Introduction to Ultracold Atoms in Optical Lattices

I.B.
ICTP *Trieste - Summer School*

Max-Planck-Institut für Quantenoptik
Ludwig-Maximilians Universität

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$ DARPA (OLE)

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Course Outline

LECTURE 1

Introduction

- Brief Review Lattice Basics
- Detection Methods
- Hubbard models

Single Atom Imaging/Control

- Single Atom Imaging Bosons/Fermions
- Probing Thermal and Quantum Fluctuations
- Single Spin Manipulation
- Light Cone Spreading of Correlations

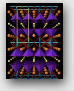
Absolute Negative Temperatures

LECTURE 2 - Quantum Magnetism with UCQG

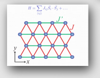
- Superexchange Interactions
- Single Spin Impurity
- Bound Magnons
- AFM Order in the Fermi Hubbard Model
- Probing Hidden AFM in 1D Hubbard Chains
- Direct Imaging of Spin-Charge Separation
- Imaging Polarons - Charge Impurities in an AFM
- Incommensurate AFM in 1D
- Quantum Magnetism with Rydberg atoms

The Challenge of Many-Body Quantum Systems

- **Understand and Design Quantum Materials** -
  one of the biggest challenge of Quantum Physics in the 21st Century
- **Technological Relevance**

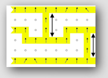



High-Tc Superconductivity (Power Delivery)



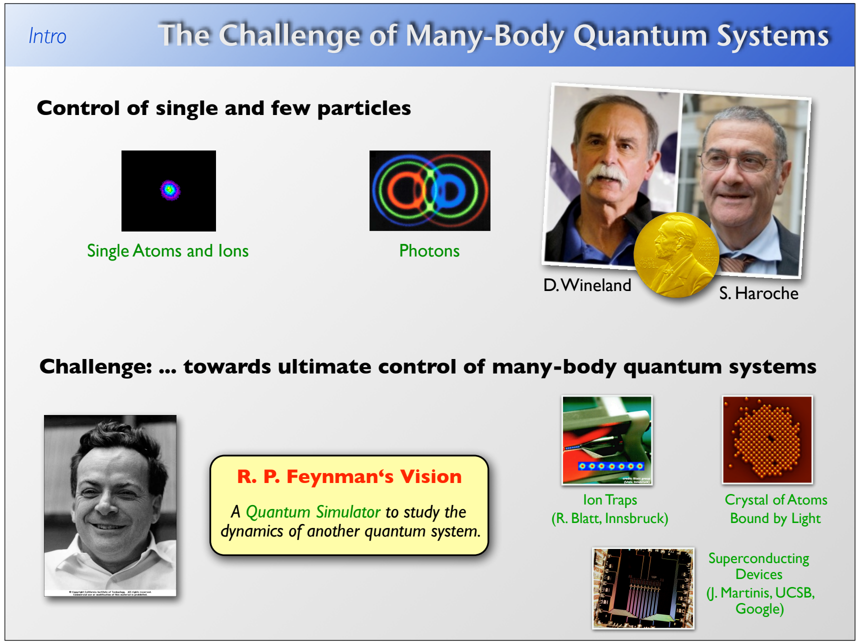
Magnetism (Storage, Spintronics...)

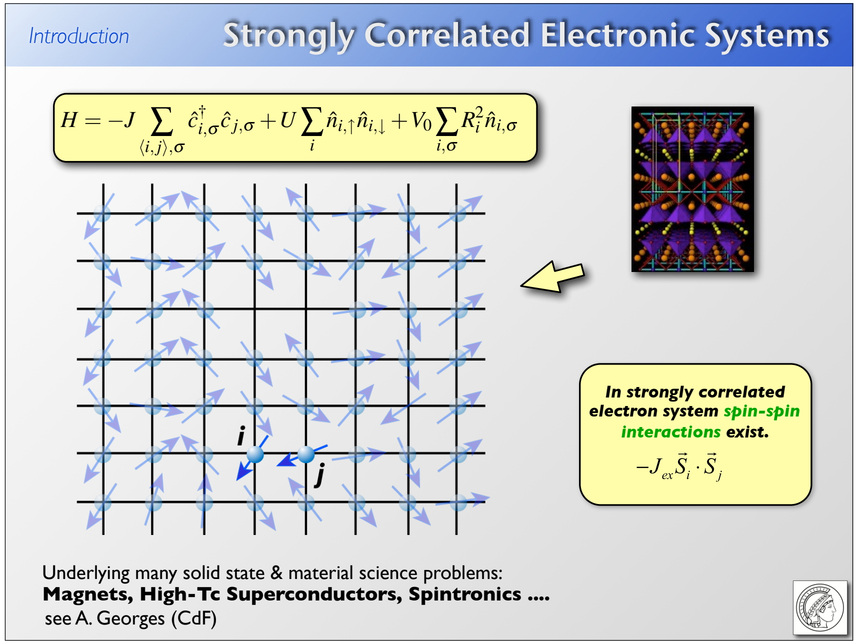
Novel Quantum Sensors (Precision Detectors)

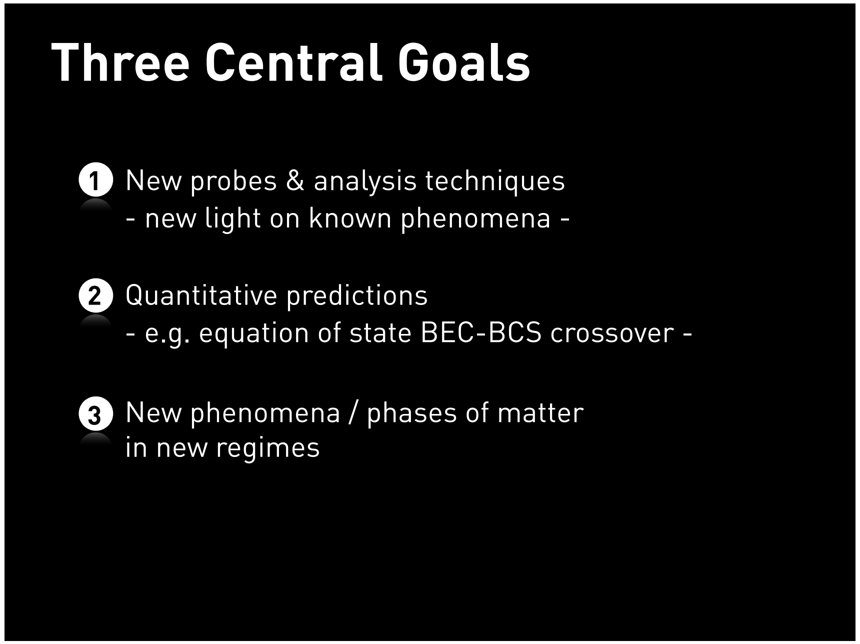


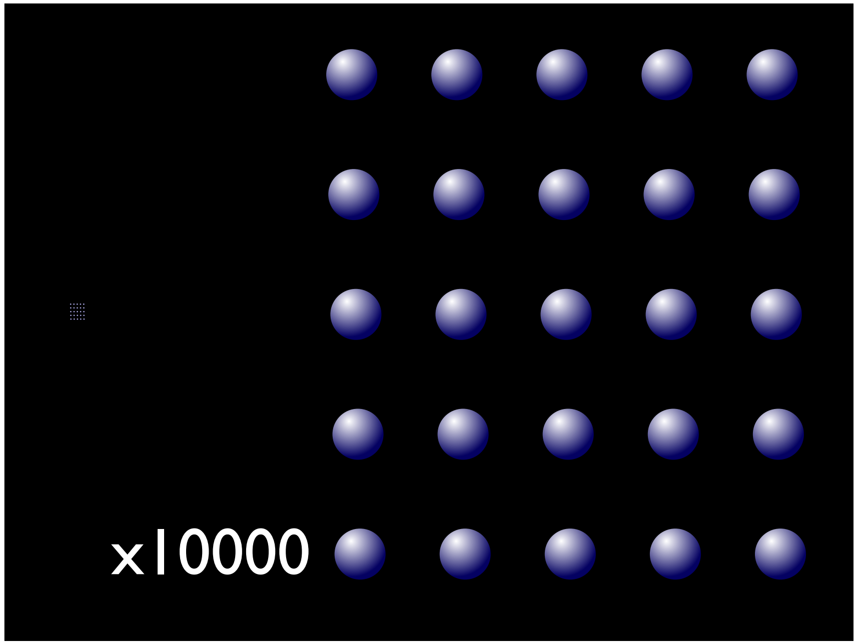
Quantum Technologies
(Quantum Computing, Metrology, Quantum Sensors,...)

Many cases: lack of basic understanding of underlying processes
Difficulty to separate effects: probe impurities, complex interplay, masking of effects...
Many cases: even simple models "not solvable"
Need to synthesize new material **to analyze effect of parameter change**

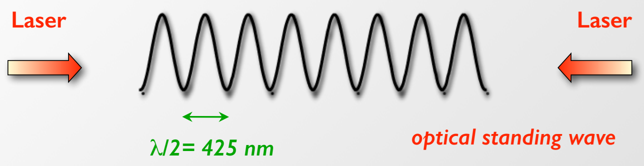

Intro
The Challenge of Many-Body Quantum Systems
Control of single and few particles
Single Atoms and Ions
Photons
D.Wineland
S. Haroche
Challenge: ... towards ultimate control of many-body quantum systems
R. P. Feynman's Vision
A Quantum Simulator to study the dynamics of another quantum system.
Ion Traps
(R. Blatt, Innsbruck)
Crystal of Atoms
Bound by Light
Superconducting
Devices
(J. Martinis, UCSB,
Google)


Introduction
Strongly Correlated Electronic Systems
$H = -J \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + V_0 \sum_{i,\sigma} R_i^2 \hat{n}_{i,\sigma}$
i
j
In strongly correlated electron system spin-spin interactions exist.
$-J_{ex}\vec{S}_i \cdot \vec{S}_j$
Underlying many solid state & material science problems:
Magnets, High-Tc Superconductors, Spintronics ....
see A. Georges (CdF)


