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Swiss Federal Institute of Technology Zurich

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Department of Physics
Institute for Theoretical Physics

Superfluidity near the Mott transition of cold bosonic atoms: validating a quantum simulator

Matthias Troyer

Collaborators

FNSNF
Swiss National Science Foundation

OLE
Optical Lattice Emulator

DARPA

- Simulations of bosons
  - Lode Pollet (Harvard)
  - Boris Svistunov (UMass)
  - Nikolay Prokof'ev (UMass)
  - Ping Nang (Tama) Ma (ETH)

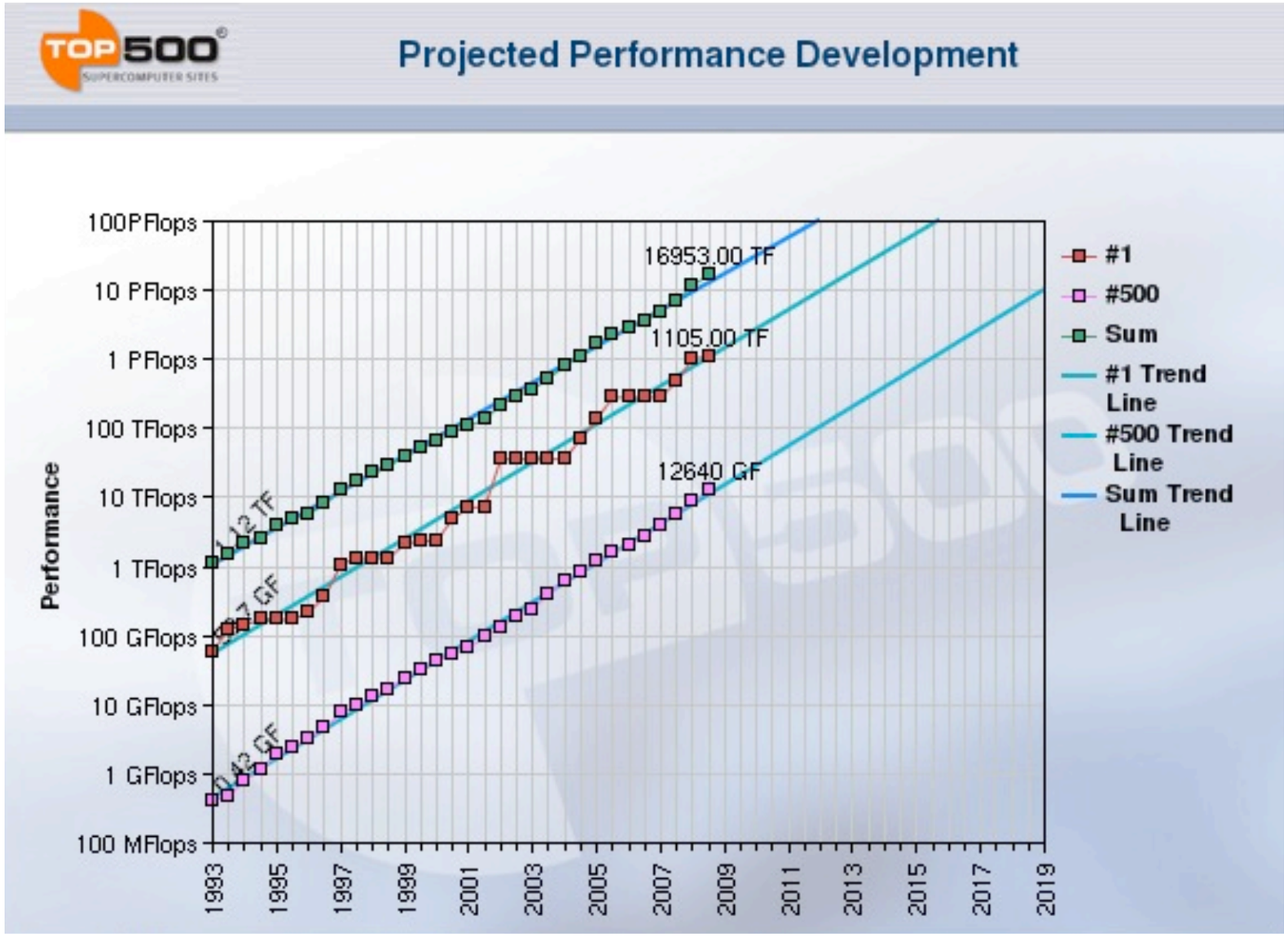
- Simulations of fermions
  - Vito Scarola (Virginia Tech)
  - Lode Pollet (Harvard)
  - E. Kozik (ETH)
  - E. Burovski (Paris)
  - Antoine Georges (Paris)
  - Corinna Kollath (Paris)
  - Lorenzo De Leo (Paris)

- Experiments on bosons
  - Stefan Trotzky (Munich)
  - Immanuel Bloch (Munich)
  - Ute Schnorrberger (Munich)
  - Fabrice Gerbier (Paris)

- Experiments on fermions
  - Robert Jördens (ETH)
  - Leticia Tarruell (ETH)
  - Tilman Esslinger (ETH)
  - Henning Moritz (ETH)
  - Niels Strohmaier (ETH)

Supercomputing: petaflop and beyond

- Supercomputing technology has broken through the petaflop-barrier and Moore's law continues to hold

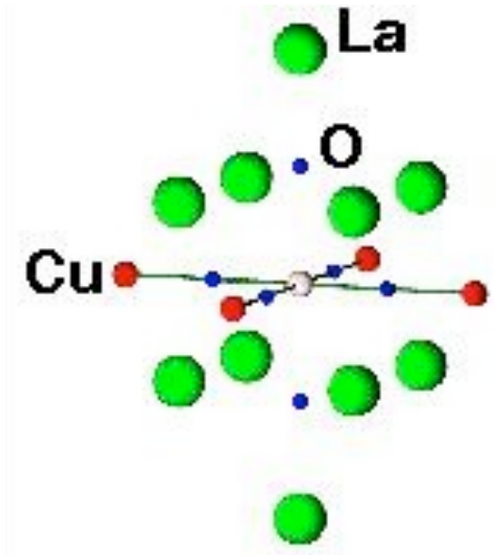


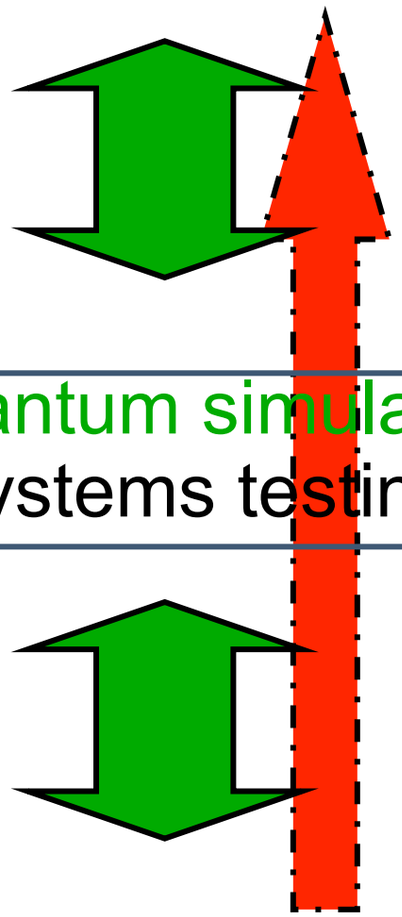
Numerical simulations

- “You let the computer solve the problem for you”
- It’s not that easy:
  - Exponentially diverging number of states ✔
    - 1 site: q states
    - *N* sites: q^N states
  - Critical slowing down of the dynamics at phase transitions ✔
  - negative sign problem for fermions (NP-hard) ?

Quantum simulators

Strongly correlated materials:
strong correlation effects in many-electron systems





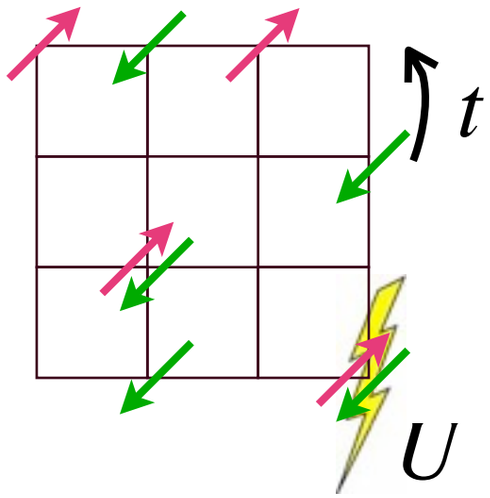
no exact solutions

approximations,

impurities,

...

Quantum simulators:
Controlled, “simple” systems testing models and verifying



Condensed matter models:
Simple models which capture the relevant mechanism

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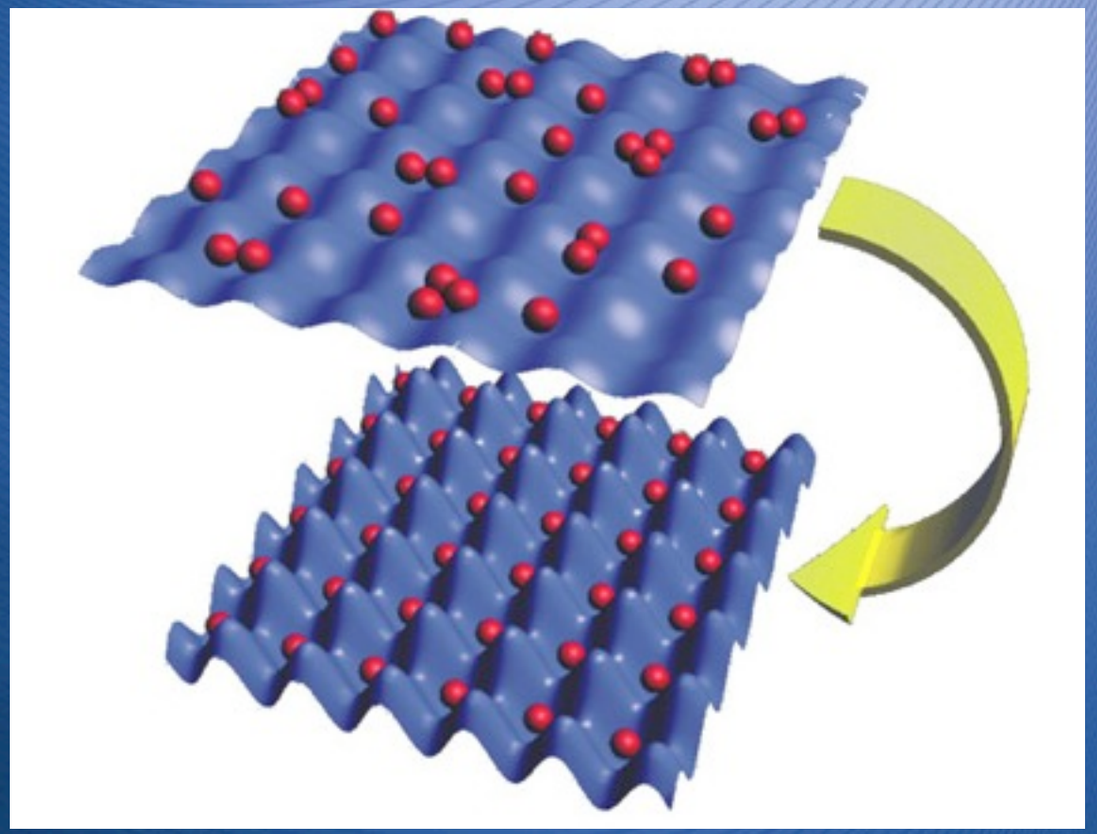
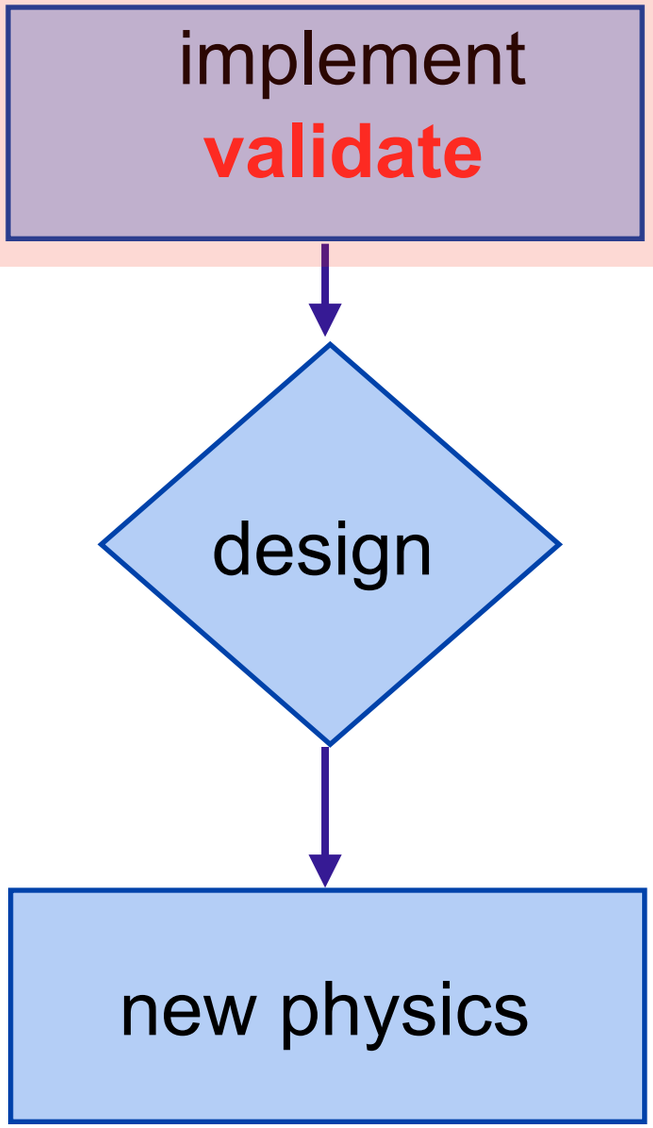
Validating a quantum simulator: does it really work?



