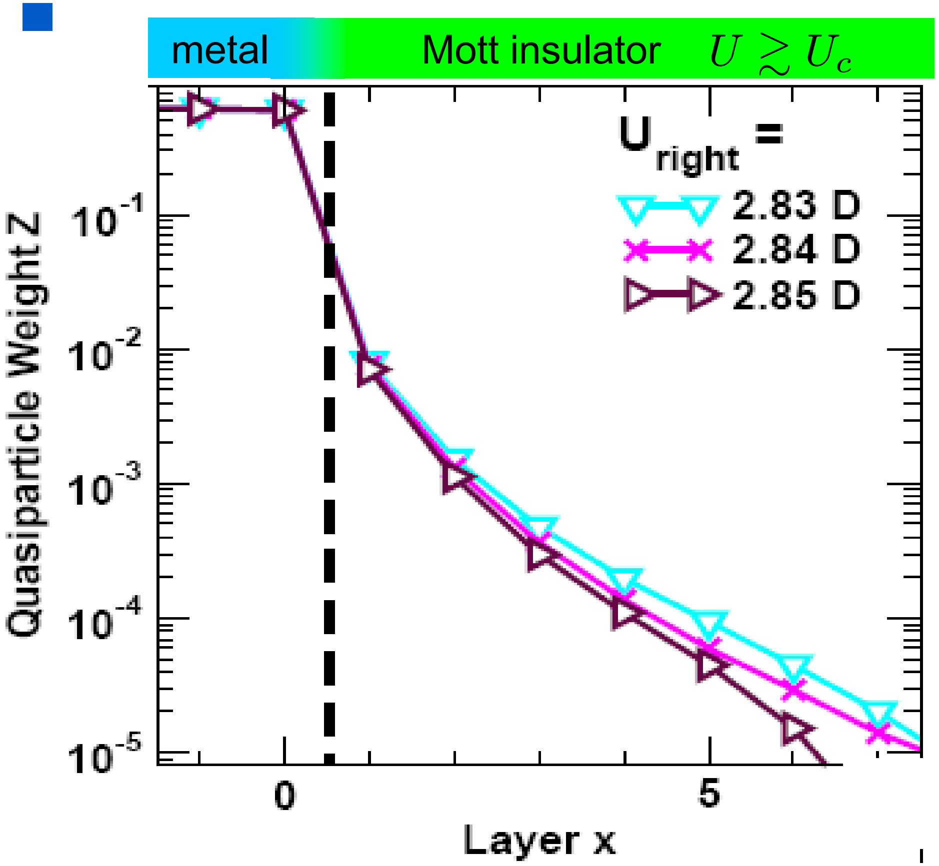
$T = 0, \quad \mathbf{U} \gtrsim \mathbf{U_c}$