Three Central Goals
1 New probes & analysis techniques
- new light on known phenomena -
2 Quantitative predictions
- e.g. equation of state BEC-BCS crossover -
3 New phenomena / phases of matter
in new regimes


x10000

Introduction **Optical Lattice Potential – Perfect Artificial Crystals**

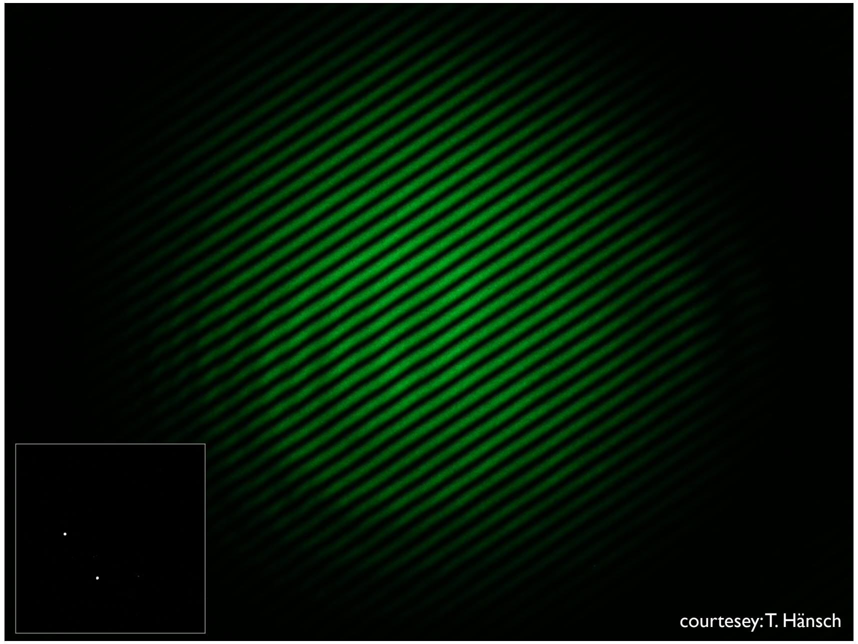


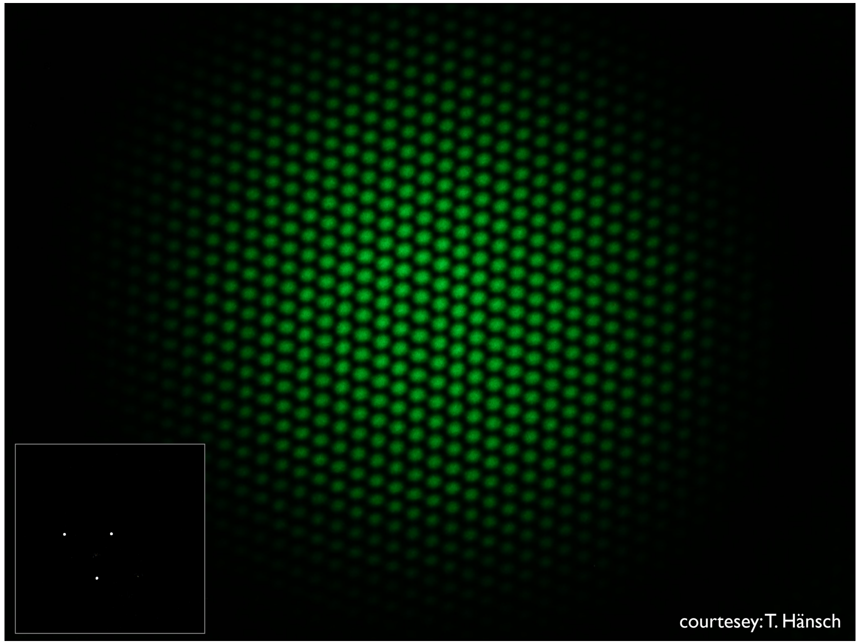
Fourier synthesize aribtrary lattices:

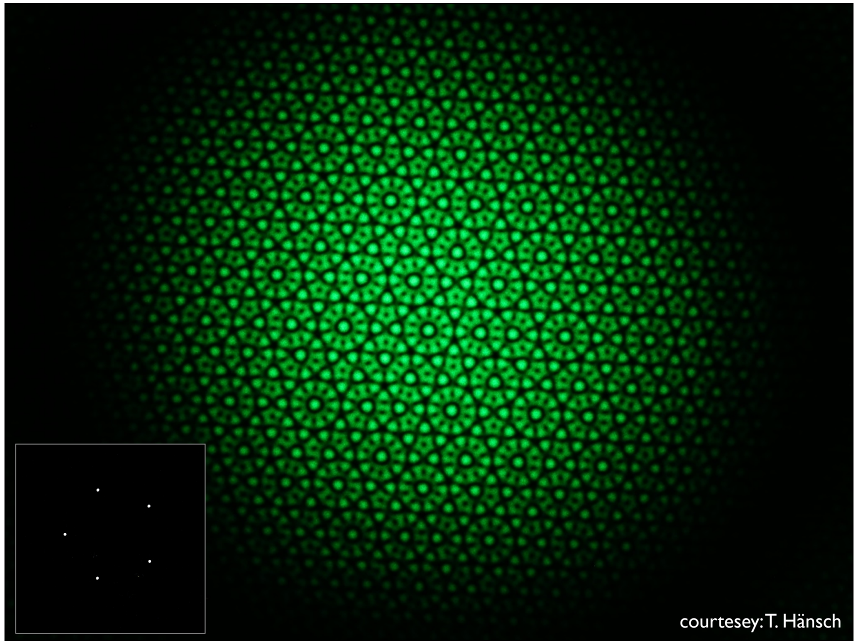
- Square
- Hexagonal/Triangular/Brick Wall
- Kagomé
- Superlattices
- *Spin dependent lattices*
- ...

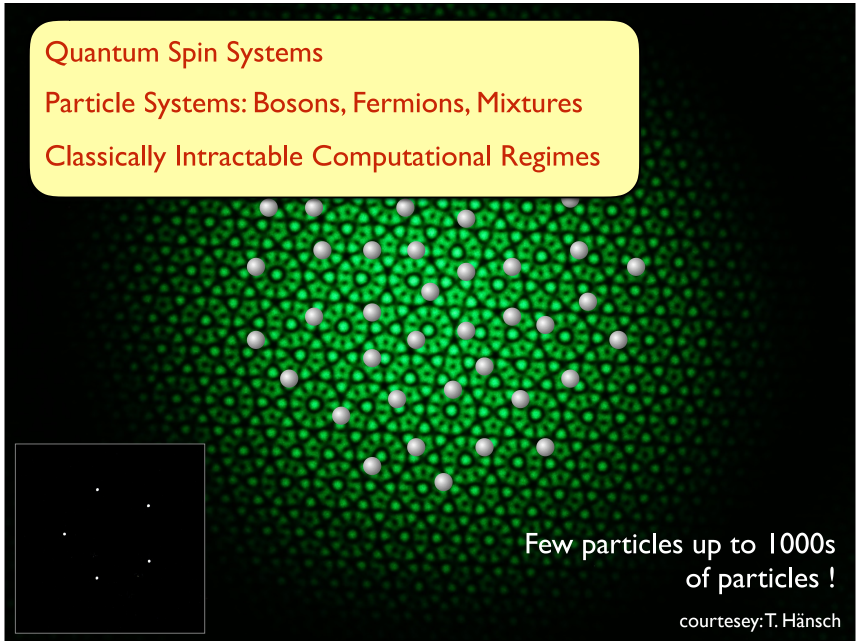
Special case: flux lattices...

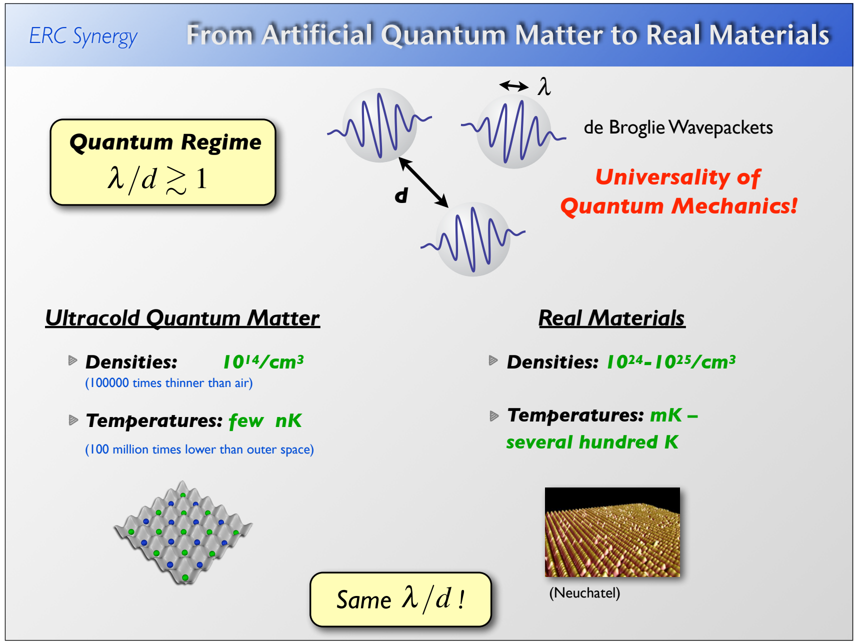
Full **dynamical** control over **lattice depth, geometry, dimensionality!**

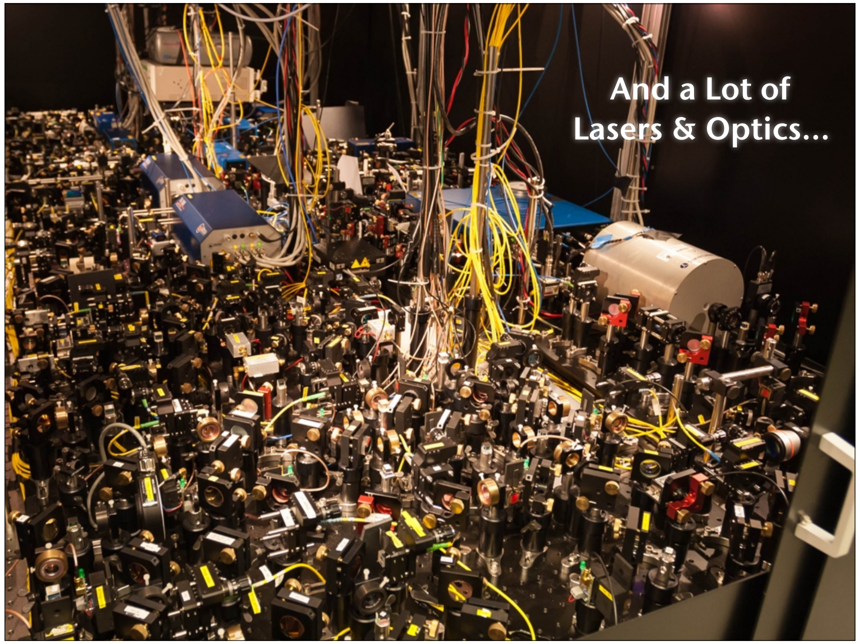







Quantum Spin Systems
Particle Systems: Bosons, Fermions, Mixtures
Classically Intractable Computational Regimes
Few particles up to 1000s of particles !
courtesey: T. Hänsch

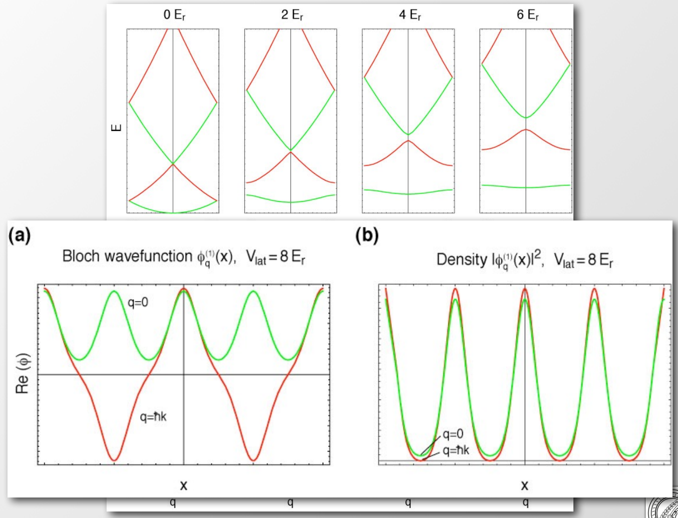

ERC Synergy
From Artificial Quantum Matter to Real Materials
Quantum Regime
$\lambda/d \gtrsim 1$
λ
d
de Broglie Wavepackets
Universality of Quantum Mechanics!
Ultracold Quantum Matter
Densities: $10^{14}/cm^3$
(100000 times thinner than air)
Temperatures: few nK
(100 million times lower than outer space)
Real Materials
Densities: 10^{24}-$10^{25}/cm^3$
Temperatures: mK – several hundred K
Same λ/d !
(Neuchatel)


And a Lot of Lasers & Optics...


Experiments isolated from environment
Not connected to reservoirs!

