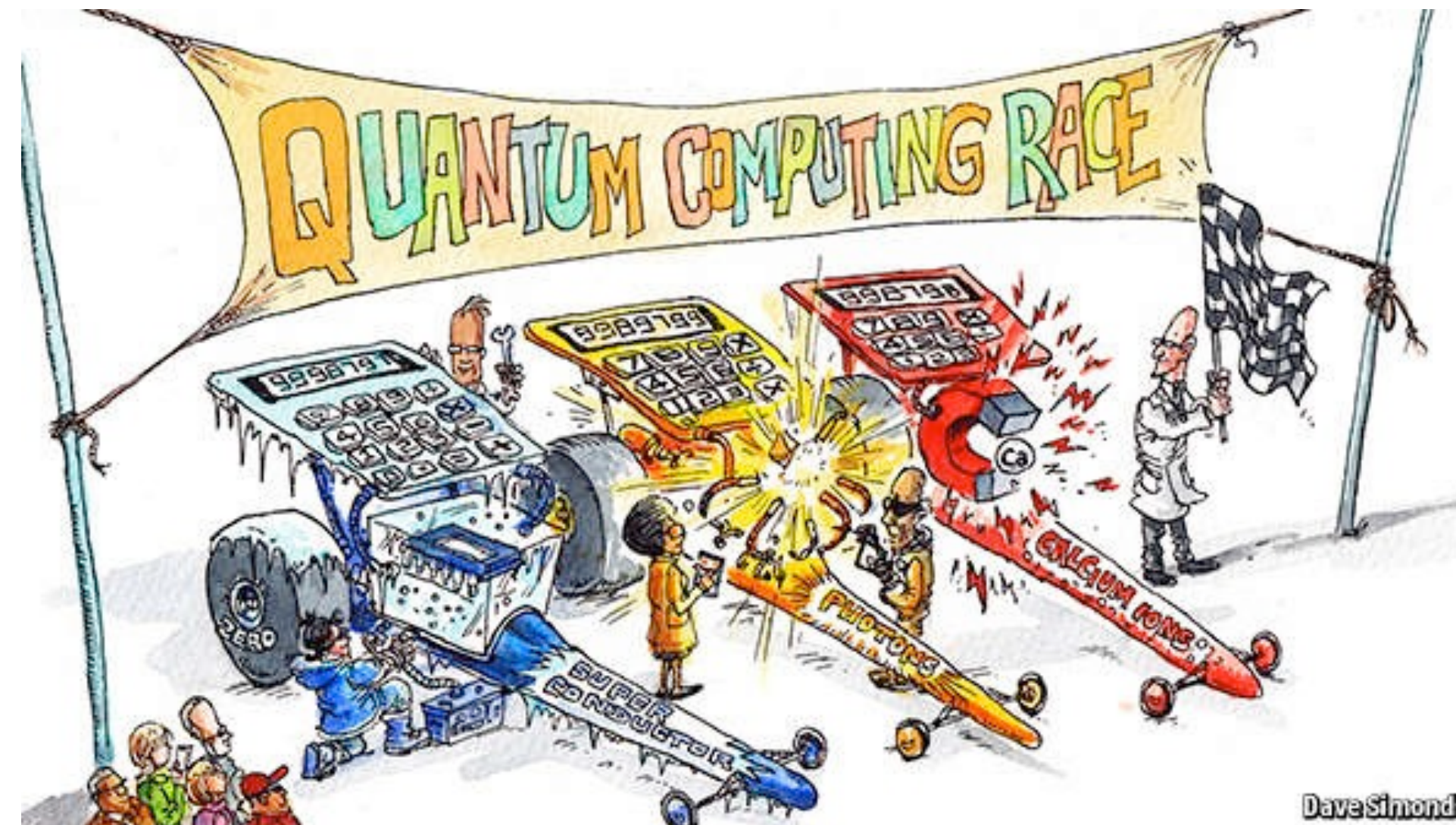




# Quantum circuits in cold atoms

Fred Jendrzejewski  
Heidelberg University, Germany

[fnj@kip.uni-heidelberg.de](mailto:fnj@kip.uni-heidelberg.de)



# Superconducting Qubits



- Superconducting electrical components
- Excitations of superconductor forms qubit

## Strengths

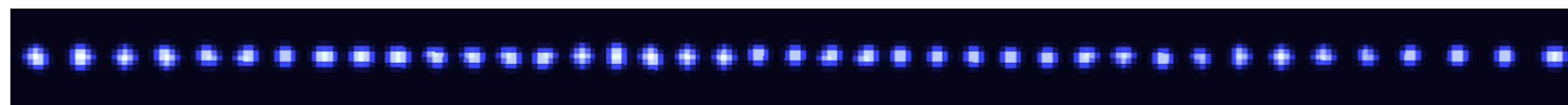
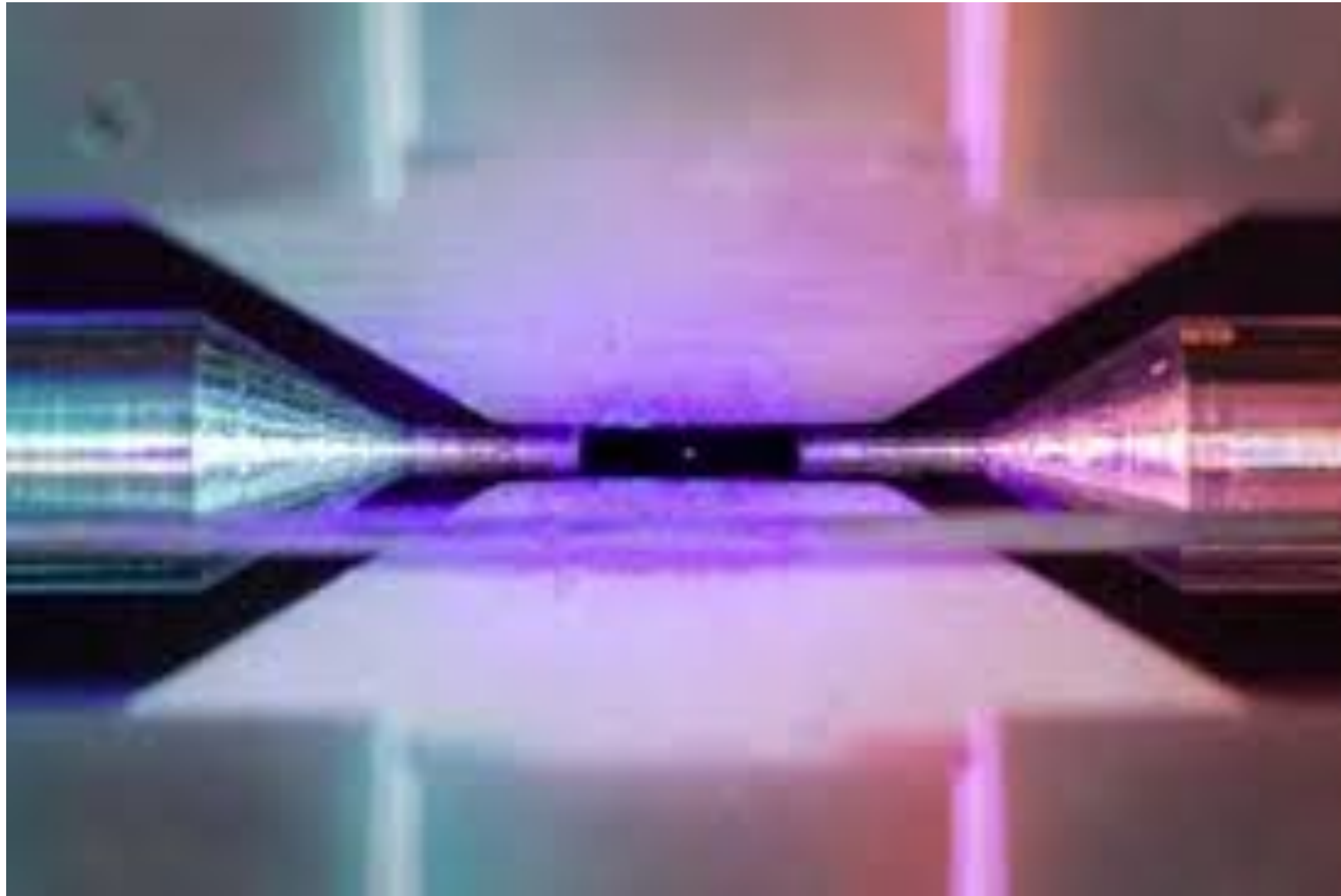
- Integrated in electrical circuit
- Control with GHz frequencies
- Great integration into software packages
- Large number of algorithms

## Open questions

- Size of system
- Fidelities
- Practical use

# Trapped Ions

Lucas group, Oxford



Monroe group, JQI Maryland

- Charged particles
- Electrostatic traps
- Laser and microwave operations

## Strengths

- Highest gate fidelities
- Fast experimental timescales

## Open questions

- Maximum size 50 qubits so far
- Challenging scalability

## Important commercial players

- IonQ (JQI)
- AQT (Innsbruck)
- Honeywell (JILA)



NYSE OPENING BELL®

OCTOBER 1, 2021

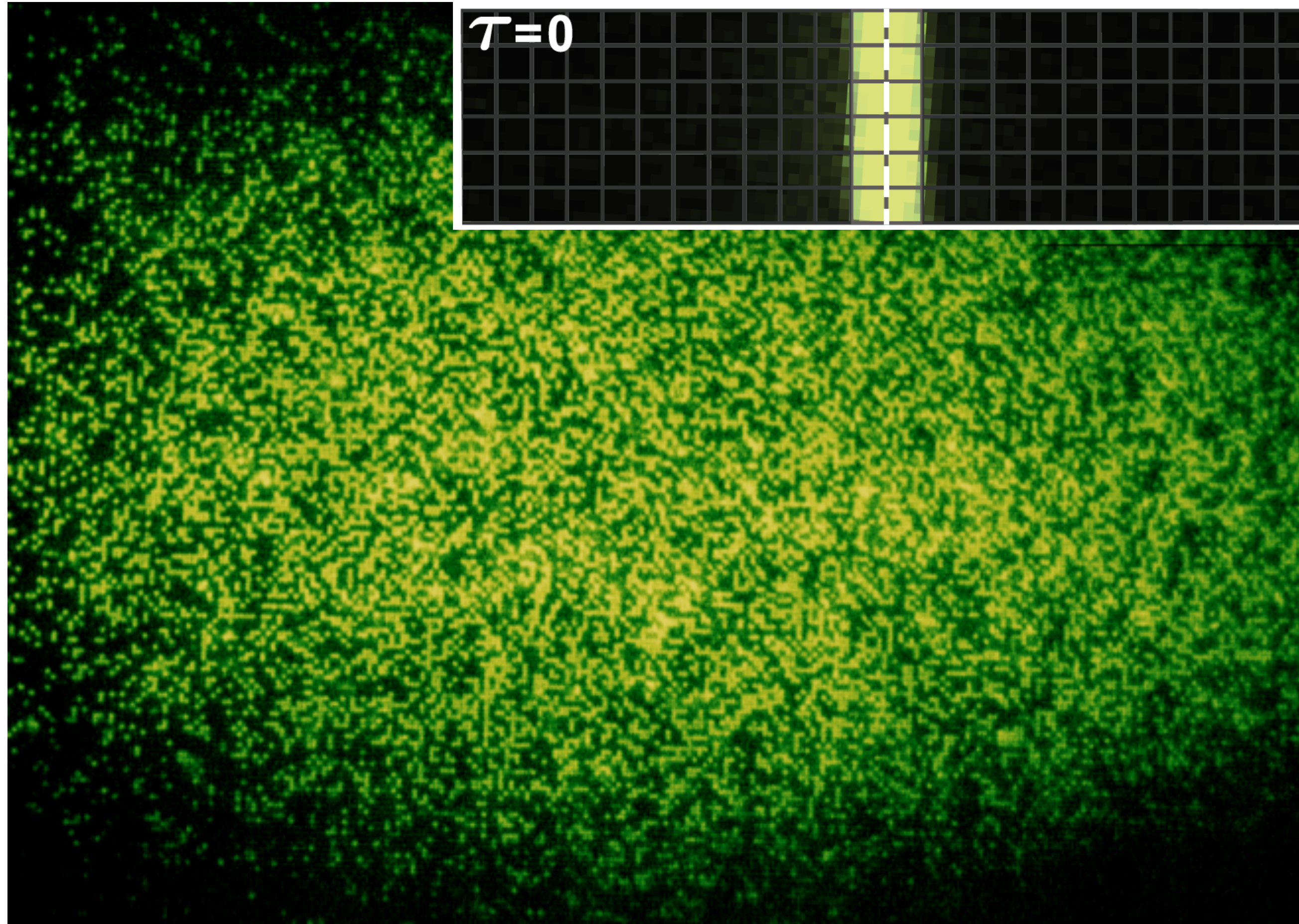


NEW YORK STOCK EXCHANGE



# Neutral atoms

Greiner group, Harvard university



- Neutral laser-cooled particles
- Optical potentials
- Single-particle readout and control

## Strengths

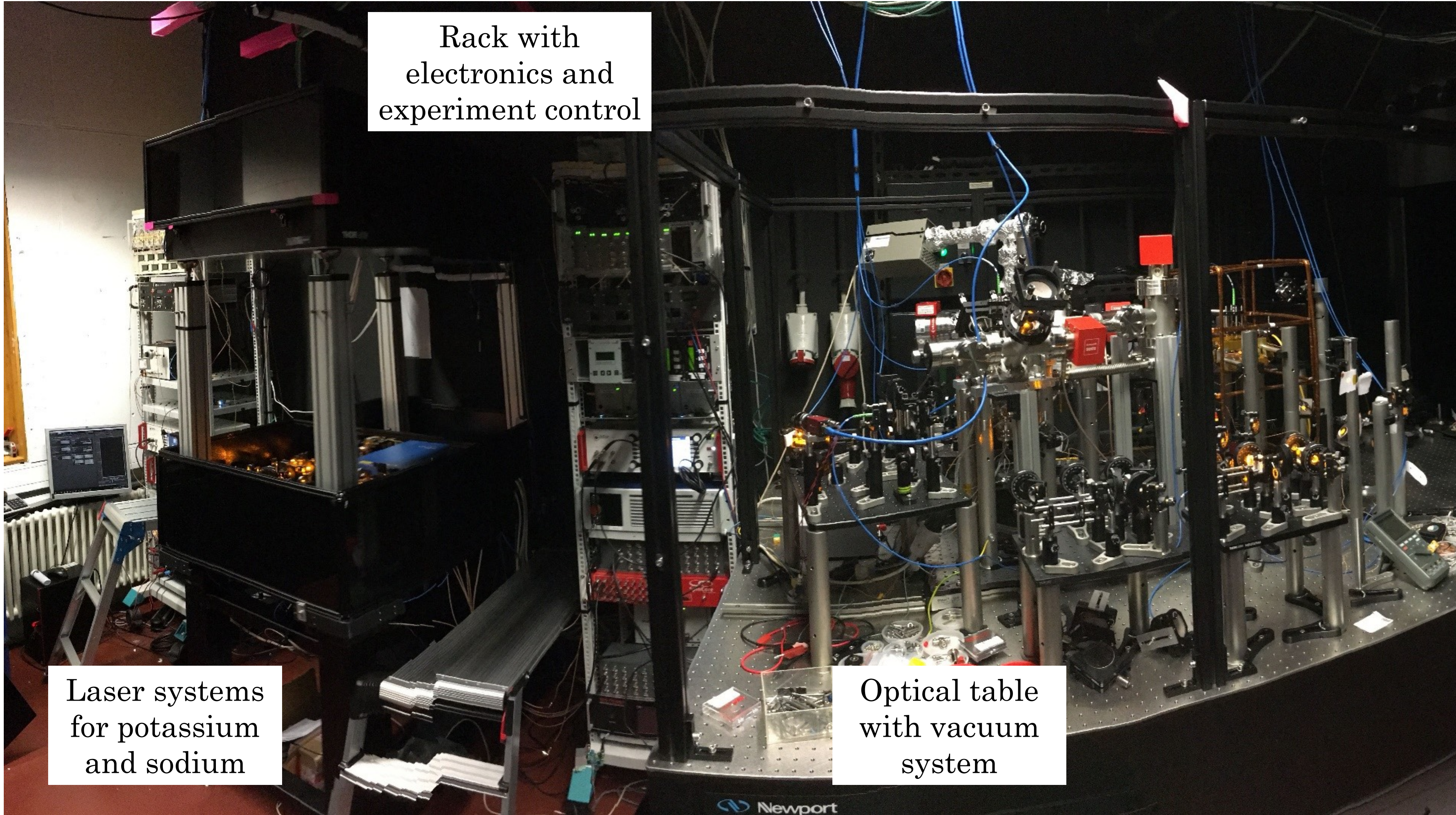
- Many hundreds of particles
- Enormous flexibility

## Open questions

- Poor software integration
- few algorithms
- few applications outside of physics studied



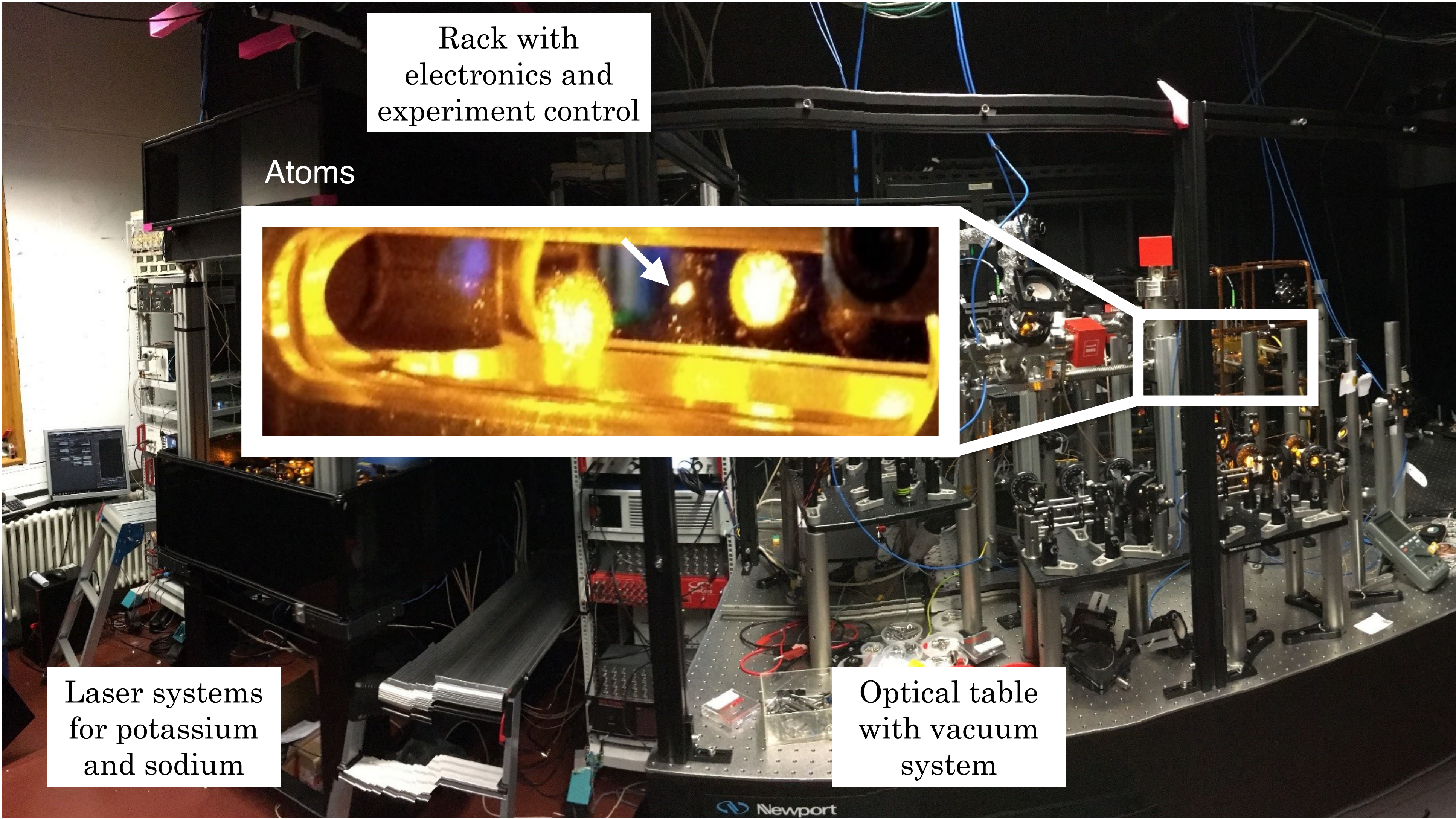
Lukin group, Harvard university



Rack with electronics and experiment control

Laser systems for potassium and sodium

Optical table with vacuum system



Rack with electronics and experiment control

Atoms



Laser systems for potassium and sodium

Optical table with vacuum system

Newport

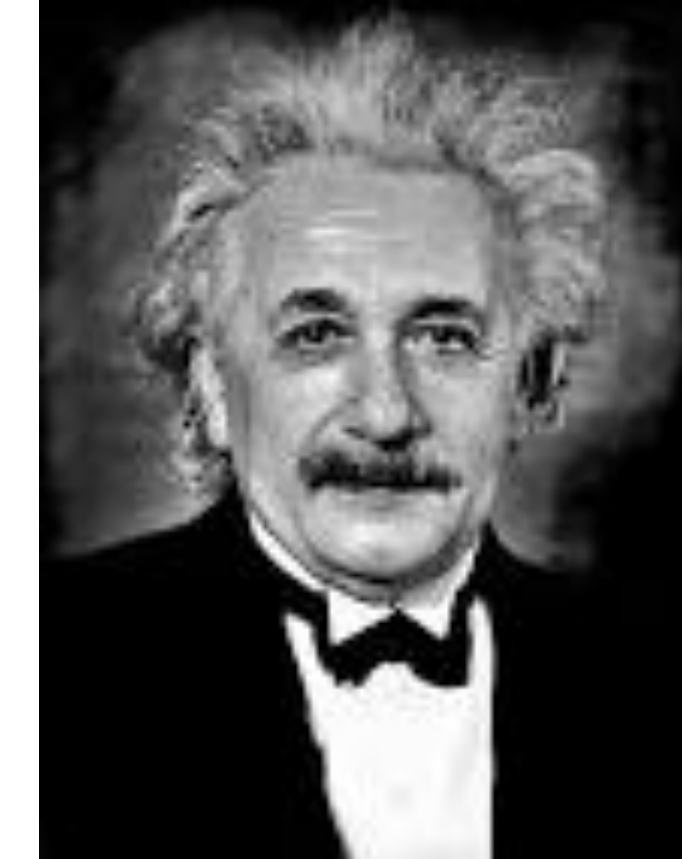
1. Atomic clocks — Qubits in cold atoms
2. Optical tweezers — Trapped qubits in atoms
3. Rydberg atoms — Large scale entanglement
4. Moving particles — Bosons vs Fermions and the link to chemistry
5. Lattice gauge theories — Working on a really hard physics problem



# What is time ?

Einsteins' special relativity:

Time is what a clock measures.



Experimentalists dilemma: What is a clock ?

Something that ,ticks', i.e. provides a regular series of events



# Traditional clocks



1 tick = 1 day



1 tick = few seconds



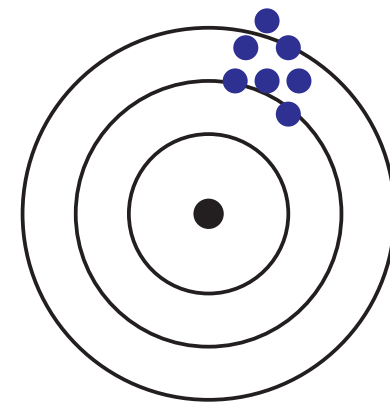
1 tick = 0.1 ms

## Problems:

- Not very stable
- Very slow ticking
- Reproducibility

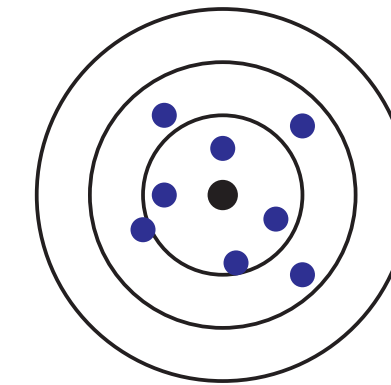
# What is a good clock ?

Stable



repeat with the same clock lots of measurements and get similar results

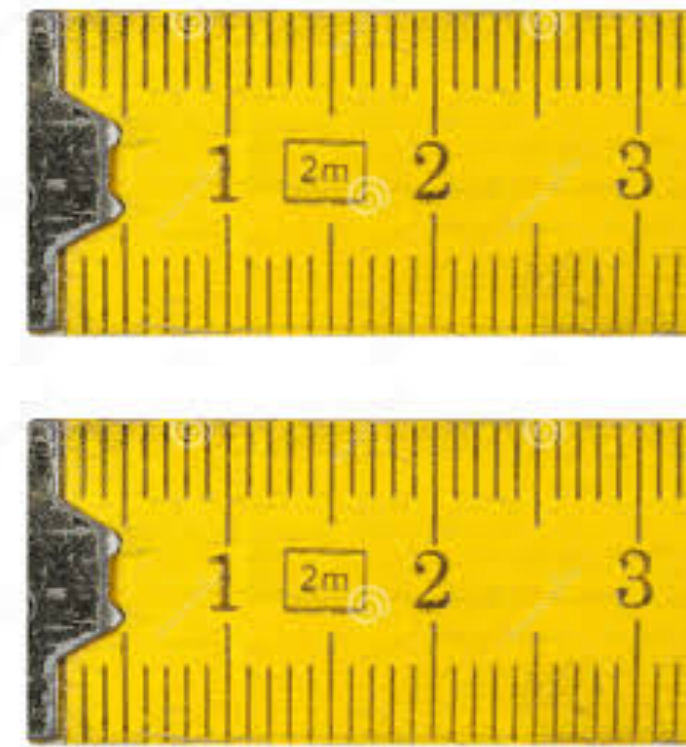
Precise



build several clocks and obtain same results

most of the time much, much harder to estimate

# Characterization of clocks



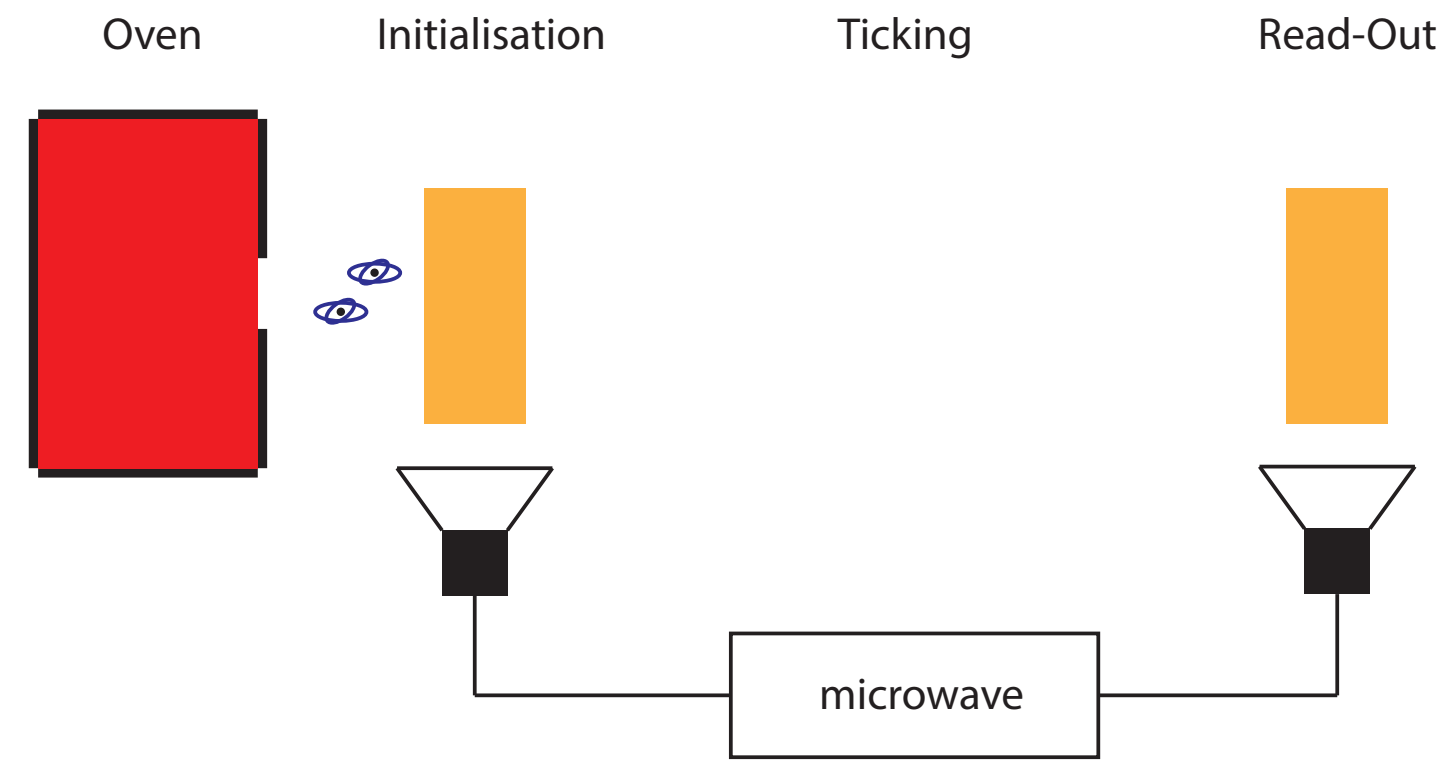
let them tick for a long time

compare the result

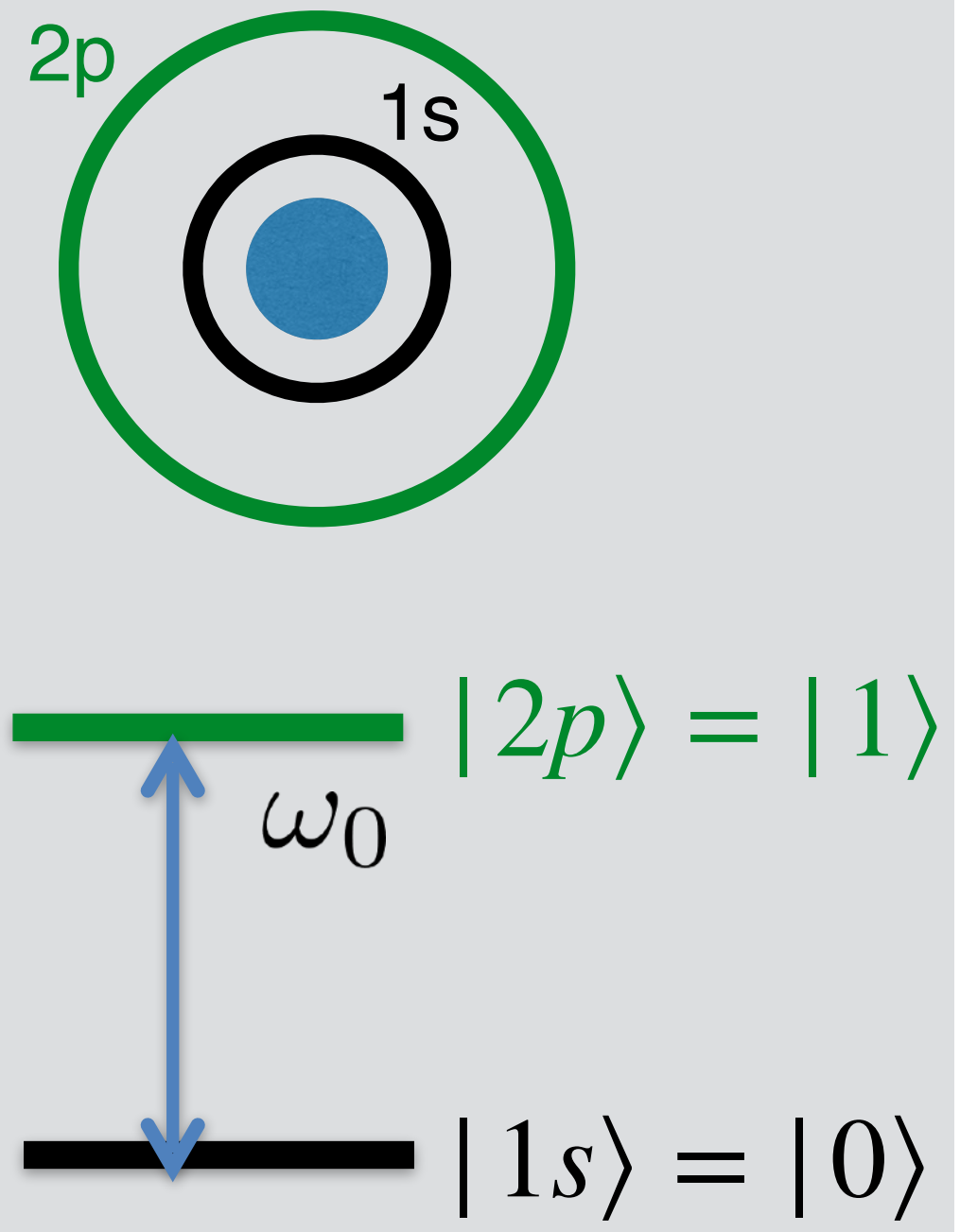
What about precision?