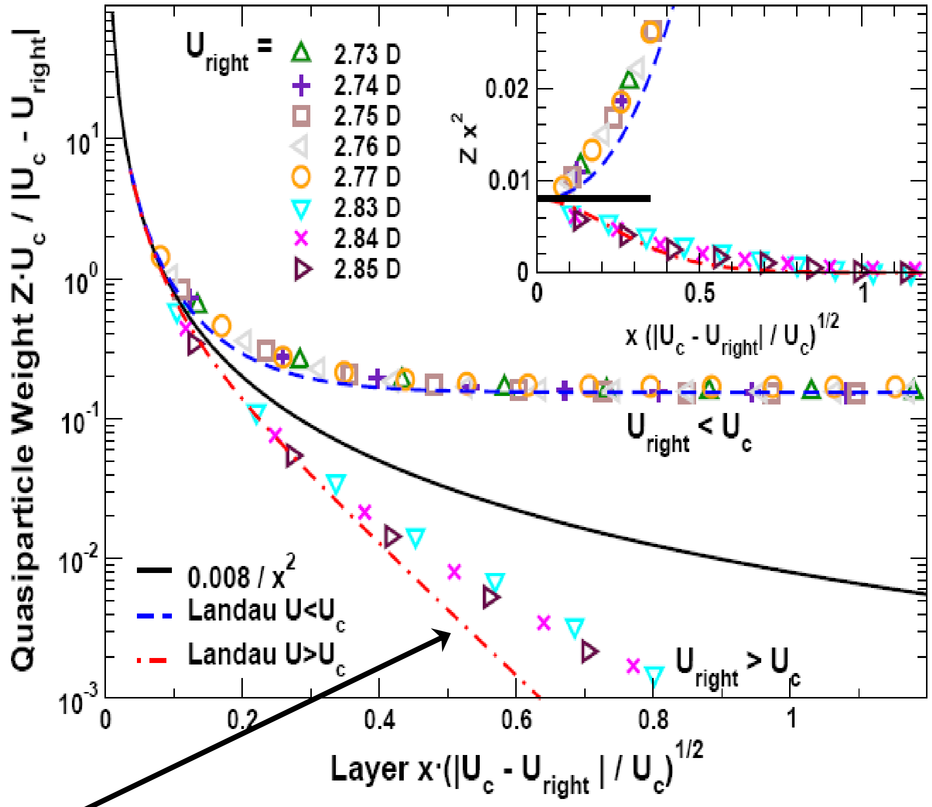
$0.01/\mathbf{x}^2$ for

for $\mathbf{x} < \xi$

exponential decay

for $\mathbf{x} > \xi$





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: $\mathbf{Z_x} \sim \frac{0.01}{x^2}$
- washed out by finite T or magnetism

Kondo proximity effect

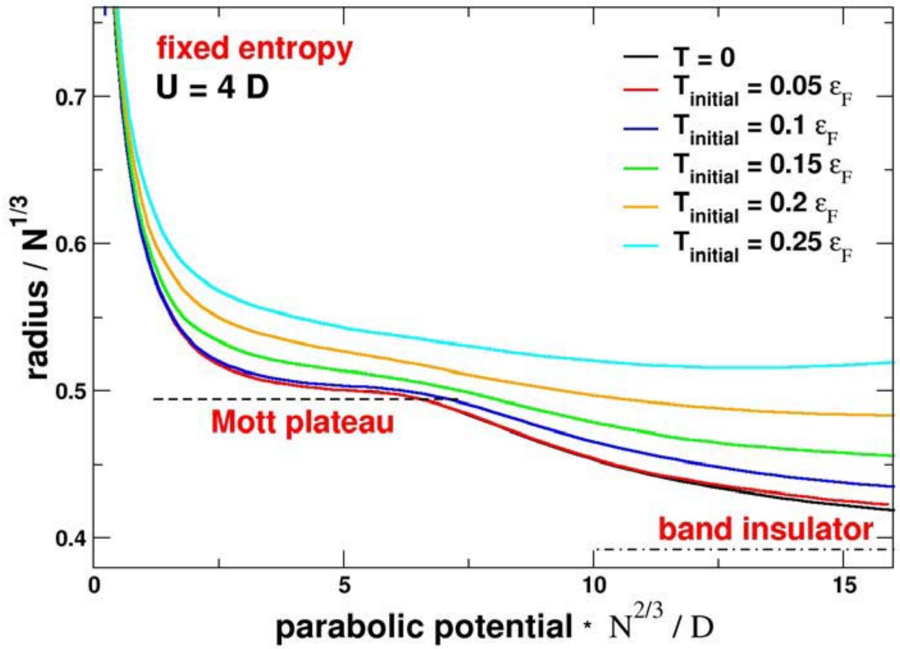
back to trapped atoms:

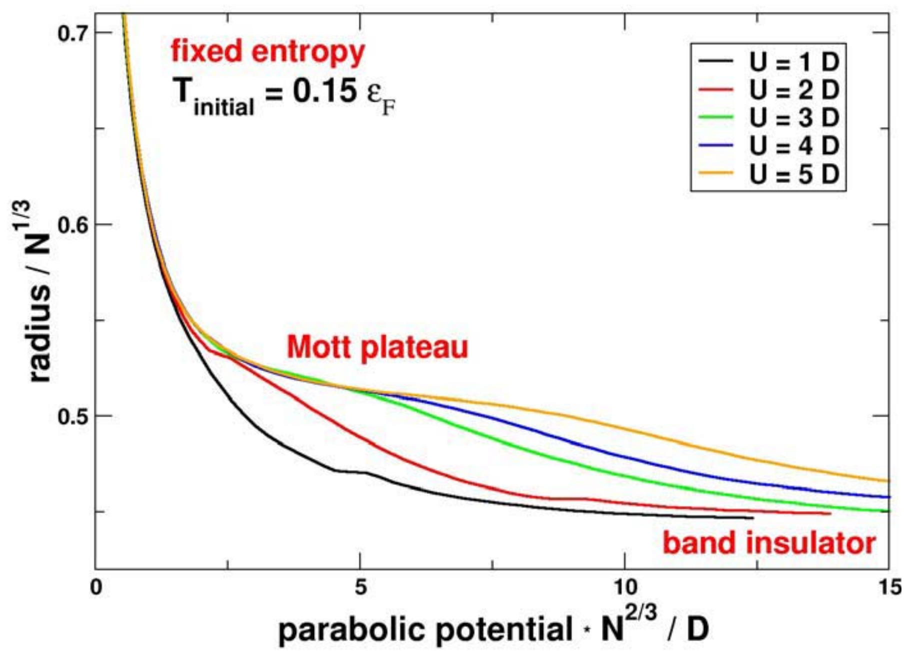
problem 1: cooling of Fermions

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)



