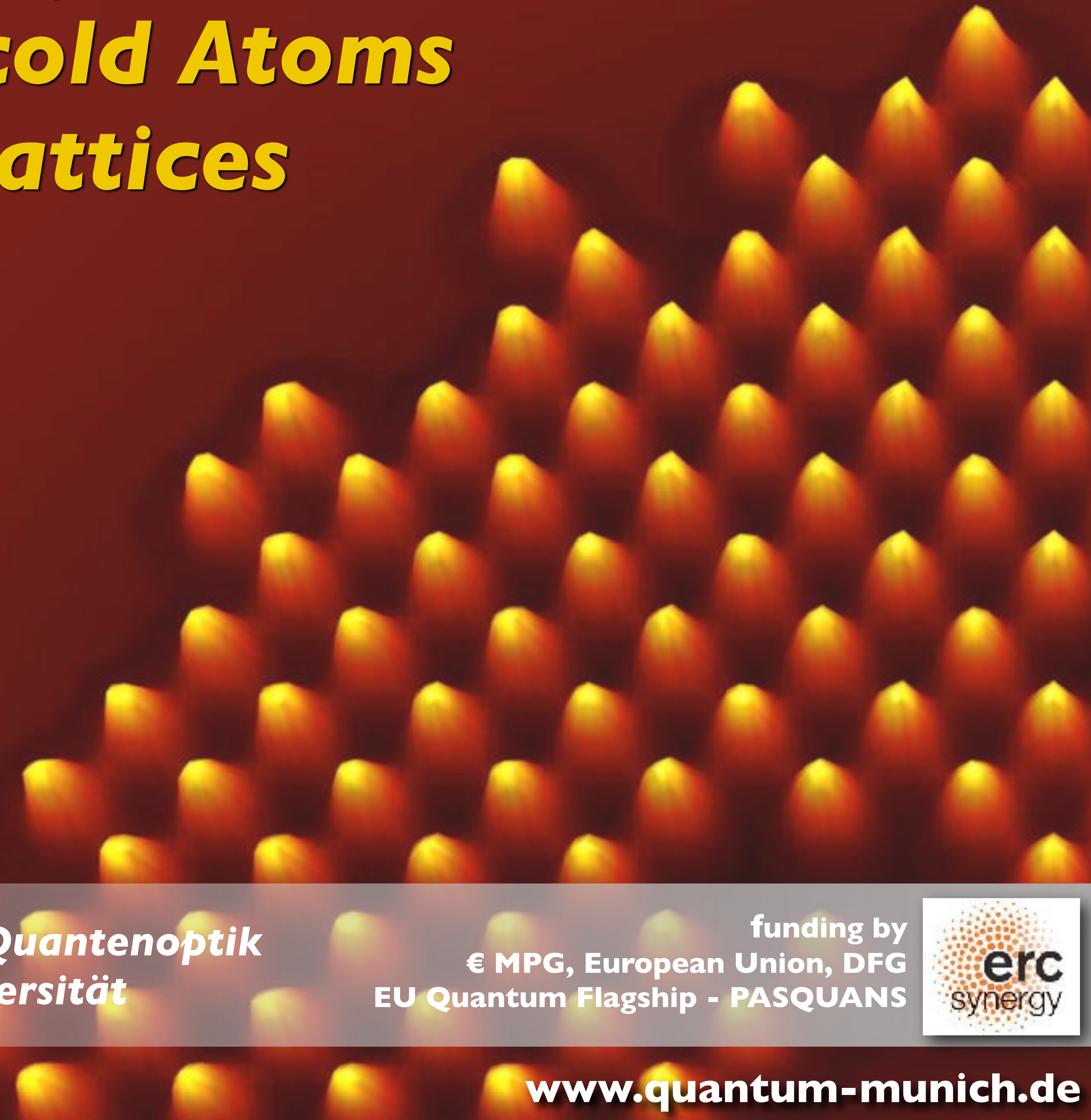
Large Scale Quantum Simulations using Ultracold Atoms in Optical Lattices

I.B.
Högberga Gård
Stockholm 2019



Max-Planck-Institut für Quantenoptik
Ludwig-Maximilians Universität

funding by
€ MPG, European Union, DFG
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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

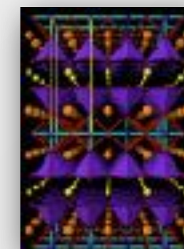
Absolute Negative Temperatures

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

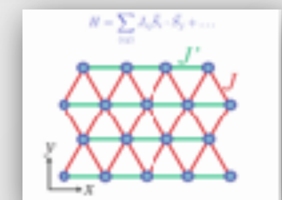
The Challenge of Many-Body Quantum Systems

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



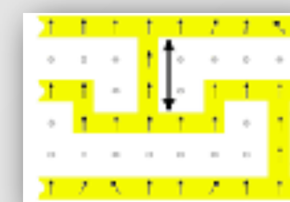
- **Technological Relevance**

  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

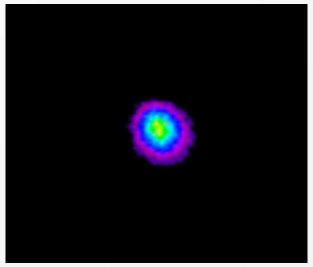
Difficulty to separate effects: probe impurities, complex interplay, masking of effects...

Many cases: even simple models "not solvable"

Need to synthesize new material **to analyze effect of parameter change**

The Challenge of Many-Body Quantum Systems

Control of single and few particles



Single Atoms and Ions

Photons

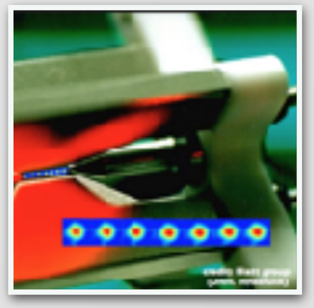
D. Wineland

S. Haroche

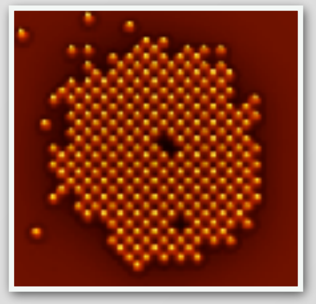
Challenge: … towards ultimate control of many-body quantum systems

R. P. Feynman's Vision

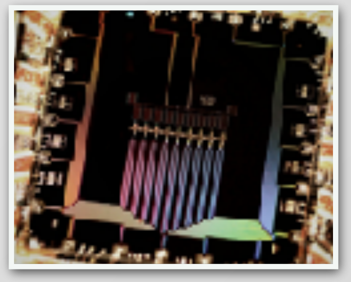
A Quantum Simulator to study the dynamics of another quantum system.



Ion Traps
(R. Blatt, Innsbruck)



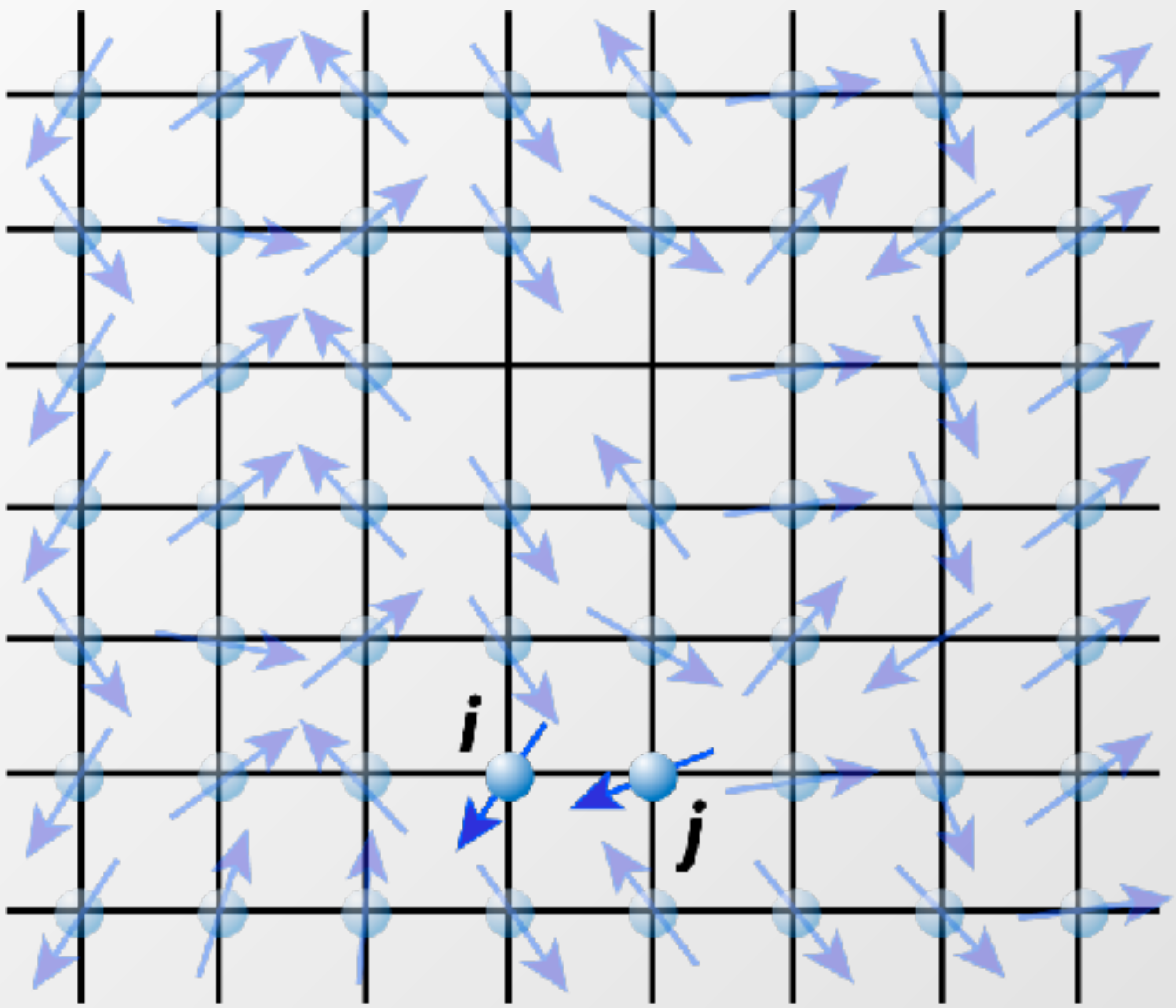
Crystal of Atoms
Bound by Light

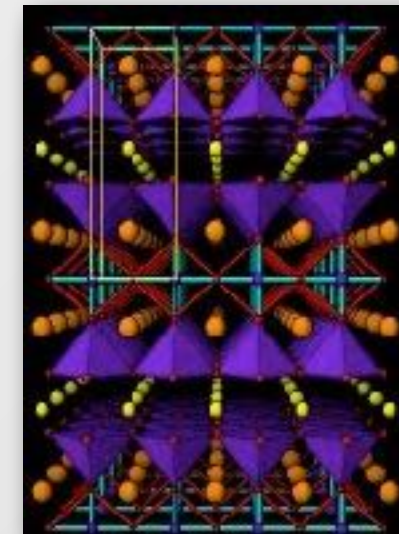


Superconducting
Devices
(J. Martinis, UCSB,
Google)

Strongly Correlated Electronic Systems

$$H = -J \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + V_0 \sum_{i,\sigma} R_i^2 \hat{n}_{i,\sigma}$$





In strongly correlated electron system spin-spin interactions exist.

$$-J_{ex} \vec{S}_i \cdot \vec{S}_j$$

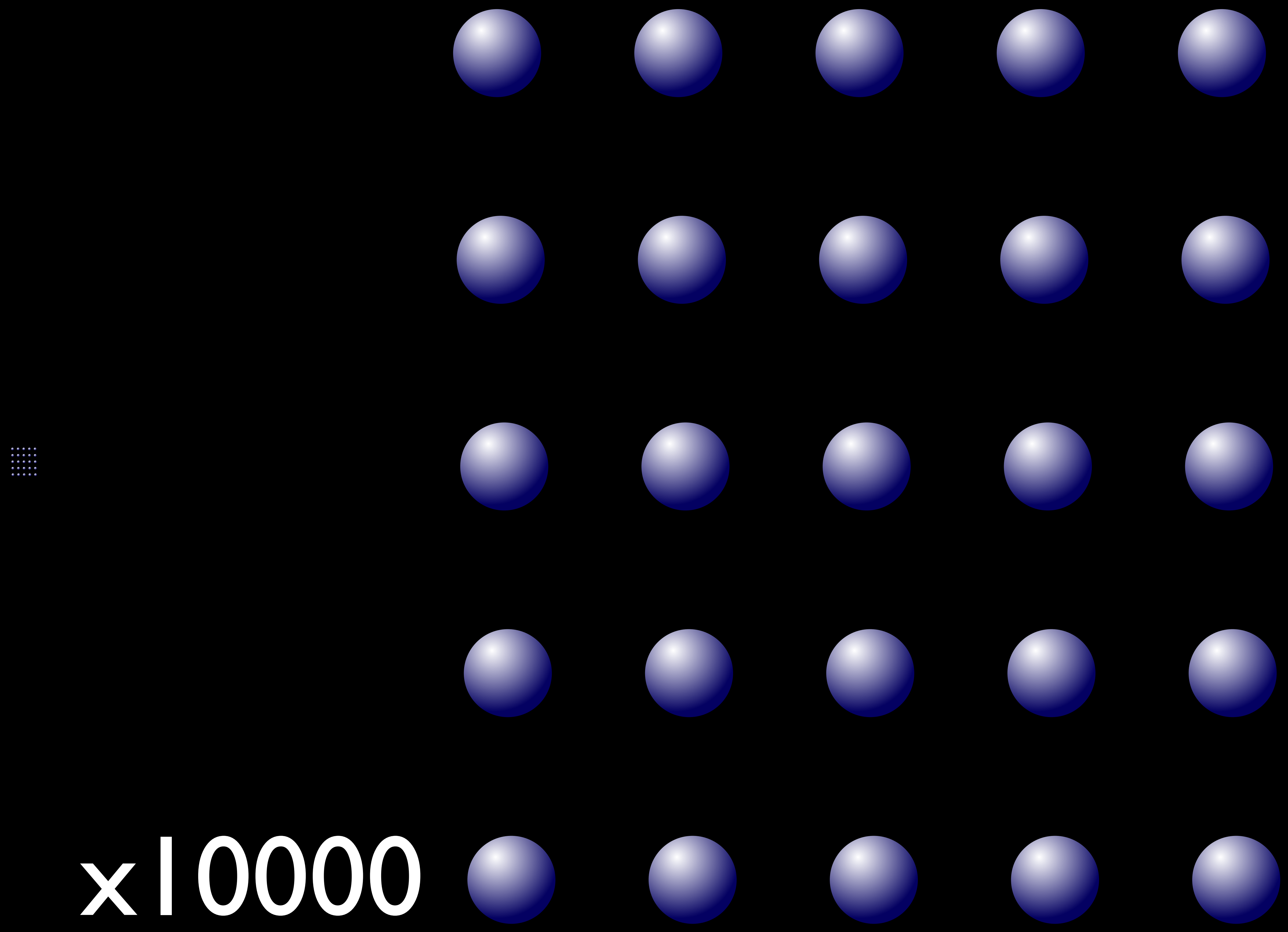
Underlying many solid state & material science problems:
Magnets, High-Tc Superconductors, Spintronics ....
see A. Georges (CdF)

Three Central Goals

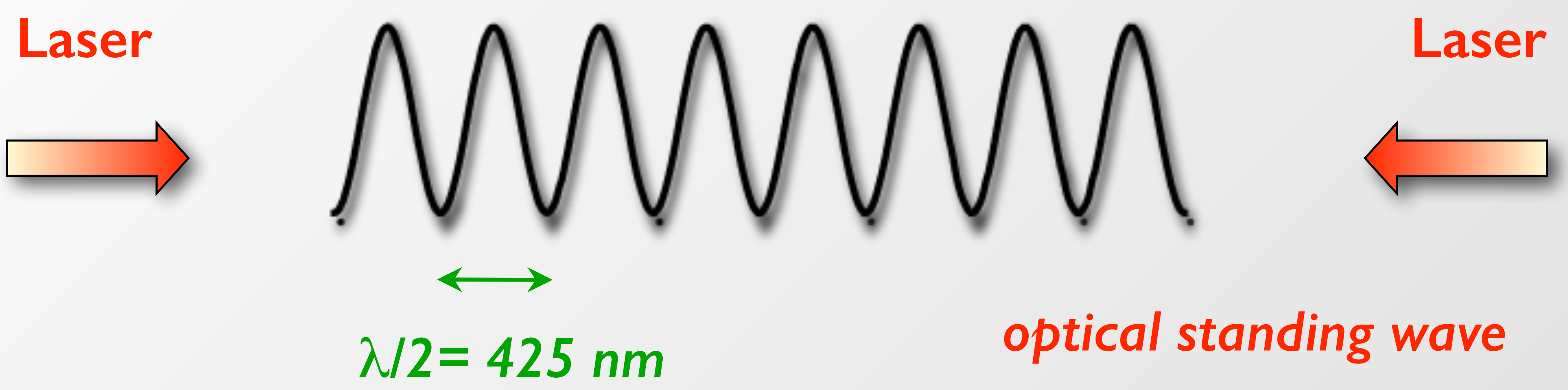
1. New probes & analysis techniques
   - new light on known phenomena -

2. Quantitative predictions
   - e.g. equation of state BEC-BCS crossover -

3. New phenomena / phases of matter
   in new regimes


x10000

Optical Lattice Potential – Perfect Artificial Crystals

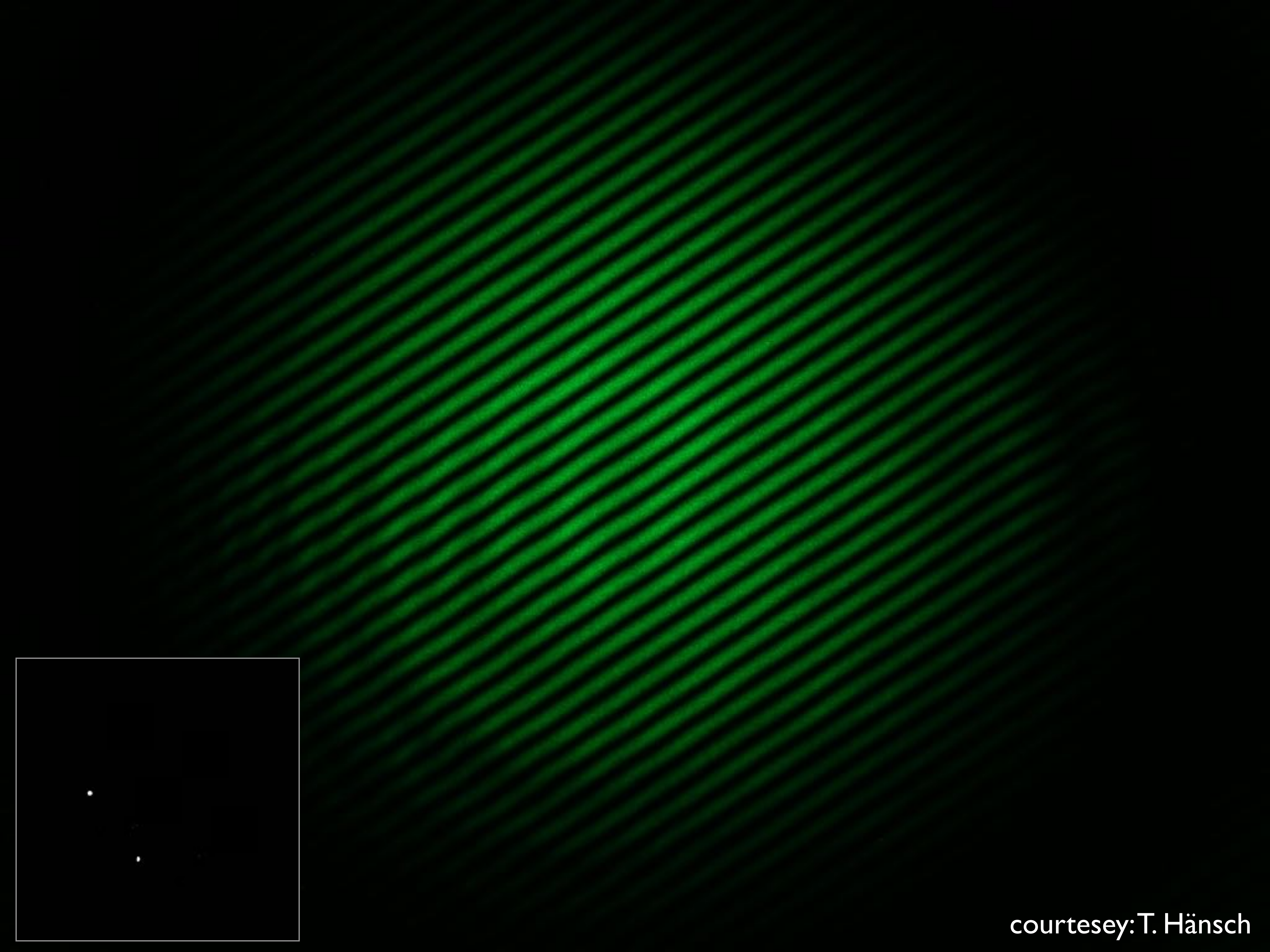


Fourier synthesize aribtrary lattices:

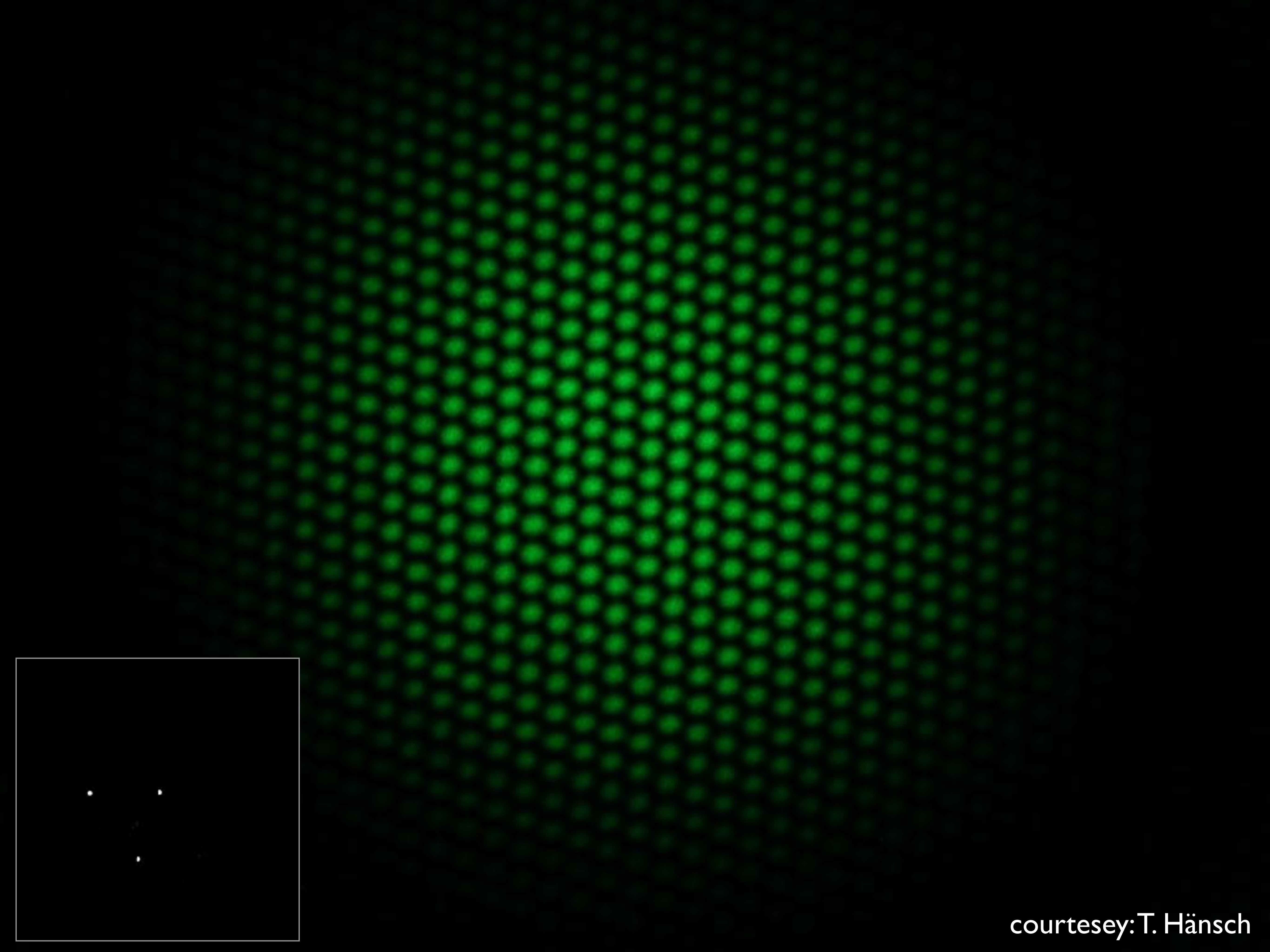
- Square
- Hexagonal/Triangular/Brick Wall
- Kagomé
- Superlattices
- *Spin dependent lattices*
- ...

Special case: flux lattices...

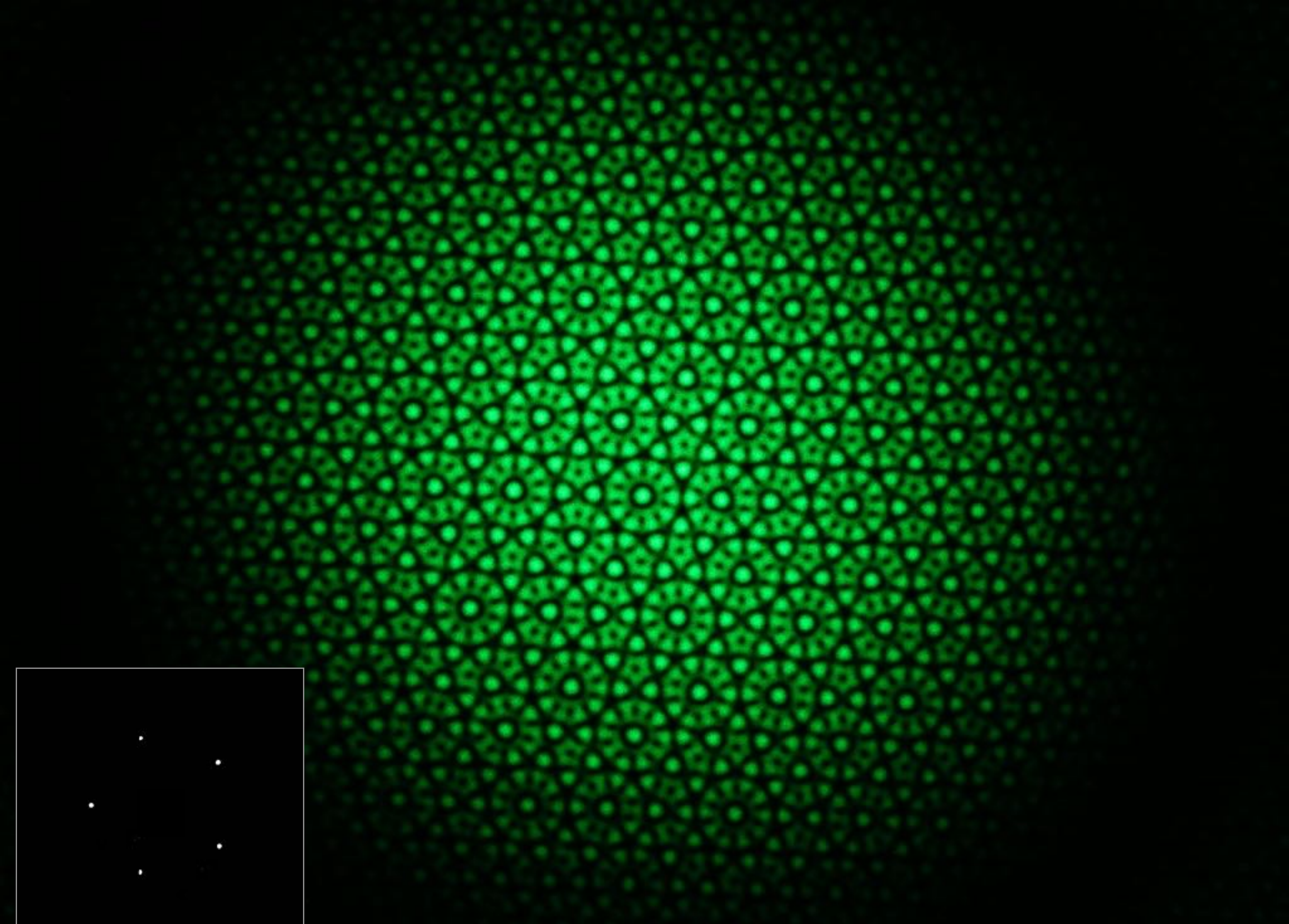
Full **dynamical** control over **lattice depth, geometry, dimensionality!**



courtesey: T. Hänsch



courtesey: T. Hänsch

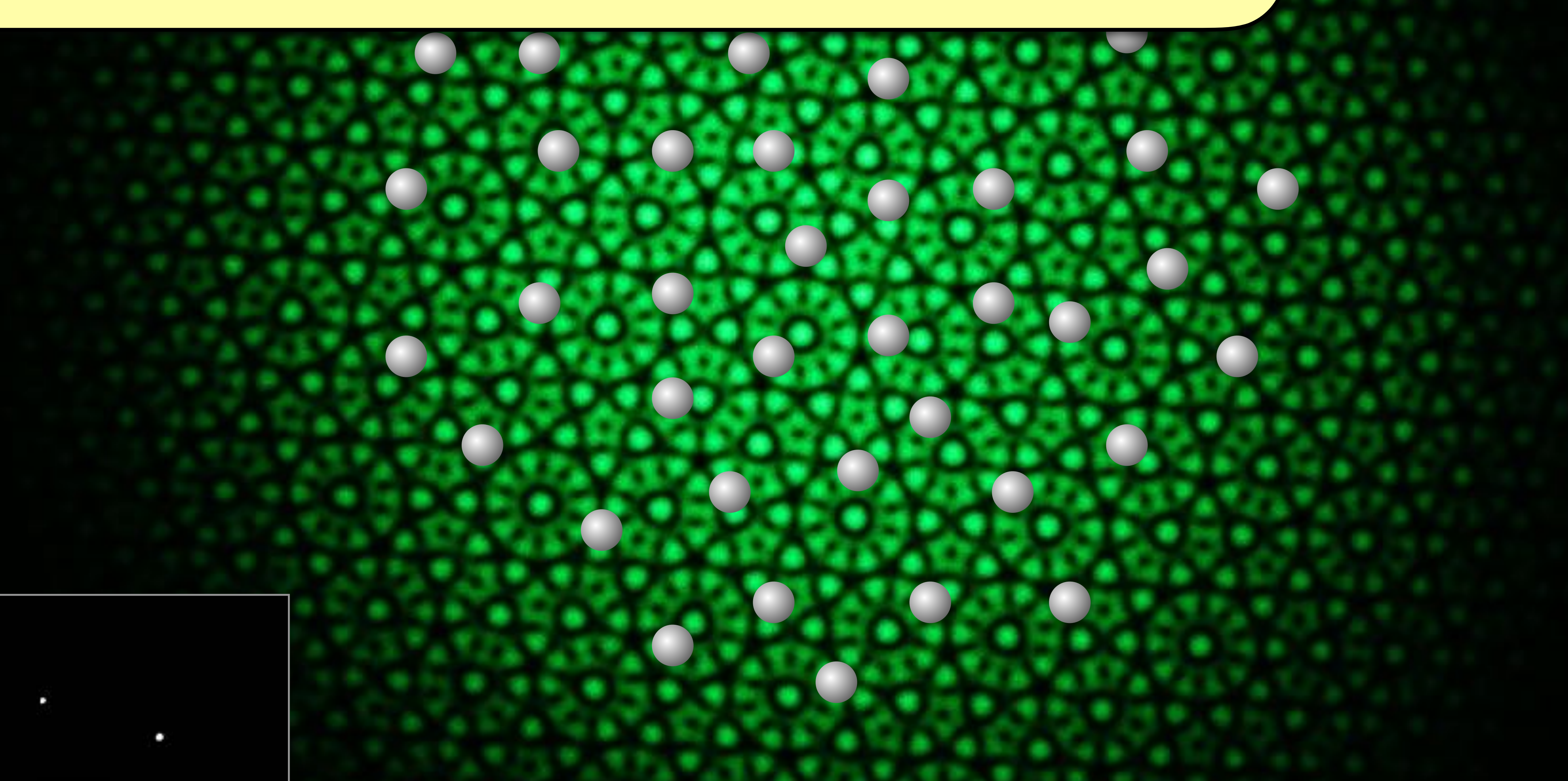


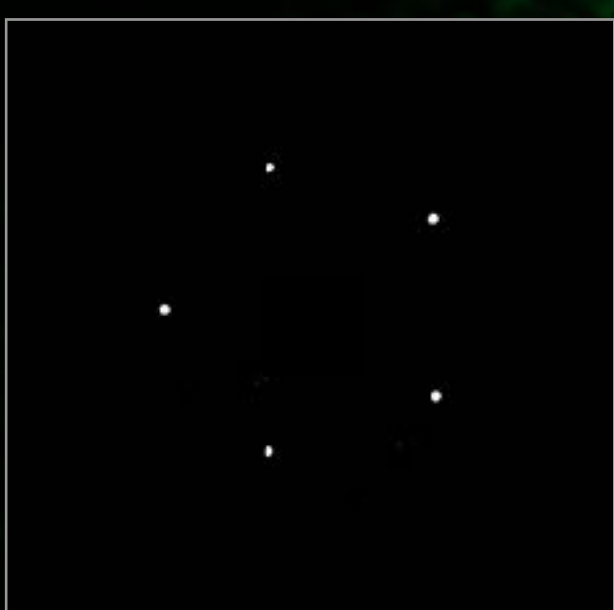
courtesey: T. Hänsch

Quantum Spin Systems

Particle Systems: Bosons, Fermions, Mixtures

Classically Intractable Computational Regimes





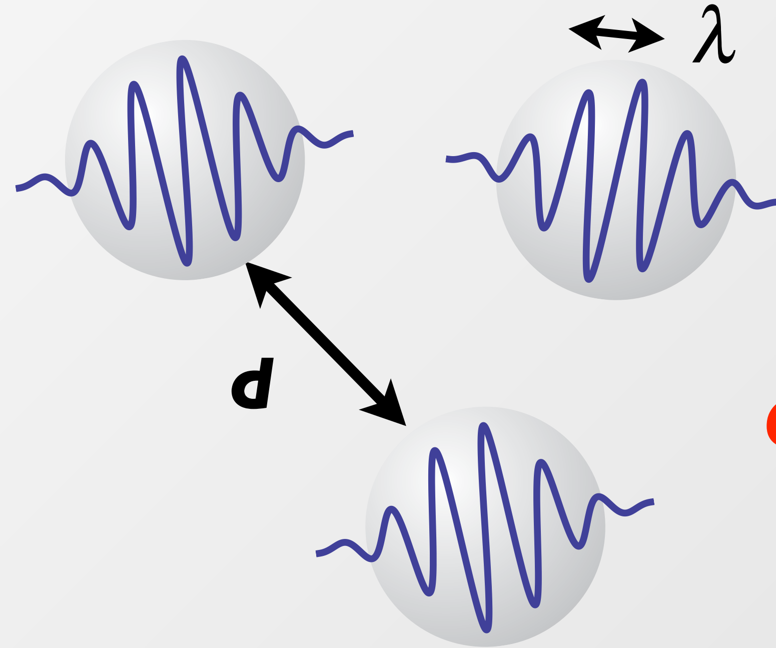
Few particles up to 1000s of particles !

courtesey: T. Hänsch

From Artificial Quantum Matter to Real Materials

Quantum Regime

$$\lambda/d \gtrsim 1$$

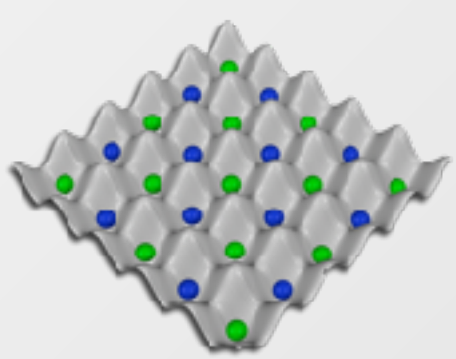


de Broglie Wavepackets

Universality of Quantum Mechanics!