Measuring Momentum Distributions

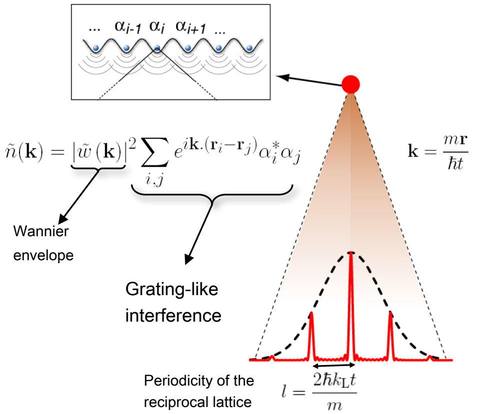
Bandstructure - Blochwaves

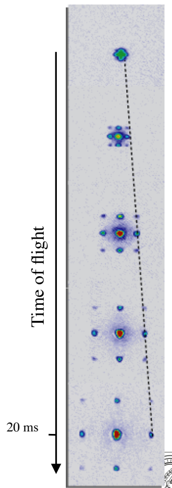


Momentum Distribution

Time of flight interference pattern

- Interference between all waves coherently emitted from each lattice site



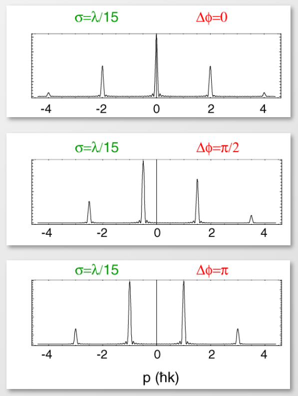


Optical Lattices

Momentum Distributions – 1D

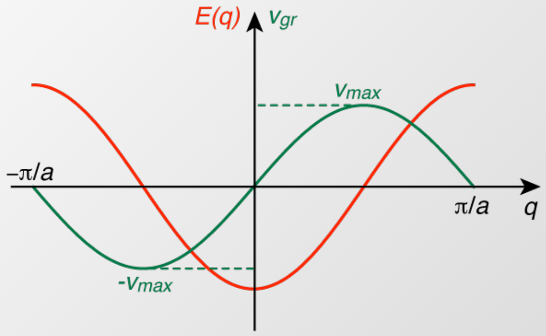
Momentum distribution can be obtained by Fourier transformation of the macroscopic wave function.

$$\Psi(x) = \sum_i A(x_j) \cdot w(x - x_j) \cdot e^{i\phi(x_j)}$$

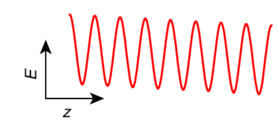


Dispersion Relation in a Square Lattice

$$E(q) = -2J\cos(qa)$$



Bloch Oscillations — Preparing Arbitrary Phase Differences Between Neighbouring Lattice Sites



$$\phi_j = E_j \cdot t / \hbar$$

Phase difference between neighboring lattice sites

$$\Delta\phi_j = (V'\lambda/2)\,\Delta t$$

(cp. Bloch-Oscillations)

$\Delta\phi = 0$ $\Delta\phi = \pi$

But: dephasing if gradient is left on for long times !

SF-MI — Bose-Hubbard Hamiltonian

Expanding the field operator in the Wannier basis of localized wave functions on each lattice site, yields :

$$\hat{\psi}(\mathbf{x}) = \sum_i \hat{a}_i w(\mathbf{x} - \mathbf{x}_i)$$

Bose-Hubbard Hamiltonian

$$H = -J\sum_{\langle i,j\rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \varepsilon_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1)$$

Tunnelmatrix element/Hopping element

$$J = -\int d^3x\, w(\mathbf{x} - \mathbf{x}_i)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{lat}(\mathbf{x})\right) w(\mathbf{x} - \mathbf{x}_j)$$

Onsite interaction matrix element

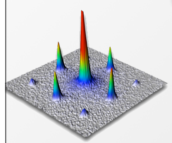
$$U = \frac{4\pi\hbar^2 a}{m}\int d^3x\, |w(\mathbf{x})|^4$$

M.P.A. Fisher et al., PRB 40, 546 (1989); D. Jaksch et al., PRL 81, 3108 (1998)

Mott Insulators now at: Munich, Mainz, NIST, ETHZ, Texas, Innsbruck, MIT, Chicago, Florence,...
see also work on JJ arrays H. Mooij et al., E. Cornell,...

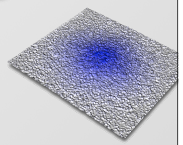
SF-MI — From Weak to Strong Interactions

$$\gamma = \frac{\text{Interaction Energy}}{\text{Kinetic Energy}} >> 1$$

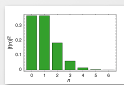


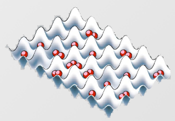
Weak Interactions

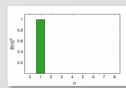
Quantum Phase Transition
See S. Sachdev & B. Keimer Phys. Today 2011

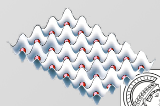


Strong Interactions





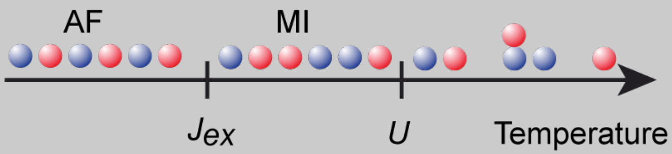




Strongly Interacting Fermions in Optical Lattices

$$\hat{H} = -J \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\downarrow}\hat{n}_{i,\uparrow} + V_t \sum_{i,\sigma} i^2 \hat{n}_{i,\sigma}$$

Predicted phases at half filling for strong interactions $U/12J > 1$



max. Entropy
$S/N = k_B\, 2 \ln 2$

R. Jördens et al., Nature **455**, 204 (2008), U. Schneider et al., Science **322,** 1520 (2008),
D. Greif et al., Science **340**, 1307 (2013)

Single Atom Detection in a Lattice

Sherson et al. Nature 467, 68 (2010),
see also Bakr et al. Nature (2009) & Bakr et al. Science (2010)

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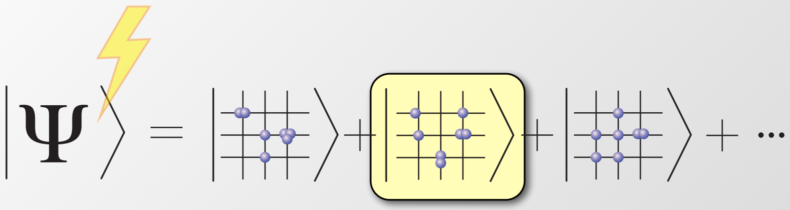
Single Atoms

Measuring a Many-Body Quantum System

Local occupation measurement

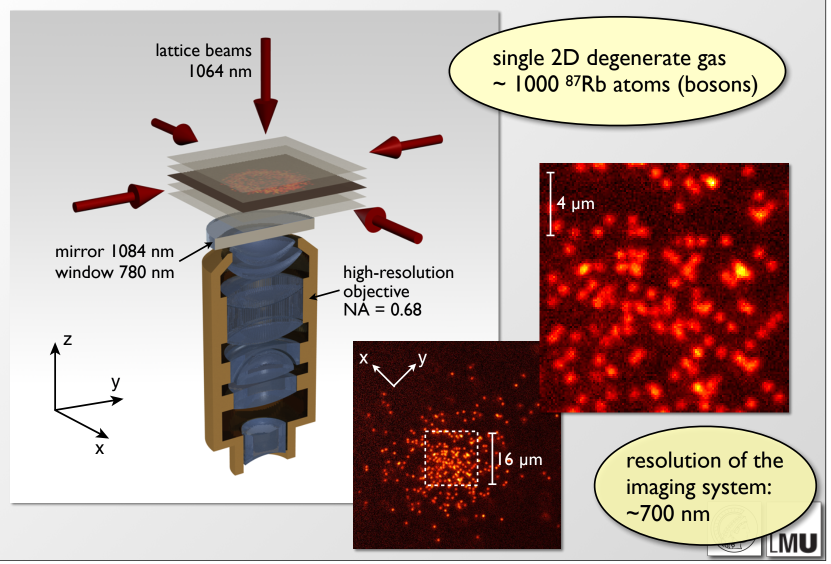


Enables access to all position correlation between particles!

Extendable to other observables (e.g. local currents etc…)

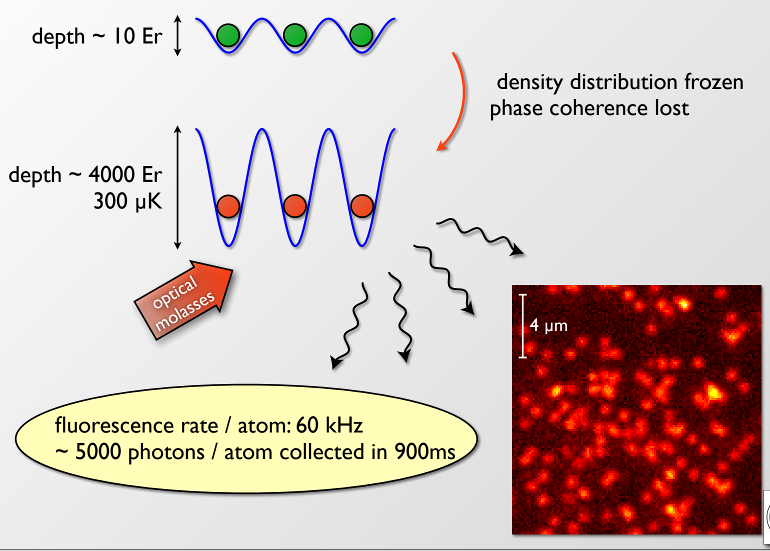
Single Atoms

Experimental Setup



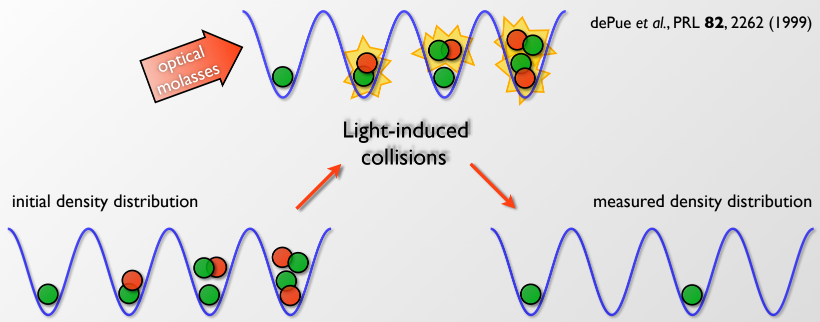
Single Atoms

Fluorescence imaging



Single Atoms

Parity projection



dePue *et al.*, PRL **82**, 2262 (1999)

measured occupation: $n_{\text{det}} = \text{mod}_2 n$

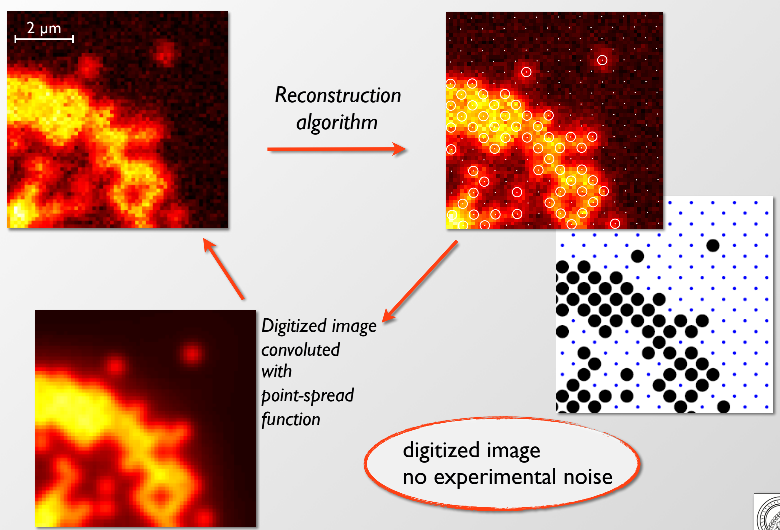
measured variance: $\sigma^2_{\text{det}} = \langle n^2_{\text{det}} \rangle - \langle n_{\text{det}} \rangle^2$

parity projection $\Rightarrow$ $\langle n^2_{\text{det}} \rangle = \langle n_{\text{det}} \rangle$

see also E. Kapit & E. Mueller, Phys. Rev. A **82**, 013644 (2010)

