



# ■ Fermionic atoms in optical lattices: Mott transition ■ and metastable superconductivity

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  - Theo Costi
  - Institute for Solid State Research, Research Centre Jülich
- experiments:  
U. Schneider, L. Hackermüller, S. Will, Th. Best, I. Bloch  
University of Mainz

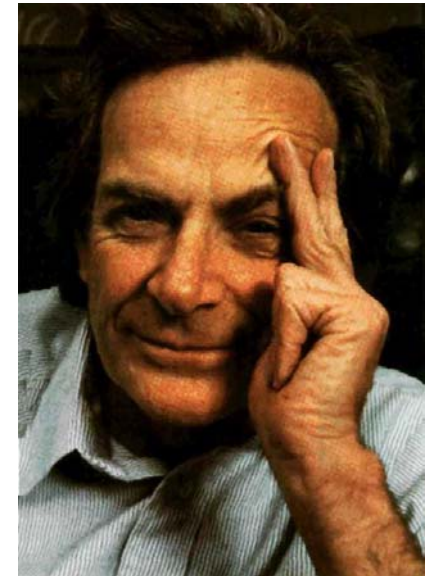
- Cold atoms as quantum simulators for solid state systems: Mott transition
- New physics out of equilibrium: exotic metastable superconductivity

## Quantum simulations for higher $T_c$ ?



best: universal quantum computers

- more efficient to solve classical problems (prime number factorization, searches, ...)
- useful to simulate **other** quantum systems (Feynman 1981)



more modest goal (while waiting...):

- simulate quantum system A (e.g. **higher- $T_c$**  superconductors) by quantum system B (e.g. cold atoms)
- useful if system B offers:
  - fewer complications (disorder, phonons, ...)
  - better control over parameters
  - other experimental probes
  - direct test of theories (!)
  - new physics (non-equilibrium)

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# Mott transition



Mott transition:

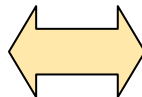


Sir Nevill Francis Mott  
1905-1996

Hubbard model

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

kinetic energy



interactions

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

**Mott insulator** for  $\mathbf{U} \gg \mathbf{J}$

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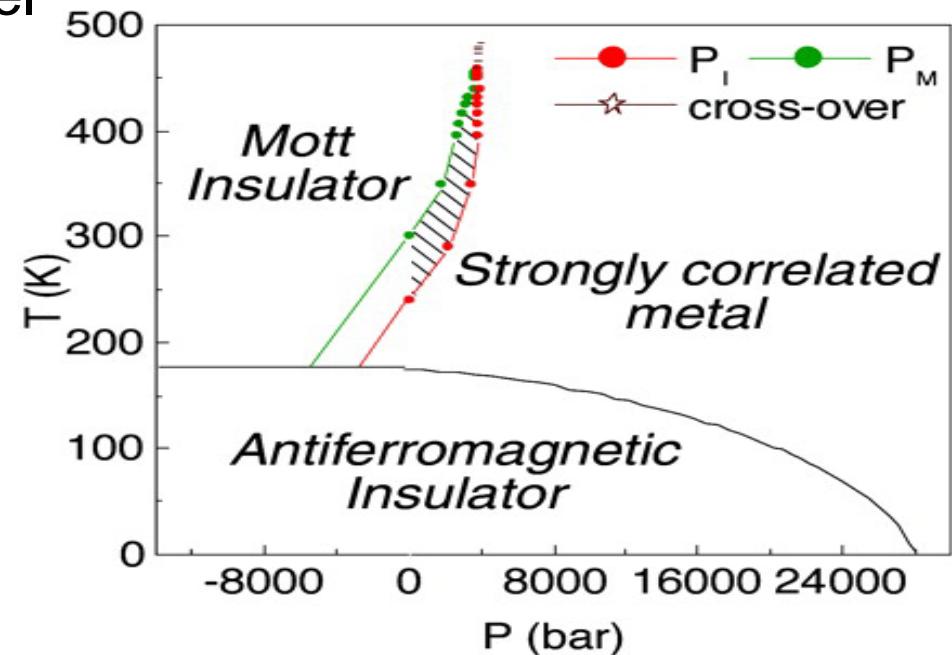
# Mott transition



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

but:

**not** described by Hubbard model  
orbitals, crystal fields, disorder  
**long-range interactions**



from Limelette *et al.* 03

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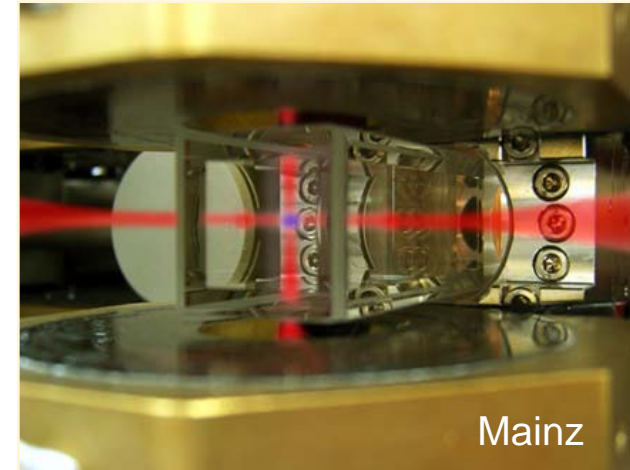
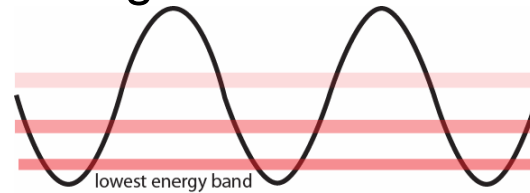
# trapped atoms in lattices made of light



- trap & cool atoms in lattice made of light
- 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