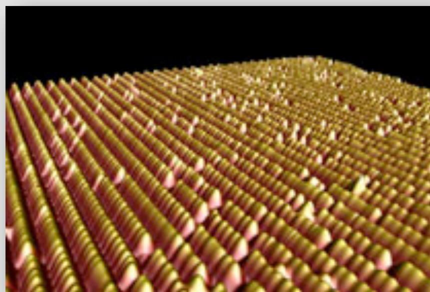
Ultracold Quantum Matter

- ***Densities:*** ***$10^{14}/cm^3$***
  (100000 times thinner than air)
- ***Temperatures:*** ***few nK***
  (100 million times lower than outer space)



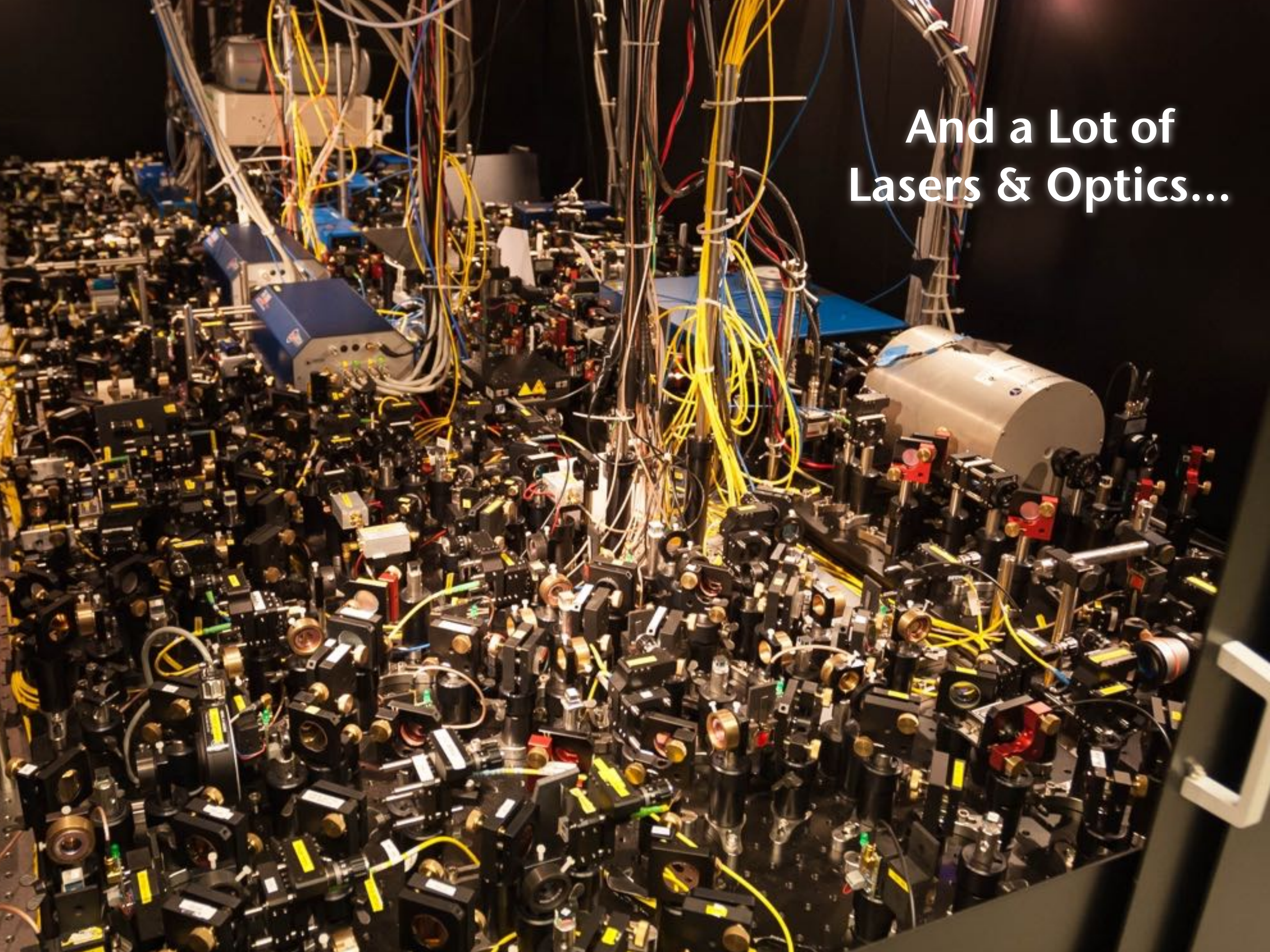
Real Materials

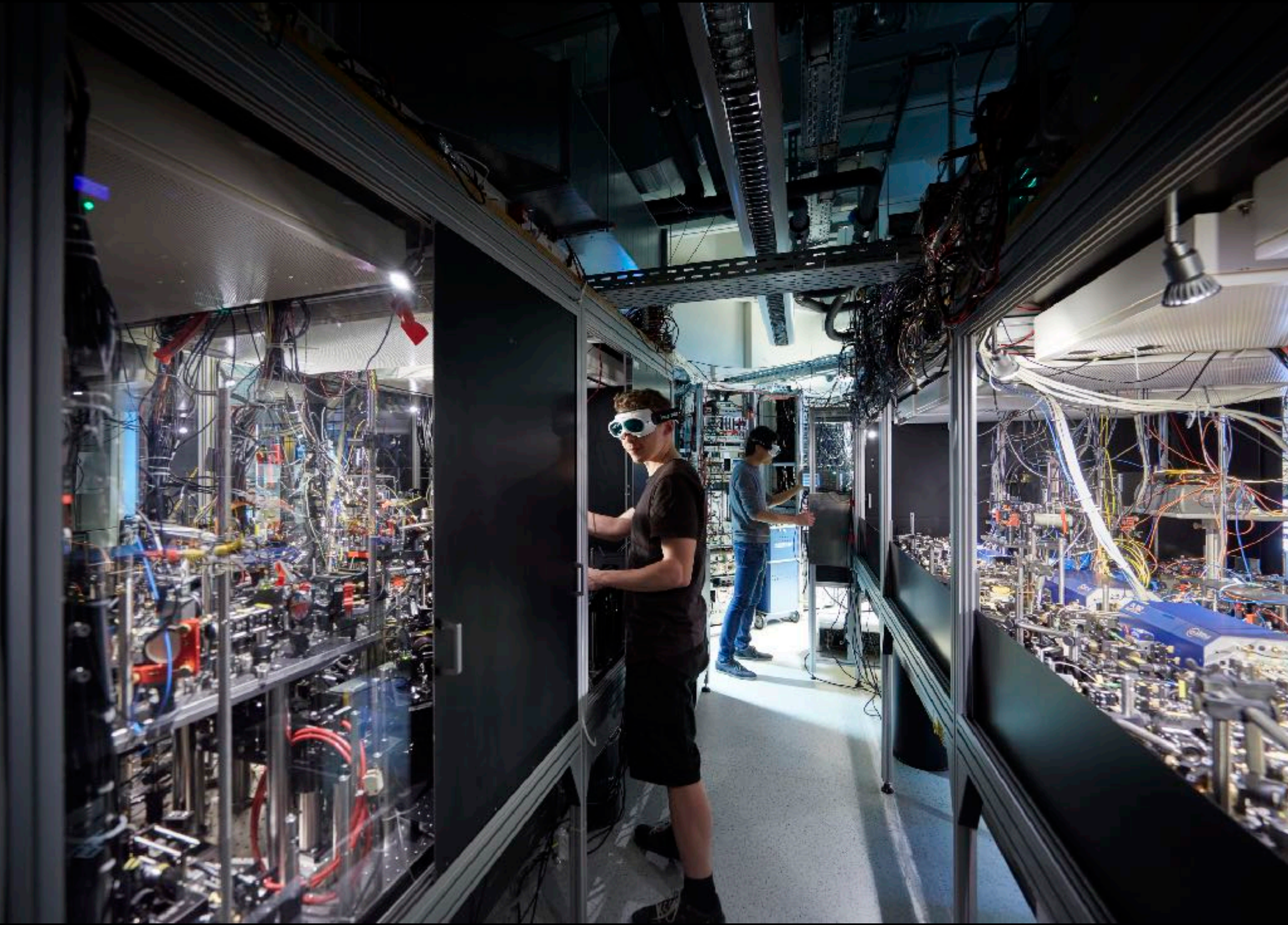
- ***Densities:*** ***10^{24}-$10^{25}/cm^3$***
- ***Temperatures:*** ***mK – several hundred K***

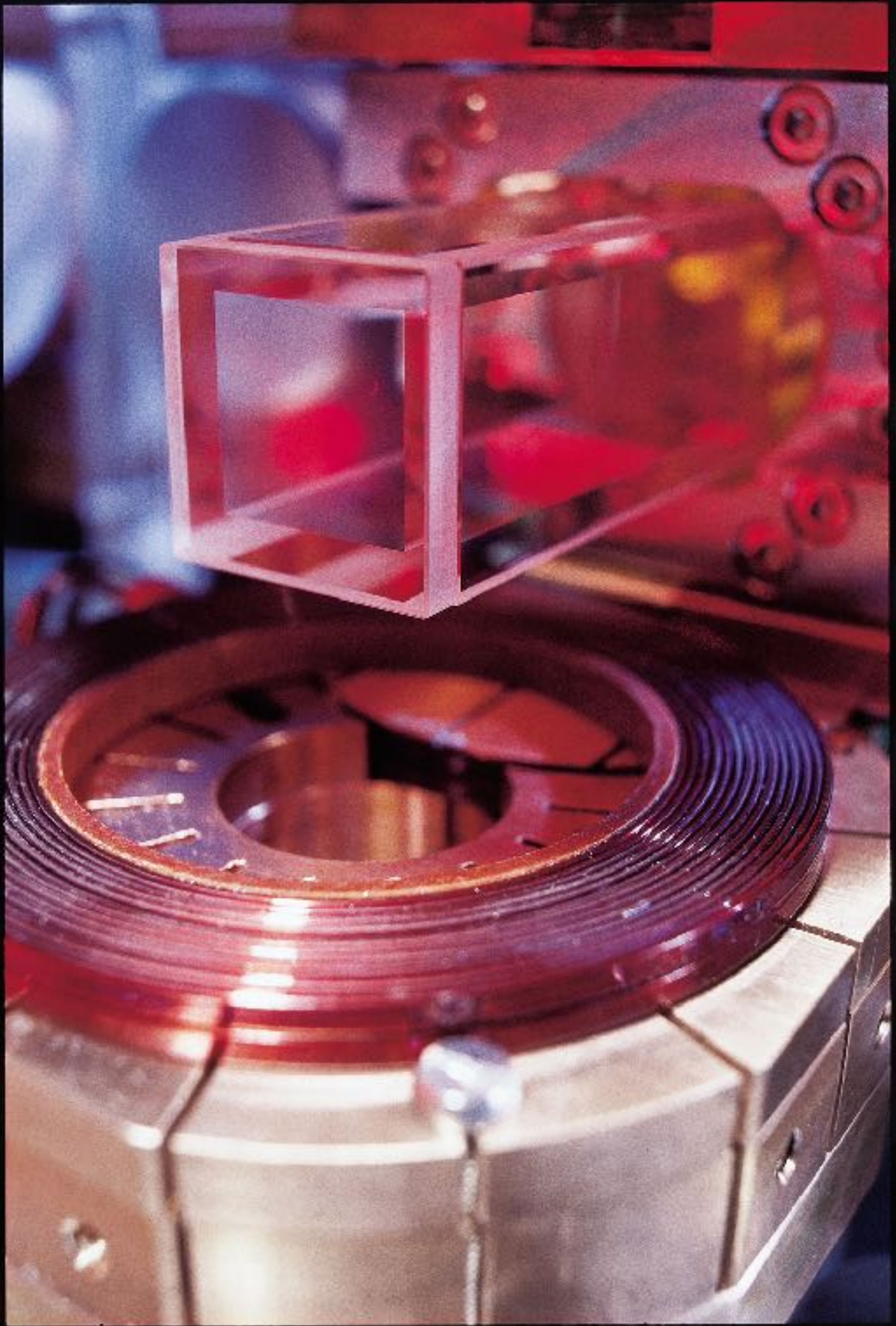


(Neuchatel)

Same λ/d !


And a Lot of
Lasers & Optics...



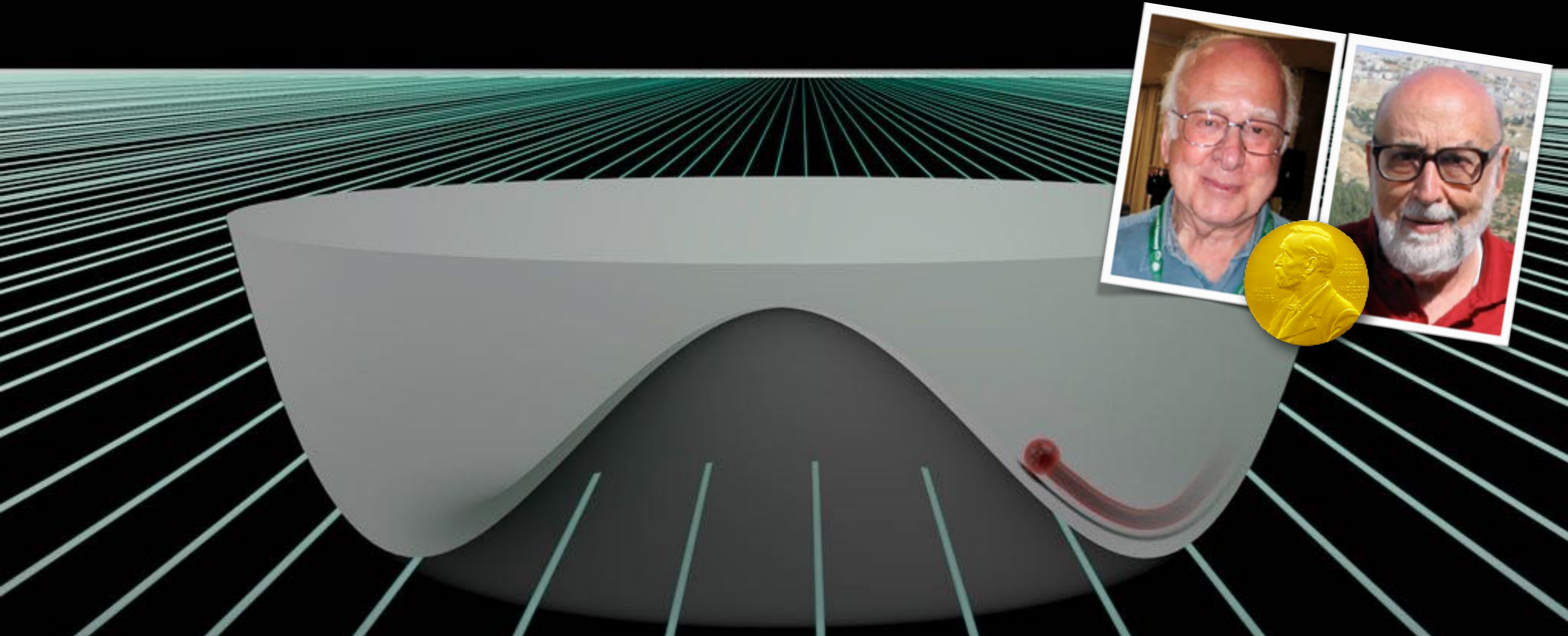


Experiments isolated from environment

Not connected to reservoirs!

Beyond Statistical Mechanics

Many-Body Localization



‘Higgs’ Amplitude Mode in Flatland

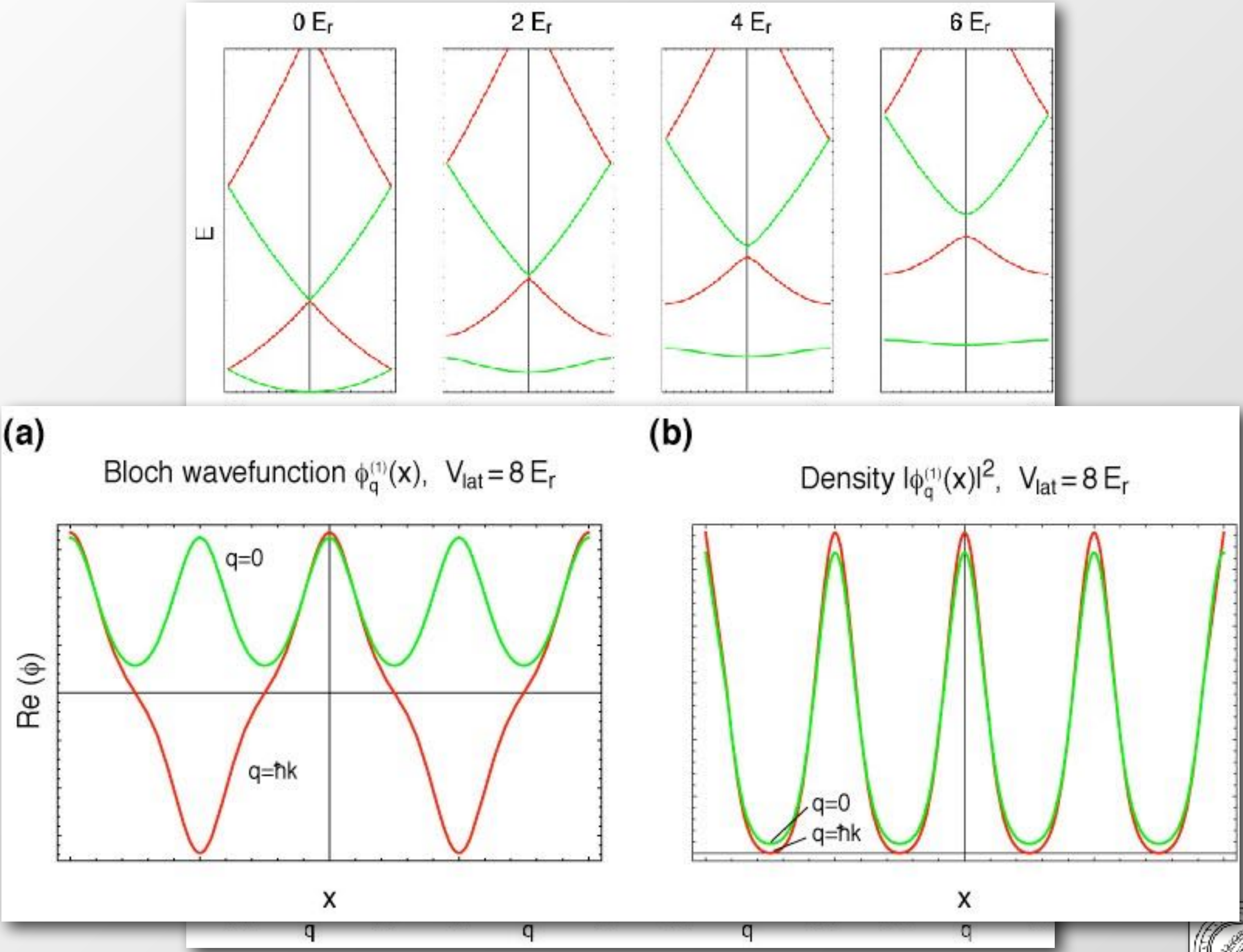
M. Endres, T. Fukuhara, M. Cheneau, P. Schauss, D. Pekker, E. Demler, S. Kuhr & I.B.

M. Endres et al. Nature (2012)

Chubukov & Sachdev, PRB 1993; Sachdev, PRB 1999; Zwerger, PRL 2004; Altman, Blatter, Huber, PRB 2007, PRL 2008; U. Bissbort et al. Phys. Rev. Lett. (2011); D. Podolsky, A. Auerbach, D. Arovas, PRB 2011

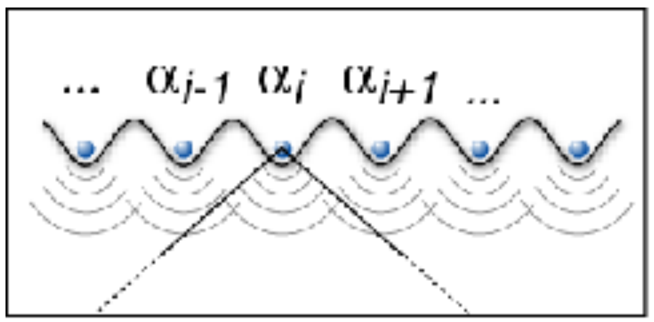
Measuring
Momentum Distributions

Bandstructure - Blochwaves



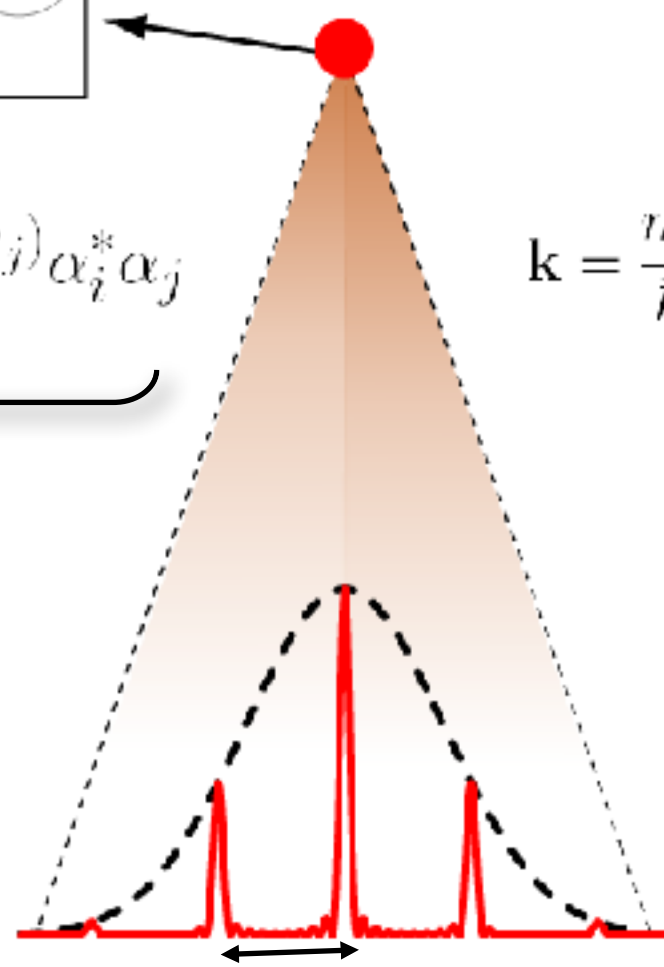
Time of flight interference pattern

- Interference between all waves coherently emitted from each lattice site



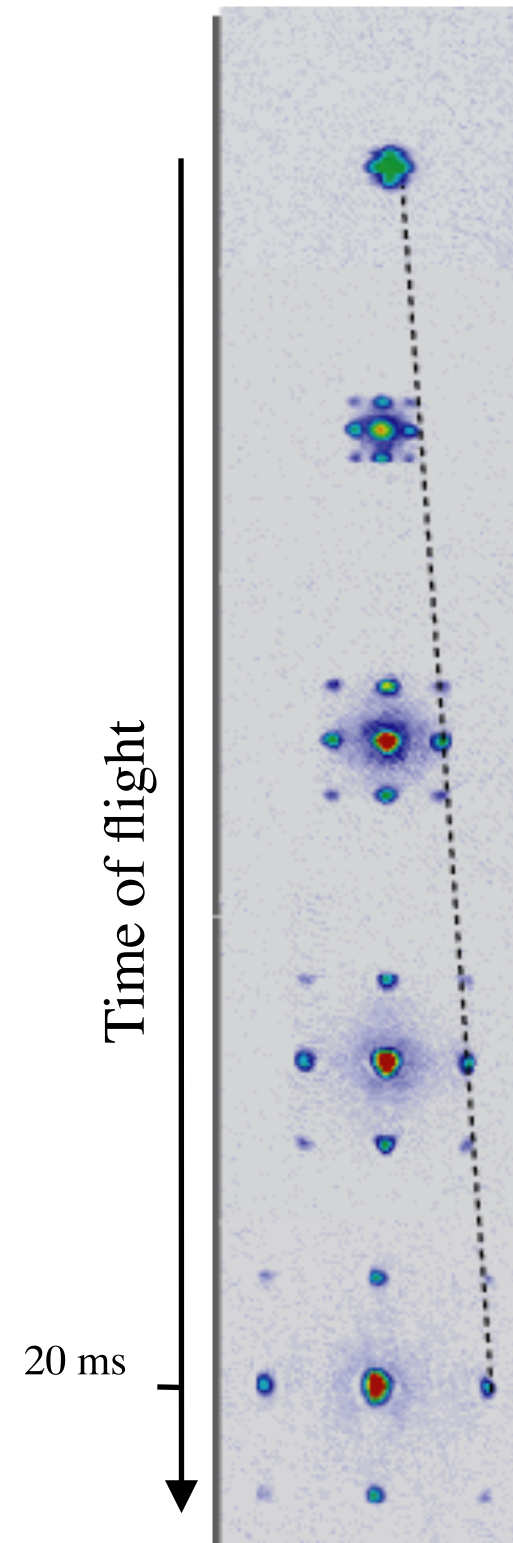
$$\tilde{n}(\mathbf{k}) = \underbrace{|\tilde{w}(\mathbf{k})|^2}_{\text{Wannier envelope}} \underbrace{\sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \alpha_i^* \alpha_j}_{\text{Grating-like interference}}$$

$$\mathbf{k} = \frac{m\mathbf{r}}{\hbar t}$$



Periodicity of the reciprocal lattice

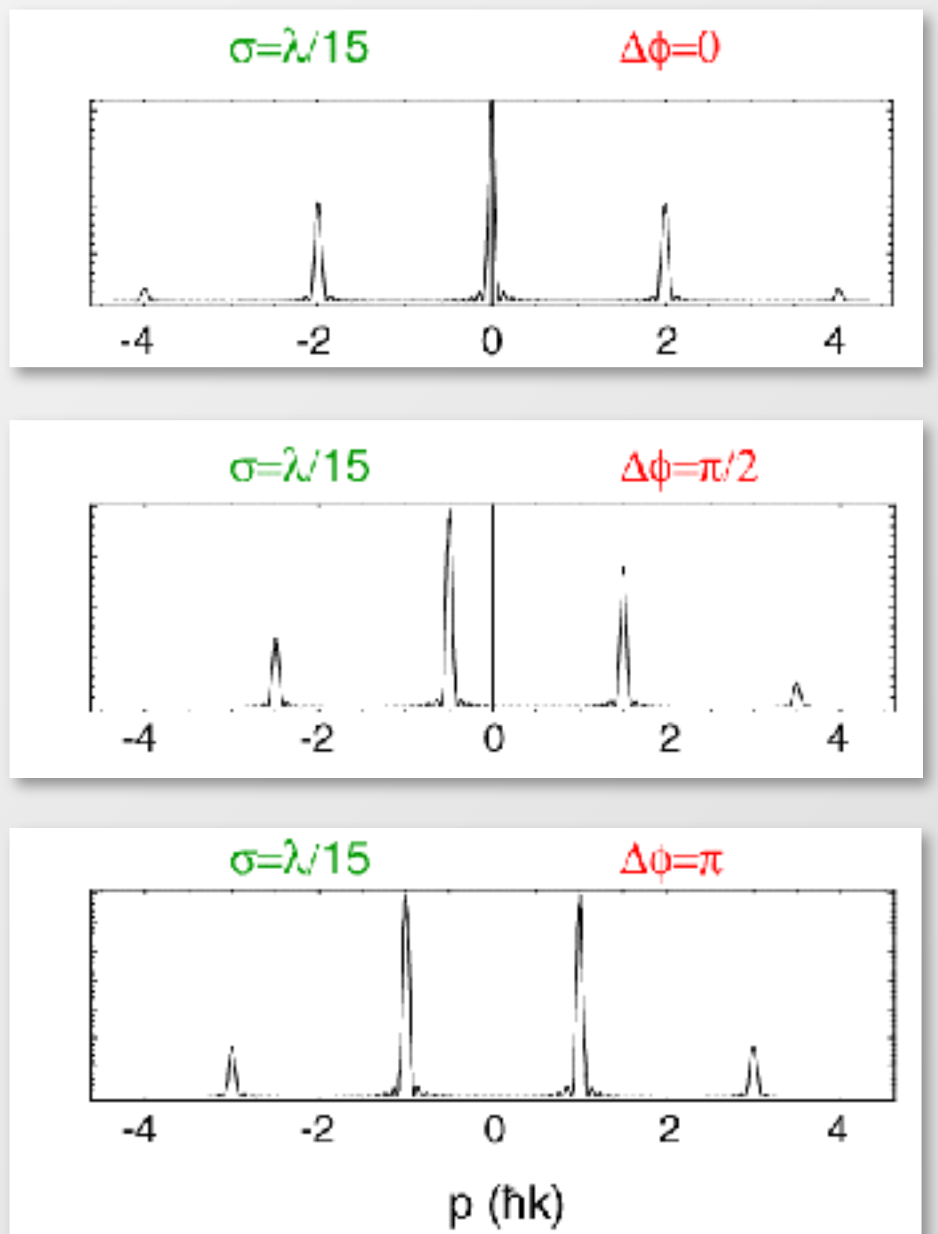
$$l = \frac{2\hbar k_{\mathrm{L}} t}{m}$$



Momentum Distributions – 1D

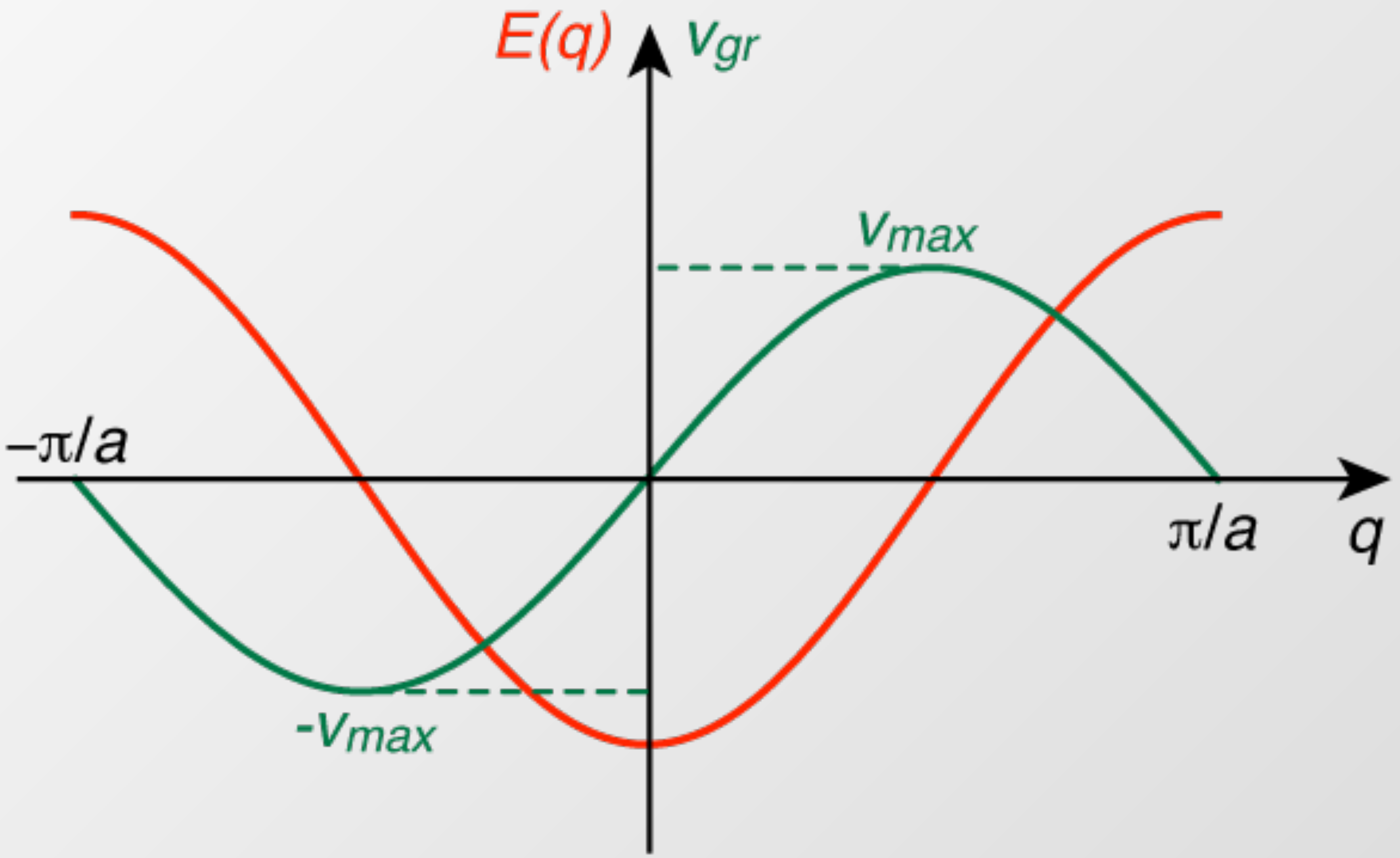
Momentum distribution can be obtained by Fourier transformation of the macroscopic wave function.

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

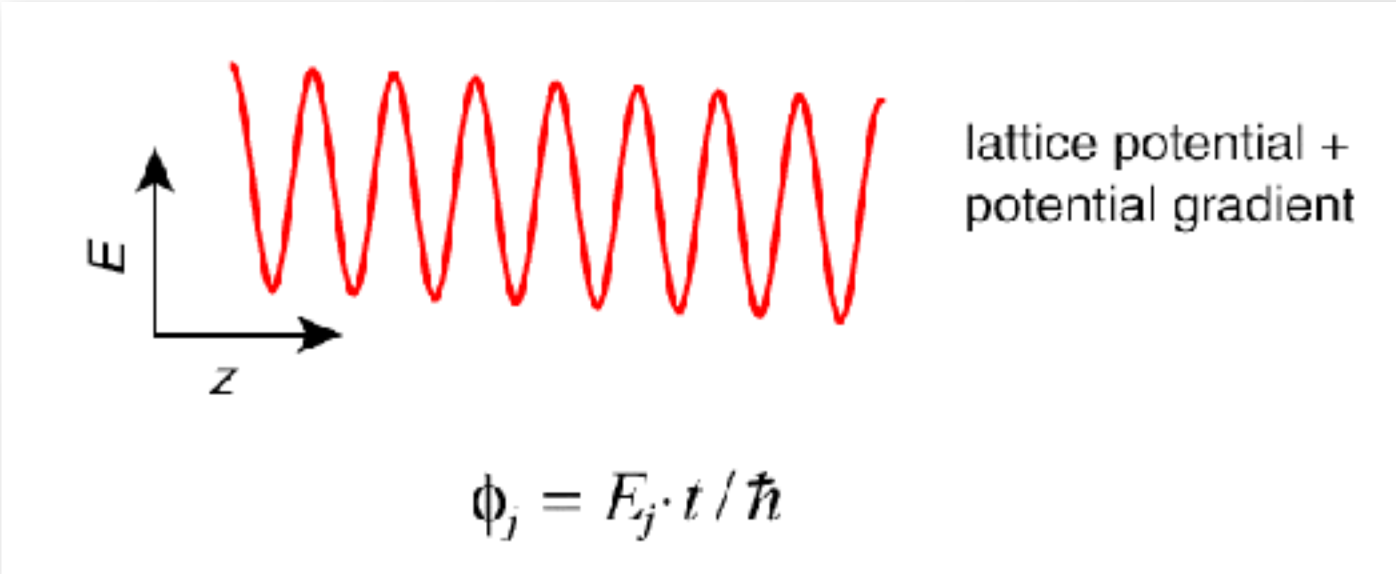


Dispersion Relation in a Square Lattice

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



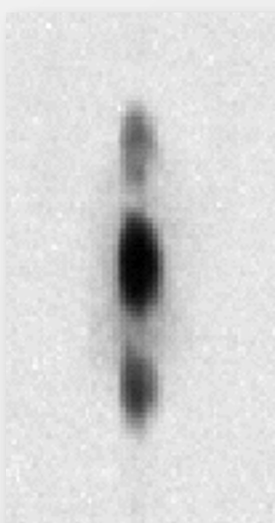
Preparing Arbitrary Phase Differences Between Neighbouring Lattice Sites



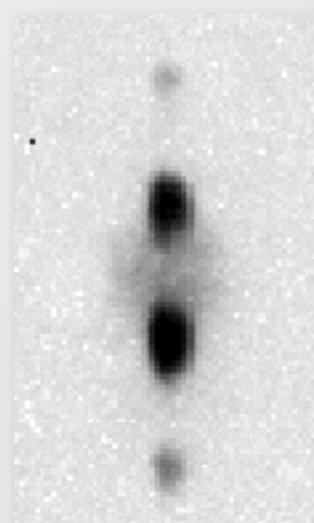
Phase difference between neighboring lattice sites

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

(cp. Bloch-Oscillations)



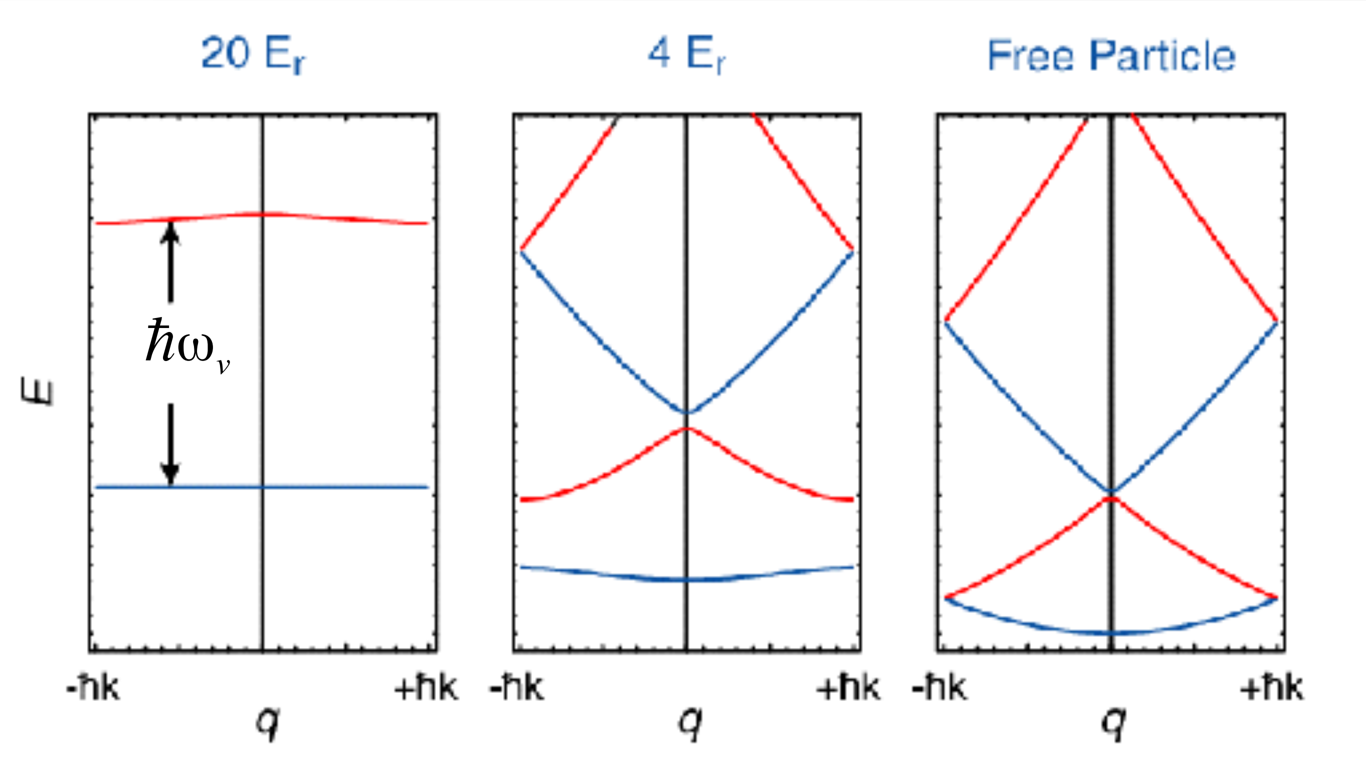
$\Delta\phi = 0$



$\Delta\phi = \pi$

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

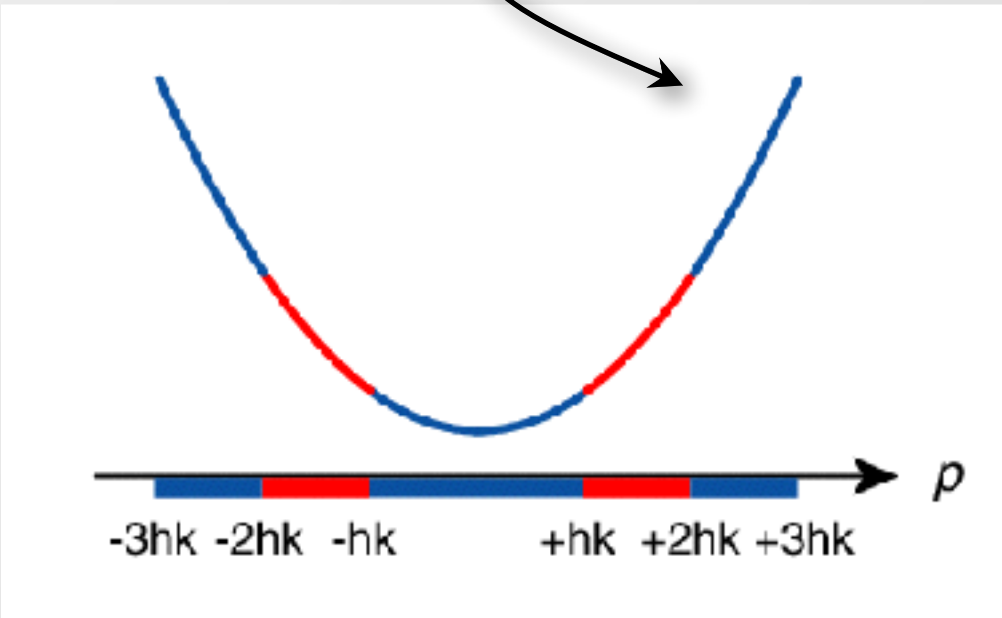
Mapping the Population of the Energy Bands onto the Brillouin Zones



Crystal momentum

Crystal momentum is conserved while lowering the lattice depth adiabatically !

Population of n^th band is mapped onto n^th Brillouin zone !