DARPA Optical Lattice Emulator program

- Goal : build an optical lattice emulator to solve the prototypical models of condensed matter physics



1. Validate / calibrate against known models (bosons)

2. Design a model with unknown physics (fermions)

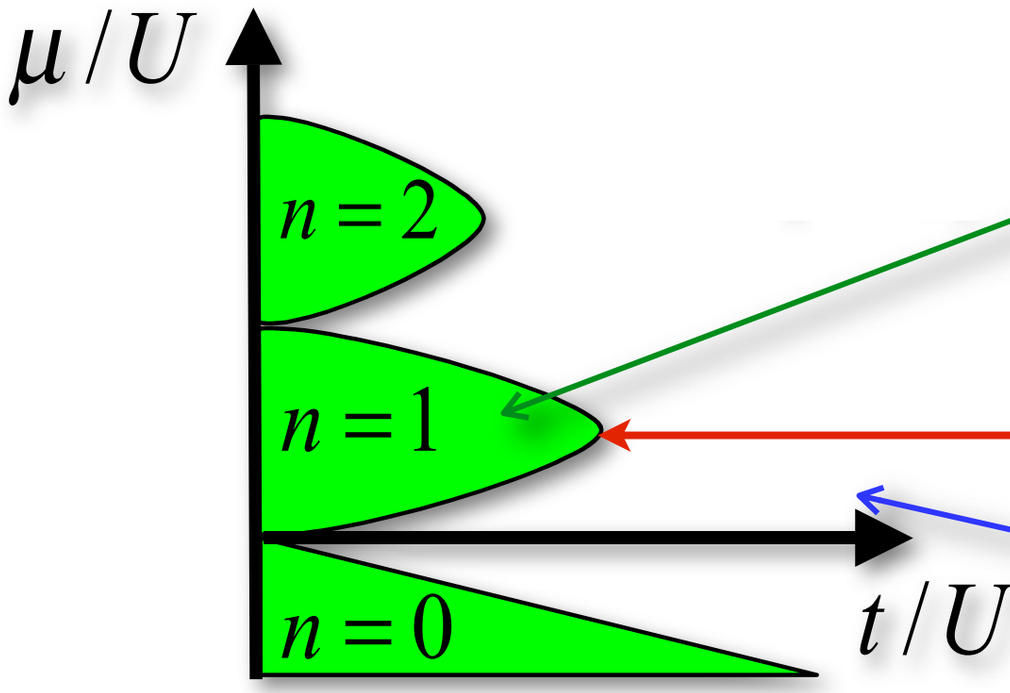
3. Learn new physics assuming all parameters of the device are still under control

Bose-Hubbard model

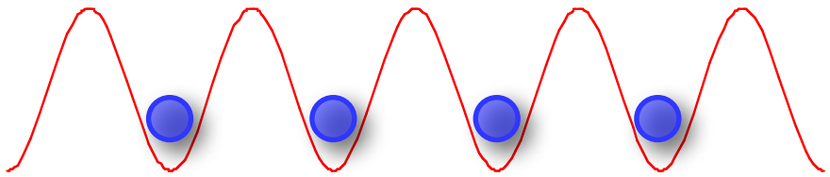
Fisher *et al*, PRB 1989

- Use bosonic atoms for validation

$$H = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + U \sum_i n_i (n_i - 1)/2 - \mu \sum_i n_i$$

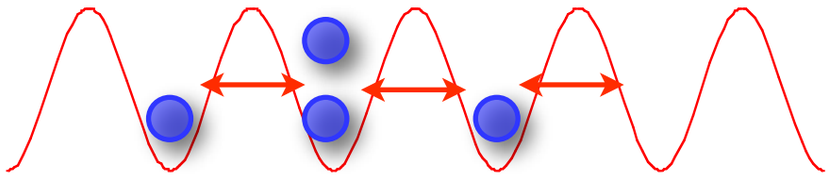


Large *U*: incompressible Mott-insulator at Integer filling

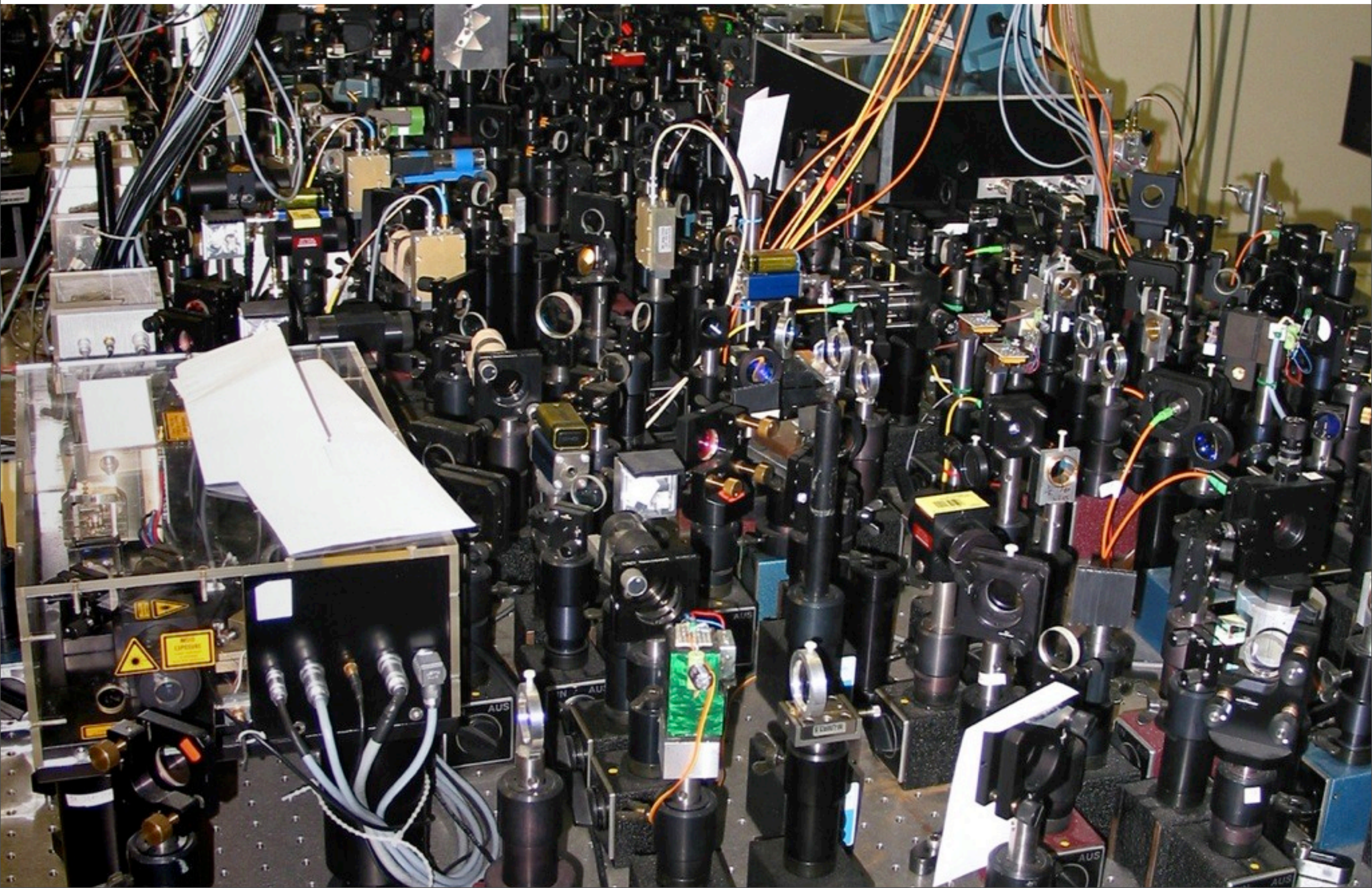


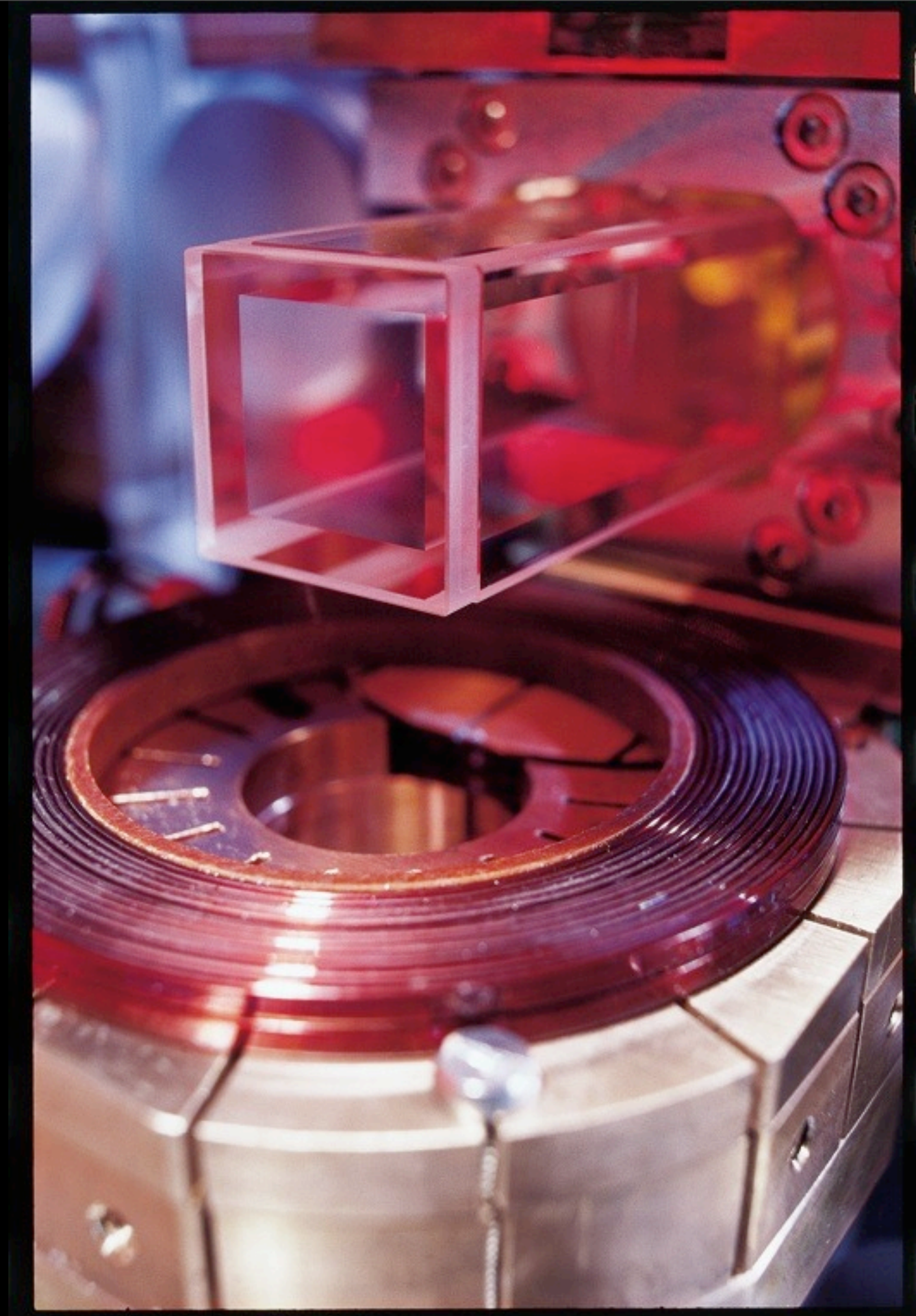
Quantum phase transition varying U/t

Large *t*: superfluid BEC



A lot of optics and electronics !



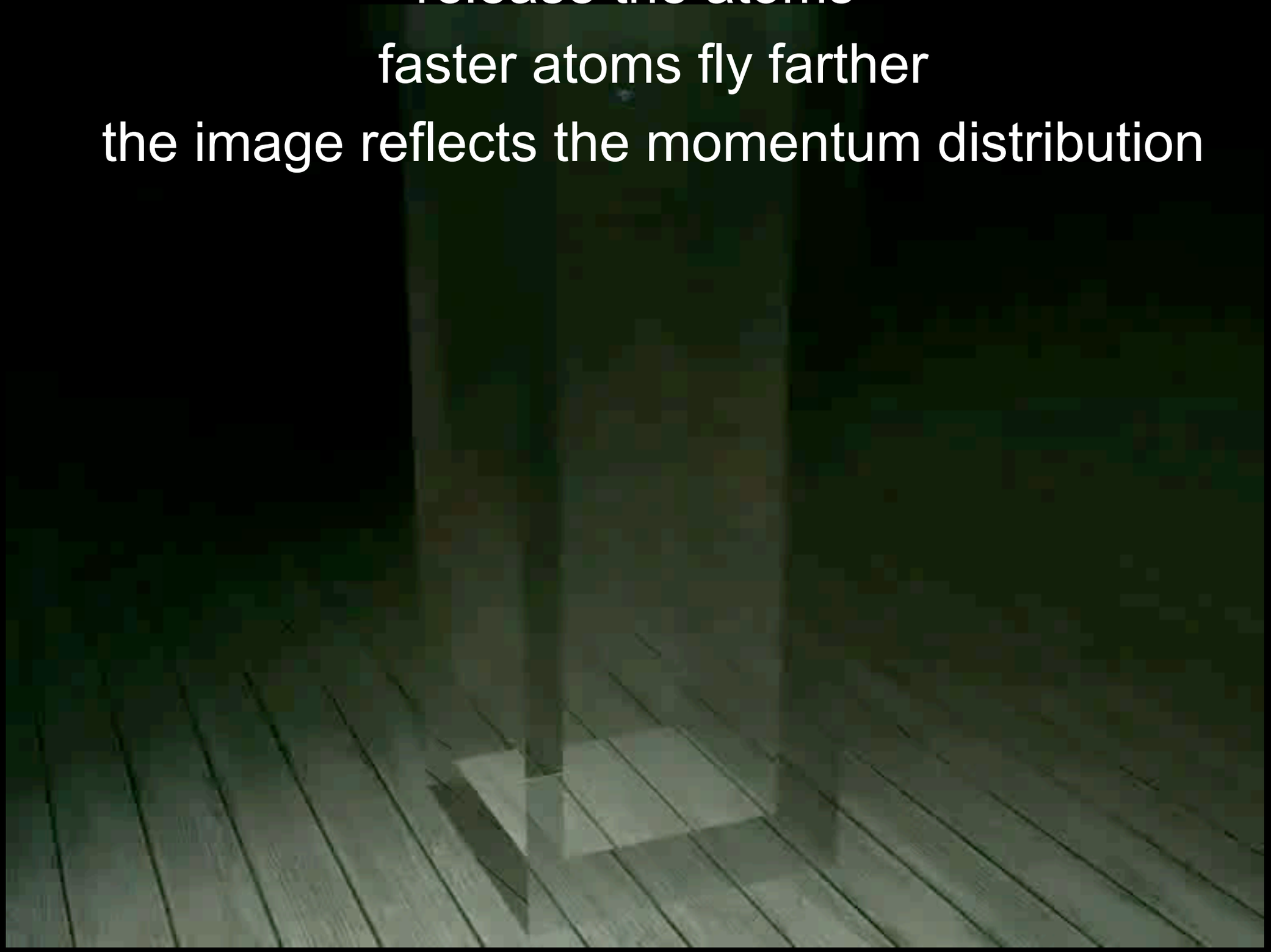


How do we detect these quantum gases ?