⇒ **perfect realization of Hubbard model**

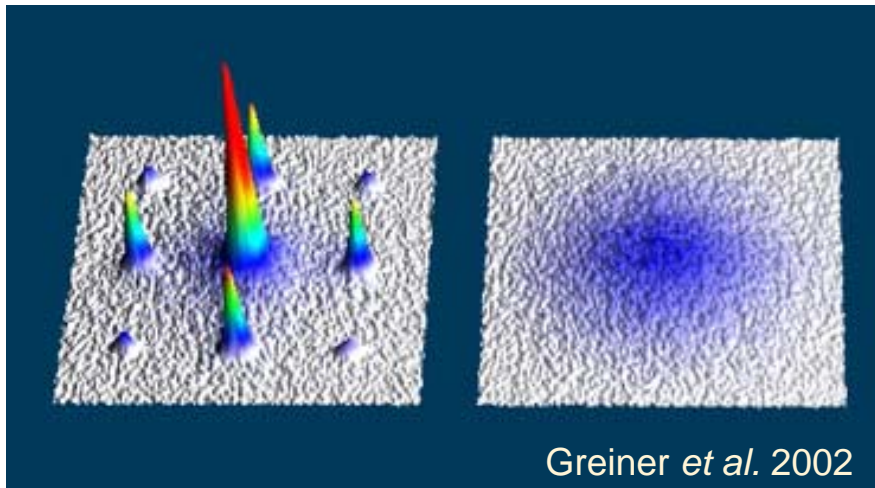
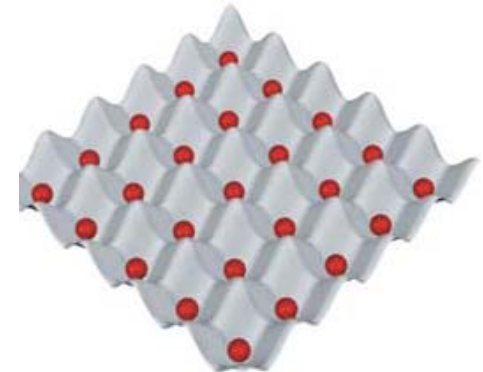
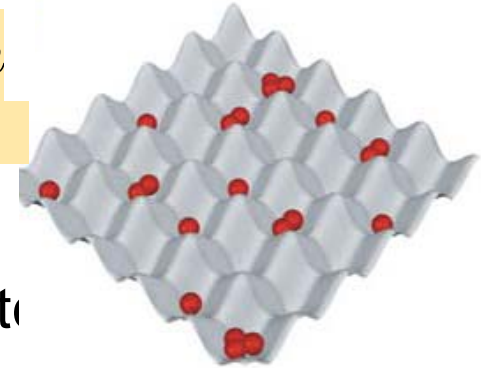
in external parabolic potential (Jaksch et al. 98)
- all parameters (**J**, **U**, parabolic potential) known and fully controllable !!
- bosons or fermions (or arbitrary mixtures)

# Mott transition of bosons



$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + U \sum_i n_i (n_i - 1) + \sum_i V_0 r_i^2 n_i$$

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



Greiner et al. 2002

superfluid

Mott insulator

- detections: **detect bose condensation!**

Bloch 05

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# Mott transition of fermions



- fermionic Mott transition in optical lattices
- more fun: magnetism, superconductivity, ...
- simulate materials
- - problem 1: cooling (less scattering due to Pauli principle)
  - problem 2: detection

experiments:

group of T. Esslinger (ETH)

R. Jördens, N. Strohmaier, K. Günter, H. Moritz, T. Esslinger, Nature 08

group of I. Bloch (Mainz)

U. Schneider, L. Hackermüller, S. Will, Th. Best,  
I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch,  
A. Rosch, Science 08

theory needed !

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# Mott transition of fermions



- Theory for Mott transition?
- no symmetry breaking, no obvious order parameter
- method of choice: **dynamical mean field theory (DMFT)**

heavily used, e.g. for ab-initio description of correlated materials  
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, Snoek Hofstetter 08,....)

mapping to N single-impurity problems coupled by self-consistency equation

solved using NRG

R. Helmes, T. Costi, A. Rosch, PRL **100**, 056403 (2008)

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# Mott transition of trapped atoms in optical lattices



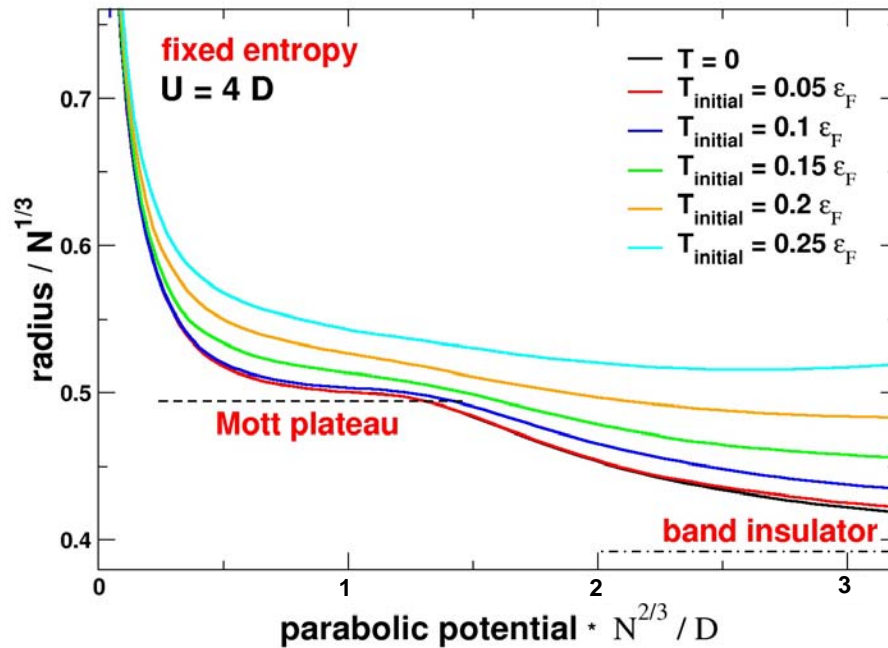
detecting Mott insulator: look for incompressible state

→ measure radius of cloud varying confining potential (I. Bloch)