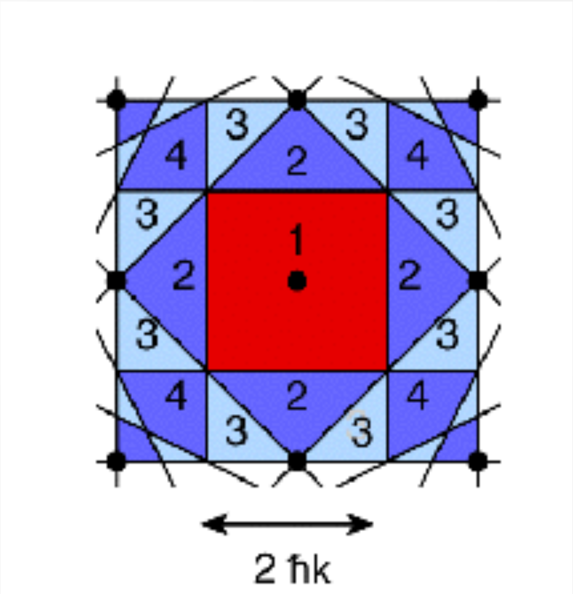


Free particle momentum

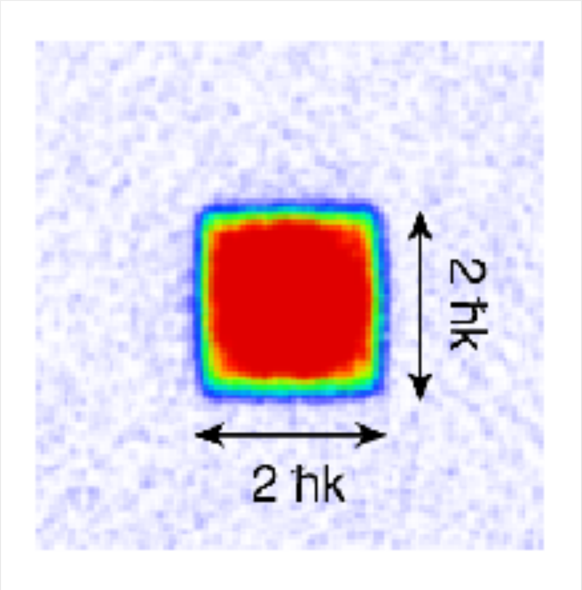
A. Kastberg et al. PRL 74, 1542 (1995)
M. Greiner et al. PRL 87, 160405 (2001)

Experimental Results

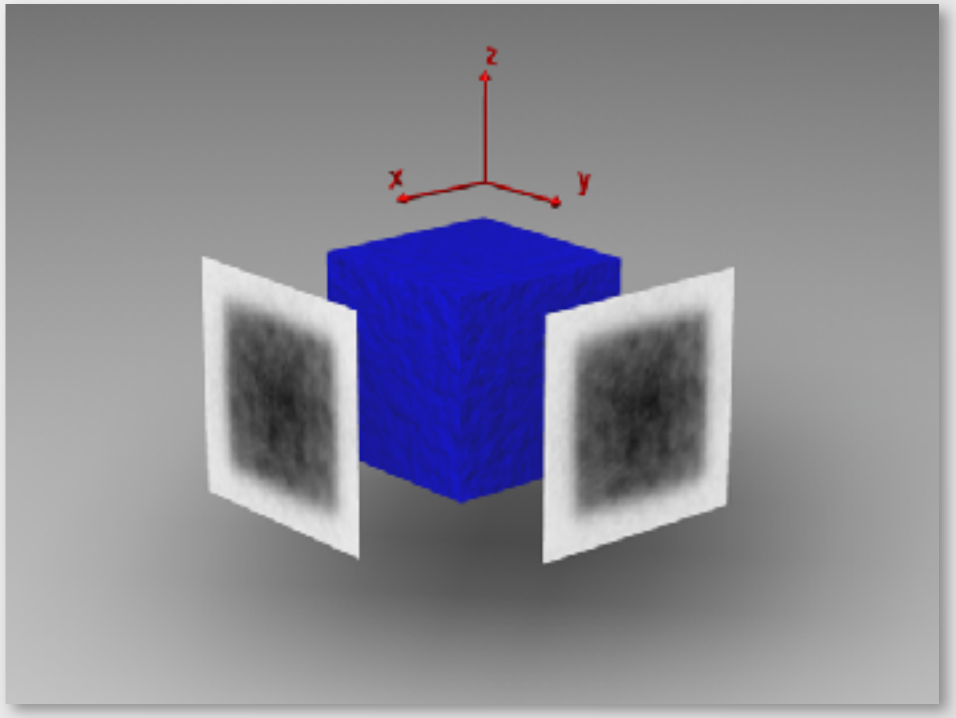
Brillouin Zones in 2D



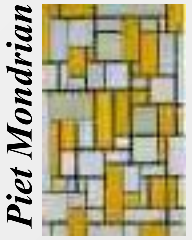
Momentum distribution of a dephased condensate after turning off the lattice potential adiabtically



2D



3D



Bose-Hubbard Hamiltonian

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

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

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

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

Onsite interaction matrix element

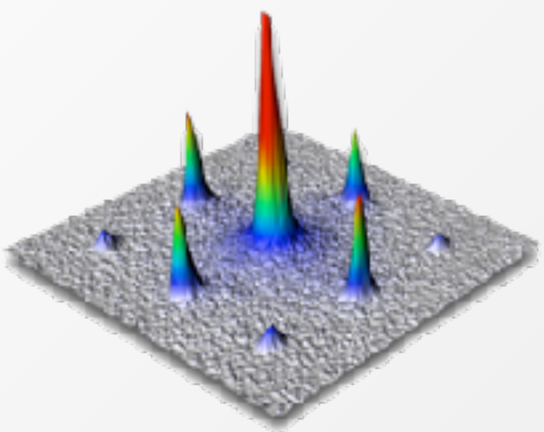
$$U = \frac{4\pi \hbar^2 a}{m} \int d^3x \left| w(\boldsymbol{x}) \right|^4$$

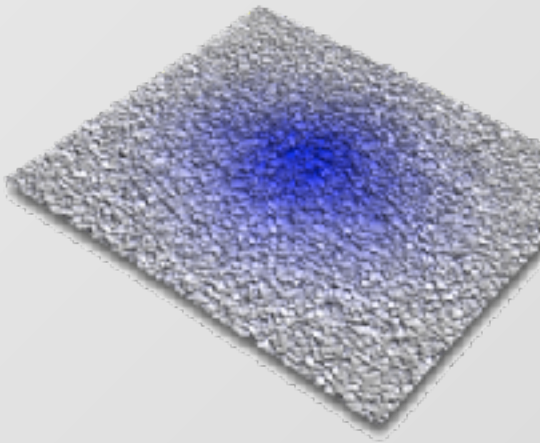
M.P.A. Fisher et al., PRB 40, 546 (1989); D. Jaksch et al., PRL 81, 3108 (1998)

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,...

From Weak to Strong Interactions

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

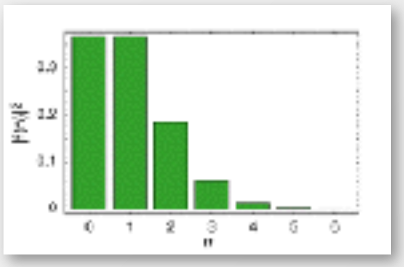


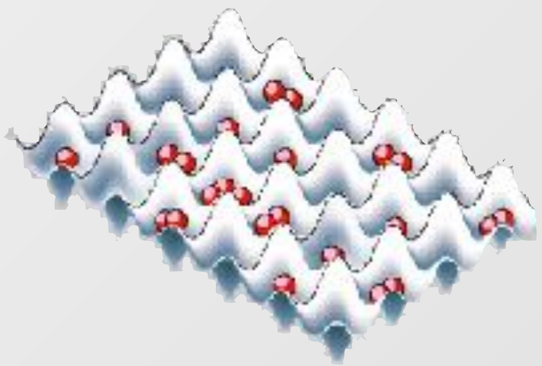


Quantum Phase Transition

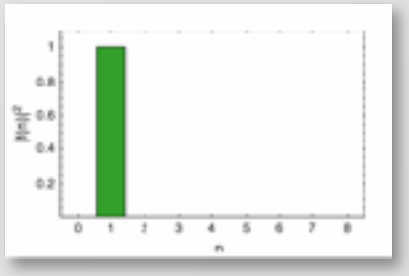
See S. Sachdev & B. Keimer Phys. Today 2011

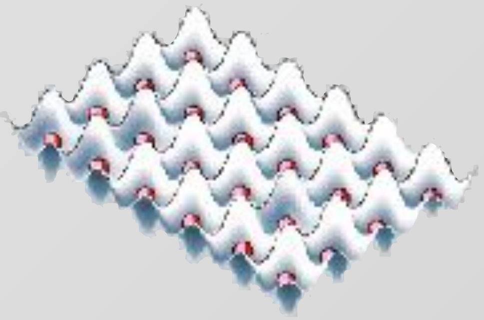
Weak Interactions





Strong Interactions

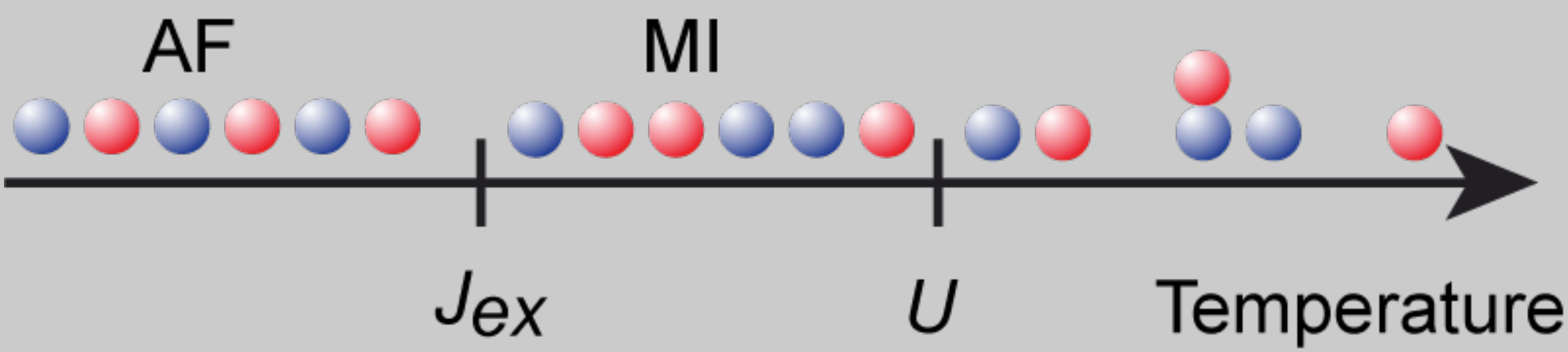




Strongly Interacting Fermions in Optical Lattices

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

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



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

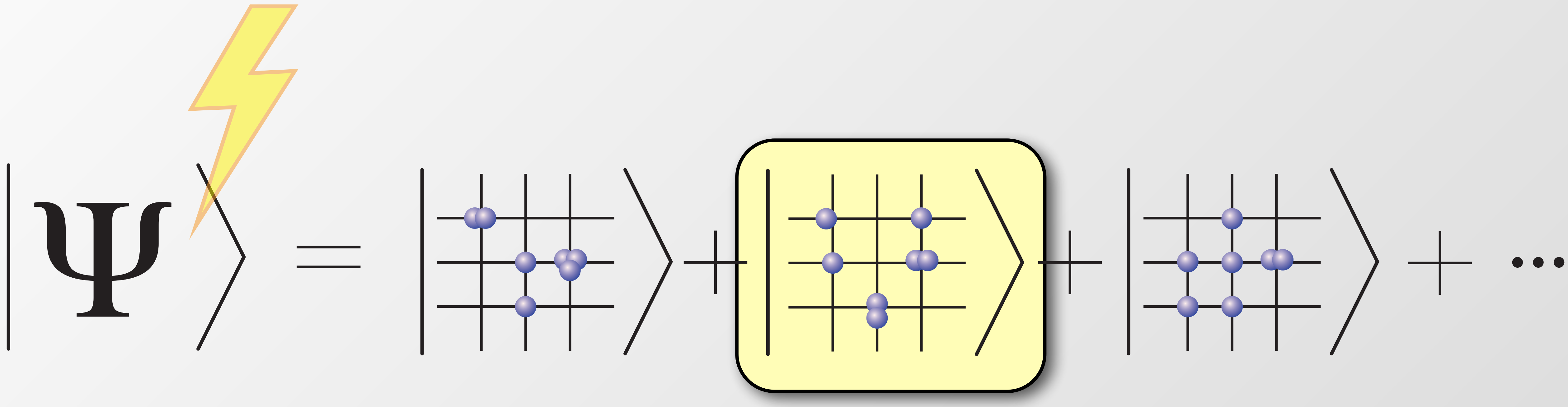
R. Jördens et al., Nature **455**, 204 (2008), U. Schneider et al., Science **322,** 1520 (2008),
D. Greif et al., Science **340**, 1307 (2013)

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)

Measuring a Many-Body Quantum System

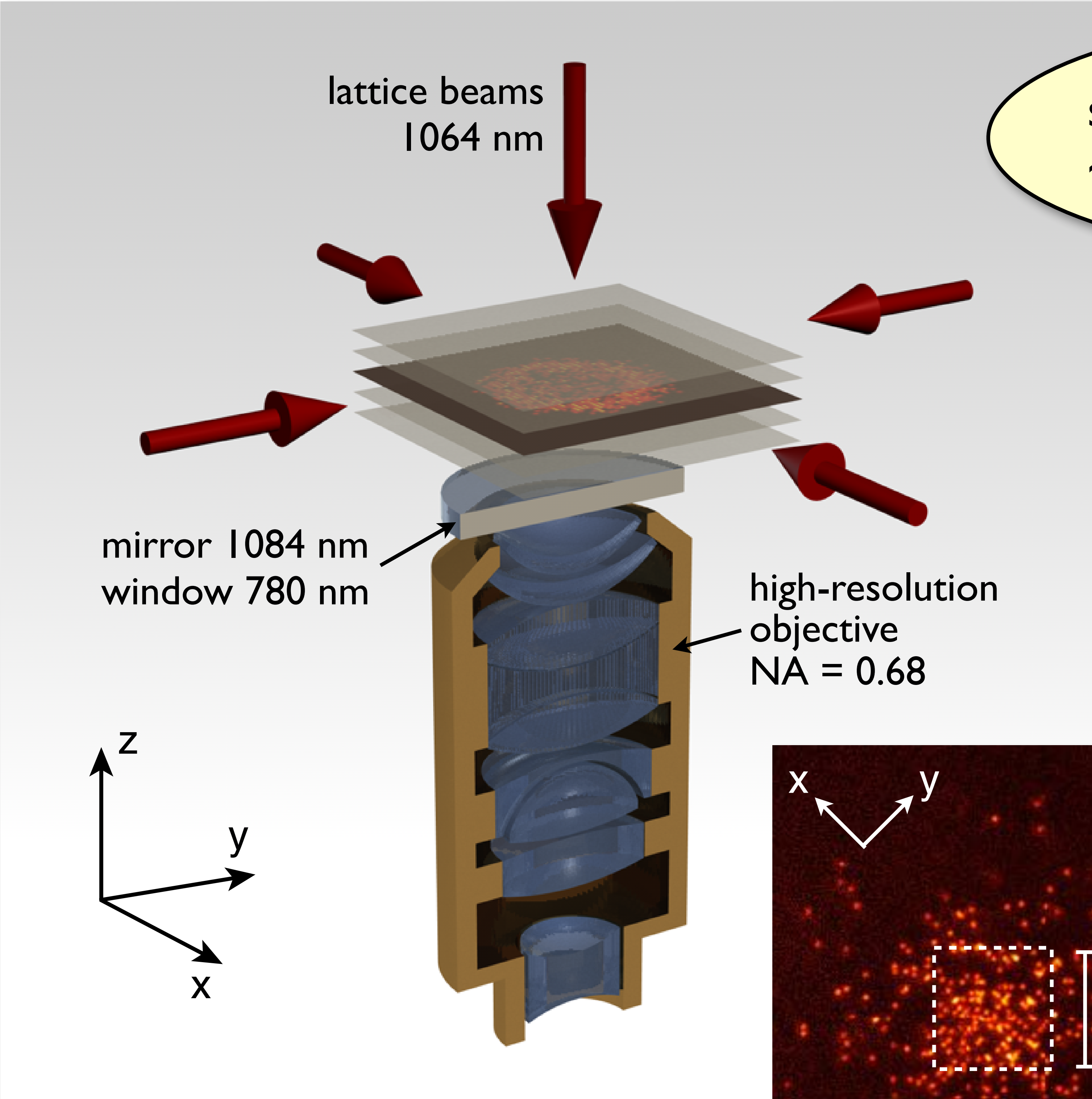
Local occupation measurement



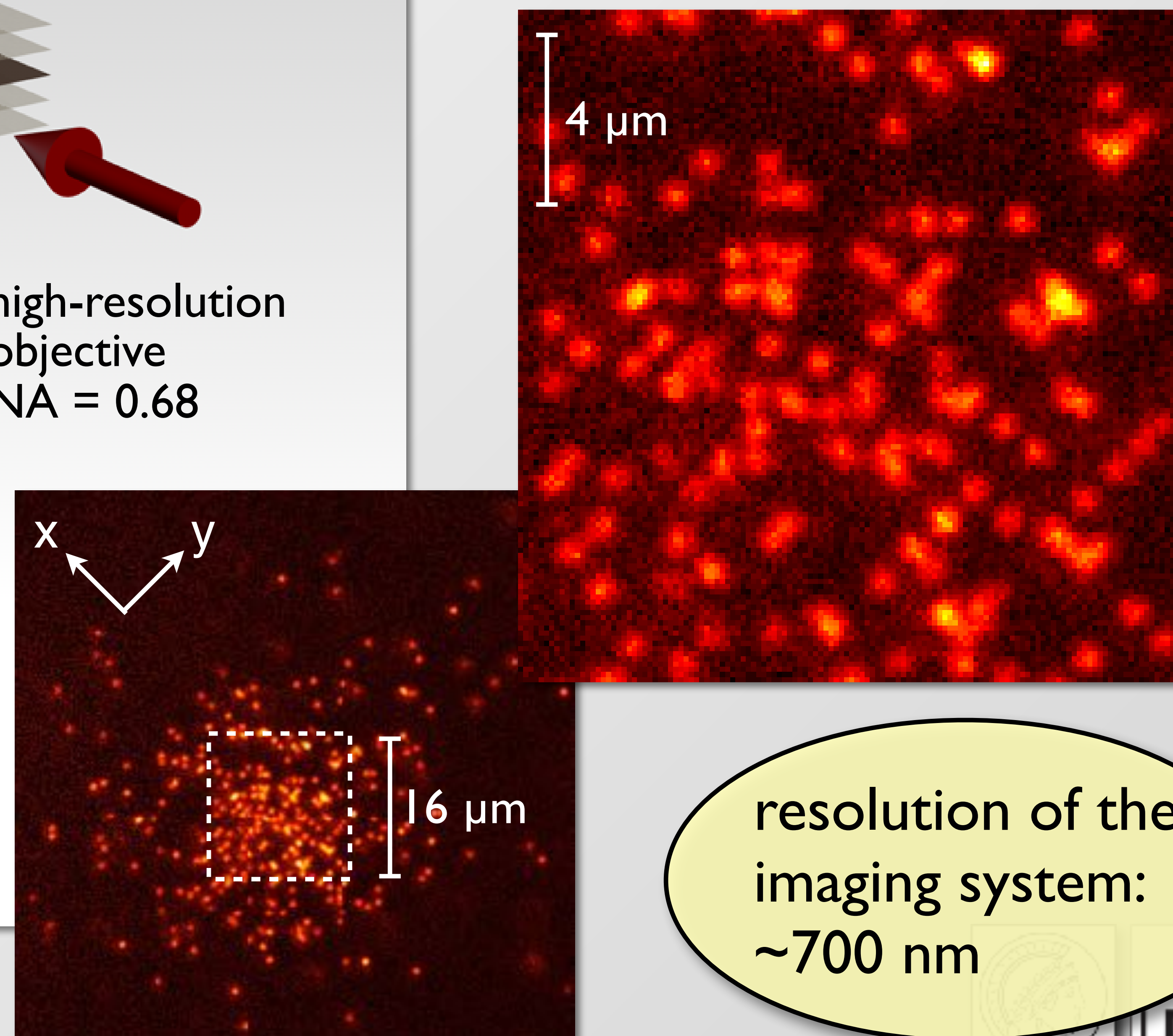
Enables access to all position correlation between particles!

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

Experimental Setup

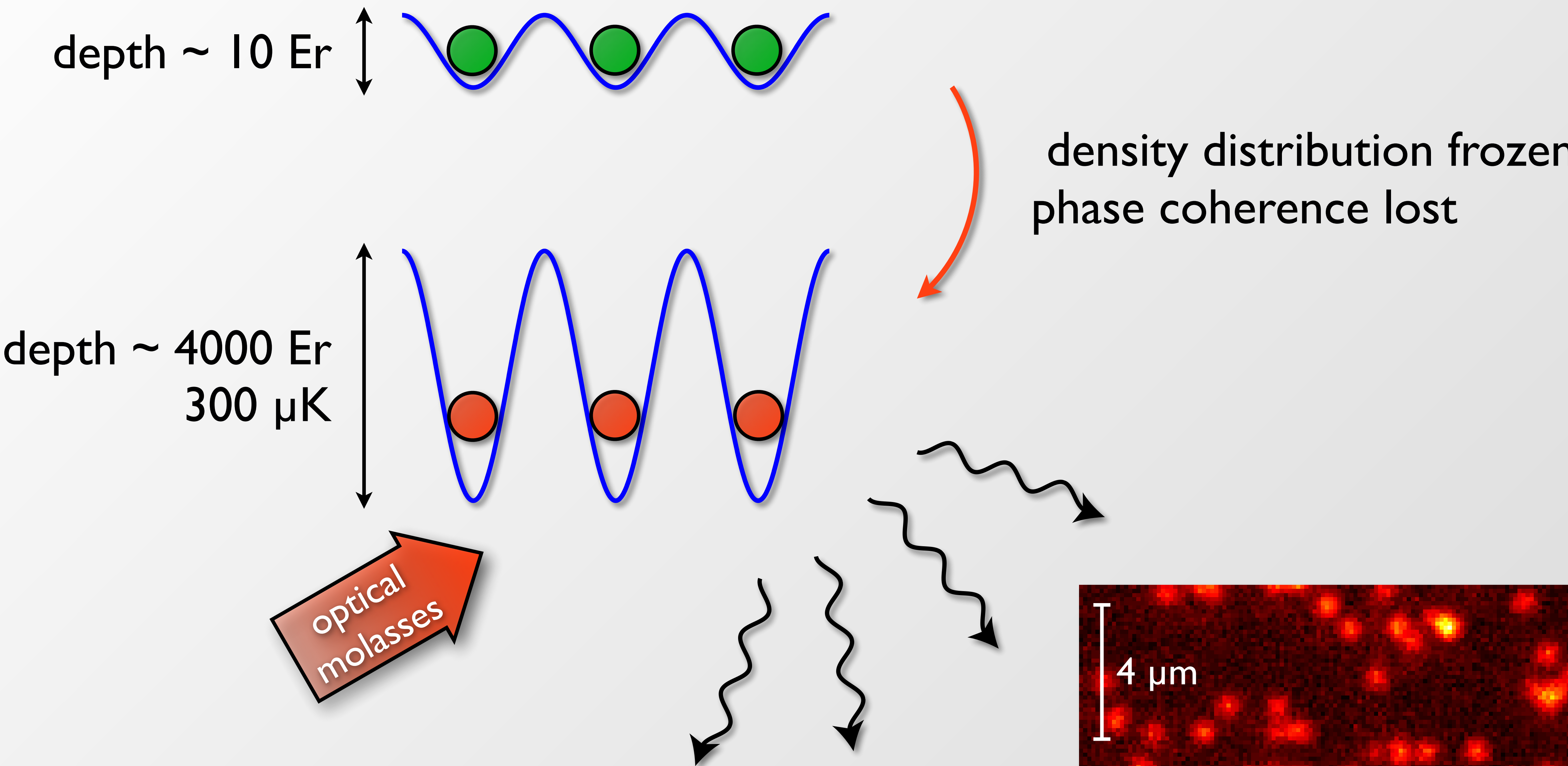


single 2D degenerate gas
~ 1000 ^{87}Rb atoms (bosons)

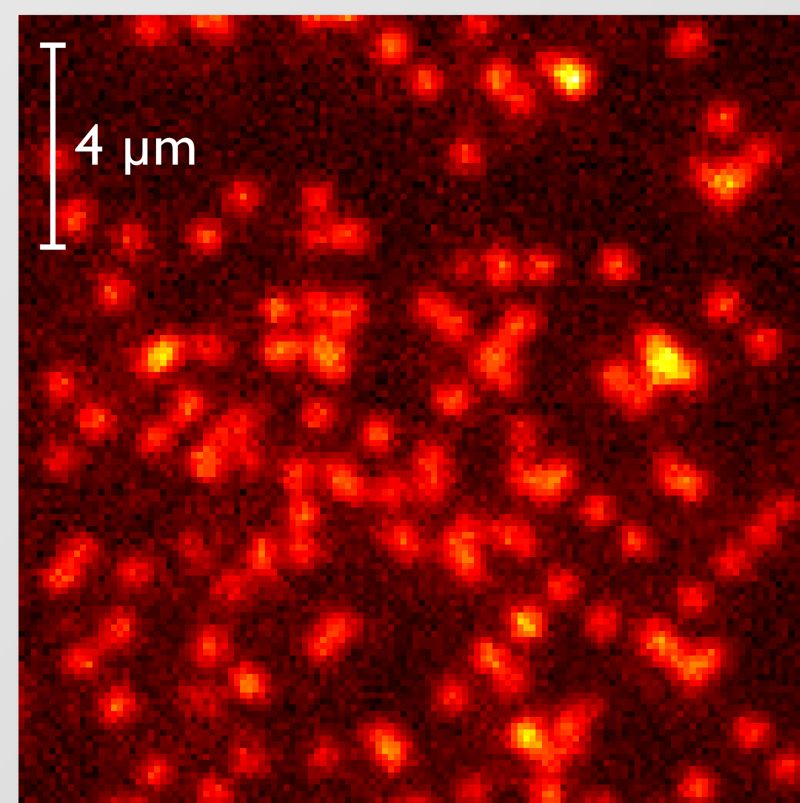


resolution of the imaging system:
~700 nm

Fluorescence imaging

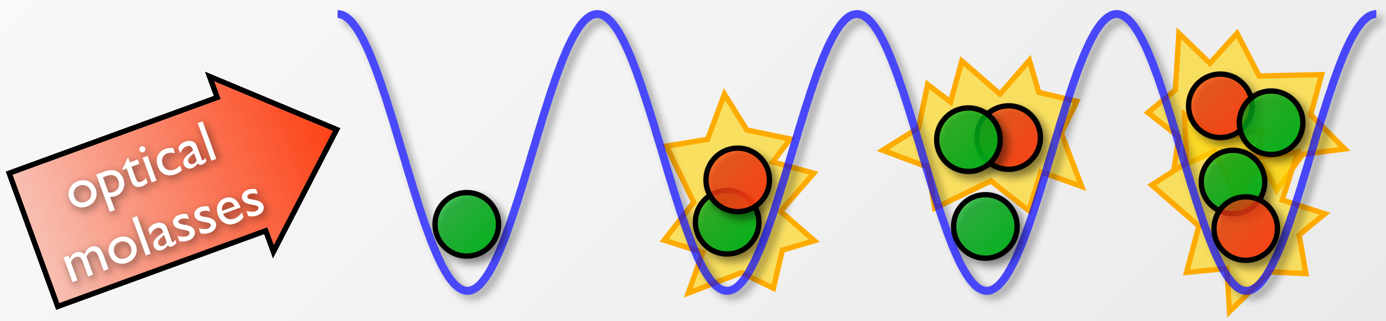


fluorescence rate / atom: 60 kHz
~ 5000 photons / atom collected in 900ms



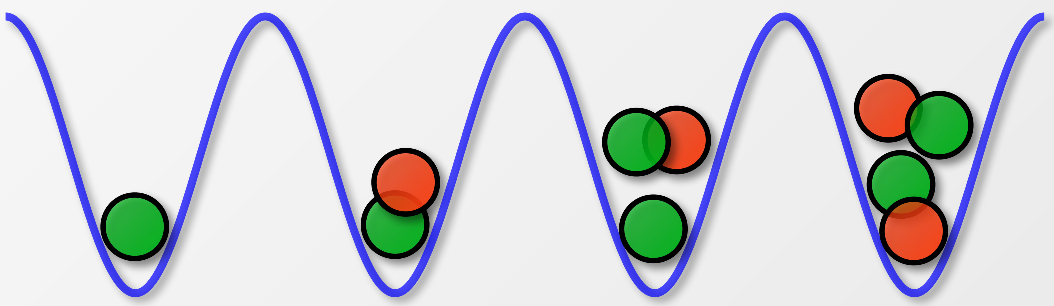
Parity projection

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

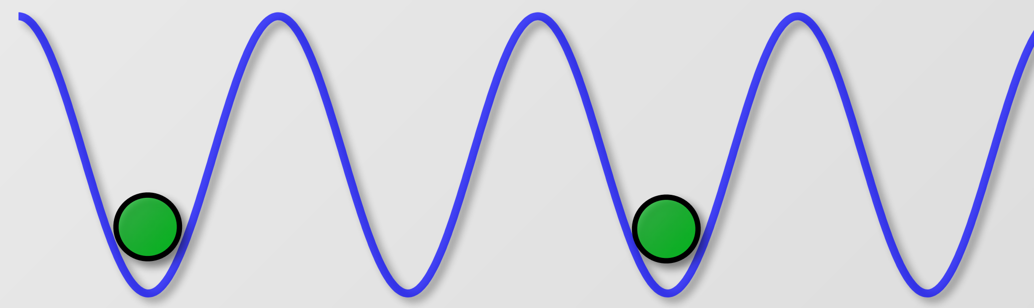


Light-induced collisions

initial density distribution



measured density distribution



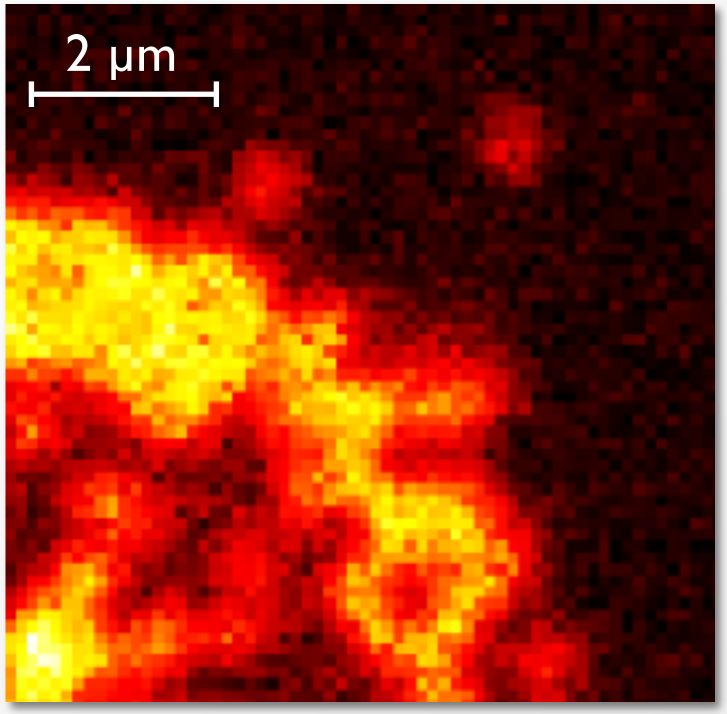
measured occupation: $n_{\text{det}} = \text{mod}_2 n$

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

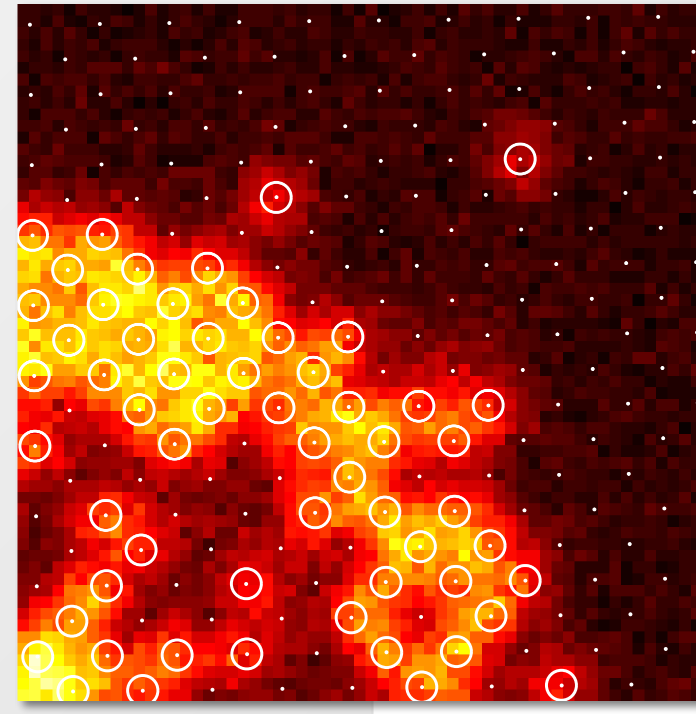
parity projection $\Rightarrow$ $\langle n^2_{\text{det}} \rangle = \langle n_{\text{det}} \rangle$

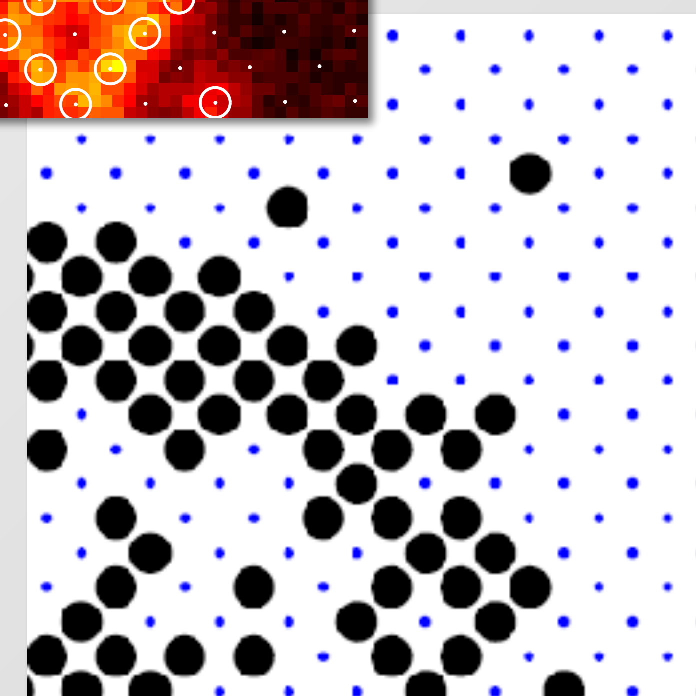
see also E. Kapit & E. Mueller, Phys. Rev. A **82**, 013644 (2010)

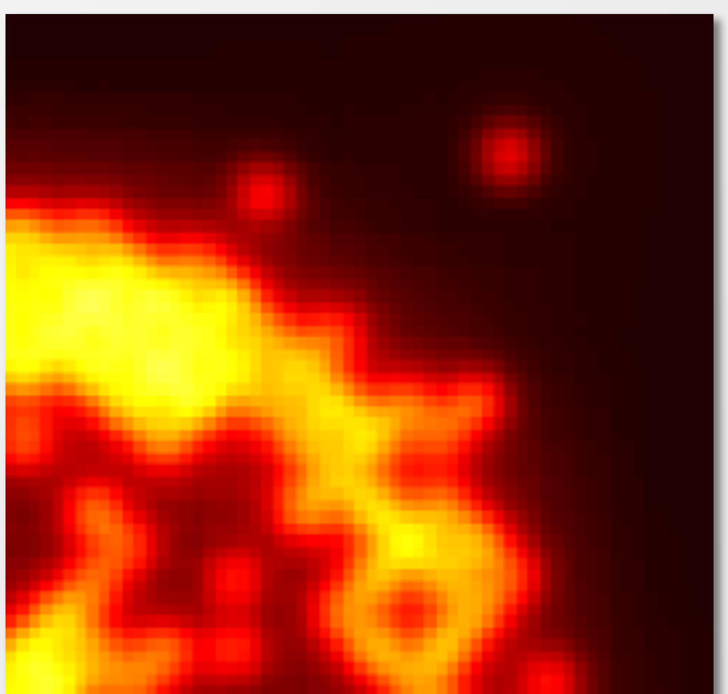
Reconstruction of site occupation



Reconstruction algorithm







Digitized image convoluted with point-spread function

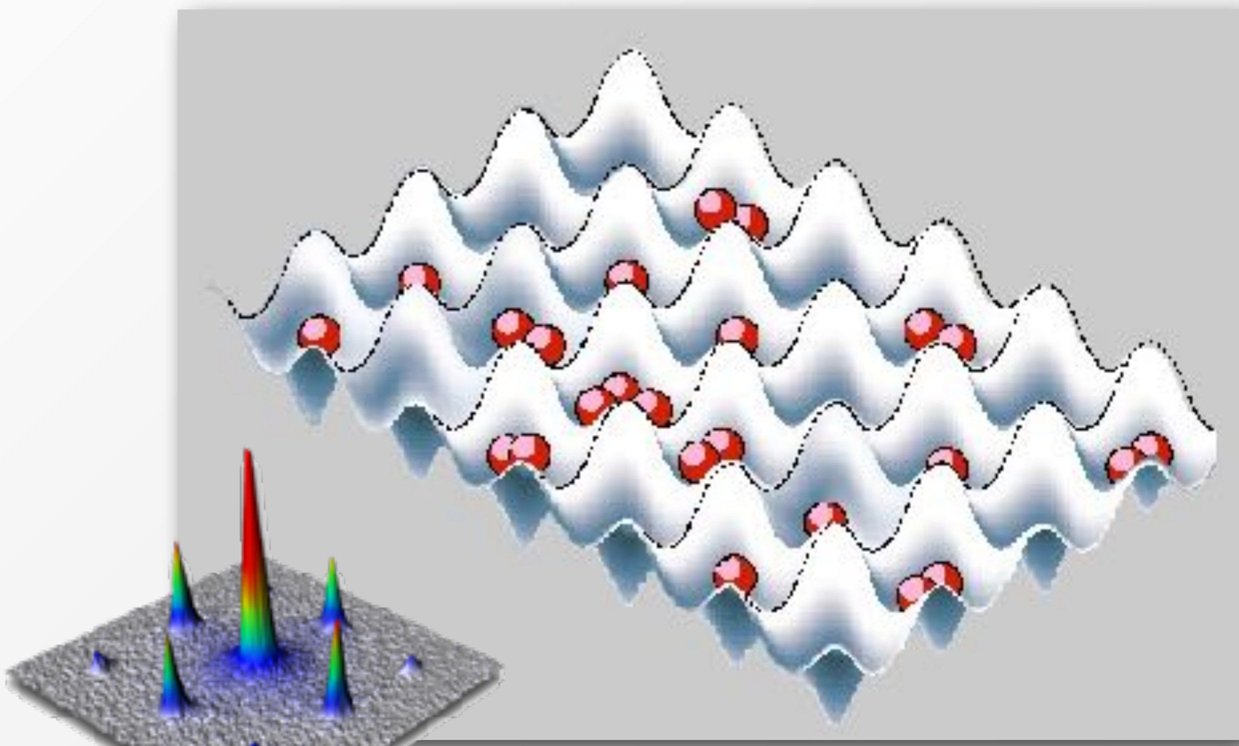
digitized image
no experimental noise

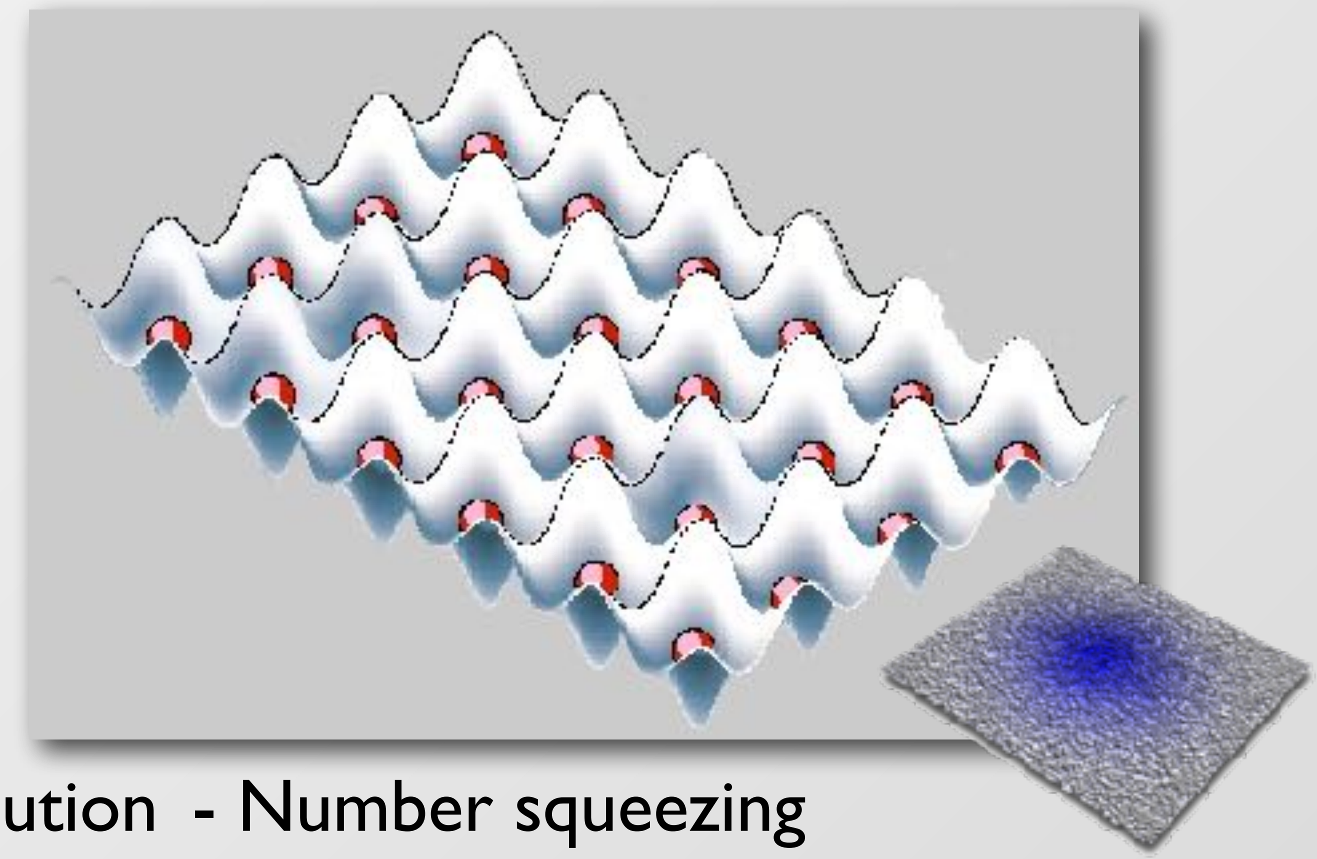
In-Situ Imaging of a Mott Insulator

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)