release the atoms

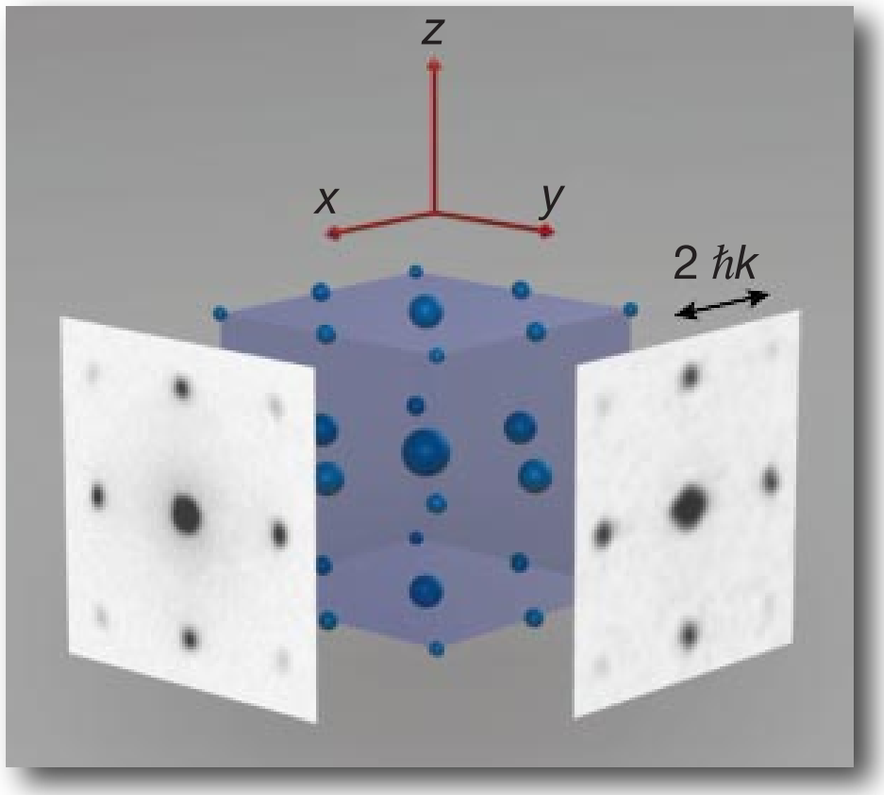
faster atoms fly farther

the image reflects the momentum distribution

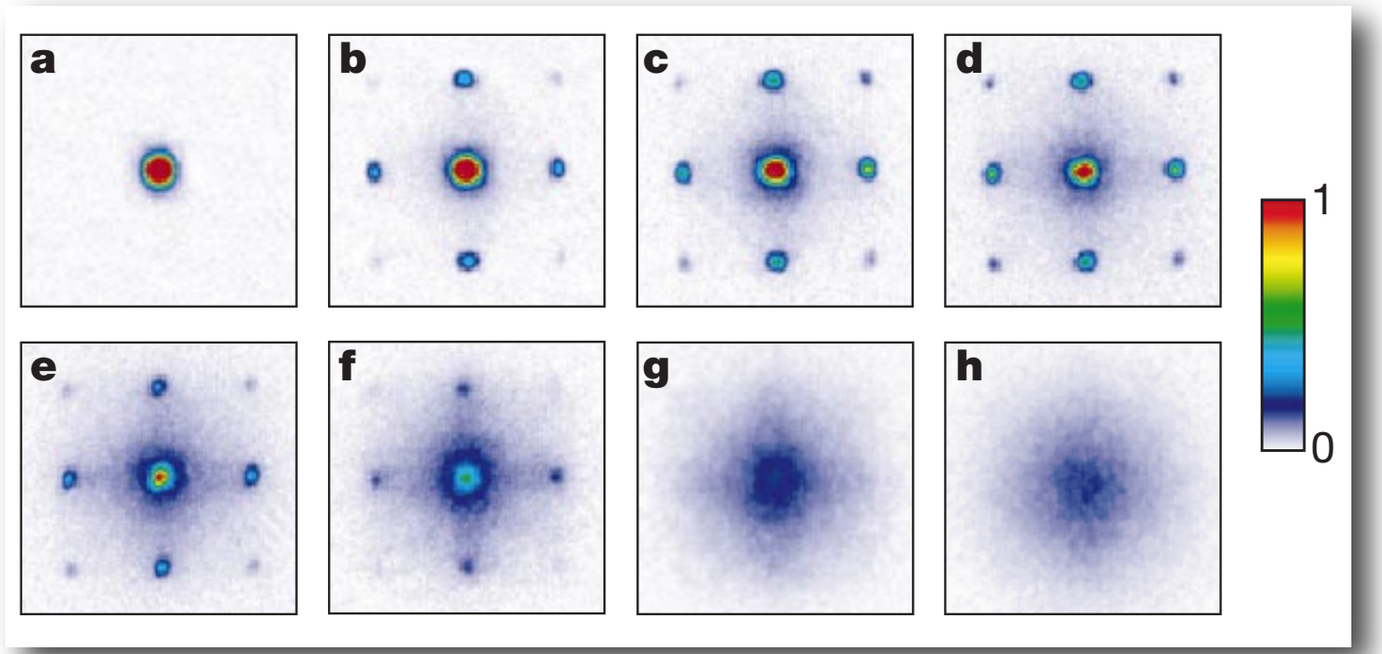


The first optical lattice experiments

- Quantum phase transition as lattice depth is increased
  - Greiner et al, Nature (2002)
  - measuring the momentum distribution function in time-of-flight images



small U/t: condensate

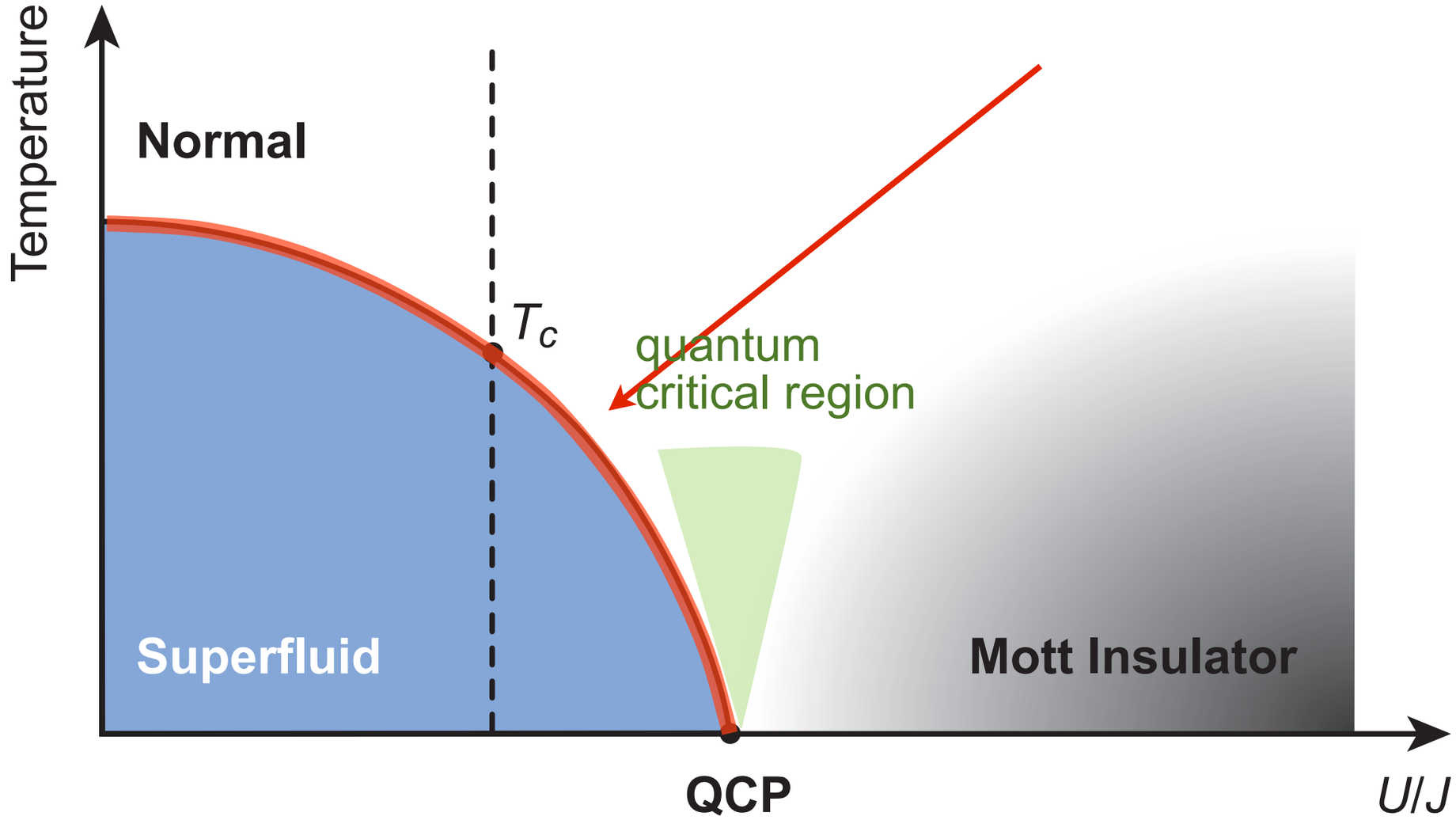


large U/t: Mott insulator

Can this be made more quantitative?

Quantitative validation: the phase diagram

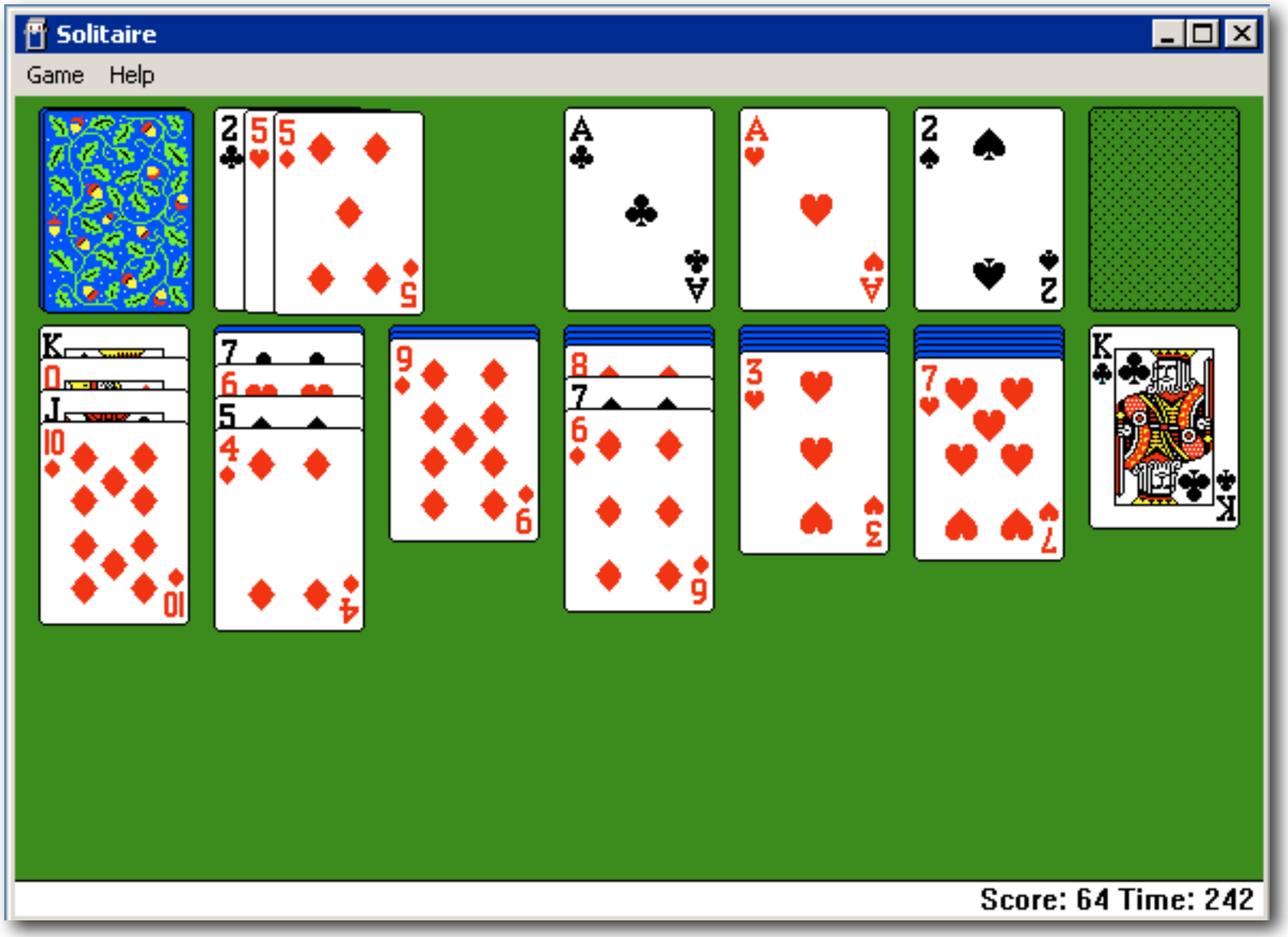
- Bosons in a 3D optical lattice at filling $n = 1$
- Measure suppression of T_c close to the Mott insulator



Quantum Monte Carlo simulations

Ulam: the Monte Carlo Method

- What is the probability to win in Solitaire?
  - Ulam's answer: play it 100 times, count the number of wins and you have a pretty good estimate



The Monte Carlo Method

observable

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{N} A_i p_i$$

statistical weight

replace the sum by the mean of a small random sample

$$\langle A \rangle \approx \overline{A} = \frac{1}{M} \sum_{i=1}^{M} A_{c_i}$$

- Need a representative sample with the correct distribution

$$P[c_i] = \frac{p_{c_i}}{Z}$$

  - fundamental problem of statistical mechanics

Monte Carlo simulations: the Metropolis algorithm

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

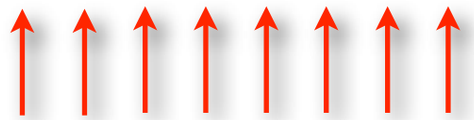
II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

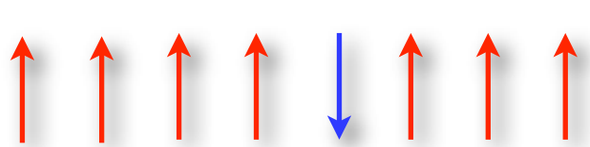
The Metropolis Algorithm

- creates a representative sample for any system

start with a configuration i



propose a small change to a configuration j



calculate the ratio of weights

$$\frac{p_j}{p_i}$$

accept the new configuration with probability

$$P = \min\left(1, \frac{p_j}{p_i}\right)$$

Monte Carlo simulations: the Metropolis algorithm

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Quantum Monte Carlo

- Feynman (1953) lays foundation for quantum Monte Carlo
- Map quantum system to classical world lines

THE
PHYSICAL REVIEW
A journal of experimental and theoretical physics established by E. L. Nichols in 1893
SECOND SERIES, VOL. 91, NO. 6 SEPTEMBER 15, 1953

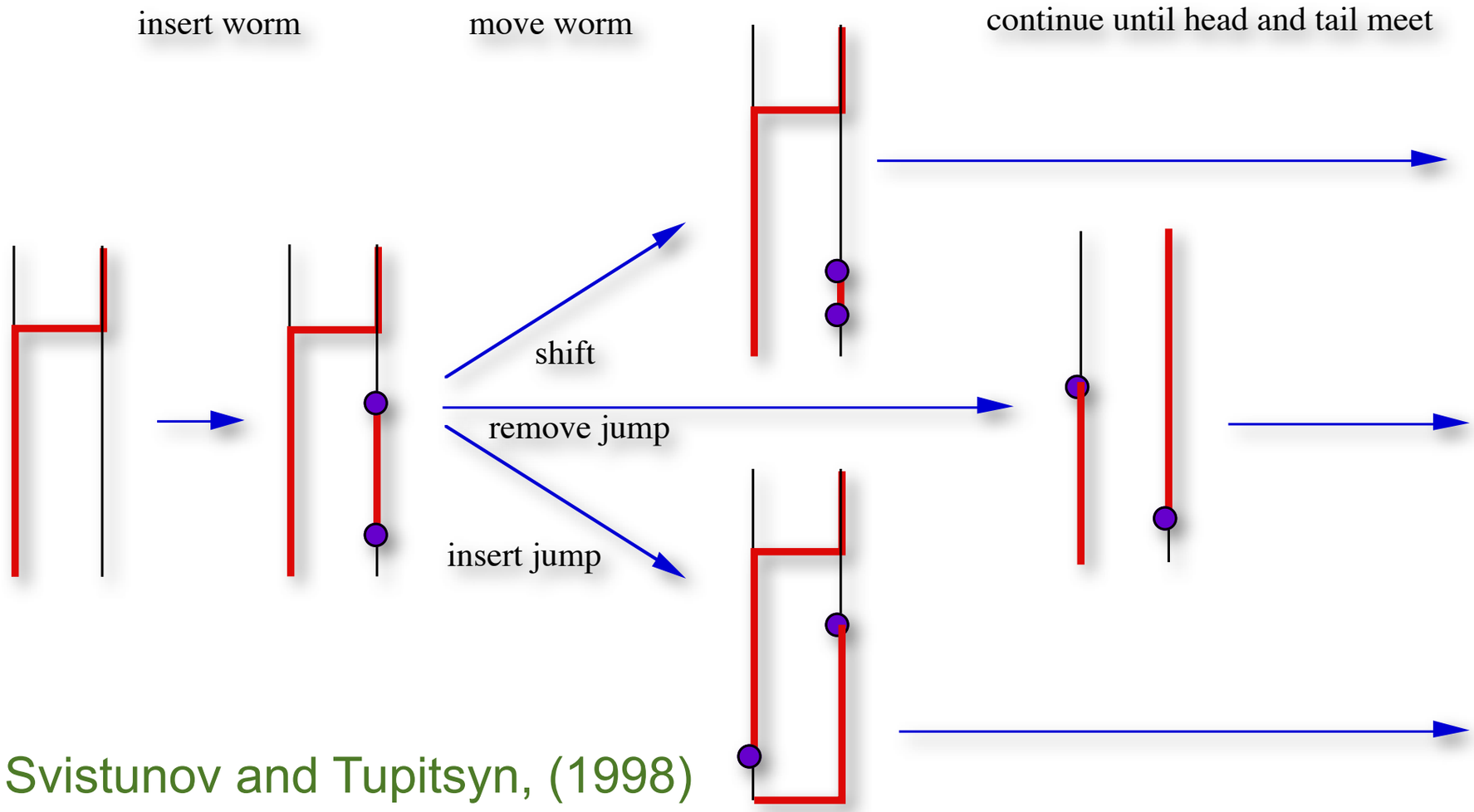
Atomic Theory of the λ Transition in Helium