**We need a good standard and atoms give this**

# Atomic clocks

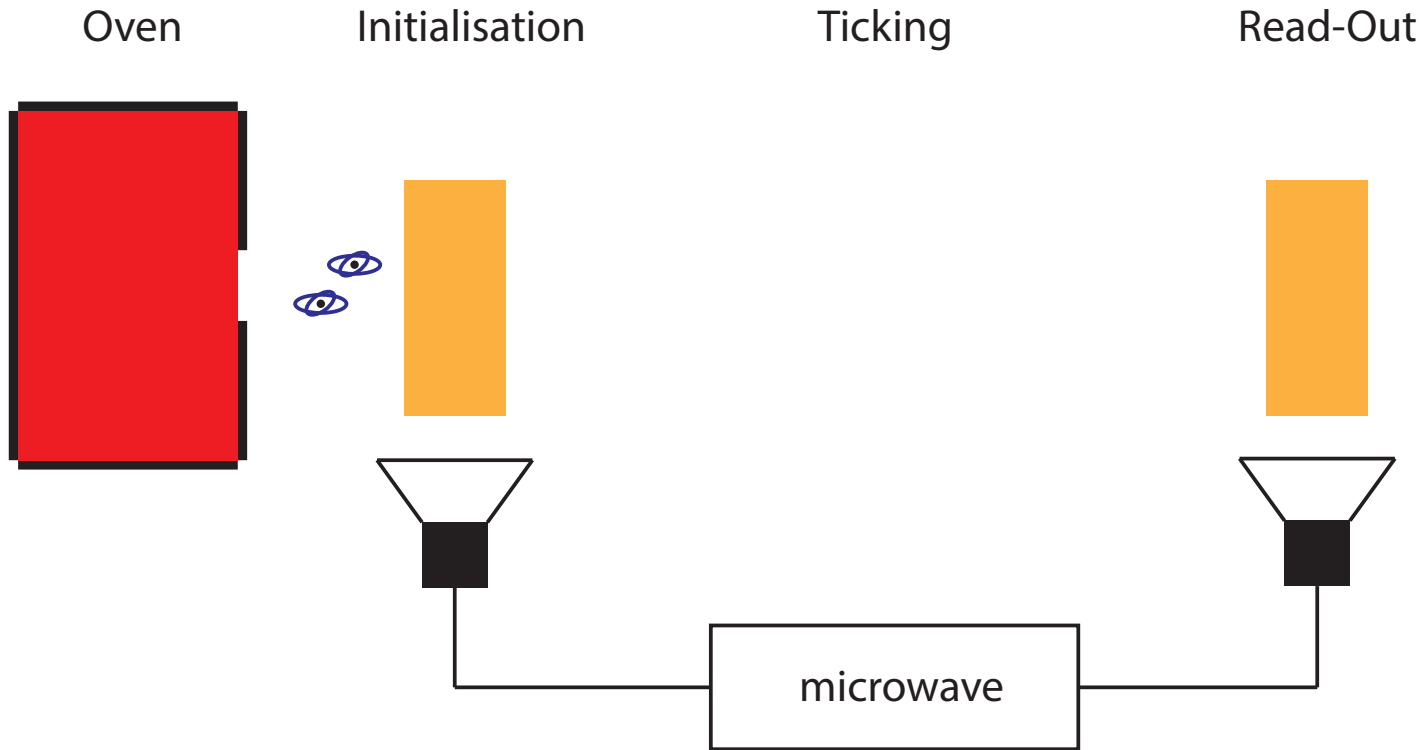


## The Atom



$$\mathcal{H} = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$$

# Atomic clocks



**The Atom**

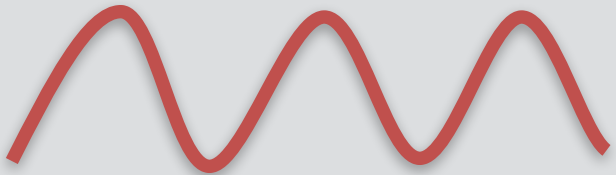
2p  
1s

$|2p\rangle = |1\rangle$   
 $\omega_0$   
 $|1s\rangle = |0\rangle$

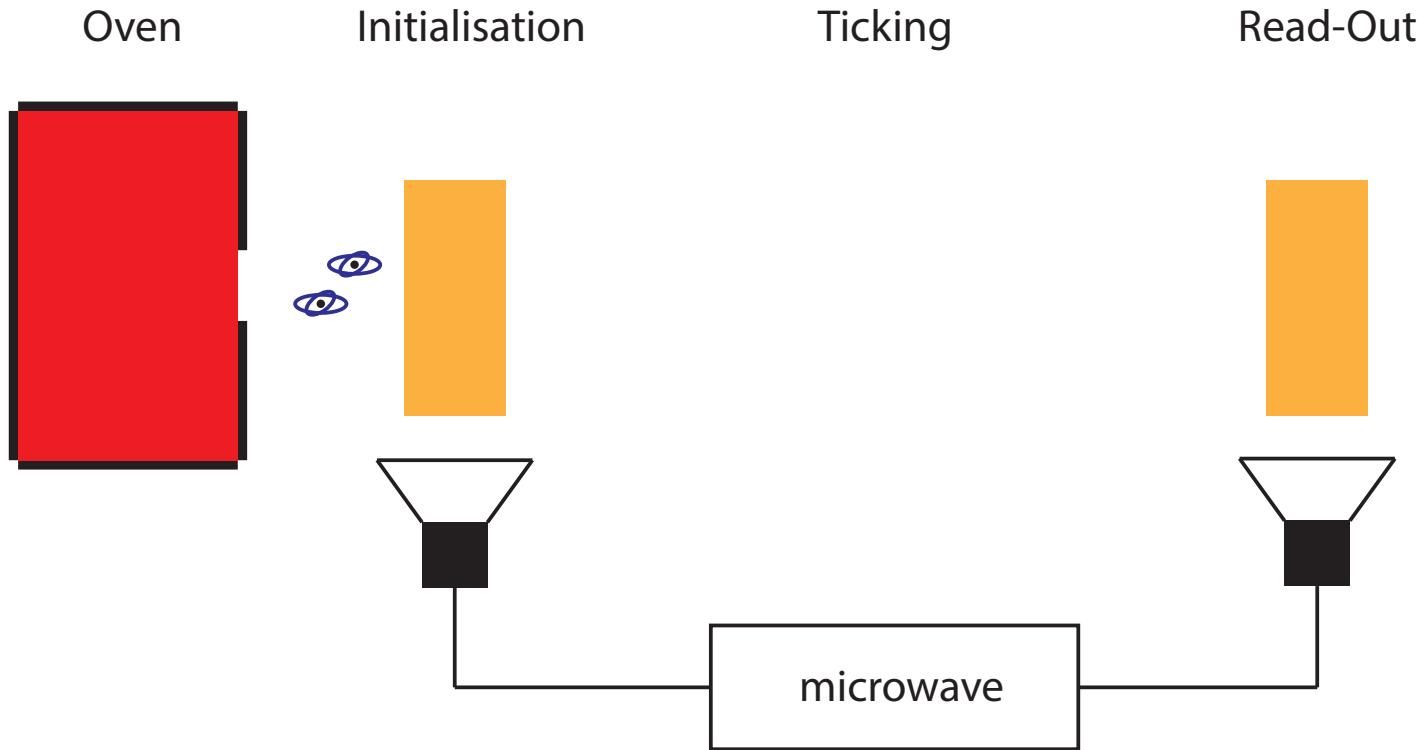
$\mathcal{H} = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$

**The electric field**

$$\mathbf{E} = E_0 (e^{i\omega_L t + i\varphi} + e^{-i\omega_L t - i\varphi})$$



# Atomic clocks

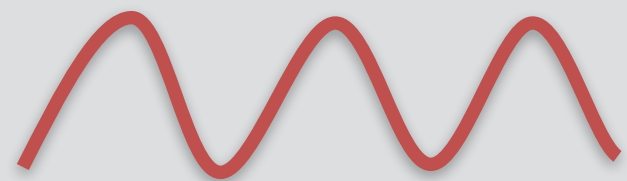


The Atom

$\mathcal{H} = E_0|0\rangle\langle 0| + E_1|1\rangle\langle 1|$

The electric field

$$\mathbf{E} = E_0 (e^{i\omega_L t + i\varphi} + e^{-i\omega_L t - i\varphi})$$



Interaction via

$$\mathcal{H} = -\mathbf{d} \cdot \mathbf{E}$$

$$\mathbf{d} = d (|0\rangle\langle 1| + |1\rangle\langle 0|)$$

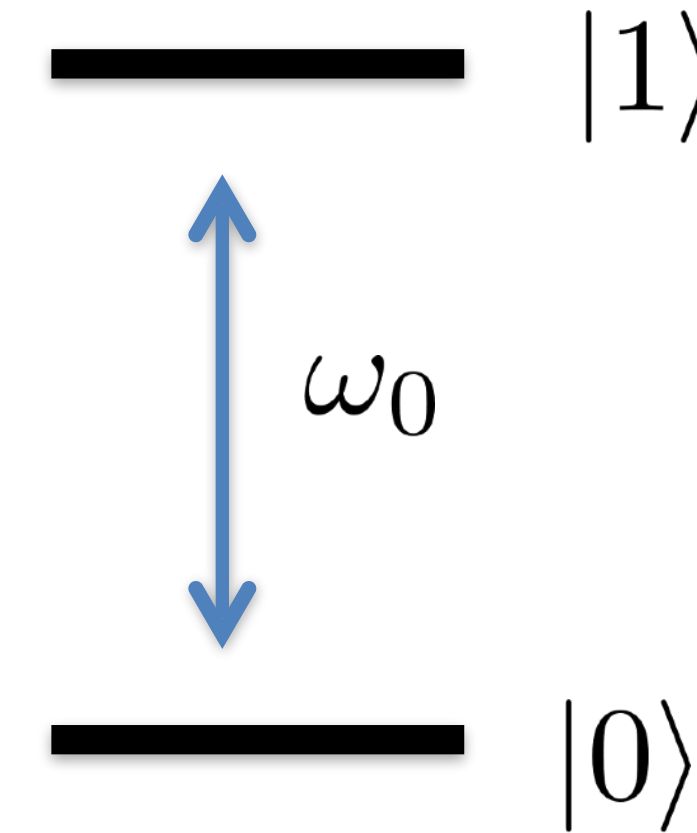
# The atom as a qubit

$$\mathcal{H} = E_0 |0\rangle \langle 0| + E_1 |1\rangle \langle 1|$$

$$\mathcal{H} = \frac{\hbar\omega_0}{2} |1\rangle \langle 1| - \frac{\hbar\omega_0}{2} |0\rangle \langle 0|$$

$$\mathcal{H} = \frac{\hbar\omega_0}{2} \sigma_z$$

→ write everything in terms of spins



$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

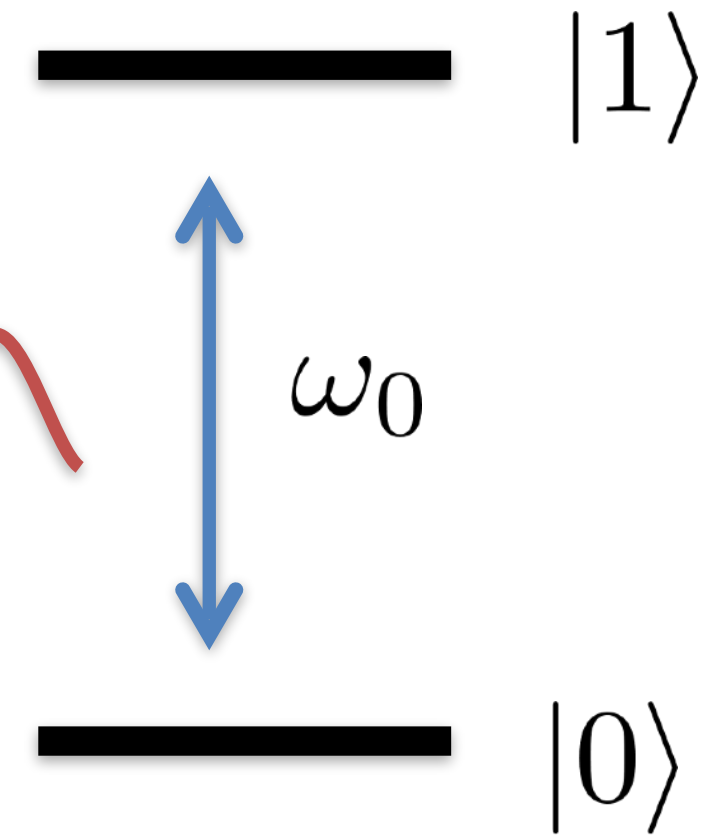


# Interaction Hamiltonian

$$\mathcal{H} = -\mathbf{d} \cdot \mathbf{E}$$

$$\mathbf{E} = E(e^{i\omega t + i\varphi} + e^{-i\omega t - i\varphi})$$

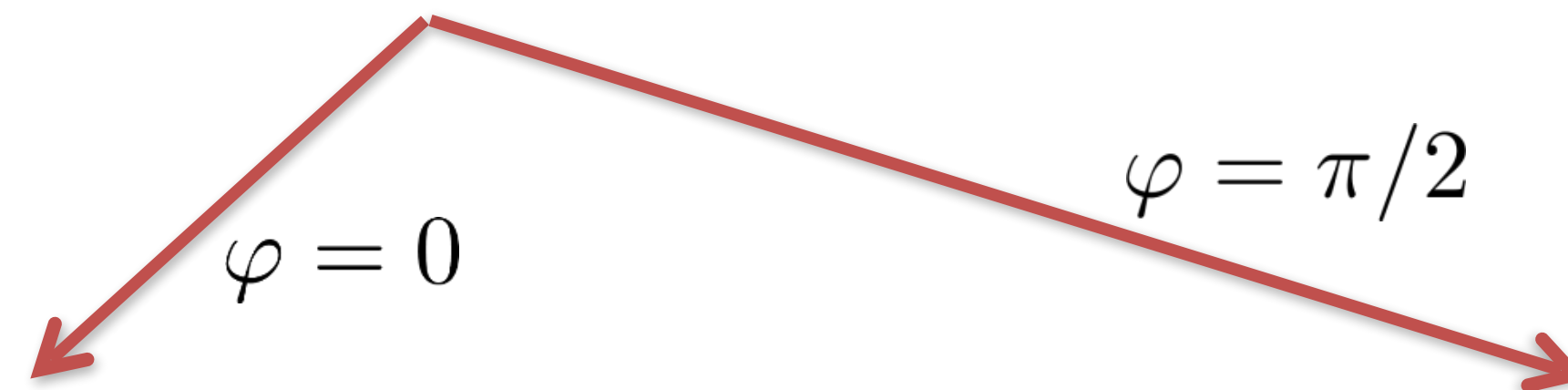
$$\mathbf{d} = d(\sigma_+ + \sigma_-)$$



Rotating frame:

$$\mathcal{H} = \frac{dE}{2}(\sigma_+ e^{i\varphi} + \sigma_- e^{-i\varphi})$$

$$\mathcal{H} \sim \hbar\Omega(\sigma_+ e^{i\varphi} + \sigma_- e^{-i\varphi})$$



$$\mathcal{H} \sim \hbar\Omega(\sigma_+ + \sigma_-)$$

$$\mathcal{H} \sim \hbar\Omega(\sigma_+ - \sigma_-)$$

$$\mathcal{H} \sim \hbar\Omega\sigma_x$$

$$\mathcal{H} \sim \hbar\Omega\sigma_y$$

# Clocks as extremely precise qubits

Rotation about z-axis  
Detuning

$$\mathcal{H} = \hbar\Delta\hat{\sigma}_z$$

Rotation about x-axis  
Laser intensity

$$\mathcal{H} = \hbar\Omega_x\hat{\sigma}_x$$

Rotation about y-axis  
Laser intensity with phase  
adjusted

$$\mathcal{H} = \hbar\Omega_y\hat{\sigma}_y$$

$$U = e^{i\mathcal{H}t/\hbar}$$

$Z_{\pi/2}$

$$\Delta t = \frac{\pi}{2}$$

$X_{\pi/2}$

$$\Omega_x t = \frac{\pi}{2}$$

$Y_{\pi/2}$

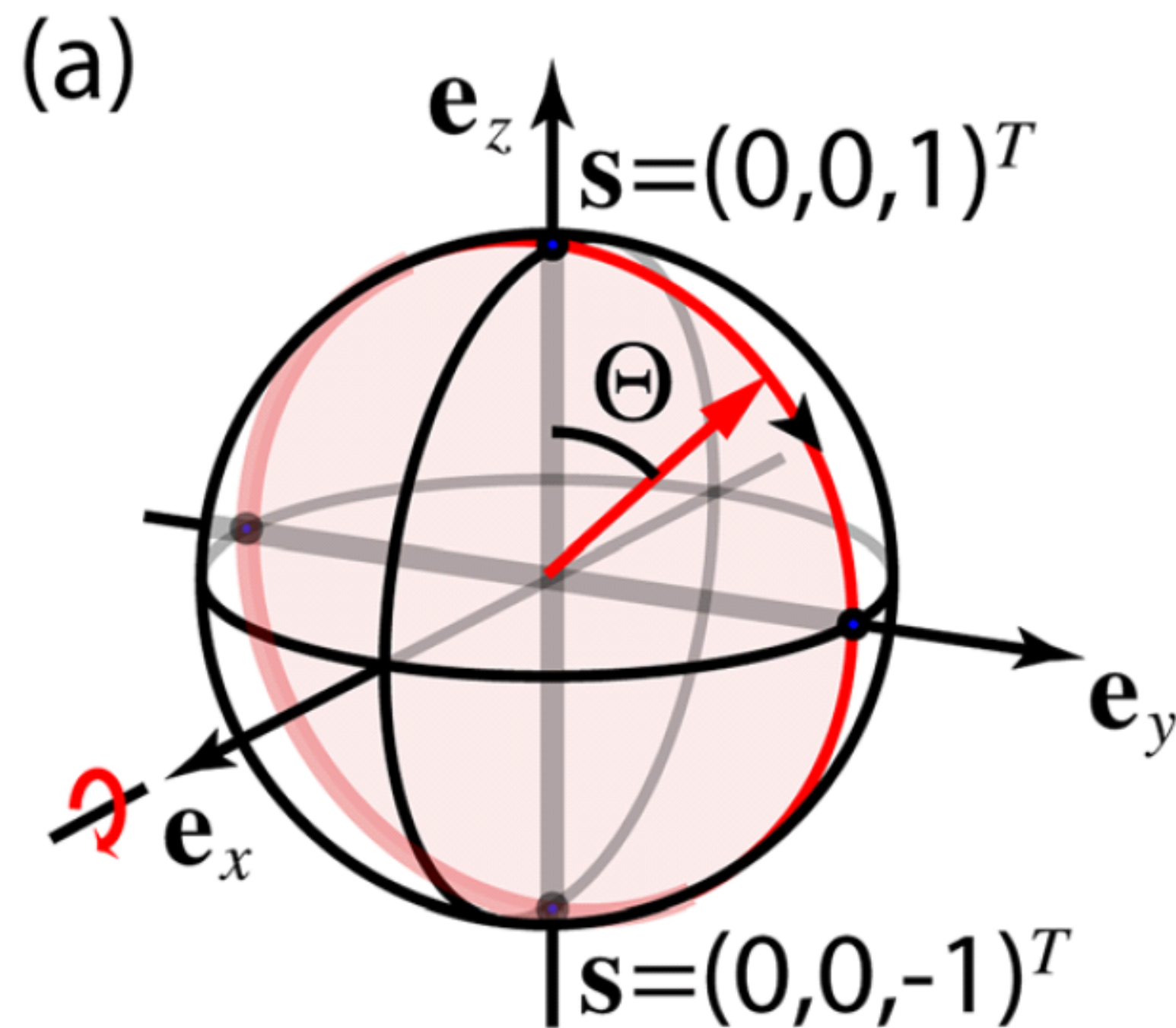
$$\Omega_y t = \frac{\pi}{2}$$

# Example: Rabi oscillations

$$\mathcal{H} = \hbar\Omega S_x$$

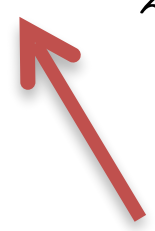
time evolution:  $e^{i\Omega\sigma_x t}$

Rotation about **x-axis** angle  $\Theta = \Omega t$

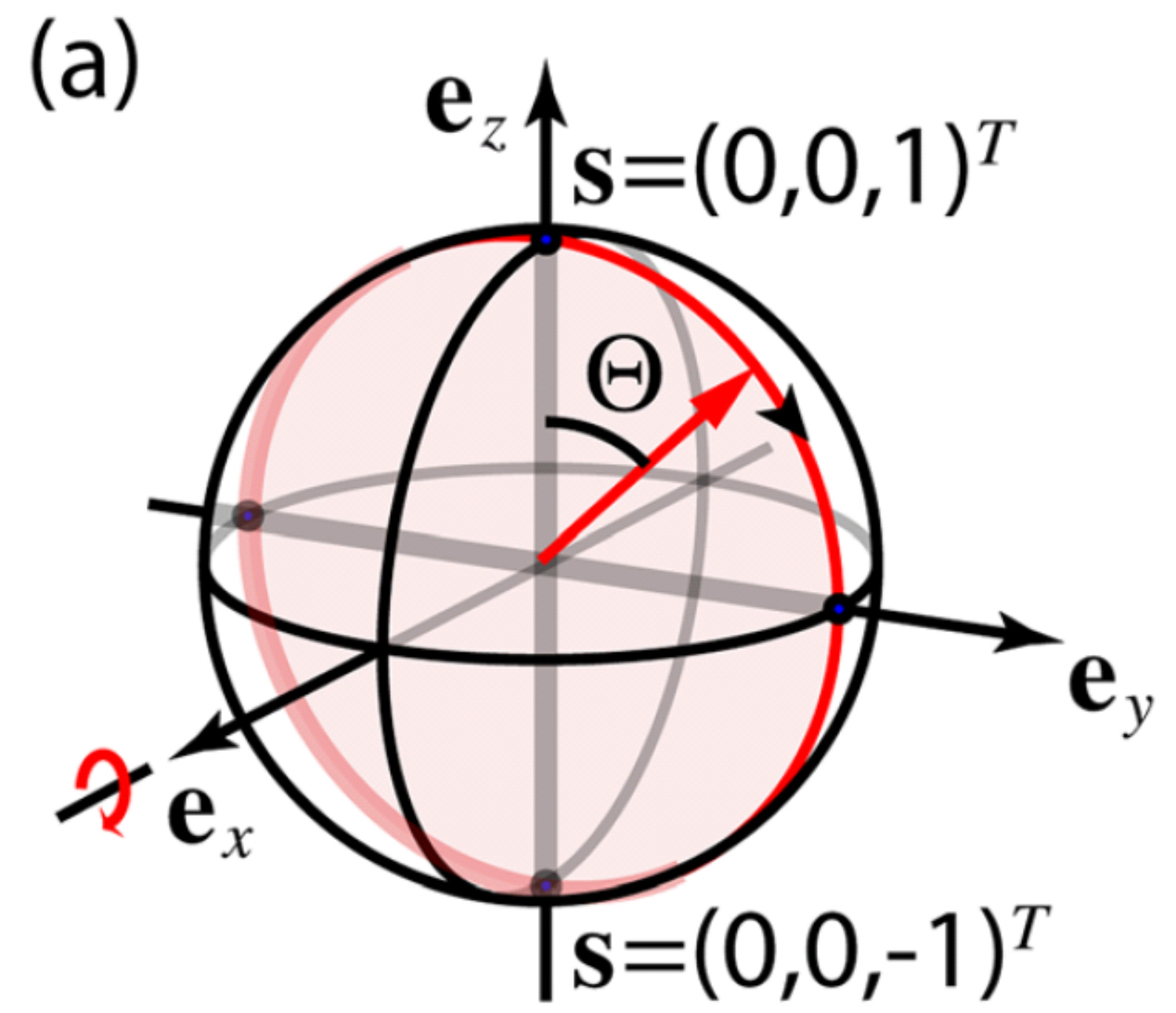
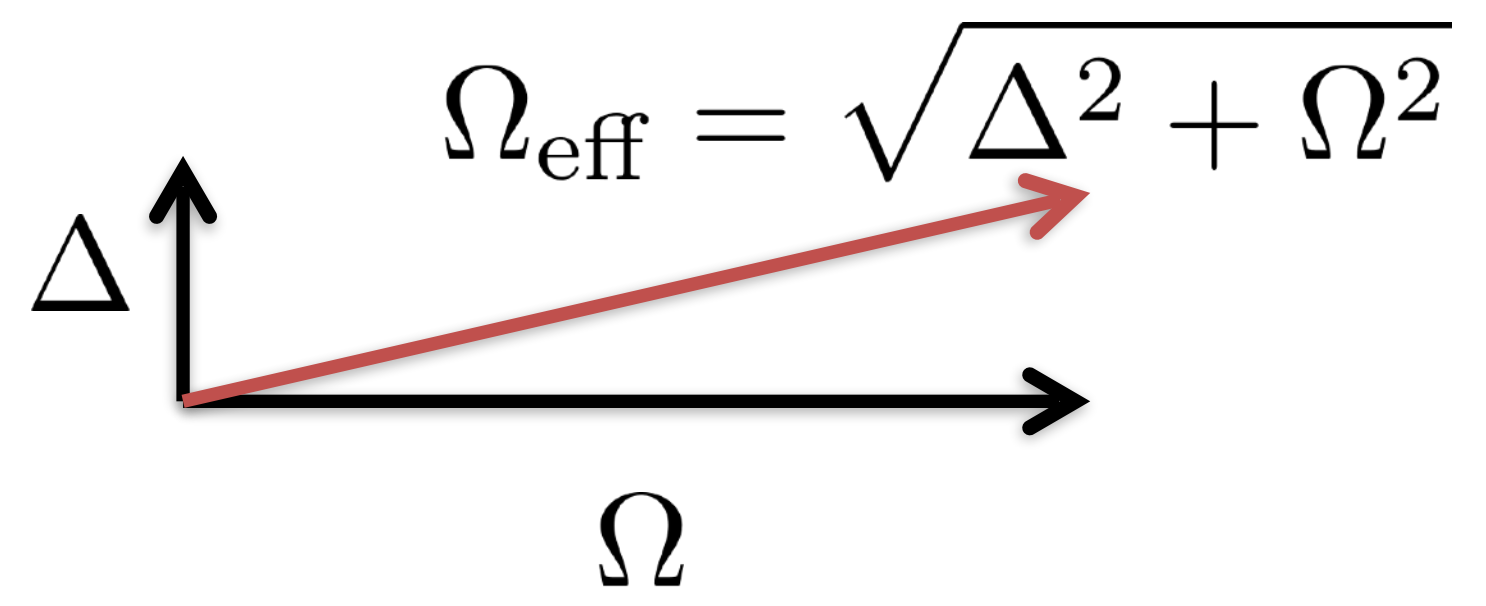


# Example: Offresonant Rabi oscillations

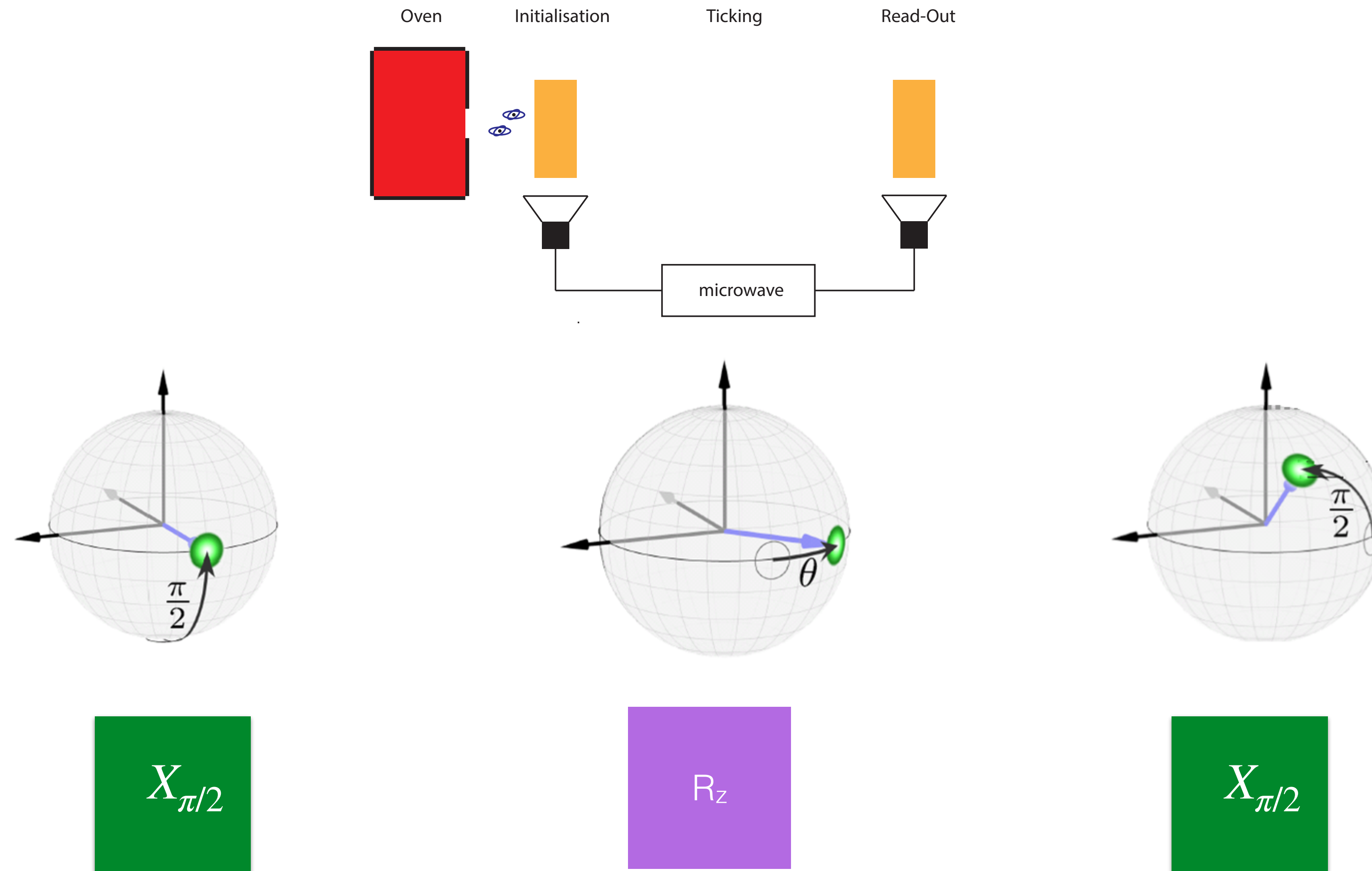
$$\mathcal{H} = \hbar\Omega S_x + \hbar\Delta S_z$$


  
**detuning**

tilted rotation axis  $J = \begin{pmatrix} \Omega \\ 0 \\ \Delta \end{pmatrix}$



# Back to our atomic clocks



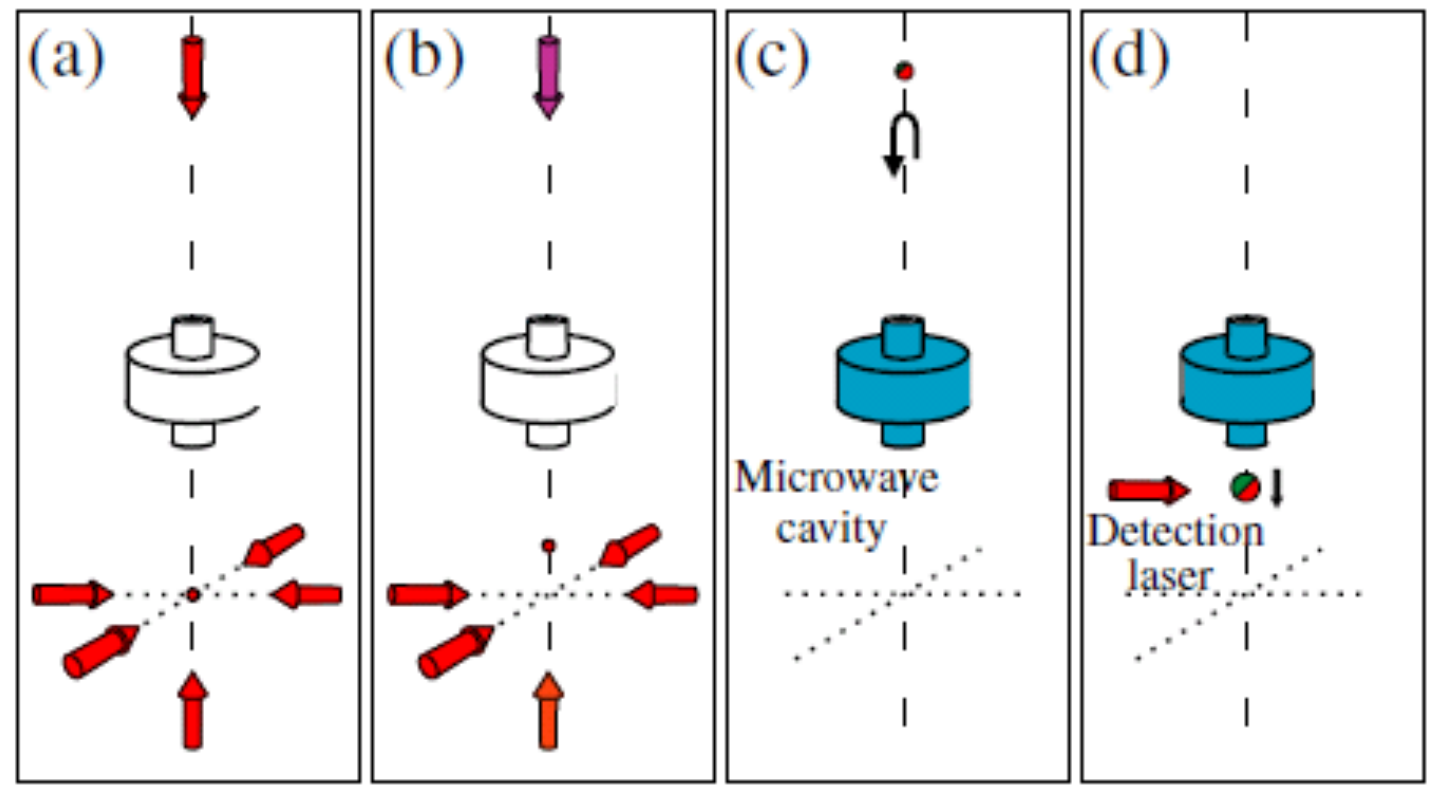
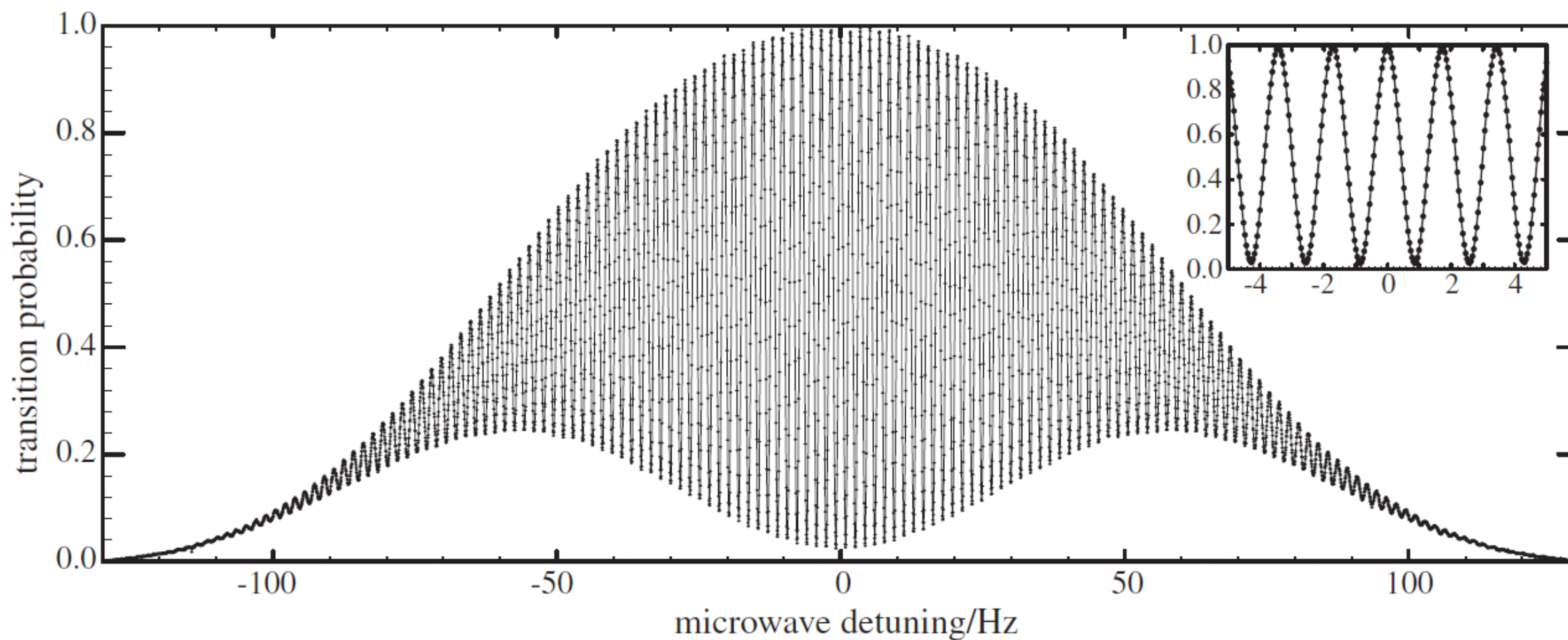
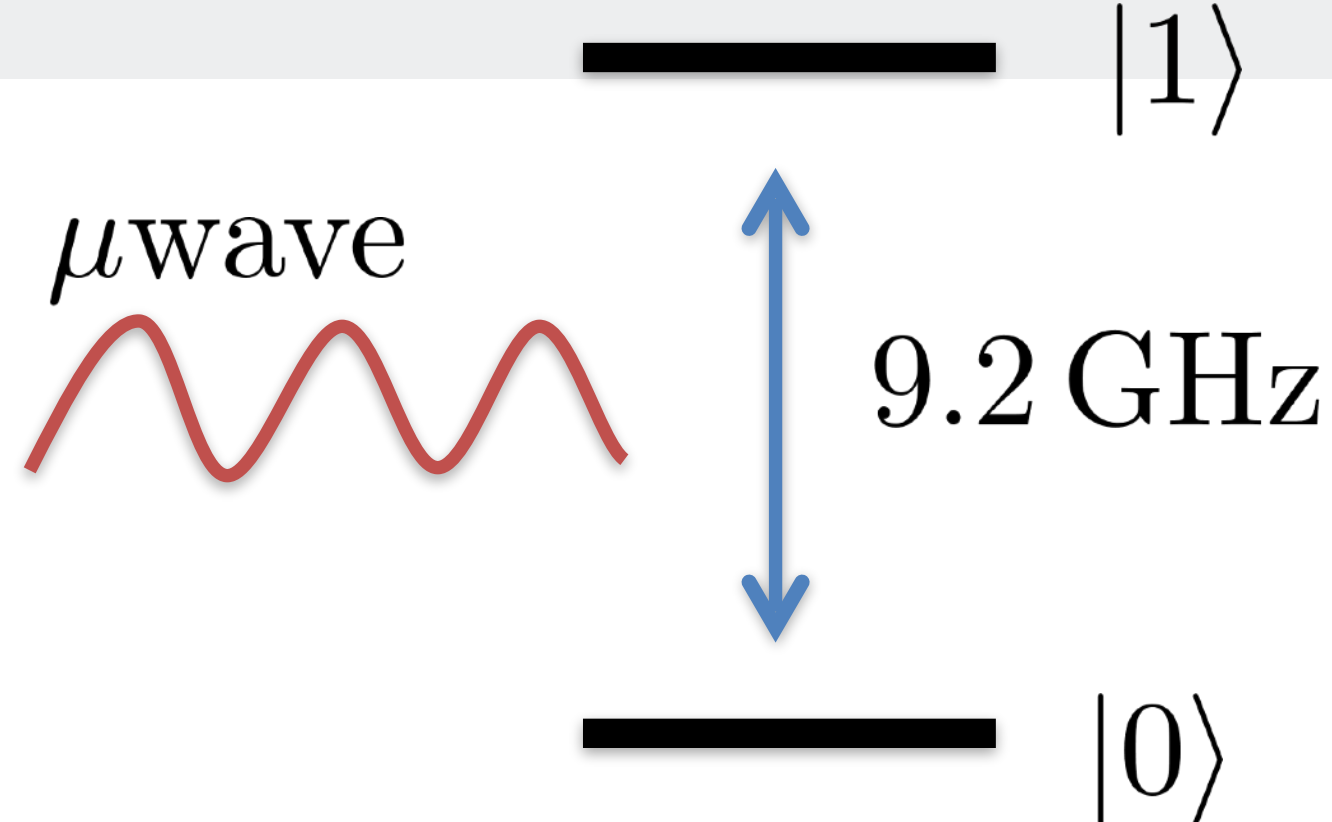
# Application: Time standard with Cesium fountain clock

$^{133}\text{Cs}$ : Hyperfine splitting 9.2 GHz

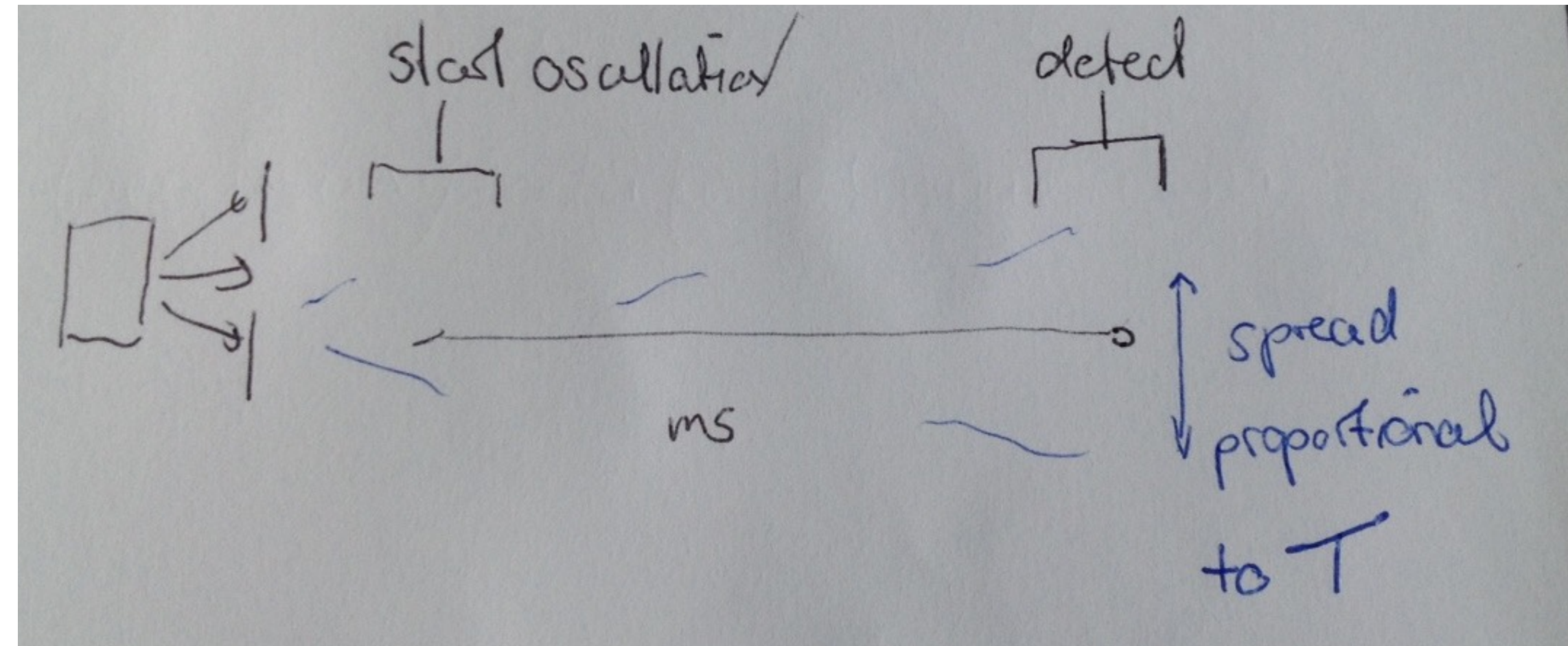
envelope  $\times \cos \Delta Et / \hbar$