Mott Insulators

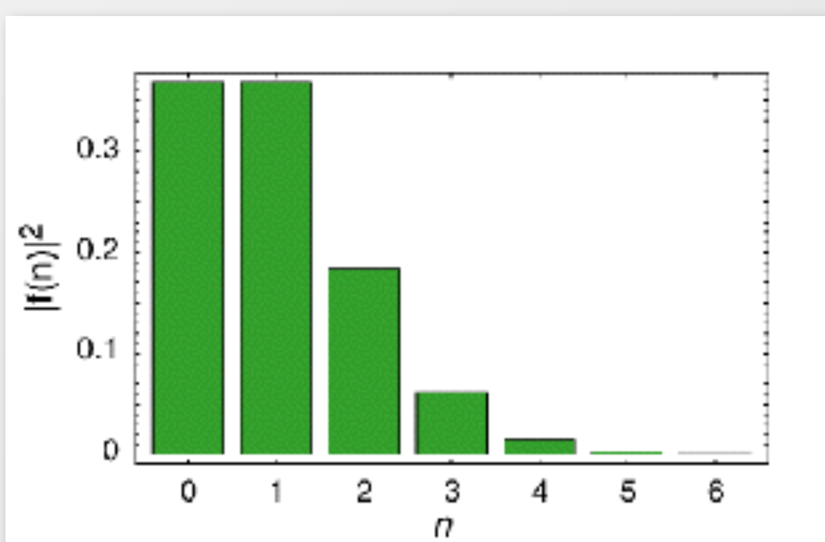
Superfluid | **Mott-Insulator**

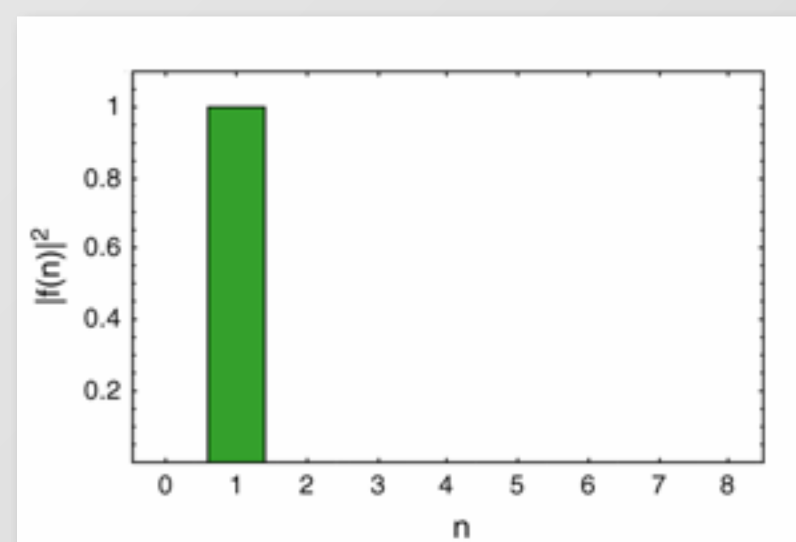




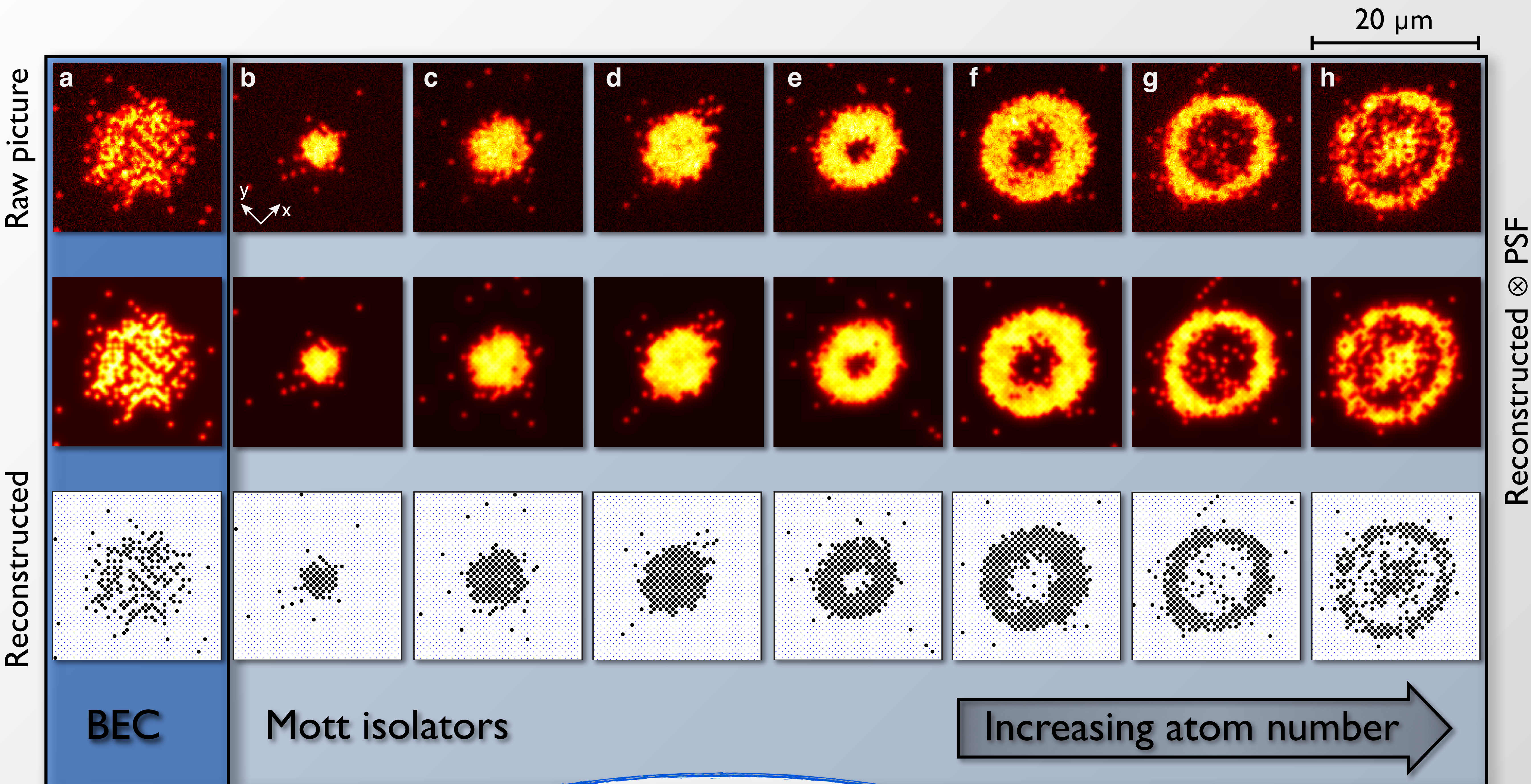
- Poissonian atom number distribution
- Long range phase coherence

- Number squeezing
- No phase coherence





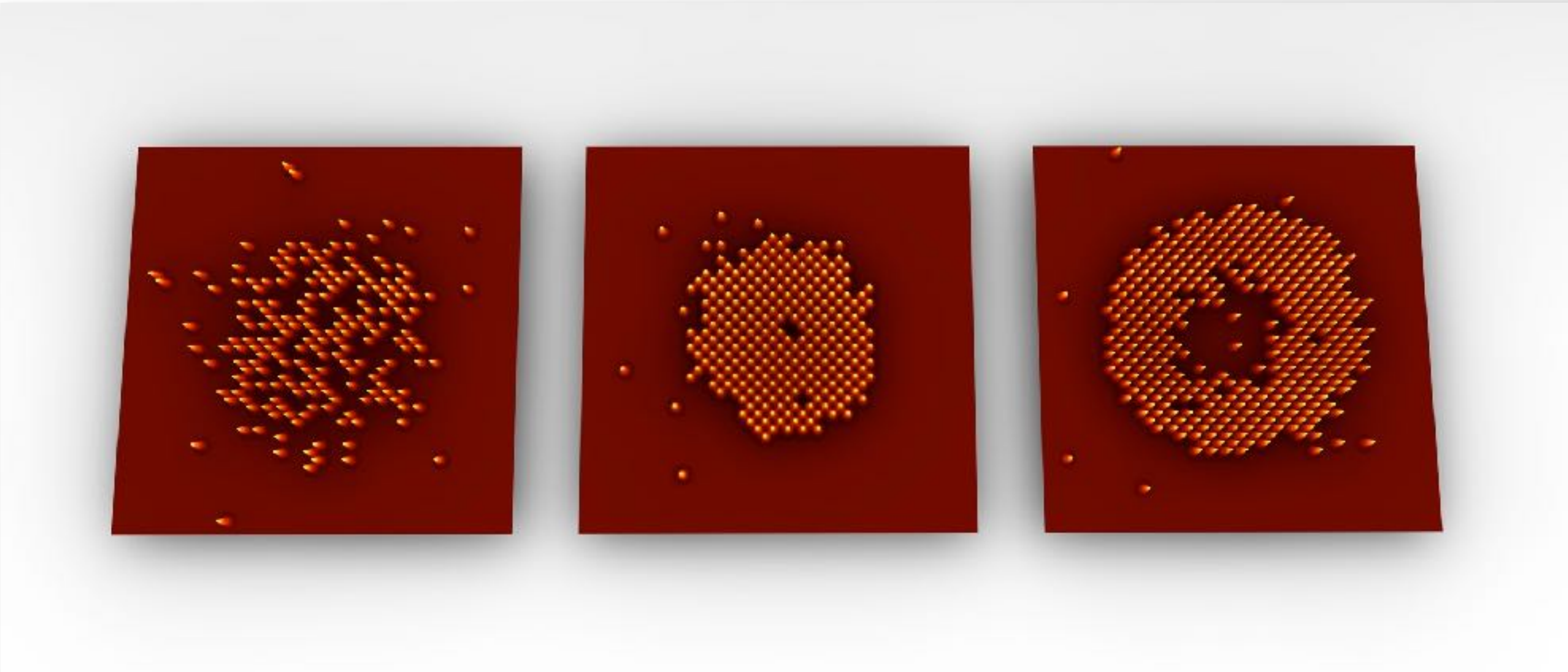
In-situ observation of a Mott insulator



for the Mott insulators: U/J ~ 300 (critical U/J ~ 16)

⇒ only thermal fluctuations

Snapshot of an Atomic Density Distribution



BEC

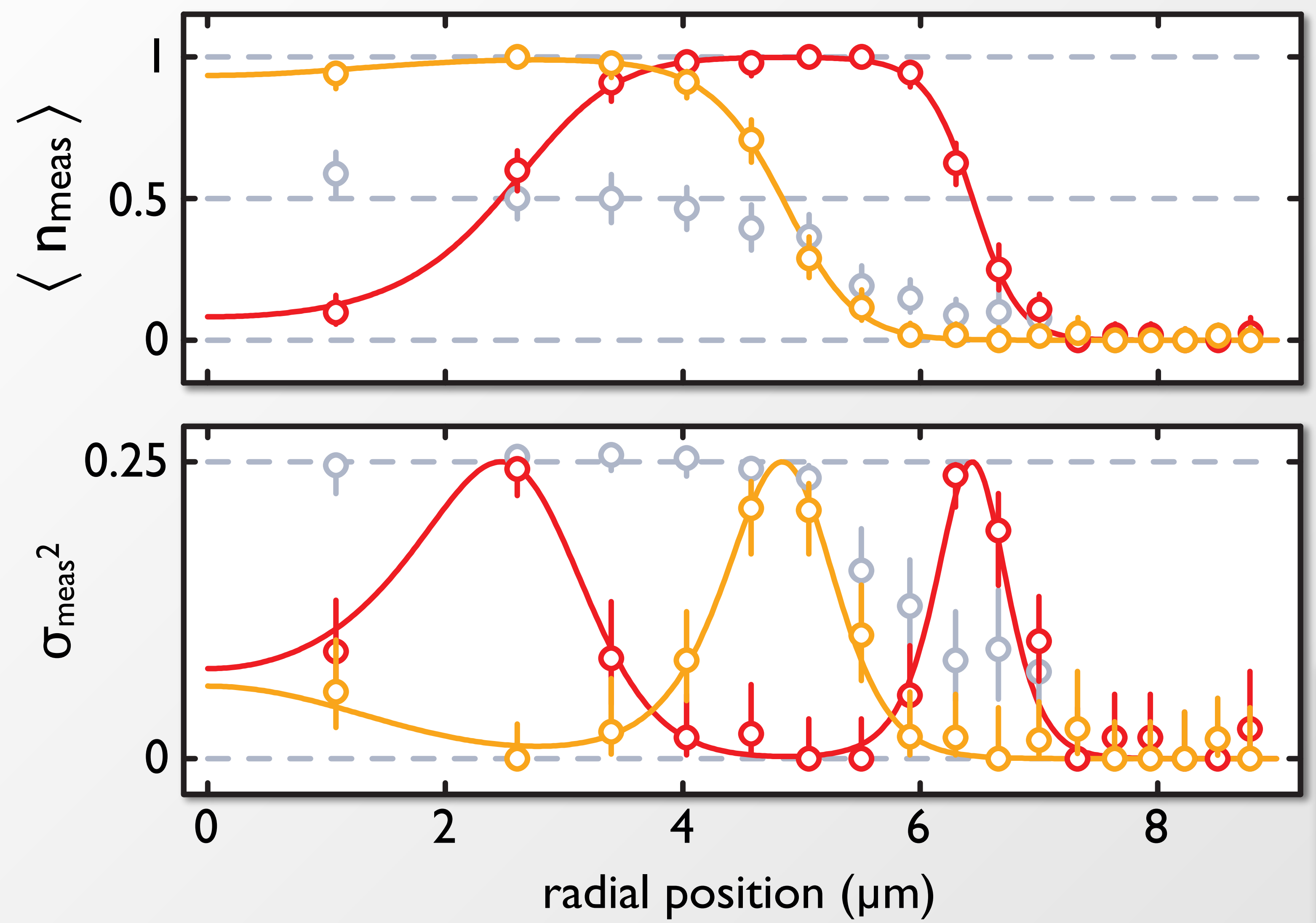
n=1
Mott Insulator

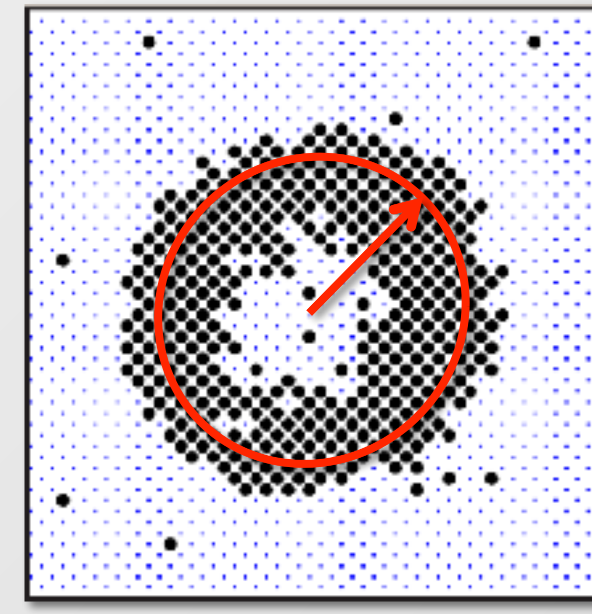
n=1 & n=2
Mott Insulator

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

LMU

Single Shot Thermodynamics



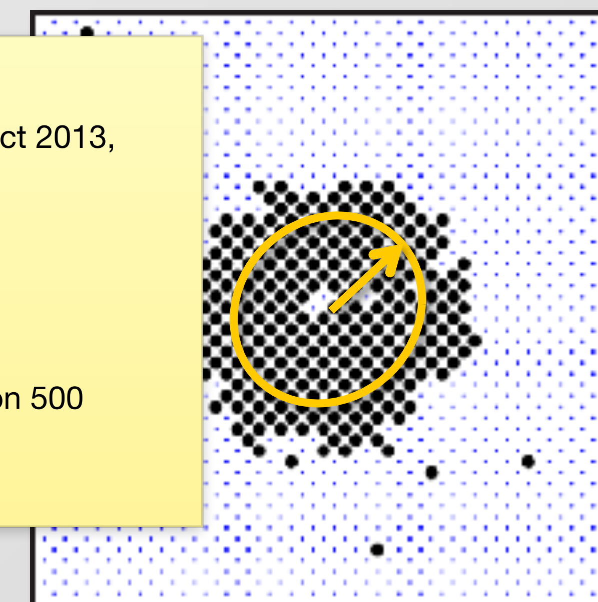


T = 0.074(5) U/k_B, μ = 1.17(1) U
N = 610(20)

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

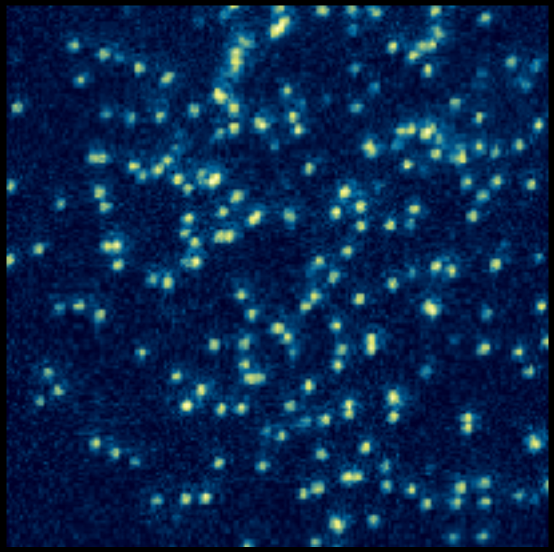
occupation probability: $$p_n(r) = \frac{e^{-\beta(E_n - \mu(r)n)}}{Z(r)}$$

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

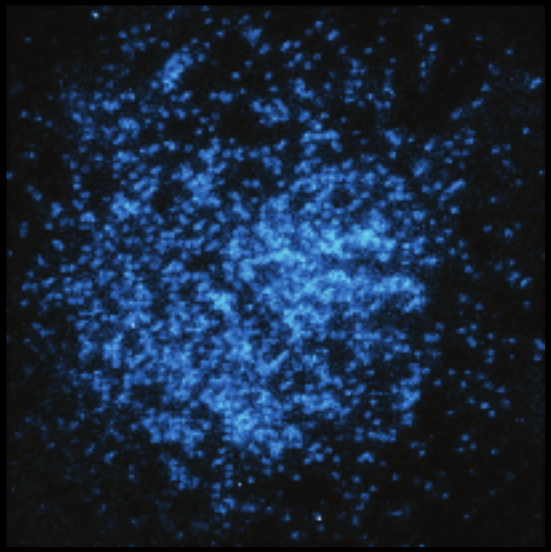
fit parameters: $$T/U, \mu/U, U/\omega^2$$

Fermionic Quantum Gas Microscopes

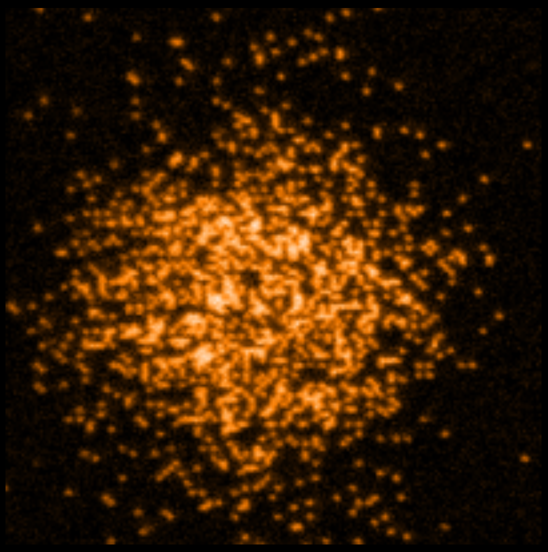
now also for fermions!



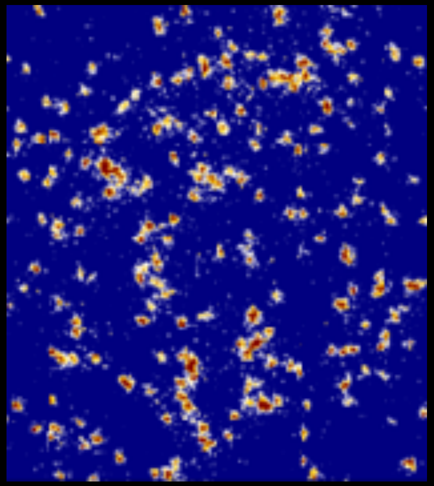
Strathclyde (^{40}K)



Harvard (^{6}Li)



MIT (^{40}K)

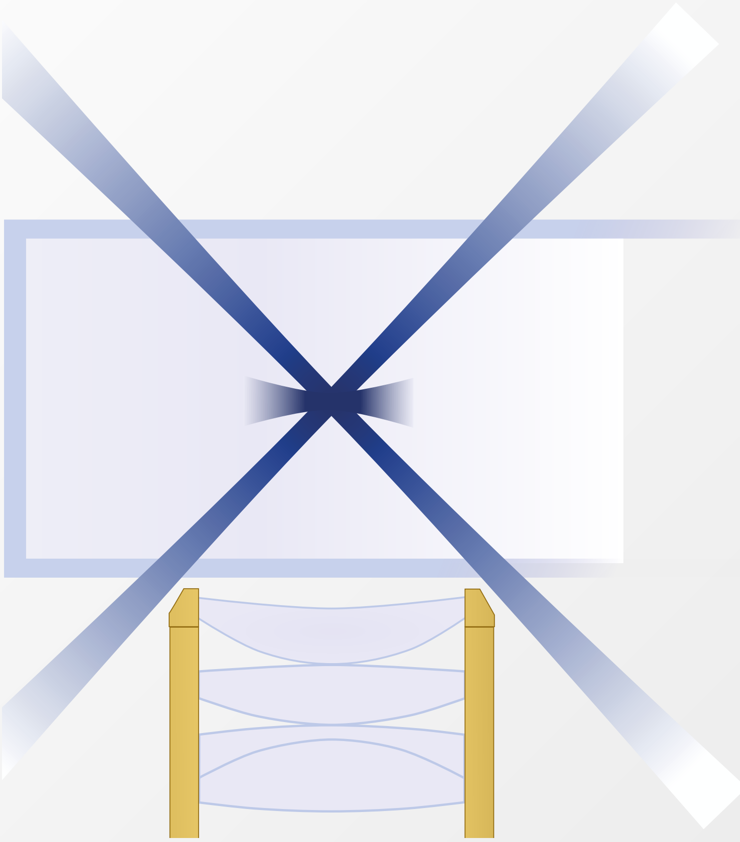


Toronto (^{40}K)

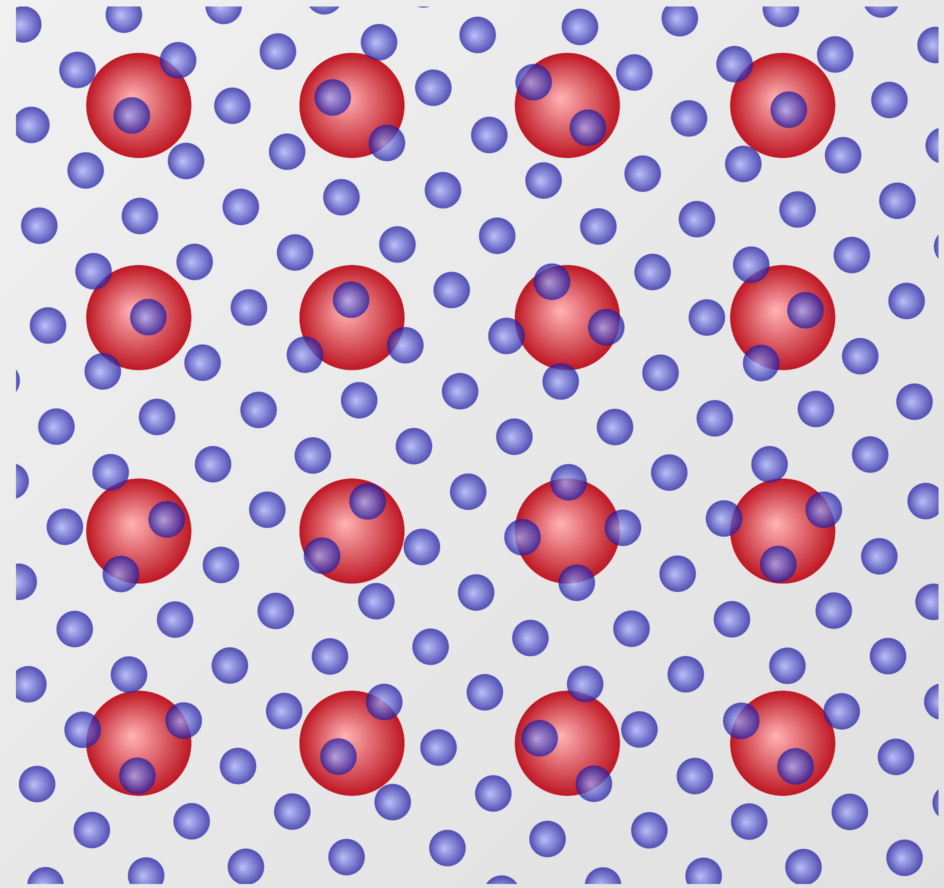
Fermionic Quantum Gas Microscopes

Detection 'Pinning' Lattice

Pinning lattice 1064 nm



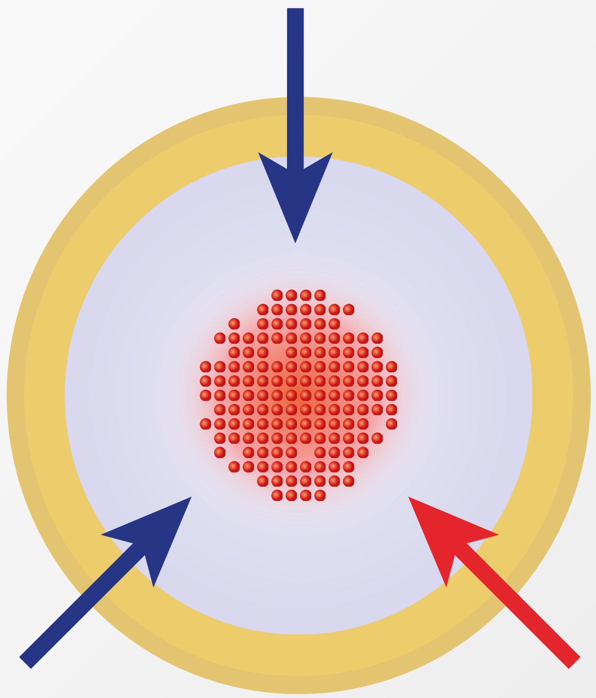
Physics Lattice + Pinning Lattice

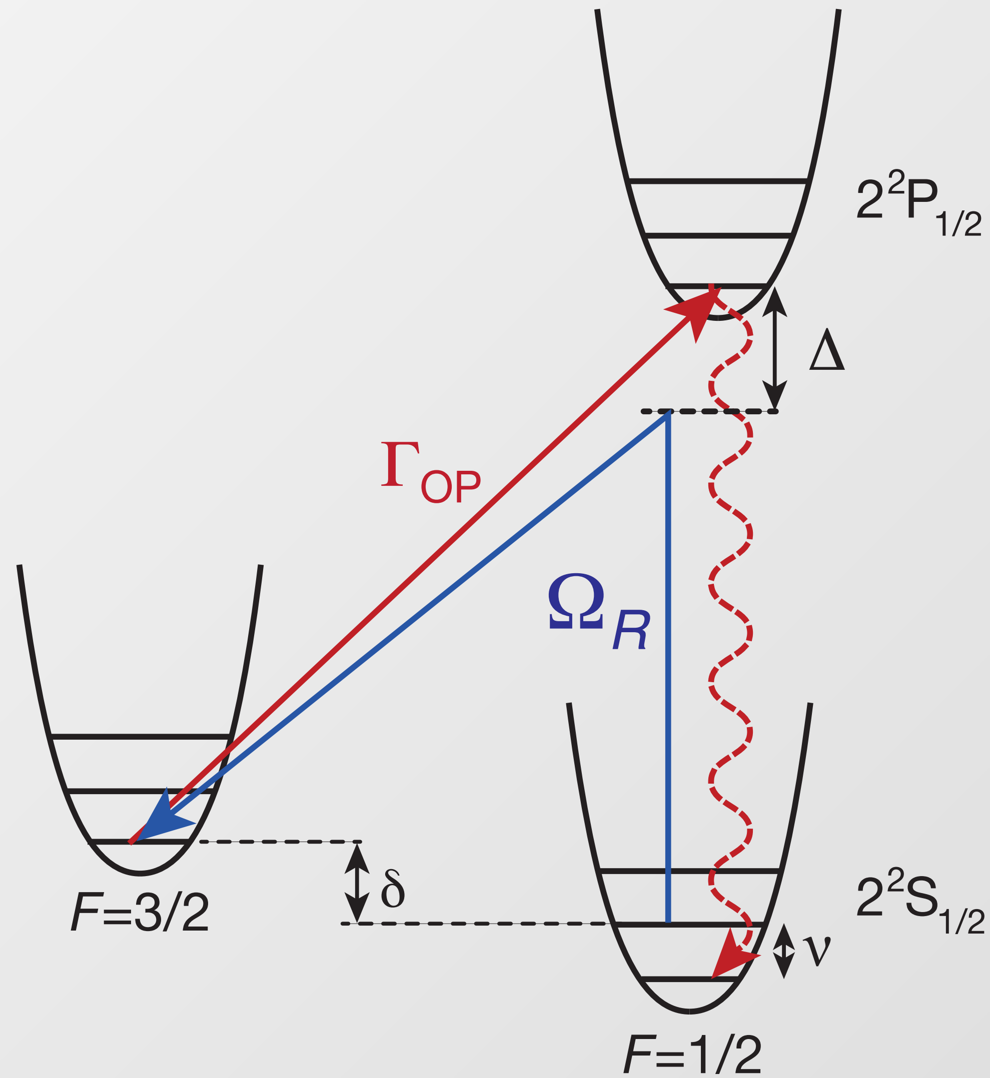


Pinning Spacing 532 nm

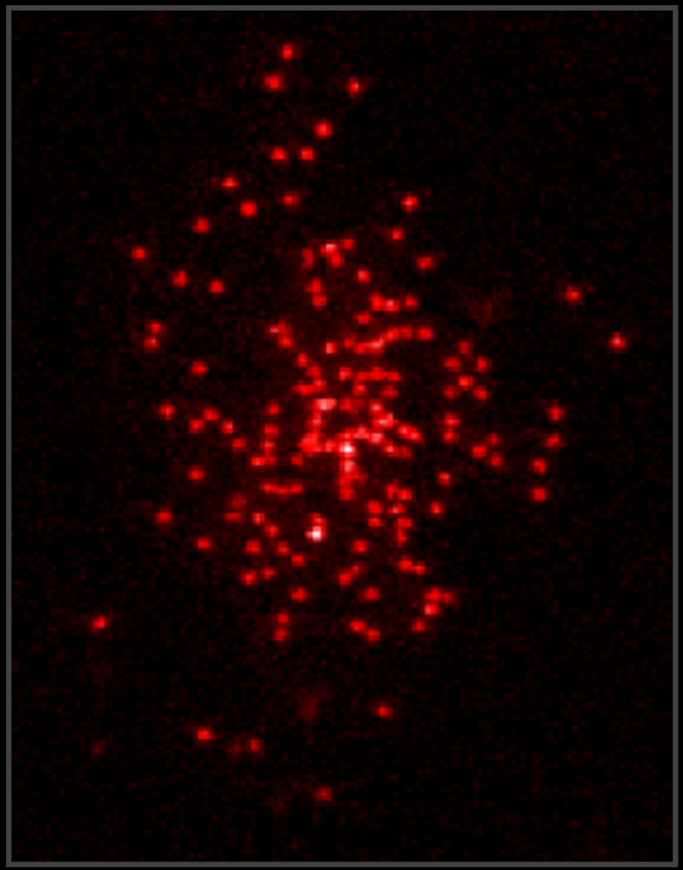
Onsite Trap Freq. 1.4 MHz

Raman Cooling in Pinning Lattice

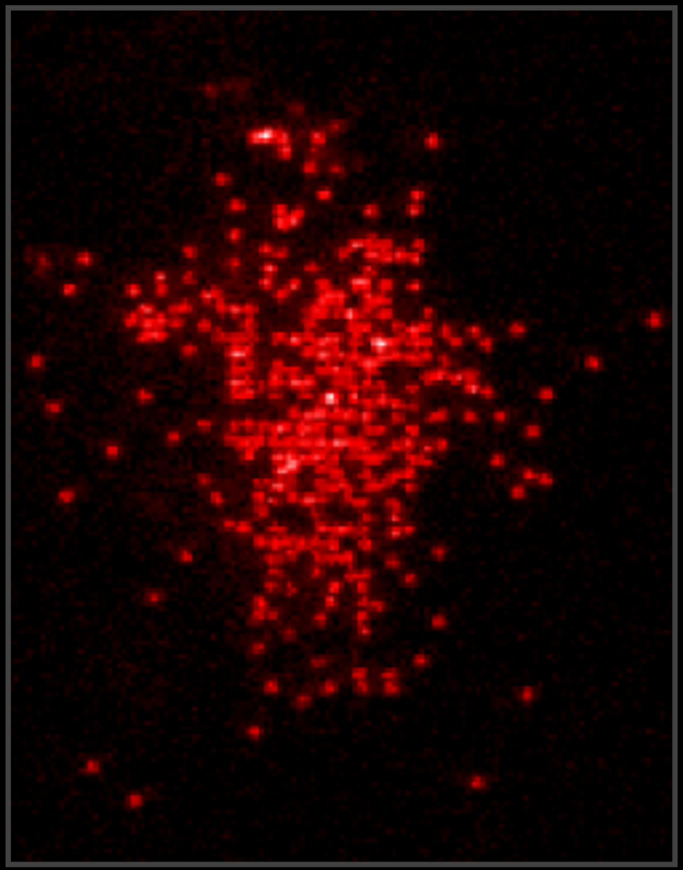




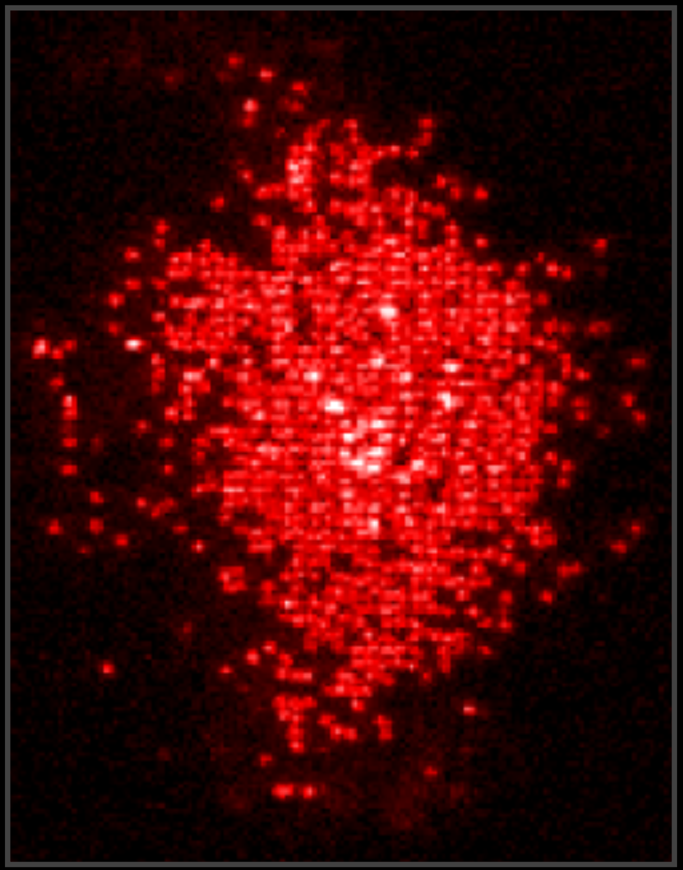
7 kHz Photon Scattering Rate!