Single Atoms

Reconstruction of site occupation



In-Situ Imaging of a Mott Insulator

J. Sherson et al. Nature **467**, 68 (2010),
see also S. Fölling et al. Phys. Rev. Lett (2006), G.K. Campbell et al. Science (2006)
N. Gemelke et al. Nature (2009), W. Bakr et al. Science (2010)

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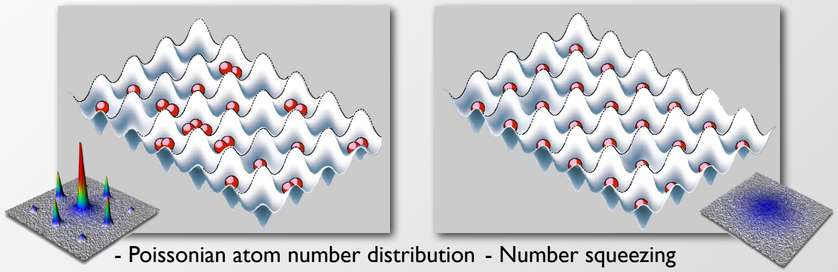
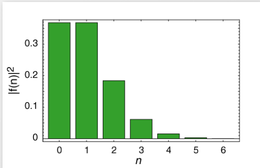
Mott Insulators

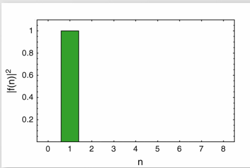
Superfluid **Mott-Insulator**



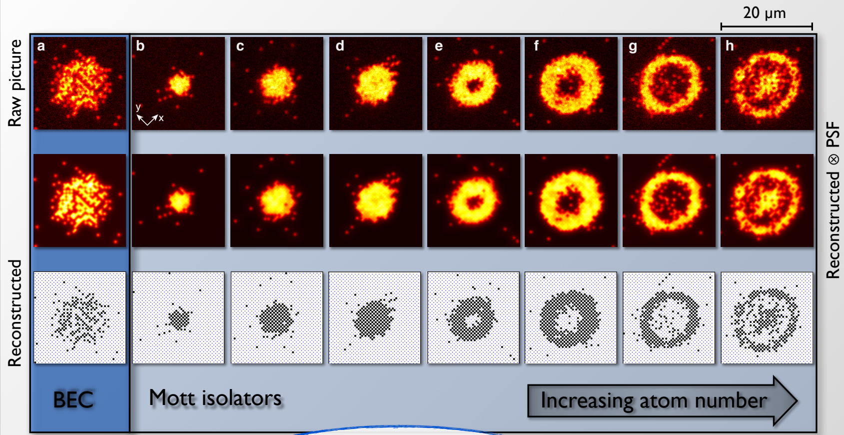
- Poissonian atom number distribution
- Long range phase coherence

- Number squeezing
- No phase coherence



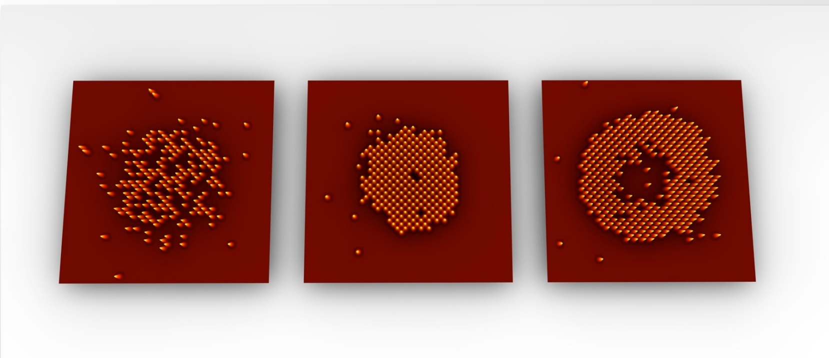


In-situ observation of a Mott insulator



for the Mott insulators: U/J ~ 300 (critical U/J ~ 16)
⇒ only thermal fluctuations

Snapshot of an Atomic Density Distribution



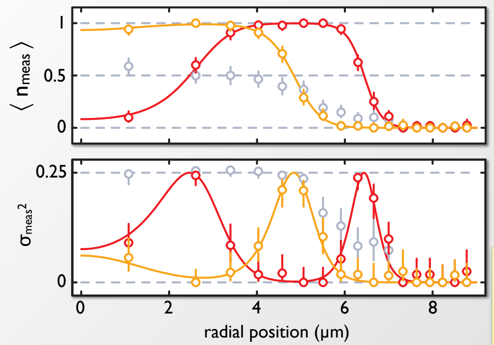
BEC

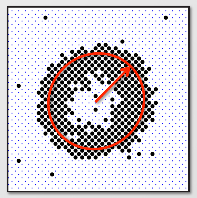
n=1
Mott Insulator

n=1 & n=2
Mott Insulator

J. Sherson *et al.* Nature **467**, 68 (2010)

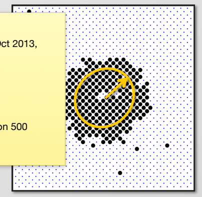
Single Shot Thermodynamics





T = 0.074(5) U/k_B, μ = 1.17(1) U
N = 610(20)

Imported Author 23 Oct 2013, 7:24
2 kHz=100nK
1 kHz=50 nK
0.1 U approx 5 nK
measurement precision 500



T = 0.090(5) U/k_B, μ = 0.73(3) U
N = 300(20)

Simple Theory - Atomic Limit Mott Insulator

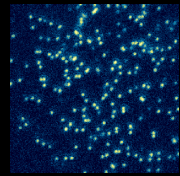
occupation probability: $p_n(r) = \frac{e^{-\beta(E_n - \mu(r)n)}}{Z(r)}$

interaction energy: $E_n = \frac{1}{2}Un(n-1)$

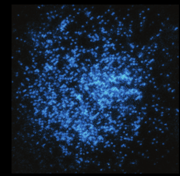
fit parameters: $T/U, \mu/U, U/\omega^2$

Fermionic Quantum Gas Microscopes

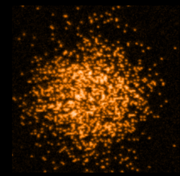
now also for fermions!



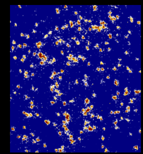
Strathclyde (^{40}K)



Harvard (^{6}Li)



MIT (^{40}K)



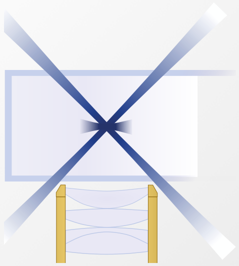
Toronto (^{40}K)