$\Delta\omega \times \Delta t \geq 1$

$\rightarrow$  precision:  $\frac{\Delta\omega}{\omega} \times \frac{1}{\sqrt{N}} \approx 10^{-13}$

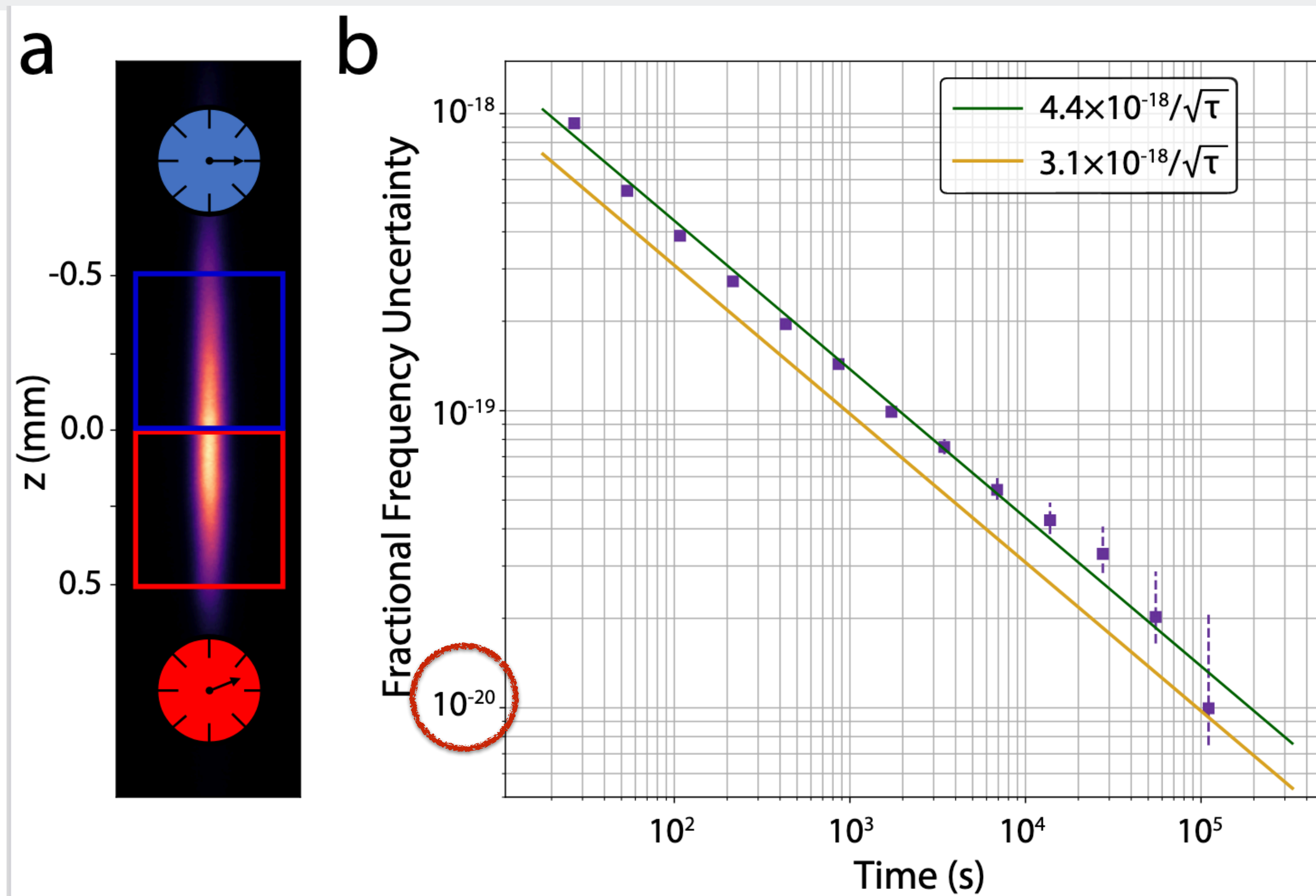


# Ramsey limitations



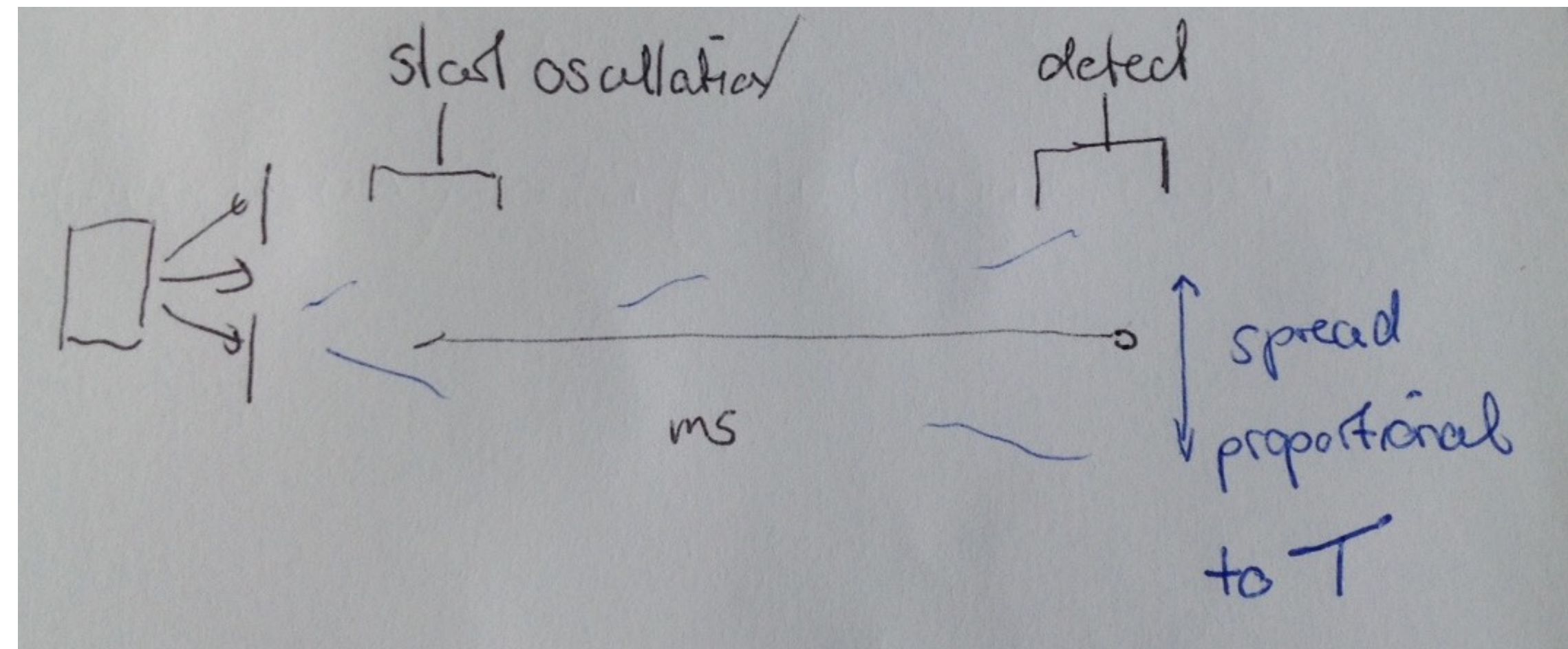
Detection better if atoms are slower

# Measuring the red-shift on the millimeter scale





# Ramsey limitations



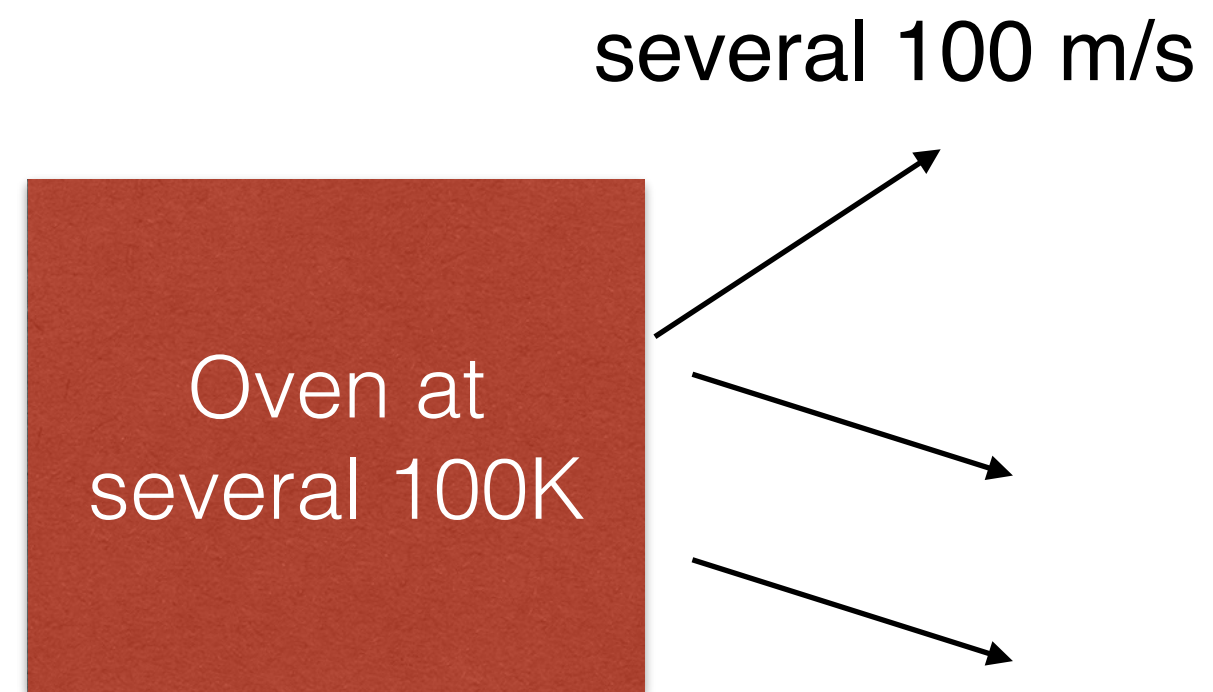
Detection better if atoms are slower

- We know how to perform qubit operation.
- How can we cool these atoms ?
- How can we trap them individually ?

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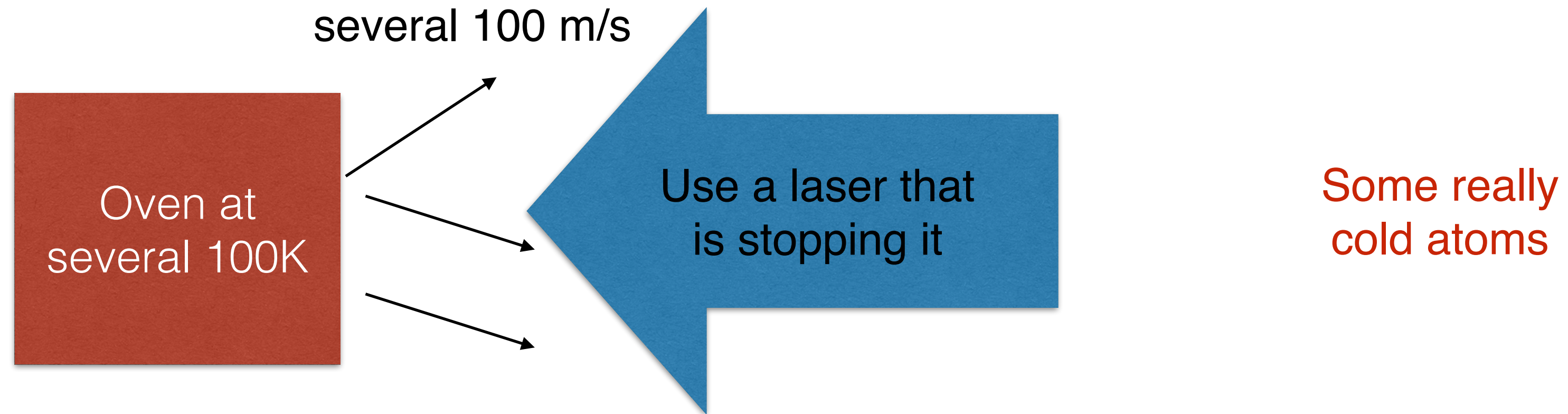
# The idea of laser cooling

How to stop the atoms?



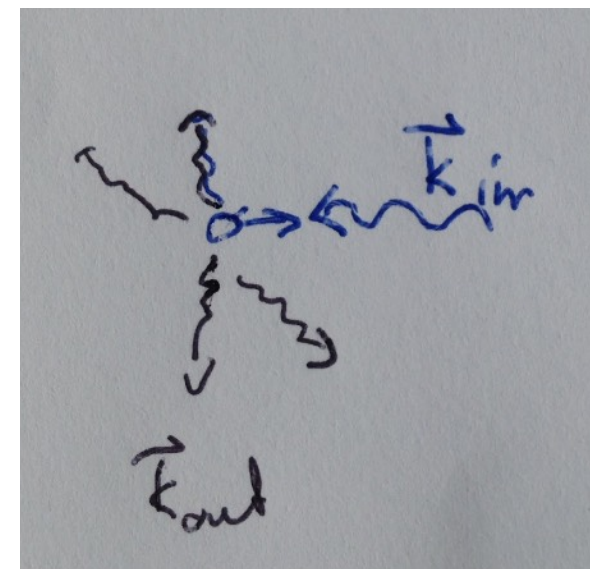
# The idea of laser cooling

How to stop the atoms?

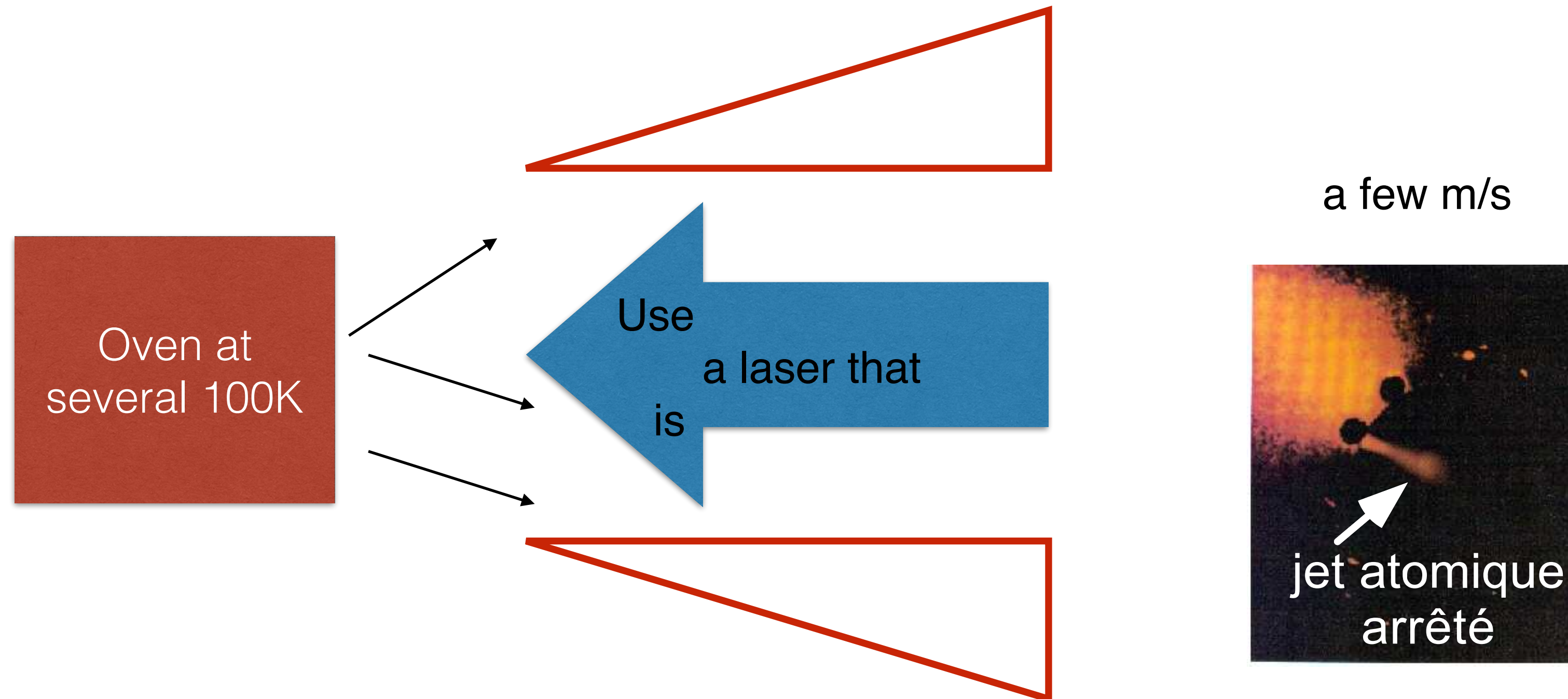


Idea of Laser cooling by Wineland, Dehmelt, Hänsch and Schawlow (1975)

Microscopic idea of radiation pressure



# The Zeeman slower



VOLUME 48, NUMBER 9

PHYSICAL REVIEW LETTERS

1 MARCH 1982

## Laser Deceleration of an Atomic Beam

William D. Phillips and Harold Metcalf<sup>(a)</sup>

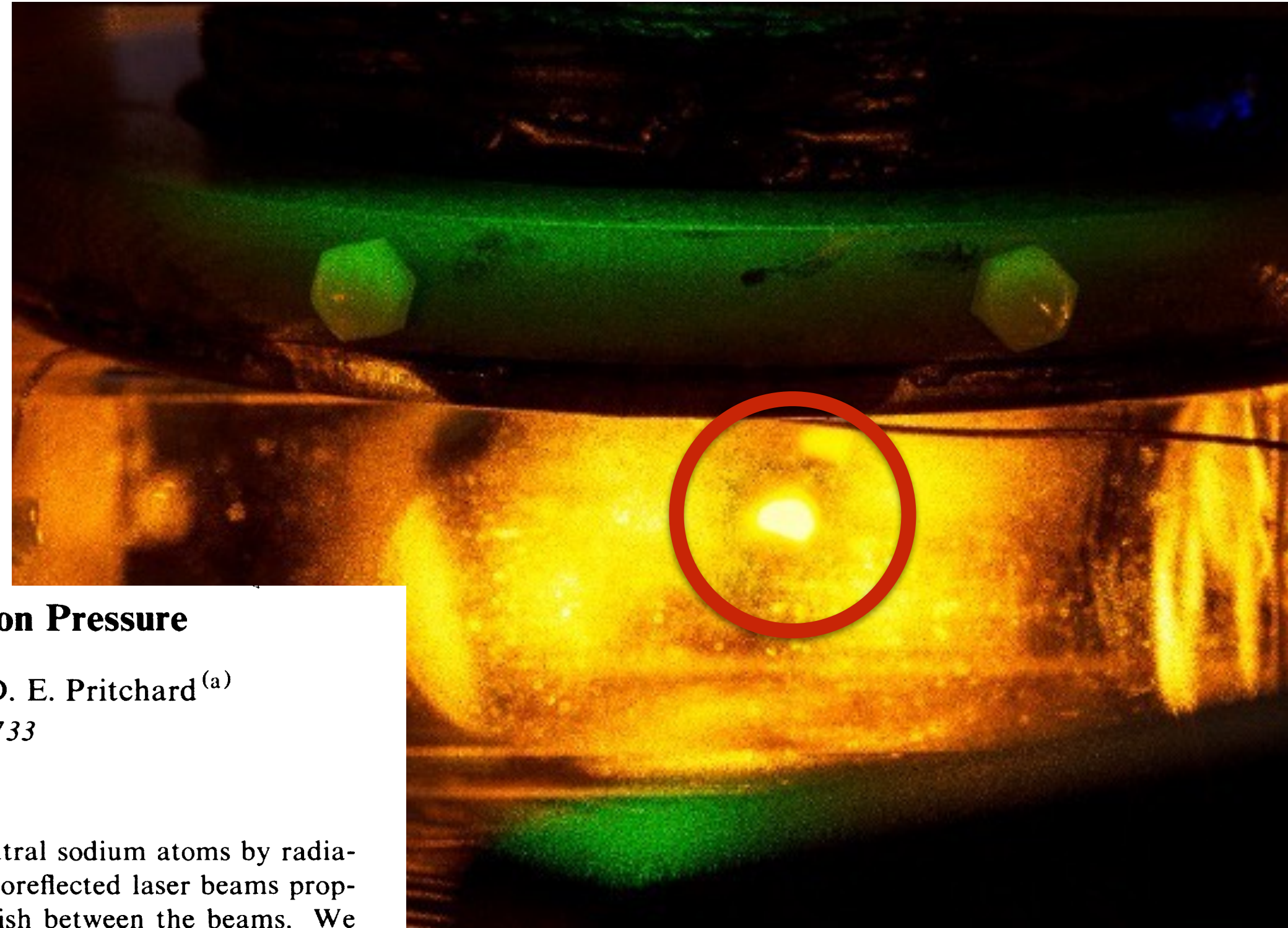
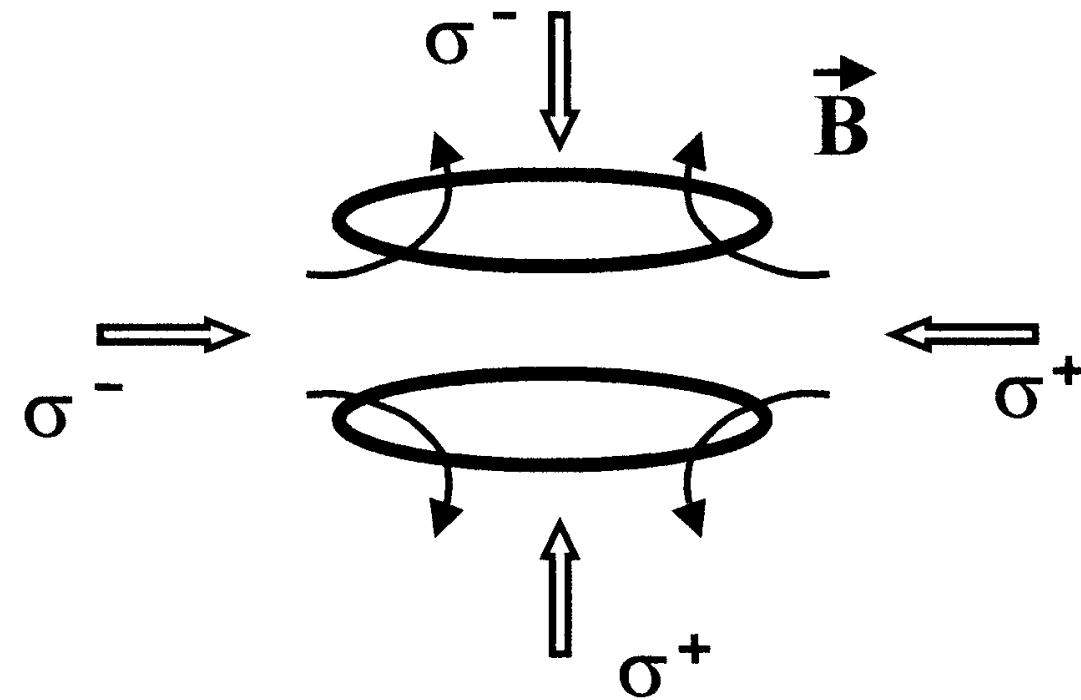
*Electrical Measurements and Standards Division Center for Absolute Physical Quantities,  
National Bureau of Standards, Washington, D. C. 20234*

(Received 23 December 1981)

Deceleration and velocity bunching of Na atoms in an atomic beam have been observed. The deceleration, caused by absorption of counterpropagating resonant laser light, amounts to 40% of the initial thermal velocity, corresponding to about 15 000 absorptions. Atoms were kept in resonance with the laser by using a spatially varying magnetic field to provide a changing Zeeman shift to compensate for the changing Doppler shift as the atoms decelerated.

# The MOT

static magnetic fields + radiation pressure



## Trapping of Neutral Sodium Atoms with Radiation Pressure

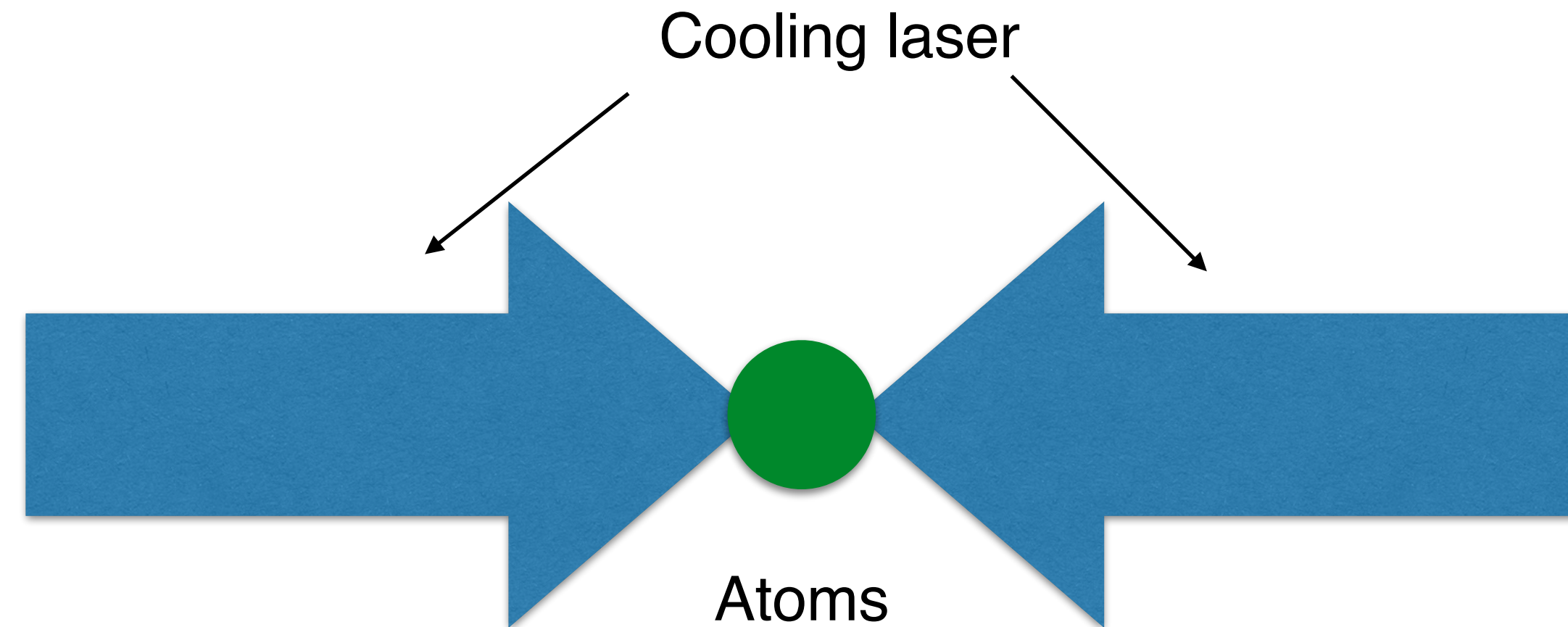
E. L. Raab,<sup>(a)</sup> M. Prentiss, Alex Cable, Steven Chu,<sup>(b)</sup> and D. E. Pritchard<sup>(a)</sup>

*AT&T Bell Laboratories, Holmdel, New Jersey 07733*

(Received 16 July 1987)

We report the confinement and cooling of an optically dense cloud of neutral sodium atoms by radiation pressure. The trapping and damping forces were provided by three retroreflected laser beams propagating along orthogonal axes, with a weak magnetic field used to distinguish between the beams. We have trapped as many as  $10^7$  atoms for 2 min at densities exceeding  $10^{11}$  atoms  $\text{cm}^{-3}$ . The trap was  $\approx 0.4$  K deep and the atoms, once trapped, were cooled to less than a millikelvin and compacted into a region less than 0.5 mm in diameter.

# Doppler Cooling/Optical Molasses



atoms undergo diffusive motion and feel 'friction' from collisions with laser

VOLUME 55, NUMBER 1

PHYSICAL REVIEW LETTERS

1 JULY 1985

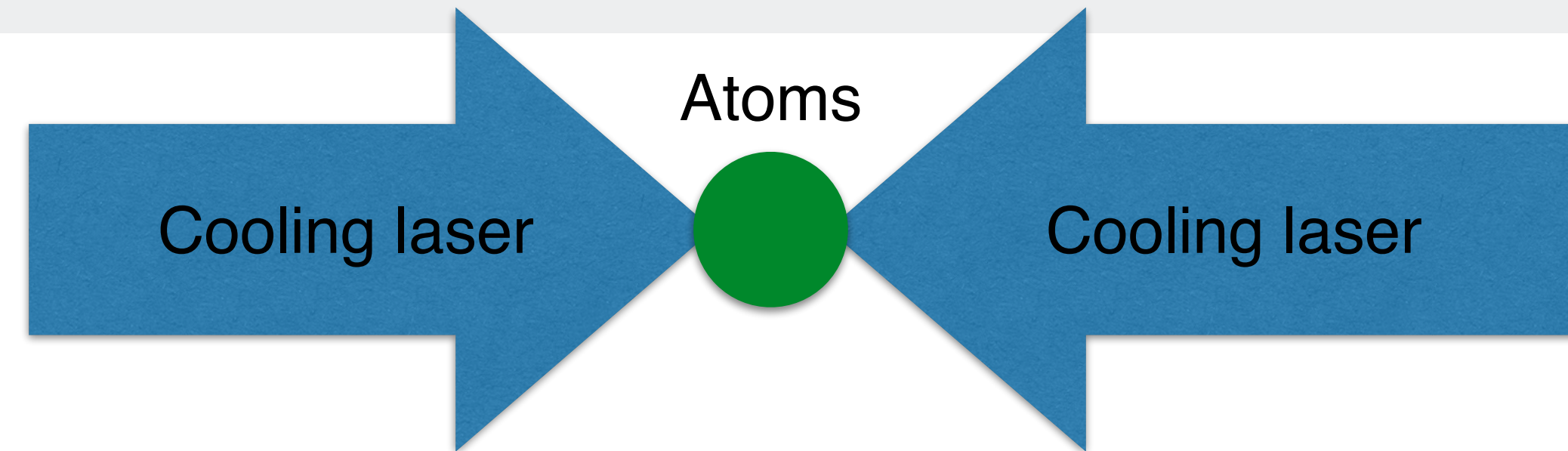
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## Three-Dimensional Viscous Confinement and Cooling of Atoms by Resonance Radiation Pressure

Steven Chu, L. Hollberg, J. E. Bjorkholm, Alex Cable, and A. Ashkin  
*AT&T Bell Laboratories, Holmdel, New Jersey 07733*  
(Received 25 April 1985)

We report the viscous confinement and cooling of neutral sodium atoms in three dimensions via the radiation pressure of counterpropagating laser beams. These atoms have a density of about  $\sim 10^6 \text{ cm}^{-3}$  and a temperature of  $\sim 240 \mu\text{K}$  corresponding to a rms velocity of  $\sim 60 \text{ cm/sec}$ . This temperature is approximately the quantum limit for this atomic transition. The decay time for half the atoms to escape a  $\sim 0.2\text{-cm}^3$  confinement volume is  $\sim 0.1 \text{ sec}$ .

# Doppler Cooling/Optical Molasses



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Doppler limit (lowest ,possible' temperature)  $T_D \approx 240 \mu\text{K}$

observed:  $T \approx 240_{-60}^{+200} \mu\text{K}$

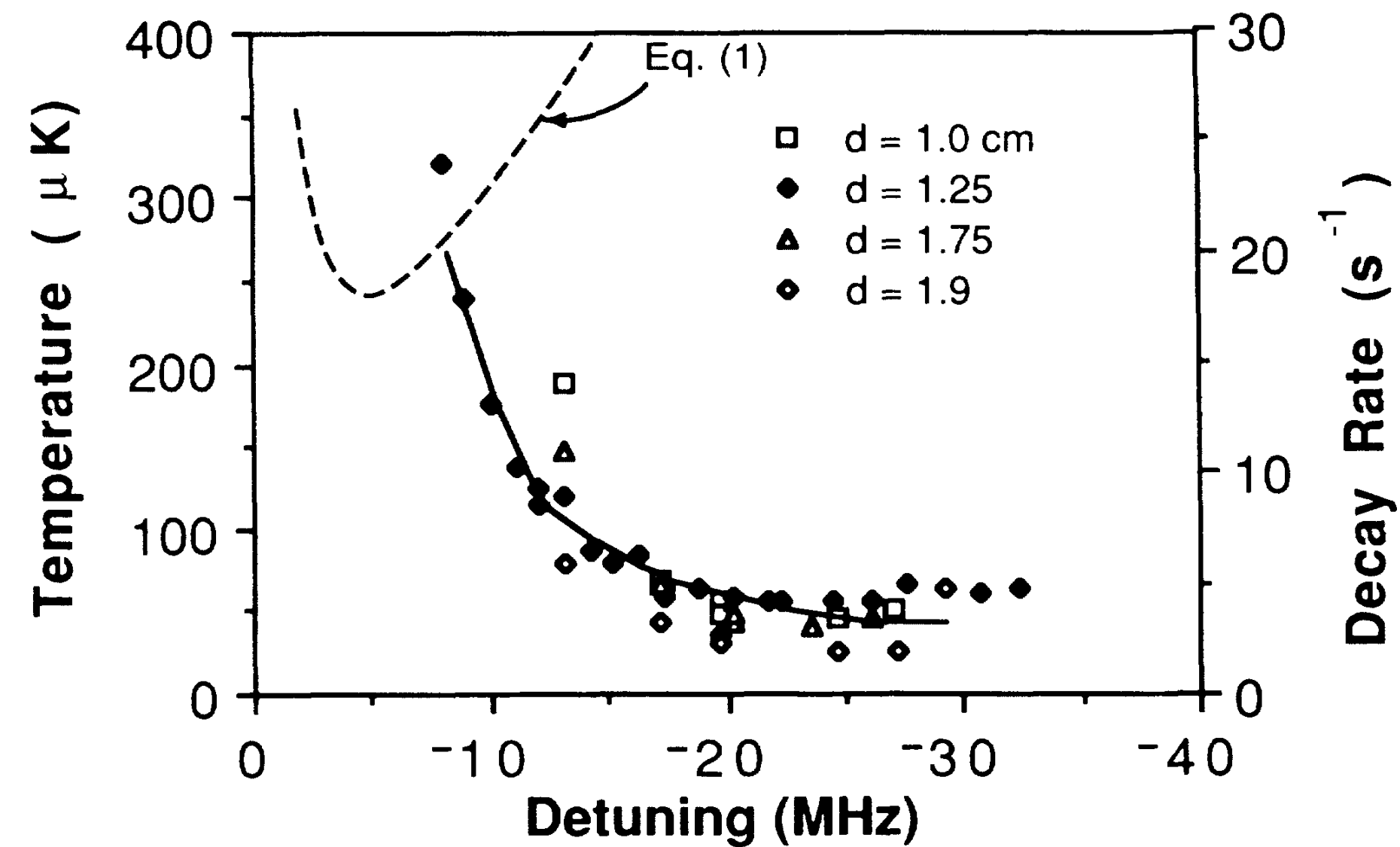


# The miracle of subdoppler cooling

## Comment by Steve Chu:

the molasses. This method allowed us to directly measure the velocity distribution. Our first measurements showed a temperature of  $185 \mu\text{K}$ , slightly lower than the minimum temperature allowed by the theory of Doppler cooling. We then made the cardinal mistake of experimental physics: instead of listening to Nature, we were overly influenced by theoretical expectations. By including a fudge factor to account for the way atoms filled the molasses region, we were able to bring our measurement into accord with our expectations.