dilute



medium

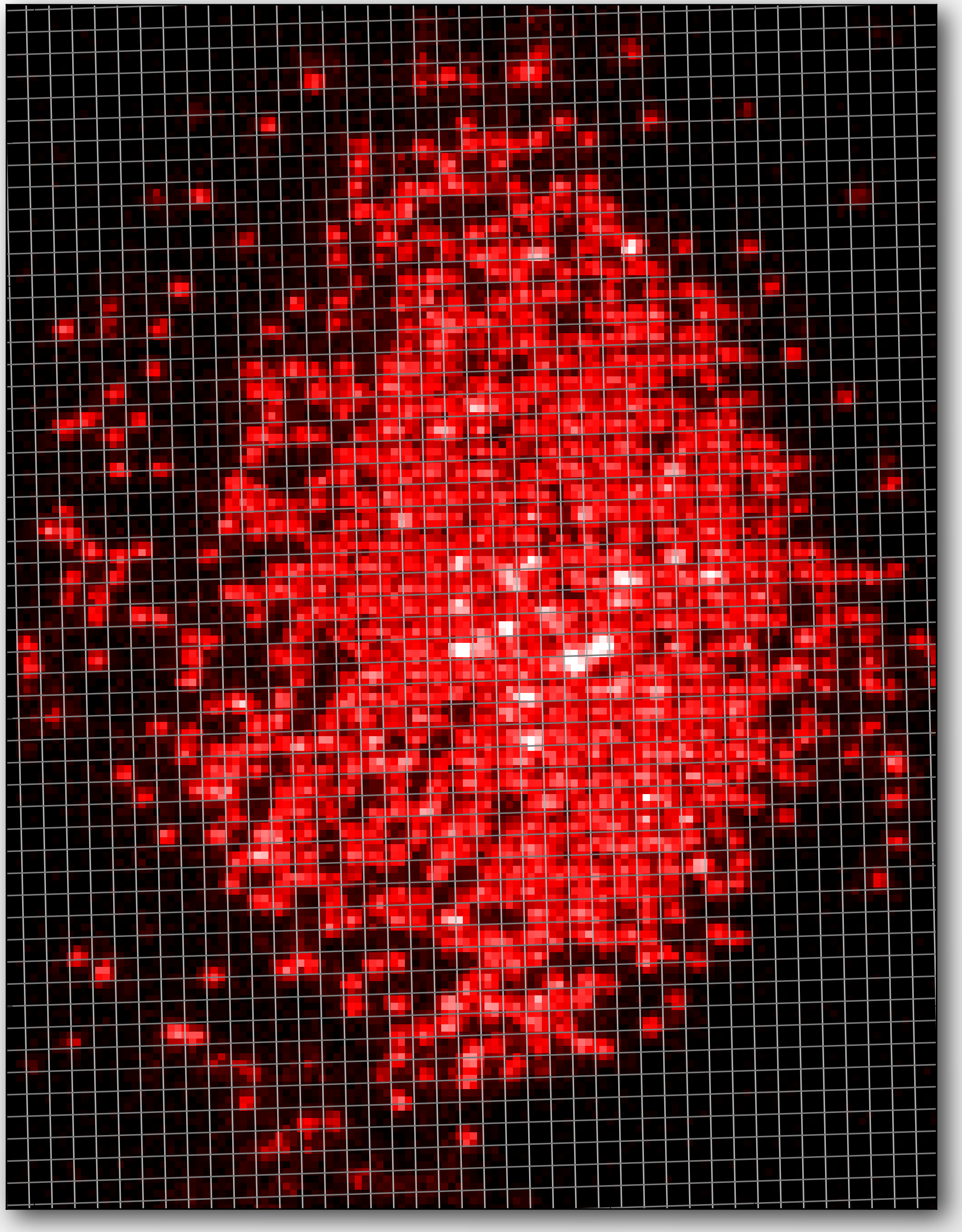


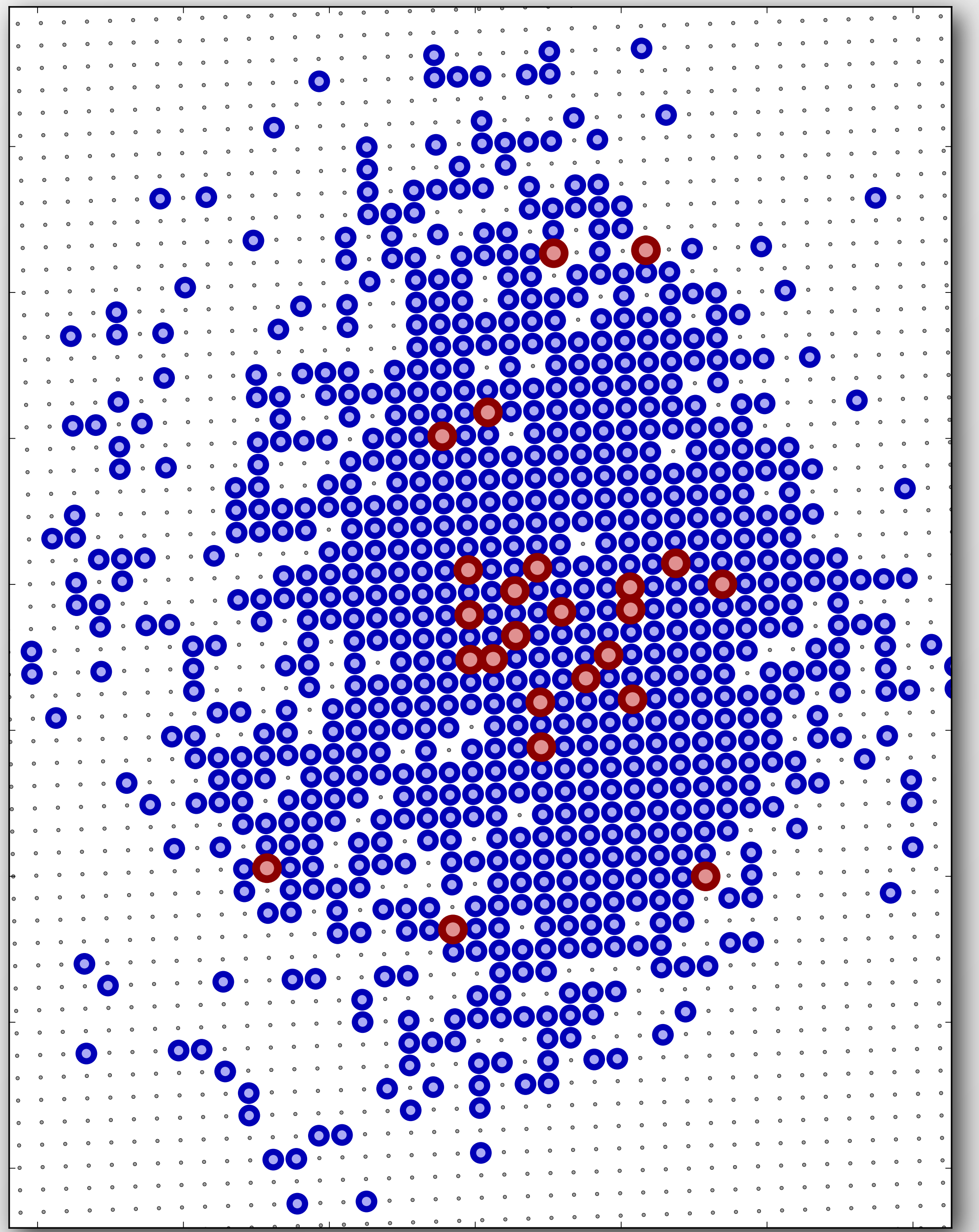
dense - Band Insulator

Single Atom Fluorescence Imaging 6-Li

A. Omran et al. PRL **115**, 263001 (2015)

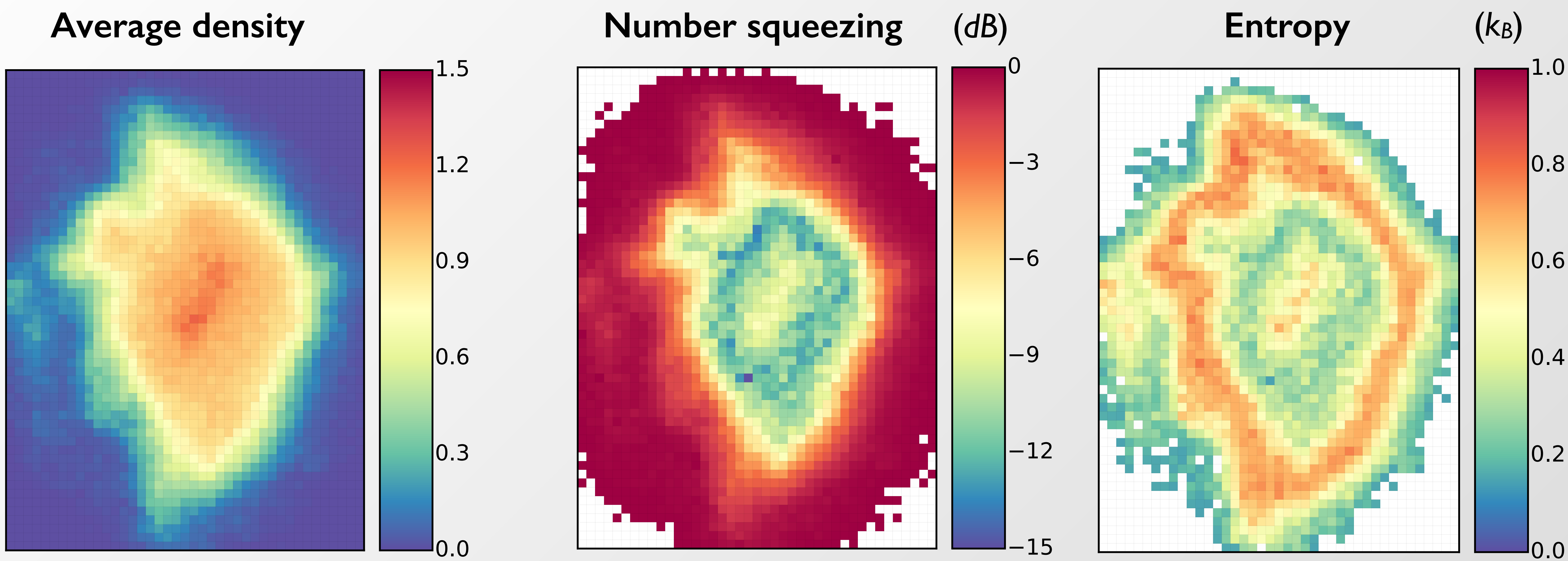
Reconstruction of BI





~800 atoms in image
field of view ~2000 lattice sites

Site Resolved Many-Body State Analysis



$\bar{n}_i$

$$\frac{\sigma_{n,i}^2}{\bar{n}_i}$$

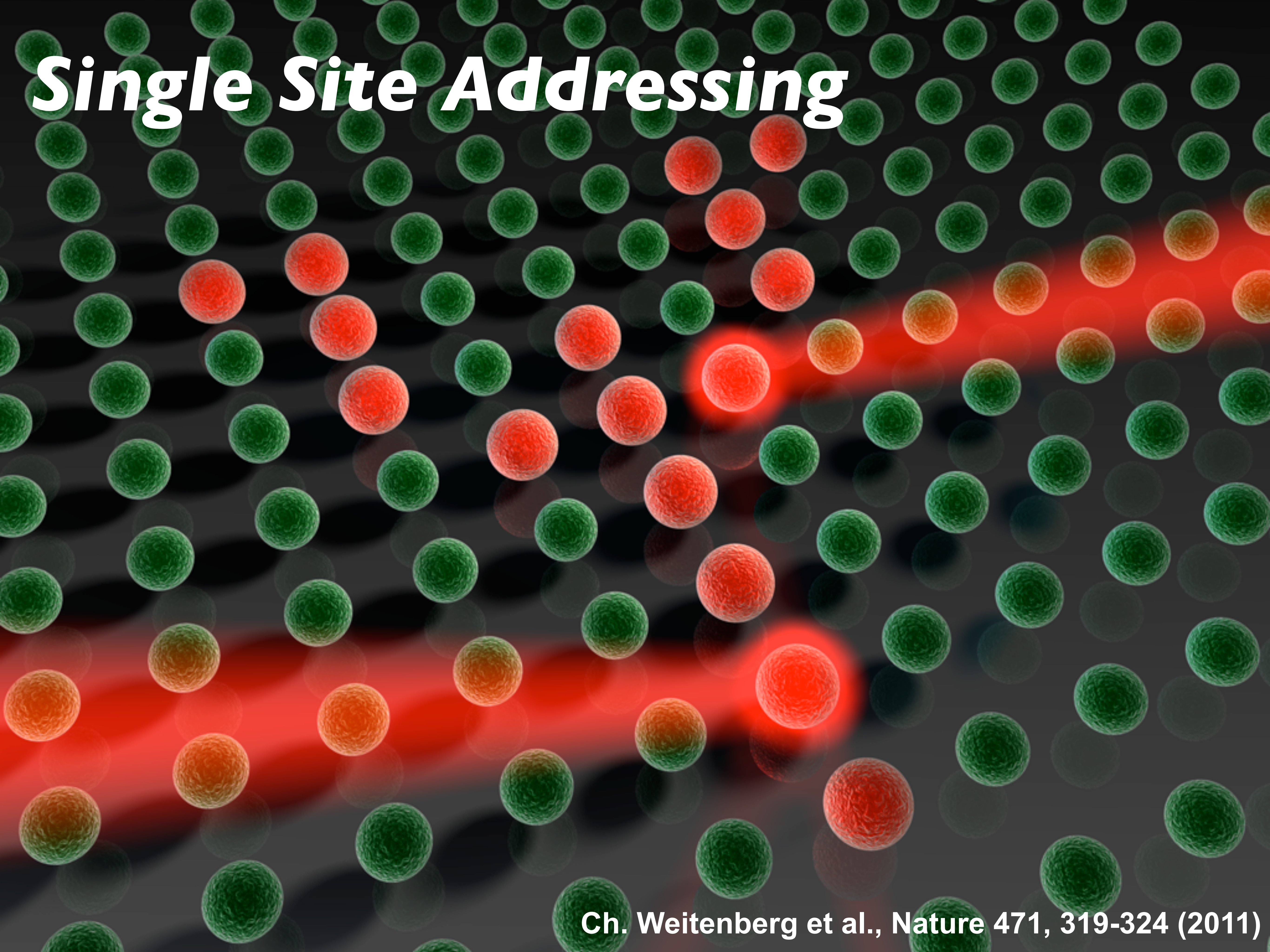
$$S_i = -k_B \sum_{j\in 0,1,2} p_{i,j} \log p_{i,j}$$

Analysis from ~500 single shot images!

Assume Grand Canonical also allows to obtain μ,T,k…

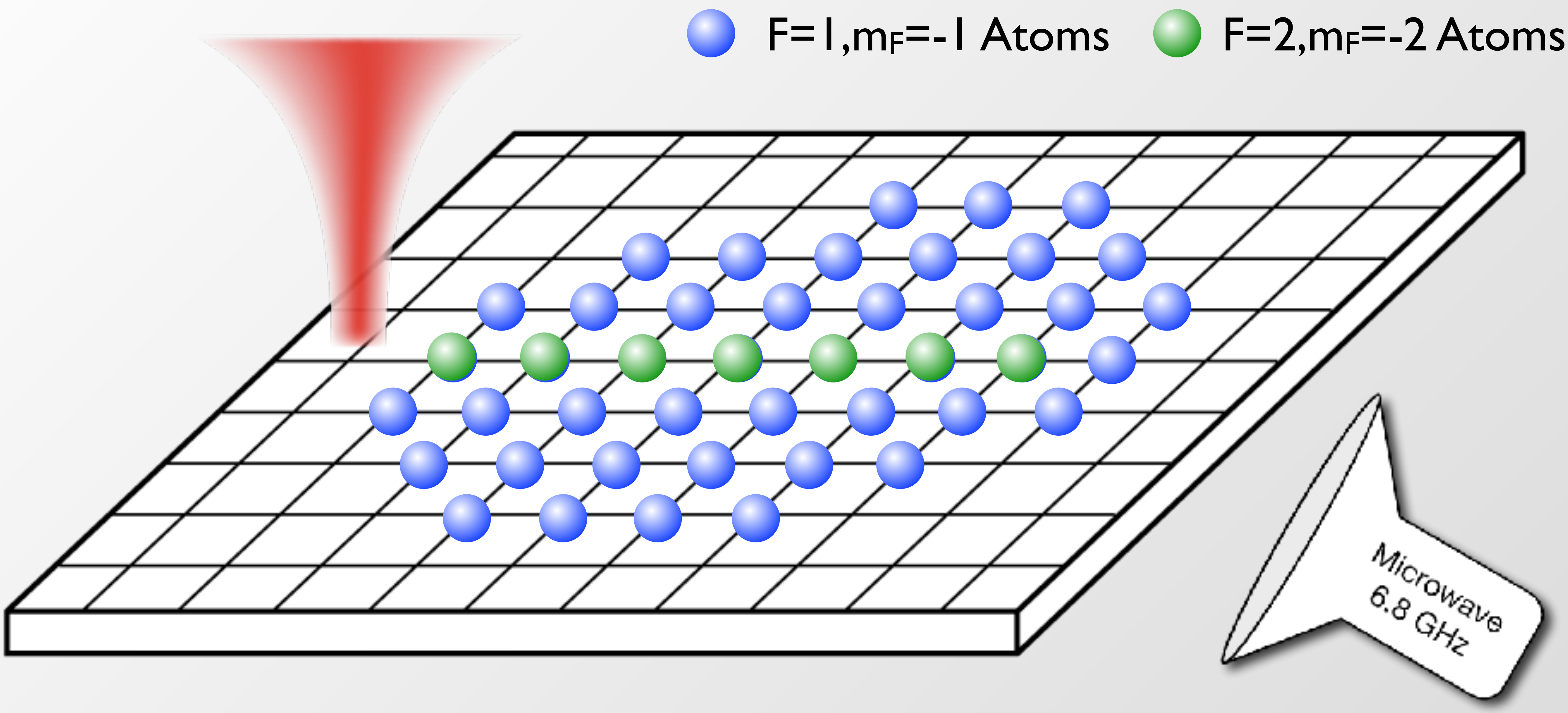
A. Omran et al. PRL **115**, 263001 (2015)

Single Site Addressing



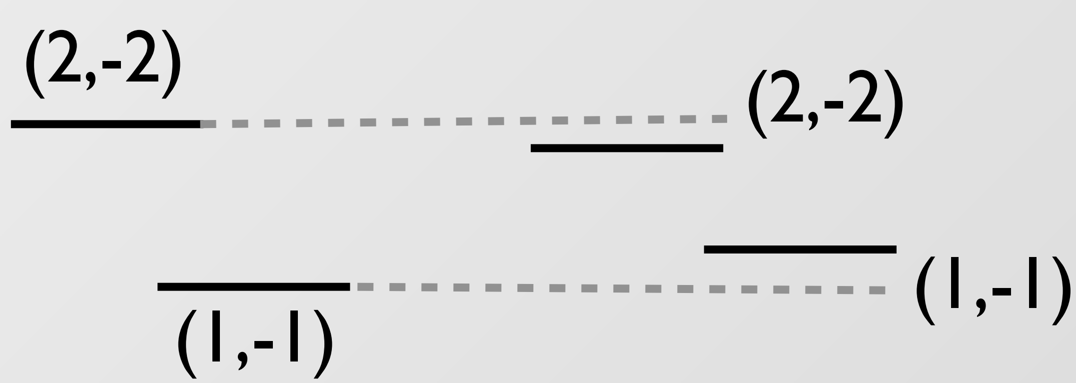
Ch. Weitenberg et al., Nature 471, 319-324 (2011)

Coherent Addressing of Atoms



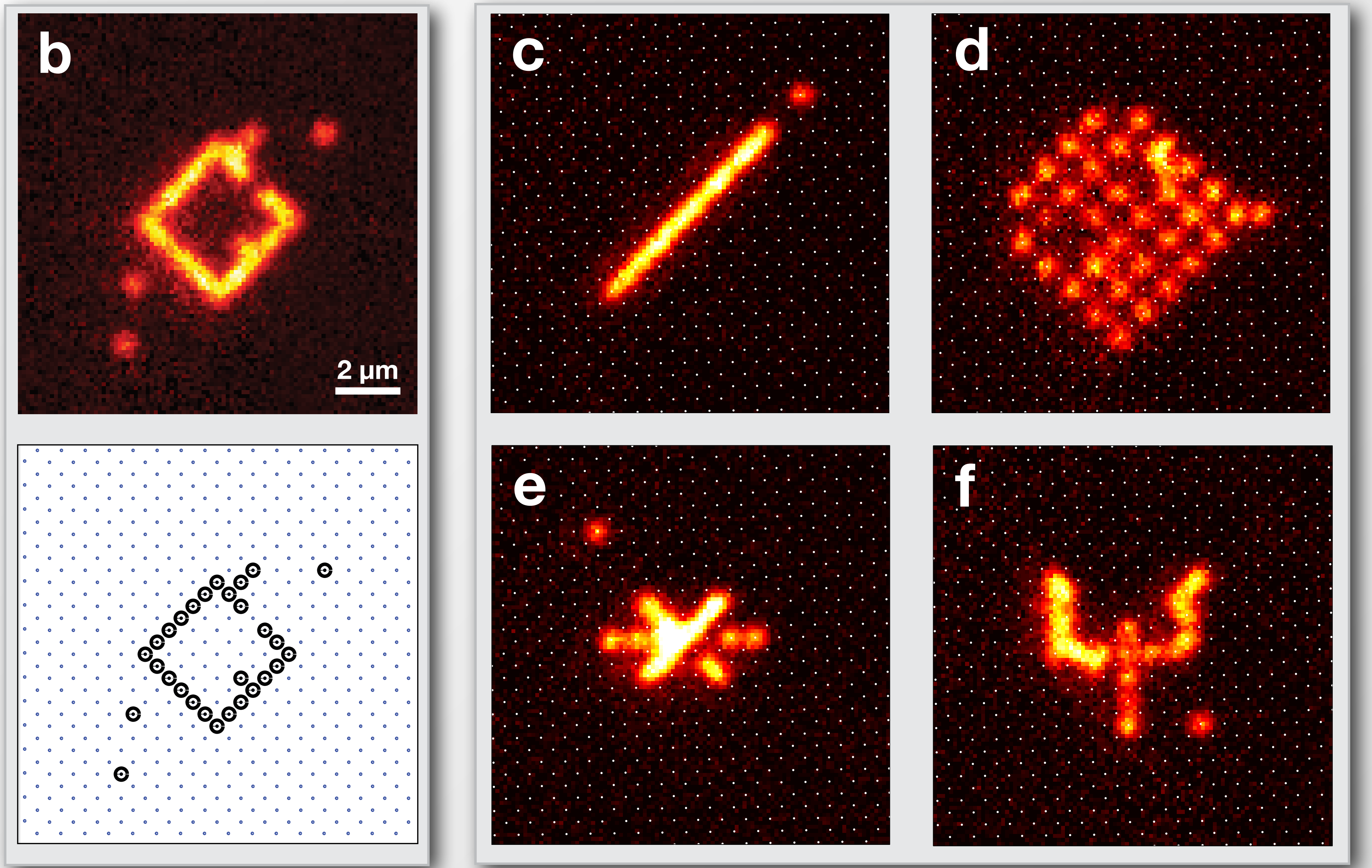
Differential light shift allows to coherently address single atoms!

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



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

Coherent Spin Flips - Positive Imaging

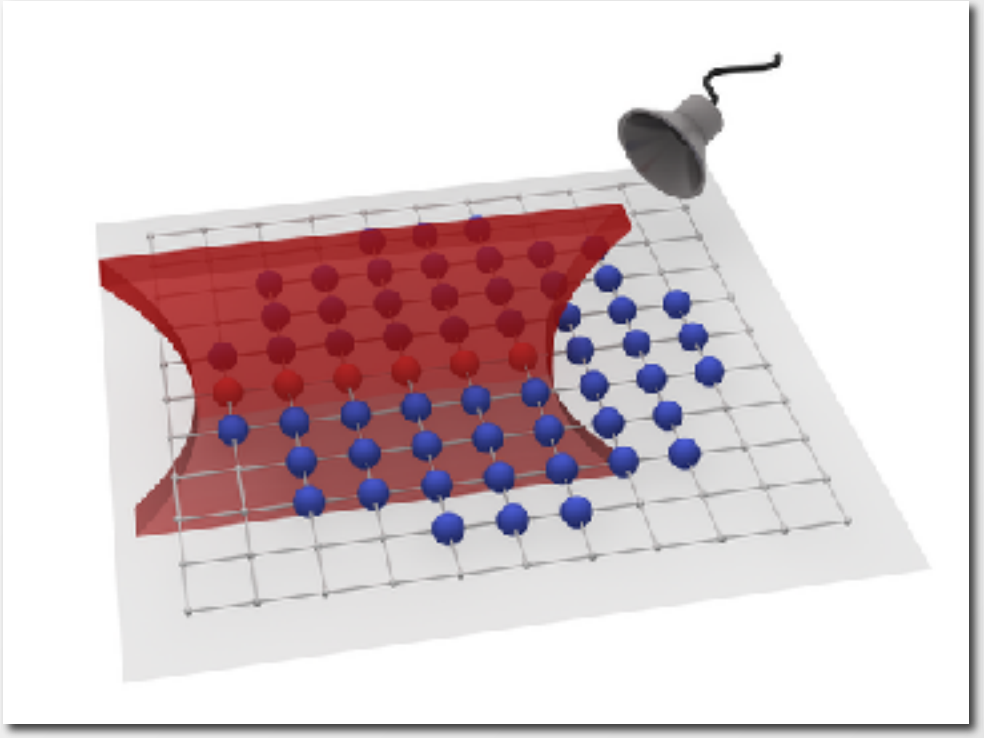


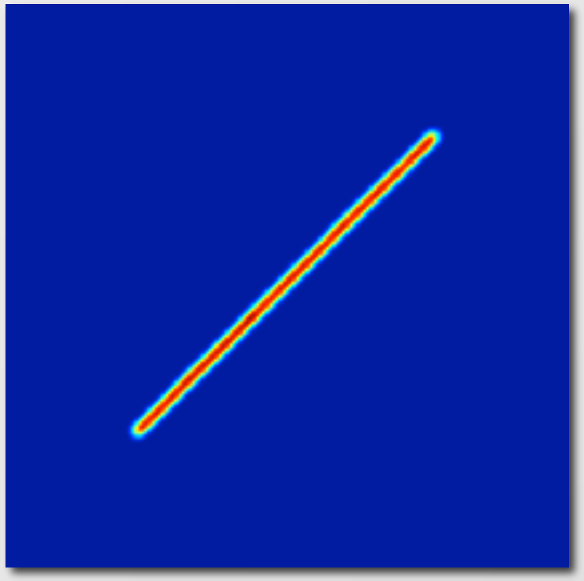
Subwavelength spatial resolution: 50 nm

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

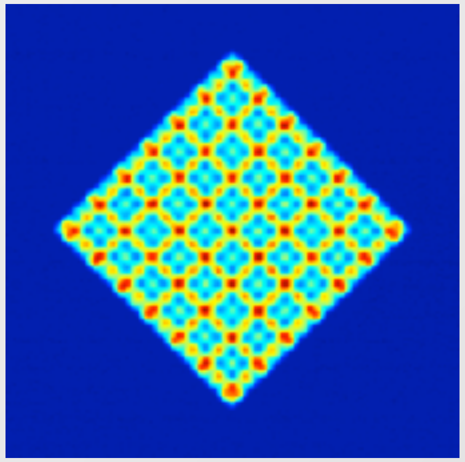
Arbitrary Light Patterns

Digital Mirror Device (DMD)

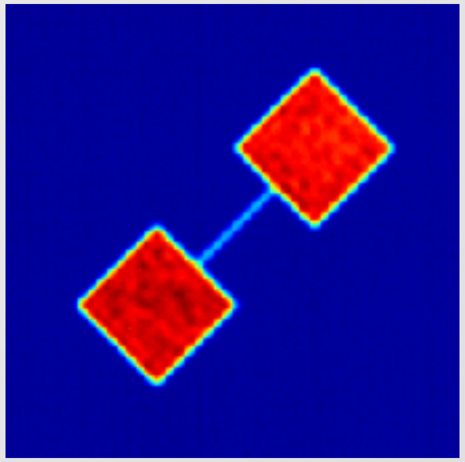




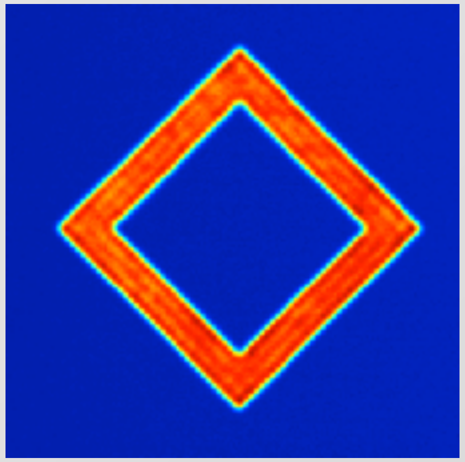
Measured Light Pattern



Exotic Lattices



Quantum Wires

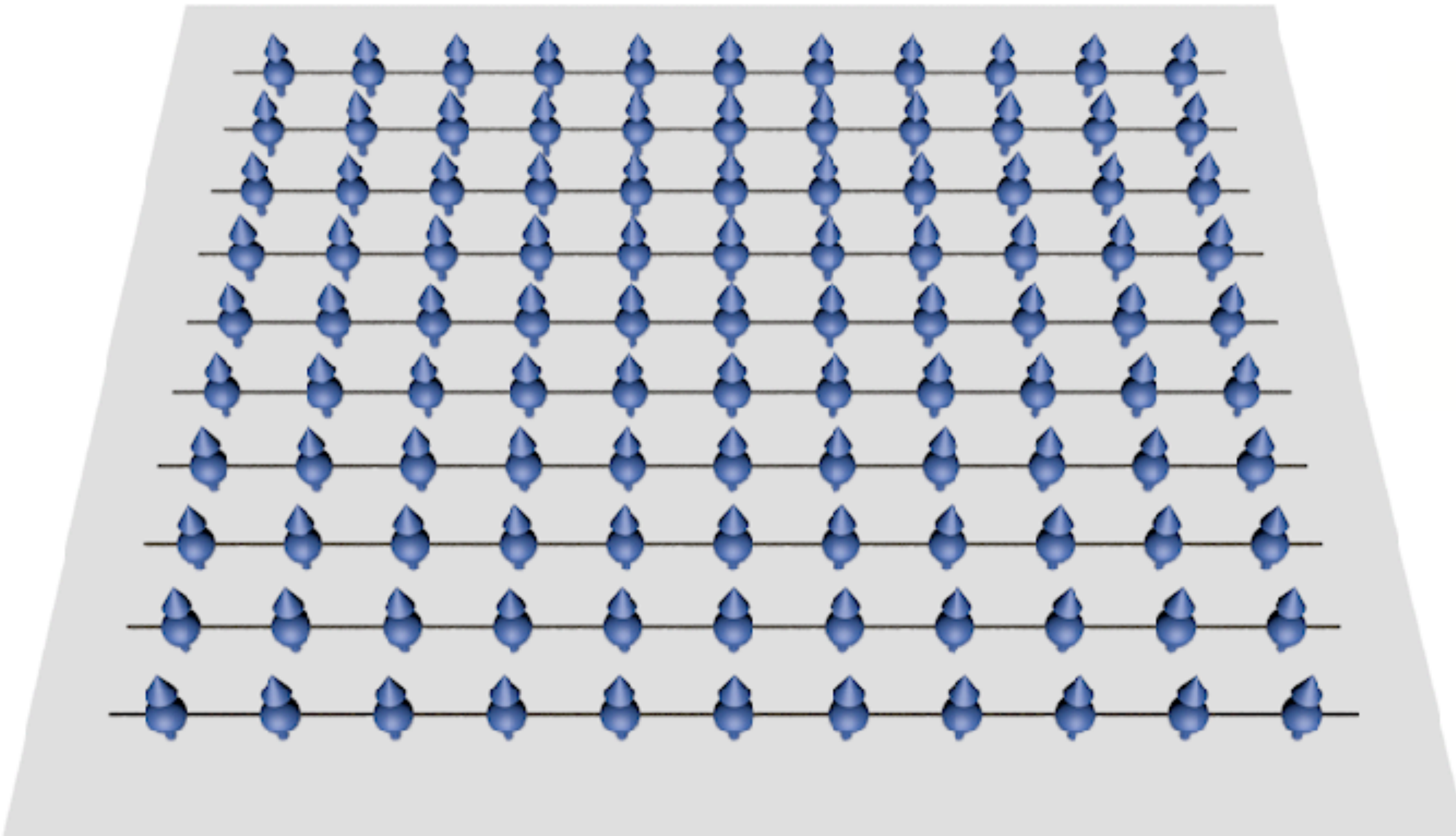


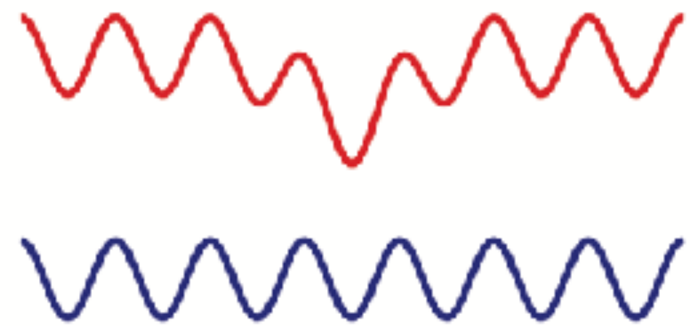
Box Potentials

Almost Arbitrary Light Patterns Possible!

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

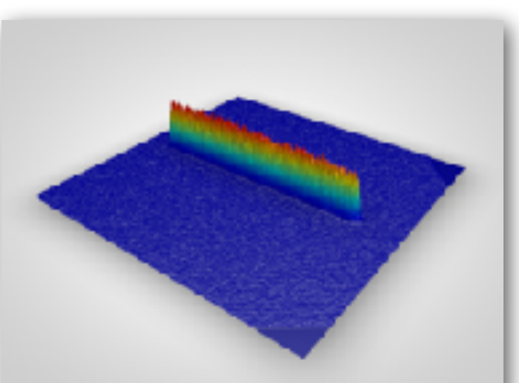
Spin impurity dynamics





$|2\rangle = |F=2, m_F=-2\rangle$

$|1\rangle = |F=1, m_F=-1\rangle$

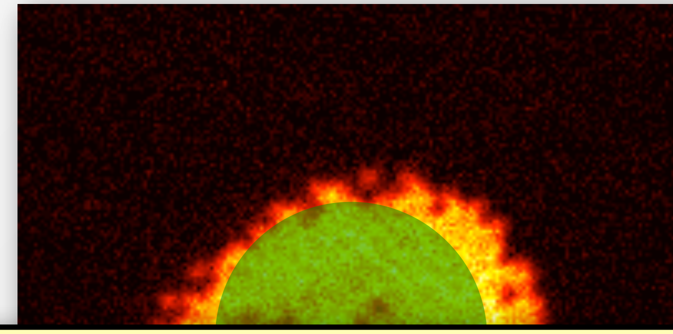


Line-shaped light field created with DMD SLM

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

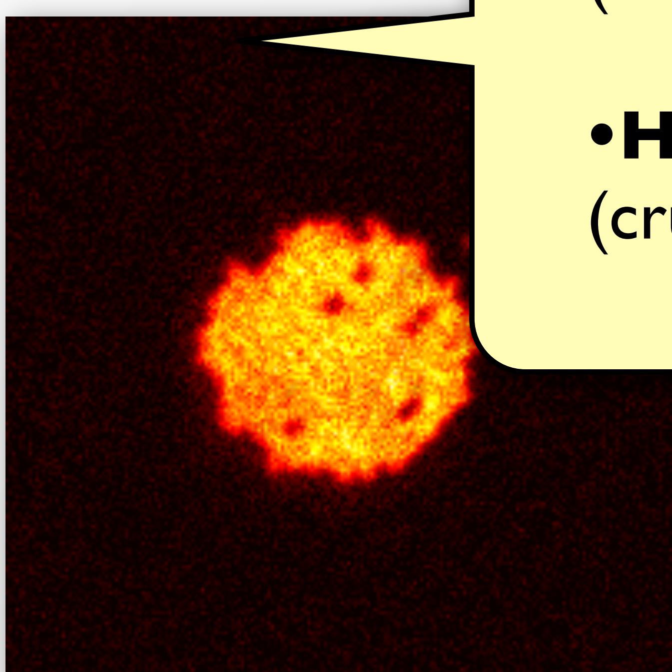
Ultimate Size Control in 2D

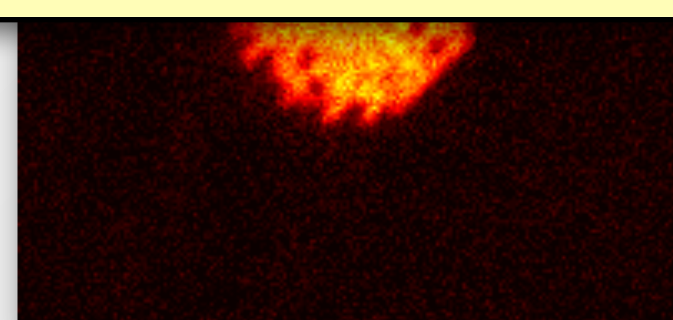
Digital Mirror
Device (Size Control)

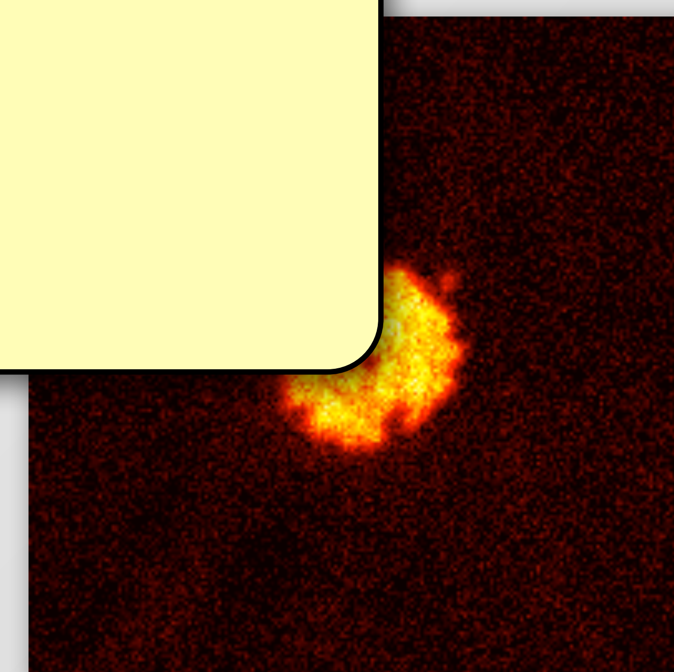


Fluctuating Size and

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

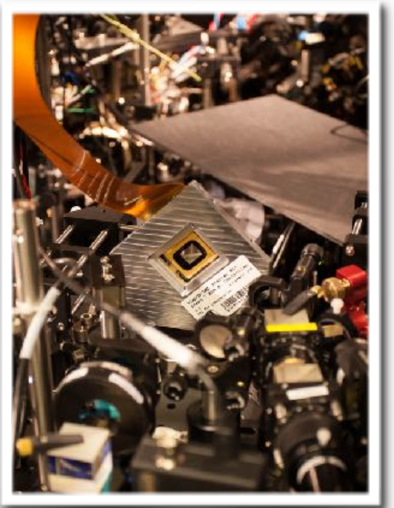




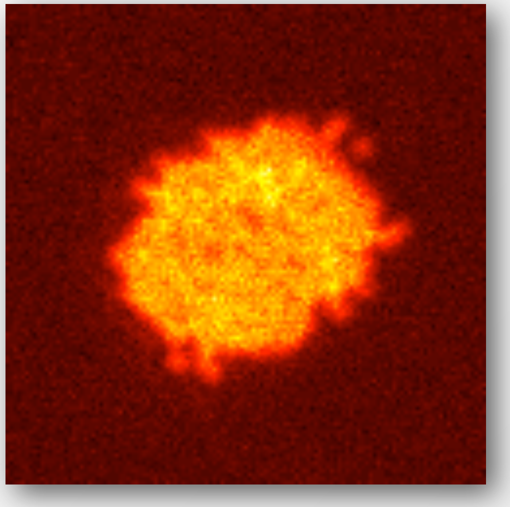


Size & atom number perfectly controlled

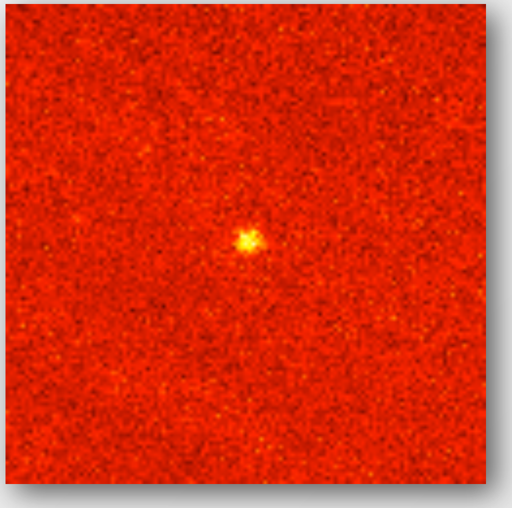
Ultimate Size Control in 2D



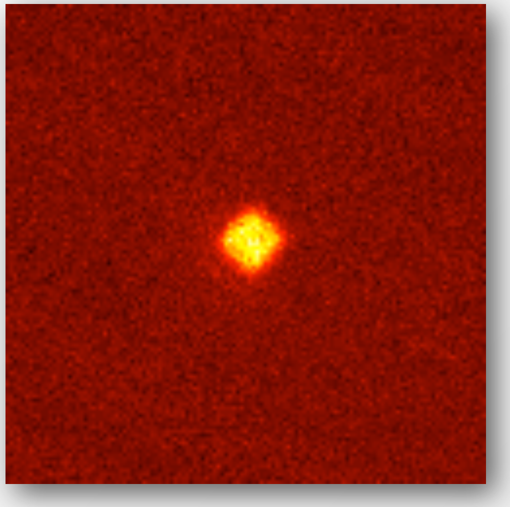
Digital Mirror Device (Size Control)