R. P. FEYNMAN
California Institute of Technology, Pasadena, California
(Received May 15, 1953)

Use Metropolis algorithm to update world lines

The worm algorithm

- Local updates are inefficient and not even ergodic (knots cannot be undone)
- Worm algorithm: cut the world lines and move the open ends



Prokof'ev, Svistunov and Tupitsyn, (1998)

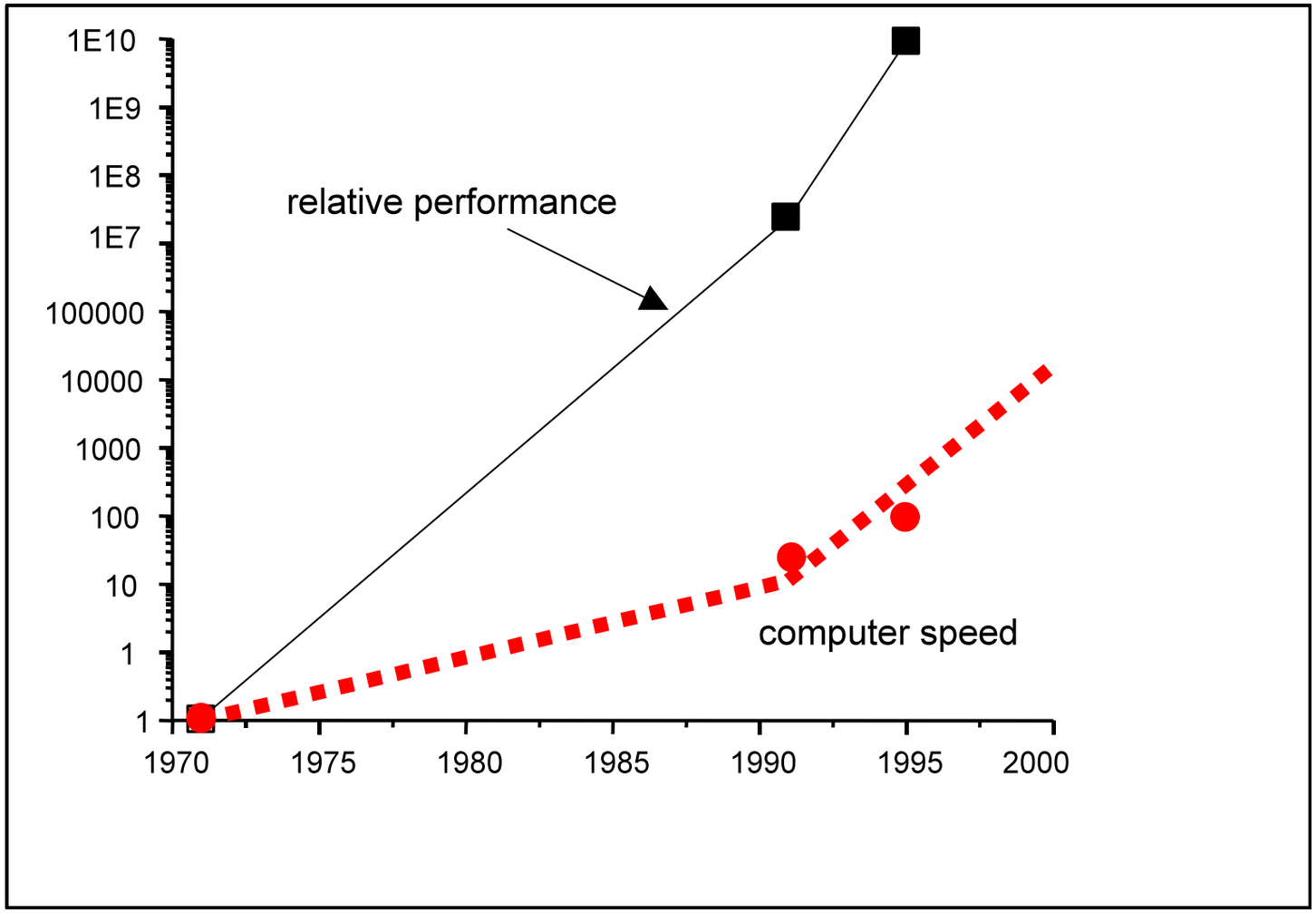
Modern quantum Monte Carlo methods

Advances in new algorithms, going beyond
Metropolis *et al* outperform Moore's law

Temperature	local updates	Modern algorithms
3D T_N	16'000 spins	16'000'000 spins
0.1 J	200 spins	1'000'000 spins
0.005 J	——	50'000 spins
3D T_c	——	1'000'000 bosons
0.1 t	32 lattice bosons	10'000 bosons

Algorithmic more important than Moore's law

- Modern algorithms on 30-year old computers are faster than 30-year old algorithms on modern computers!
- Example from D.P. Landau, simulating the Ising model



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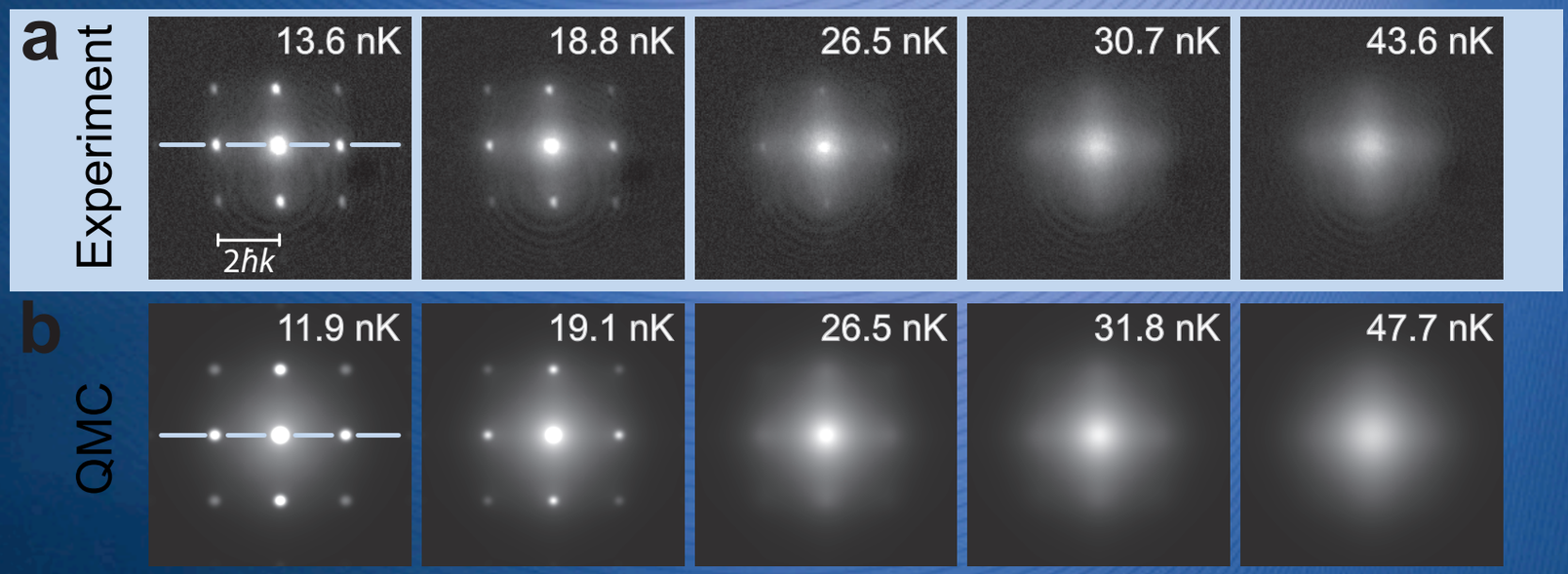
Simulating the experiment



Validation by Quantum Monte Carlo simulations

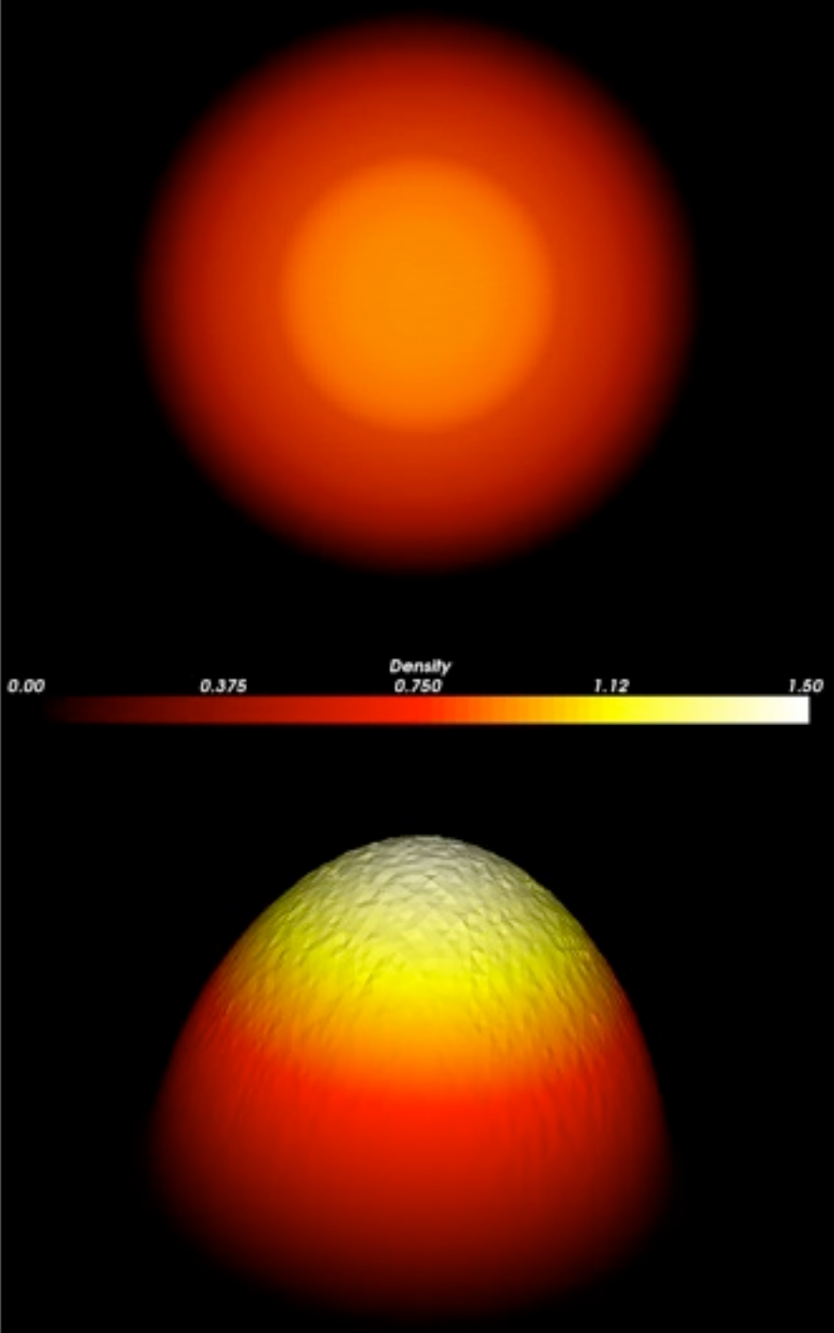
- Approximation-free QMC simulations
  - worm algorithm, Prokof'ev, Svistunov and Tupitsyn, (1998)
  - up to 500,000 atoms, 220 x 220 x 200 ≈ 10 million sites
  - a single simulation takes only 10 hours on one CPU core

- We can model all details of the experiment
  - accurate microscopic model
  - same system size, particle numbers
  - temperature and entropy matched to experiment
  - measure quantities as observed in experiment

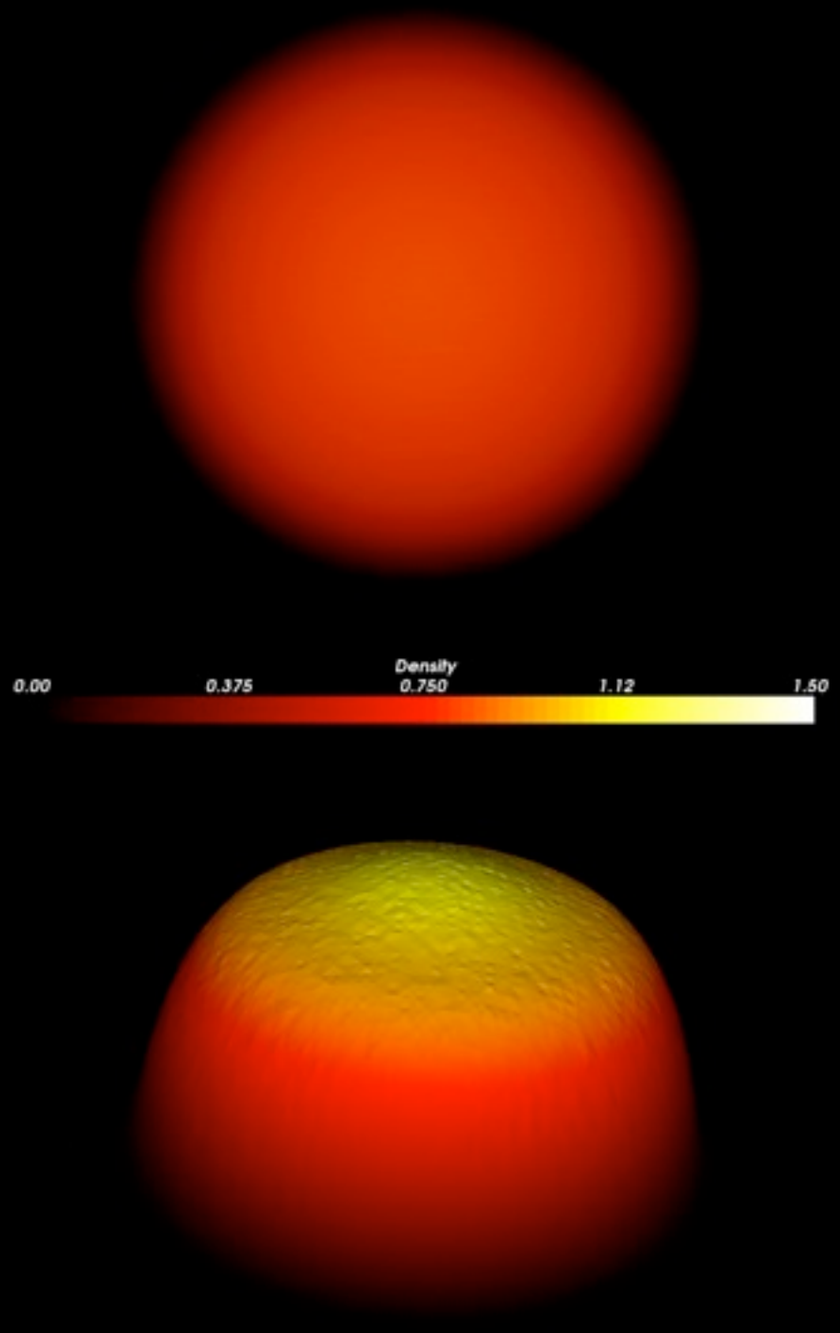
- Issues that can be addressed
  - Test new theoretical ideas (e.g. thermometry)
  - Validate experiment against QMC simulations