## The result by the Phillips group:



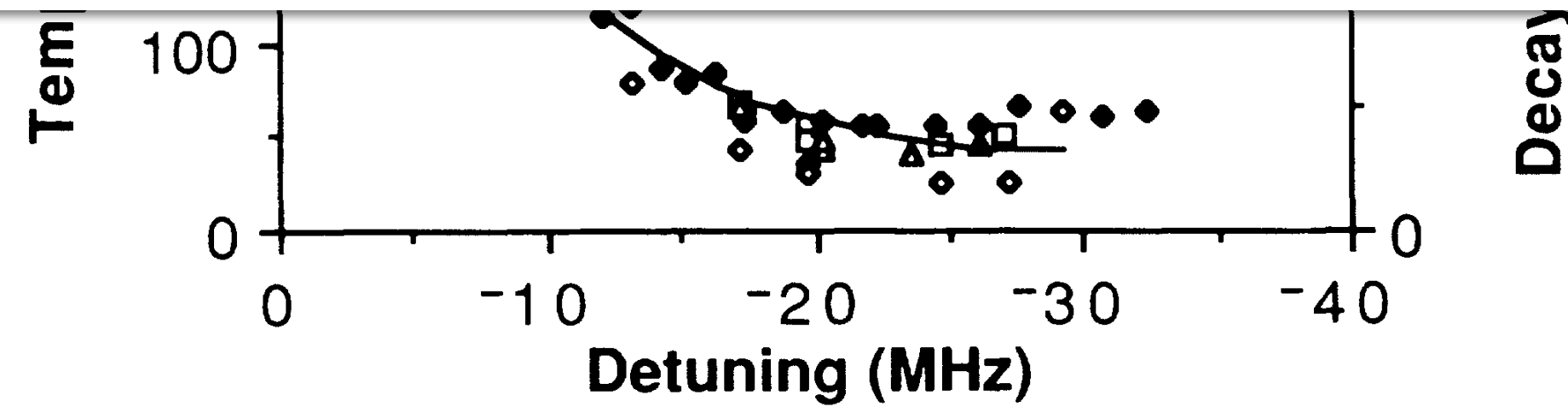
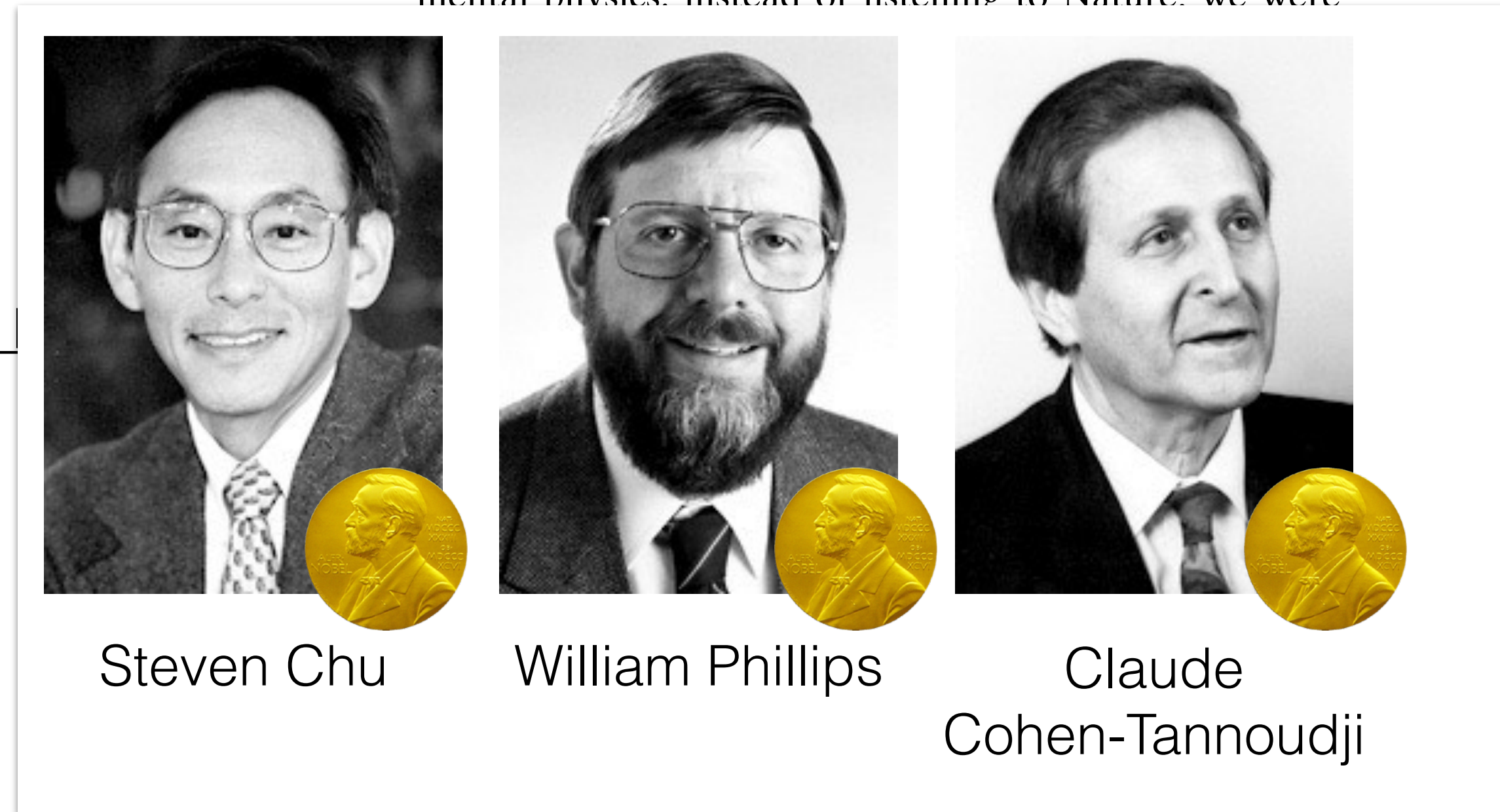
Lett *et al.* PRL **61** 169 (1988)

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Lett *et al.* PRL **61** 169 (1988)

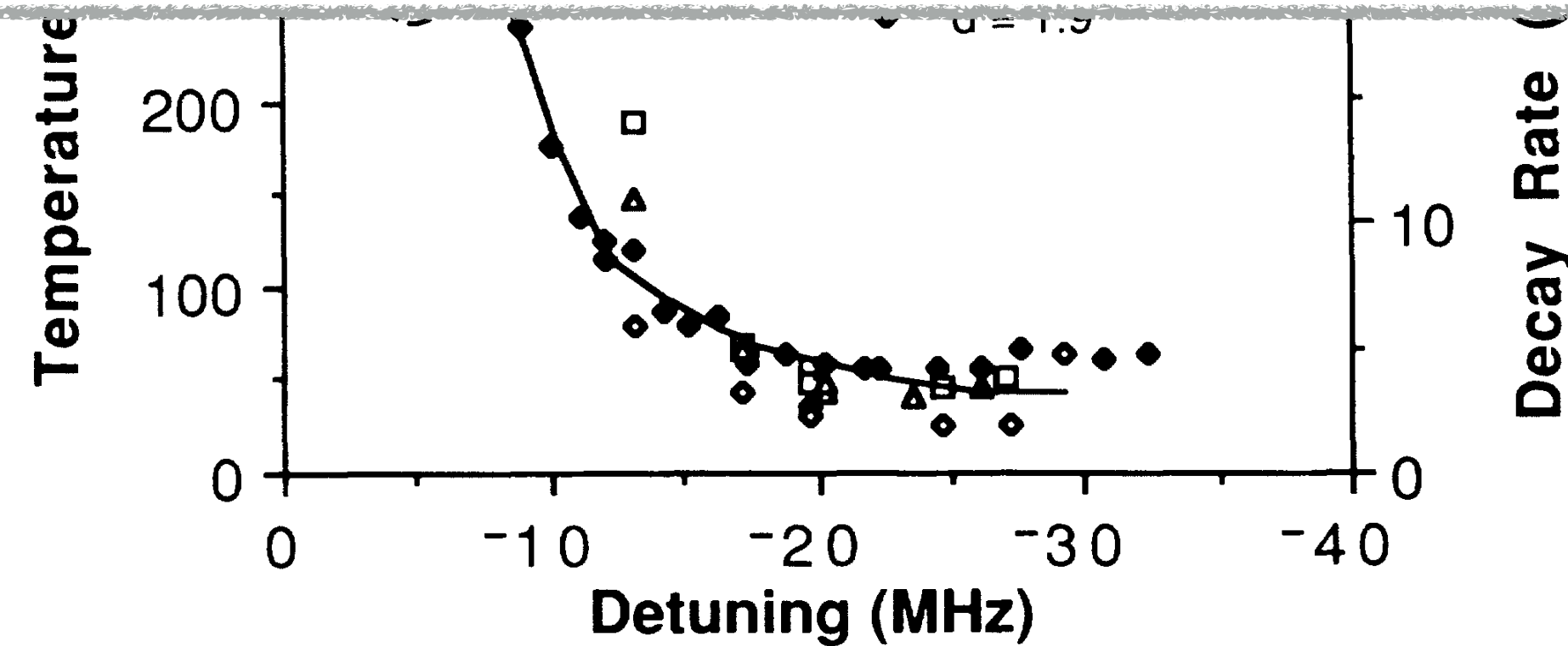
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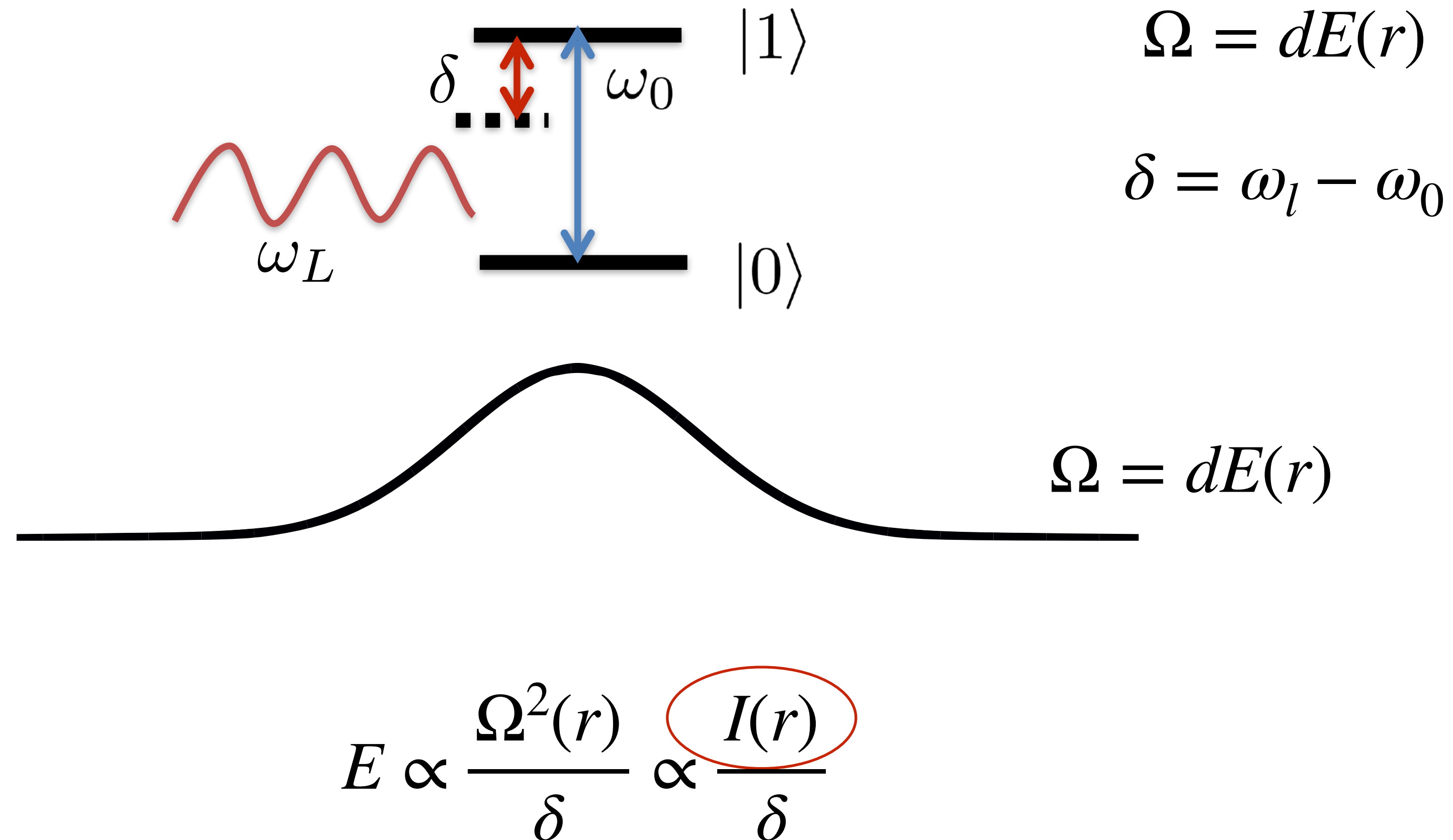
The result by

- We know how to perform qubit operation.
- Atoms are really cold.
- How can we trap them individually ?



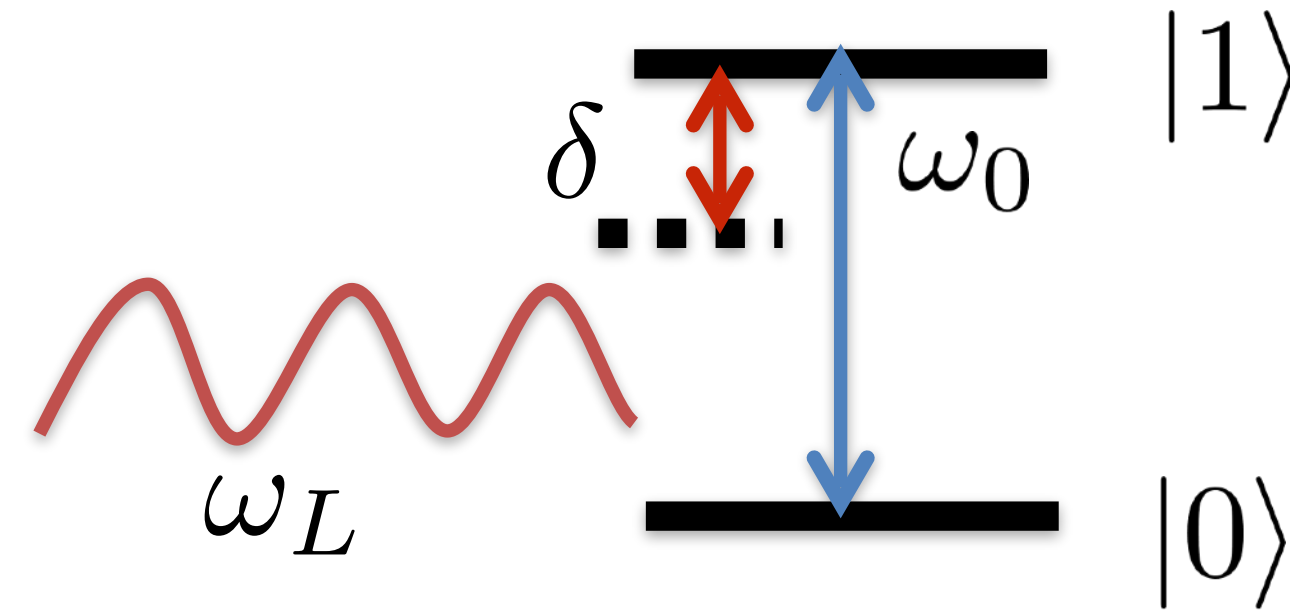
Lett *et al.* PRL **61** 169 (1988)

# The dipole potential - making optical tweezers



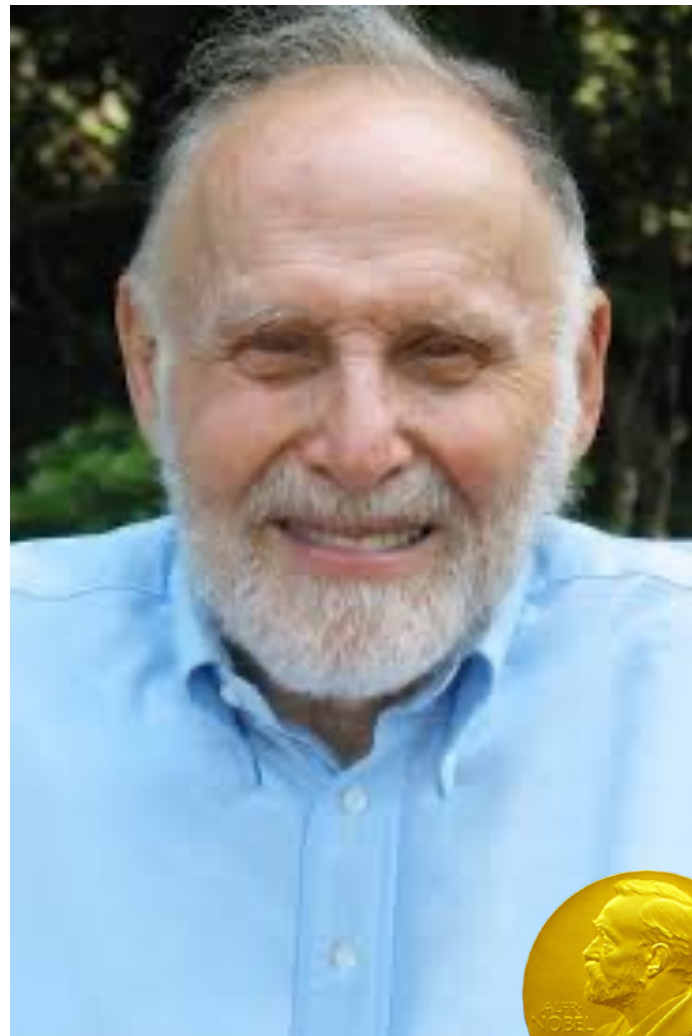
**The dipole potential is directly proportional to the intensity !**

# The dipole potential - making optical tweezers



$$\Omega = dE(r)$$

$$\delta = \omega_l - \omega_0$$

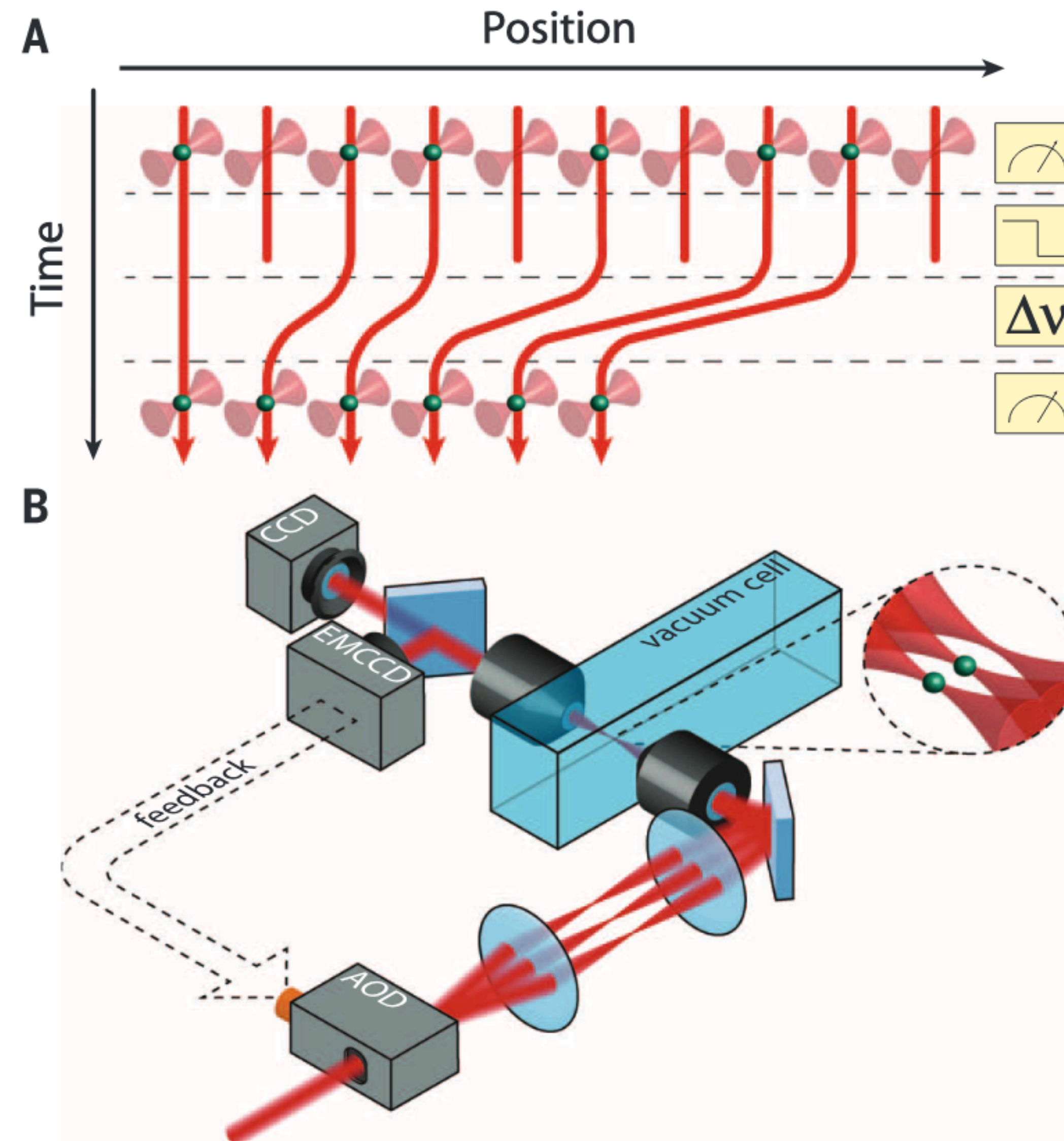


$$\Omega = dE(r)$$

$$E \propto \frac{\Omega^2(r)}{\delta} \propto \frac{I(r)}{\delta}$$

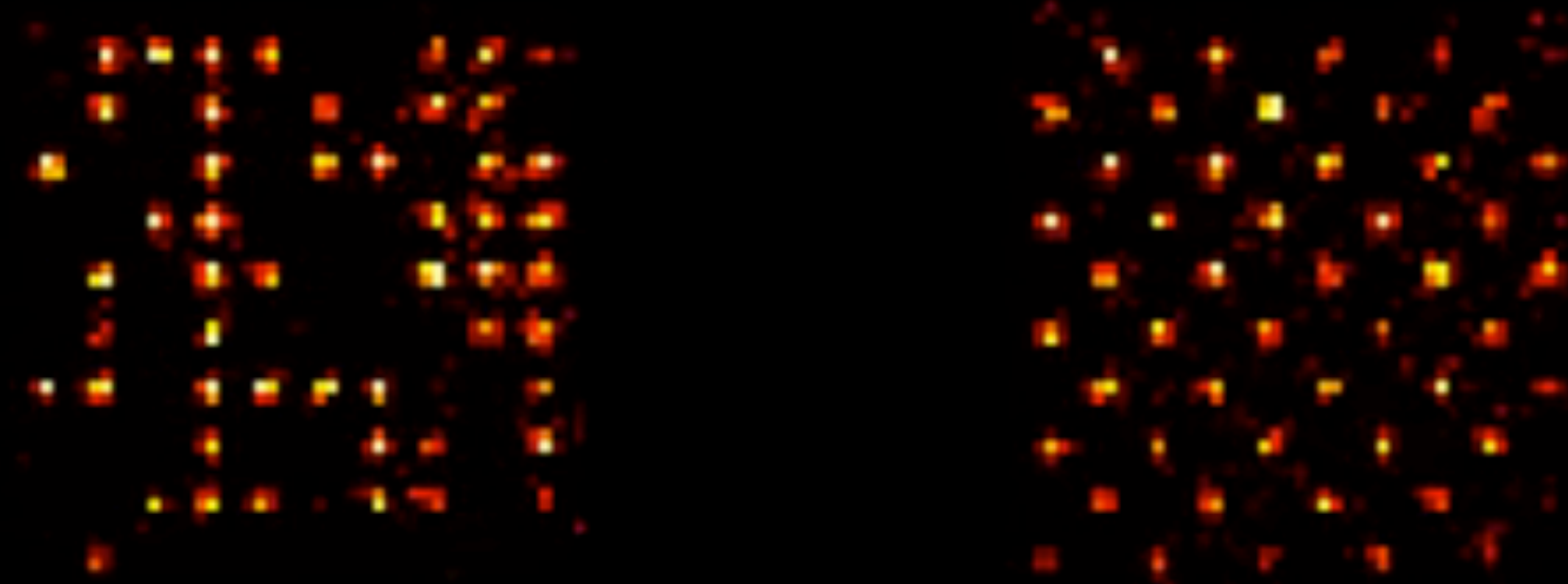
**The dipole potential is directly proportional to the intensity !**

# Tweezers and atom sorting



# Tweezers and atom sorting

An atom-by-atom assembler  
of defect-free arbitrary 2d atomic arrays



Daniel Barredo, Sylvain de Léséleuc, Vincent Lienhard,  
Thierry Lahaye, Antoine Browaeys

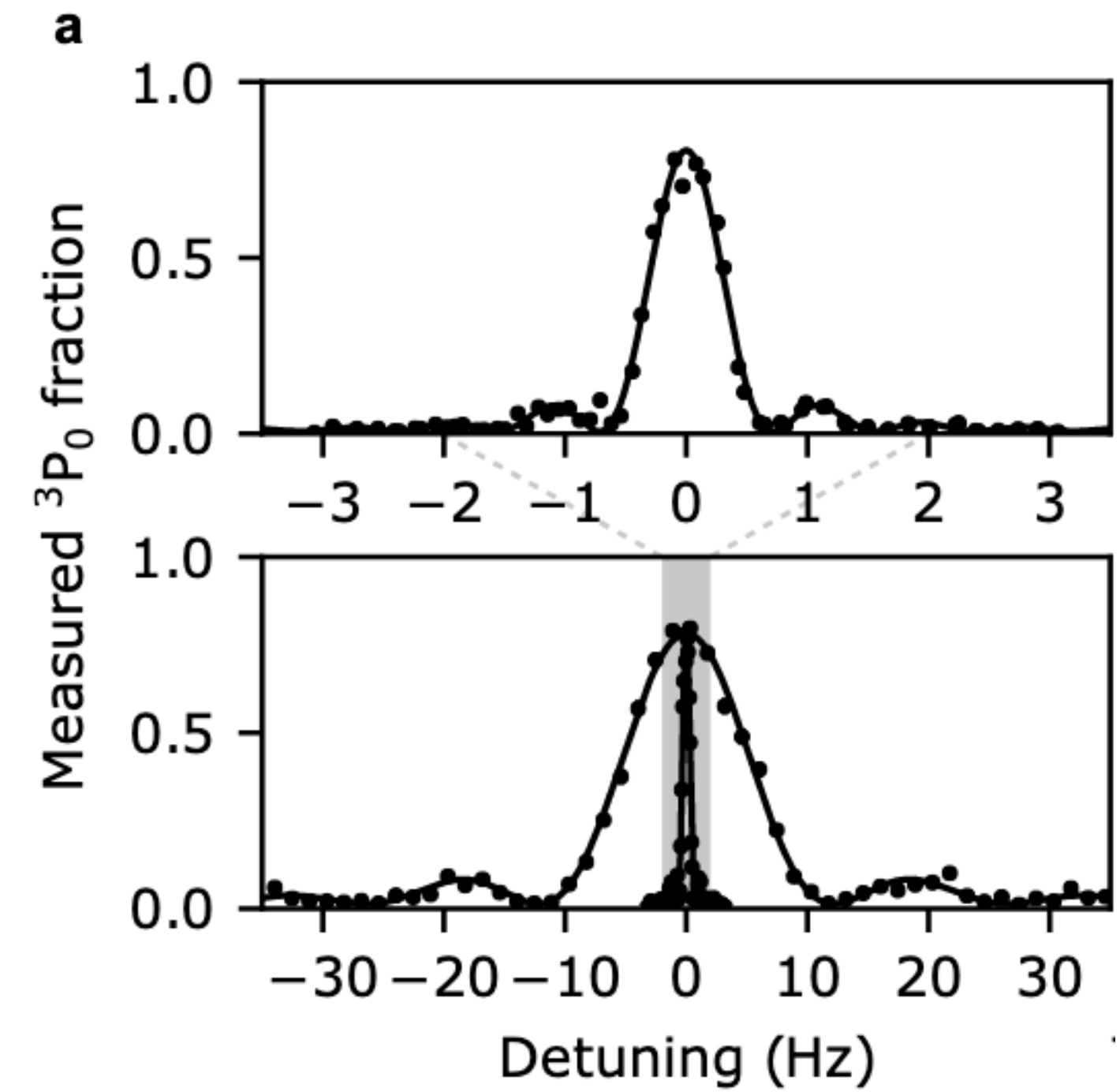
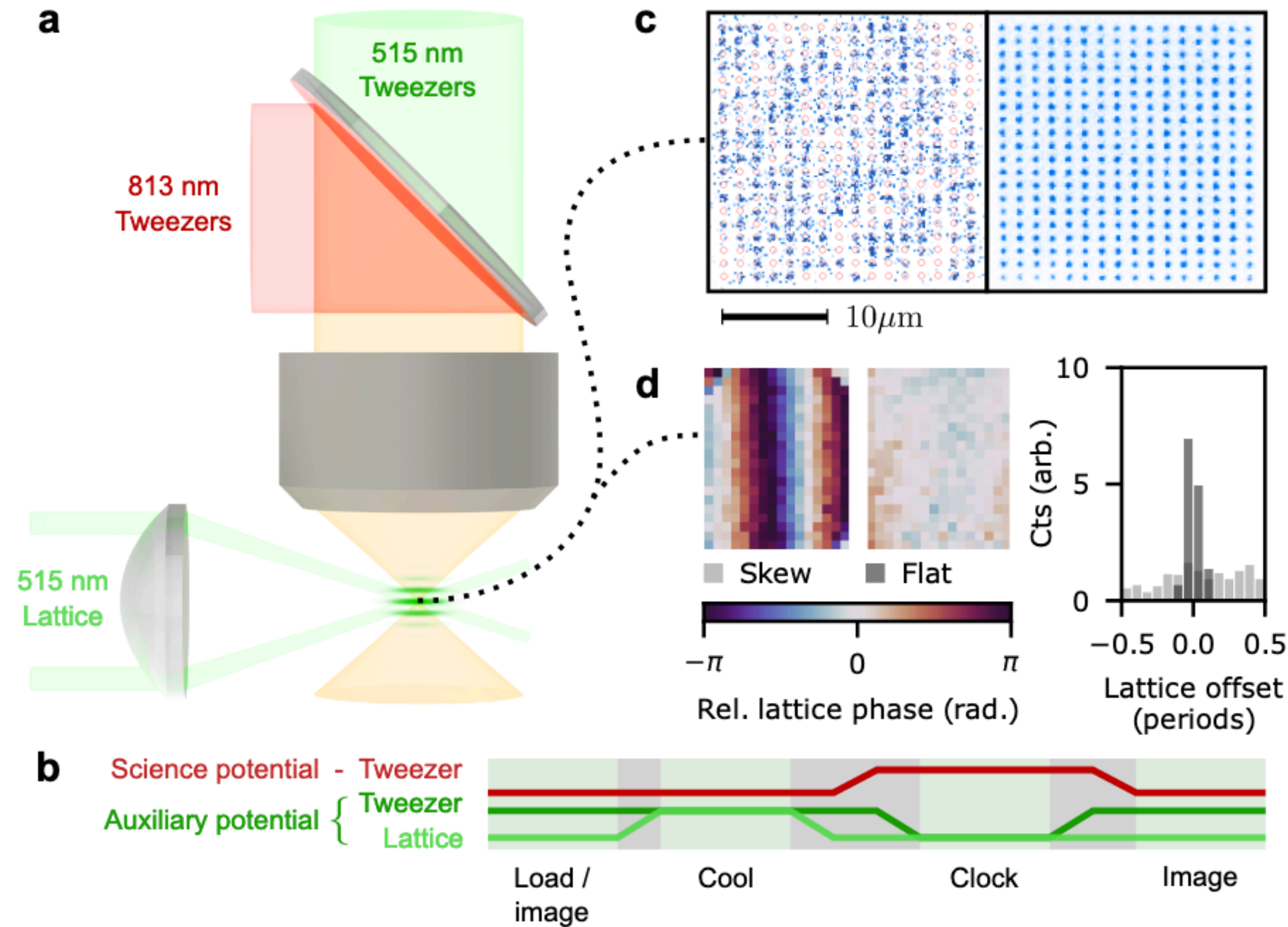
INSTITUT  
d'OPTIQUE  
GRADUATE SCHOOL  
ParisTech

*Institut d'Optique, CNRS*



# Tweezer clocks

A. Young et al. arXiv:2004.06095 (2020)

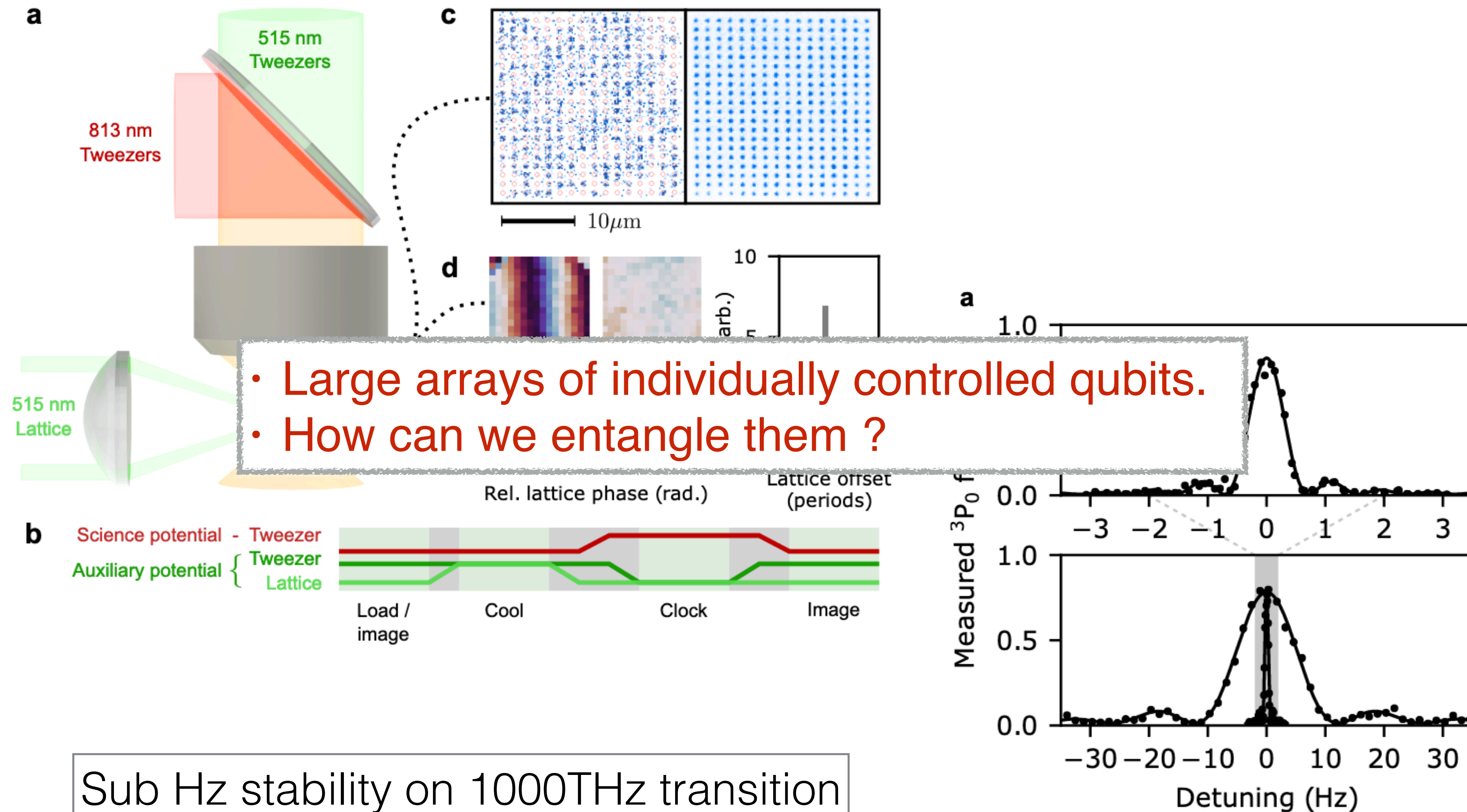


Sub Hz stability on 1000THz transition



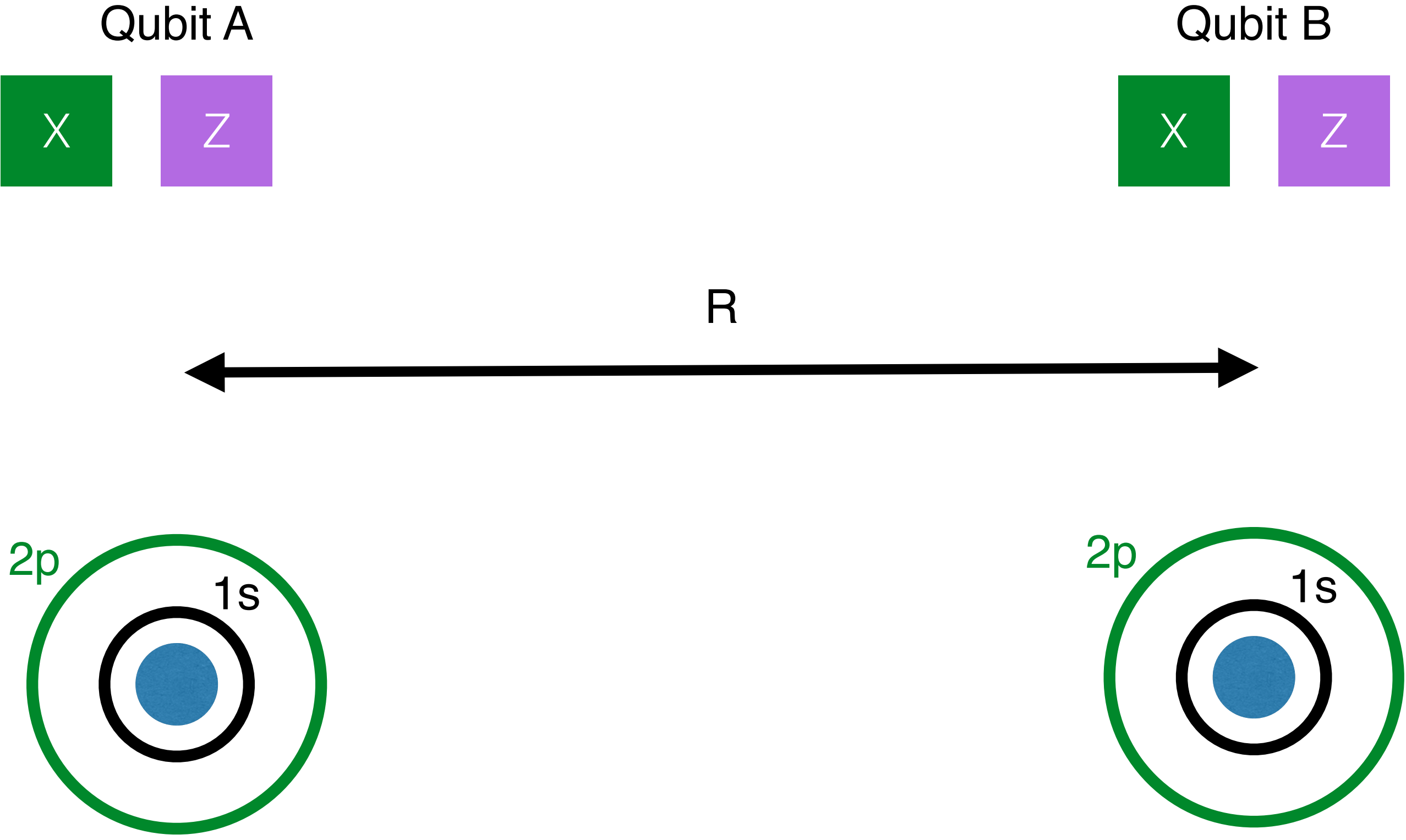
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A. Young et al. arXiv:2004.06095 (2020)