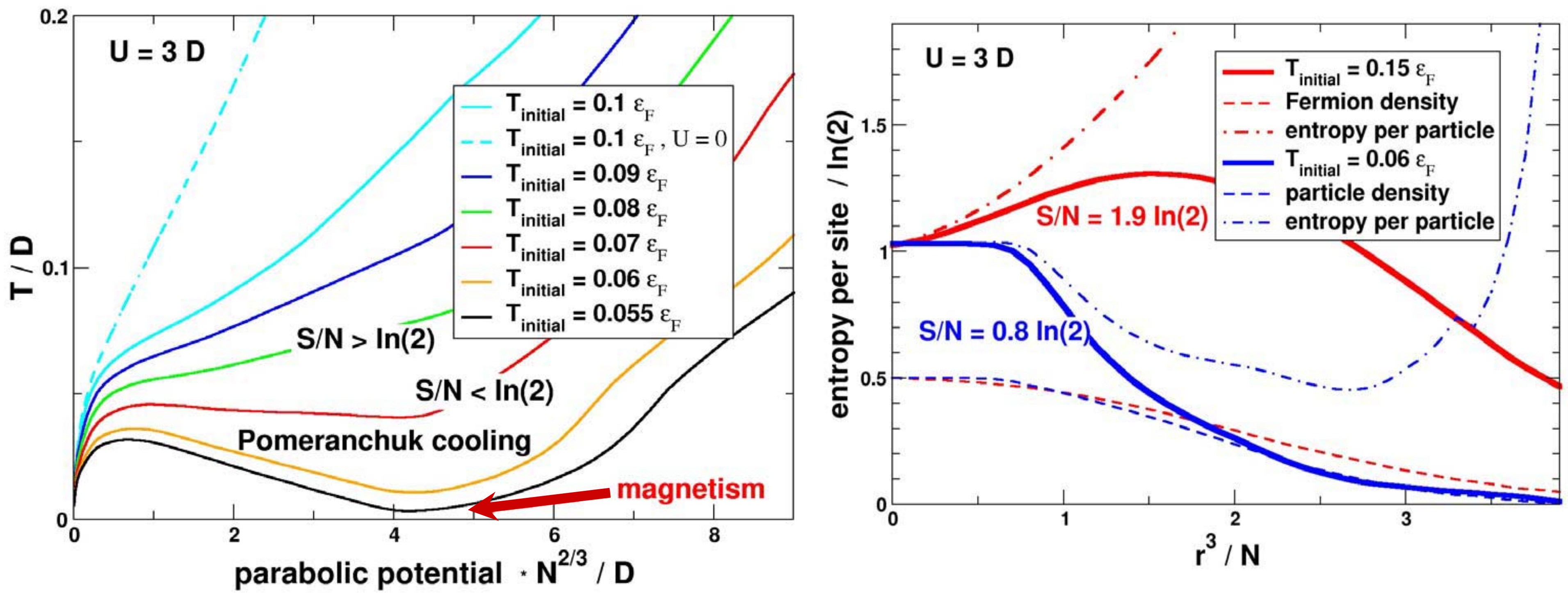


Calculation: DMFT using Thomas Fermi approx.

Mott transition 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



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

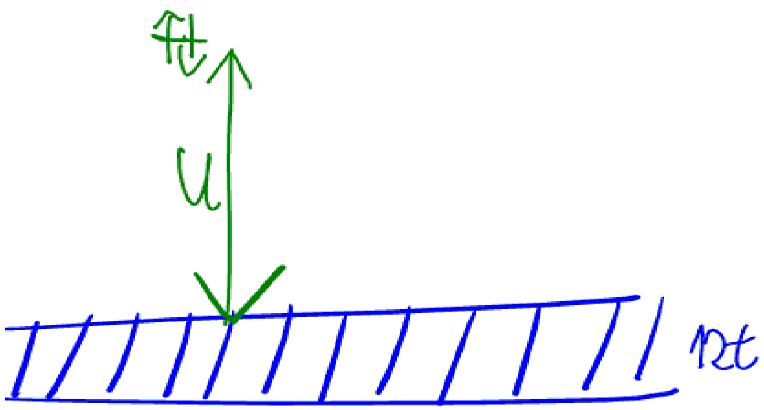
Metastable superconductivity

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

$$H_h = -t \sum_{\langle ij \rangle, \sigma = \uparrow\downarrow} c^\dagger_{i\sigma} c_{j\sigma} + \mathbf{U} \sum_i n_{i\uparrow} n_{i\downarrow}$$

Lifetime of doubly occupied site for $\mathbf{U} \gg t$?

Get rid of huge energy $\mathbf{U}$: Create O($\mathbf{U}/t$) excitations with energy ***t***



lifetime **exponentially** large

$$t_d \sim \exp(c(n)\mathbf{U}/t)$$

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

experiment: Winkler *et al.* (2006)

Metastable superconductivity

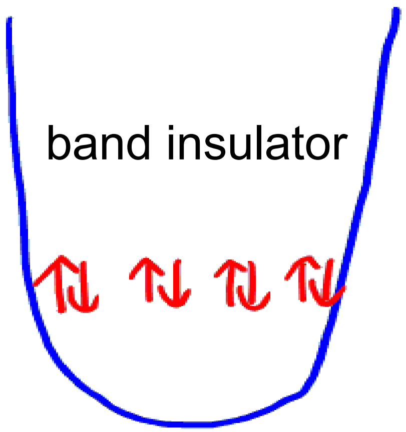
Include again trapping potential $\mathbf{H}_{\text{trap}} = \sum \mathbf{V_0} r_i^2 n_i$