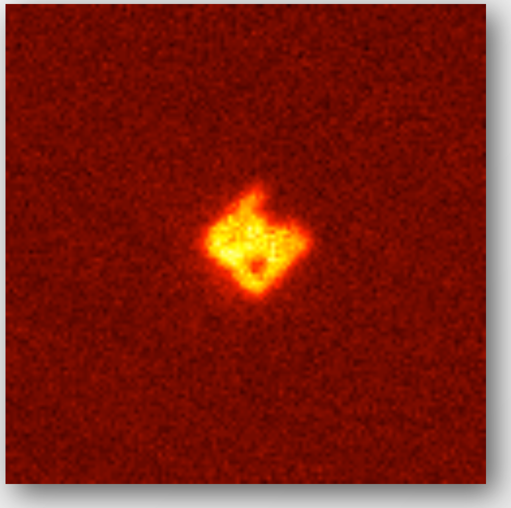
Initial MI



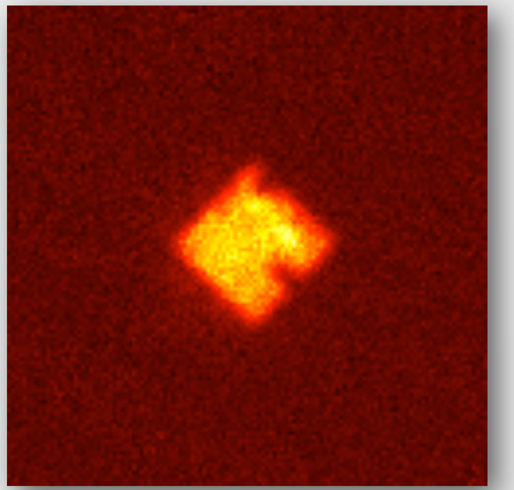
Single Atom



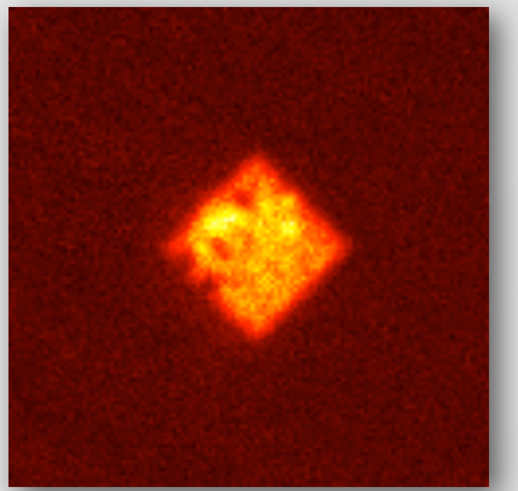
3x3



5x5



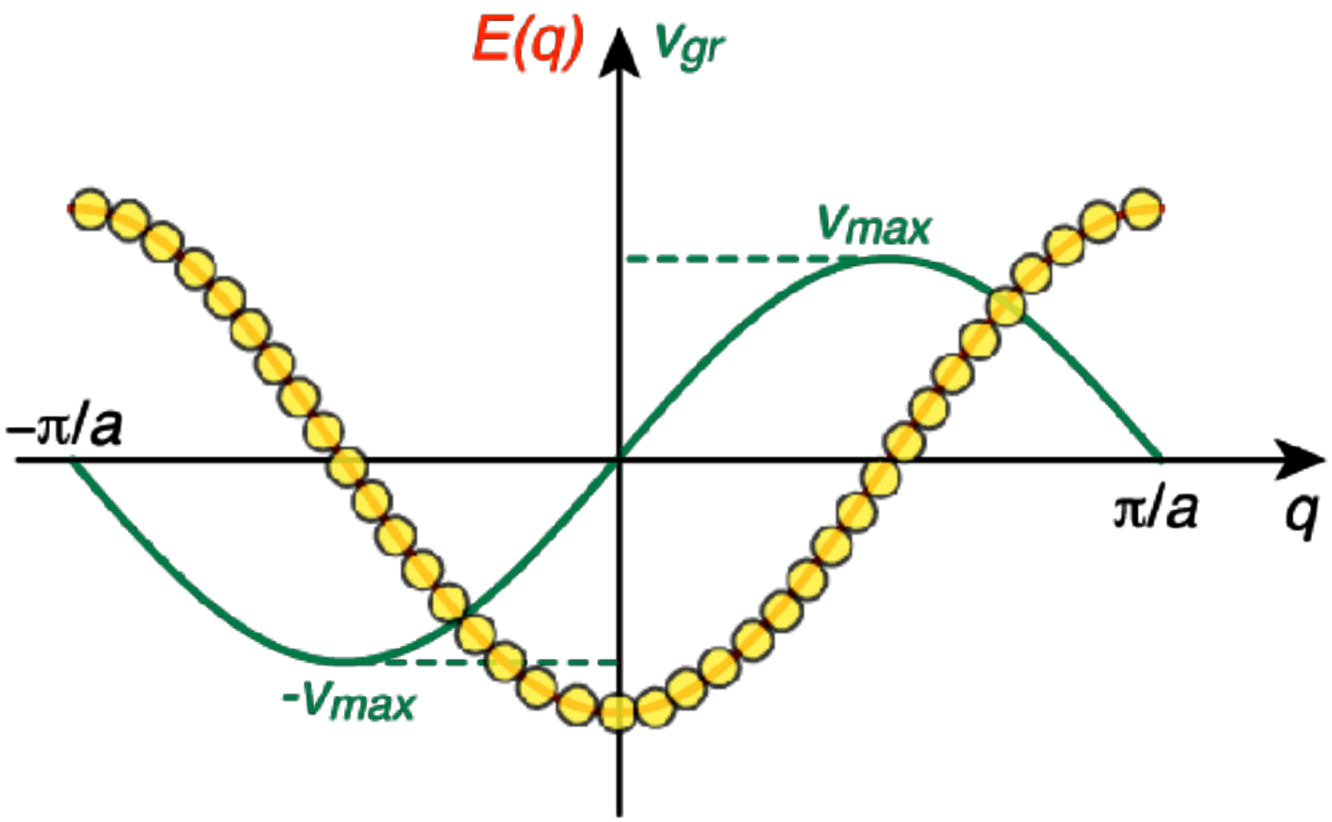
7x7



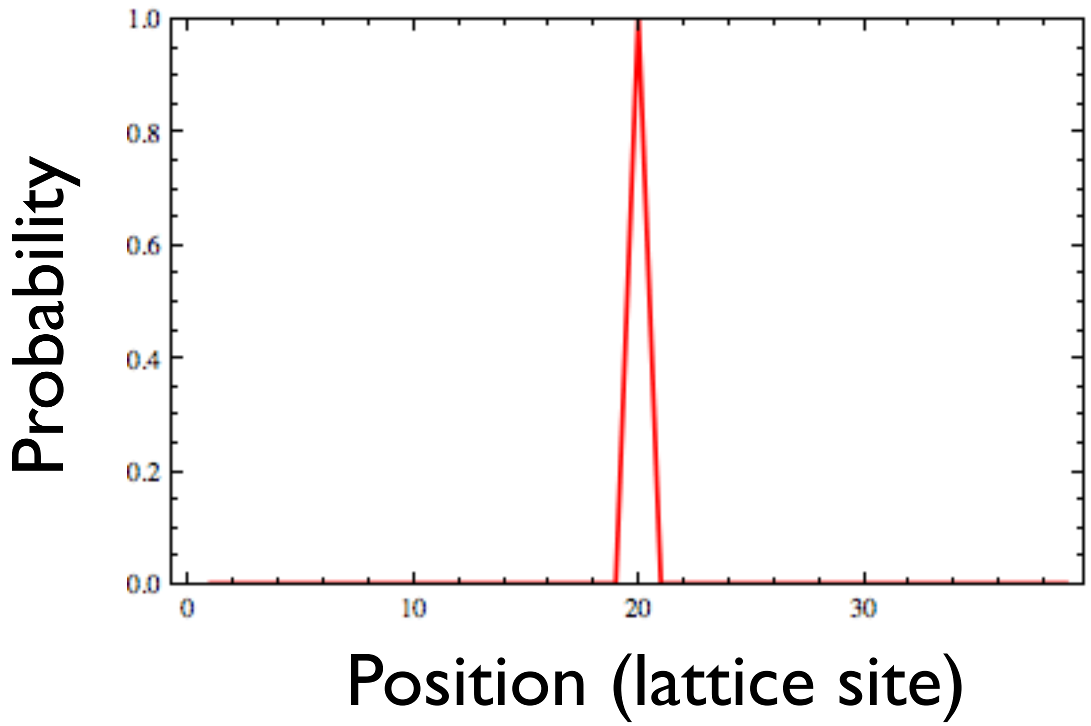
8x8

atoms

Tunneling of a Single Atom

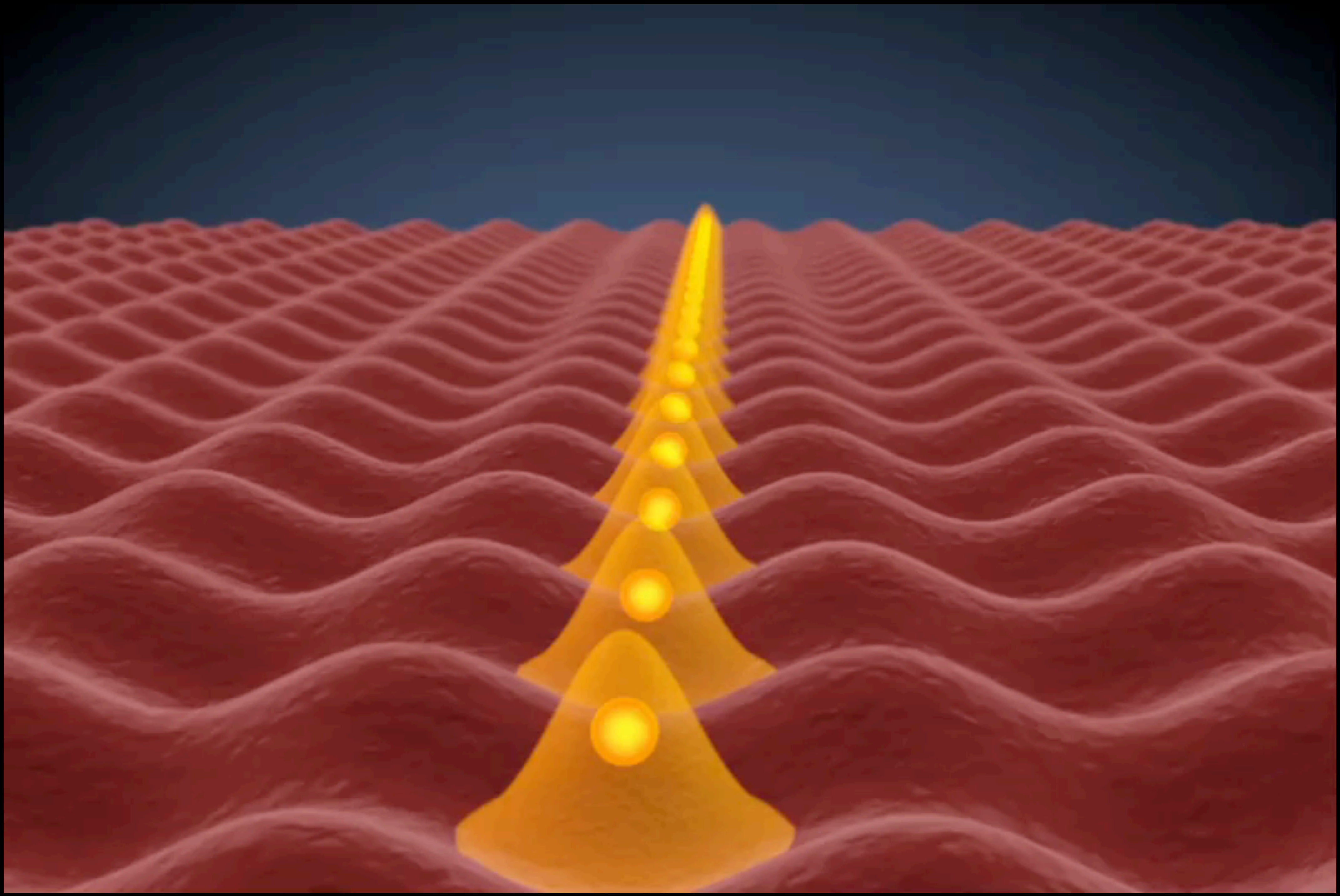


$$v_{max} = \frac{2Ja}{\hbar}$$

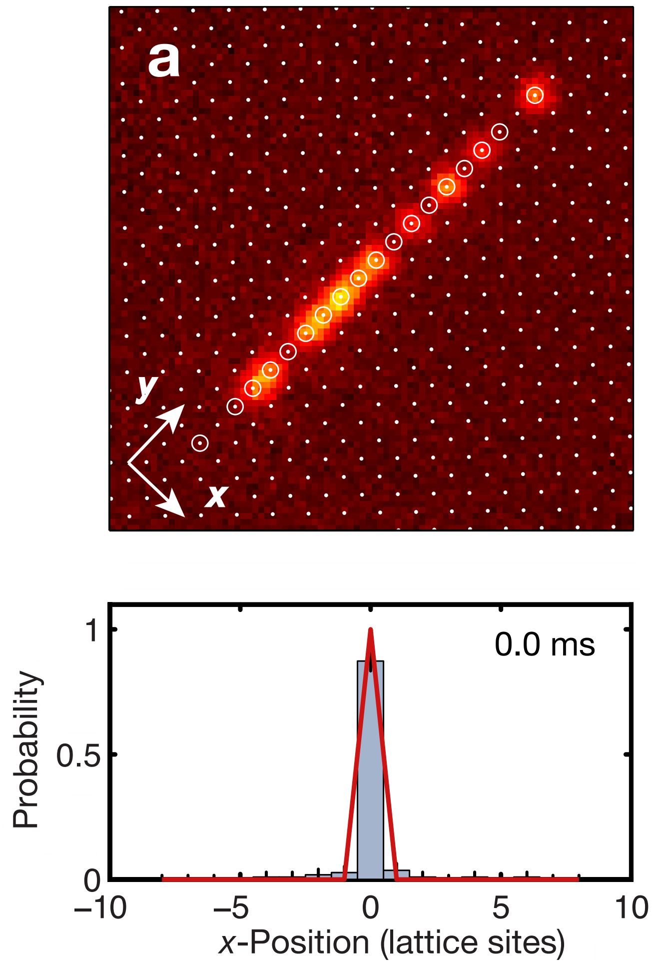


$$H = -J^{(0)} \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \frac{1}{2} m\omega^2 a_{\rm lat}^2 i^2 \hat{n}_i$$

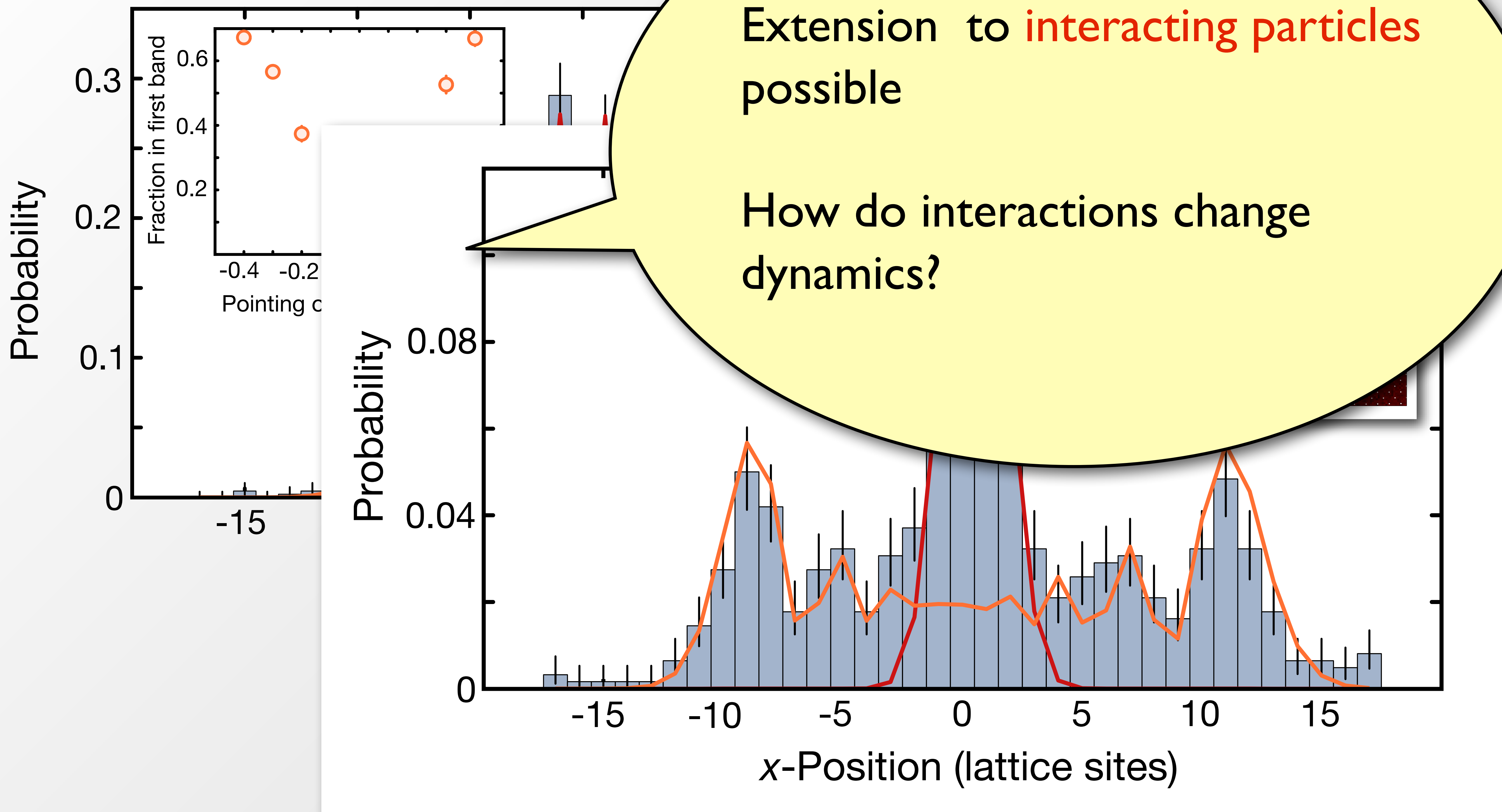
Single Atom Tunnelling



Motional State Affected?



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



Extension to interacting particles possible

How do interactions change dynamics?

Excellent agreement with simulation.

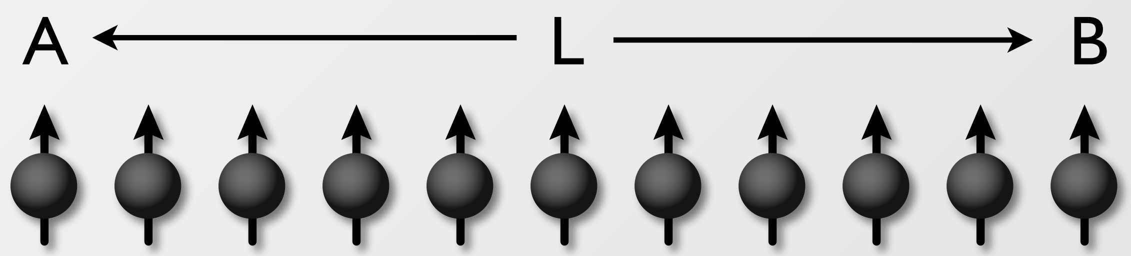
Light-Cone Like Spreading of Correlations in a Many-Body System

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)

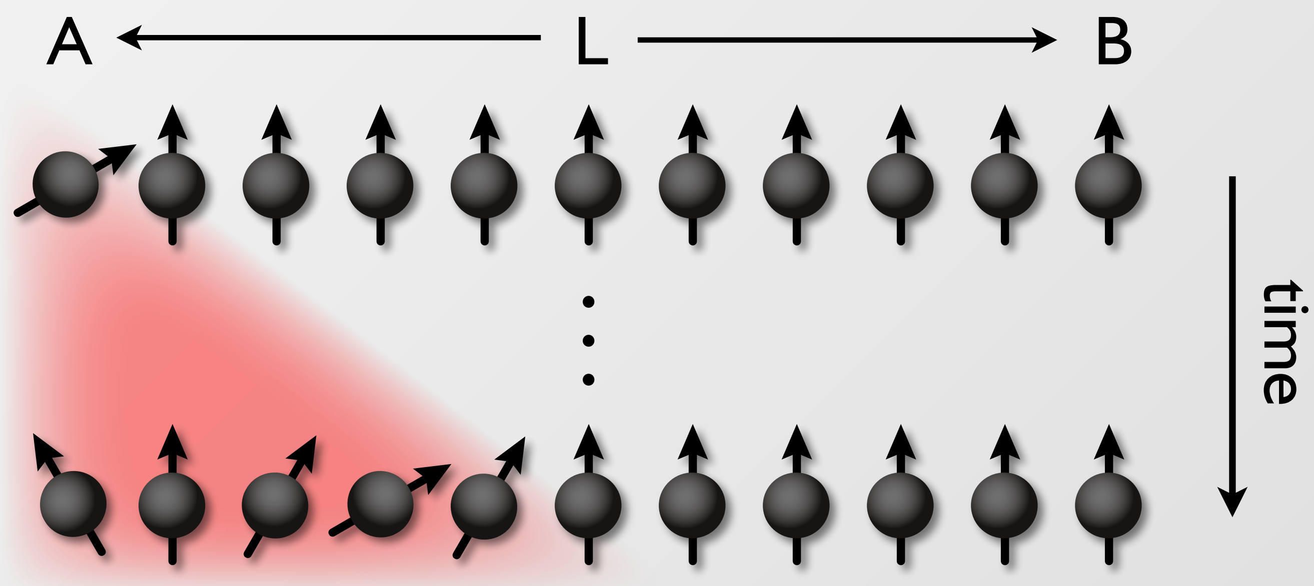
Lieb-Robinson bounds

Spin chain
short-range interactions



Lieb-Robinson bounds

Spin chain
short-range interactions

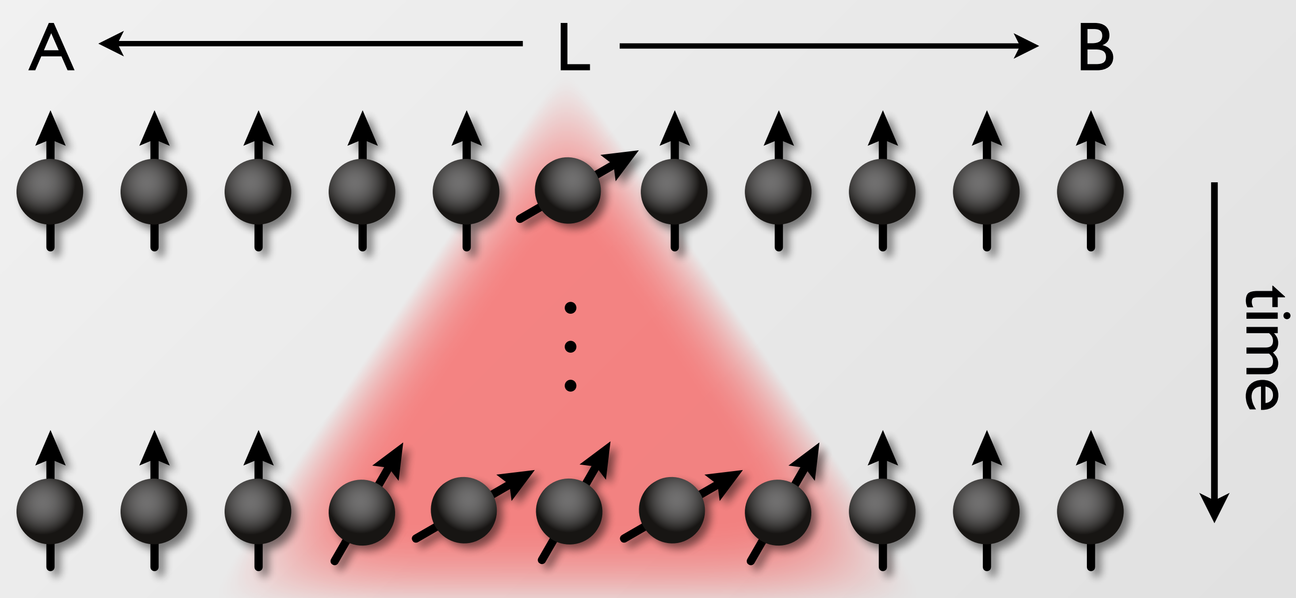


Lieb and Robinson (1972)

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

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

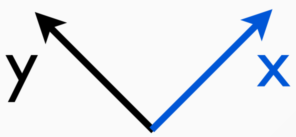
$$\left| \langle A(t)B(t)\rangle - \langle A(t)\rangle\langle B(t)\rangle \right| \leq \lambda' \exp\left(\frac{vt - L/2}{\zeta'}\right)$$

the propagation of correlations is bounded by an effective light cone

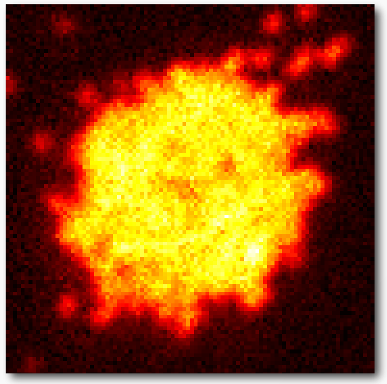
1D Mott insulator out of equilibrium

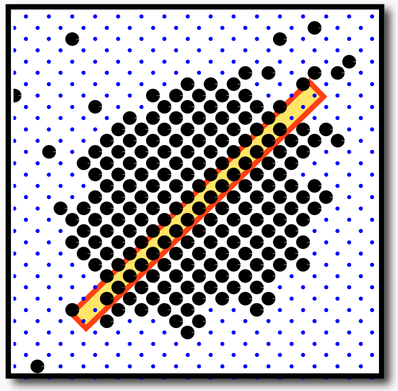
1. Prepare 1D Mott insulator with $U/J \gg 1$

deep lattice (20 E_r)
no tunnelling



variable
lattice depth

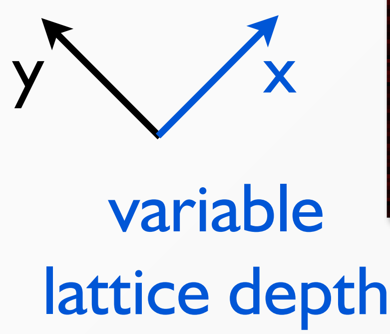


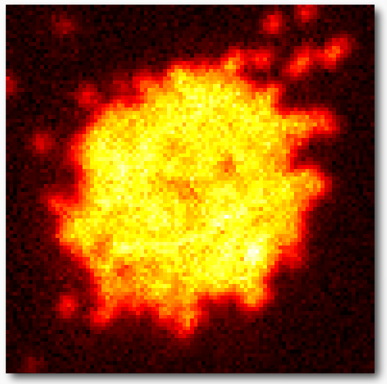


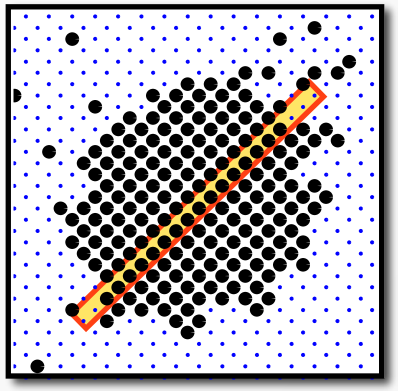
1D Mott insulator out of equilibrium

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

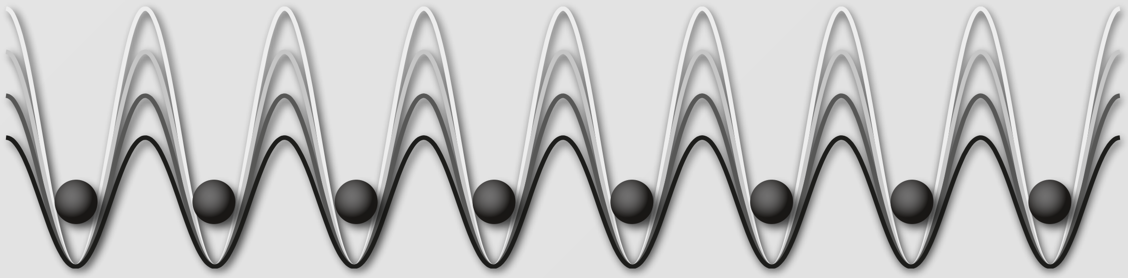
deep lattice (20 E_r)
no tunnelling

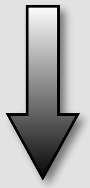






2. Lower U/J abruptly

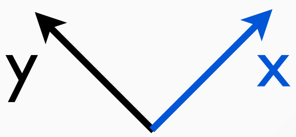




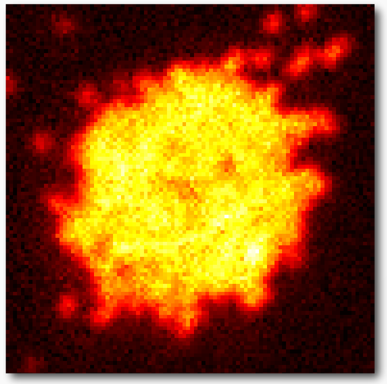
1D Mott insulator out of equilibrium

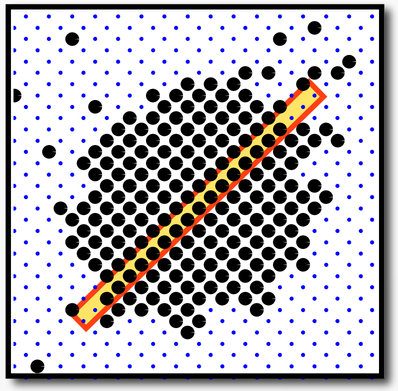
1. Prepare 1D Mott insulator with U/J ≫ 1

deep lattice (20 E_r)
no tunnelling

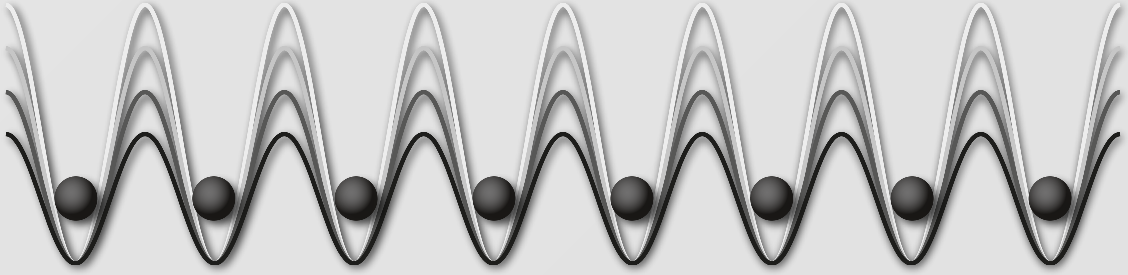


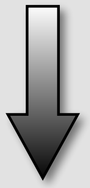
variable
lattice depth





2. Lower U/J abruptly





quench

3. Record the dynamics

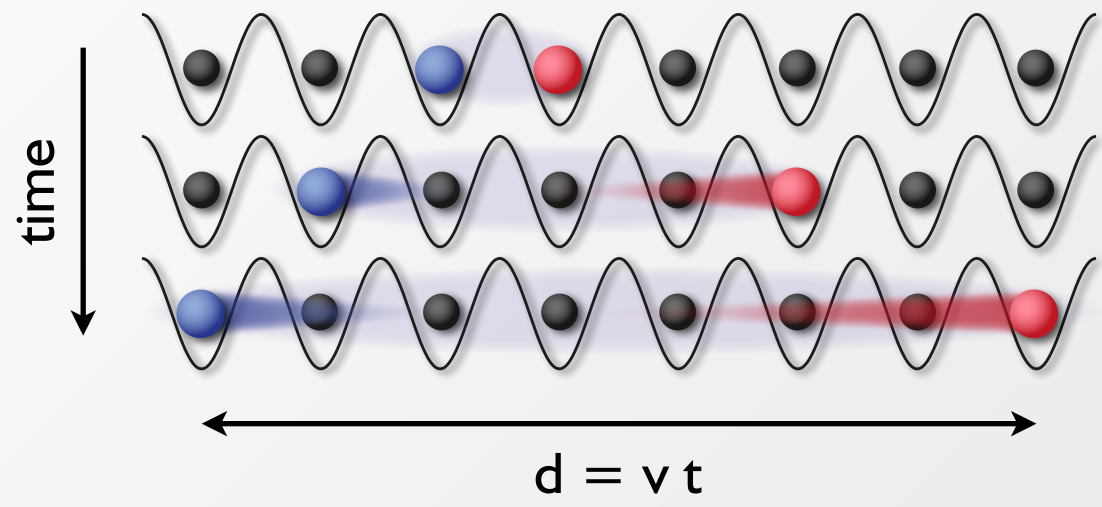
The initial state is highly excited.