Fermionic Quantum Gas Microscopes

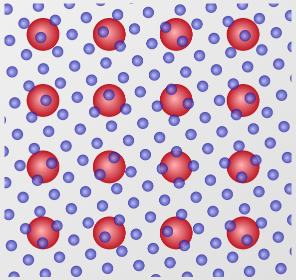
Li-Microscope

Detection 'Pinning' Lattice

Pinning lattice 1064 nm



Physics Lattice
Pinning Lattice

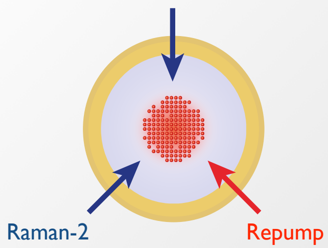


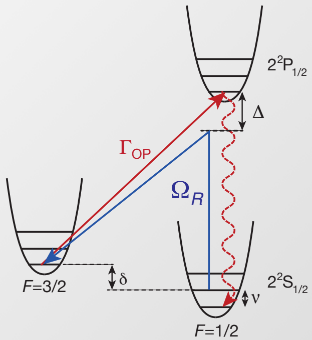
Pinning Spacing 532 nm

Onsite Trap Freq. 1.4 MHz

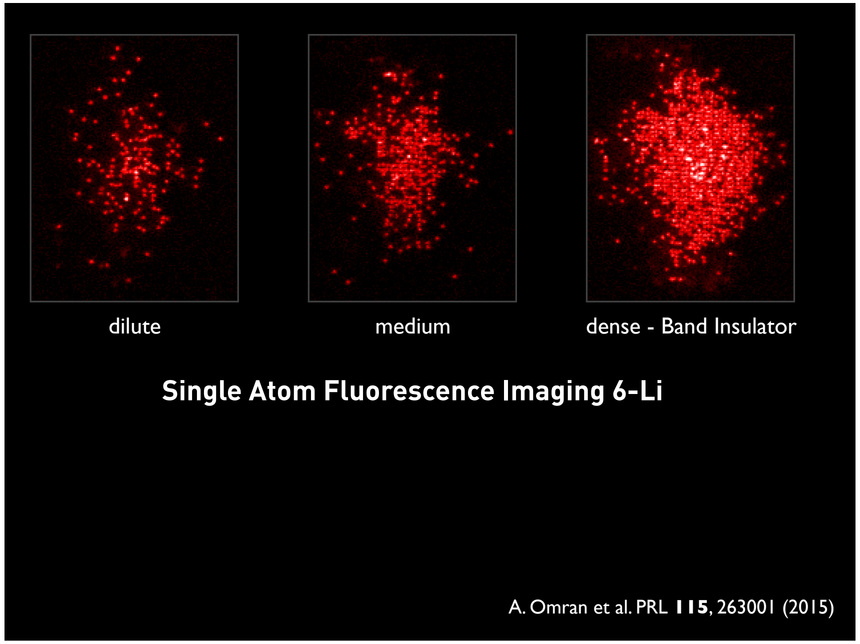
Li-Microscope

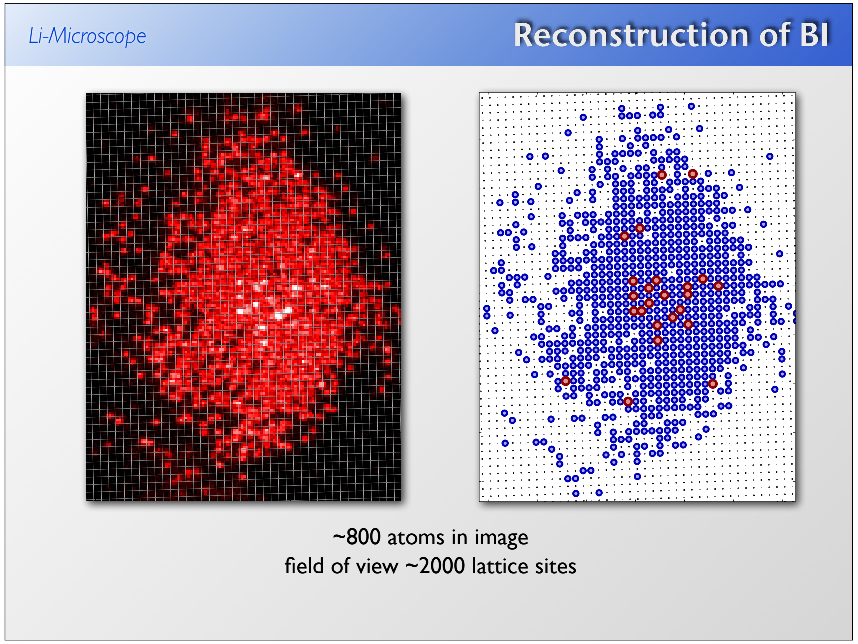
Raman Cooling in Pinning Lattice

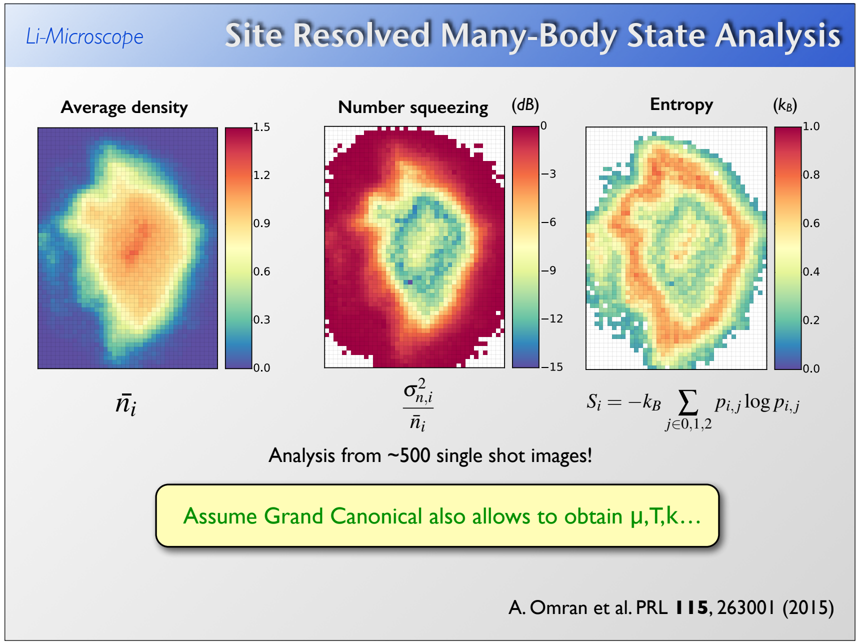


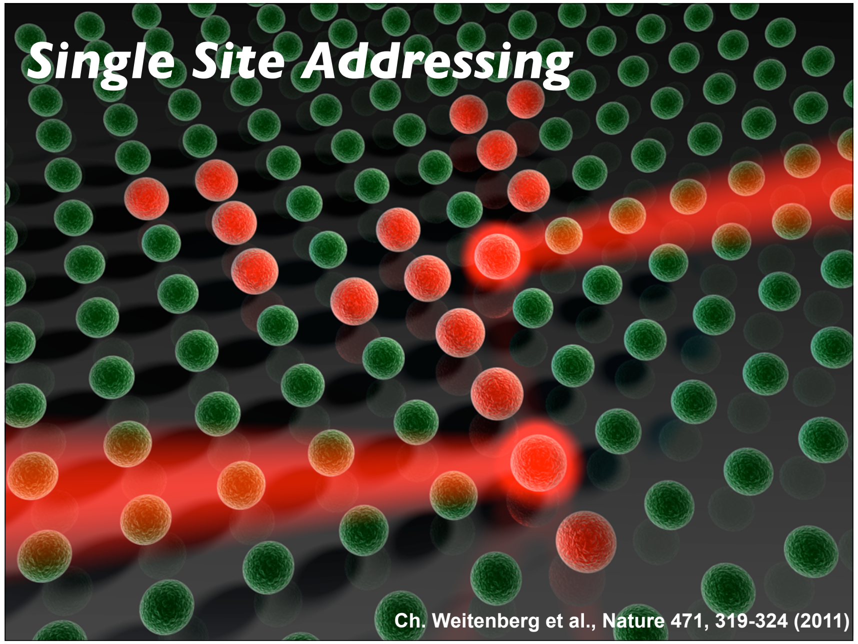


7 kHz Photon Scattering Rate!


dilute
medium
dense - Band Insulator
Single Atom Fluorescence Imaging 6-Li
A. Omran et al. PRL **115**, 263001 (2015)

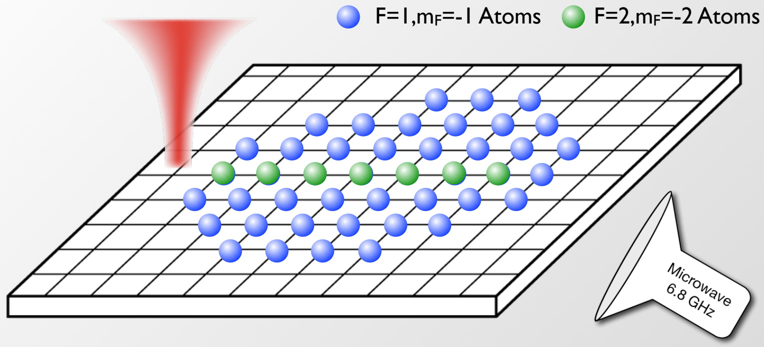

Li-Microscope
Reconstruction of BI
~800 atoms in image
field of view ~2000 lattice sites


Li-Microscope
Site Resolved Many-Body State Analysis
Average density
Number squeezing
(dB)
Entropy
(k_B)
$\bar{n}_i$
$\frac{\sigma^2_{n,i}}{\bar{n}_i}$
$S_i = -k_B \sum_{j \in 0,1,2} p_{i,j} \log p_{i,j}$
Analysis from ~500 single shot images!
Assume Grand Canonical also allows to obtain μ,T,k…
A. Omran et al. PRL **115**, 263001 (2015)


Single Site Addressing
Ch. Weitenberg et al., Nature 471, 319-324 (2011)

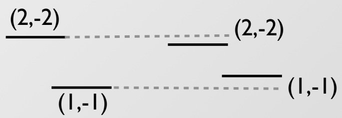
Addressing

Coherent Addressing of Atoms



Differential light shift allows to coherently address single atoms!

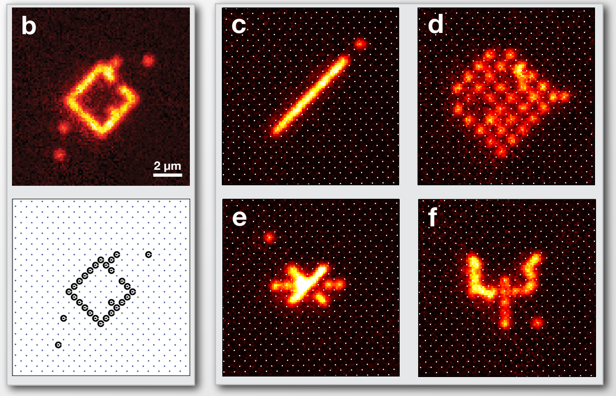
Landau-Zener Microwave sweep to coherently convert atoms between spin-states.



D.S.Weiss et al., PRA (2004),
Zhang *et al.*, PRA (2006)

Addressing

Coherent Spin Flips - Positive Imaging

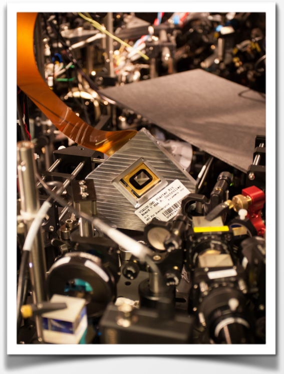


Subwavelength spatial resolution: 50 nm

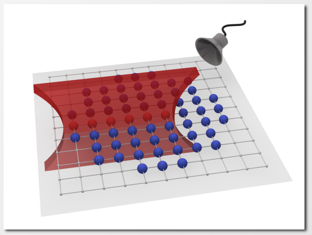
Ch. Weitenberg et al., Nature **471**, 319-324 (2011)

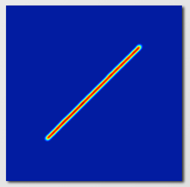
Addressing

Arbitrary Light Patterns

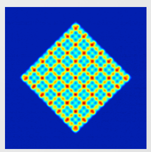


Digital Mirror Device (DMD)

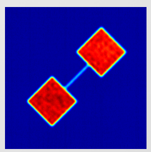




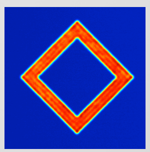
Measured Light Pattern



Exotic Lattices



Quantum Wires



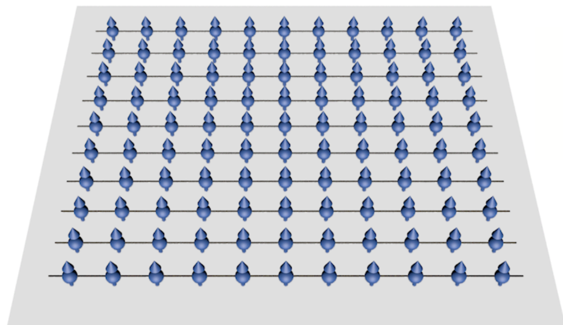
Box Potentials

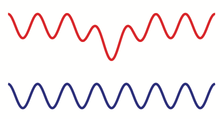
Almost Arbitrary Light Patterns Possible!

Single Spin Impurity Dynamics, Domain Walls, Quantum Wires, Novel Exotic Lattice Geometries, ...

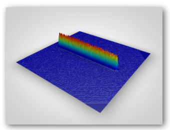
DMD Adressing

Spin impurity dynamics





|2> = |F=2, m$_F$=-2>
|1> = |F=1, m$_F$=-1>

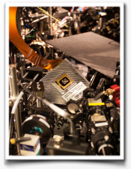


Line-shaped light field created with DMD SLM

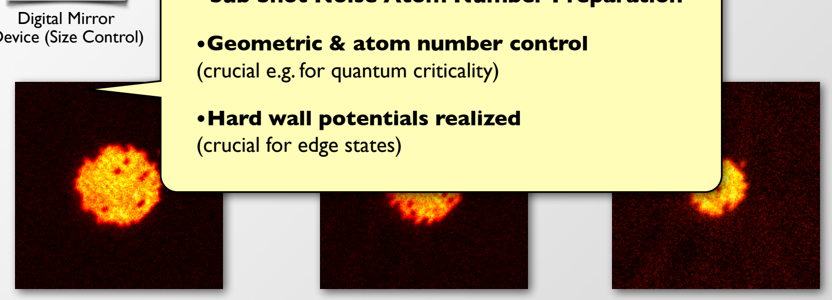
T. Fukuhara et al., Nature Physics **9**, 235 (2013)

DMD Adressing

Ultimate Size Control in 2D



Digital Mirror Device (Size Control)



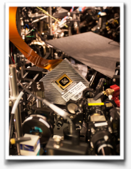
Fluctuating Size and

- **Sub Shot Noise Atom Number Preparation**
- **Geometric & atom number control** (crucial e.g. for quantum criticality)
- **Hard wall potentials realized** (crucial for edge states)

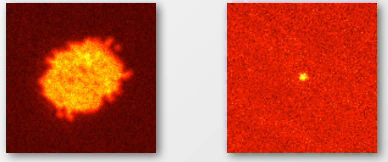
Size & atom number perfectly controlled

DMD Adressing

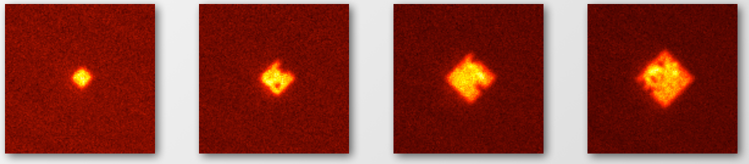
Ultimate Size Control in 2D



Digital Mirror Device (Size Control)