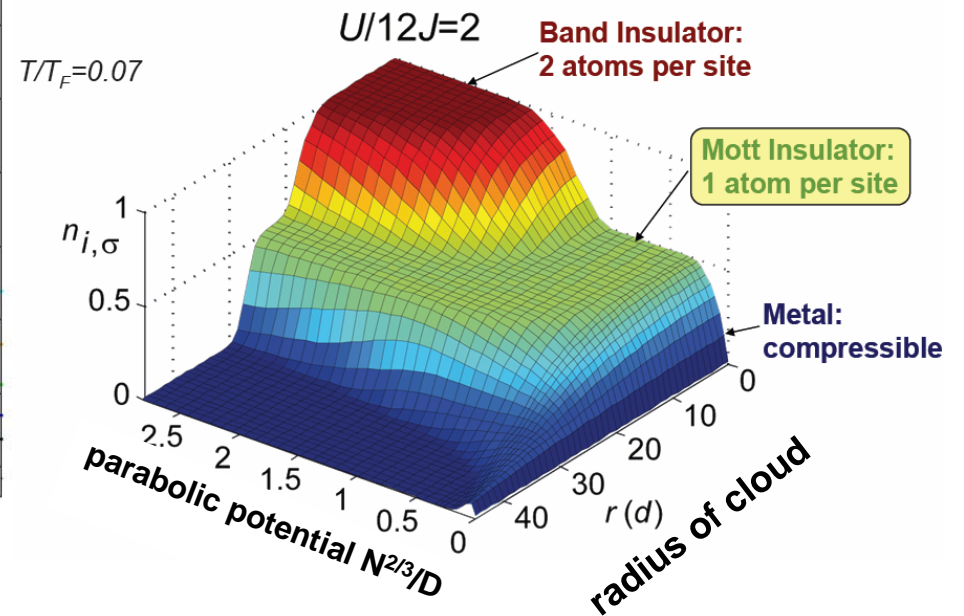
important: **fixed entropy S**

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 'LDA' approx.



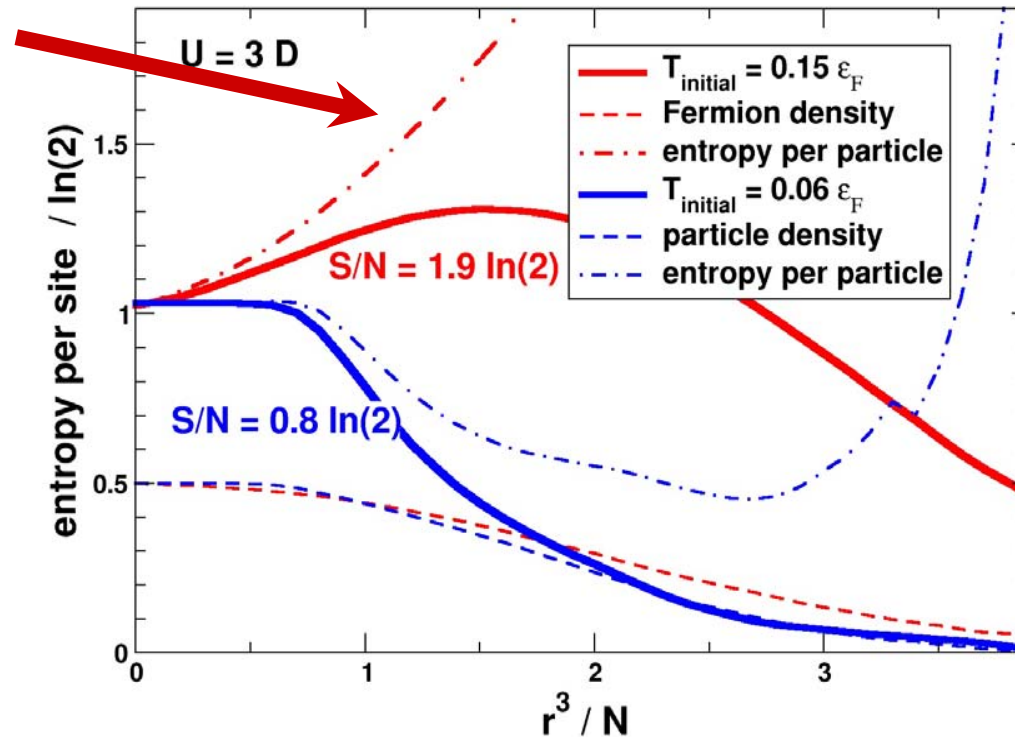
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# Mott transition of trapped atoms in optical lattices



Problem: large entropy per particle  $\frac{S}{N} \gtrsim 2 \ln 2$   
Solution: dump entropy