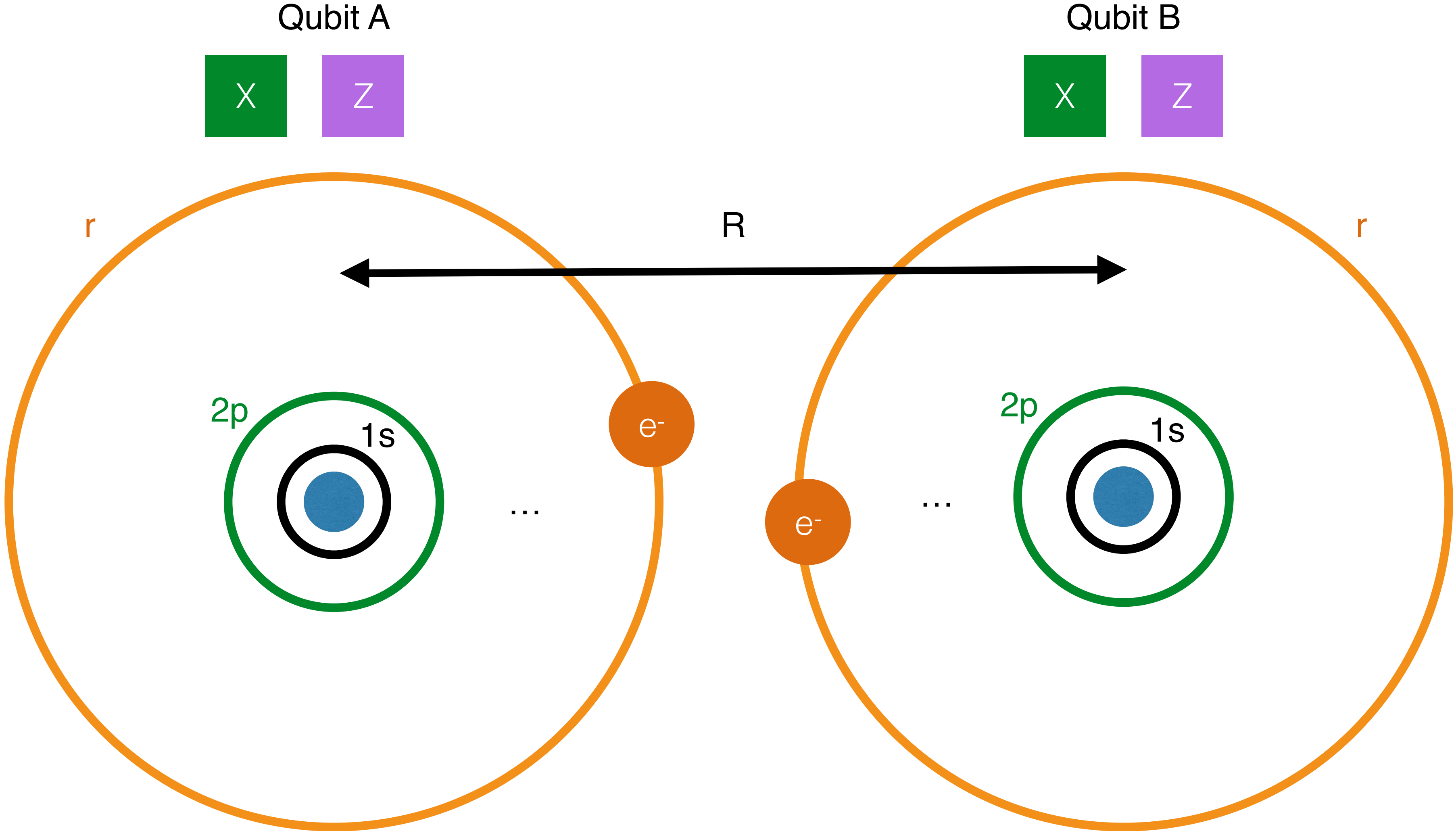


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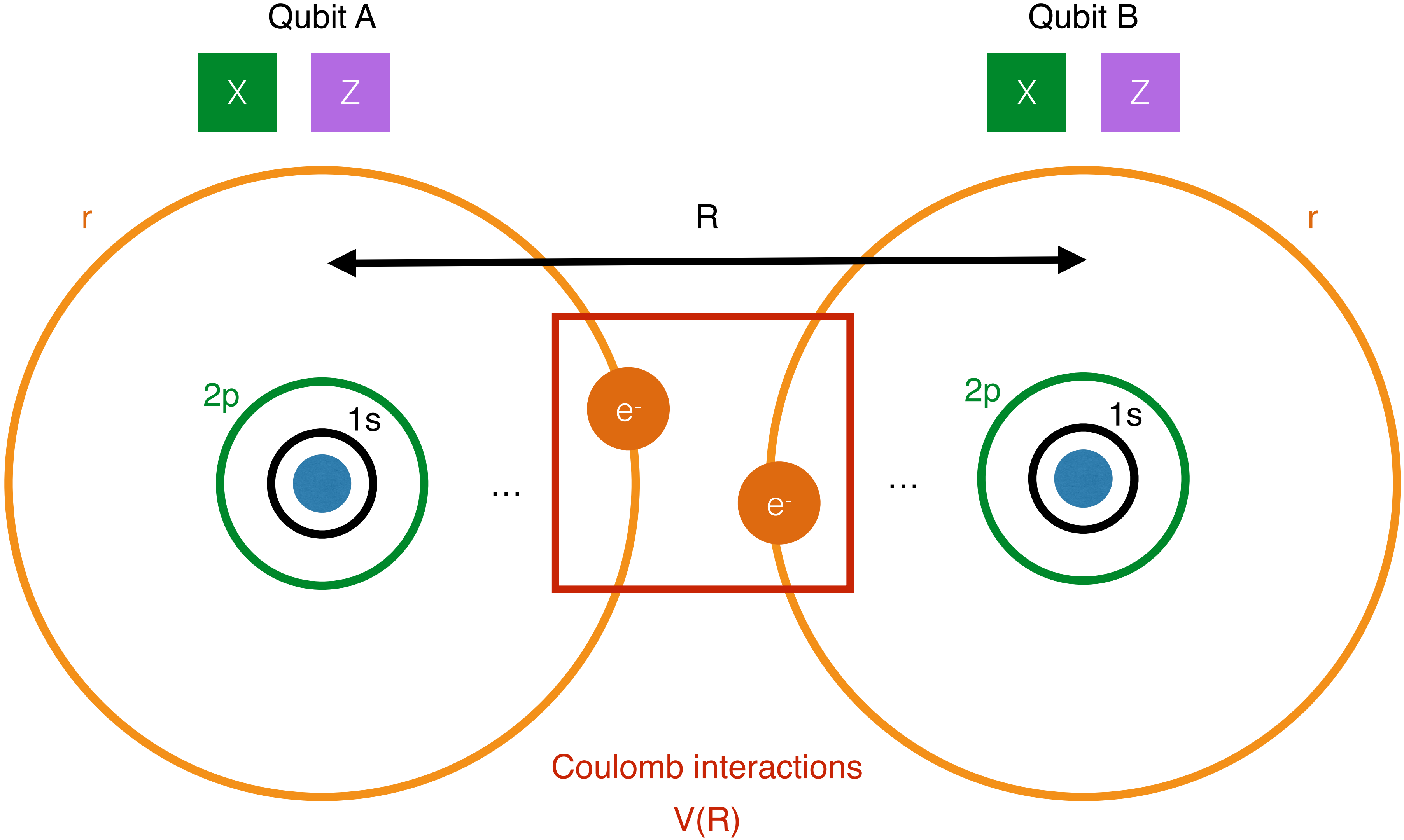
# Rydberg atoms - Fast entanglement of neutral atoms



# Rydberg atoms - Fast entanglement of neutral atoms

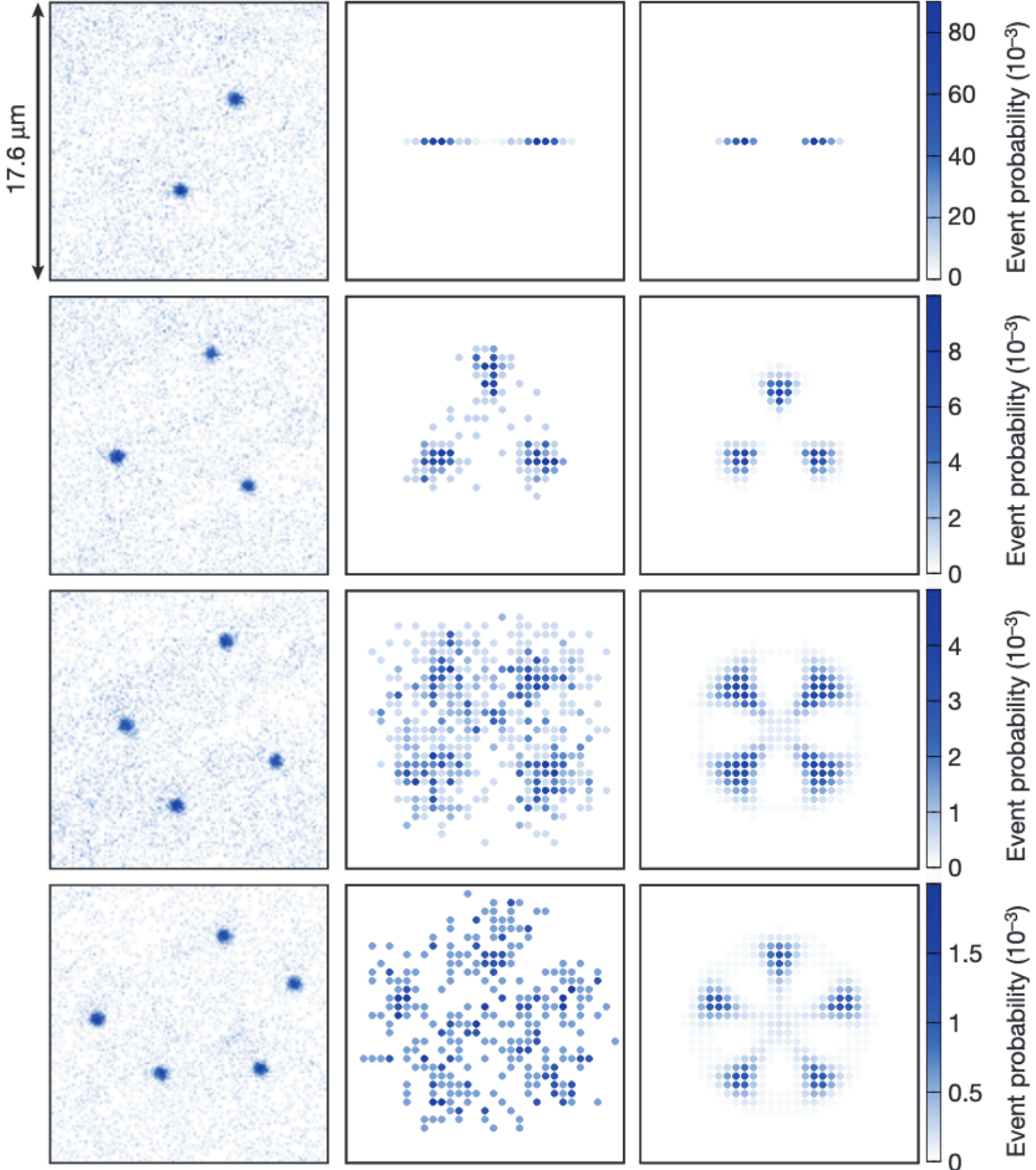
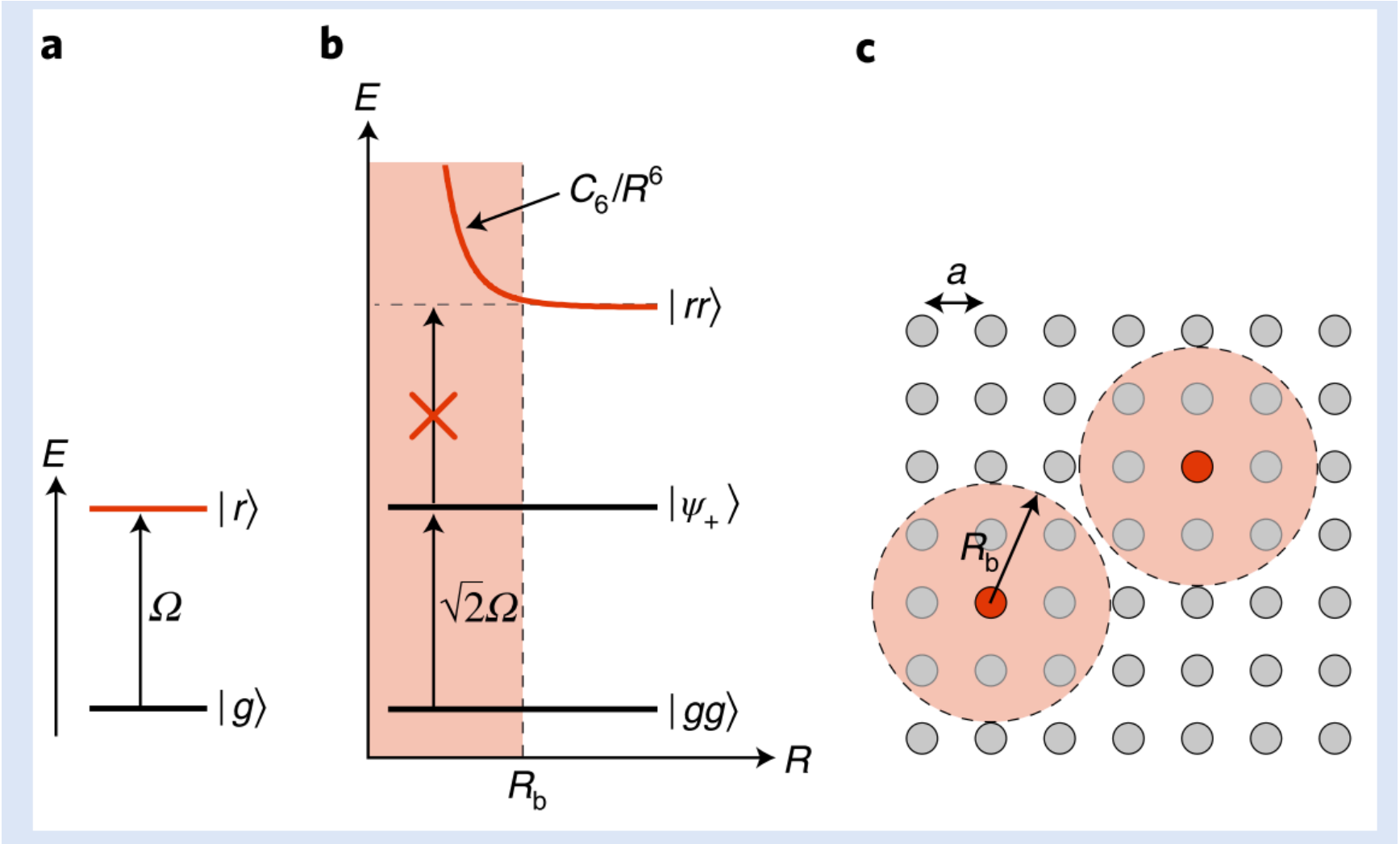


# Rydberg atoms - Fast entanglement of neutral atoms



# Rydberg atoms - Fast entanglement of neutral atoms

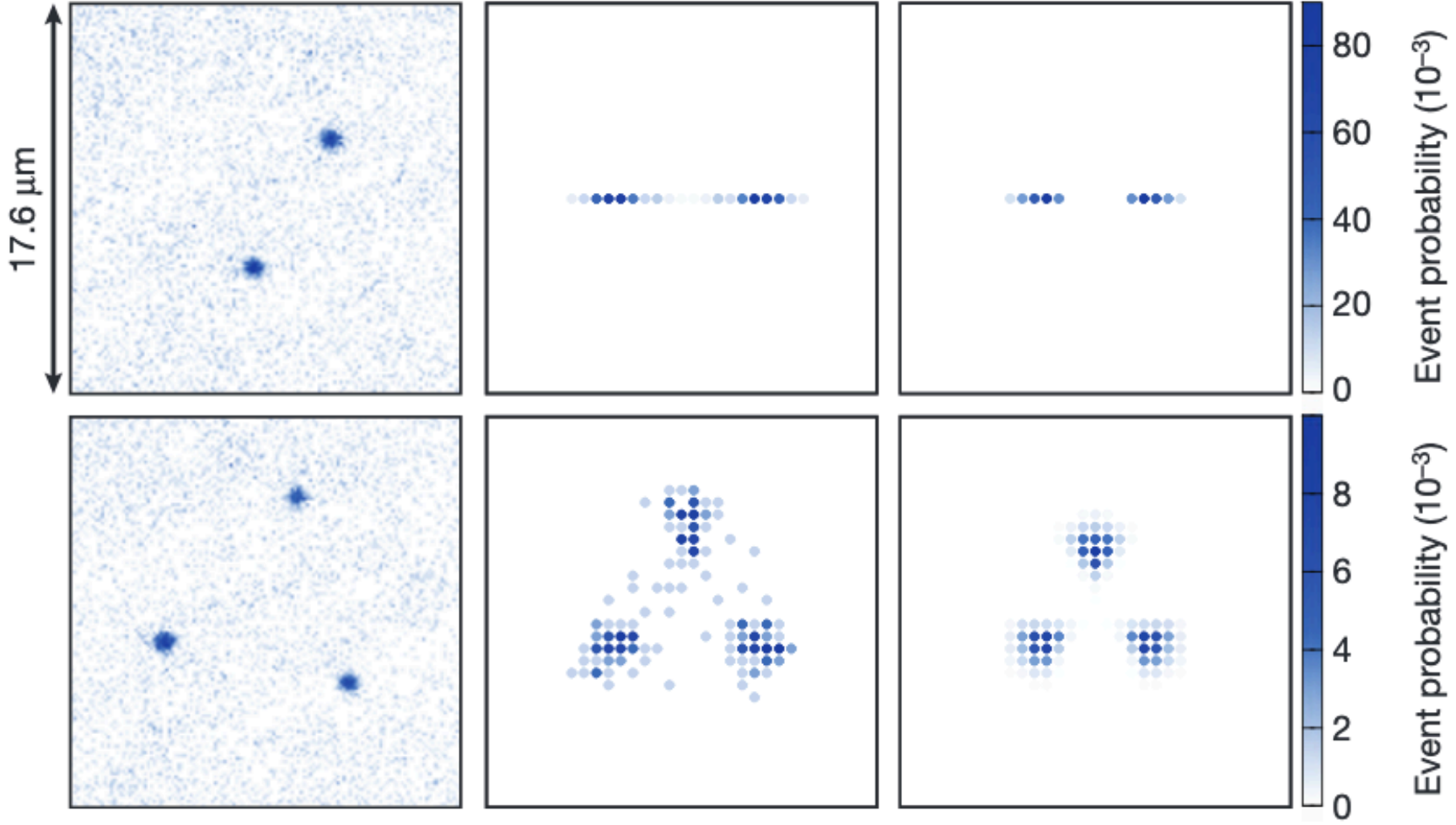
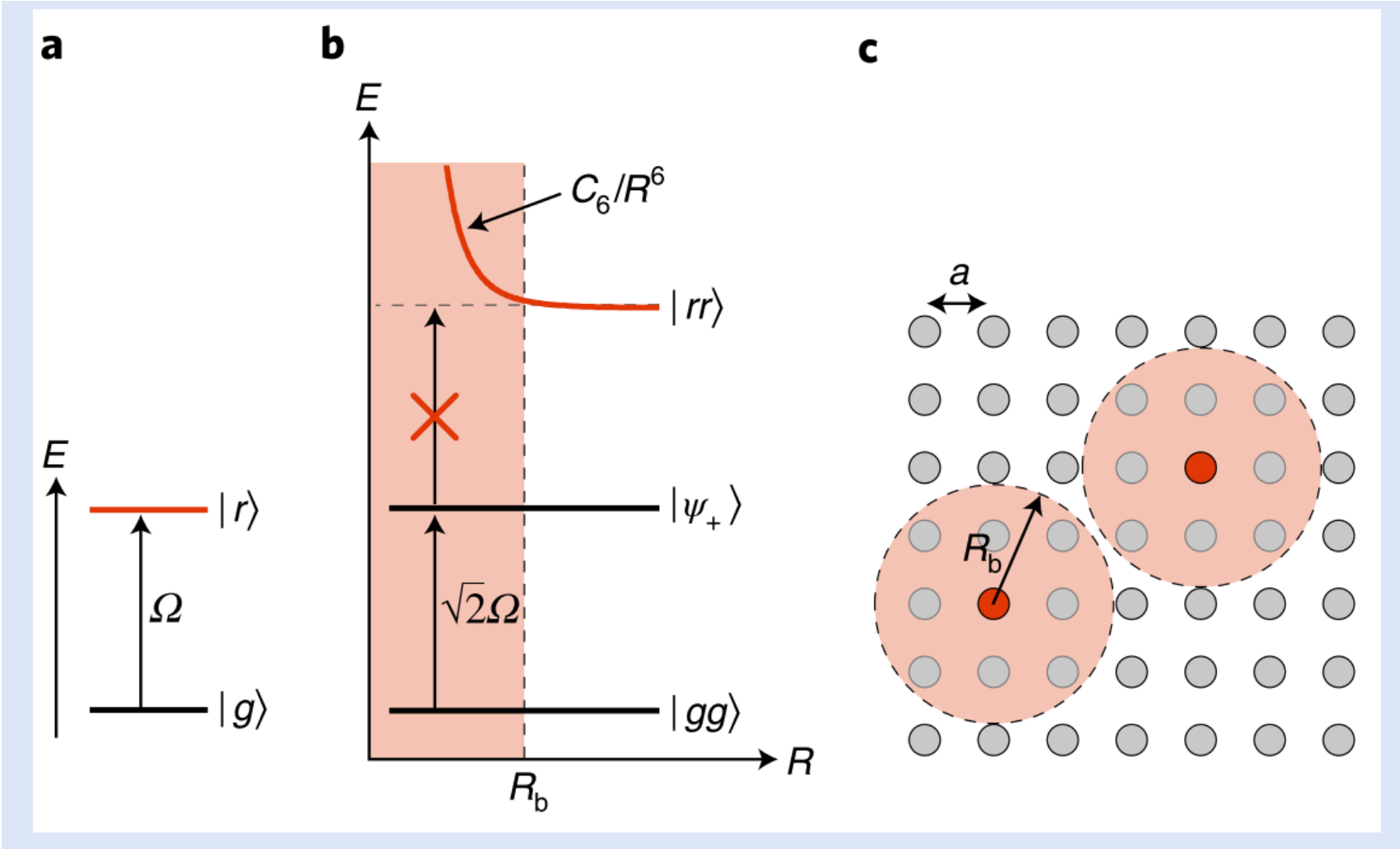
A. Browaeys and T. Lahaye, Nat. Phys. 16, 132 (2020).



P. Schauß et al. Nature 491, 87 (2012).

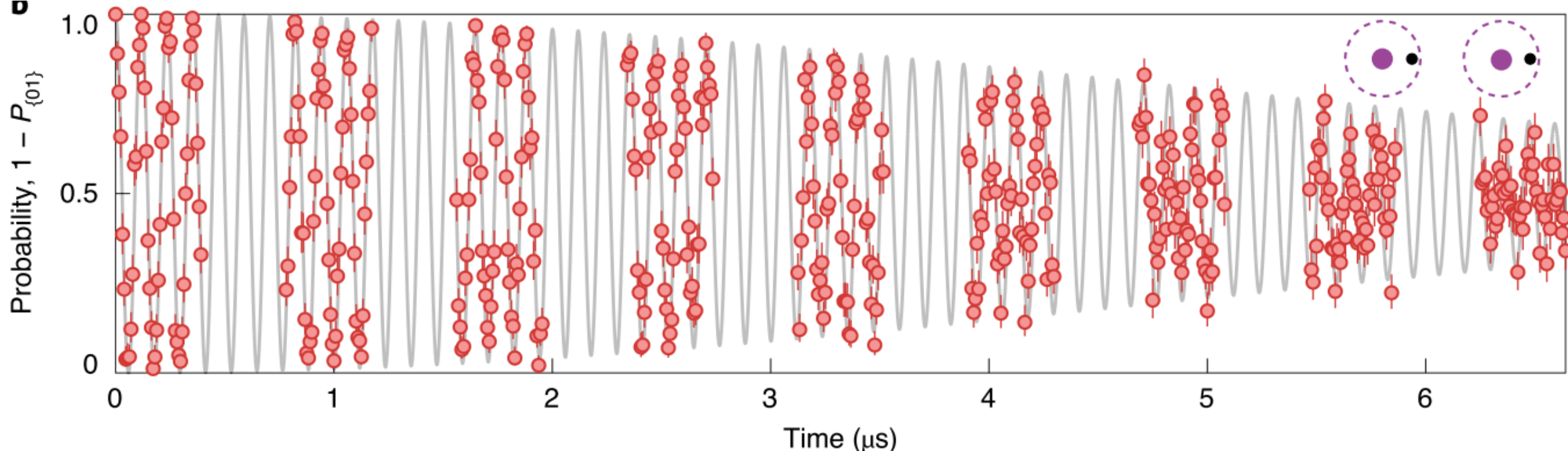
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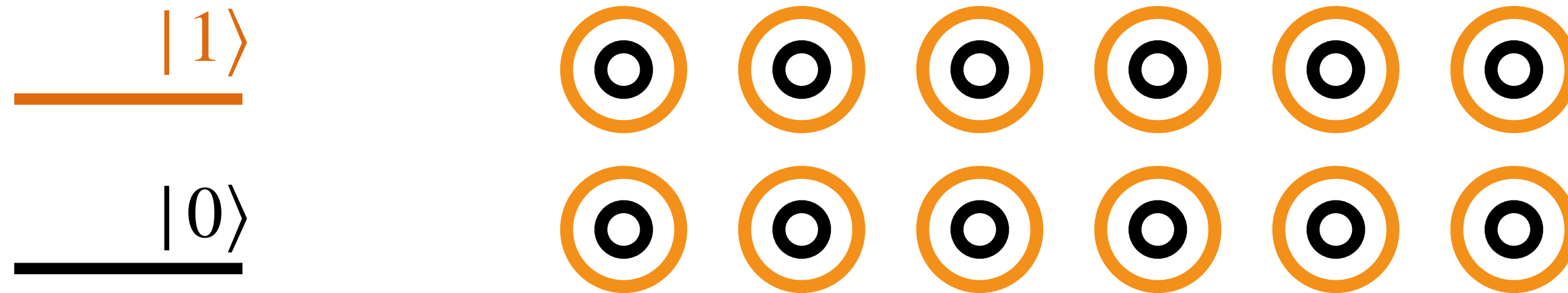
High fidelity entanglement

I. S. Madjarov et al. Nat. Phys. 16, 857 (2020).



# Rydberg atoms as quantum simulators

**Until now:** Use the control to implement a universal gate set



$$\mathcal{H} = \frac{\hbar\Omega}{2} \sum_j \sigma_j^x + \frac{\hbar\Delta}{2} \sum_j \sigma_j^z + \sum_{i \neq j} \frac{C_6}{r_{ij}^6} n_i n_j \quad n_j = \frac{1}{2} + \sigma_j^z$$


Single qubit control

Two qubit interaction

**Now:** Use full control over the parameters of the Hamiltonian to solve specific problems.

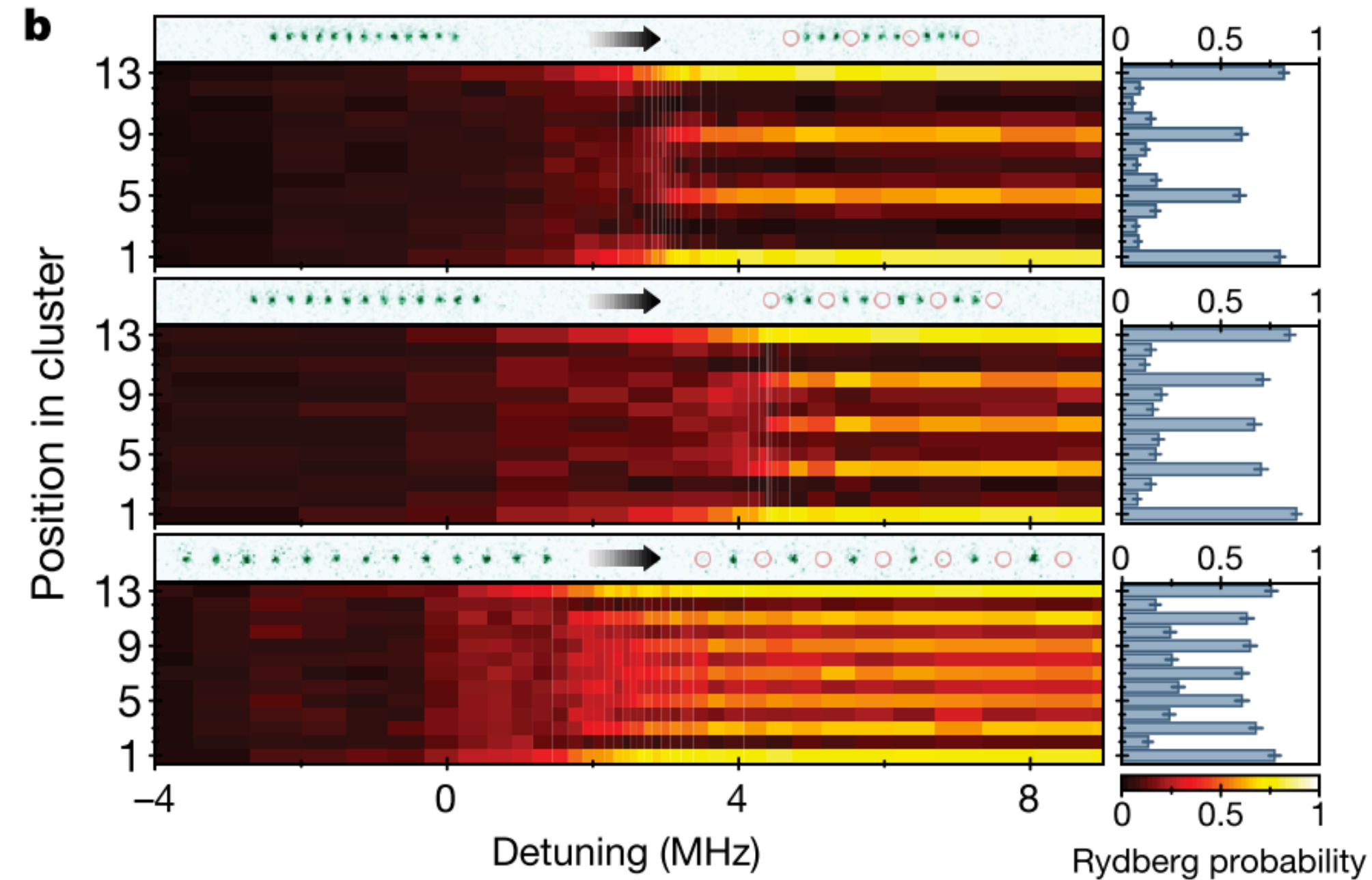
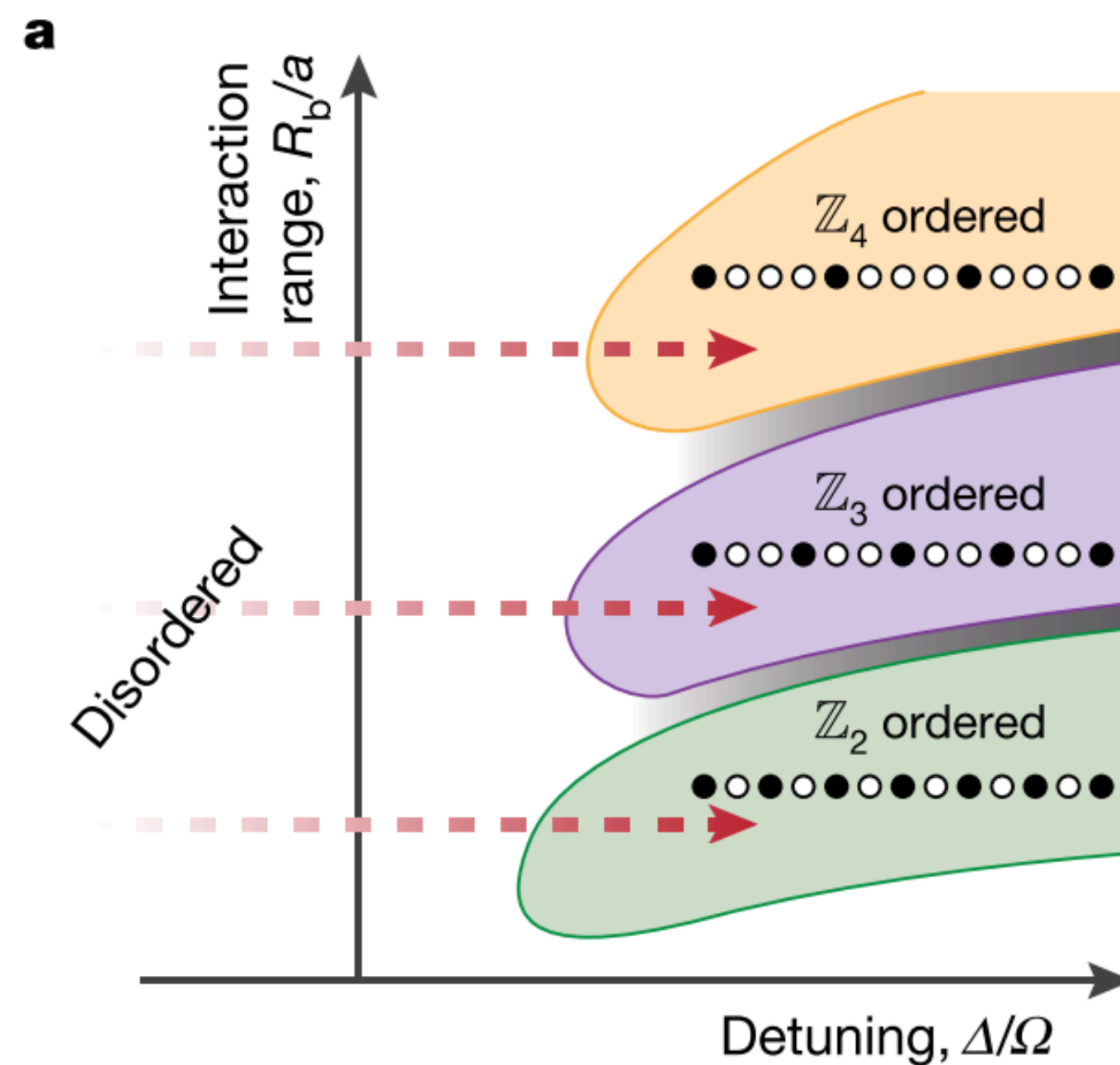


# Rydberg atoms as quantum simulators

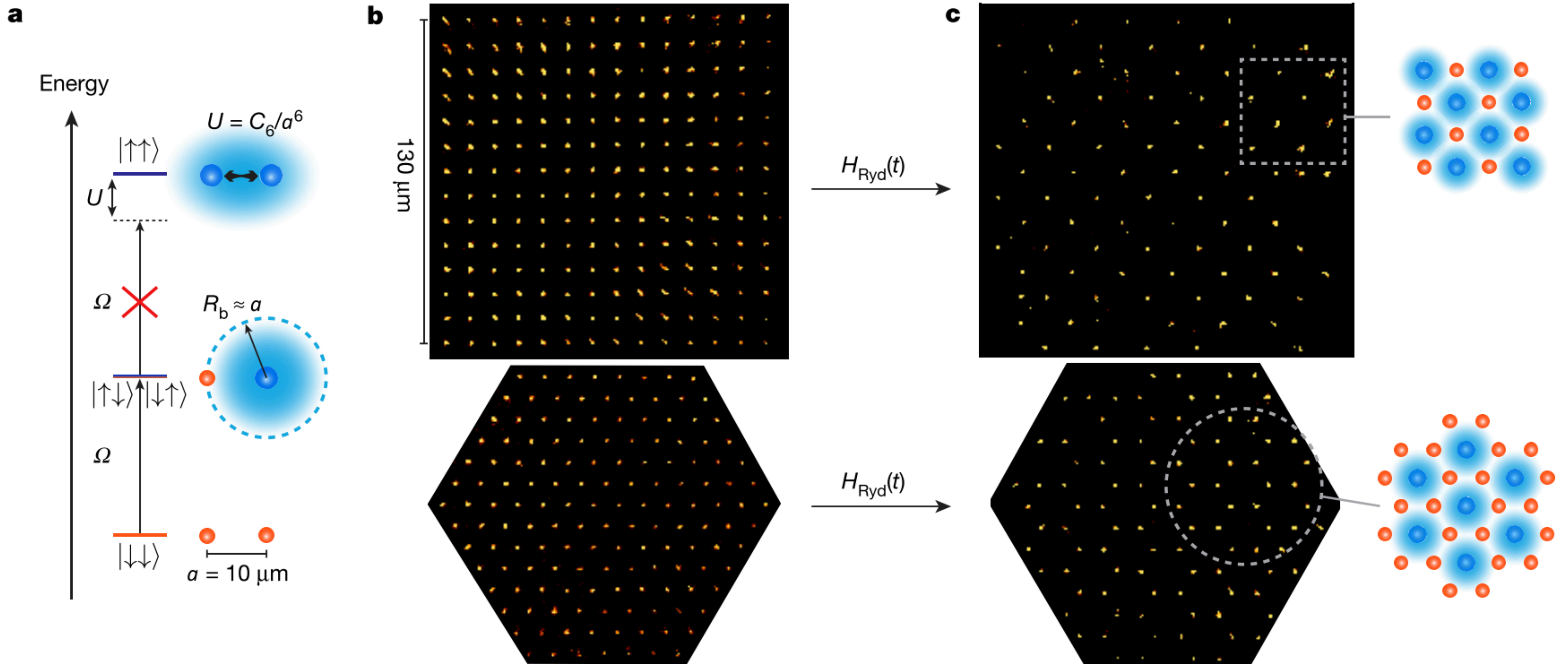


$$\mathcal{H} = \frac{\hbar\Omega}{2} \sum_j \sigma_j^x + \frac{\hbar\Delta}{2} \sum_j \sigma_j^z + \sum_{i \neq j} \frac{C_6}{r_{ij}^6} n_i n_j$$