Initial MI — Single Atom

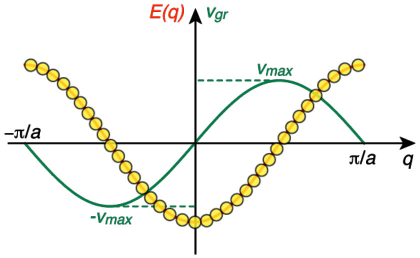


3x3 — 5x5 — 7x7 — 8x8

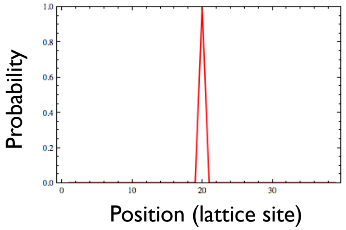
atoms

Addressing

Tunneling of a Single Atom

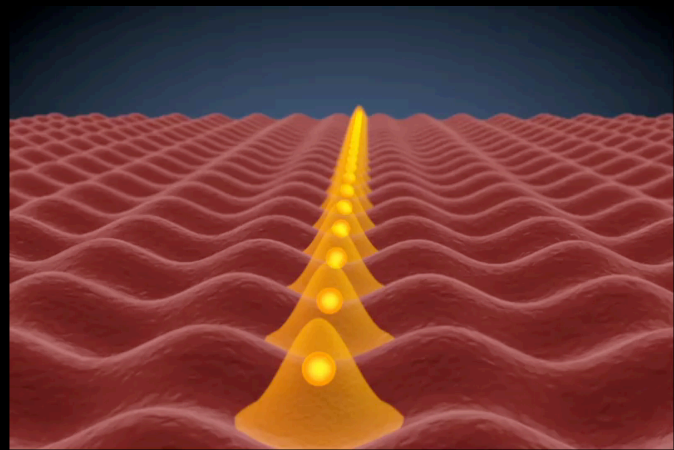


$$v_{max} = \frac{2Ja}{\hbar}$$



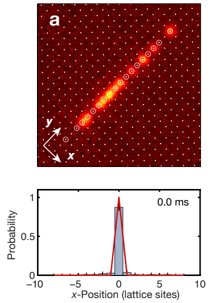
$$H = -J^{(0)} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{1}{2} m\omega^2 a_{\text{lat}}^2 i^2 \hat{n}_i$$

Single Atom Tunnelling



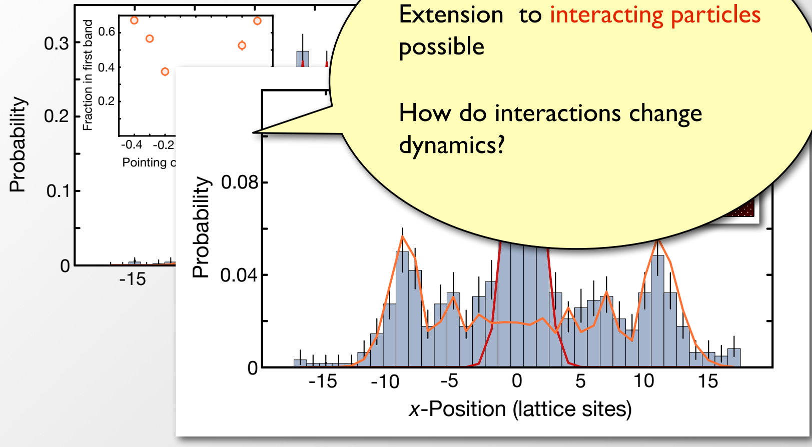
Addressing

Motional State Affected?



see exp: Y. Silberberg (photonic waveguides), D. Meschede & R. Blatt (quantum walks)...

Addressing



Extension to interacting particles possible

How do interactions change dynamics?

Excellent agreement with simulation.

Light-Cone Like Spreading of Correlations in a Many-Body System

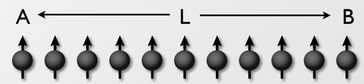
M. Cheneau, P. Barmettler, D. Poletti, M. Endres, P. Schauß, T. Fukuhara, Ch. Gross, I. Bloch, C. Kollath, S. Kuhr

M. Cheneau et al., Nature **481**, 484 (2012)
T. Langen et al. Nat. Physics **9**, 640 (2013)
P. Jurcevic et al. Nature (2014), Ph. Richerme et al. Science (2014)

www.quantum-munich.de

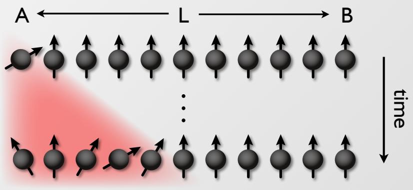
Lieb-Robinson bounds

Spin chain
short-range interactions



Lieb-Robinson bounds

Spin chain
short-range interactions

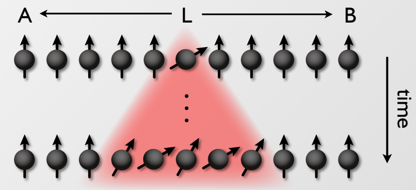


Lieb and Robinson (1972)

$$\left|[A, B(t)]\right| \leq \lambda \exp\left(\frac{vt - L}{\zeta}\right)$$

Lieb-Robinson bounds

Spin chain
short-range interactions



Bravyi, Hastings and Verstraete (2006)
Calabrese and Cardy (2006)
Eisert and Osborne (2006)
Nachtergaele, Ogata and Sims (2006)
... and many others since then

$$\left|\langle A(t)B(t)\rangle - \langle A(t)\rangle\langle B(t)\rangle\right| \leq \lambda' \exp\left(\frac{vt - L/2}{\zeta'}\right)$$

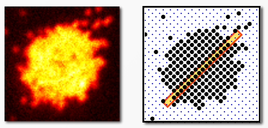
the propagation of correlations is bounded by an effective light cone

1D Mott insulator out of equilibrium

1. Prepare 1D Mott insulator with $U/J \gg 1$

deep lattice (20 E_r)
no tunnelling

variable
lattice depth



1D Mott insulator out of equilibrium

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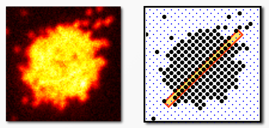
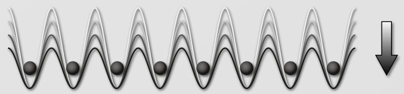
lattice depth



2. Lower U/J abruptly



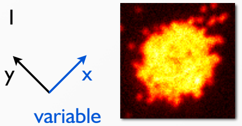
quench

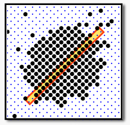
1D Mott insulator out of equilibrium

1. Prepare 1D Mott insulator with $U/J \gg 1$

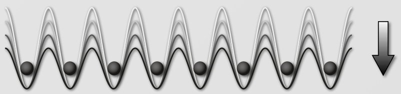
deep lattice (20 E_r)
no tunnelling

variable lattice depth





2. Lower U/J abruptly



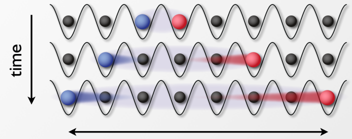
3. Record the dynamics

The initial state is highly excited. Calabrese and Cardy (2006)

Quasiparticles are emitted and propagate ballistically, carrying correlations across the system.

Light-cone like spreading of correlations

- Quasiparticle dynamics



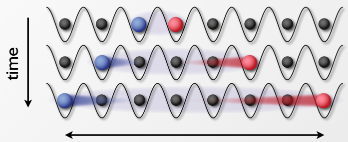
- Two-point parity correlation function

$$C_d(t) = \langle s_j(t) s_{j+d}(t)\rangle - \langle s_j(t)\rangle\langle s_{j+d}(t)\rangle \longrightarrow \begin{cases} \simeq 0 & \text{in the initial state} \\ > 0 & \text{when } t \simeq d/v \end{cases}$$

$$s_j(t) = e^{i\pi[n_j(t)-\bar{n}]} \begin{cases} +1 & \text{if (one atom)} \\ -1 & \text{if (empty) or (two atoms)} \end{cases}$$

Light-cone like spreading of correlations

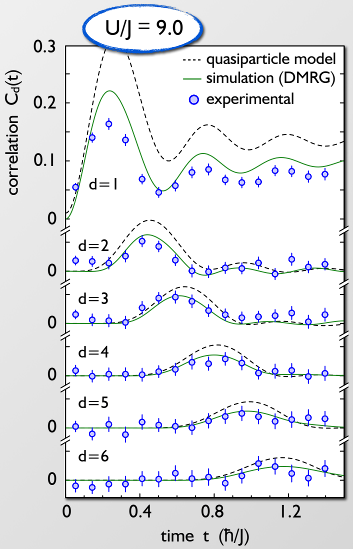
- Quasiparticle dynamics



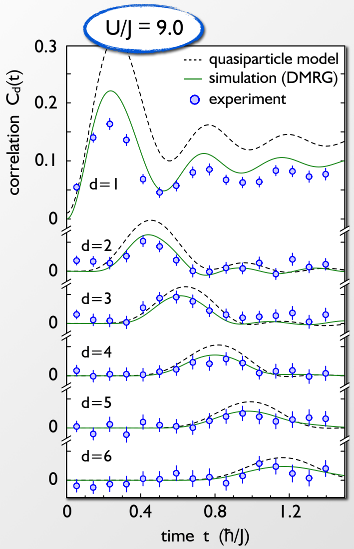
- Two-point parity correlation function

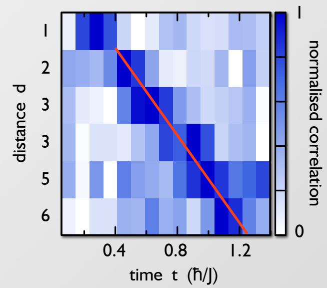
$$C_d(t) = \langle s_j(t) s_{j+d}(t)\rangle - \langle s_j(t)\rangle\langle s_{j+d}(t)\rangle$$

$$s_j(t) = e^{i\pi[n_j(t)-\bar{n}]} \begin{cases} +1 & \text{if (one atom)} \\ -1 & \text{if (empty) or (two atoms)} \end{cases}$$



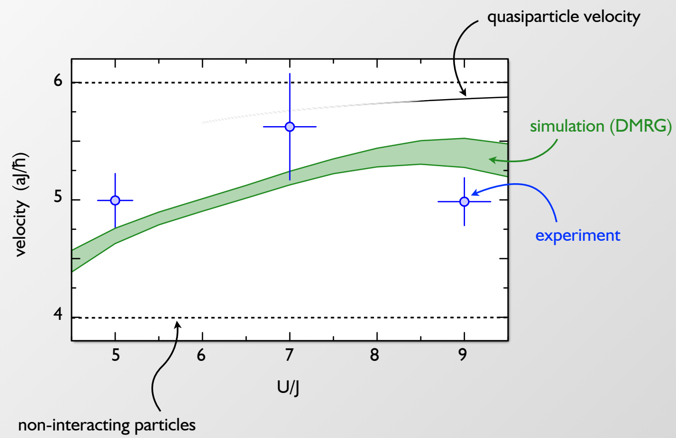
Light-cone like spreading of correlations

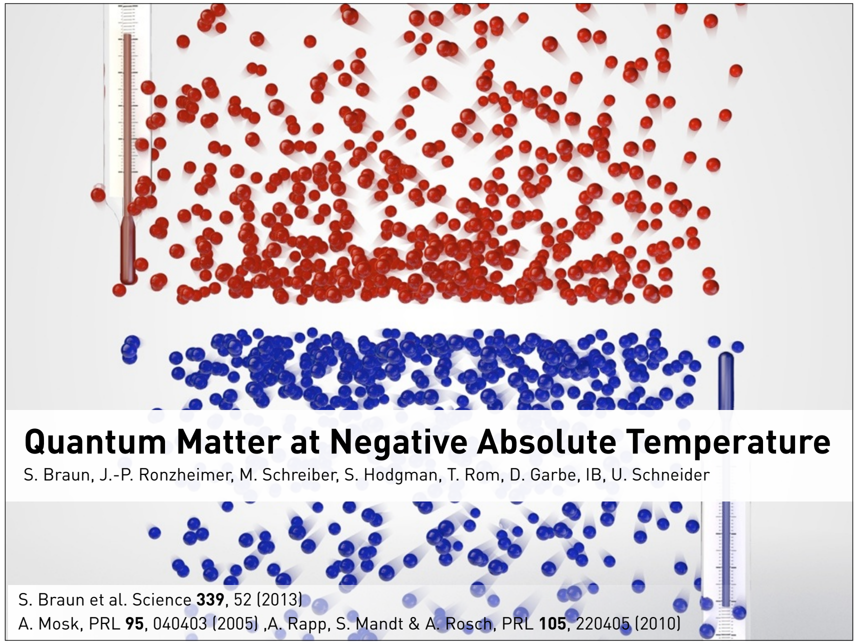




effective light-cone!