QMC “images” of the boson cloud

U/t = 10



U/t = 25



U/t = 50

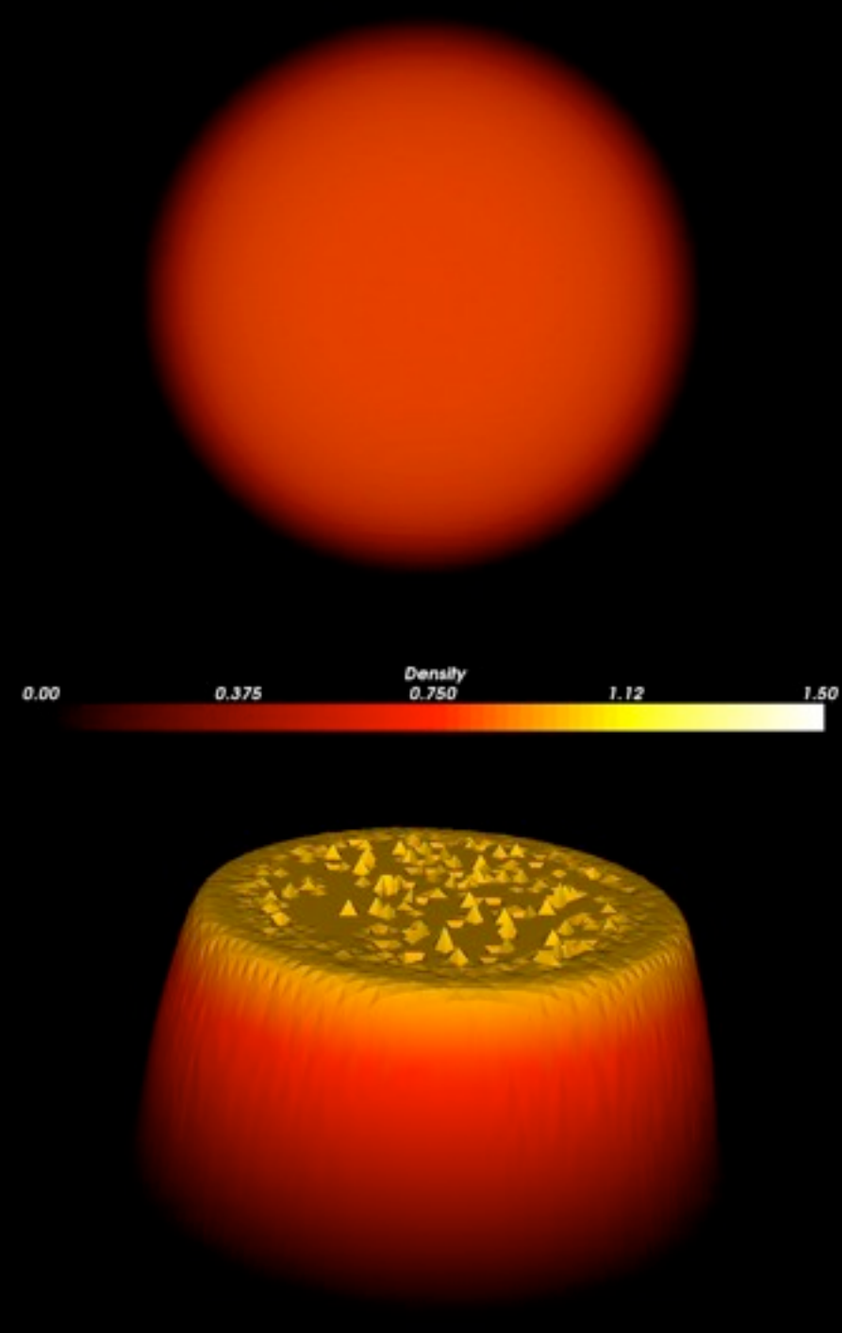
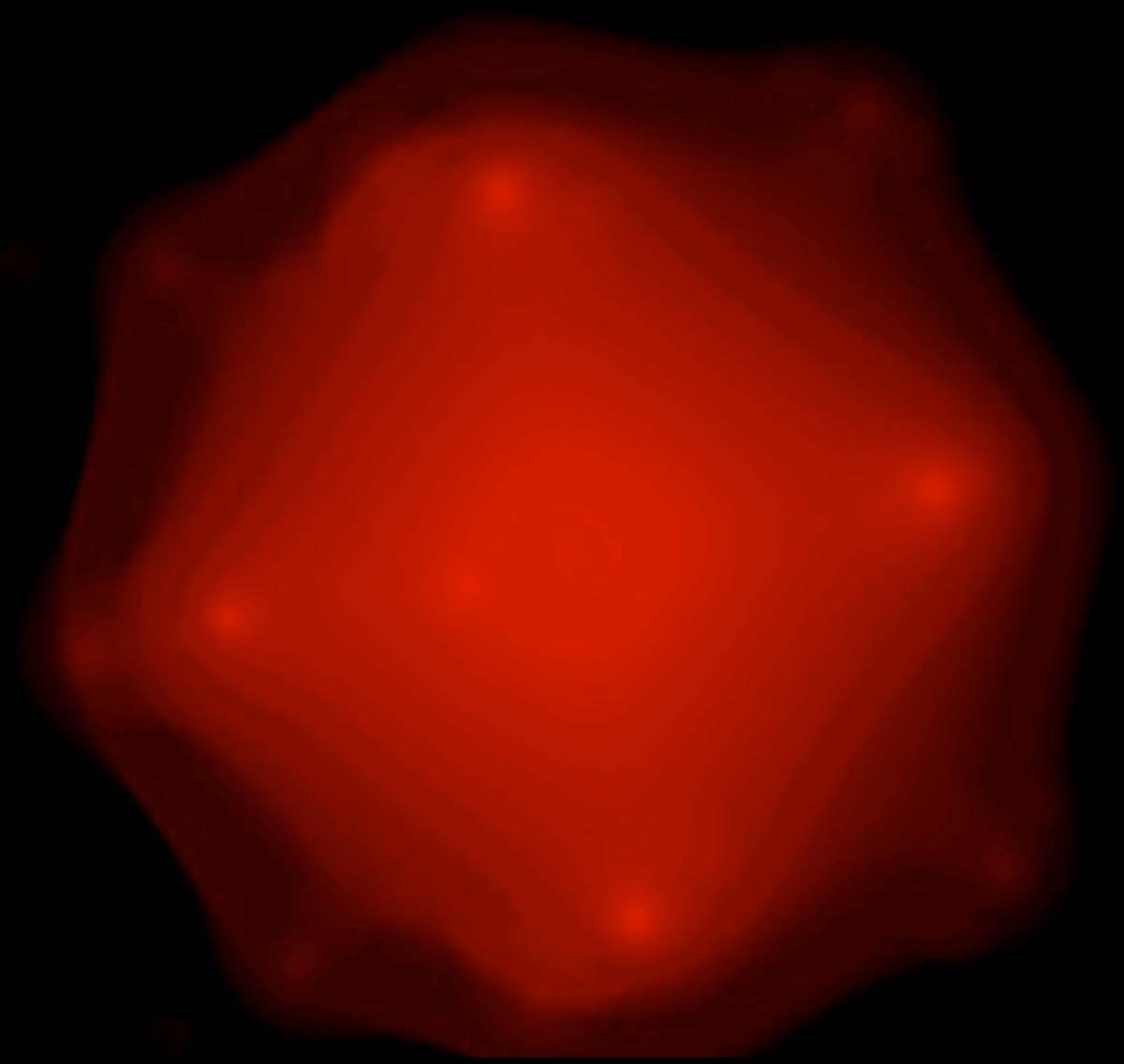
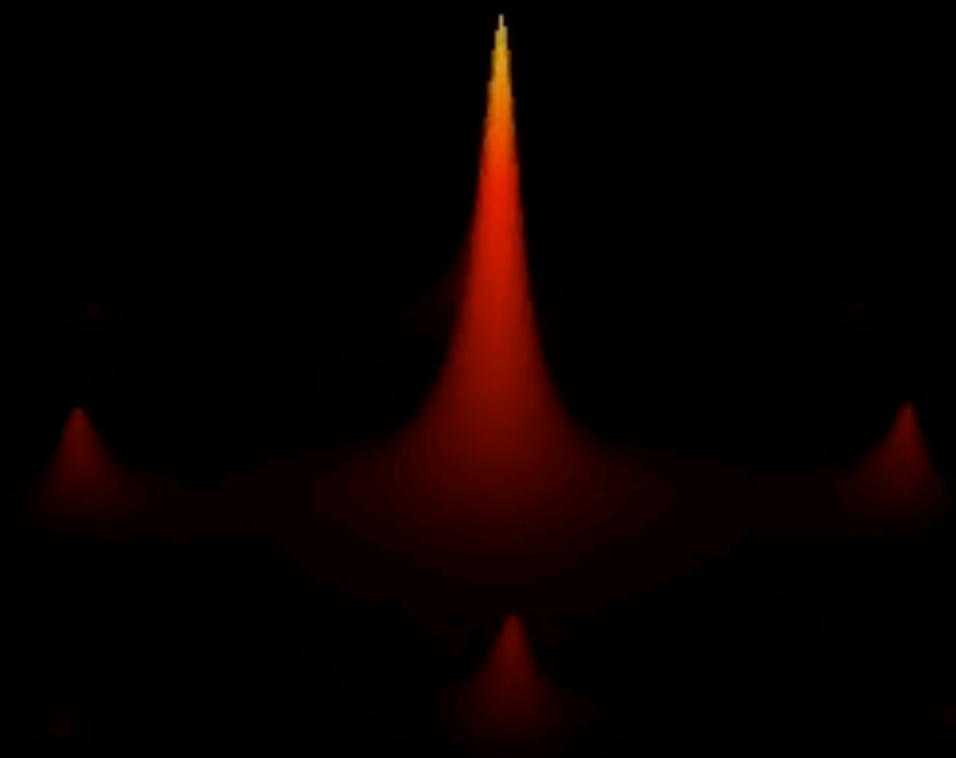


Image after expansion – momentum distribution

3D image



Crosssection

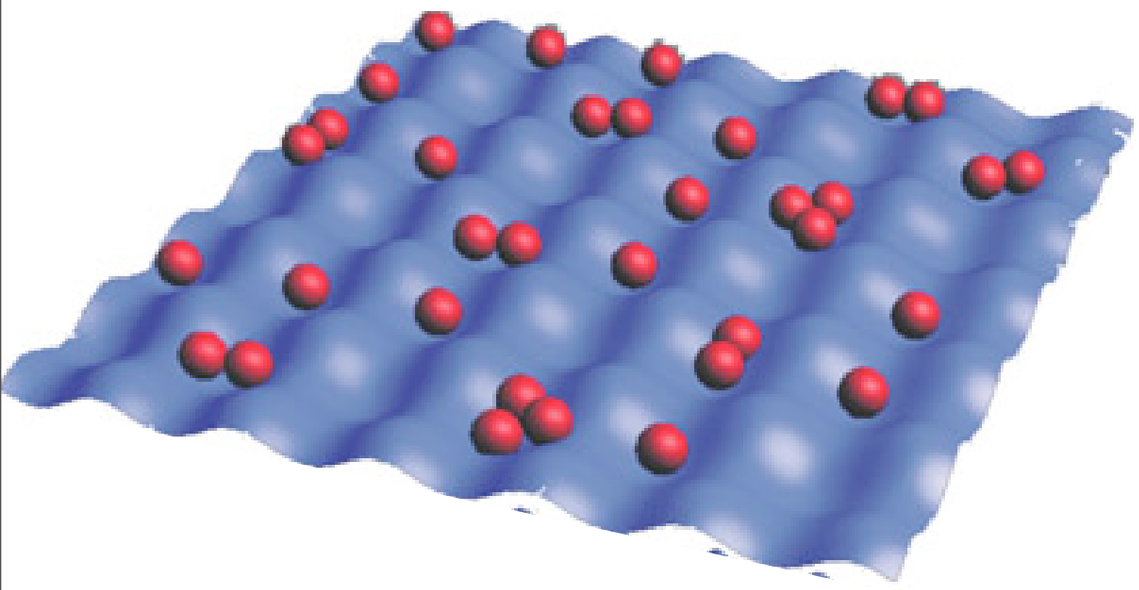


1. microscopic model from experiment

$$H = \int d^3r \psi^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m}\Delta + V_{\text{opt}}(\vec{r}) \right) \psi(\vec{r}) + \frac{g}{2} \int d^3r \psi^\dagger(\vec{r})\psi^\dagger(\vec{r})\psi(\vec{r})\psi(\vec{r})$$

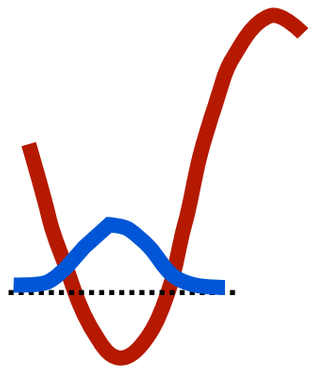
$$V_{\text{opt}}(r,z) = -V_0 e^{-2r^2/w^2(z)} \sin^2(kz)$$

$$g = \frac{4\pi\hbar^2 a_s}{m}$$



$$\psi(\vec{r}) = \sum_i w(\vec{r} - \vec{r}_i) b_i$$

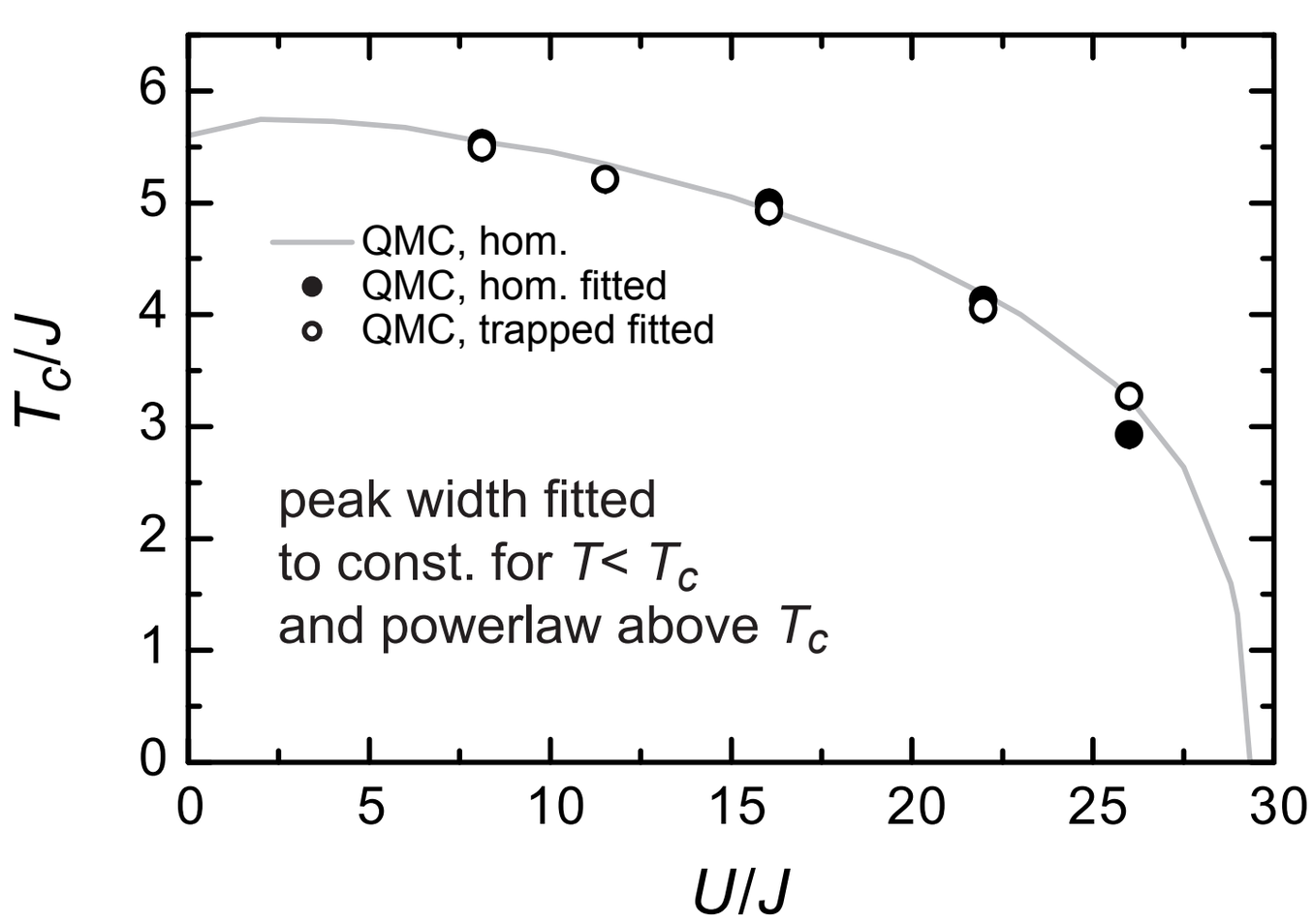
express the bosonic field operator in terms of Wannier functions



$$H = -t \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + \text{h.c.} \right) + U \sum_i n_i(n_i - 1)/2 - \mu \sum_i n_i + V \sum_i r_i^2 n_i$$