Quantum simulators with up to 51 atoms




# Rydberg simulators in 2D

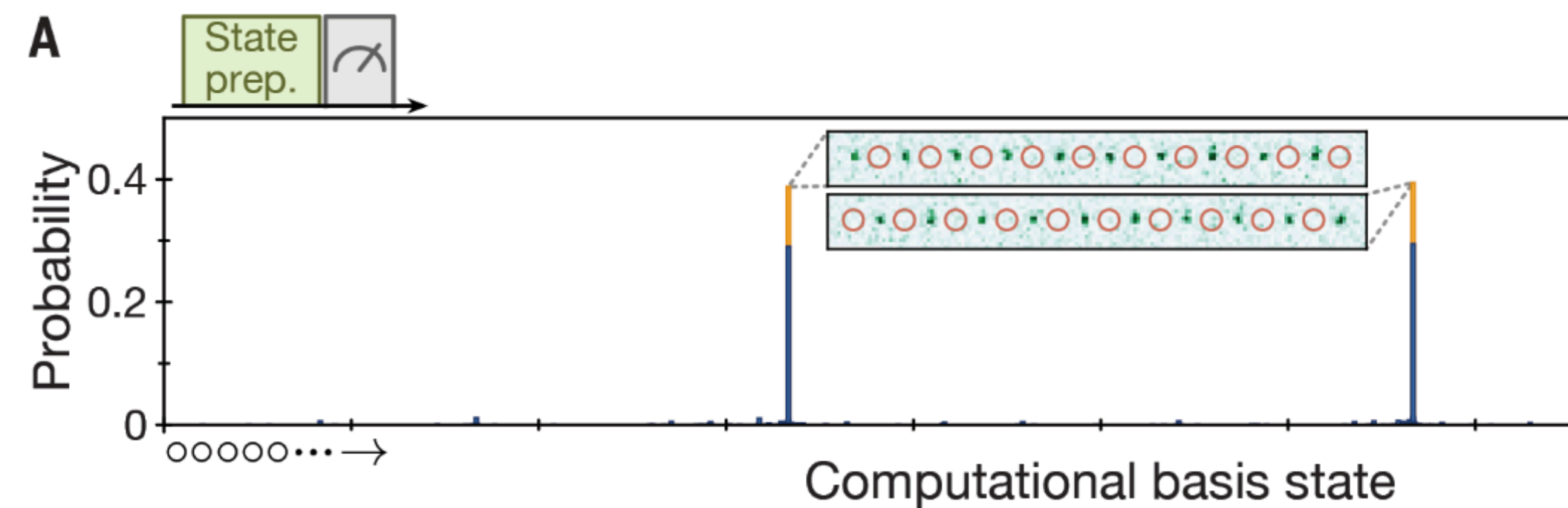
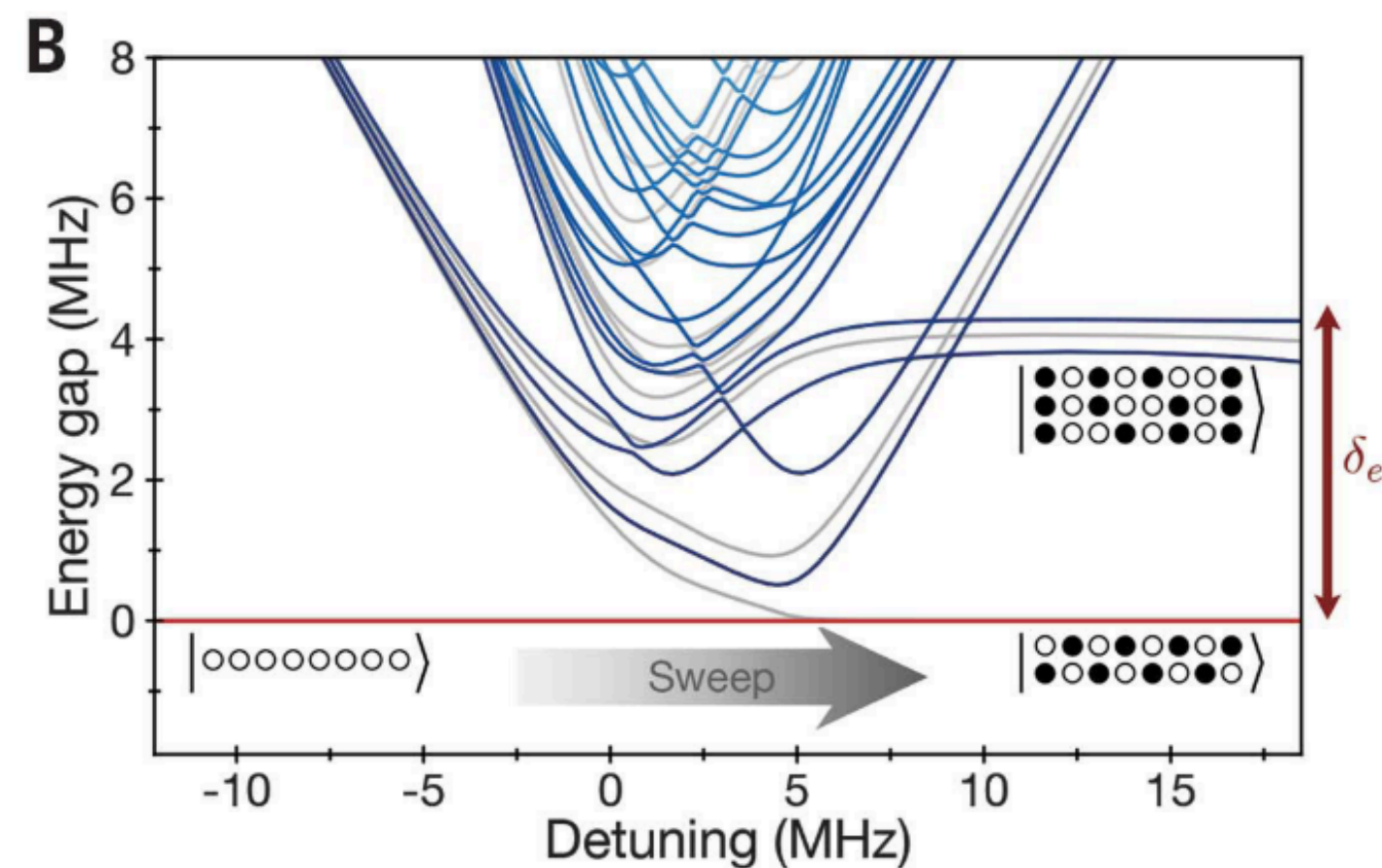


# Rydberg atoms as quantum simulators



$$\mathcal{H} = \frac{\hbar\Omega}{2} \sum_j \sigma_j^x + \frac{\hbar\Delta}{2} \sum_j \sigma_j^z + \sum_{i \neq j} \frac{C_6}{r_{ij}^6} n_i n_j$$


Schrödinger cats with 20 atoms

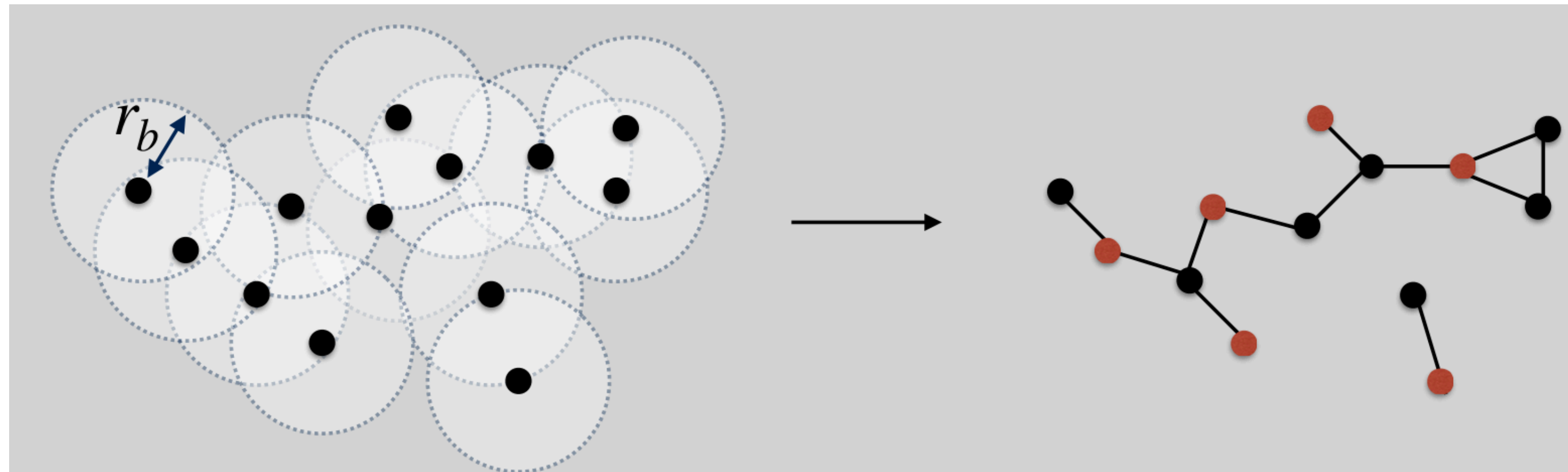


A. Omran et al. Science 365, 570 (2019).

# Maximum Independent Sets

L. Henriot et al. Quantum 4, 327 (2020).

H. Pichler et al., ArXiv 1808.10816 (2018).



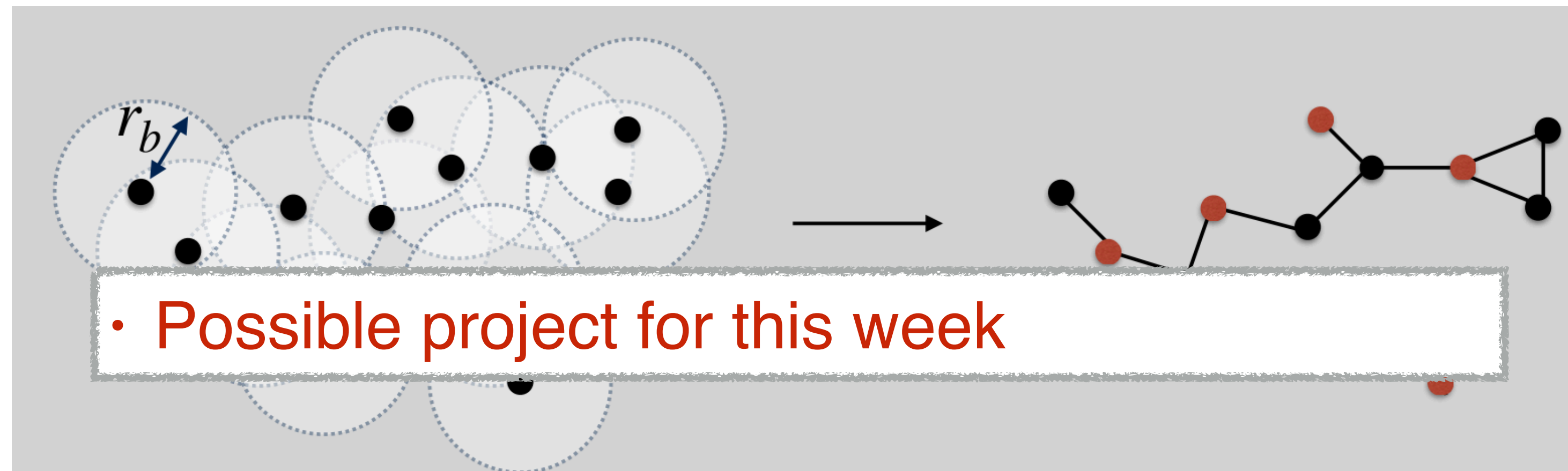
Possible applications to finance, network design



# Maximum Independent Sets

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Possible applications to finance, network design

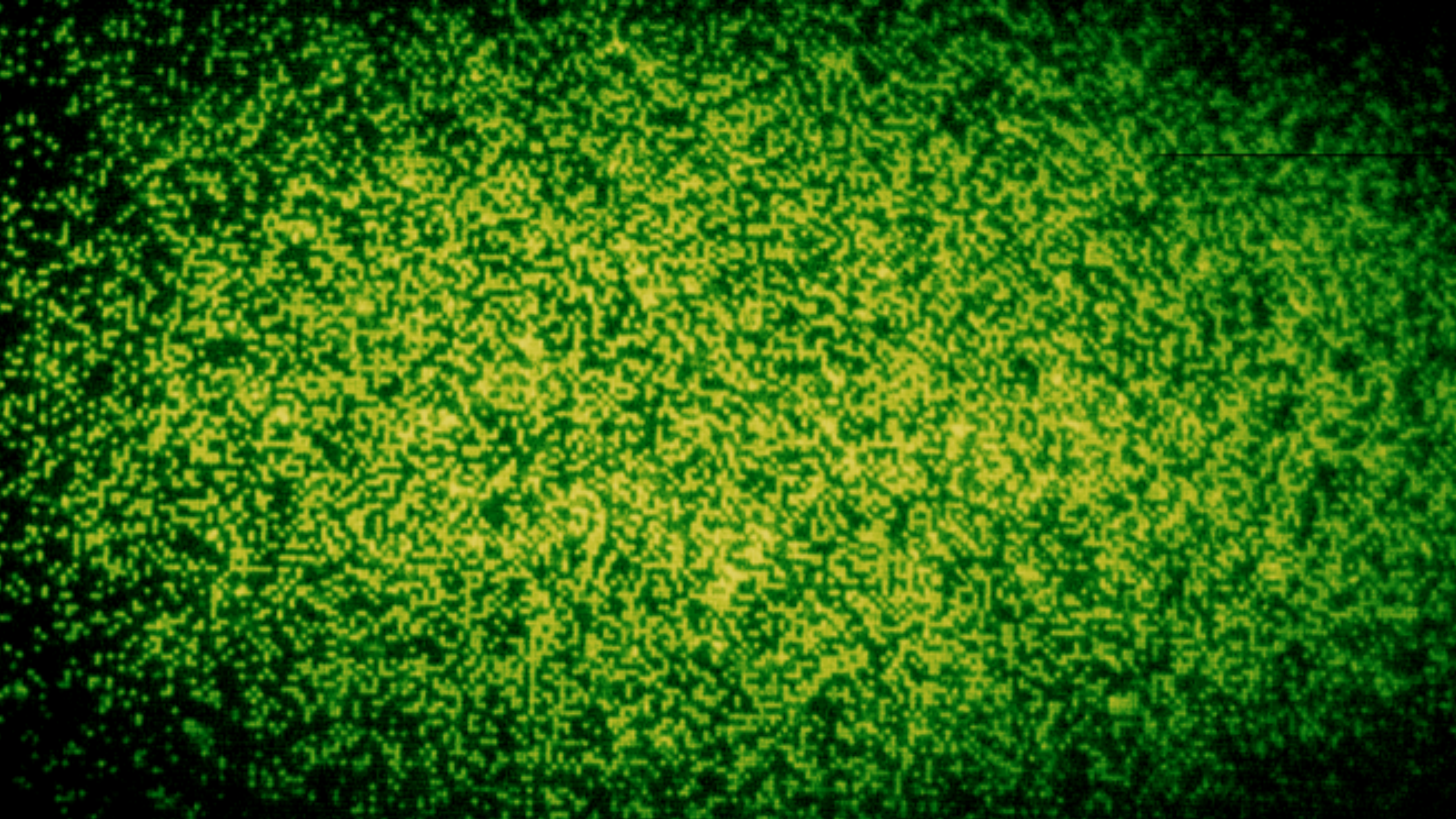


# Digital vs analog

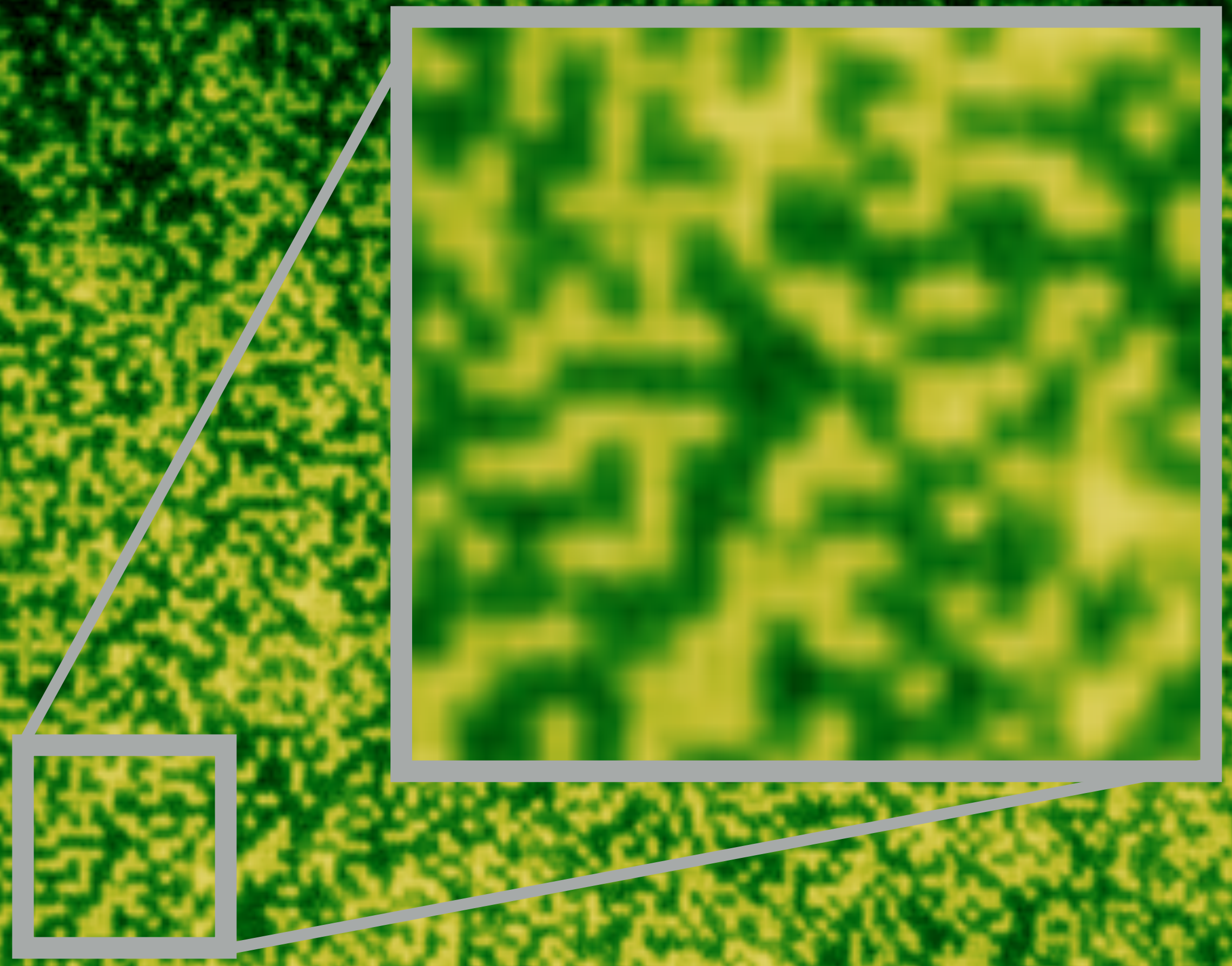
	<b>Analog Quantum Simulation</b>	<b>Digital Quantum Simulation</b>
<b>Resource used for simulation</b>	Hamiltonians	Gates
<b>Key advantages</b>	Promising hybrid quantum-classical approaches	Universal approach
<b>Shortcomings</b>	Limited number of available configurations	Requires a large number of gates
<b>Status</b>	Quantum advantage already achieved	Academic research

L. Henriet et al. Quantum 4, 327 (2020).

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# What happens when you cool a gas?

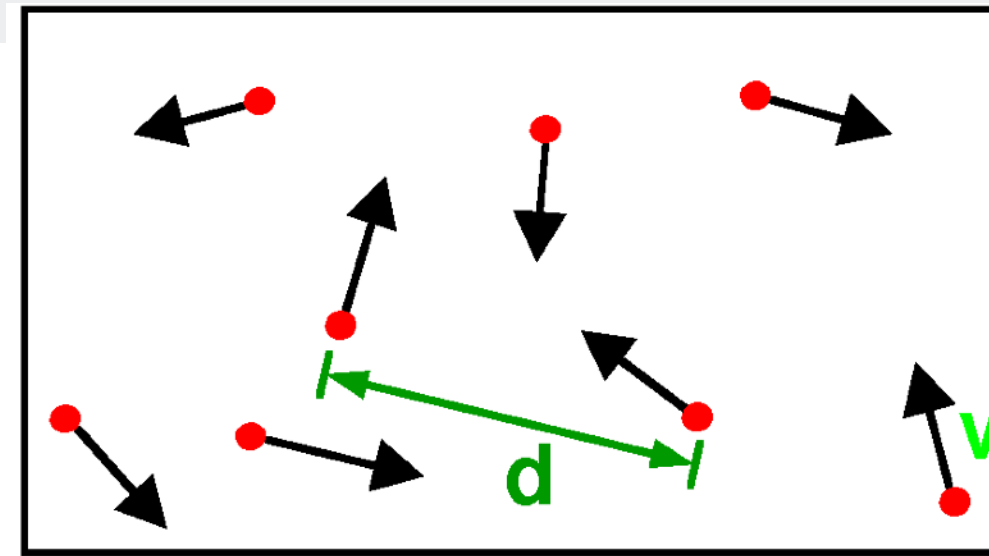
Average velocity of thermal atoms:

$$\langle |v| \rangle = \sqrt{\frac{3k_B T}{m}}$$

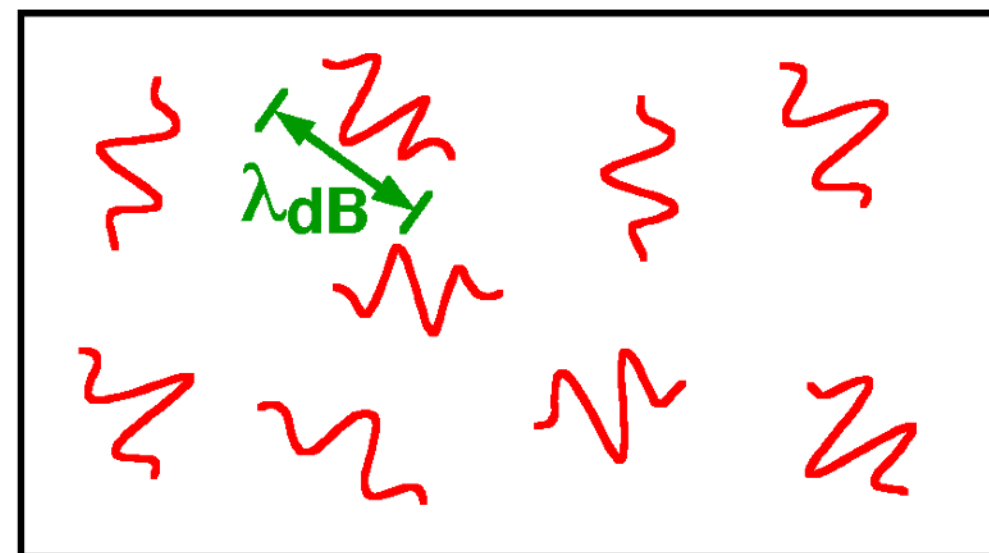
atoms = wave packets

$$\lambda_{dB} = \frac{h}{mv} = \sqrt{\frac{h^2}{3mk_B T}}$$

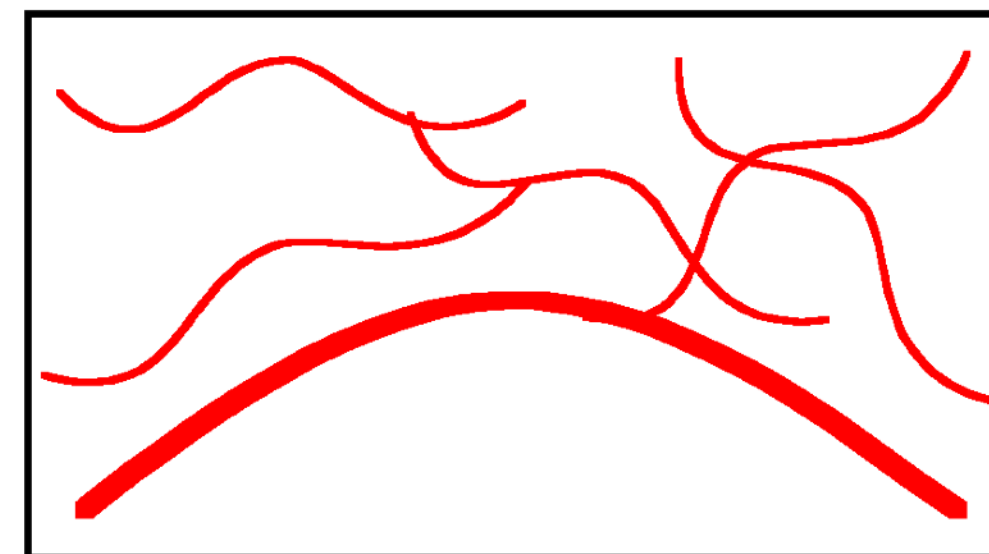
Thermal de Broglie wavelength



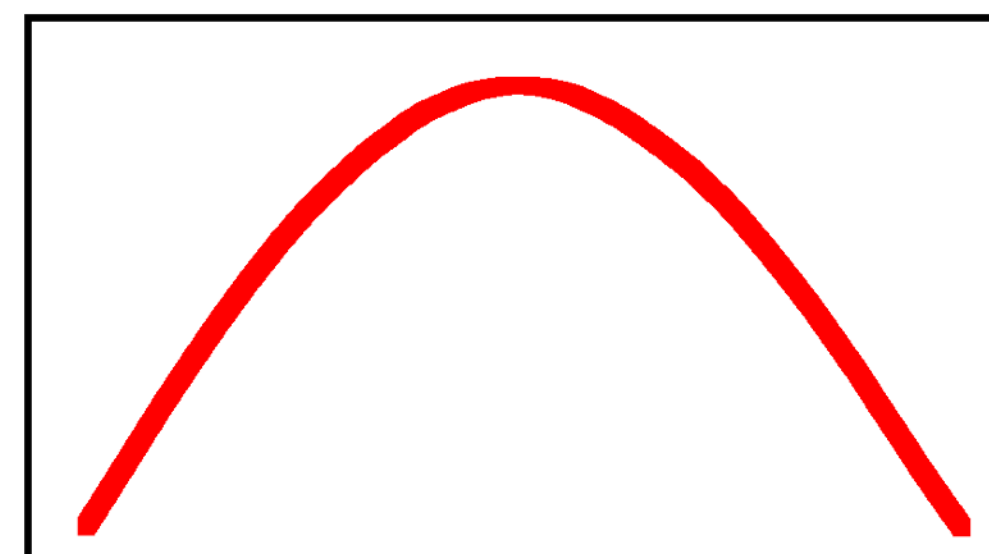
**High Temperature T:**  
 thermal velocity  $v$   
 density  $d^{-3}$   
 "Billiard balls"



**Low Temperature T:**  
 De Broglie wavelength  
 $\lambda_{dB} = h/mv \propto T^{-1/2}$   
 "Wave packets"



**T = T\_{crit}:**  
 Bose-Einstein Condensation  
 $\lambda_{dB} \approx d$   
 "Matter wave overlap"



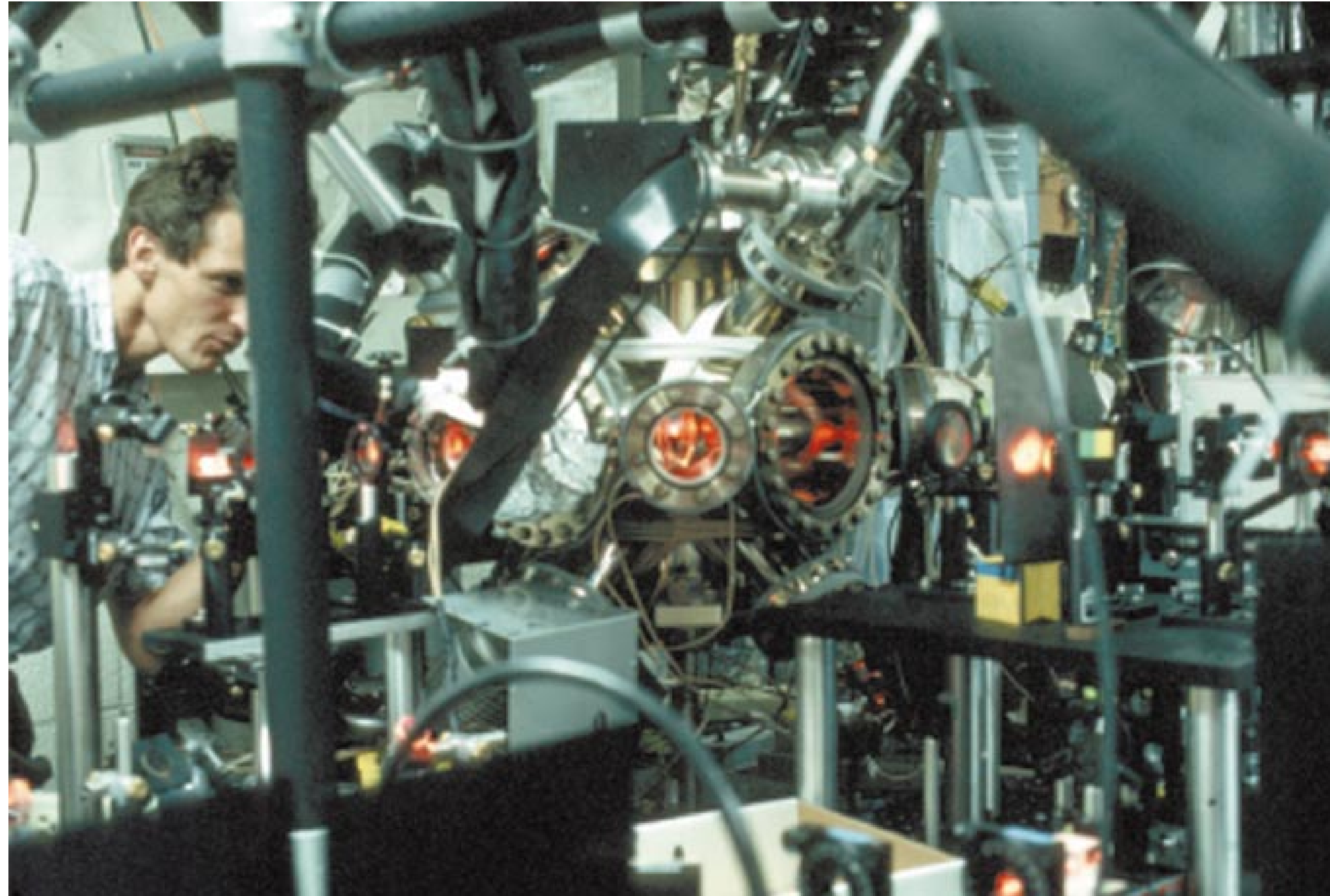
**T = 0:**  
 Pure Bose condensate  
 "Giant matter wave"

How to get colder?