Spreading velocity





Quantum Matter at Negative Absolute Temperature

S. Braun, J.-P. Ronzheimer, M. Schreiber, S. Hodgman, T. Rom, D. Garbe, IB, U. Schneider

S. Braun et al. Science **339**, 52 (2013)
A. Mosk, PRL **95**, 040403 (2005) ,A. Rapp, S. Mandt & A. Rosch, PRL **105**, 220405 (2010)

Thermodynamic Definition of Temperature

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right.$$

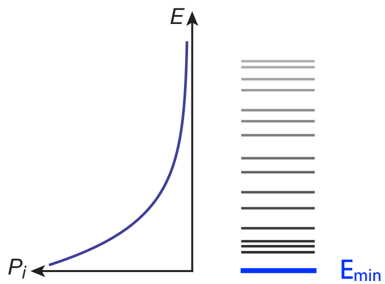
...mperature
...ith Energy

Warning:
Temperature does not measure energy content!!!

...erature
...s with Energy

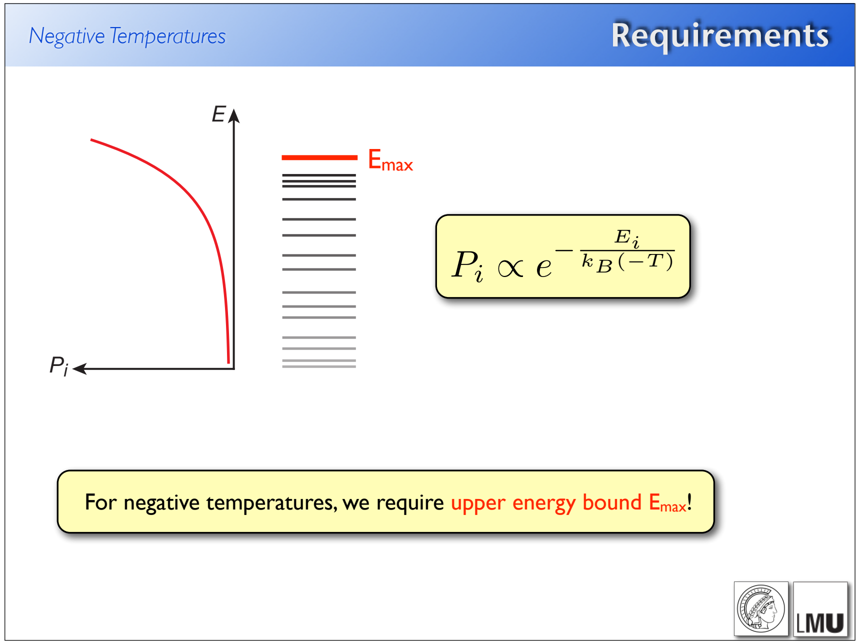
Thermodynamic theorems apply in negative as well as positive temperature regime!

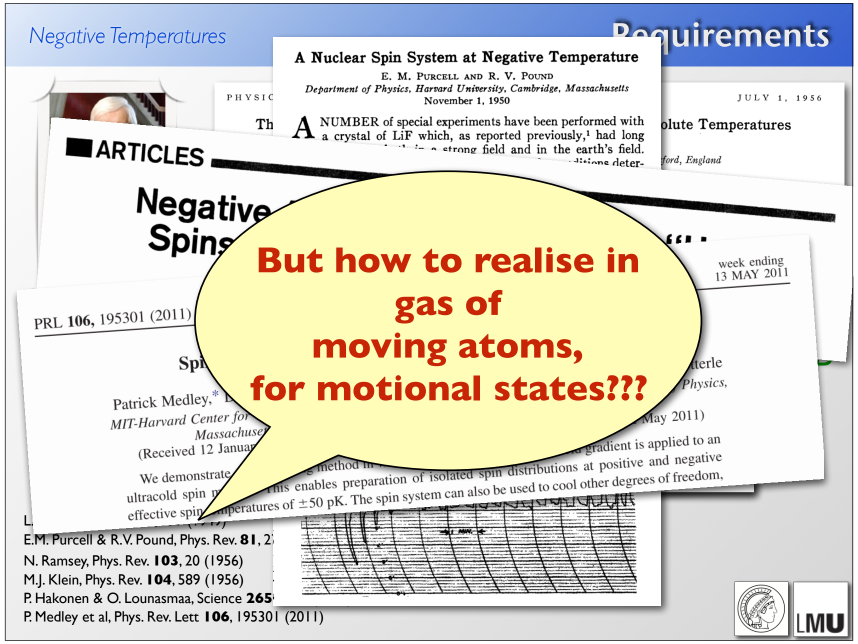
Requirements

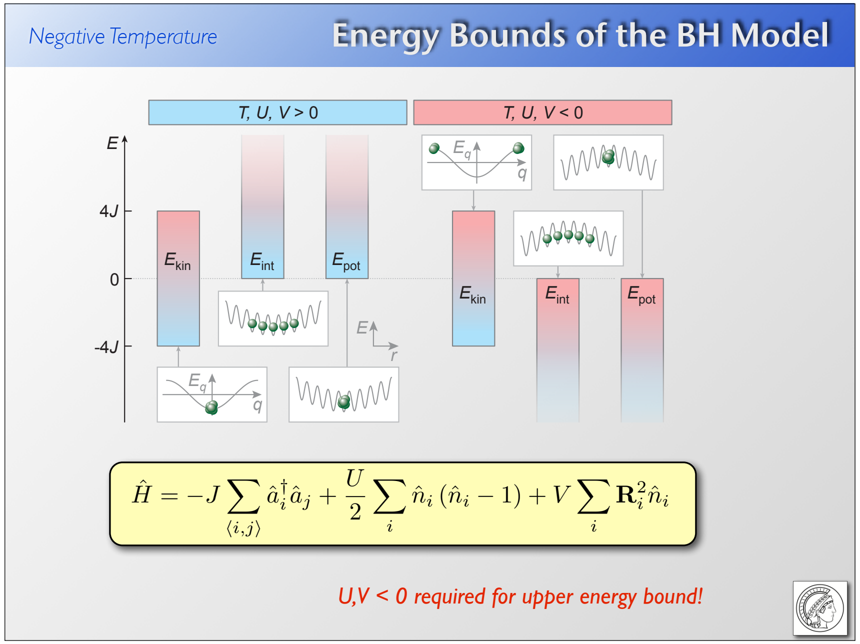


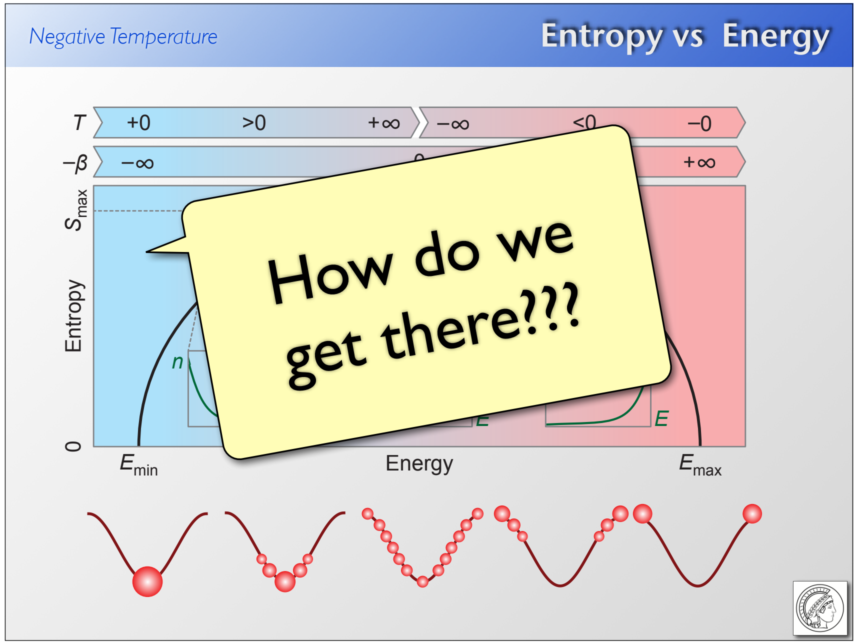
$$P_i \propto e^{-\frac{E_i}{k_B T}}$$

For positive temperatures, we require lower energy bound E_{min}!

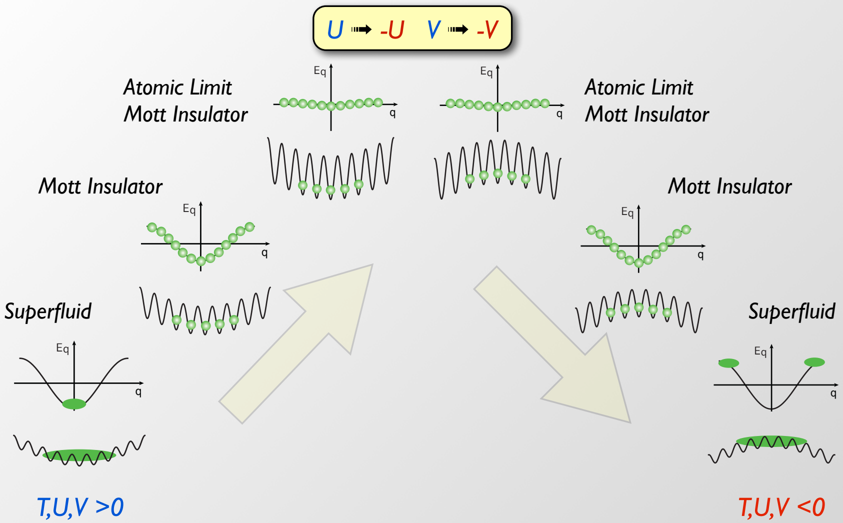

Negative Temperatures
Requirements
E
E_{max}
P_i
$P_i \propto e^{-\frac{E_i}{k_B(-T)}}$
For negative temperatures, we require upper energy bound E_{max}!


Negative Temperatures
Requirements
A Nuclear Spin System at Negative Temperature
E. M. Purcell and R. V. Pound
Department of Physics, Harvard University, Cambridge, Massachusetts
November 1, 1950
ARTICLES
Negative
Spins
PRL 106, 195301 (2011)
Patrick Medley,
MIT-Harvard Center for
week ending
13 MAY 2011
But how to realise in gas of moving atoms, for motional states???
E.M. Purcell & R.V. Pound, Phys. Rev. 81, 2
N. Ramsey, Phys. Rev. 103, 20 (1956)
M.J. Klein, Phys. Rev. 104, 589 (1956)
P. Hakonen & O. Lounasmaa, Science 265
P. Medley et al, Phys. Rev. Lett 106, 195301 (2011)


Negative Temperature
Energy Bounds of the BH Model
T, U, V > 0
T, U, V < 0
E
4J
0
-4J
E_{kin}
E_{int}
E_{pot}
E_q
q
E
r
$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + V \sum_i \mathbf{R}_i^2 \hat{n}_i$
U,V < 0 required for upper energy bound!


Negative Temperature
Entropy vs Energy
T
+0
>0
+∞
−∞
<0
−0
−β
−∞
+∞
S_{max}
Entropy
0
n
E
E_{min}
Energy
E_{max}
How do we get there???