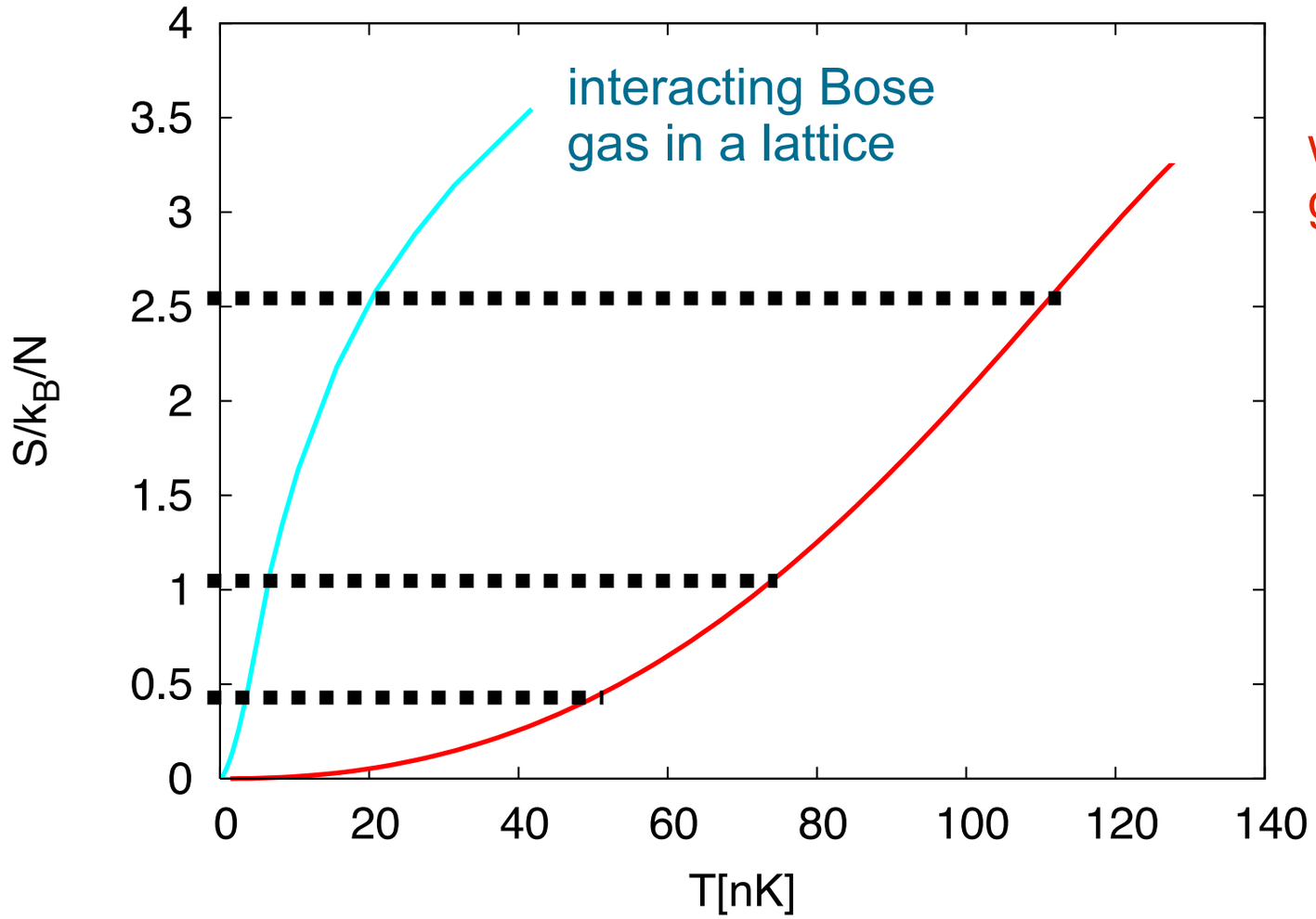
2. use QMC to fix the particle number in the center

- Use QMC to find total particle number *N* that gives density *n*=1 in the center at Tc then perform experiment with that particle number *N*
- QMC comparison of a trapped and homogeneous system: trap effects are negligible in this case



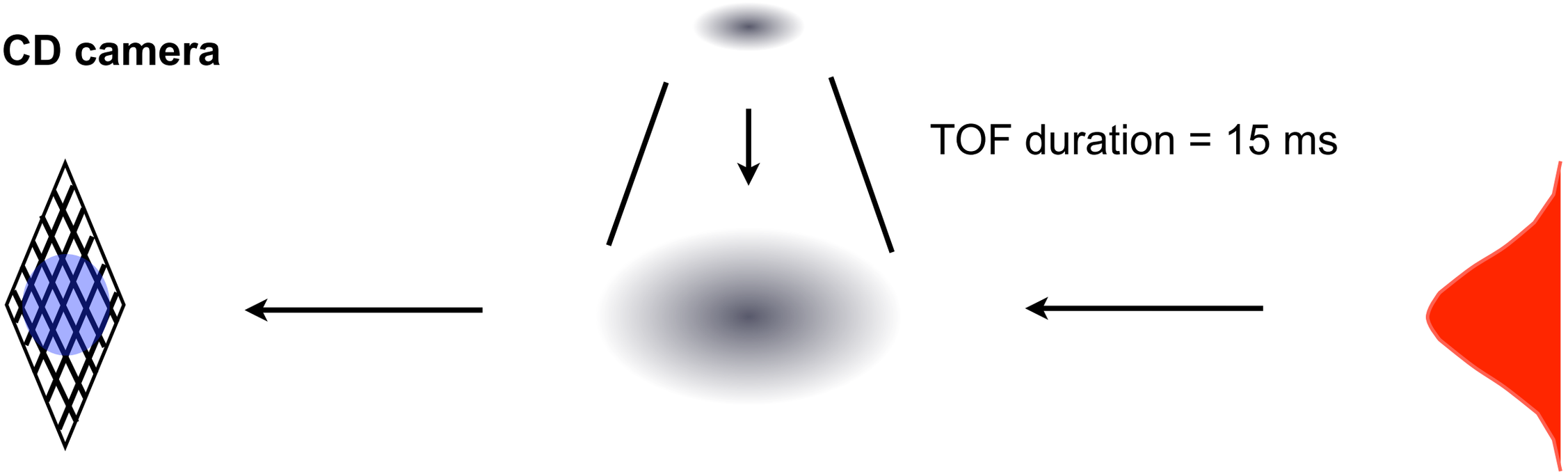
3. Use QMC simulations for thermometry

- Experiments work at constant entropy!
  - Measure the momentum distribution before loading the gas into the lattice
  - Get its temperature and entropy fitting to a dilute Bose gas
  - Use QMC simulations to find the temperature for that entropy once loaded into an optical lattice



4. accurately model time of flight (TOF) images

CCD camera



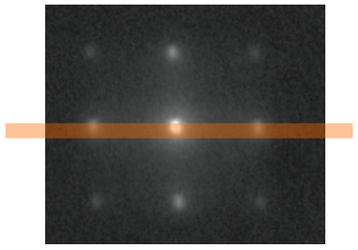
pixel size : 4.4 micron

further broadening
by optical elements

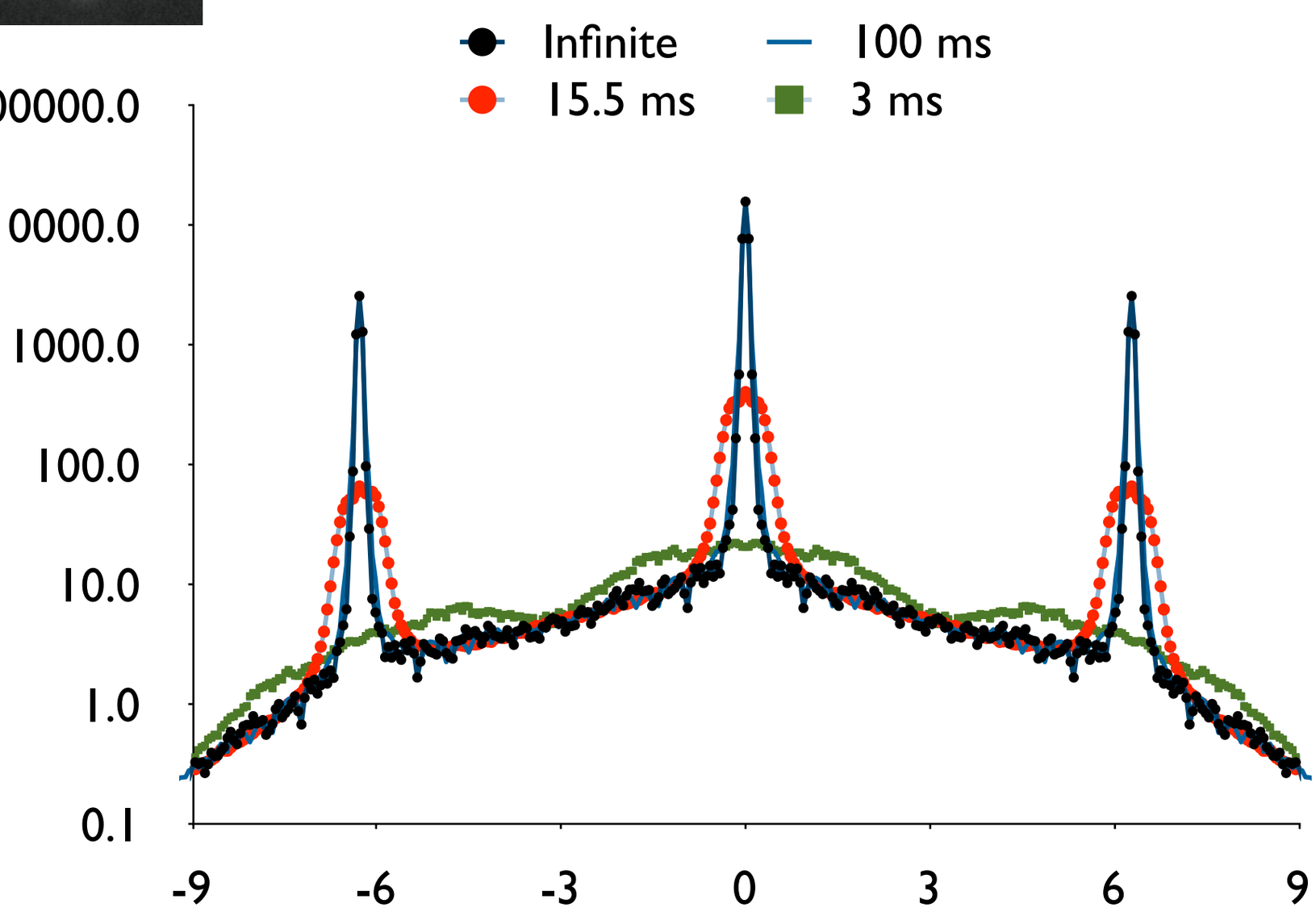
faster atoms fly farther

records the momentum distribution

Finite time of flight broadens the peaks



F. Gerbier *et al*, PRL (2008)



finite time of flight cuts off spatial correlations

broadens peaks

F. Gerbier *et al*, accepted in PRL

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Swiss Federal Institute of Technology Zurich

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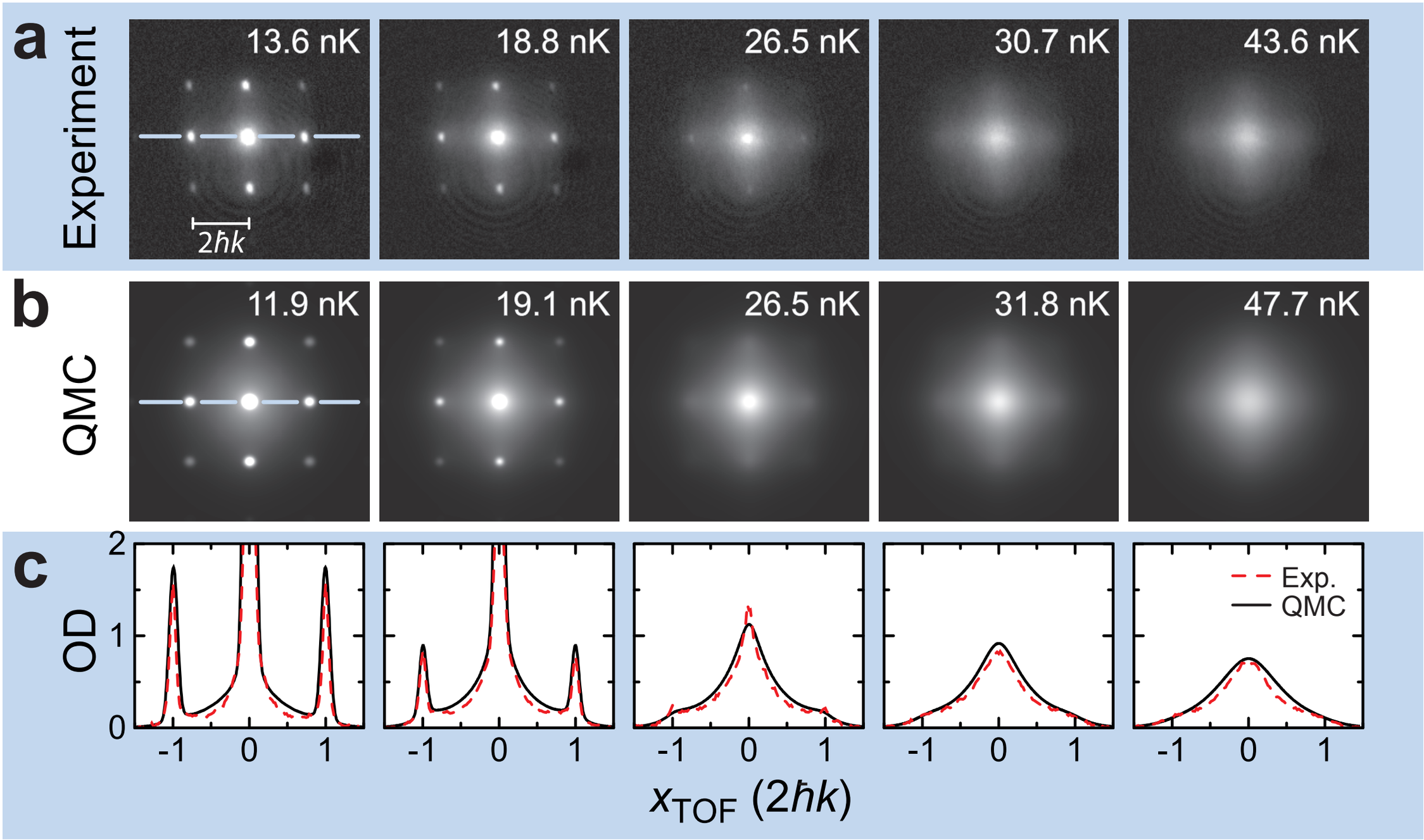
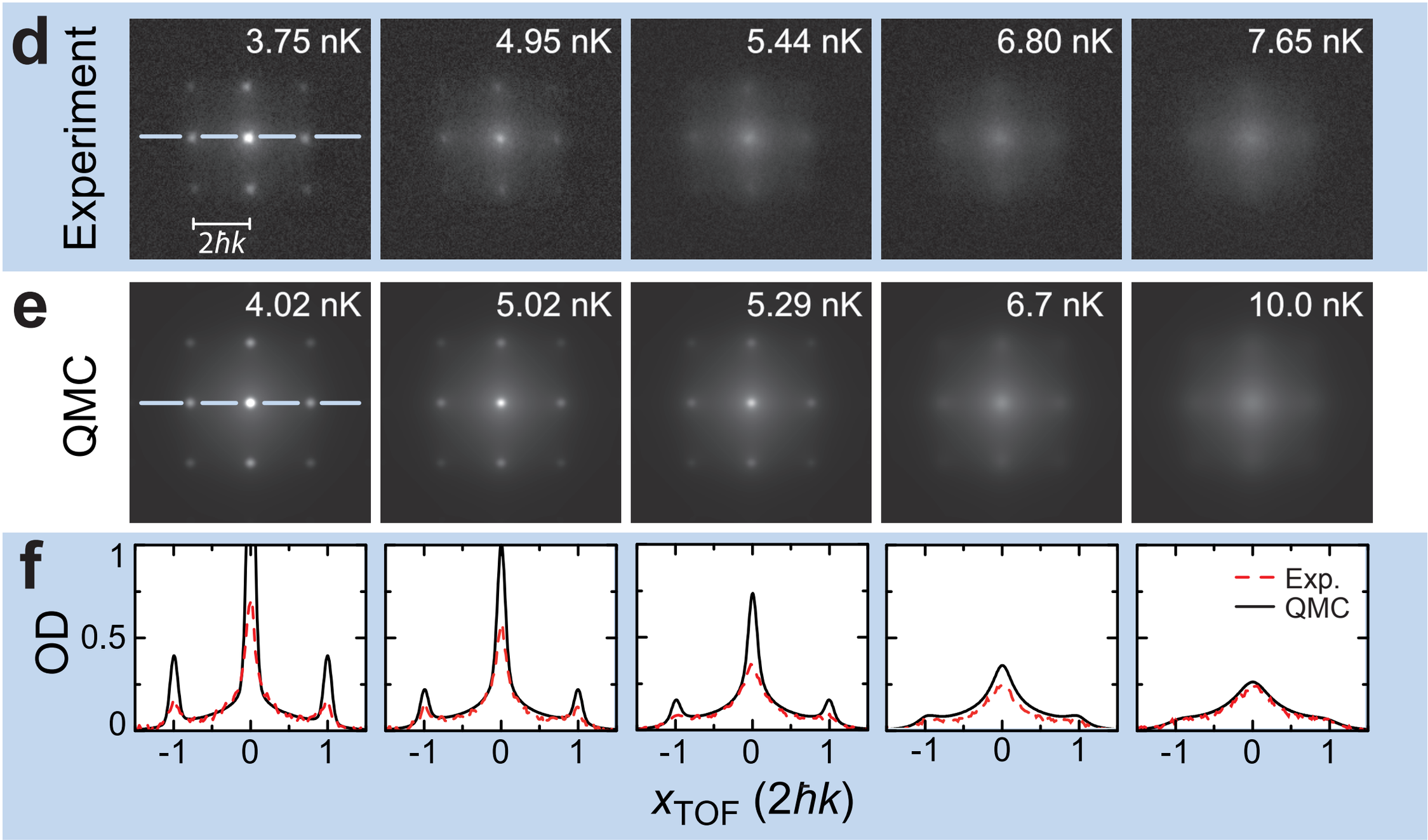
Validation of experiment by QMC: small *U/t*