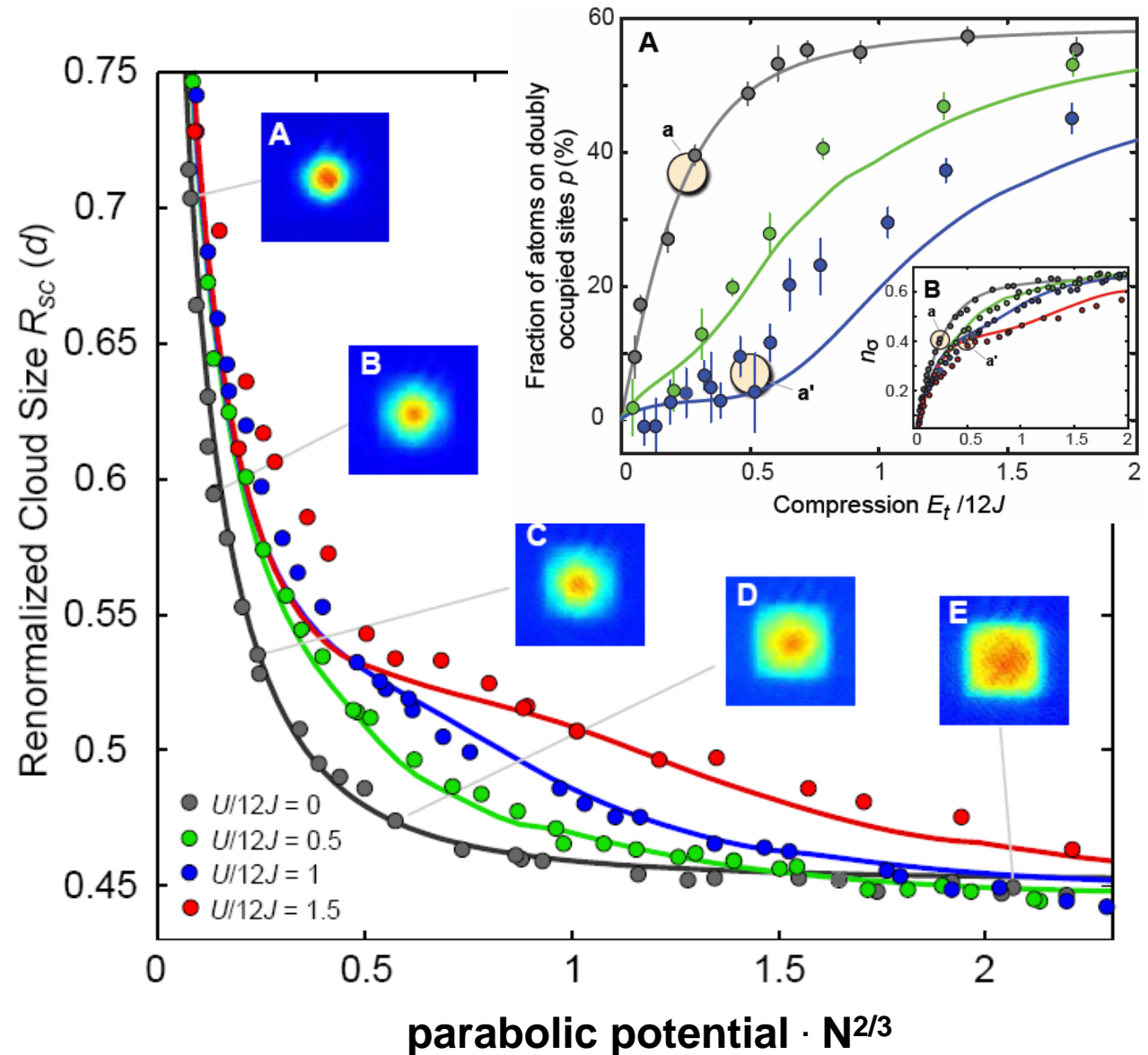
in metallic belt



# Mott transition of trapped atoms in optical lattices



- experimental results:
  - U. Schneider, L. Hackermül
  - S. Will, Th. Best, I. Bloch
  - about  $10^5$   $^{40}\text{K}$  atoms
  - in optical lattice
  - initial  $T \sim 0.15 E_F$
- detection of fermionic Mott insulator
  - real **experimental test** of DMFT without free parameters
  - main experimental problem: adiabaticity



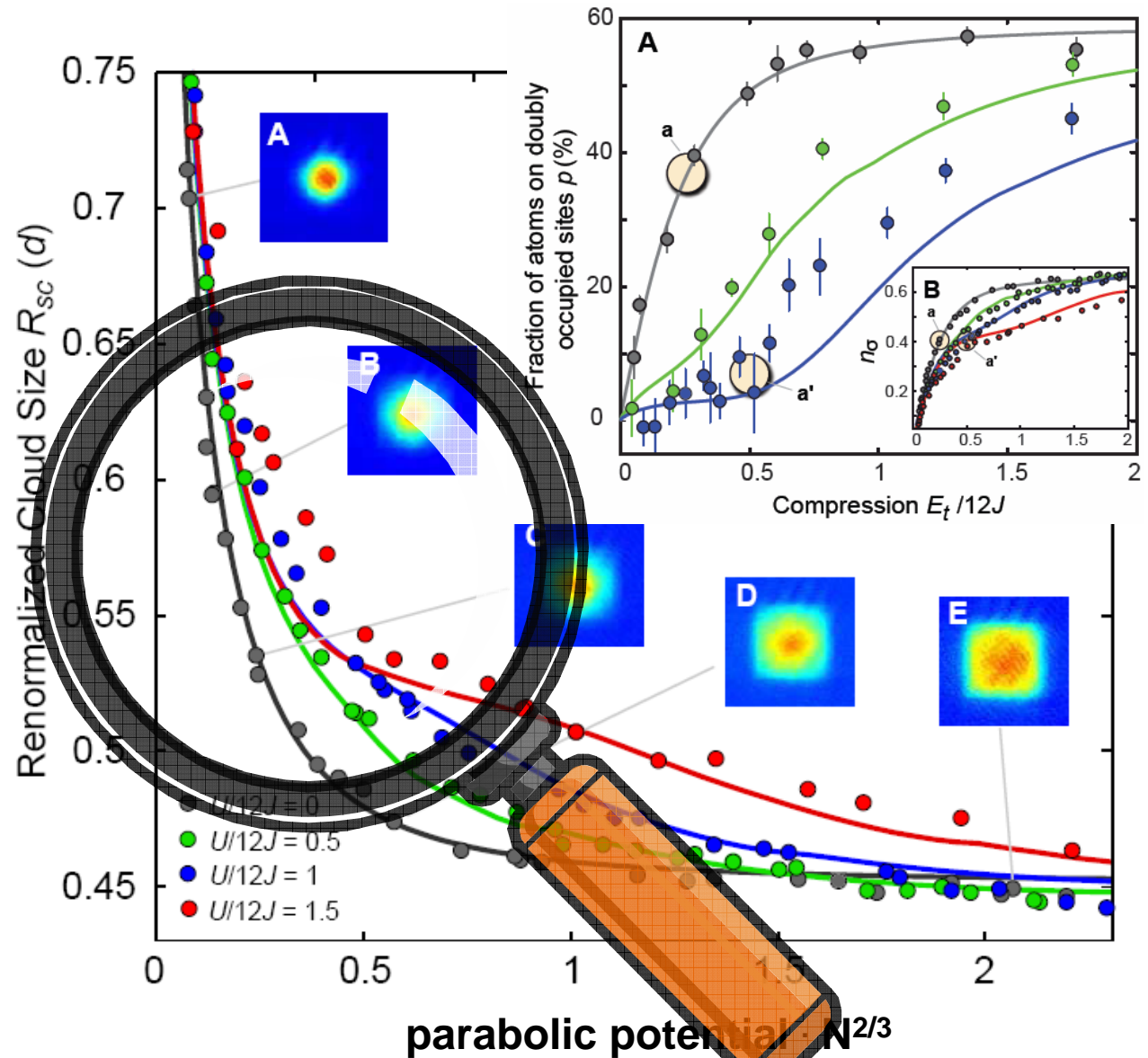
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# Mott transition of trapped atoms in optical lattices



- 
- 
- Deviations of theory and experiment for large  $U$ ?
- 

Experiment non-adiabatic for large  $U$ ?