Calabrese and Cardy (2006)

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

Light-cone like spreading of correlations

- Quasiparticle dynamics



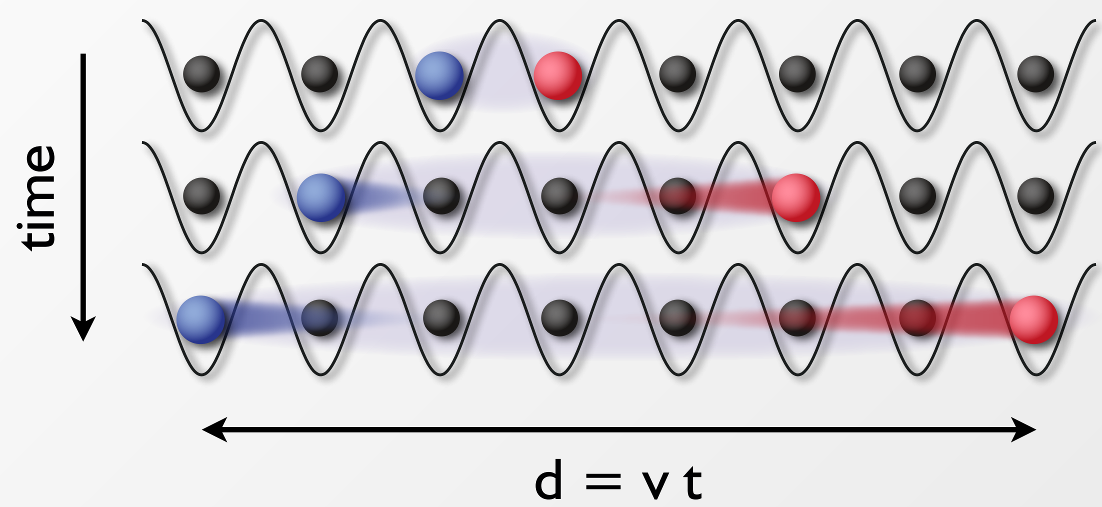
- Two-point parity correlation function

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

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

Light-cone like spreading of correlations

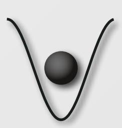
- Quasiparticle dynamics

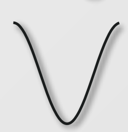
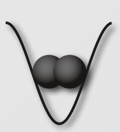


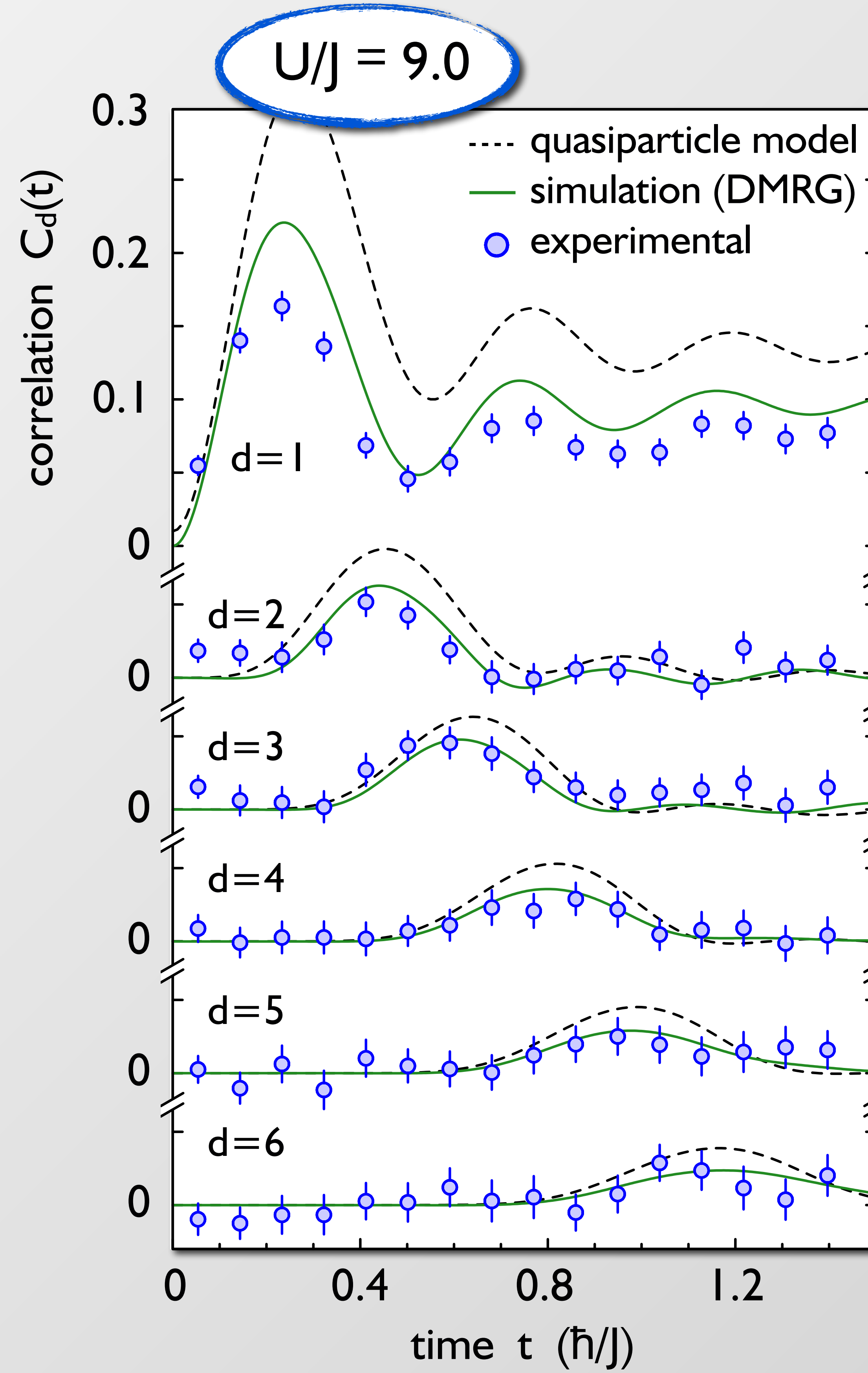
- Two-point parity correlation function

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

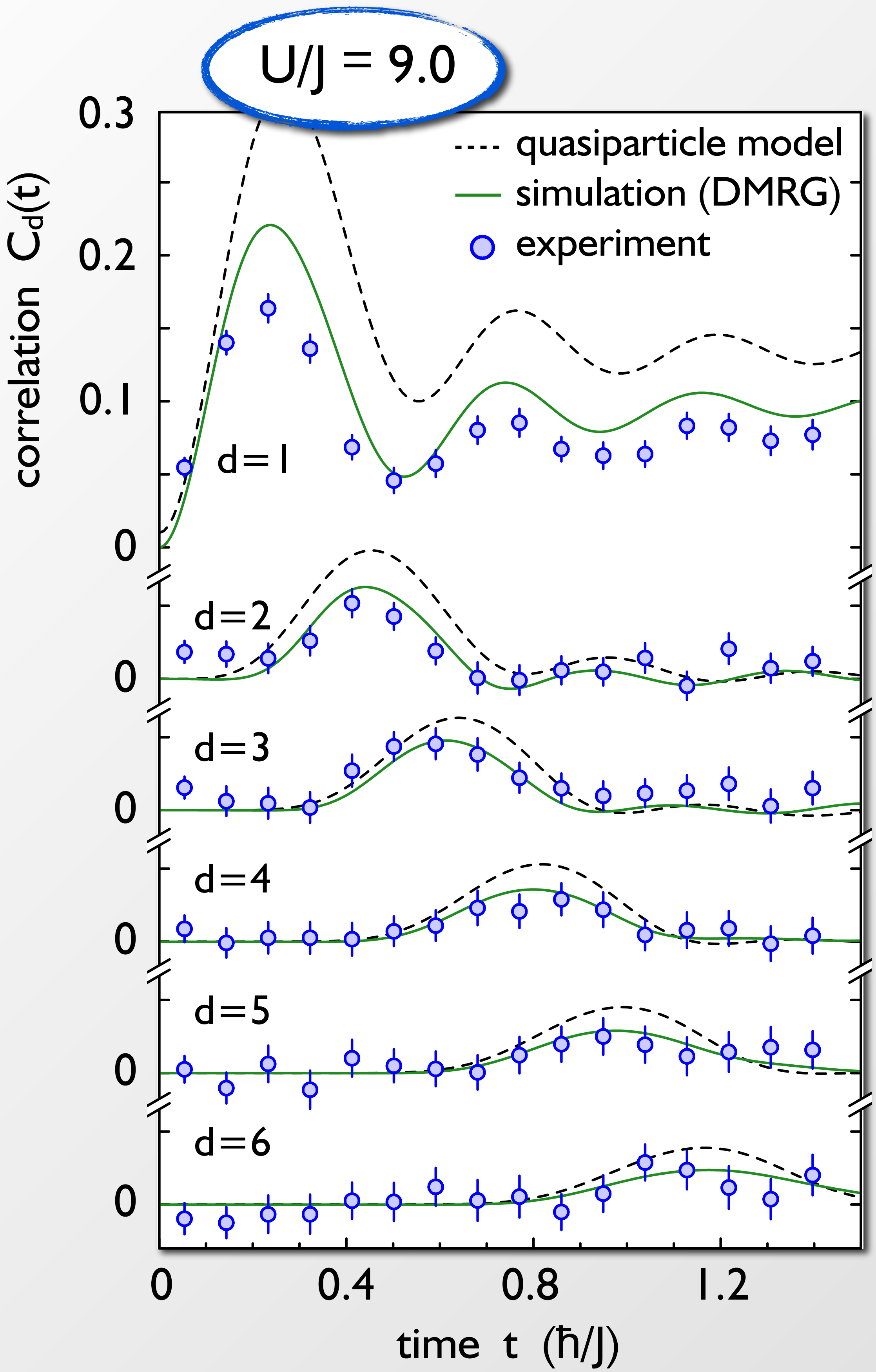
$$s_j(t) = e^{i\pi[n_j(t)-\bar{n}]}$$

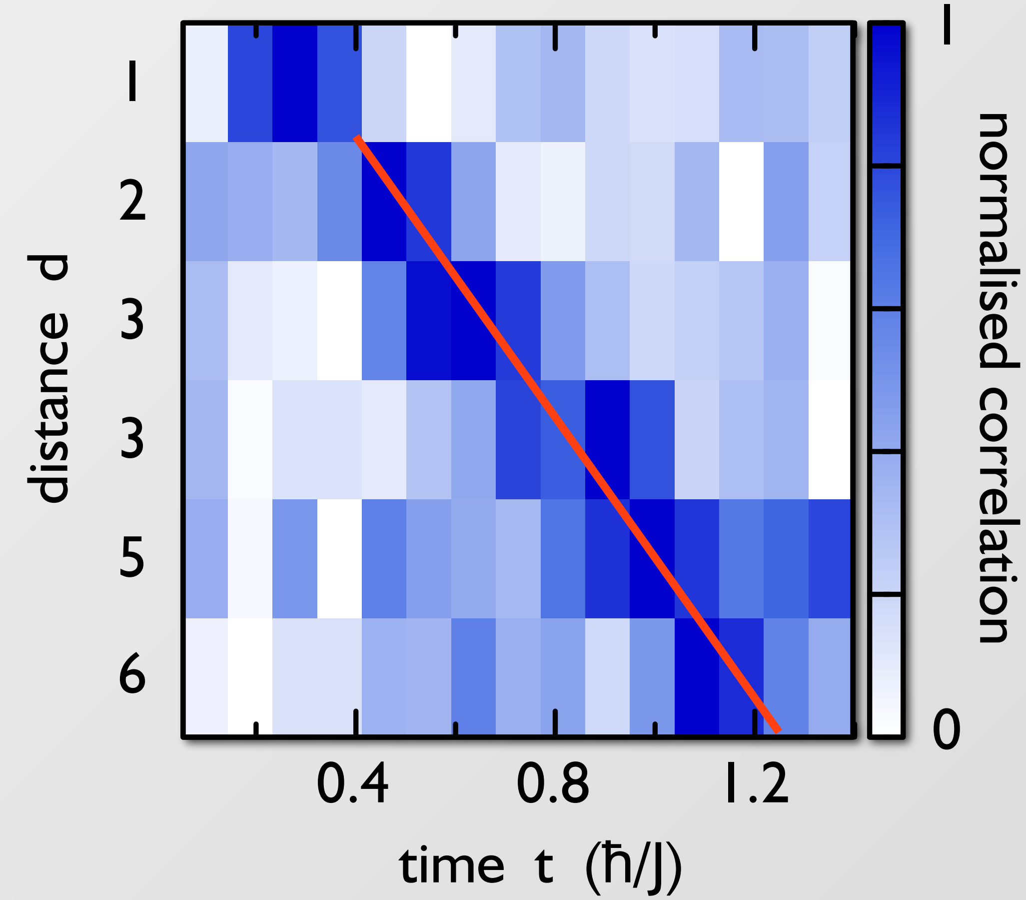
$\{$ +1 if 

-1 if  or 



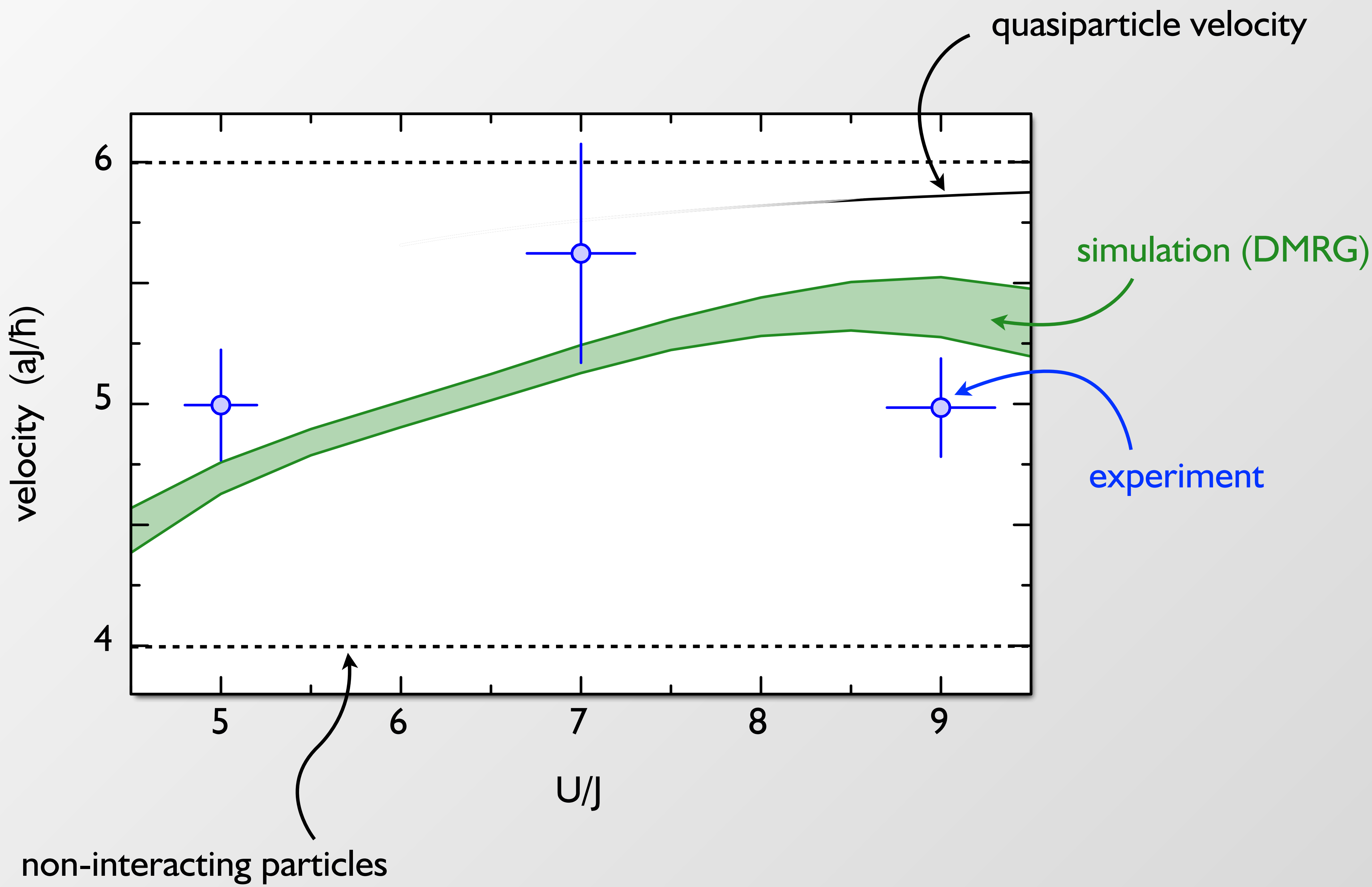
Light-cone like spreading of correlations

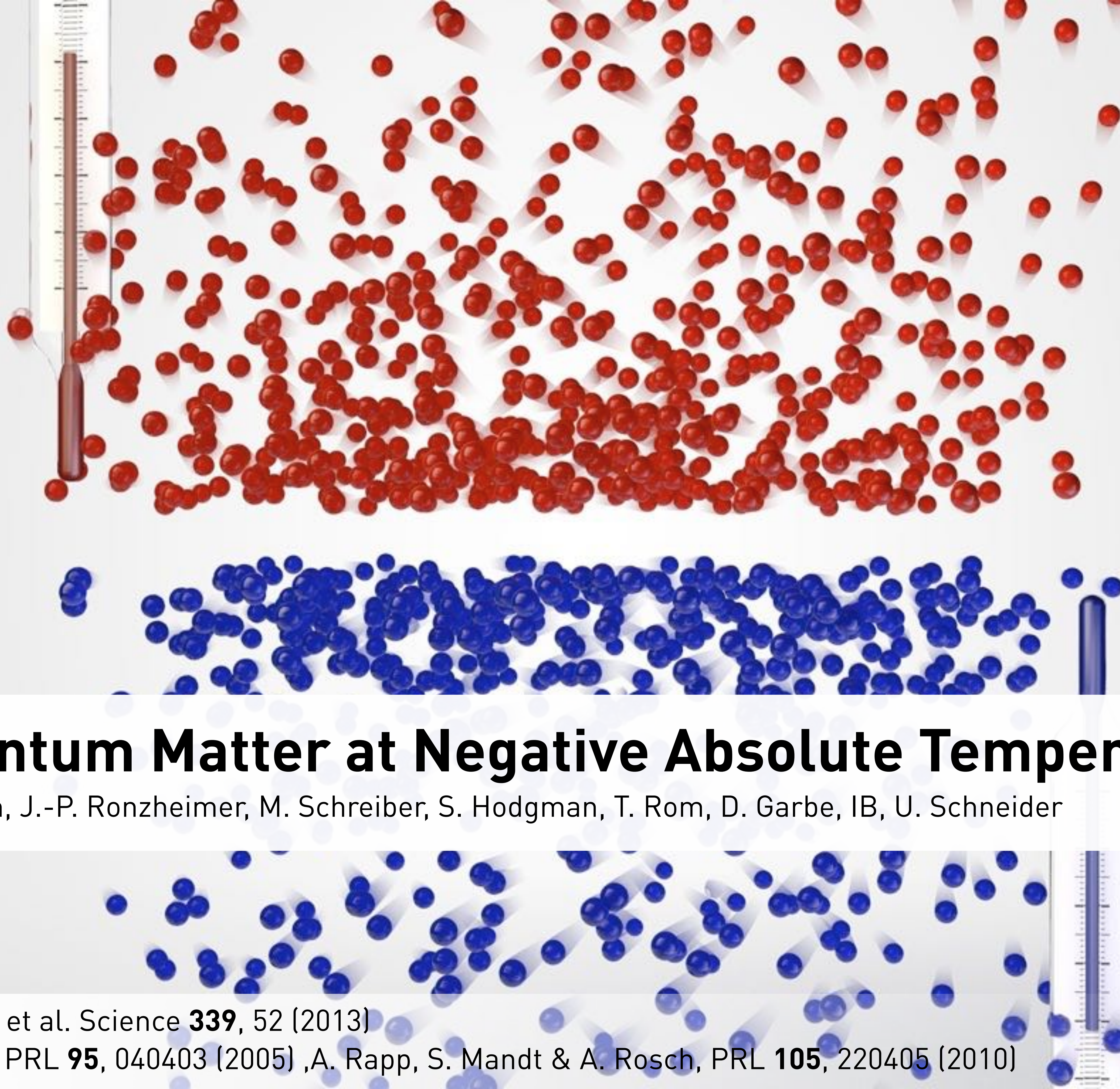




effective light-cone!

Spreading velocity





Quantum Matter at Negative Absolute Temperature

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

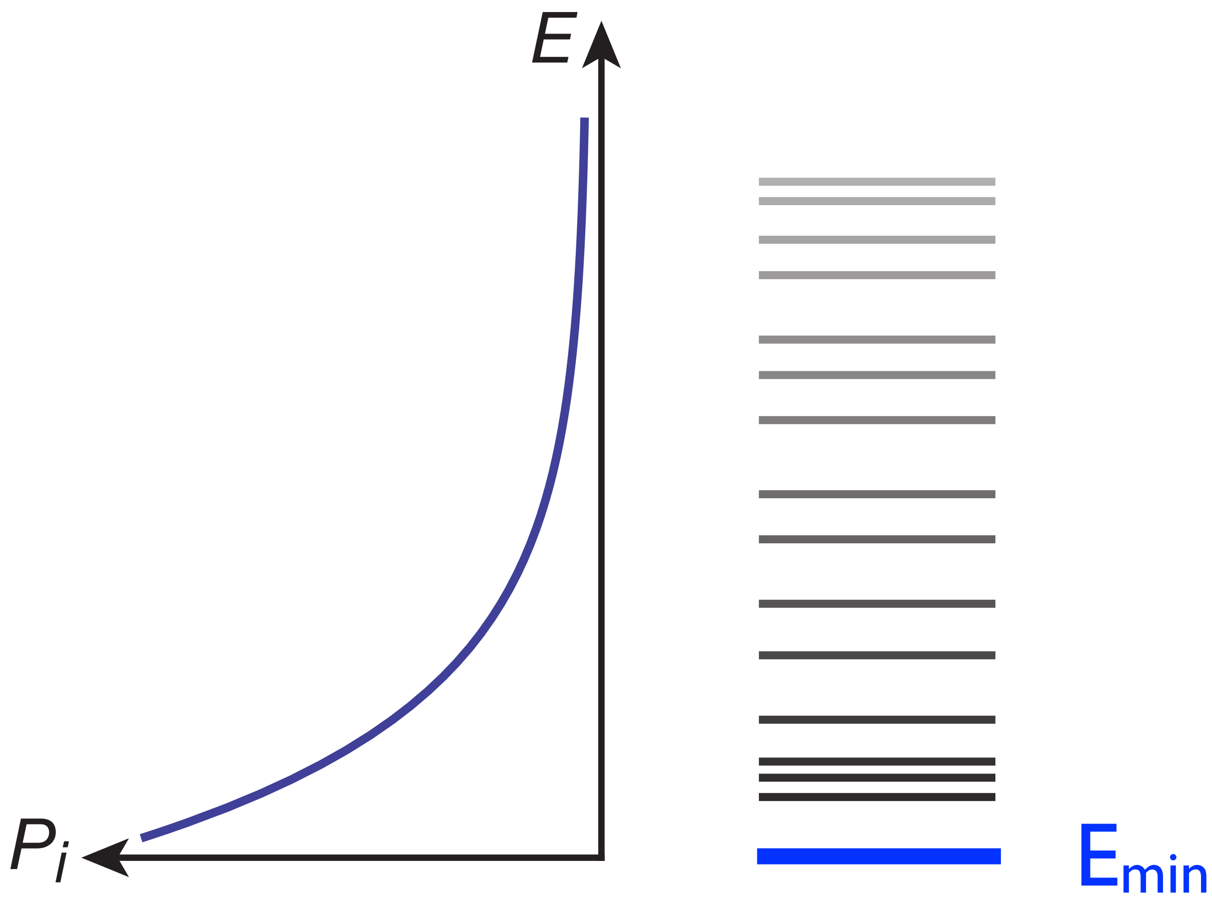
S. Braun et al. Science **339**, 52 (2013)
A. Mosk, PRL **95**, 040403 (2005) ,A. Rapp, S. Mandt & A. Rosch, PRL **105**, 220405 (2010)

Thermodynamic Definition of Temperature

Warning:
Temperature
does not measure
energy content!!!

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

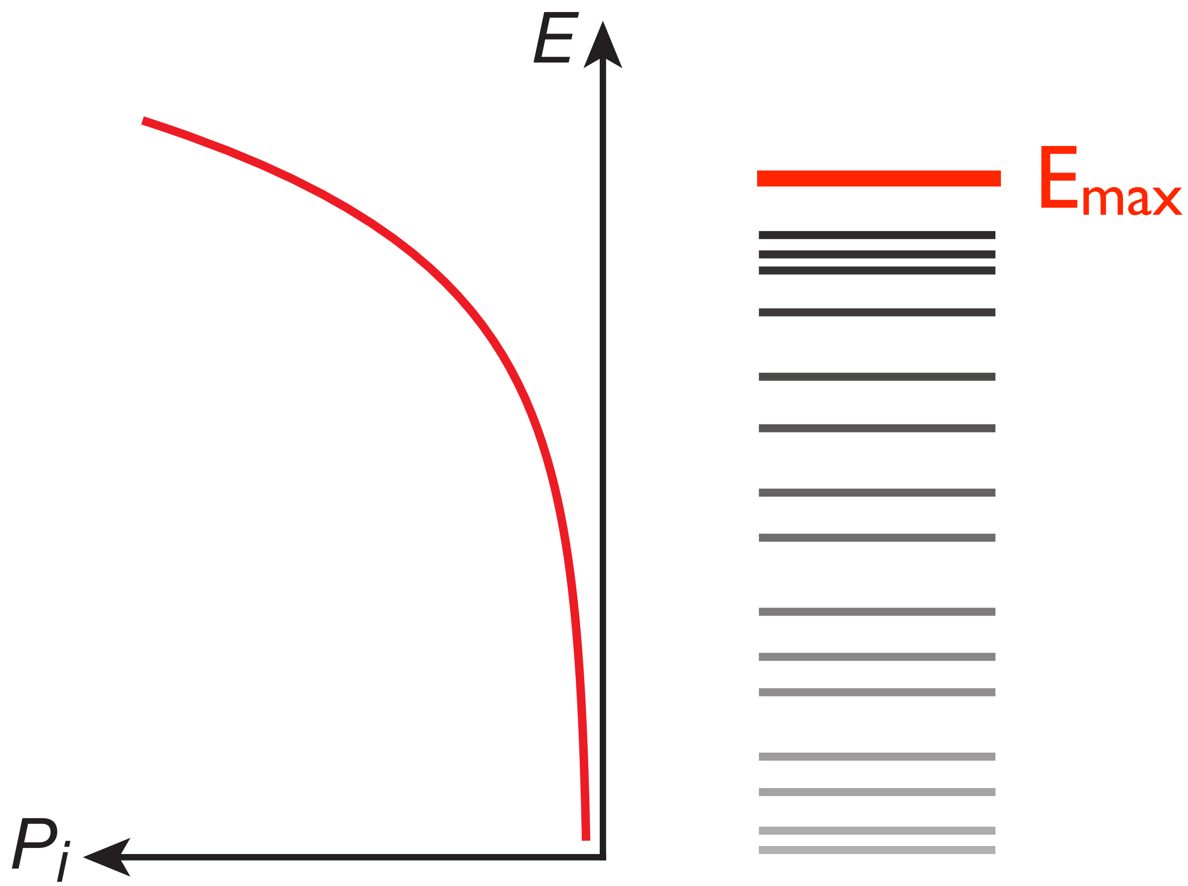
Requirements



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

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

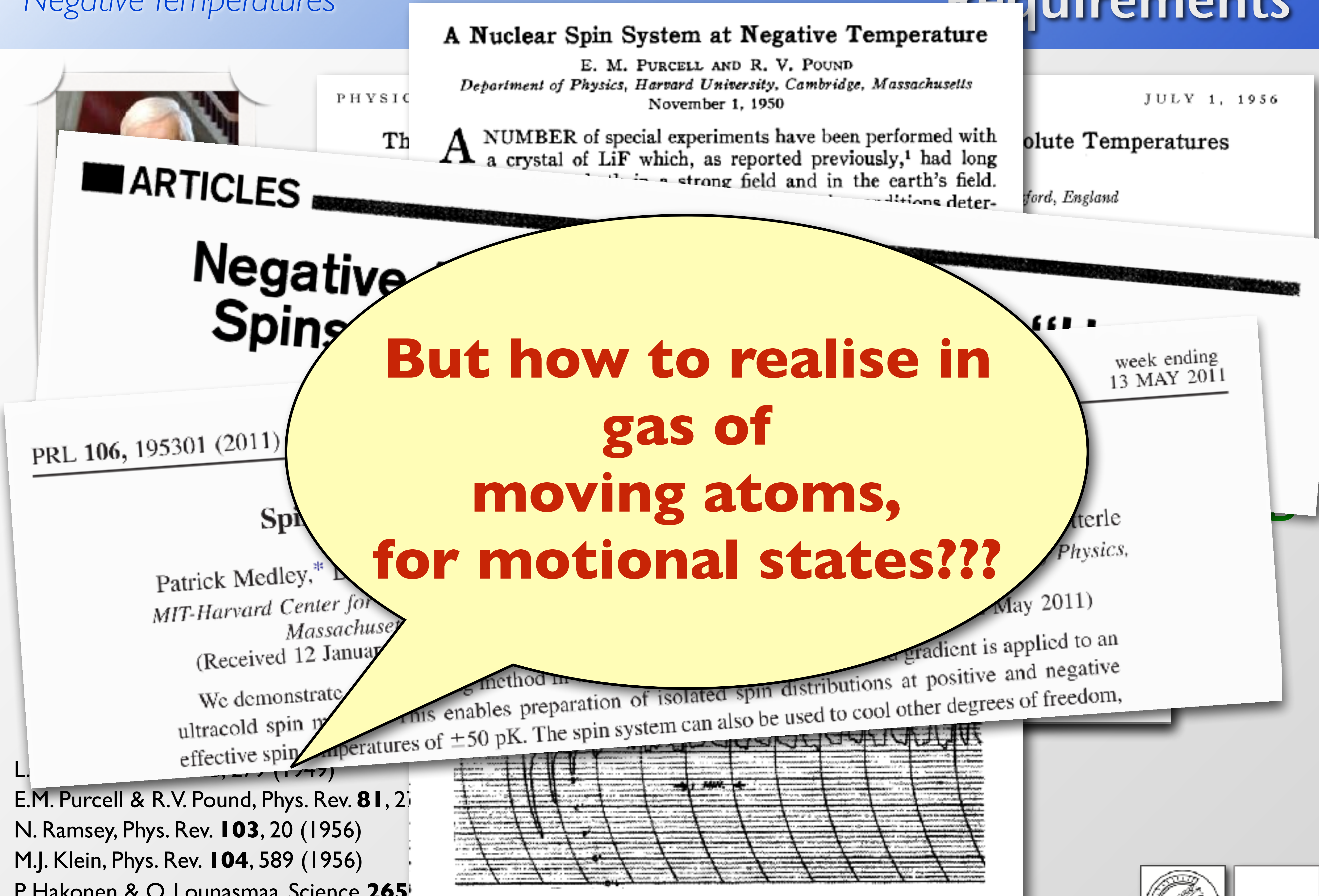
Requirements



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

For negative temperatures, we require upper energy bound E_{max}!

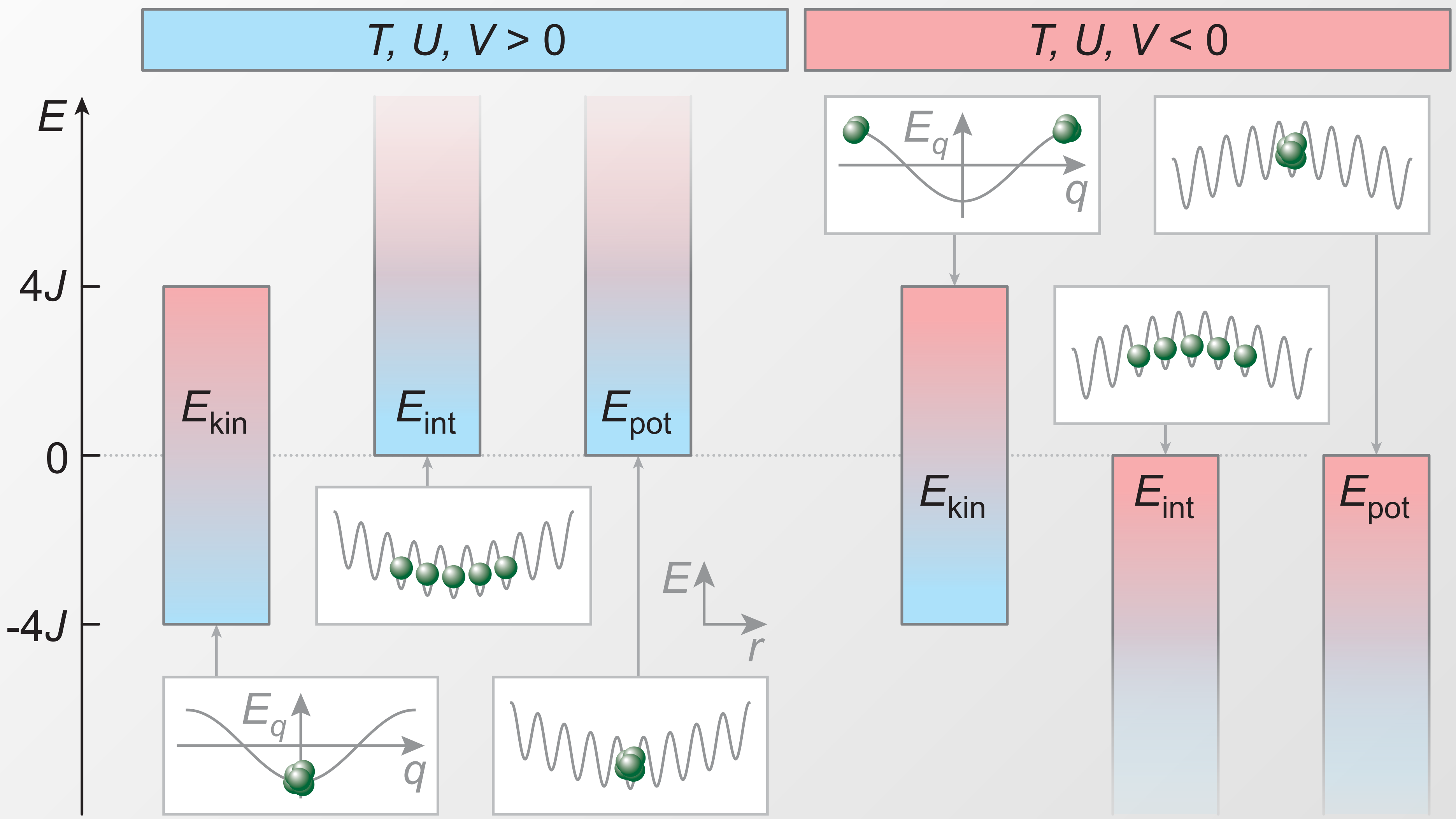
Requirements



But how to realise in gas of moving atoms, for motional states???

L. ... , 279 (1949)
E.M. Purcell & R.V. Pound, Phys. Rev. **81**, 27...
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)

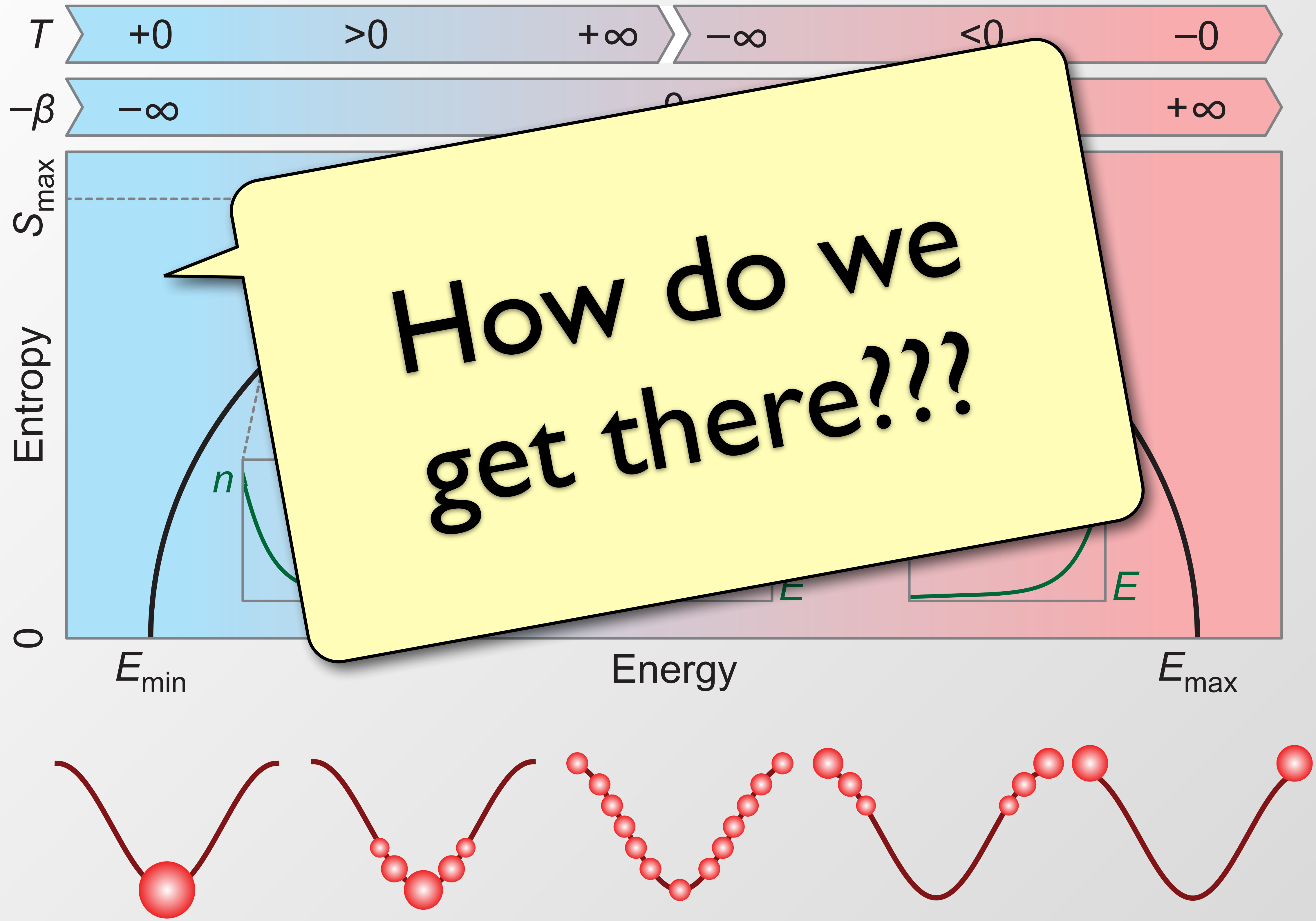
Energy Bounds of the BH Model



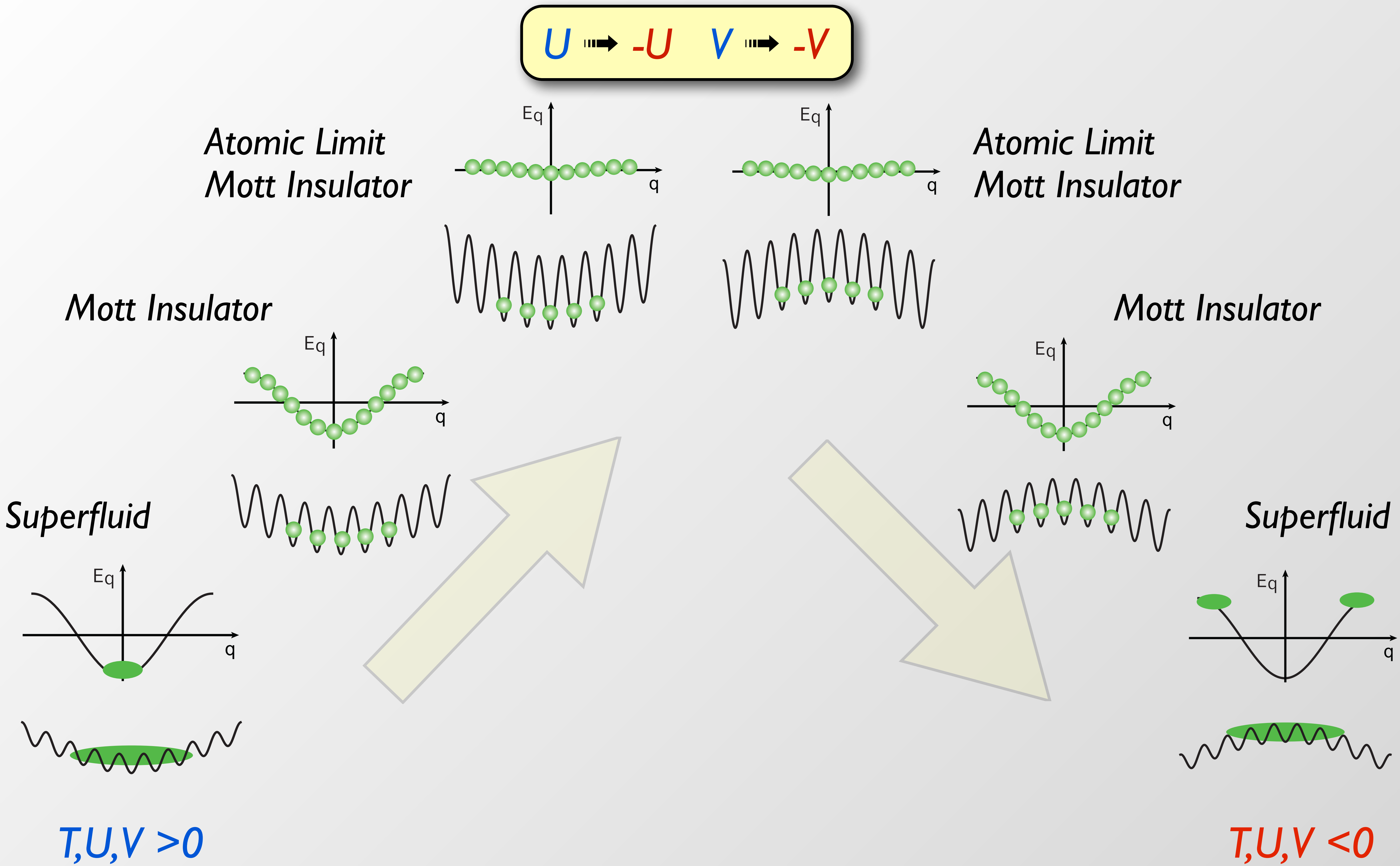
$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) + V \sum_i \mathbf{R}_i^2 \hat{n}_i$$

U,V < 0 required for upper energy bound!