$$V_0 = 8E_r\,,\quad U/J = 8.11\,,\quad T_c = 26.5\text{nK}$$

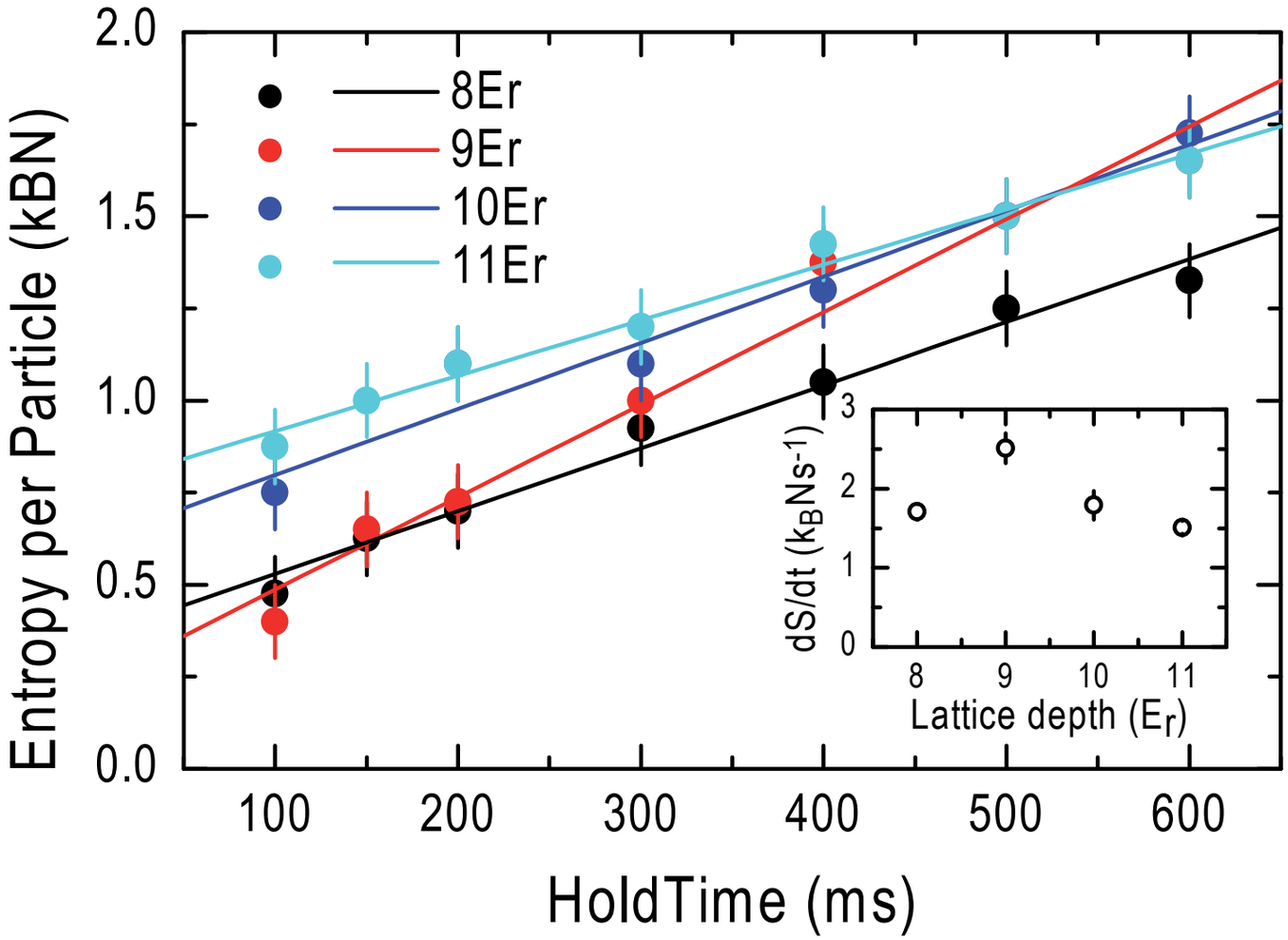


Validation of experiment by QMC: large *U/t*

$$V_0 = 11.75E_r\,,\quad U/J = 27.5\,,\quad T_c = 5.31\text{nK}$$



Non-adiabaticity: heating from lattice laser

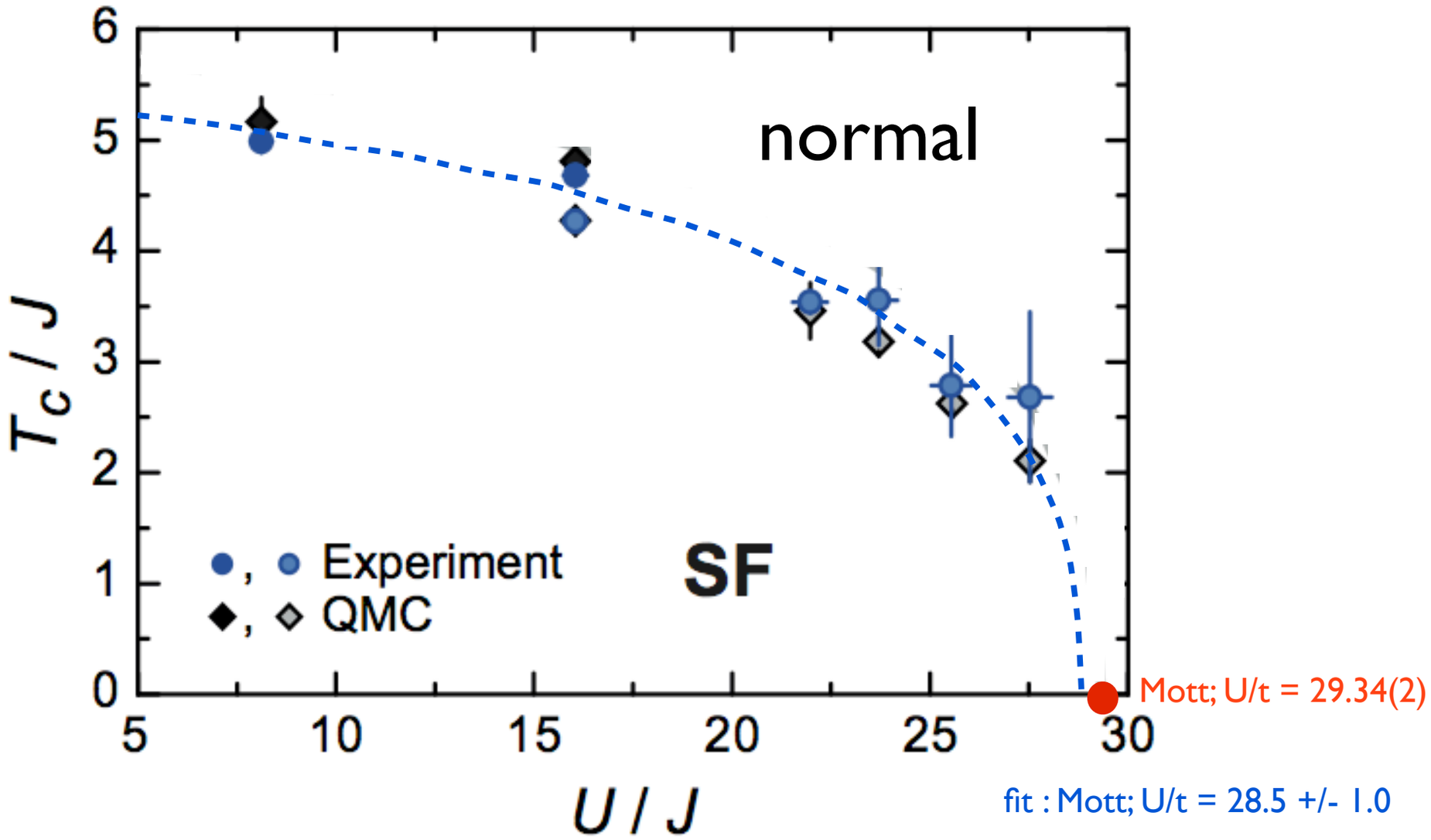


Entropy determined by comparing TOF images to QMC simulations

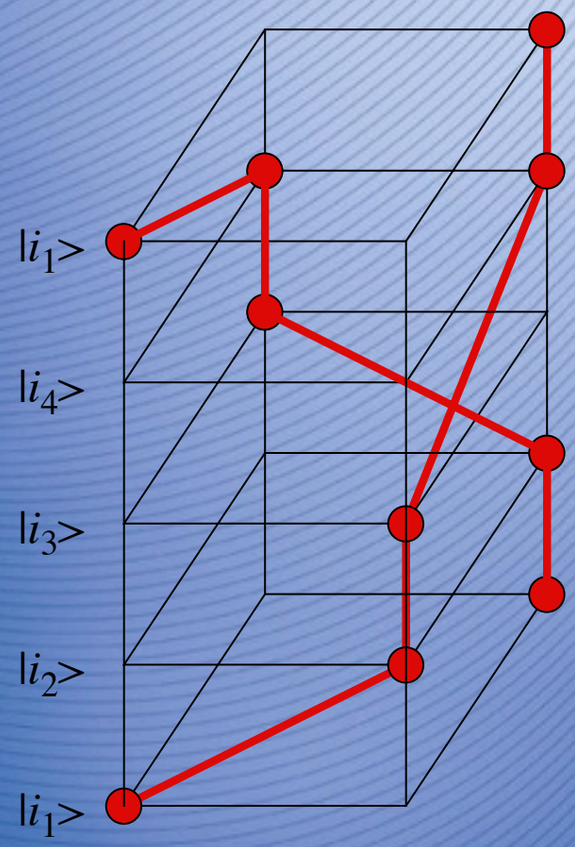
Heating due to spontaneous emission > 1 k_B / s / particle!

Severe limitation on accessible temperatures in experiments

Phase diagram obtained by the quantum simulation

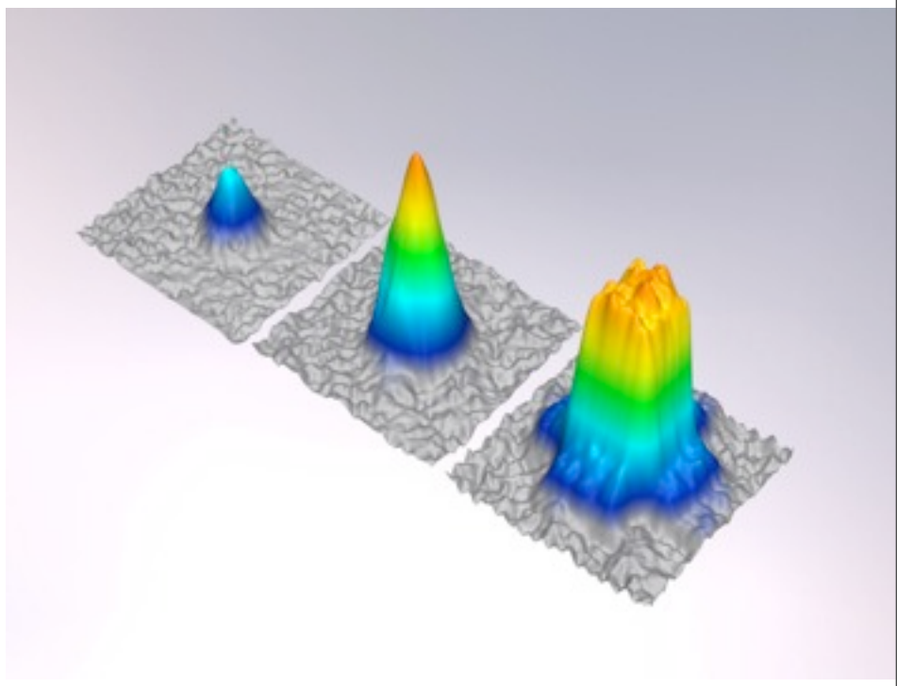


Fermions



The big challenge: fermions

- Detection of Fermi surface in ^{40}K
  - M. Köhl *et al*, PRL **94**, 080403 (2005)
- Fermionic Mott insulator
  - R. Jördens *et al*, Nature **455**, 204 (2008)
  - U. Schneider *et al*, Science **322**: 1520 (2008)

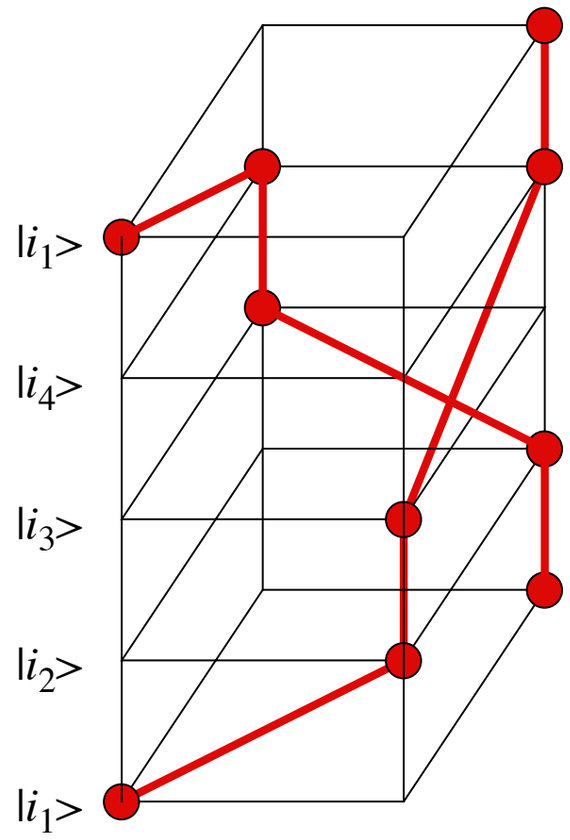


The fermion sign problem in QMC

- Quantum systems mussed first be mapped to classical systems

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_i p_i$$

- There is a “sign problem” if two fermions exchange: $p_i < 0$
  - cannot sample using negative weights
  - “ignoring” sign in sampling gives exponentially growing errors