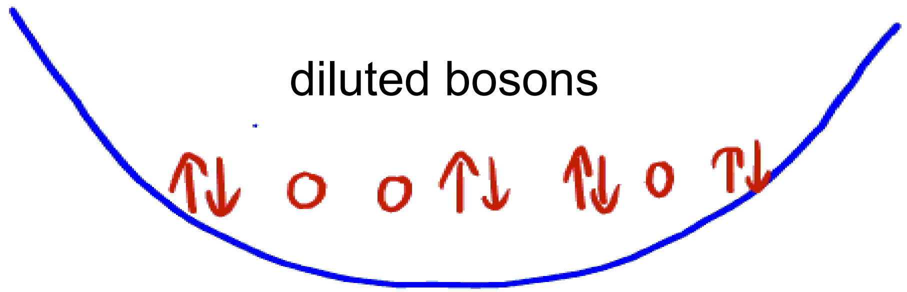
large $\mathbf{V_0}$ ⇨ band insulator

reduce $\mathbf{V_0}$ **slowly** compared

to $1/t$ or $\mathbf{U}/t^2$

but **fast** compared to $\frac{1}{t}\exp[c\mathbf{U}/t]$





Bose condensation of diluted doubly occupied sites

⇨ **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:

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

Trick: rewrite as spin Hamiltonian: $\downarrow$ empty site

$\uparrow$ doubly occupied site

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

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 –paring, C.N. Yang 1989)

uniform system with m=0: phase separation and superconductivity degenerate

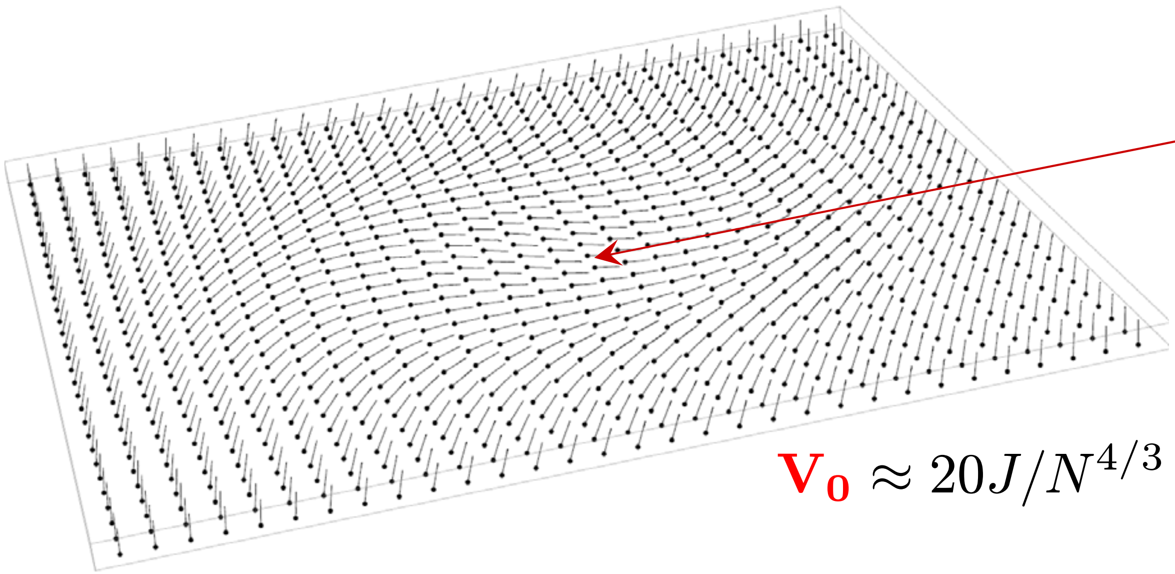
Metastable superconductivity

- with trapping and chemical potential:

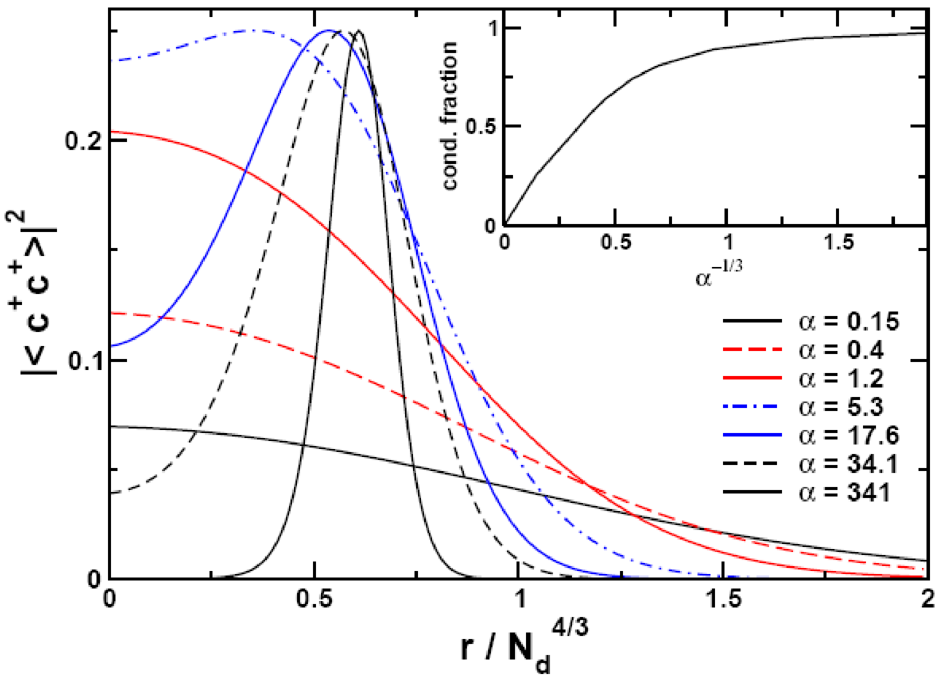
$$H_{\text{eff}} = -\frac{2t^2}{\mathbf{U}}\sum_{\langle ij\rangle}\mathbf{S_i}\cdot\mathbf{S_j} + \sum_i(\mathbf{V_0}r_i^2-\mu)S_i^z$$

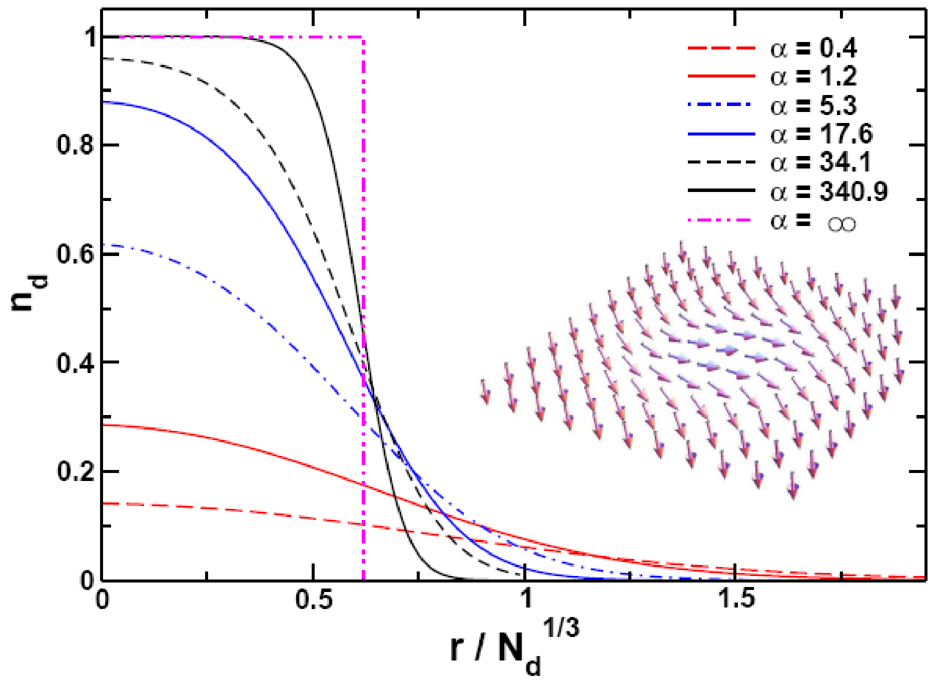
- fixed by initial state: number of doubly occupied size $\sum(2S_i^z+1)$