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## Cold atoms as quantum simulator for Hubbard model?



- now: onset of Mott physics
- most needed: new cooling mechanism to reduce entropy by factor 4 for magnetism, factor 10 for d-wave superconductivity
- many ideas...
- • **likely** within 2-3 years: detection of d-wave superconductivity in the 2d Hubbard model (if existent)  
**not likely**: any decent precision measurement (Tc as function of doping, T, ...)
- already: useful as test for theories!  
see also: De Leo, Kollath, Georges, Ferrero, Parcollet, PRL 2008  
Snoek, Titvinidze, Toke, Byczuk, Hofstetter, New J. Phys. 2008  
Scarola, Pollet, Oitmaa, Troyer, PRL 2009,

**more fun with cold atoms:  
physics out of equilibrium**

simple example: metastable finite momentum superconductivity

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usually:

high energy states in interacting many body systems:

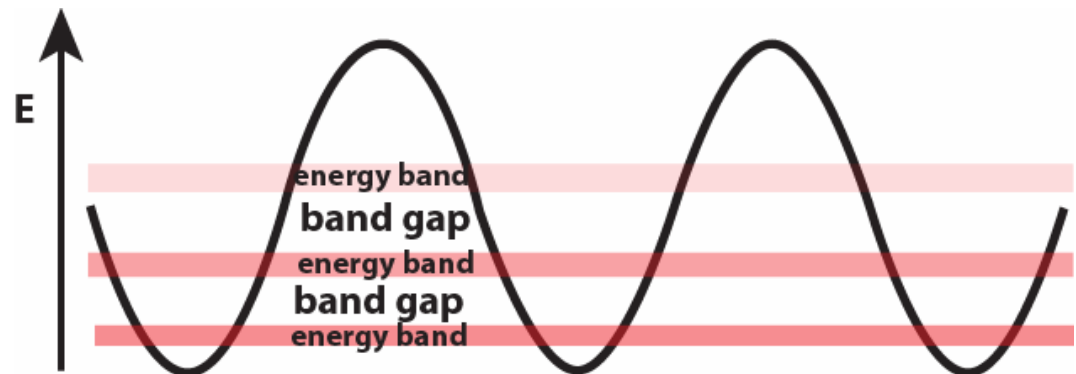
decay rapidly due to huge phase space

(exception: topologically stable states, solitons, domainwalls... of ordered phases)

periodic potential:  
formation of bands and  
**band-gaps**

→ regions **without**  
single-particle excitations

→ possibility for (meta-) stable **high energy states**  
protected by energy conservation (not by topology)



# Lifetime of doubly occupied lattice sites

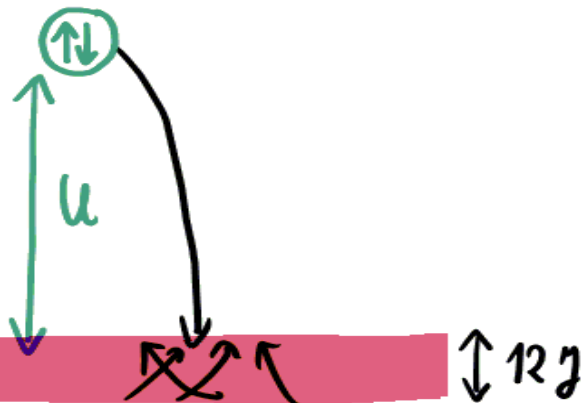
Hubbard model: band-gap  $\gg U \gg J$

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

single particle states:  $E_{\mathbf{k}} = -2J \sum_{i=x,y,z} \cos(k_i a)$

maximal single-particle energy:  $12J$

energy of doubly occupied site:  $U$



How can doubly occupied state decay?

necessary to create **many**,  $N \gtrsim \frac{U}{12J}$ ,  
single particles excitation to absorb energy