The negative sign problem

- Sample with respect to absolute values of the weights

$$\langle A\rangle = \sum_i A_i p_i \Big/ \sum_i p_i = \frac{\sum_i A_i \operatorname{sgn} p_i |p_i| \Big/ \sum_i |p_i|}{\sum_i \operatorname{sgn} p_i |p_i| \Big/ \sum_i |p_i|} \equiv \frac{\langle A \cdot sign\rangle_{|p|}}{\langle sign\rangle_{|p|}}$$

- Exponentially growing cancellation in the sign

$$\langle sign\rangle = \frac{\sum_i p_i}{\sum_i |p_i|} = Z/Z_{|p|} = e^{-\beta V(f-f_{|p|})}$$

- Exponential growth of errors

$$\frac{\Delta sign}{\langle sign\rangle} = \frac{\sqrt{\langle sign^2\rangle - \langle sign\rangle^2}}{\sqrt{M}\langle sign\rangle} \approx \frac{e^{\beta V(f-f_{|p|})}}{\sqrt{M}}$$

- NP-hard problem (no general solution) [Troyer and Wiese, PRL 2005]

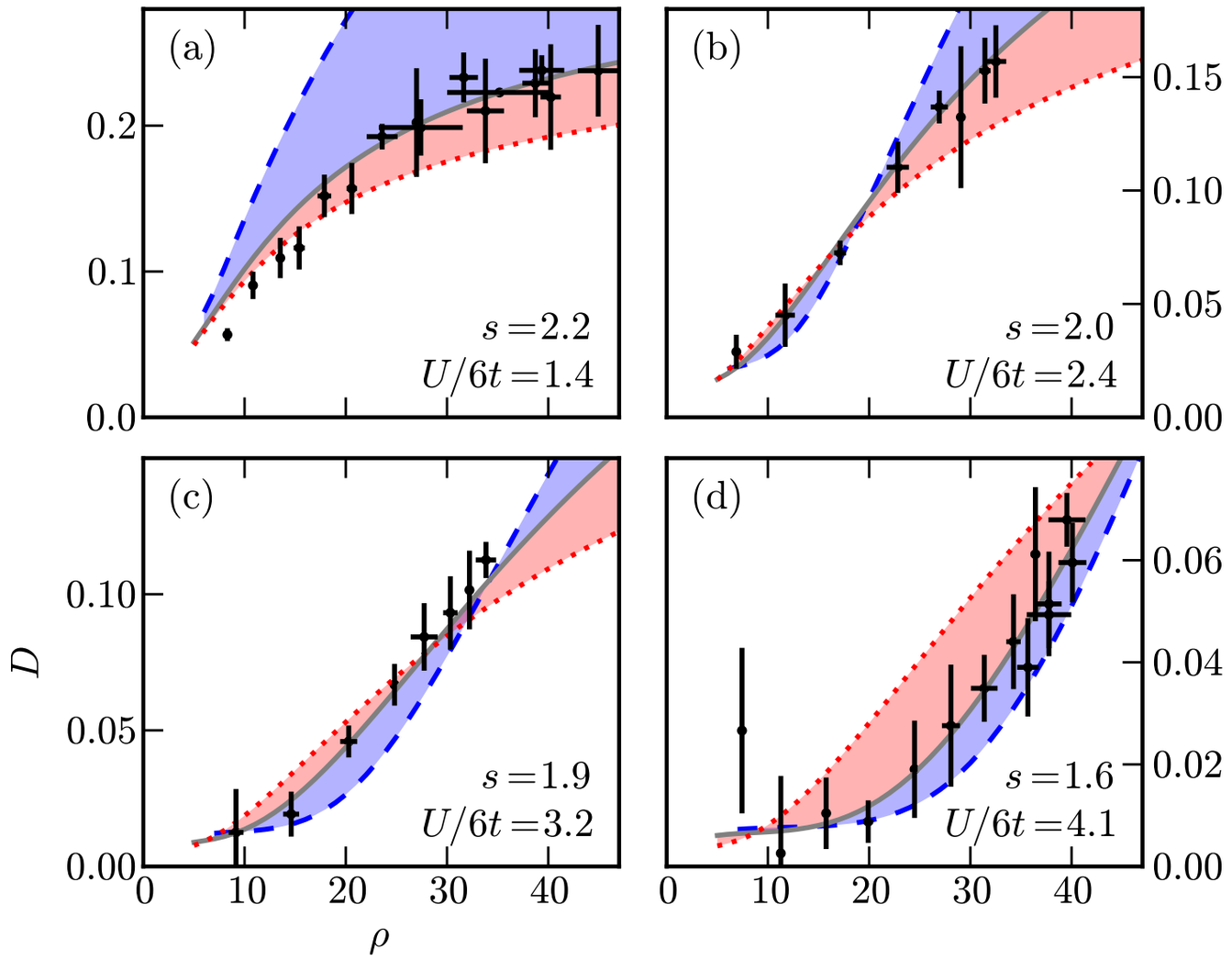
Simulating fermions

- There is no “black box” solution for all fermion problems
  - We need to think hard and find good approximate methods
  - The good news: we’ll never be out of business

- We can still simulate fermions in experimentally relevant regimes:
  - High-temperature expansions: valid down to T ≈ t
    - Scarola, Pollet, Oitmaa, Troyer, Phys. Rev. Lett. 102, 135302 (2009)
  - Dynamical mean field theory approximation
    - see lectures by Antoine Georges
  - New diagrammatic QMC methods

Determining the temperature for fermions

- Fit to high-temperature series expansions to measurements of double occupancy gives temperature and entropy
  - R. Jördens, L. Tarruell, D. Greif, T. Uehlinger, N. Strohmaier, H. Moritz, T. Esslinger, L. De Leo, C. Kollath, A. Georges, V. Scarola, L. Pollet, E. Burovski, E. Kozik, M. Troyer, PRL (2010)



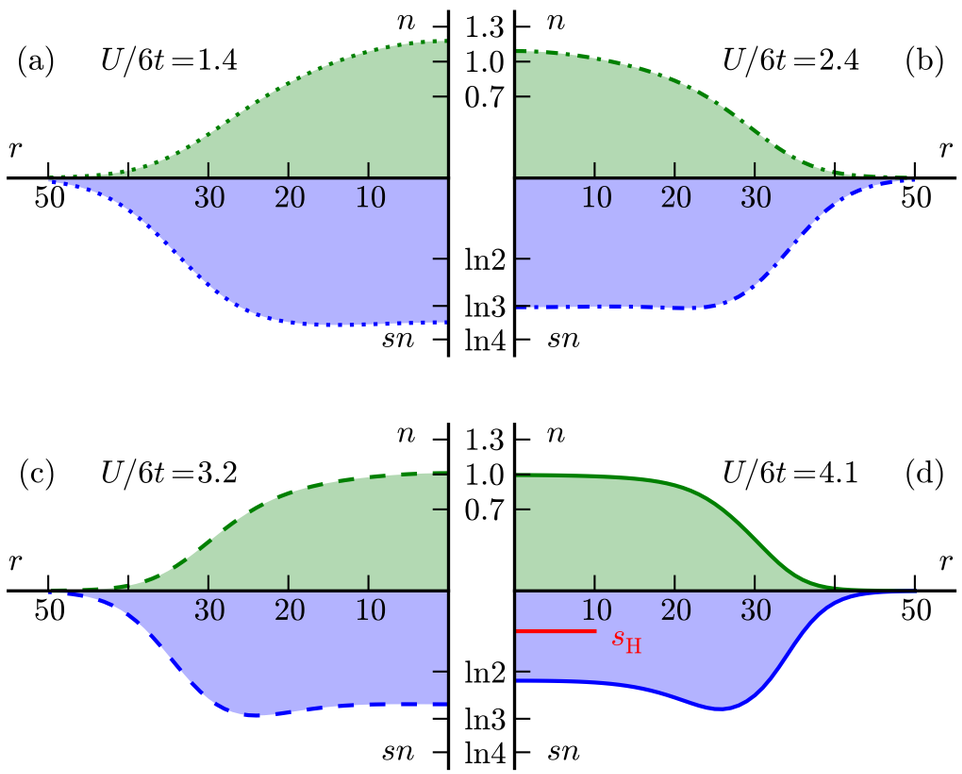
$$T / T_F \approx 0.15 - 0.2$$

$$\rho = N / N_0$$

$$N_0 = (12t / m\omega^2 a^2)^{3/2} \approx 7400$$

Reaching the Néel state

- At large *U/t* a Mott-insulating phase has been reached in the center but the entropy is still 3x too high to see the Néel state
- The Néel state still seems reachable, but lower temperature phases will be a very hard challenge – if not impossible



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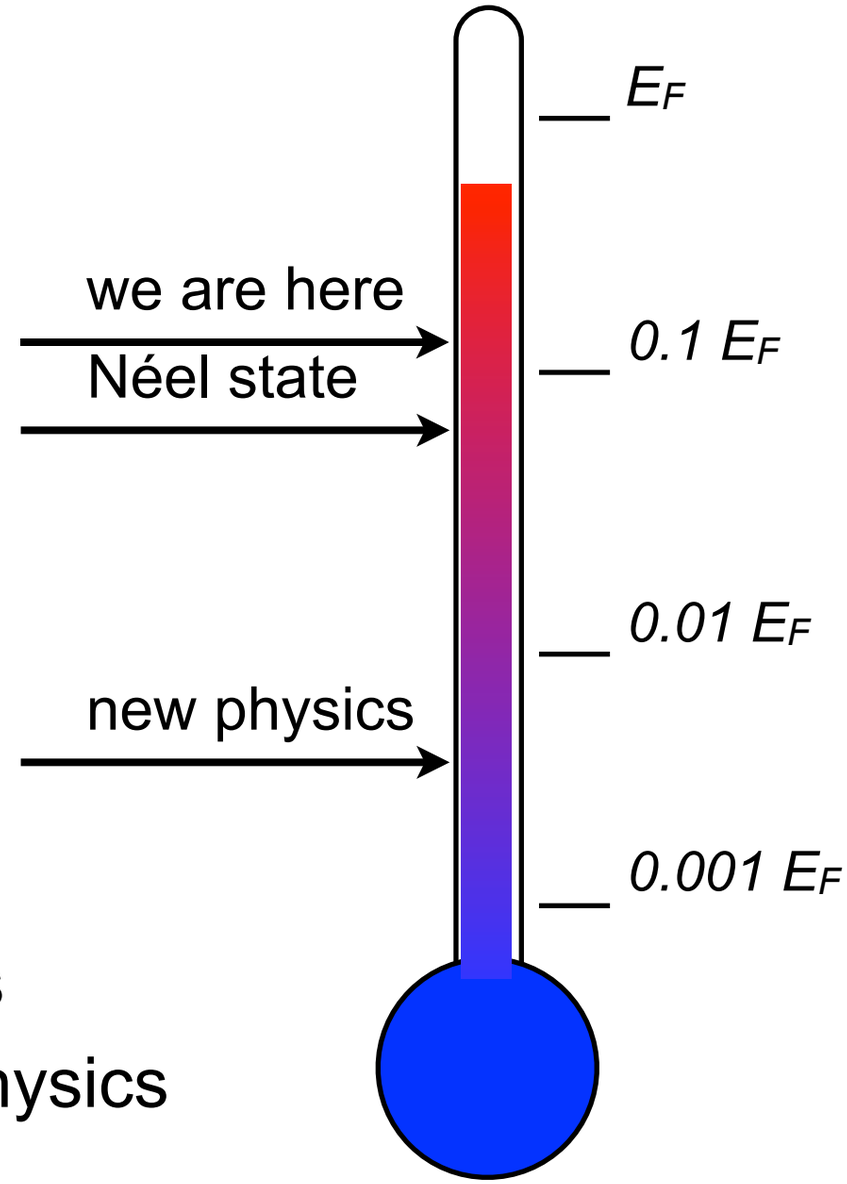
- But the temperature is still high
  - equivalent to 5000K in cuprate superconductors
  - need to cool 10-100x lower to see interesting physics
- Major engineering challenges are ahead of us



The challenges for experiments

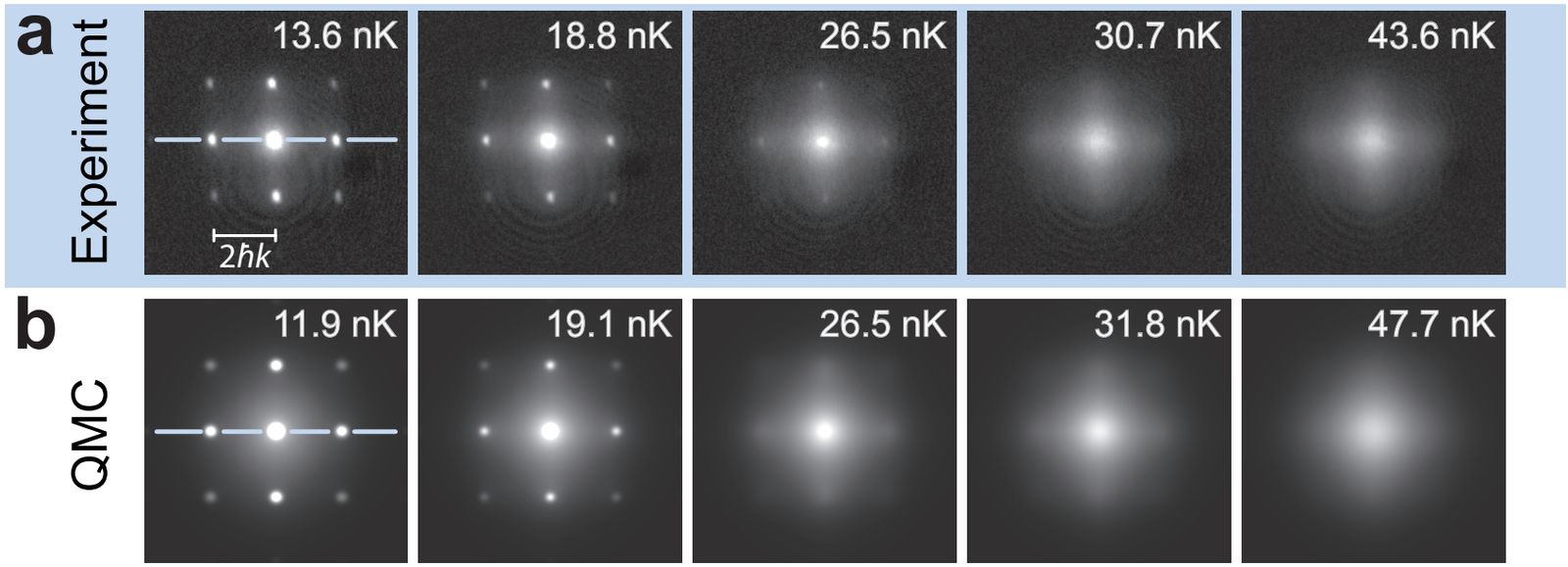
- We need to develop methods to measure
  - the local density in the middle of the trap
  - the temperature in the trap

- We need to improve the accuracy in calibrating
  - the laser amplitude (5% uncertainty gives 20% uncertainty in U/t)
  - the total atom number count (estimated 10% systematic error)

- We need to improve cooling and avoid heating
  - Still at rather high temperatures $T \approx t$
  - Heating rates measured in the lattice are bad news for low-T physics

Successes and challenges for simulations

- Bosonic simulations of millions of particles are feasible on PCs
- Can be used to validate experiments on ultracold bosonic gases



- Fermions still are a challenge
  - Good approximate methods are needed
  - Collaboration between analytical and computational methods