variational solution in the 3d scaling limit: **superconductivity**



Metastable superconductivity





$$\alpha = \mathbf{V_0} N_d^{4/3} \mathbf{U} / t^2$$

large α: condensation only at domain wall
small α: superfluid fraction 100%

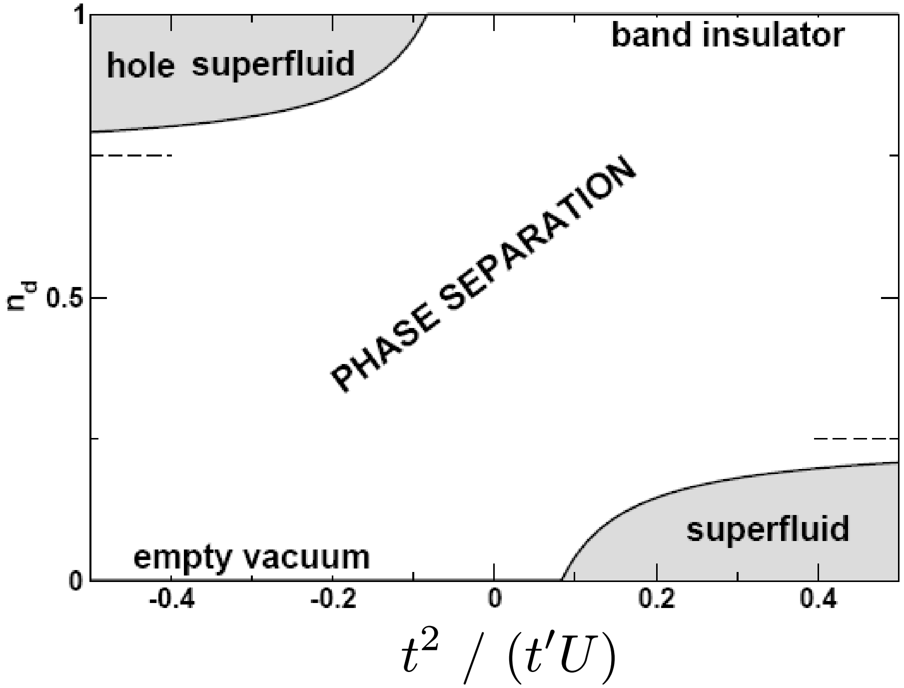
Metastable superconductivity

- 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/(12 U)
superfluid phase with finite stiffness stable



$$E_{\rm eff}[\hat n] \approx \int \frac{2t^2}{\mathbf{U}}(\nabla \hat n)^2 + \mathbf{V_0} r_i^2 \hat n^z - \frac{\mathbf{t'}^2}{2\mathbf{U}}\hat n_z^2 - 6\frac{t^2\mathbf{t'}}{\mathbf{U}^2}\hat n_z^3$$