$$t_d \gtrsim (const.)^N \sim \frac{1}{J} \exp[const. U/J]$$

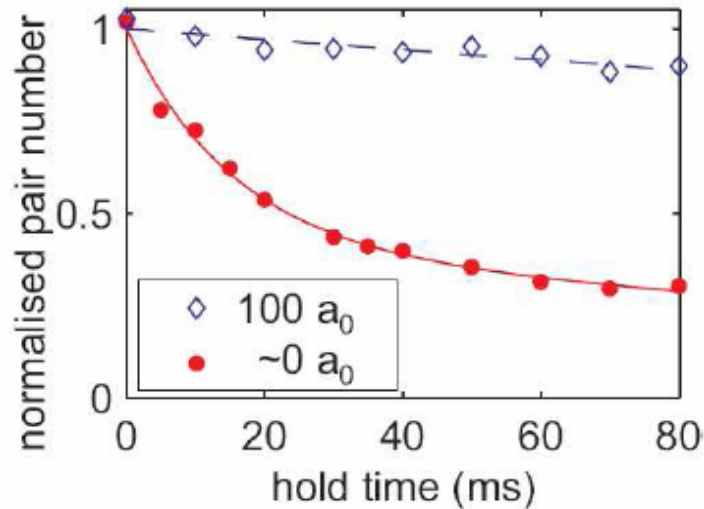
**exponentially large** life time

# Exponentially large lifetime of doubly occupied lattice sites

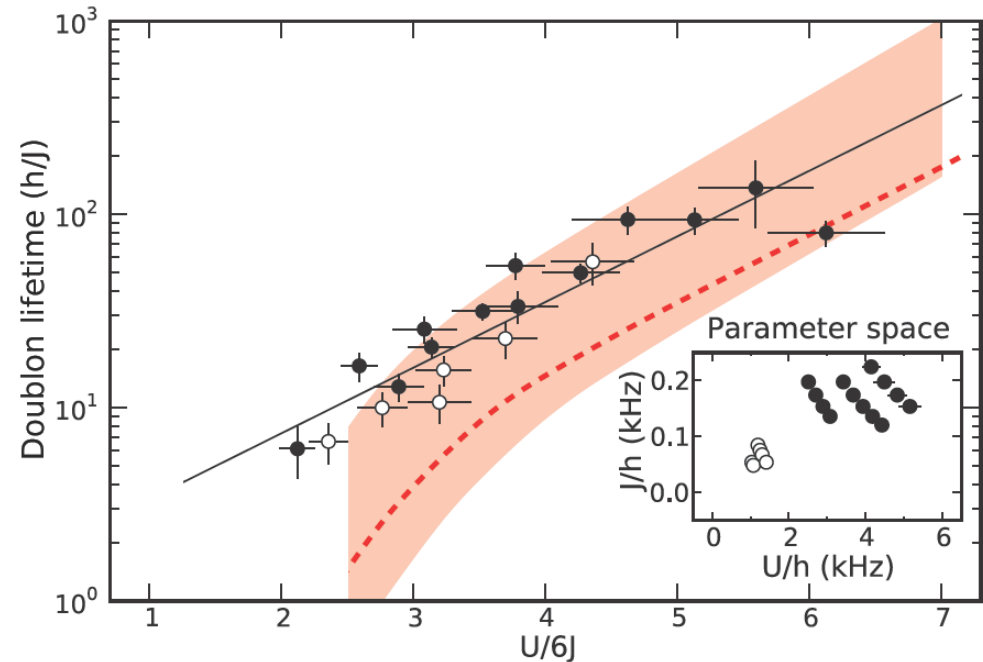


Winkler, Thalhammer, Lang, Grimm, Denschlag, Daley, Kantian, Büchler, Zoller, Nature 2006

Strohmaier, Greif, Jördens, Tarruell, Moritz, Sensarma, Pekker, Altman, Demler, arXiv:0905.2963



lifetime 700 ms probably restricted by scattering from lattice photons



numerics in 1d: quasistationary state within time-dependent DMRG for large  $U$ : Kollath, Läuchli, Altmann, PRL 2007

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# metastable superconductivity

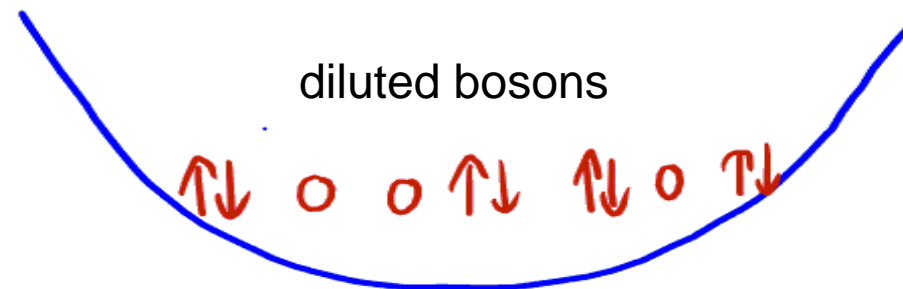
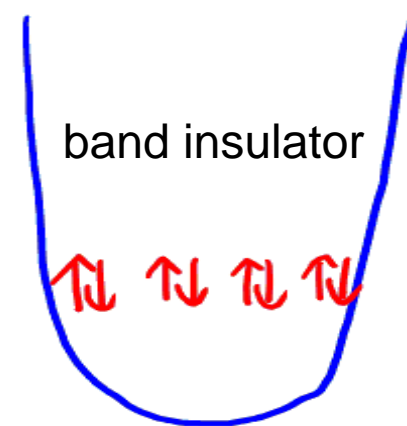
Include again trapping potential  $H_{\text{trap}} = \sum V_0 r_i^2 n_i$

large  $V_0 \implies$  band insulator with large  $U$

reduce  $V_0$  slowly compared

to  $1/J$  or  $U/J^2$

but fast compared to  $\frac{1}{J} \exp[cU/J]$



Bose condensation of diluted doubly occupied sites



**s-wave superconductivity**

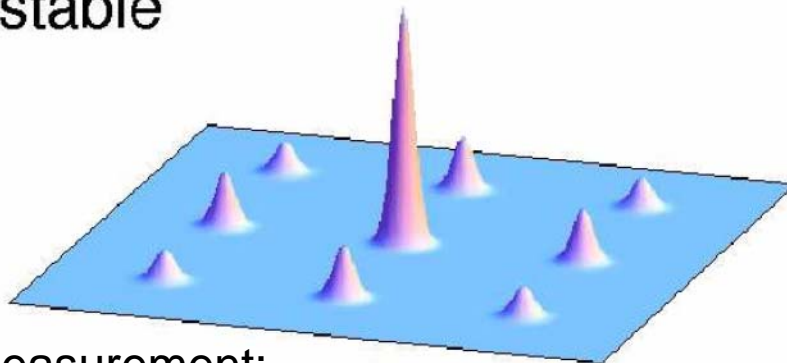
in strongly repulsive Hubbard model !

# detection of metastable superfluidity

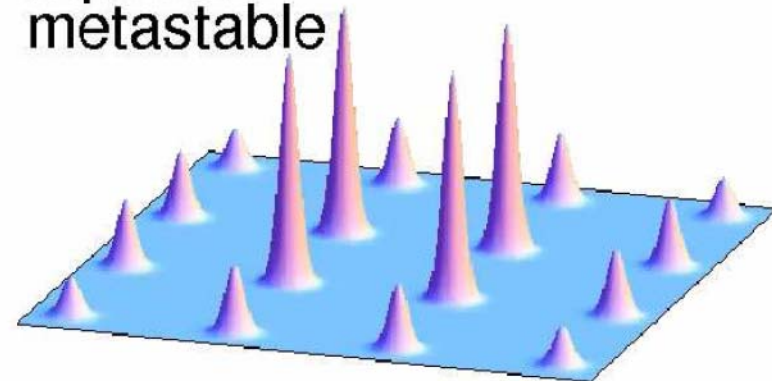
- Difference of repulsively from attractively bound states?
- Hopping via **virtual low-energy** rather than **high-energy** states
- $\Rightarrow$  sign change of hopping rate of pairs
- attractively bound pairs ( $U \ll -J$ ):
- $\Rightarrow$  condensation at momentum  $(0,0,0)$
- repulsively bound pairs ( $U \gg J$ ):
- $\Rightarrow$  condensation at momentum  $(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$



attractive  
stable



repulsive  
metastable



measurement:

convert to chemically bound pairs by rapid sweep through Feshbach resonance, measure momentum distribution of molecules (Regal, Greiner, Jin 04)