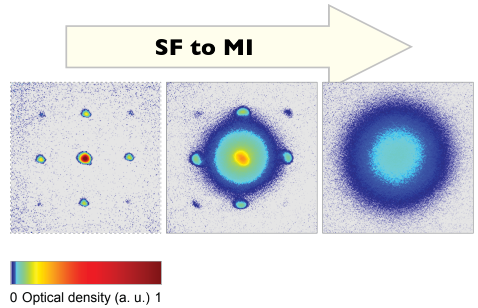
Experimental Sequence



Sequence: A. Rapp, S. Mandt & A. Rosch, PRL (2010)

Experimental Results

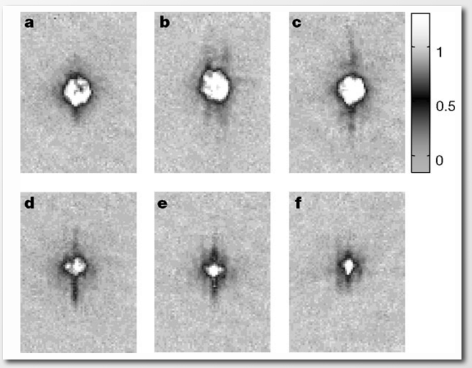
Positive Temperature w/o switching



Negative Temperature w switching

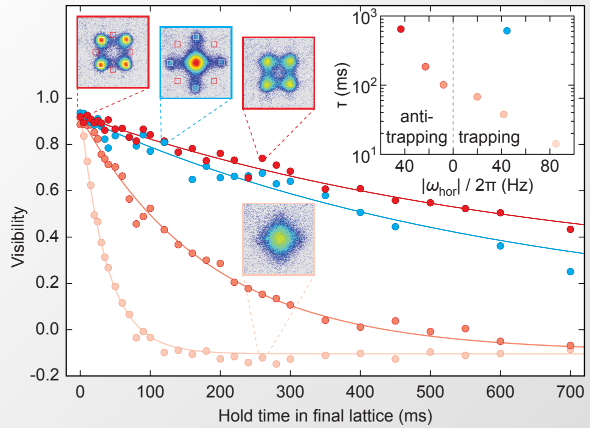
Collapse of Condensate

For attractive interactions (a<0), condensate collapses!



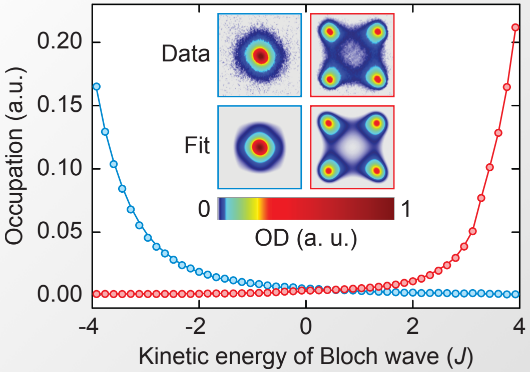
E.A. Donley et al. *Nature* **412,** 295-299 (2001)
J. M. Gerton et al. *Nature* 408, 692 (2000)

Stability



Negative Temperature State as Stable as Positive Temperature State!

Occupation of Energy States



T=-2.2J/k_B

Kinetic energy well fitted by Bose-Einstein distribution

$$n(q_x,q_y)=\frac{1}{e^{(E_{kin}(q_x,q_y)-\mu)/k_BT}-1}$$

$$E_{kin}(q_x,q_y)=-2J\left[\cos(q_xd)+\cos(q_yd)\right]$$

Implications

Gases with **negative temperature** possess **negative pressure**!

$$\left.\frac{\partial S}{\partial V}\right|_E \geq 0 \qquad \text{and} \qquad dE=TdS-PdV$$

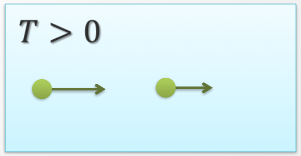
$$\Rightarrow \left.\frac{\partial S}{\partial V}\right|_E = \frac{P}{T} \geq 0$$

Carnot engines **above unit efficiency!** **(but no perpetuum mobile!)**

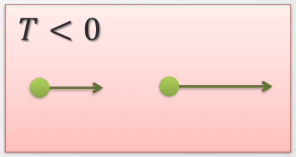
$$\eta=\frac{W}{Q_1}=1-\frac{T_2}{T_1}$$

Some statements for the second law of thermodynamics become invalid!

Anti-Friction at Negative Temperature



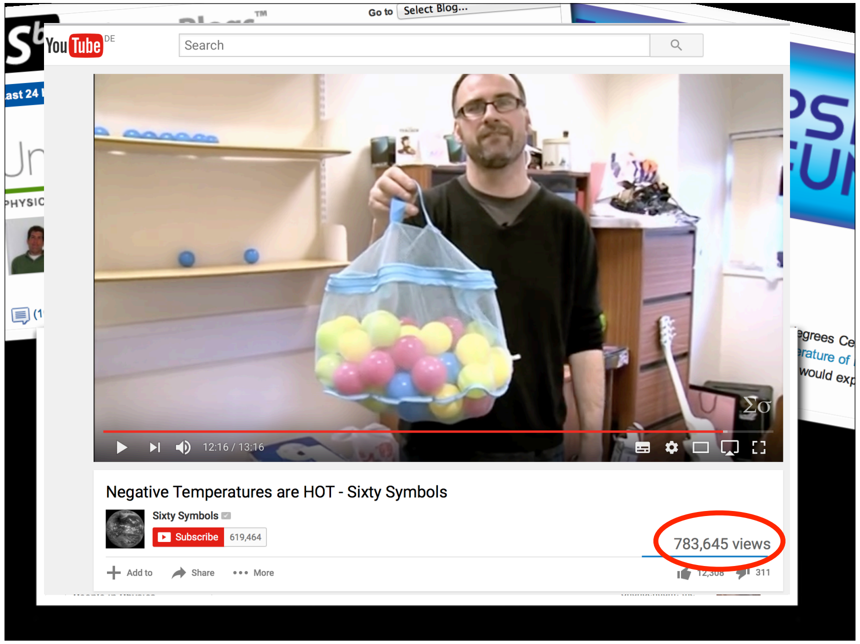
Friction:
- entropy increases
  - → Medium heats up
- Particle slows down



Anti-Friction:
- entropy increases
  - → Medium cools down
- Particle accelerates

(but direction is randomized in long-term limit)

particle spectrum is assumed to be unbounded



Atoms in Periodic Potentials

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Single Particle in a Periodic Potential - Band Structure (1)

$$H\phi_q^{(n)}(x) = E_q^{(n)}\phi_q^{(n)}(x) \qquad \text{with} \qquad H = \frac{1}{2m}\hat{p}^2 + V(x)$$

Solved by Bloch waves (periodic functions in lattice period)

$$\phi_q^{(n)}(x) = e^{iqx}\cdot u_q^{(n)}(x)$$

q = Crystal Momentum or Quasi-Momentum

n = Band index

Plugging this into Schrödinger Equation, gives:

$$H_B u_q^{(n)}(x) = E_q^{(n)} u_q^{(n)}(x) \qquad \text{with} \qquad H_B = \frac{1}{2m}(\hat{p}+q)^2 + V_{lat}(x)$$

Single Particle in a Periodic Potential - Band Structure (2)

Use Fourier expansion

$$V(x) = \sum_r V_r e^{i2rkx} \qquad \text{and} \qquad u_q^{(n)}(x) = \sum_l c_l^{(n,q)} e^{i2lkx}$$

yields for the potential energy term

$$V(x)u_q^{(n)}(x) = \sum_l \sum_r V_r e^{i2(r+l)kx} c_l^{(n,q)}$$

and the kinetic energy term

$$\frac{(\hat{p}+q)^2}{2m} u_q^{(n)}(x) = \sum_l \frac{(2\hbar k l + q)^2}{2m} c_l^{(n,q)} e^{i2lkx}.$$

In the experiment standing wave interference pattern gives

$$V(x) = V_{lat}\sin^2(kx) = -\frac{1}{4}\left(e^{2ikx} + e^{-2ikx}\right) + \text{c.c.}$$

Single Particle in a Periodic Potential - Band Structure (3)

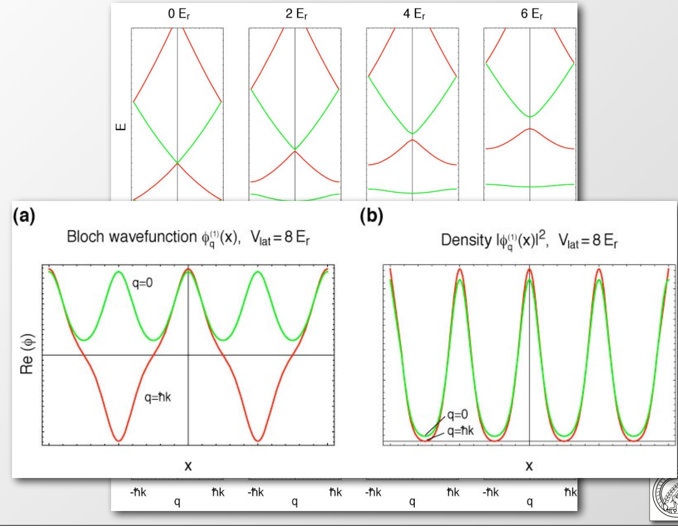
Use Fourier expansion

$$\sum_l H_{l,l'} \cdot c_l^{(n,q)} = E_q^{(n)} c_l^{(n,q)} \quad \text{with} \quad H_{l,l'} = \begin{cases} (2l + q/\hbar k)^2 E_r & \text{if } l = l' \\ -1/4 \cdot V_0 & \text{if } |l - l'| = 1 \\ 0 & \text{else} \end{cases}$$

$$\begin{pmatrix} (q/\hbar k)^2 E_r & -\frac{1}{4}V_0 & 0 & 0 & \cdots \\ -\frac{1}{4}V_0 & (2+q/\hbar k)^2 E_r & -\frac{1}{4}V_0 & 0 & \\ 0 & -\frac{1}{4}V_0 & (4+q/\hbar k)^2 E_r & -\frac{1}{4}V_0 & \\ & & -\frac{1}{4}V_0 & \ddots & \end{pmatrix} \begin{pmatrix} c_0^{(n,q)} \\ c_1^{(n,q)} \\ c_2^{(n,q)} \\ \vdots \end{pmatrix} = E_q^{(n)} \begin{pmatrix} c_0^{(n,q)} \\ c_1^{(n,q)} \\ c_2^{(n,q)} \\ \vdots \end{pmatrix}$$

Diagonalization gives us Eigenvalues and Eigenvectors!

Bandstructure - Blochwaves

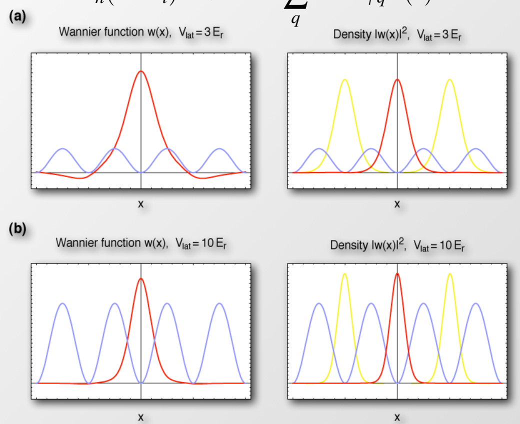


Topic

Wannier Functions

An alternative basis set to the Bloch waves can be constructed through localized wave-functions: Wannier Functions!

$$w_n(x - x_i) = \mathcal{N}^{-1/2} \sum_q e^{-iqx_i} \phi_q^{(n)}(x)$$



Dispersion Relation in a Square Lattice

$$E(q) = -2J\cos(qa)$$