conclusions

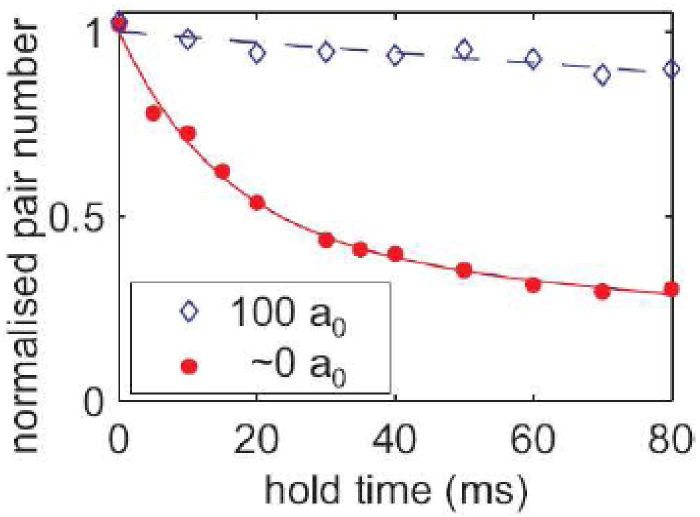
- implementation of DMFT+NRG for inhomogeneous systems: domains and domains walls, heterostructures, disorder effects, trapped atoms …
- How does metal penetrate into a quantum critical Mott insulator? Almost not! Prefactors small
- fermionic Mott transition of cold atoms: soon to be “discovered”
- High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

R. Helmes, T. Costi, A. Rosch, PRL **100,** 056403 (2008)
R. Helmes, T. Costi, A. Rosch, arXiv:0805.0566, PRL (2008)
A. Rosch, D. Rasch, B. Binz, 2008

Repulsively bound atom pairs in an optical lattice

K. Winkler, G. Thalhammer, F. Lang, R. Grimm[1], and J. Hecker Denschlag
Institute for Experimental Physics, University of Innsbruck, A-6020 Innsbruck, Austria and
[1] *Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria*

A. J. Daley, A. Kantian, H. P. Büchler, and P. Zoller
Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria and
Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria
(Dated: 8 May 2006)



lifetime 700 ms probably restricted by scattering from lattice photons

Ginzburg-Ladau style description

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

$$\mathbf{Z}'_{\mathbf{x}} = \frac{3}{22}\left(\mathbf{Z}_{\mathbf{x-1}} + \frac{16}{3}\mathbf{Z}_{\mathbf{x}} + \mathbf{Z}_{\mathbf{x+1}}\right)$$

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

$$\mathbf{Z}_{\mathbf{x}} = \mathbf{Z}'_{\mathbf{x}} - \alpha\frac{\mathbf{U}-\mathbf{U}_{\mathbf{c}}}{\mathbf{U}_{\mathbf{c}}}\mathbf{Z}'_{\mathbf{x}} - \beta\mathbf{Z}'^{\,2}_{\mathbf{x}}$$

mass and interaction term

- reproduces DMFT exponents, 2 free parameters α, β
  determined from $\mathbf{Z} = \frac{\alpha}{\beta}\frac{\mathbf{U}-\mathbf{U}_{\mathbf{c}}}{\mathbf{U}_{\mathbf{c}}}$, $\mathbf{Z}_{\mathbf{x}} = \frac{9\beta}{11x^2}$ for $\mathbf{U} = \mathbf{U}_{\mathbf{c}}$

- asymptotics analytically solvable, e.g.

$$\xi = \sqrt{\frac{3}{22\alpha}}\left(\frac{\mathbf{U}-\mathbf{U}_{\mathbf{c}}}{\mathbf{U}_{\mathbf{c}}}\right)^{1/2} \approx 0.09\left(\frac{\mathbf{U}-\mathbf{U}_{\mathbf{c}}}{\mathbf{U}_{\mathbf{c}}}\right)^{1/2}$$

- Does it fit in scaling regime? Probably not (non-trivial ω dependence not captured)

Metastable superconductivity

include both singly and doubly occupied sites:
assisted hopping of doubly occupied sites (bosonic field d):

$$H = -t \sum_{\langle ij \rangle} \tilde{f}_{i\sigma}^{\dagger} \tilde{f}_{j\sigma} + d_i^{\dagger} \tilde{f}_{i\sigma} \tilde{f}_{j\sigma}^{\dagger} d_j + \mathrm{constraint} + O(\frac{t^2}{\mathbf{U}})$$

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