Entropy vs Energy



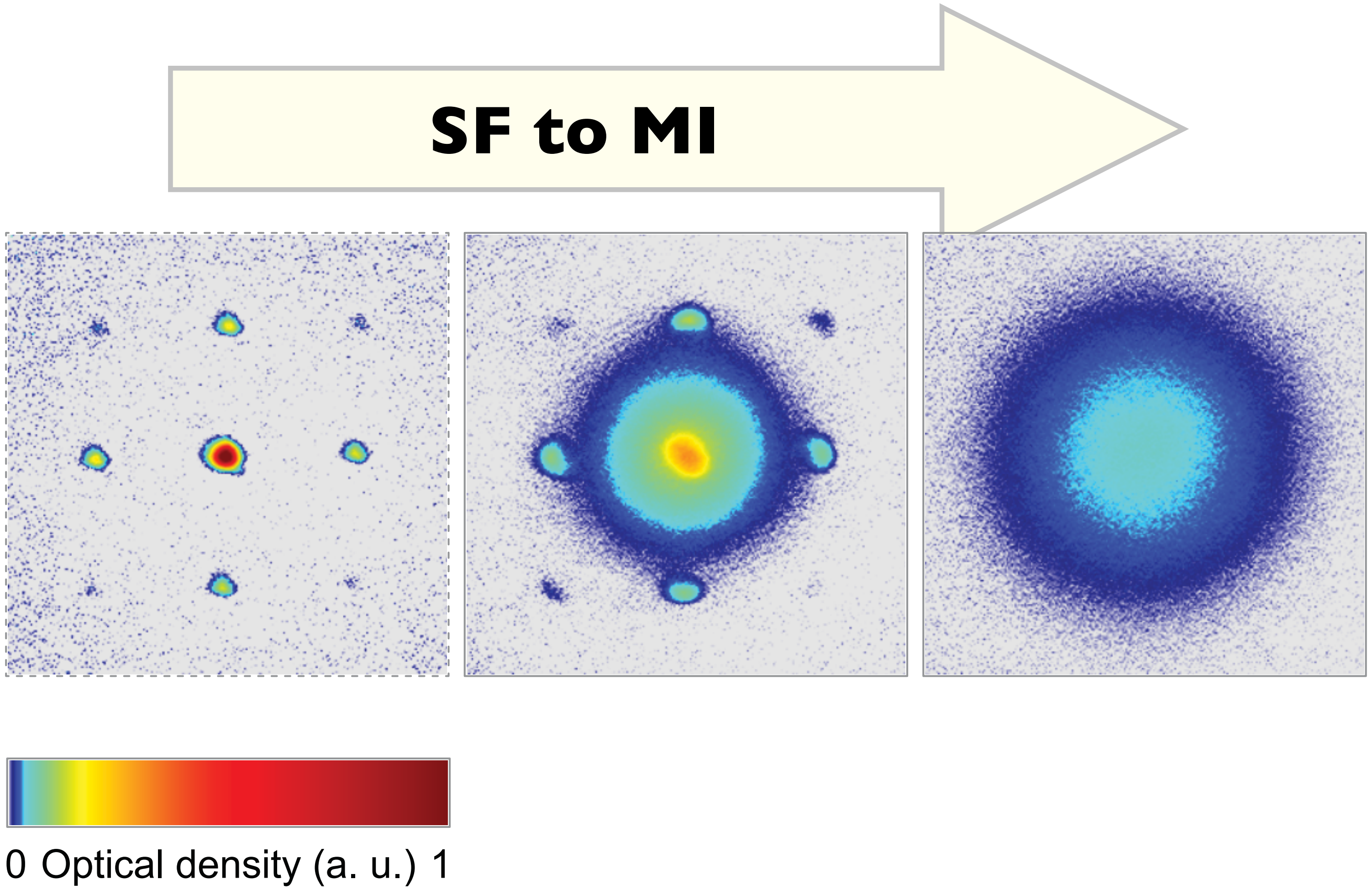
Experimental Sequence



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

Experimental Results

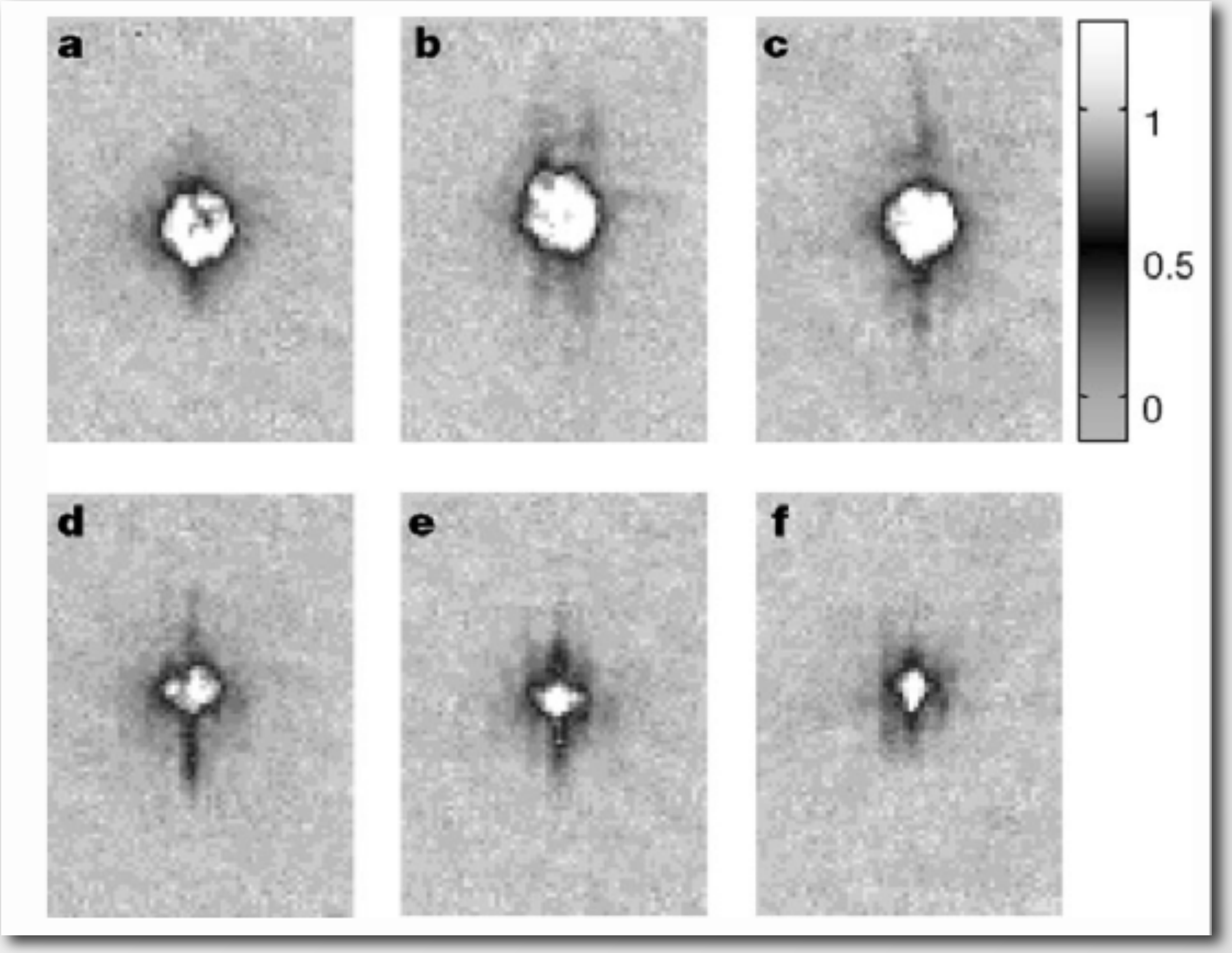
Positive Temperature w/o switching



Negative Temperature w switching

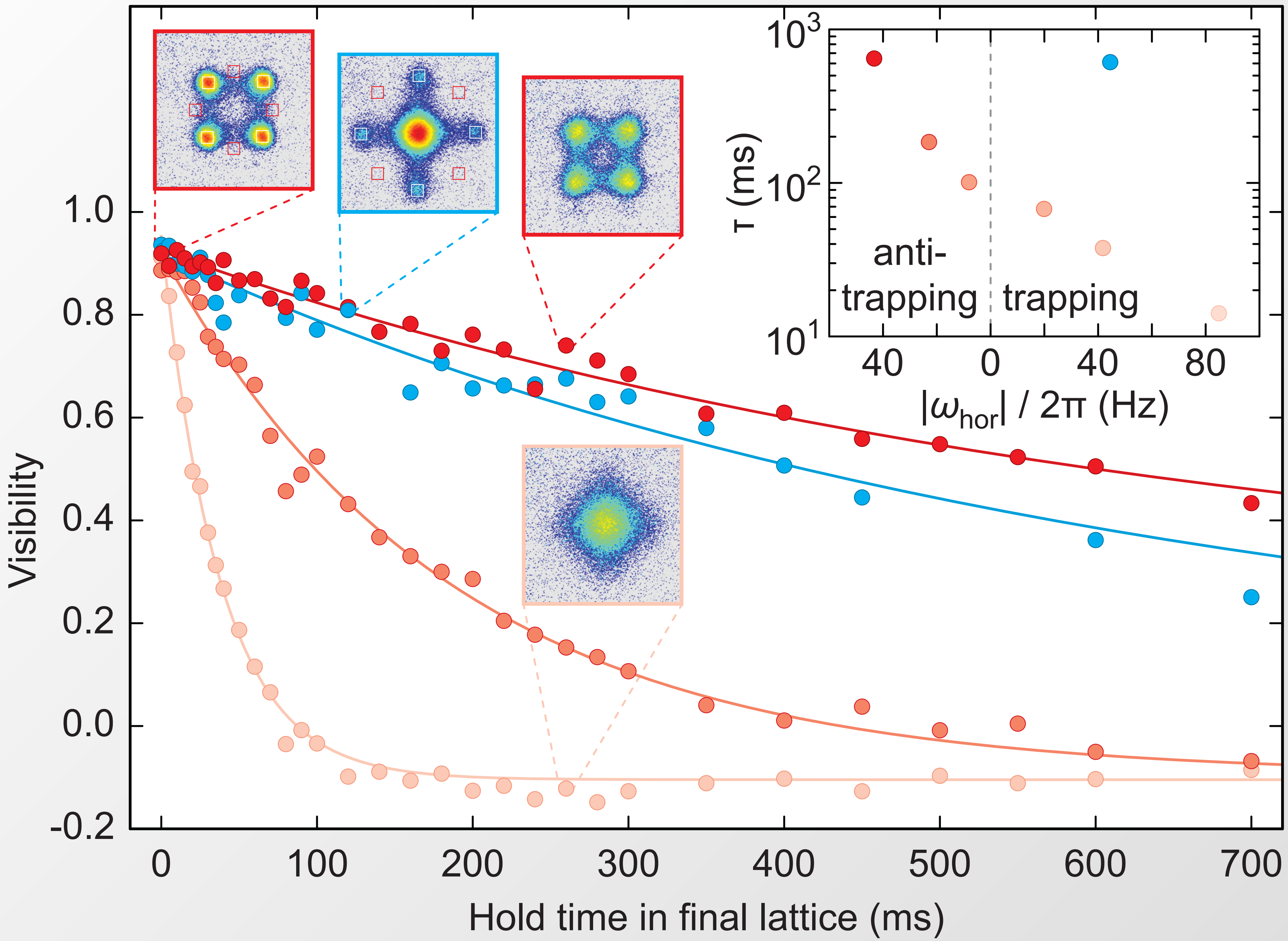
Collapse of Condensate

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)

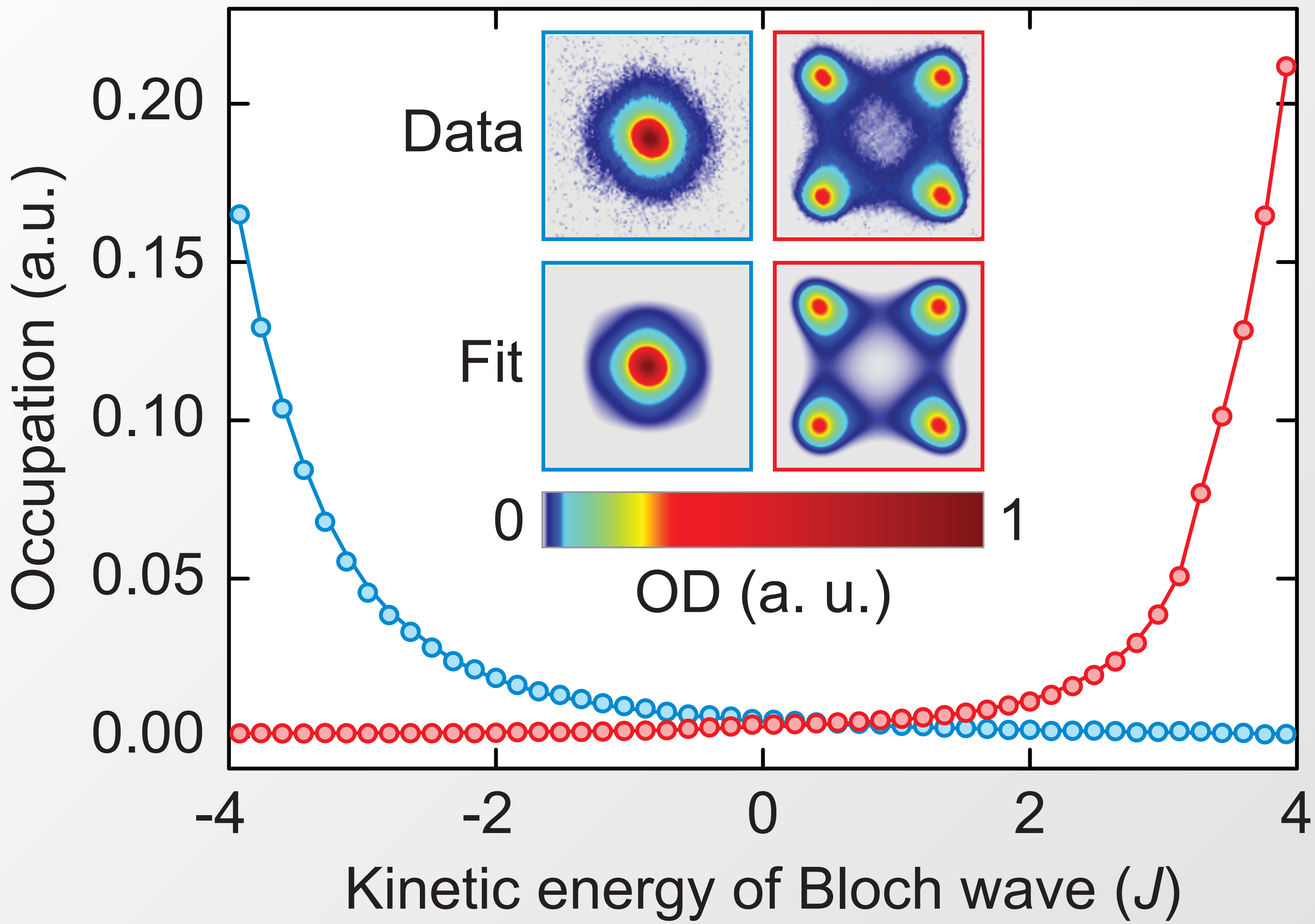
Stability



Negative Temperature State as Stable as Positive Temperature State!

LMU

Occupation of Energy States



T=-2.2J/k$_B$

Kinetic energy well fitted by Bose-Einstein distribution

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

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

Implications

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

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

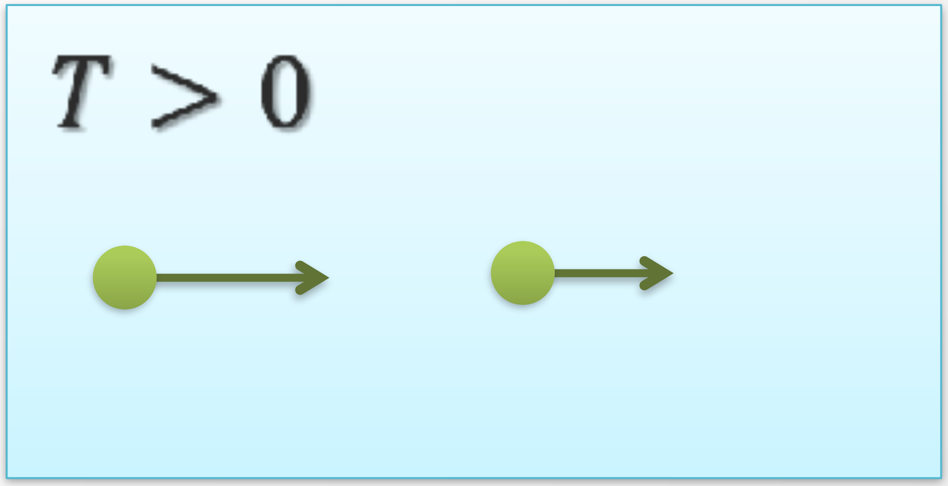
$$\Rightarrow \quad \left.\frac{\partial S}{\partial V}\right|_E = \frac{P}{T} \geq 0$$

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

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

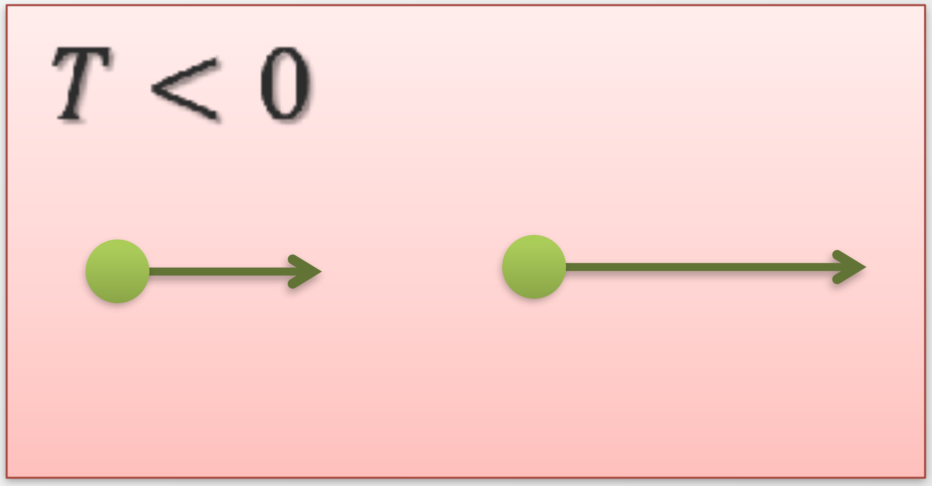
Some statements for the second law of thermodynamics become invalid!

Anti-Friction at Negative Temperature



Friction:

- entropy increases
  → Medium heats up
- Particle slows down



particle spectrum is
assumed to be unbounded

Anti-Friction:

- entropy increases
  → Medium cools down
- Particle accelerates

(but direction is randomized
in long-term limit)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What is the correct form of the entropy?

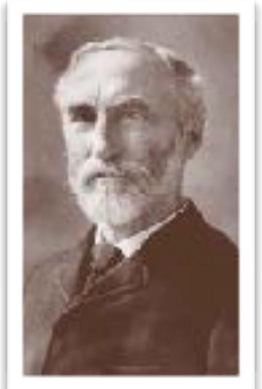
- Observation: Cold atoms are thermally isolated
  → *microcanonical ensemble?*

- Equivalence of ensembles not a priori clear for bounded systems.

- Two possible entropy definitions:

Boltzmann / Surface entropy:

$$S_B = k_B \log(\rho(E) dE)$$



Gibbs / Hertz / Volume entropy:

$$S_G = k_B \log(\int_0^E \rho(E')\ dE')$$

- Typically in unbounded systems:

$$\rho(E) \propto \exp(E) \rightarrow \int \rho(E)\, dE \propto \exp(E)$$

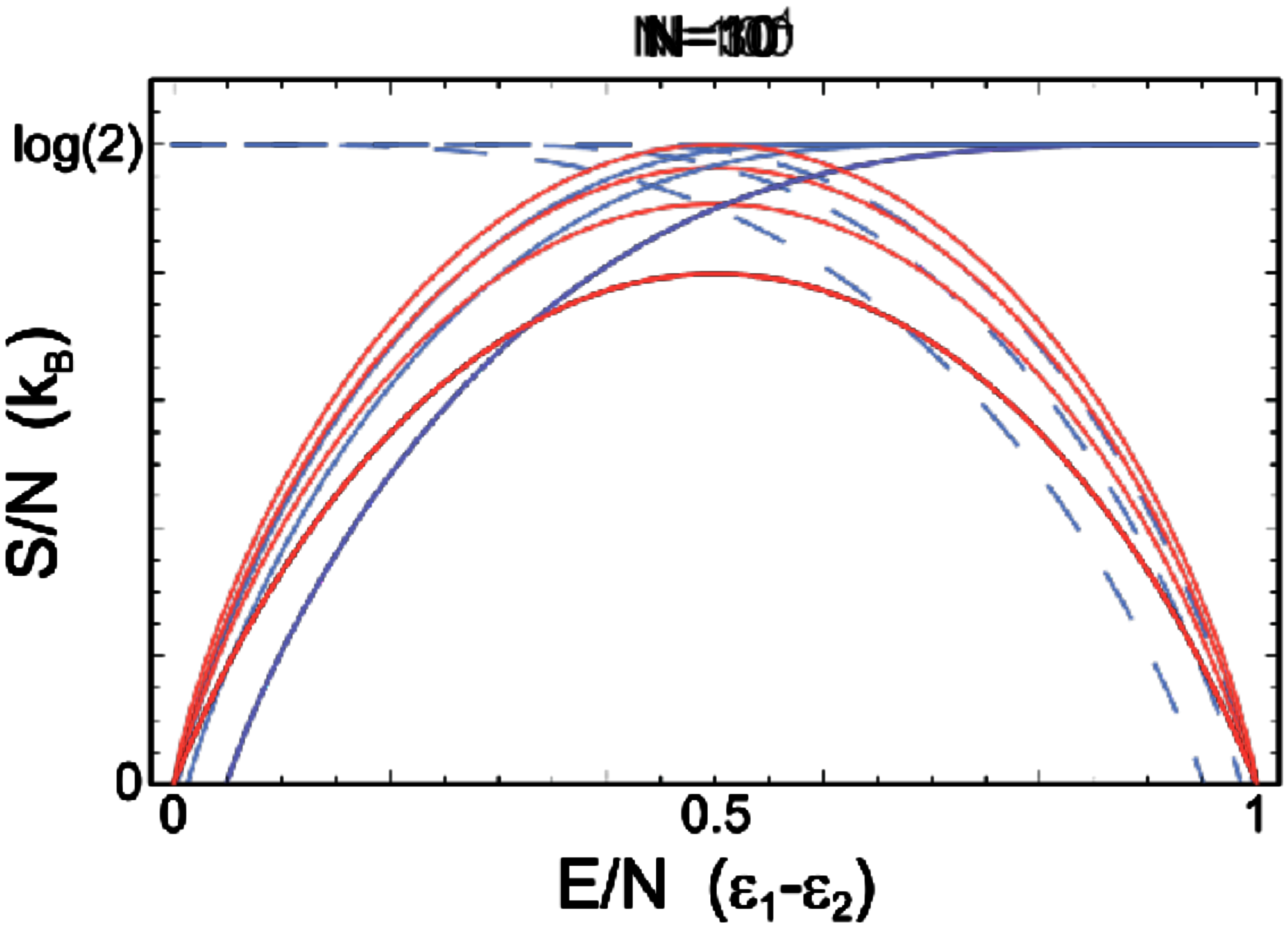
  → *no real difference*

What is the correct form of the entropy?

- Neccesary condition for consistent thermodynamics:
  dS=... must be a total differential (needed for e.g. Maxwell relations)
- Boltzmann entropy: $S_B = k_B \log(\rho(E)dE)$ does *not* fulfill above requirement for the *microcanonical ensemble*
- Need to use Gibbs / Hertz entropy: $S_G = k_B \log(\int_0^E \rho(E')\ dE')$
- $\rho(E) \geq 0 \ \rightarrow S_G$ monotonously increasing ➔ $T \geq 0$ ☹ ??

Dunkel, Hilbert Nat. Phys. **10**, 67 (2014)

Example: N two-level atoms



- Boltzmann entropy:

$$S_B = k_B \log(\rho(E)\, dE)$$

- Gibbs / Hertz entropy:

$$S_G = k_B \log\left(\int_0^E \rho(E')\; dE'\right)$$

- New: Inverted Gibbs:

$$\overline{S_G} = k_B \log\left(\int_E^{E_{max}} \rho(E')\; dE'\right)$$

→ $d\overline{S_G}$ is also total differential!

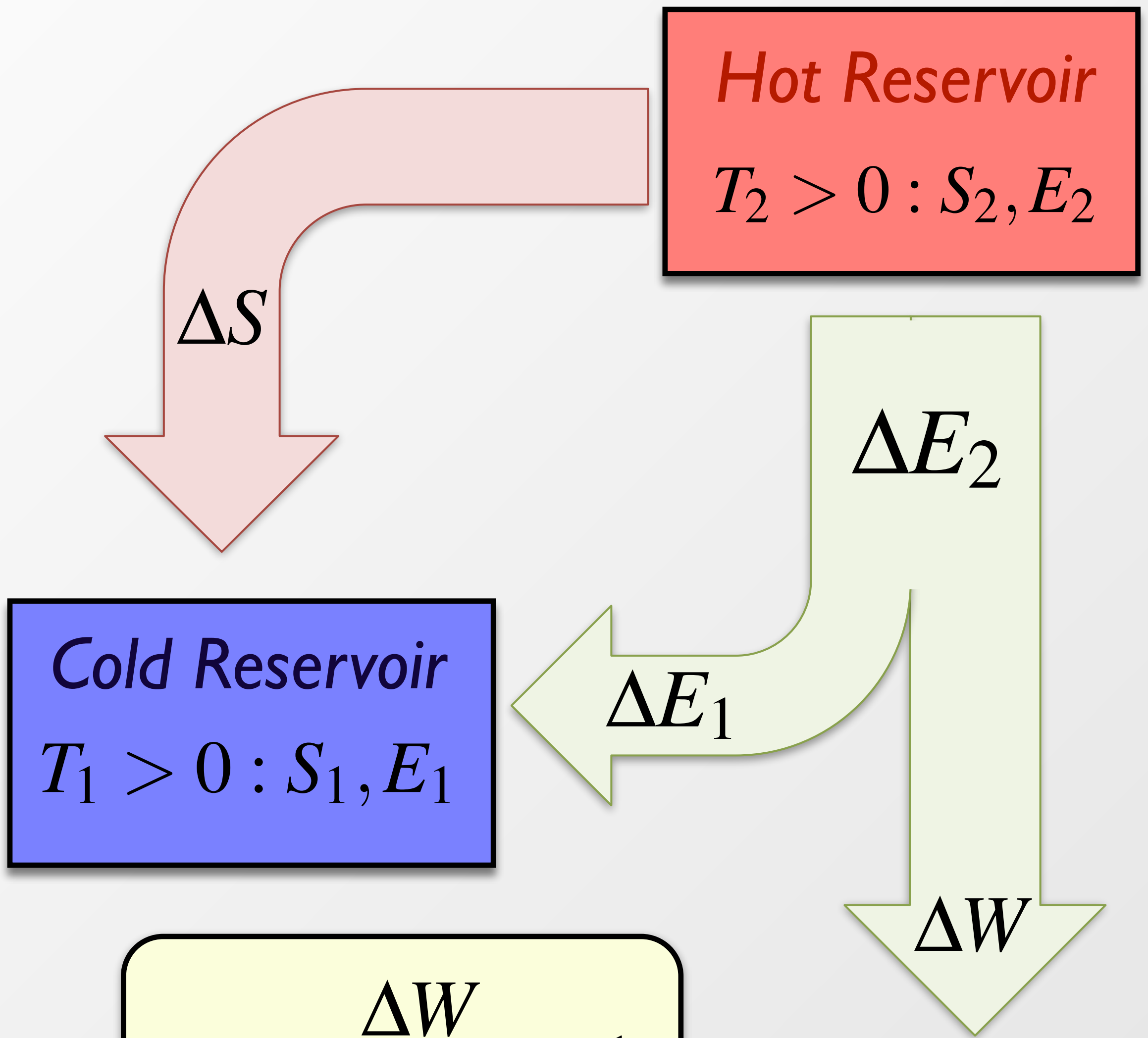
Proposal: $\boldsymbol{S_m = \min\{S_G, \overline{S_G}\}}$

- dS_m is also total differential (except at $E = \frac{E_{max}}{2}$)
- thermodynamic limit: $\lim_{N\to\infty} S_m = \lim_{N\to\infty} S_B$

➔ Equivalence of Ensembles

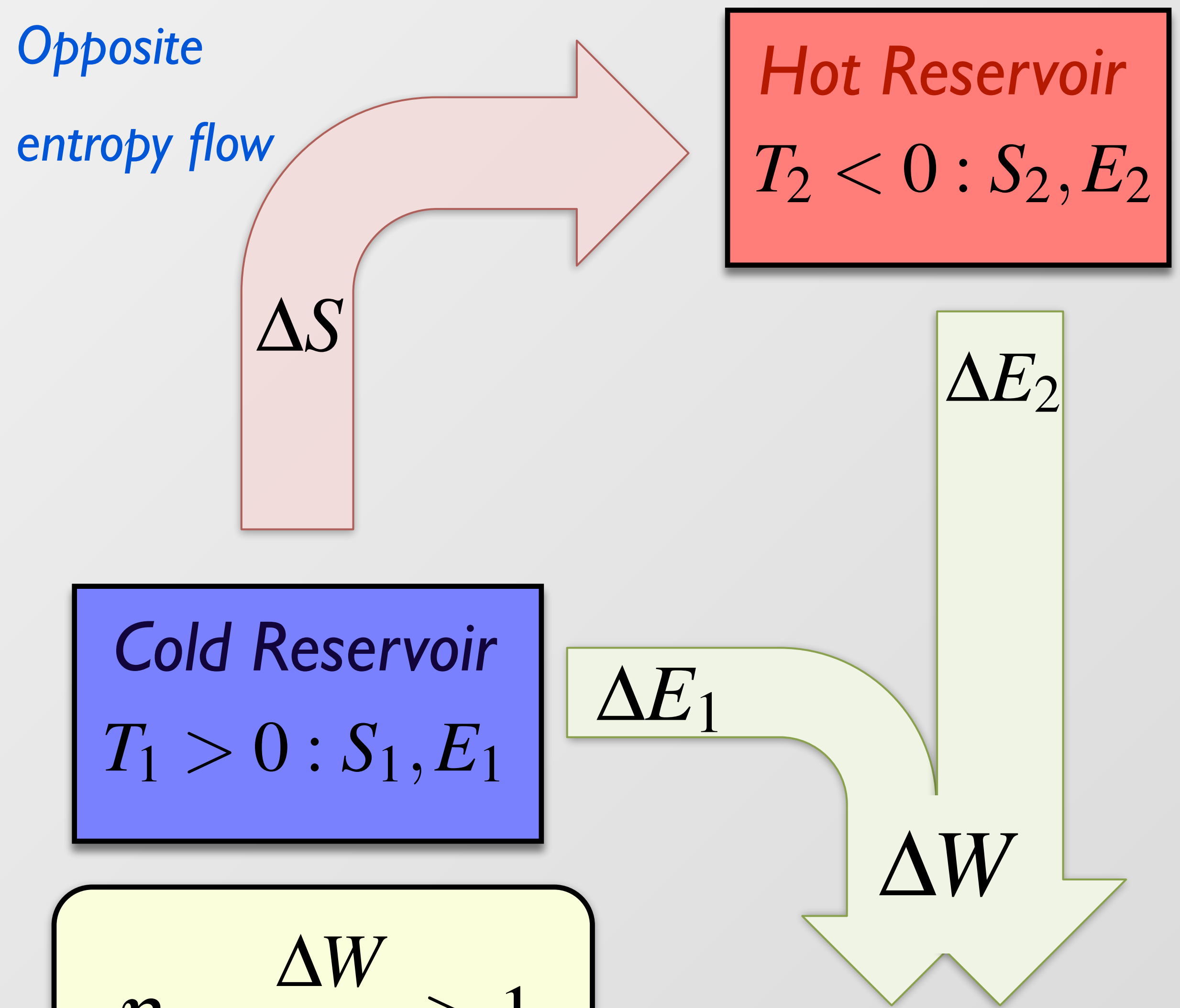
Carnot limits

$T_1 > 0, T_2 > 0$



$$\eta = \frac{\Delta W}{\Delta E_2} < 1$$

$T_1 > 0, T_2 < 0$



$$\eta = \frac{\Delta W}{\Delta E_2} > 1$$

- *Energy and Entropy are globally conserved!*
- *No violation of thermodynamic laws* → *No solution to energy problem!*

Atoms in Periodic Potentials

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)

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

q = Crystal Momentum or Quasi-Momentum

n = Band index

Plugging this into Schrödinger Equation, gives:

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

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

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

In the experiment standing wave interference pattern gives

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

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

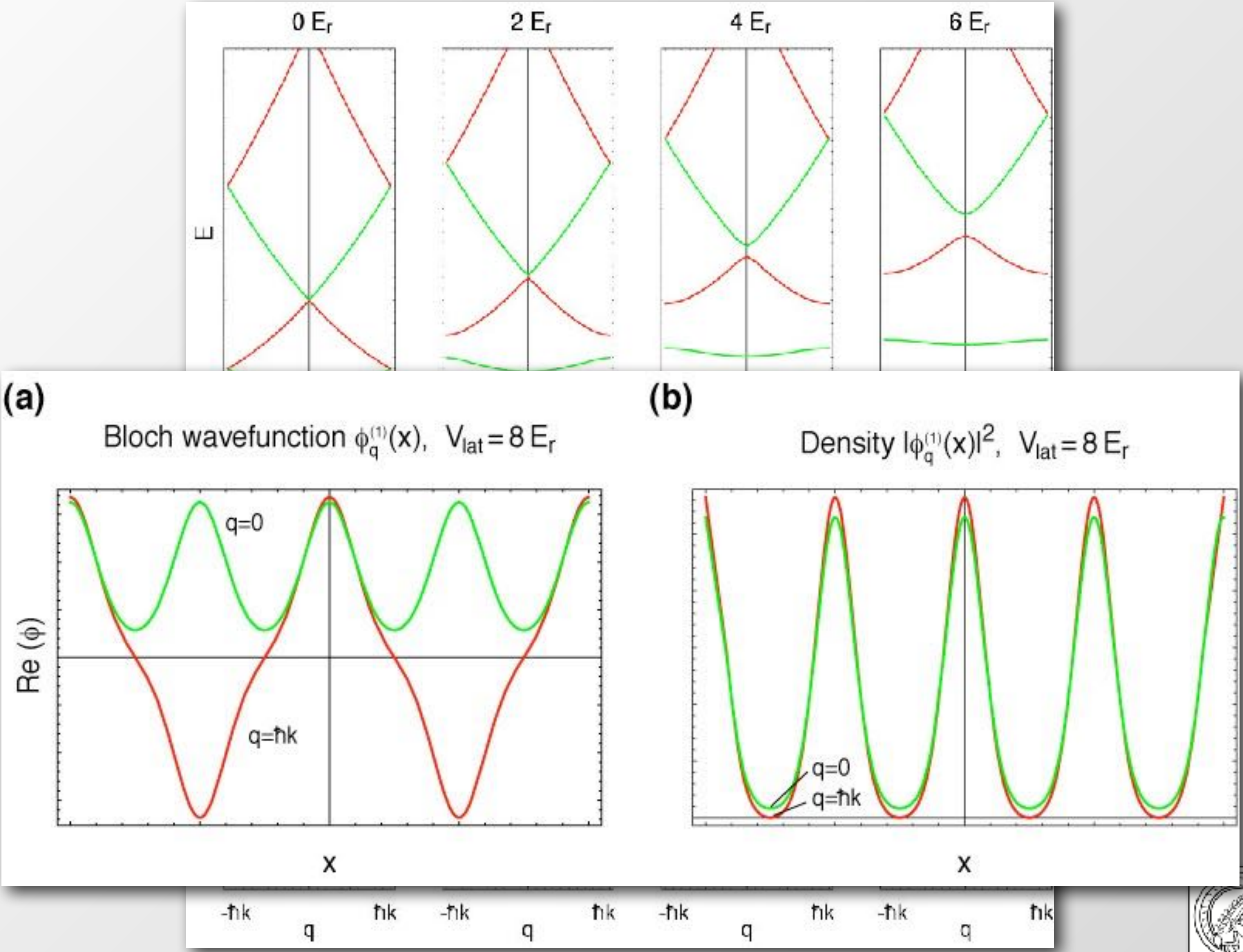
Use Fourier expansion

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

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

Diagonalization gives us Eigenvalues and Eigenvectors!

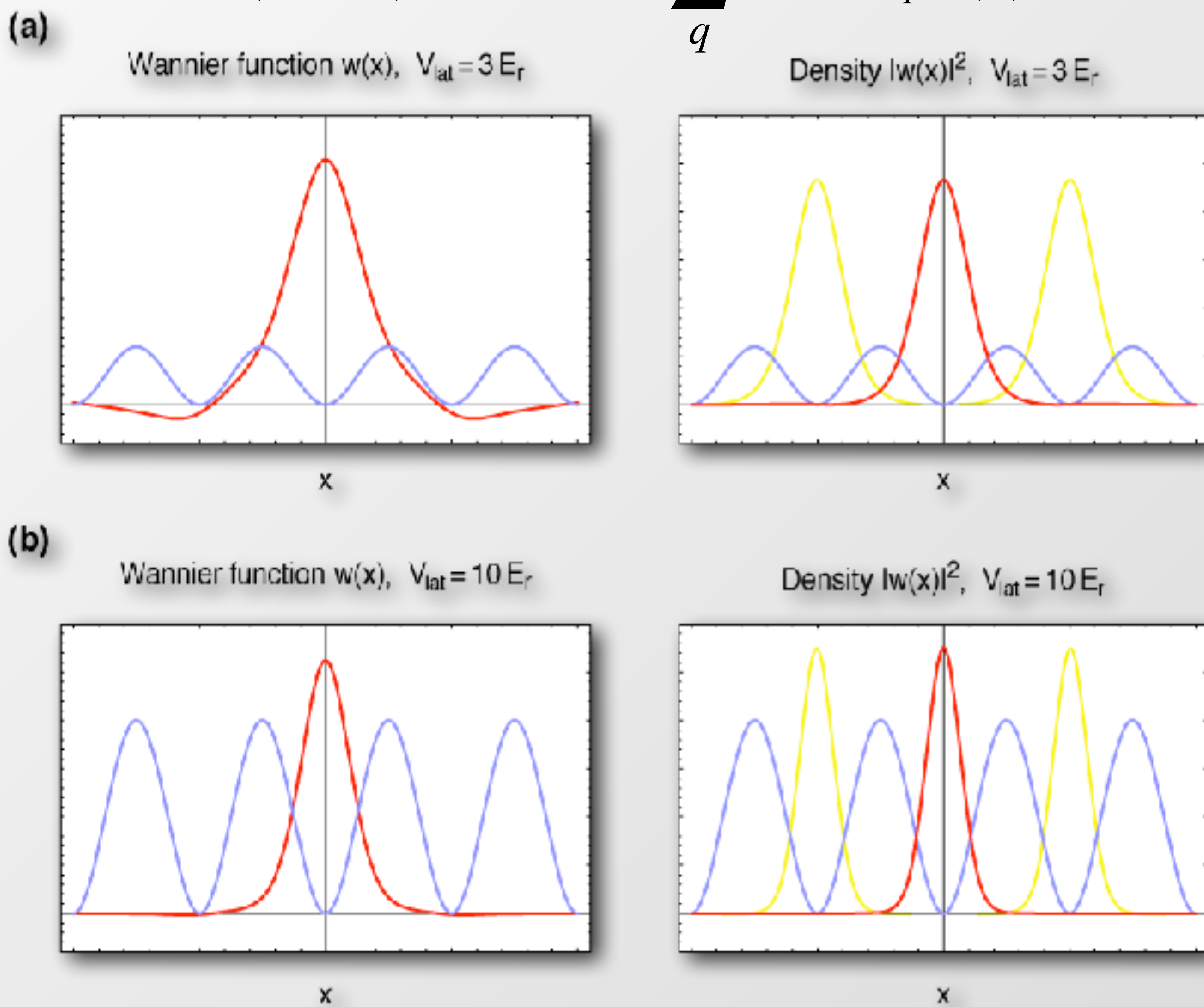
Bandstructure - Blochwaves



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

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