Evaporative Cooling

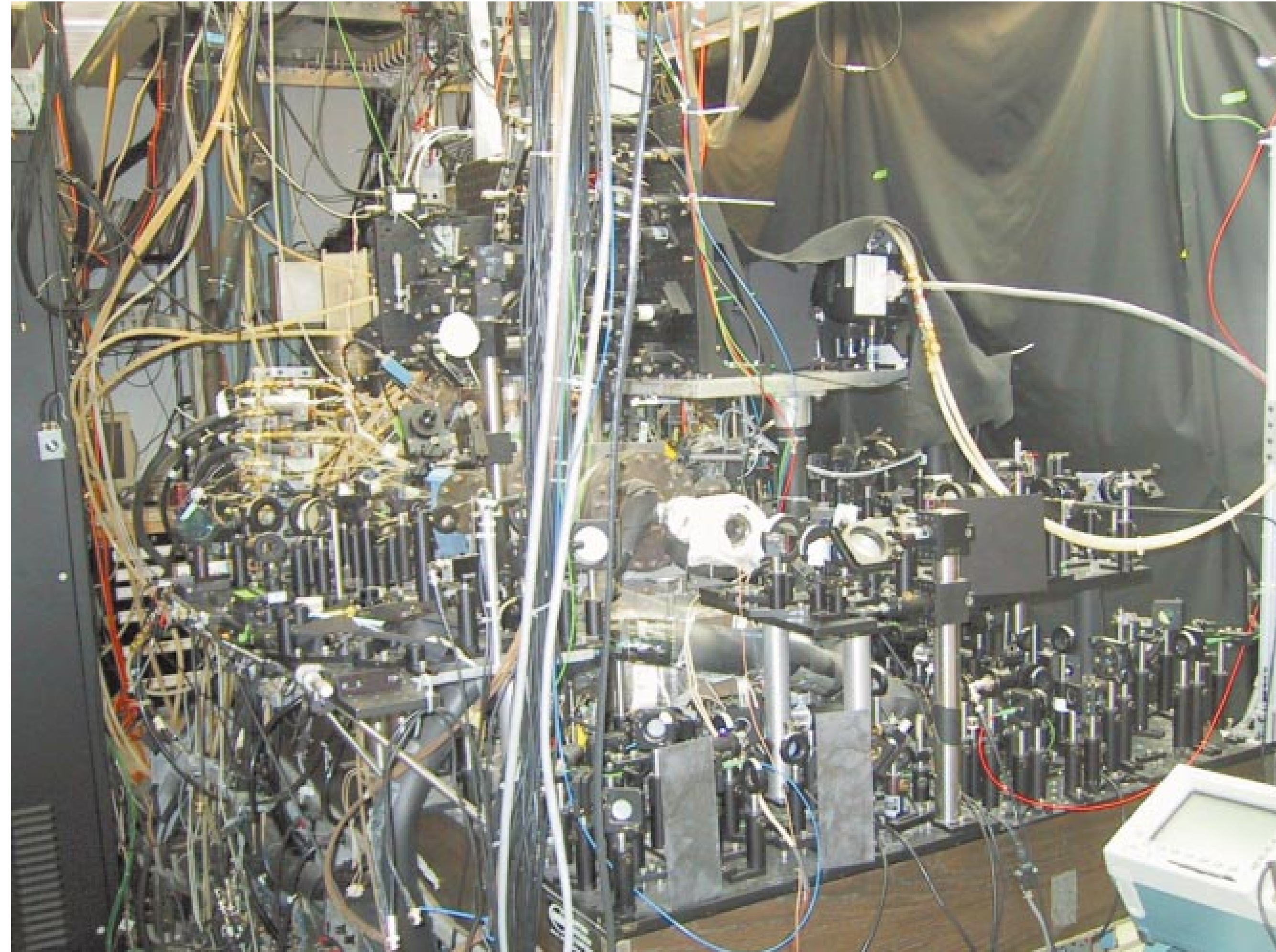
# How do you create a BEC ?

before BEC

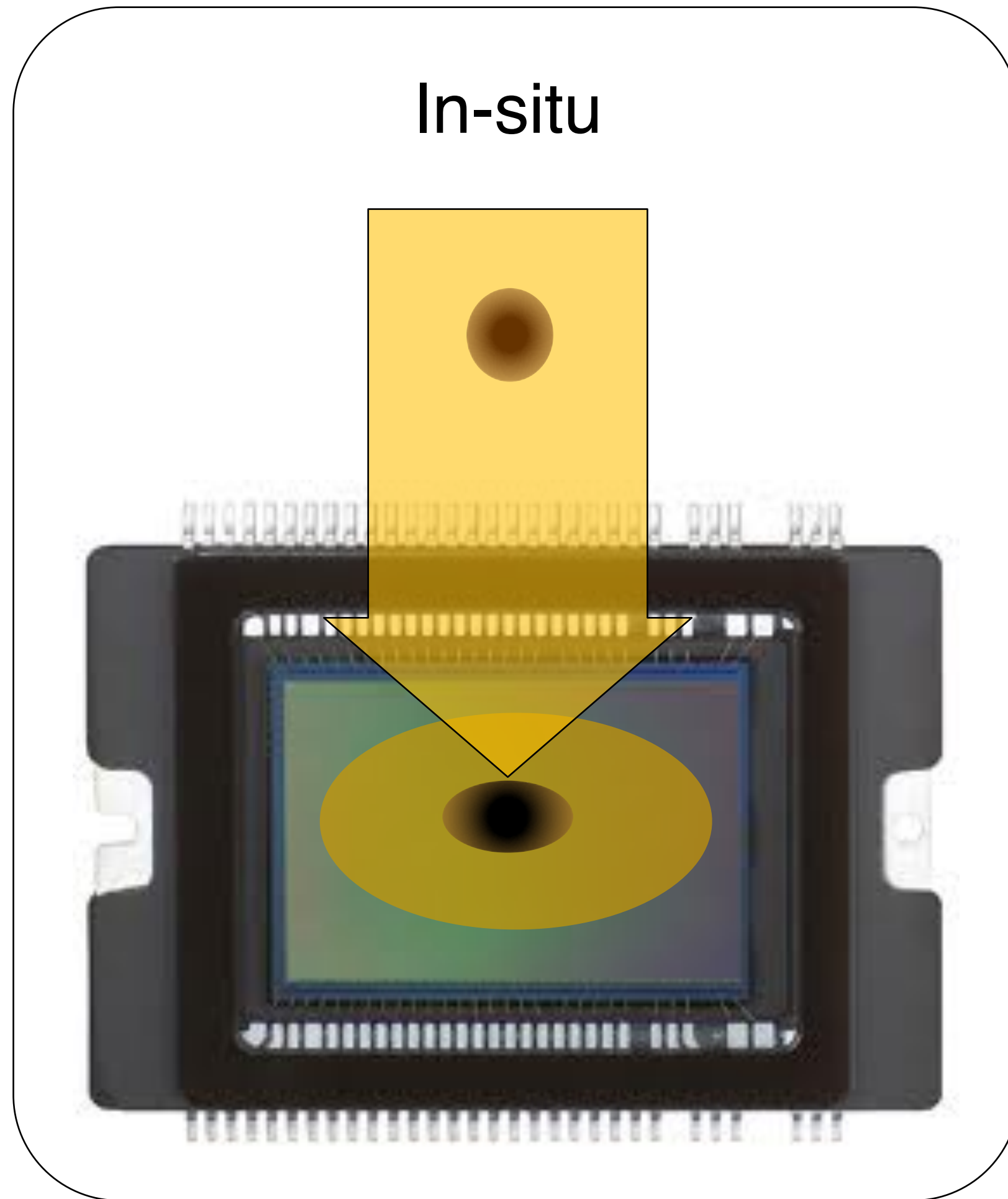


# How do you create a BEC ?

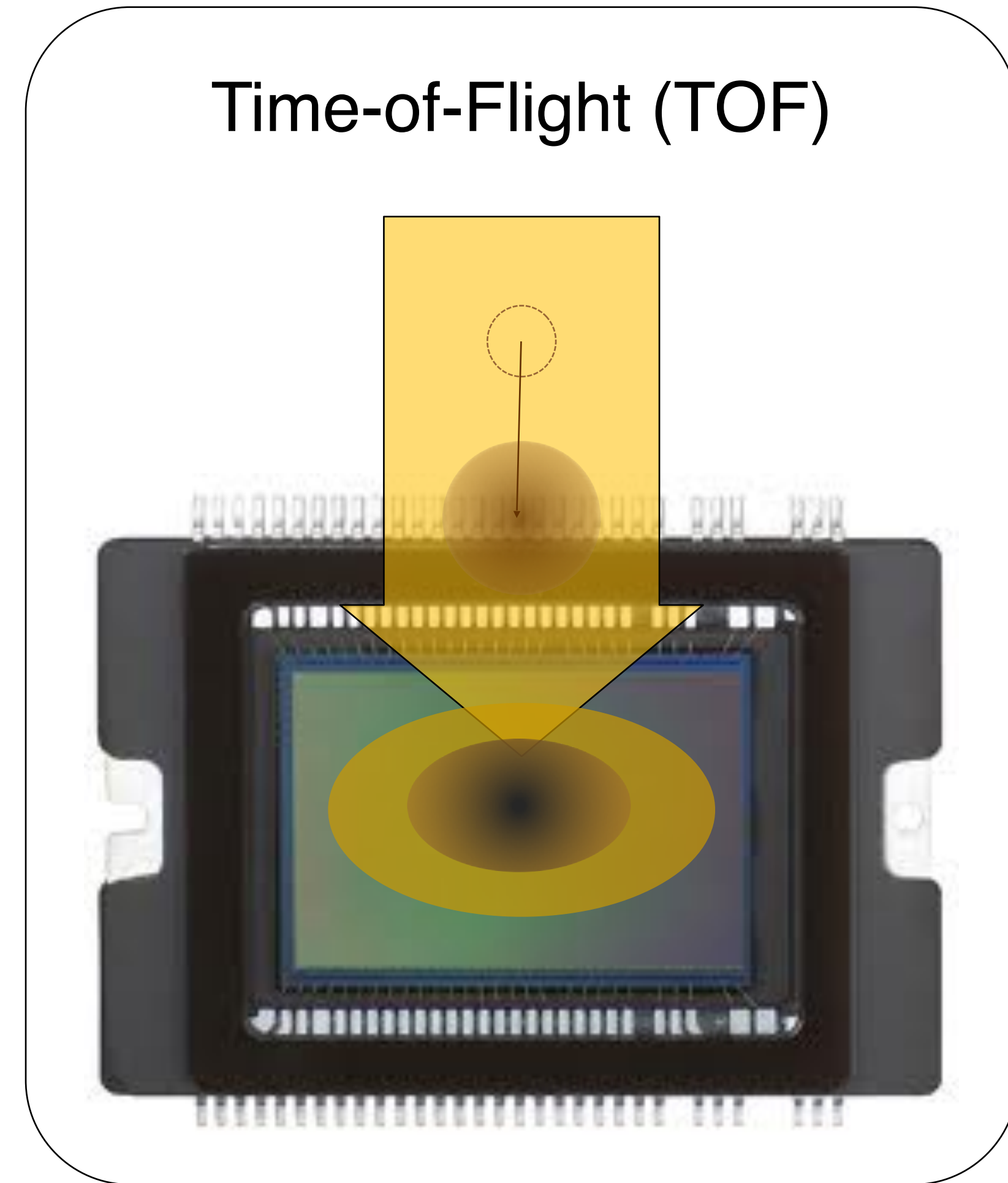
with BEC



# Absorption Imaging



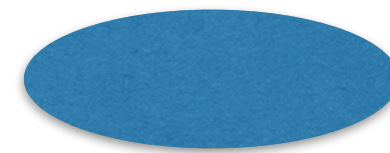
Spatial Information



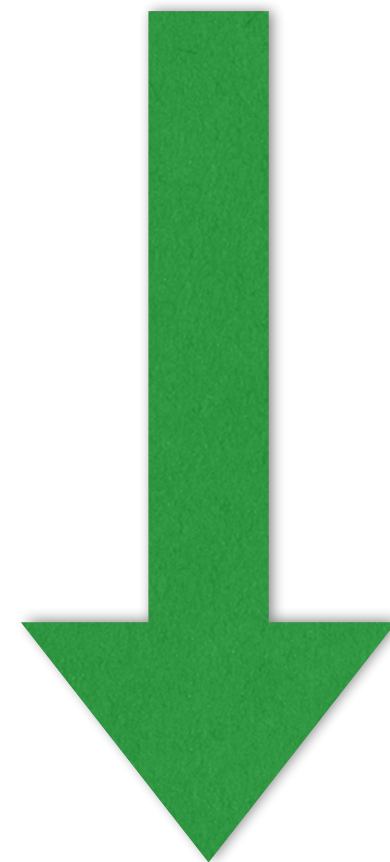
Momentum Information

# How do you see a BEC ?

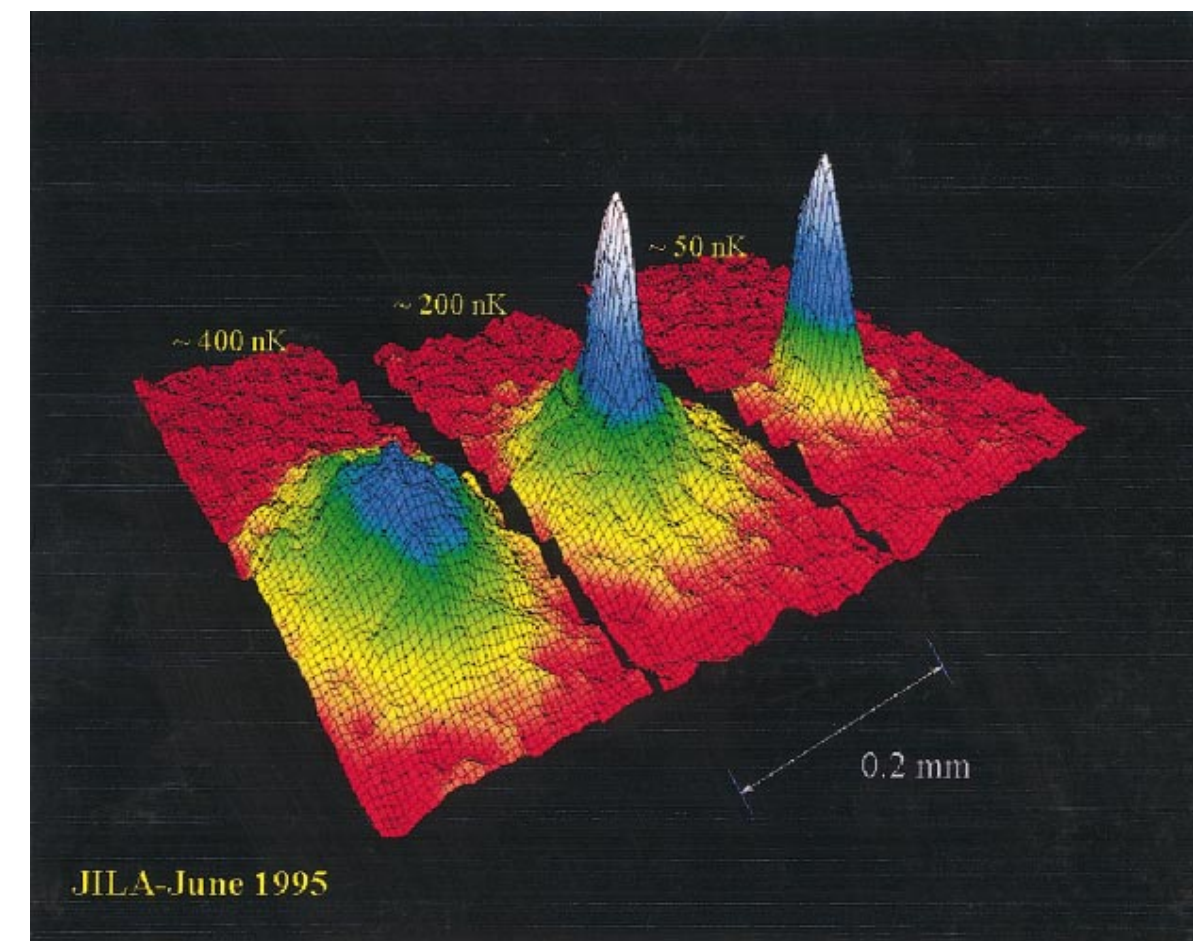
Initial trap (Real space):

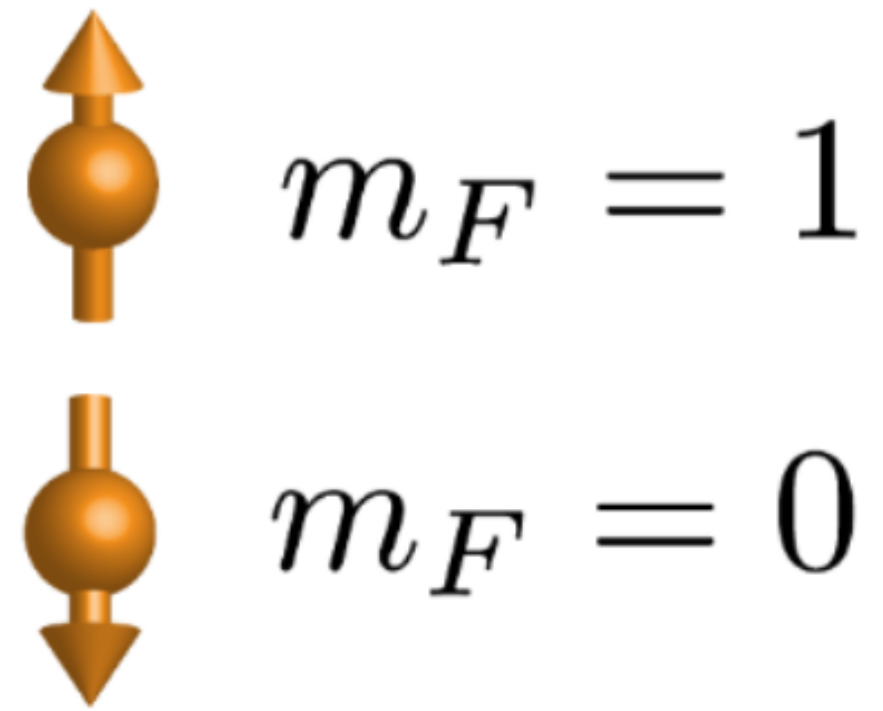


Time of flight  
cut the trap and  
let it expand freely



Momentum distribution:





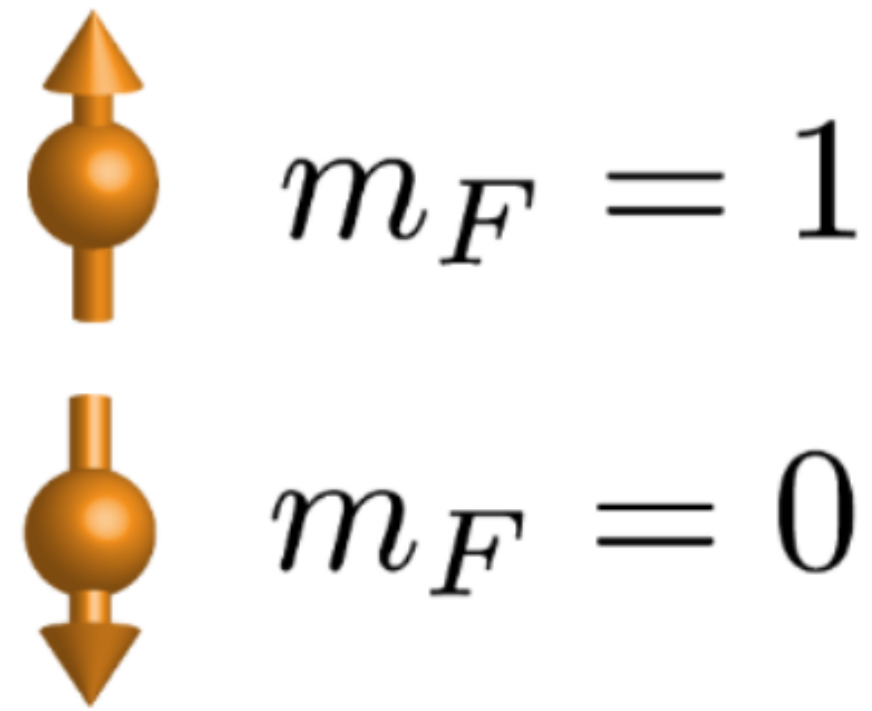
single atom — qubit —  $\ell = 1/2$

$$|\psi\rangle = \alpha_{-1/2} | - 1/2 \rangle + \alpha_{1/2} | 1/2 \rangle$$

$$\hat{L}_z |n\rangle = n |n\rangle \text{ with integer } |n| \leq \ell$$

$$[\hat{L}_x, \hat{L}_y] = i\hat{L}_z$$



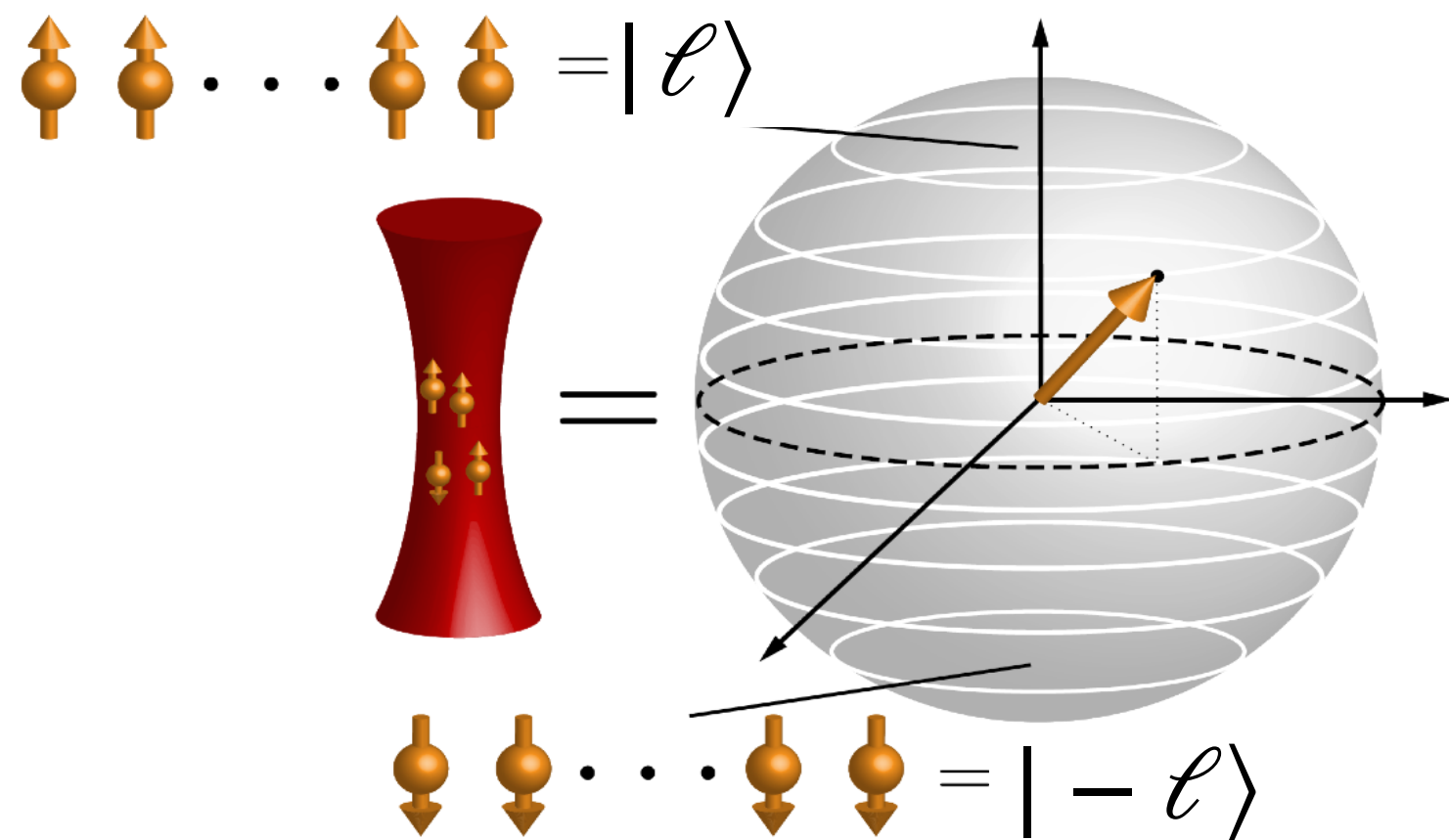


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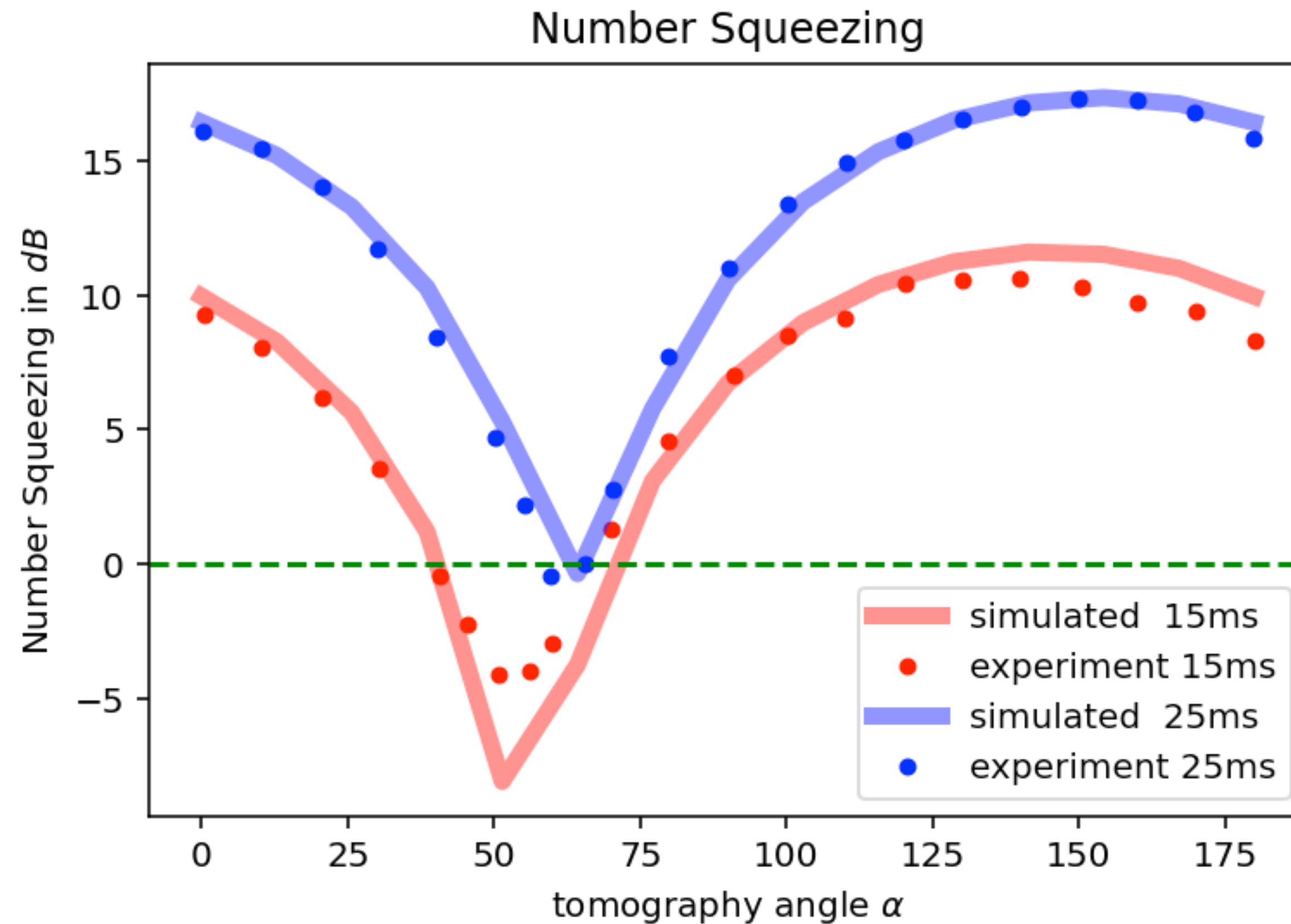
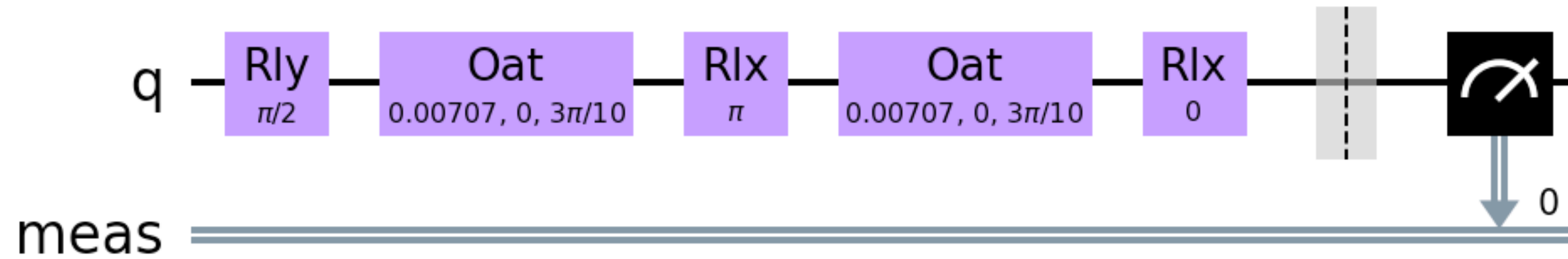
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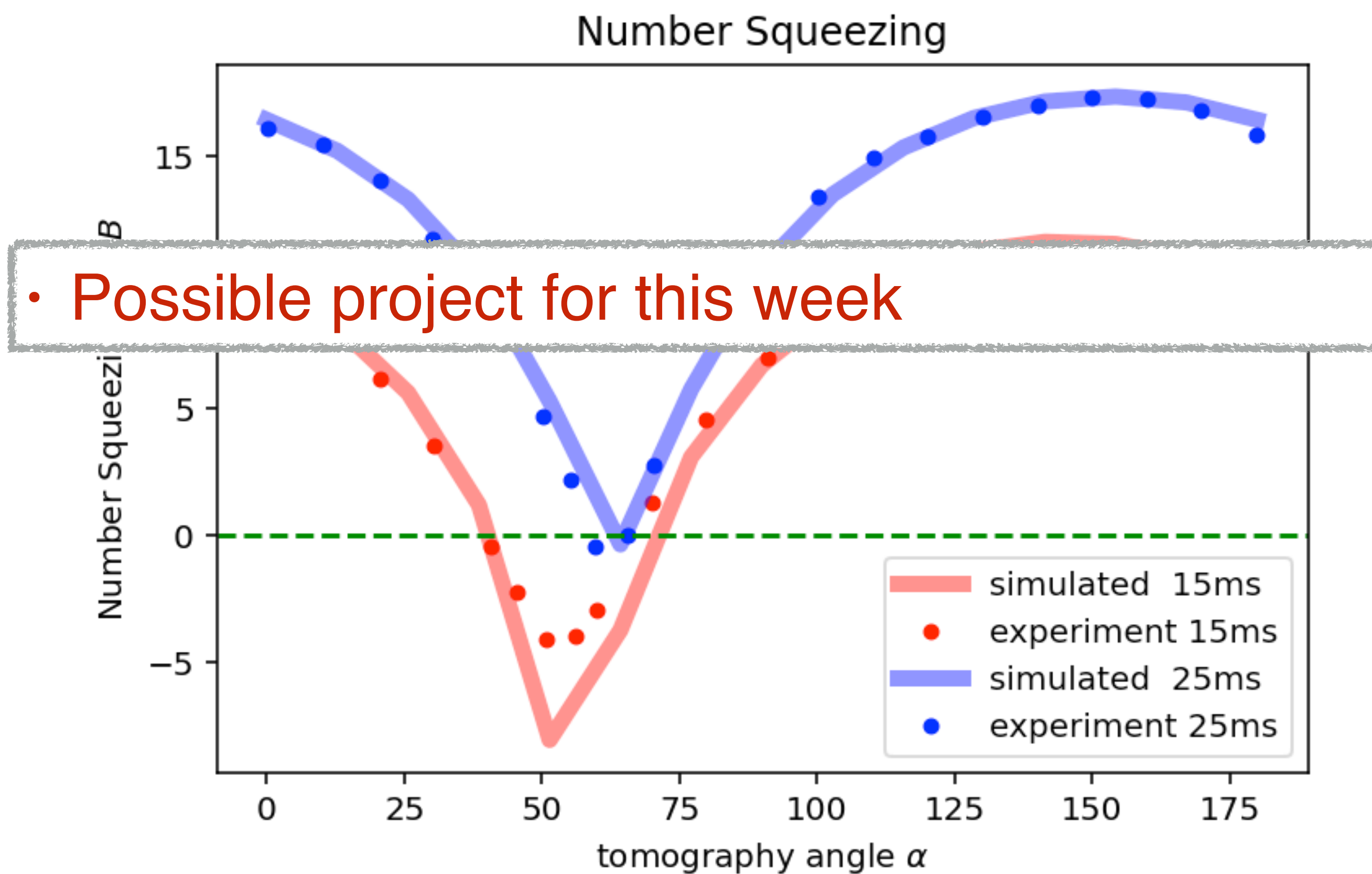
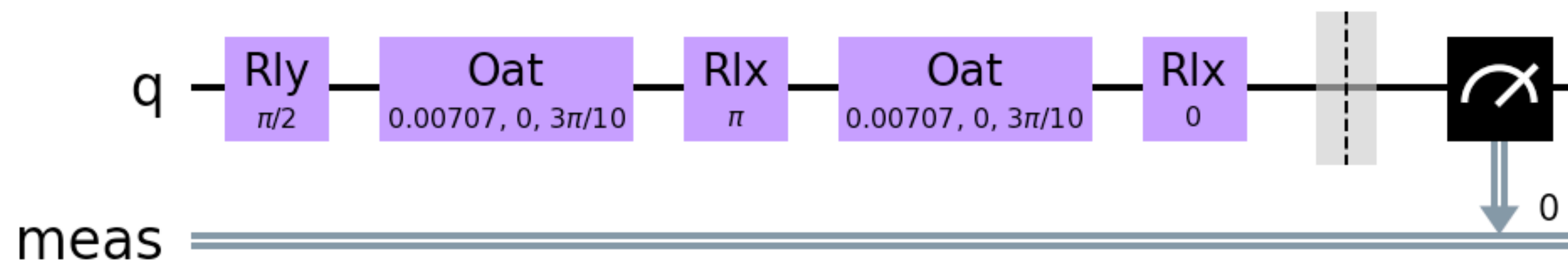
N indistinguishable atoms — qudit —  $\ell = N/2$

$$|\psi\rangle = \alpha_{-\ell} | - \ell\rangle + \dots + \alpha_{\ell} | \ell\rangle$$

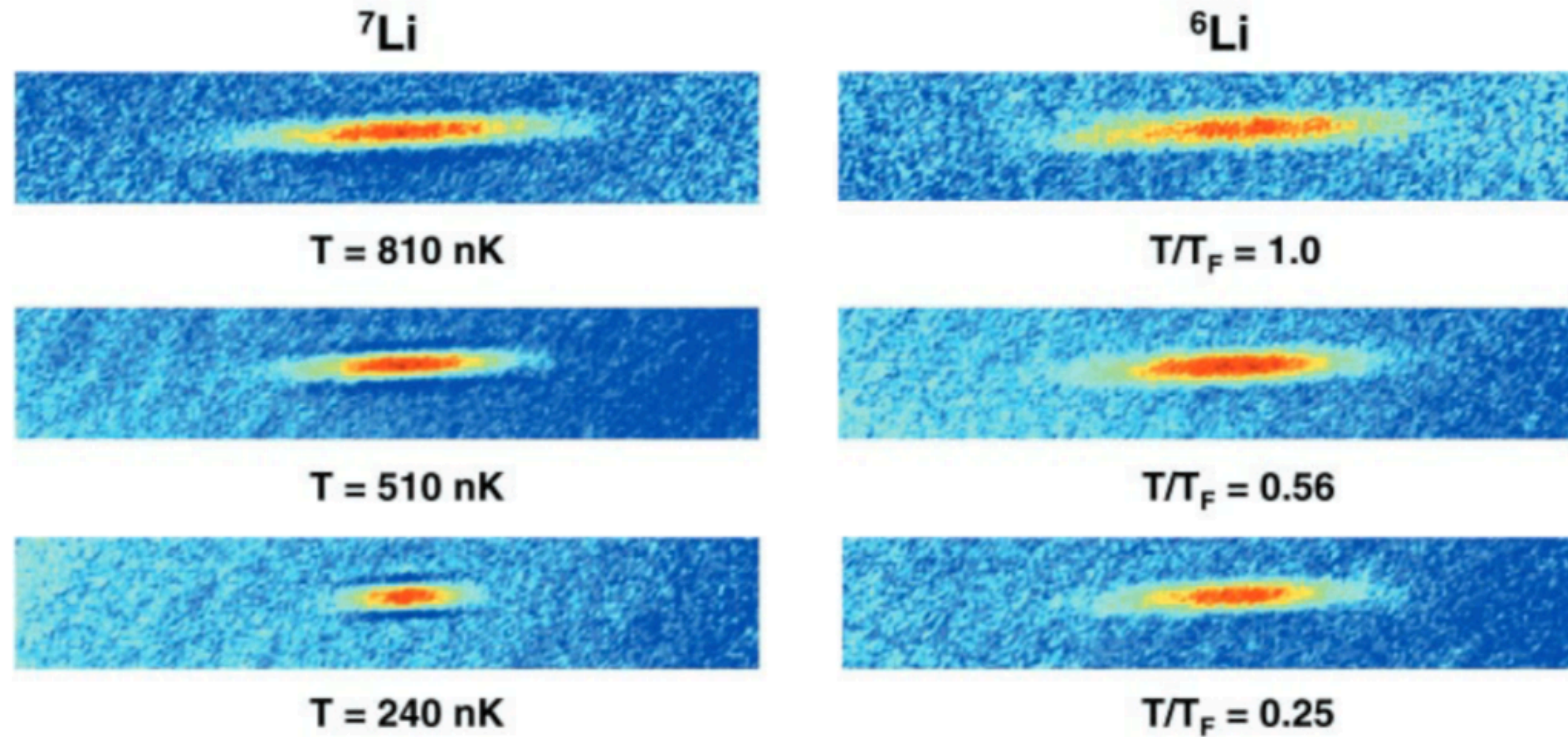
# Squeezing with cold atoms



# Squeezing with cold atoms

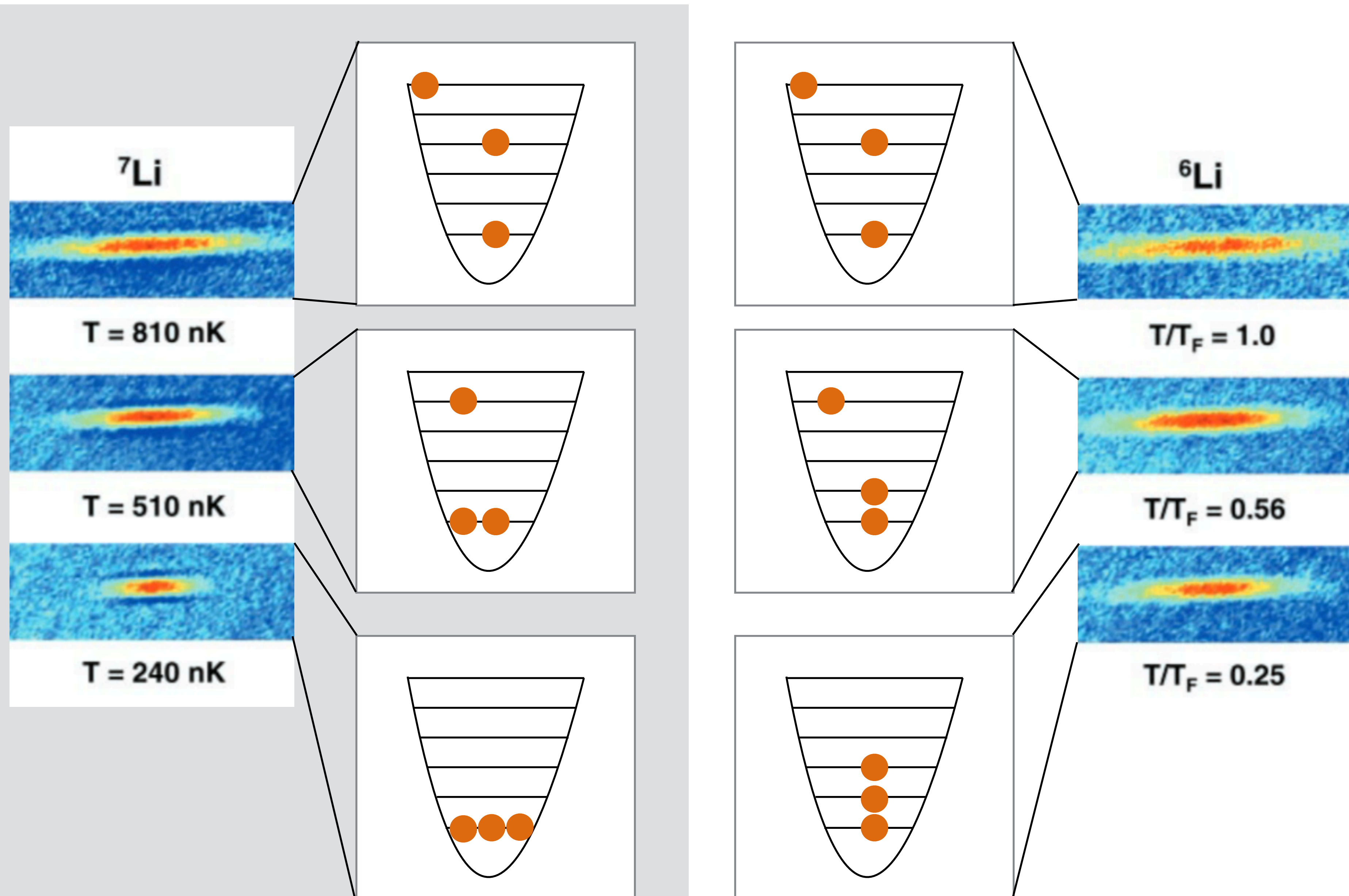


# On fermion vs bosons



A. G. Truscott et al. Science 291, 2570 (2001).

# On fermion vs bosons



# Second quantization

Many particles: full wave-function has to be properly symmetrized

Bosons

$$\psi(1, 2) = \psi(2, 1)$$

Fermions

$$\psi(1, 2) = -\psi(2, 1)$$

Second quantization: work with creation operators at the given states

orthonormal base

$$\hat{\psi} = \sum_i \varphi_i(x) \hat{a}_i$$

lowering operator

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

$$[\hat{a}_i, \hat{a}_k^\dagger] = \delta_{ik}$$

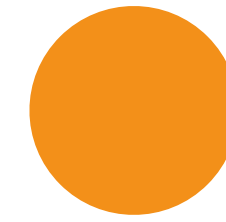
$$[\hat{\psi}(x), \hat{\psi}(x')^\dagger] = \delta(x - x')$$

$$\{\hat{a}_i, \hat{a}_k^\dagger\} = \delta_{ik}$$

$$\{\hat{\psi}(x), \hat{\psi}(x')^\dagger\} = \delta(x - x')$$

# Number states of bosons and fermions

Single orbit



Bosons

$$\hat{a}^\dagger |0\rangle = |1\rangle$$

$$\hat{a}^\dagger |1\rangle = \sqrt{2} |2\rangle$$

$\vdots$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

Hilbert space infinite on each site

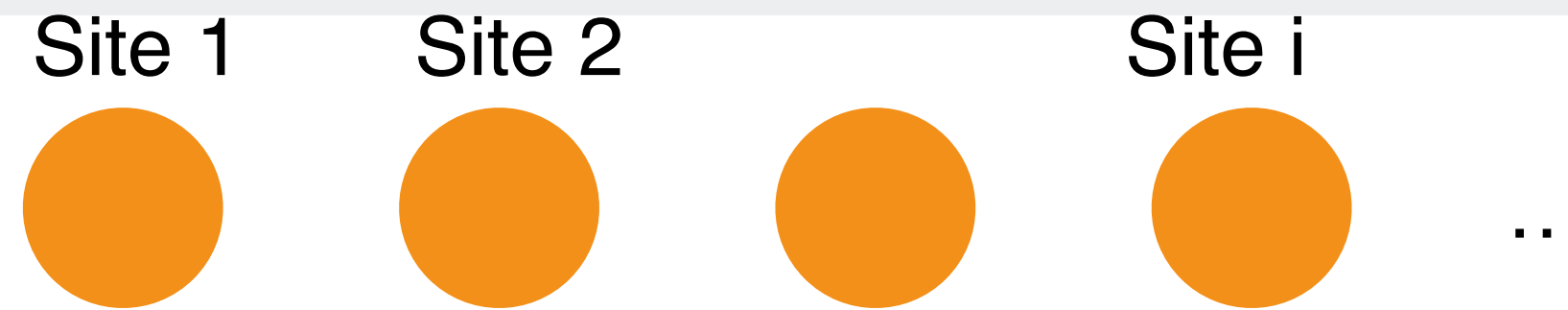
Fermions

$$\hat{a}^\dagger |0\rangle = |1\rangle$$

$$\hat{a}^\dagger |1\rangle = 0$$

Only two states (like for qubits)