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## metastable superfluidity



- 
- alternative to bose-condensation of pairs:
- phase separation (pairs clump together)
- 
- e.g. analog situation for Bosons analyzed by D. Petrosyan, B. Schmidt, J. R. Anglin, M. Fleischhauer, Phys. Rev. A 76, 033606 (2007)

phase separation seems to be unavoidable for bosons

**controlled** calculation needed for fermionic case !  
**usually** difficult, here: symmetries help

# Metastable superconductivity



Simple case: only doubly occupied and empty sites:

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

Trick:

rewrite as spin Hamiltonian:

↓ empty site

↑ doubly occupied site

$$S_i^+ = (-1)^i c_{\uparrow i}^\dagger c_{\downarrow i}^\dagger$$

$$H_{\text{eff}} = -\frac{2J^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

ferromagnetic Heisenberg model

due to SU(2) symmetry in the charge sector

**exact** groundstates for uniform systems:

magnetization in +z direction: band insulator

magnetization in -z direction: no particles

magnetization in x/y direction: s-wave superconductivity with momentum  $(\pi, \pi, \pi)$ ,

( $\eta$  -paring, C.N. Yang 1989)

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# Metastable superconductivity

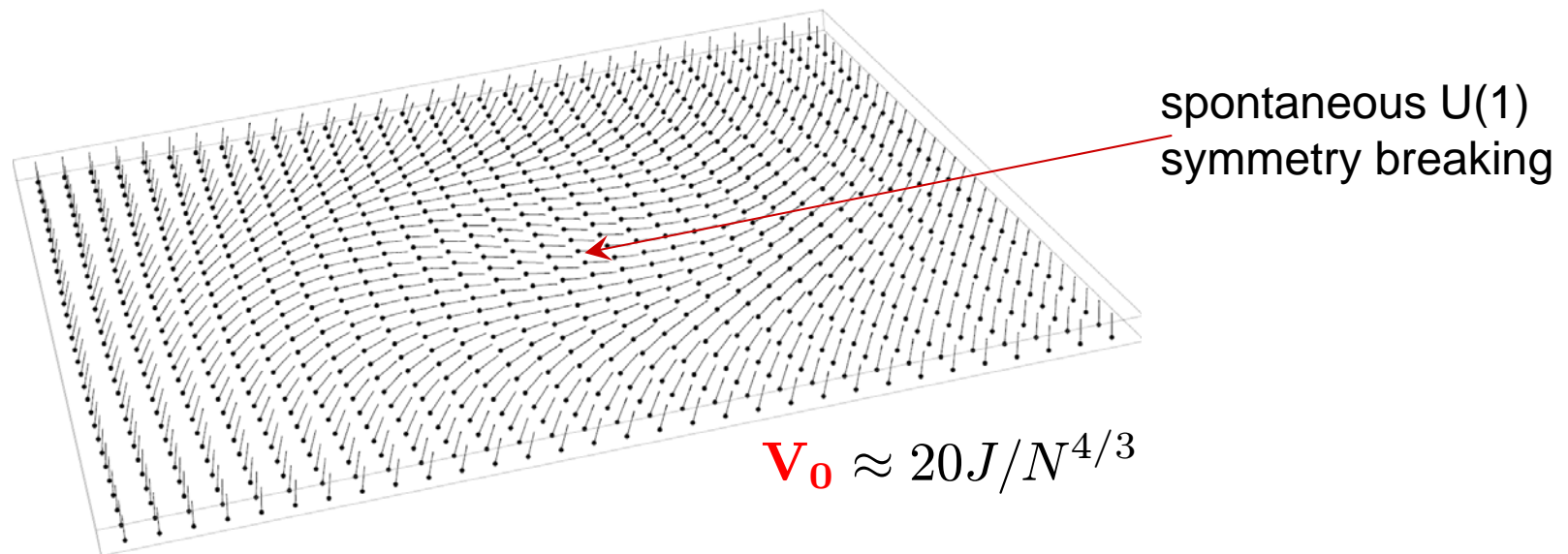


- with trapping and chemical potential:

$$H_{\text{eff}} = -\frac{2J^2}{U} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_i (\mathbf{V}_0 r_i^2 - \mu) S_i^z$$

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

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



# Metastable superconductivity



- Is this a true superfluid with phase stiffness? **NO** (not yet)
- ferromagnet: quadratic dispersion of spin-waves,  $\omega \sim k^2$
- superfluid: linear dispersion (necessary for superfluidity)
- no superfluid  $\sim$  exact cancellation of attractions and hard-core repulsion of bosons

similarly:

up to domain wall energy

phase separation & superconductivity degenerate



 **Leading correction can change physics!**

Calculations: stabilized by corrections to Hubbard model

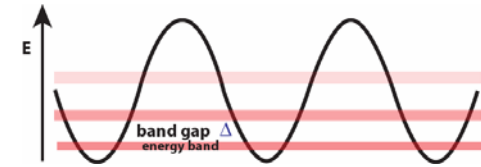
(e.g. nearest neighbor interactions)

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# breaking of $SU_c(2)$ symmetry of Hubbard model



Analyze leading corrections to  $SU_c(2)$  from **corrections** to Hubbard model



next nearest neighbor hopping favors phase separation but only to 2nd order  $O(J^4 / (\text{gap}^2 U))$



assisted hopping



pair hopping



dominant:  
nearest neighbor interaction

$$U' \sim U (J / \text{gap})^2 \gg J^4 / (\text{gap}^2 U)$$

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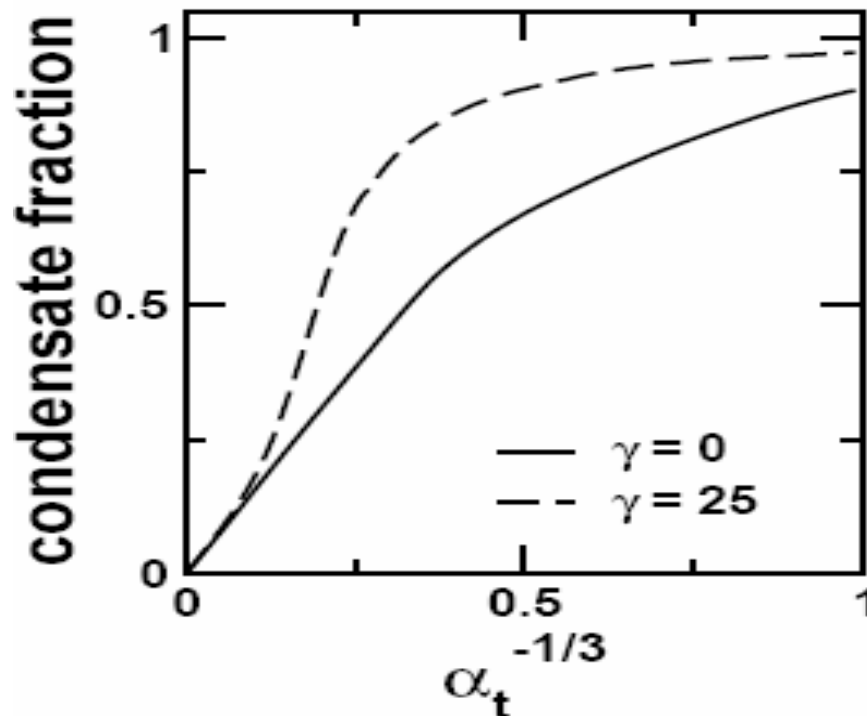
# breaking of $SU_C(2)$ symmetry of Hubbard model

trapping potential

$$\alpha_t = \mathbf{V} N^{4/3} \mathbf{U} / J^2$$

corrections to Hubbard model

$$\gamma = \mathbf{U}' \mathbf{U} N^{2/3} / J^2 \gg 1$$



cloud expands  $\rightarrow$   
 exotic metastable s-wave superfluidity stabilized in strongly repulsive Hubbard model

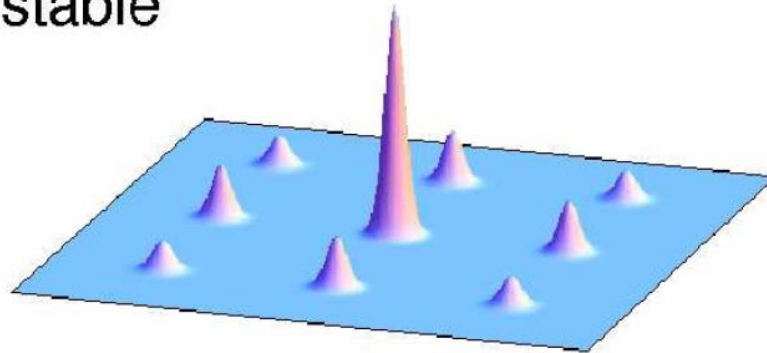


# Metastable superfluidity

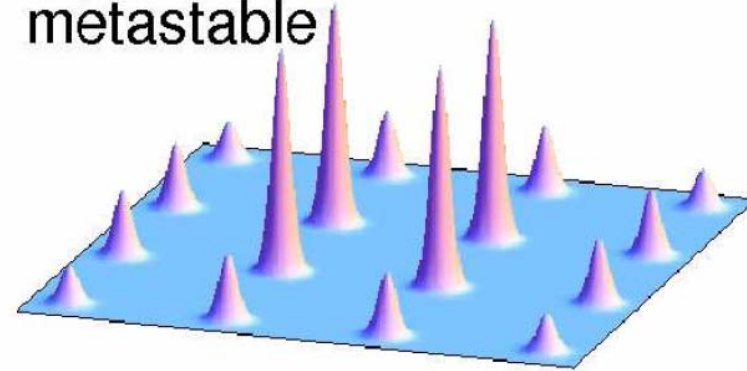


metastable superconductivity easy to realize and detect?

attractive  
stable



repulsive  
metastable



**crude** estimate:

Bose condensation in trap for entropie per boson  $S < 3.6 k_B$

corresponding entropy per Fermion:  $S < 1.8 k_B$

corresponding initial temperature before loading in trap:  $0.22 T_F$

presently reached (e.g. group of Bloch):  $0.15 T_F$

Main question: effect of singly occupied sites!

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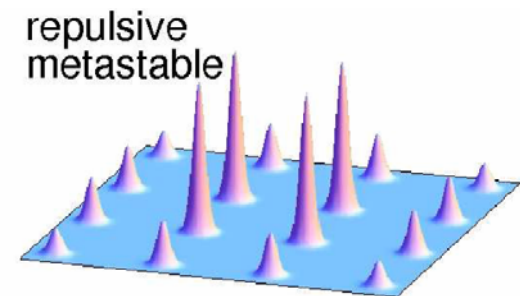
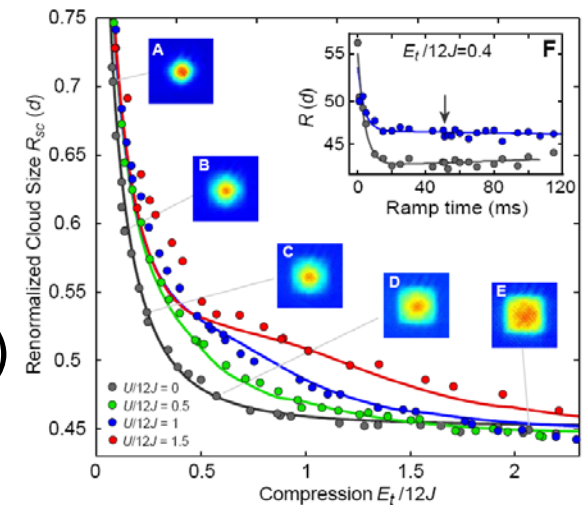
# Quantum simulations with cold atoms



- first simulations of correlated fermions in lattices: Mott transition
- next steps: quantum magnetism (with 1/4th of entropy) d-wave superconductivity

new phenomena out of equilibrium:

- metastable superconductivity



Helmes, Costi, Rosch, PRL **100**, 056403 (2008)

Helmes, Costi, Rosch, PRL **101**, 066802 (2008)

Schneider, Hackermüller, Will, Best, Bloch, Costi, Helmes, Rasch, A. Rosch, Science (2008)

Rosch, Rasch, Binz, Vojta, PRL **101**, 265301 (2008)

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