# Number states of bosons and fermions



Bosons

$$\hat{a}_j^\dagger |n_0, \dots, n_j, \dots\rangle = \sqrt{n_j + 1} |n_0, \dots, n_j + 1, \dots\rangle$$

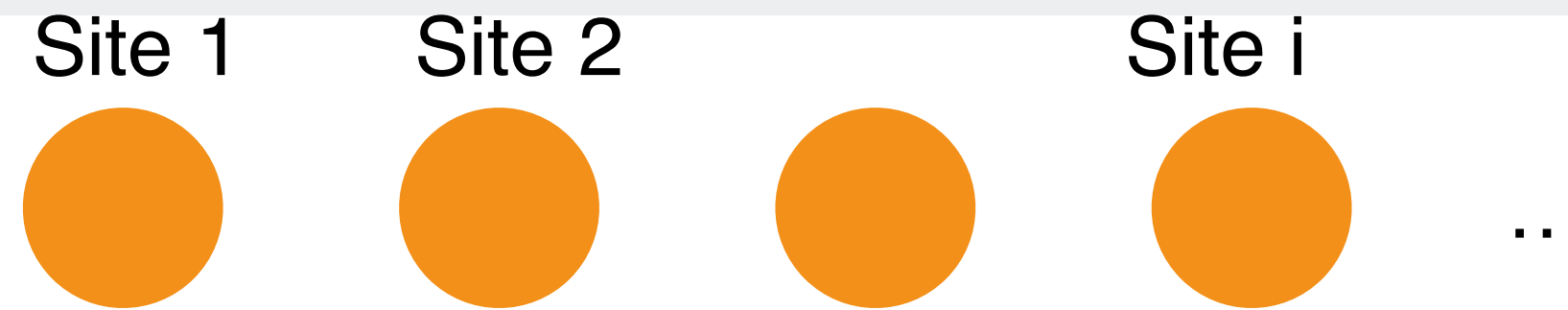
Fermions

$$\hat{a}_j^\dagger |n_0, \dots, n_j, \dots\rangle = (-1)^{\sum_{i < j} n_i} \sqrt{1 - n_j} |n_0, \dots, n_j + 1, \dots\rangle$$

Sign problem



# Number states of bosons and fermions



Bosons

Fermions

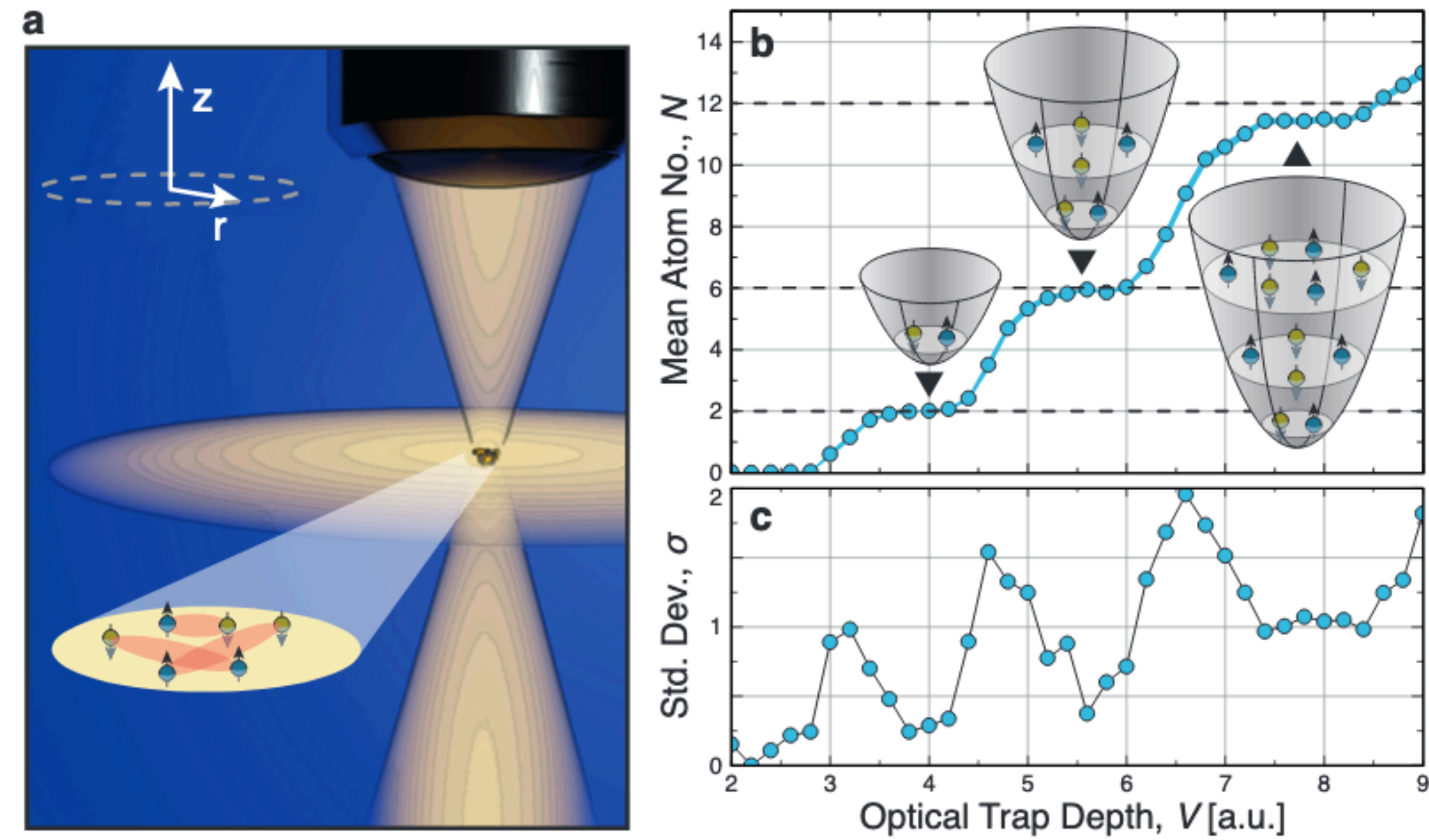
- Quite complicated even on quantum computers
- Solve this in natural implementations ?

$$\hat{a}_j^\dagger |n_0, \dots, n_j, \dots\rangle = \sqrt{n_j + 1} |n_0, \dots, n_j + 1, \dots\rangle$$

$$a_j |n_0, \dots, n_j, \dots\rangle = (-1)^{i_{<j}} \sqrt{1 - n_j} |n_0, \dots, n_j - 1, \dots\rangle$$

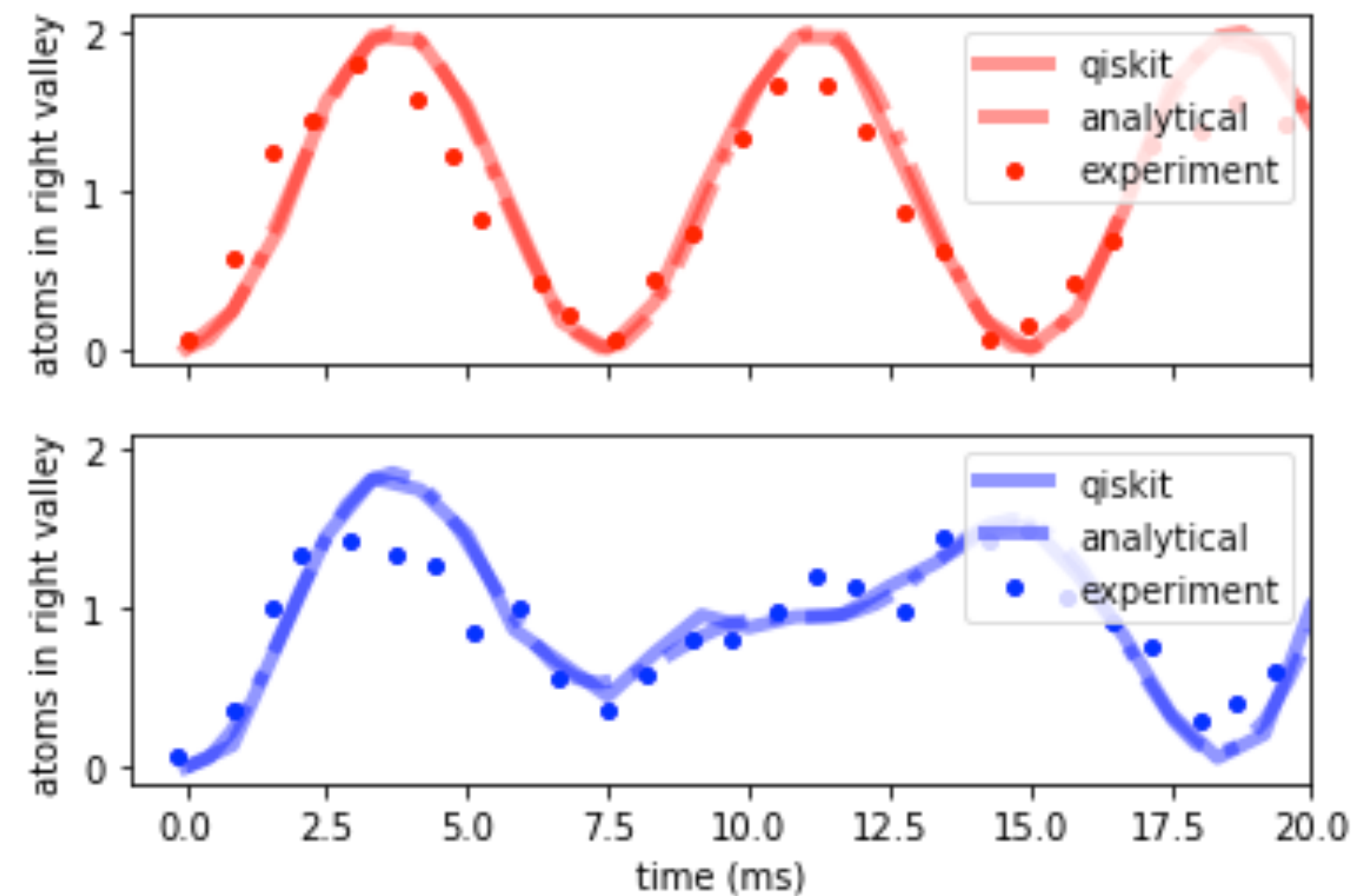
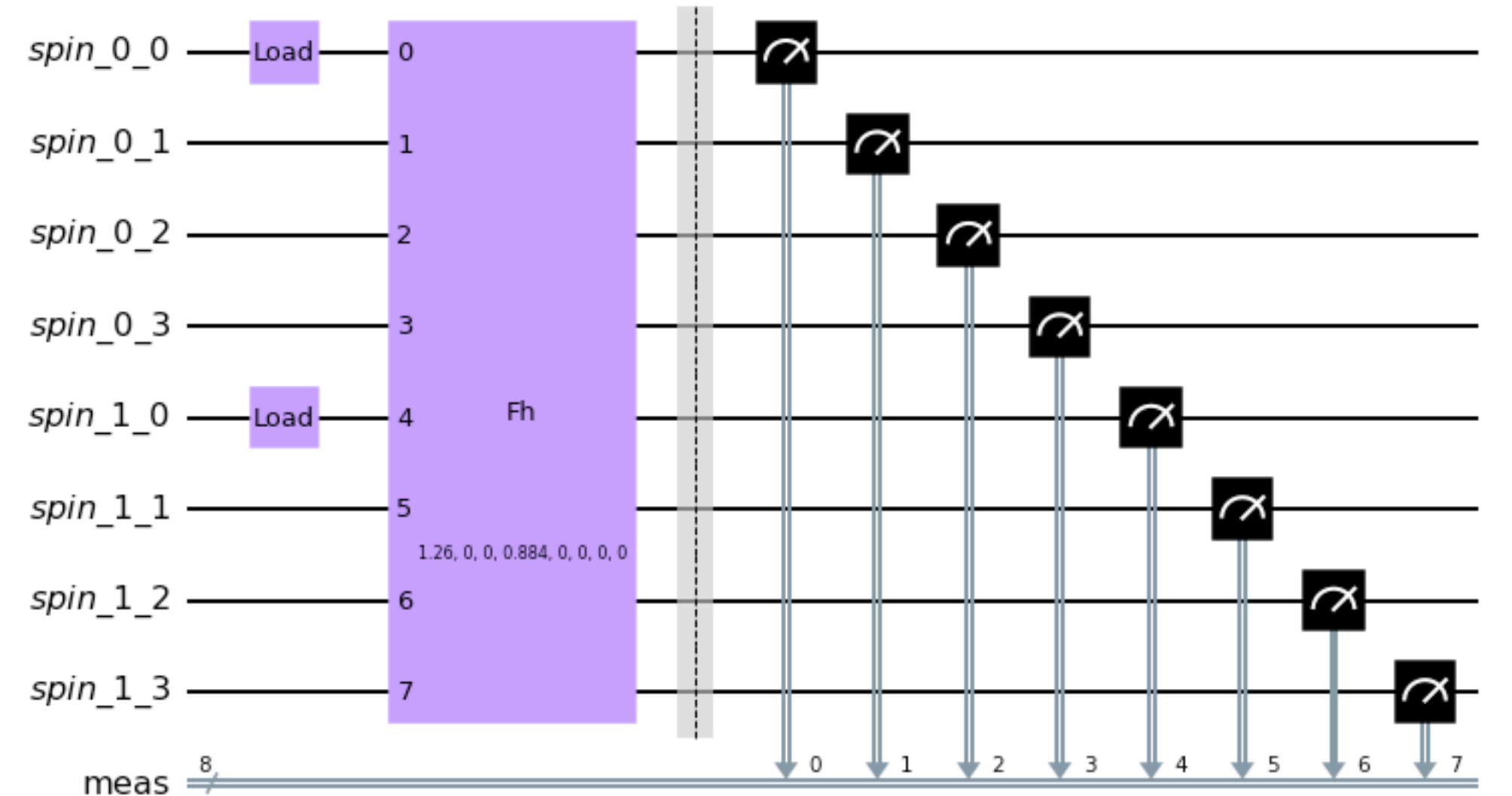
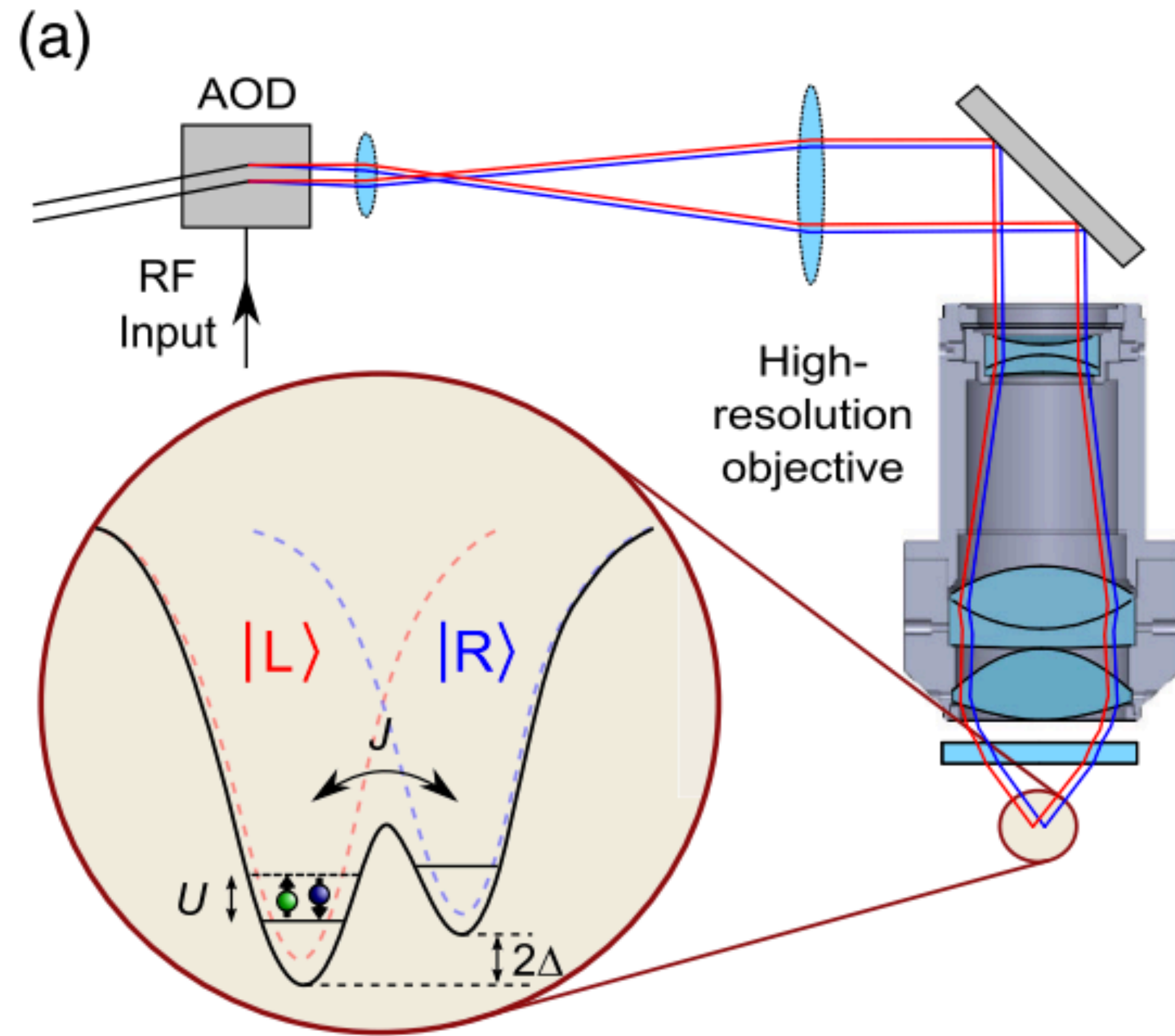
Sign problem

# One fermion at a time

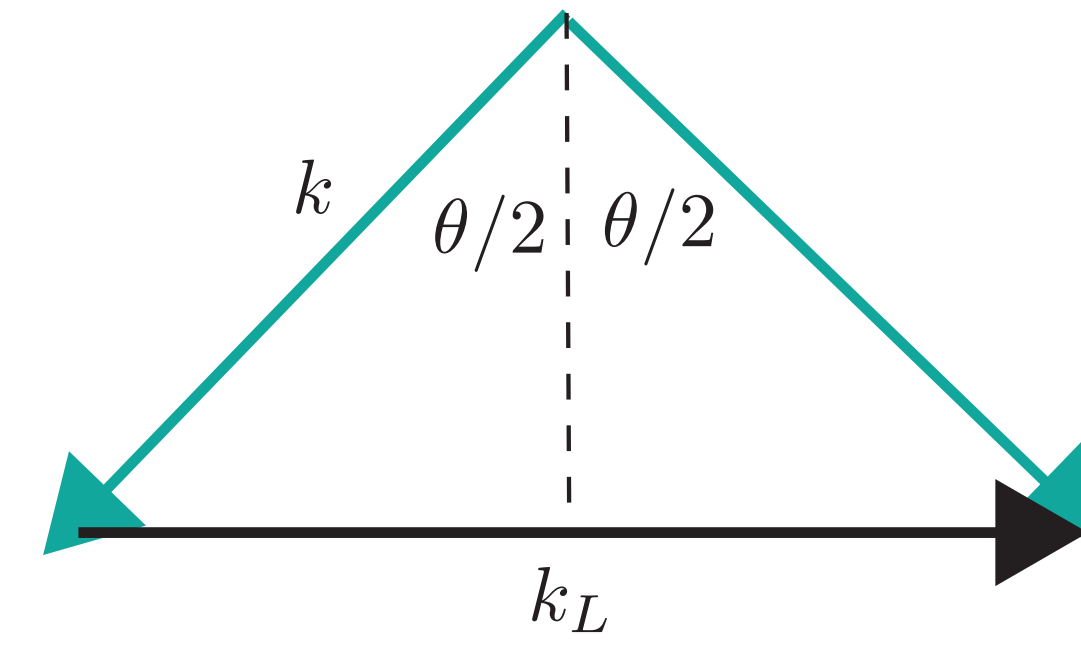
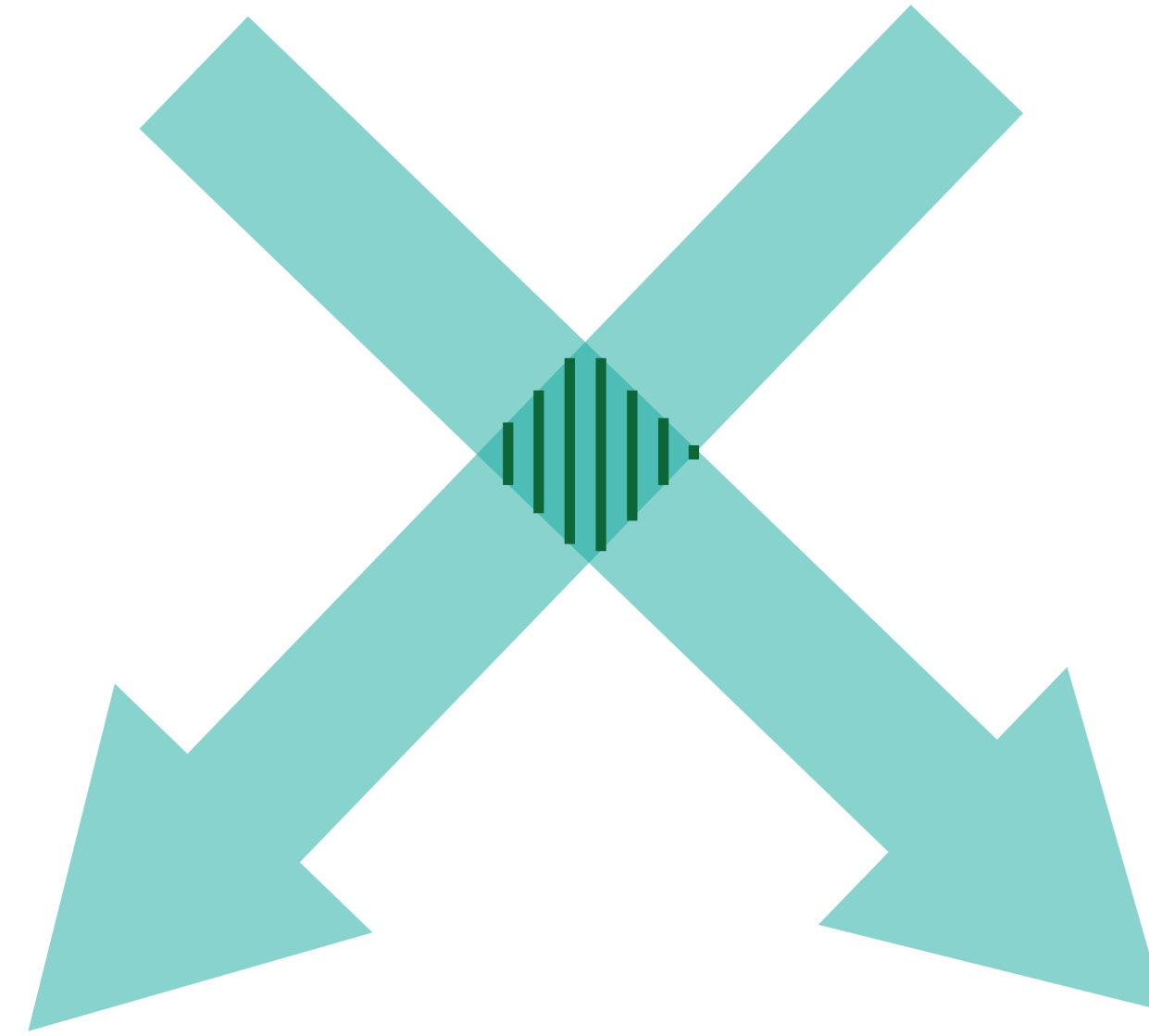


L. Bayha et al., arXiv 2004.14761 (2020).

# Fermions in different tweezers



# Now let's go real big - the optical lattice



$$\sin(\theta/2) = \frac{k_L/2}{k}$$

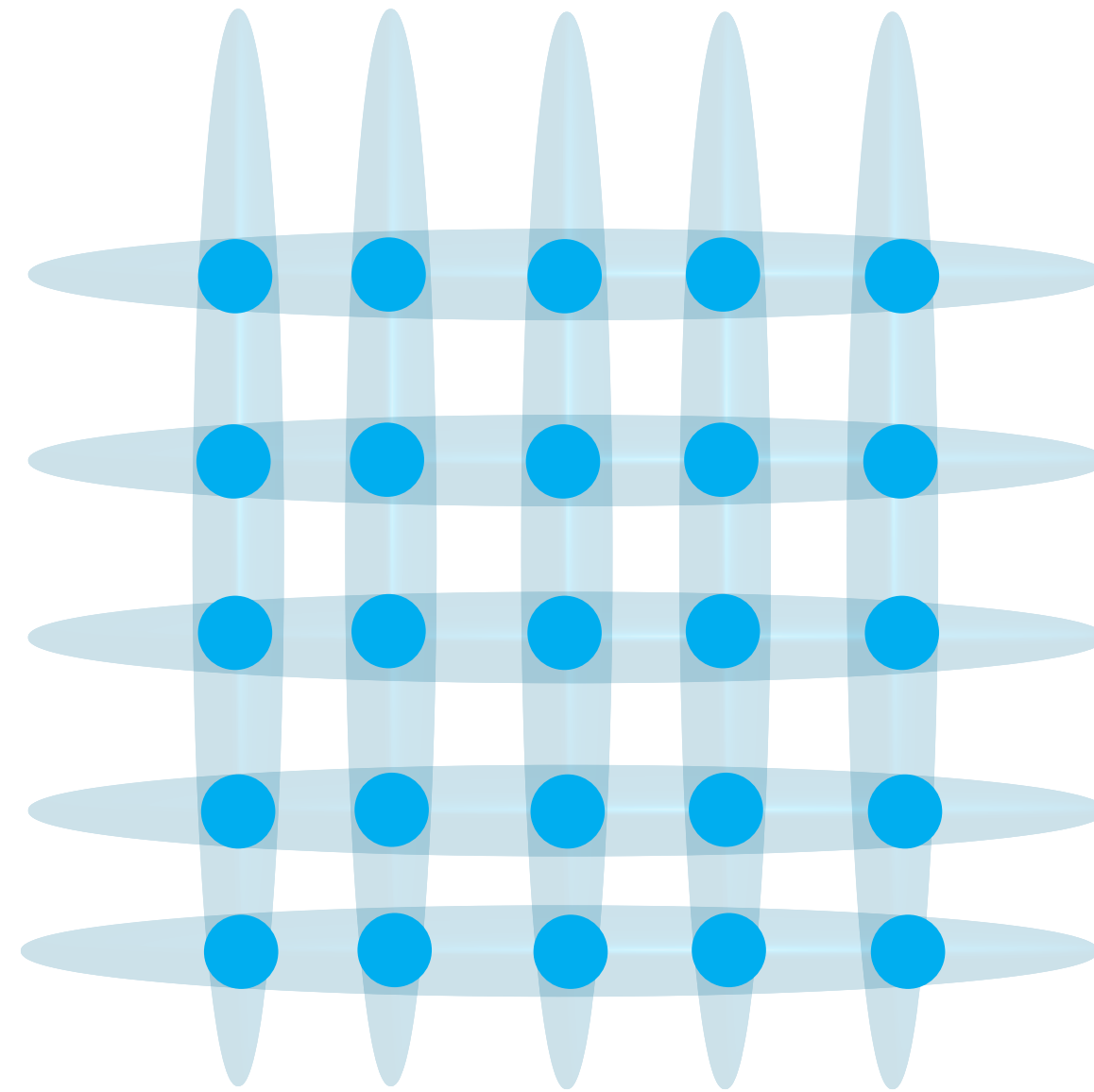
Lattice spacing:

$$a_L = \frac{\lambda}{2 \sin(\theta/2)}$$

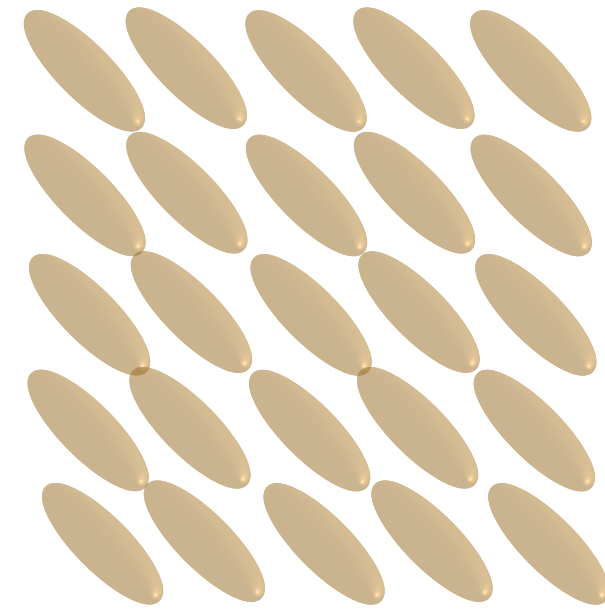
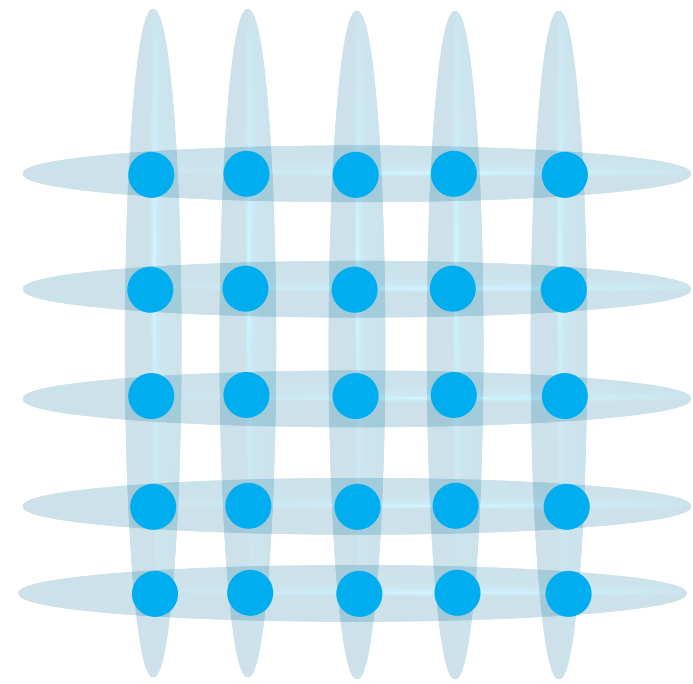
Optical lattice with potential:  $V_L = V_0 \sin^2(k_L x)$        $k_L = \frac{\pi}{a_L}$

# Higher dimensional lattice

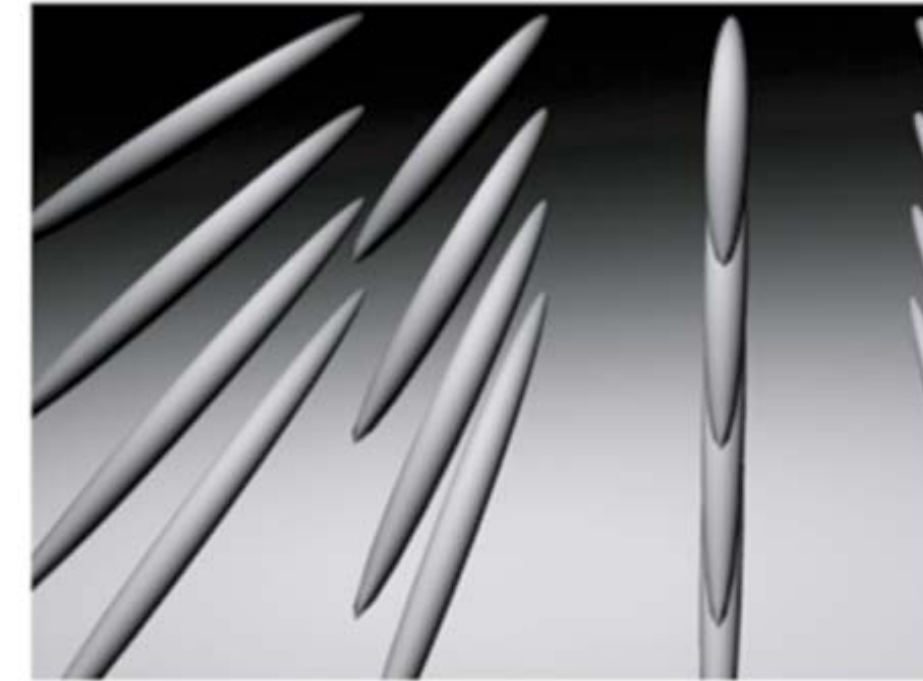
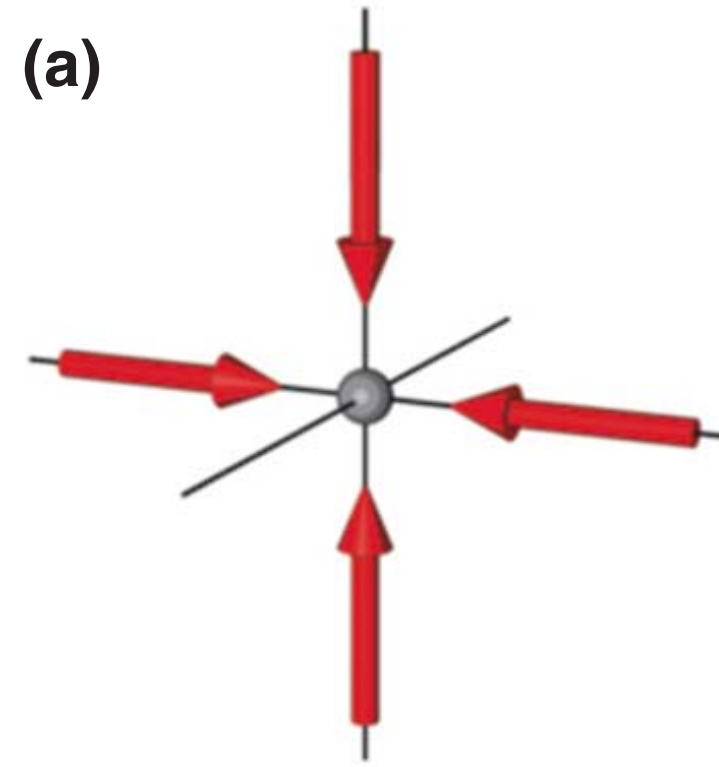
Cross the polarization !



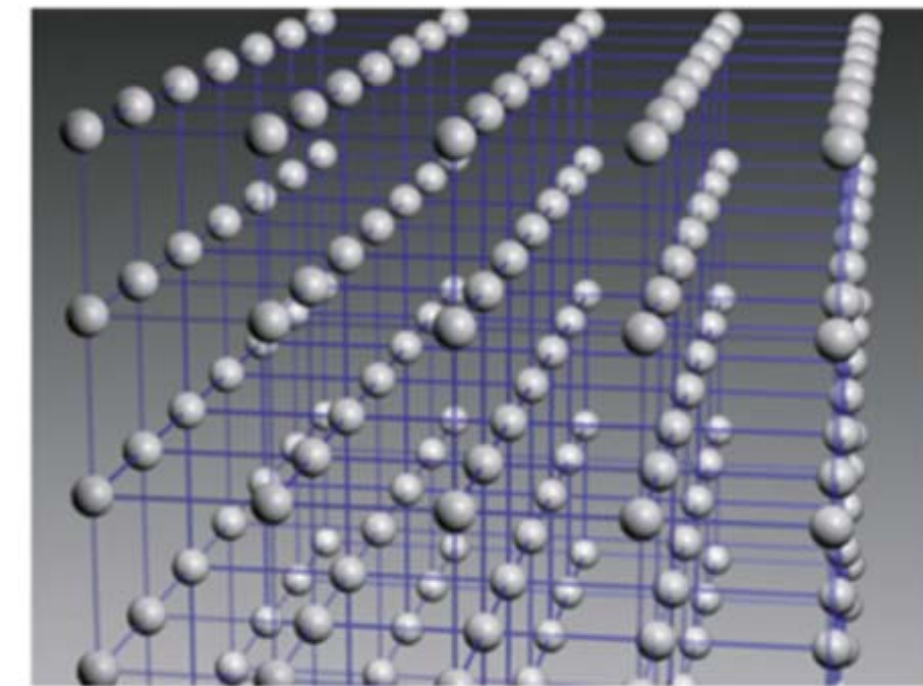
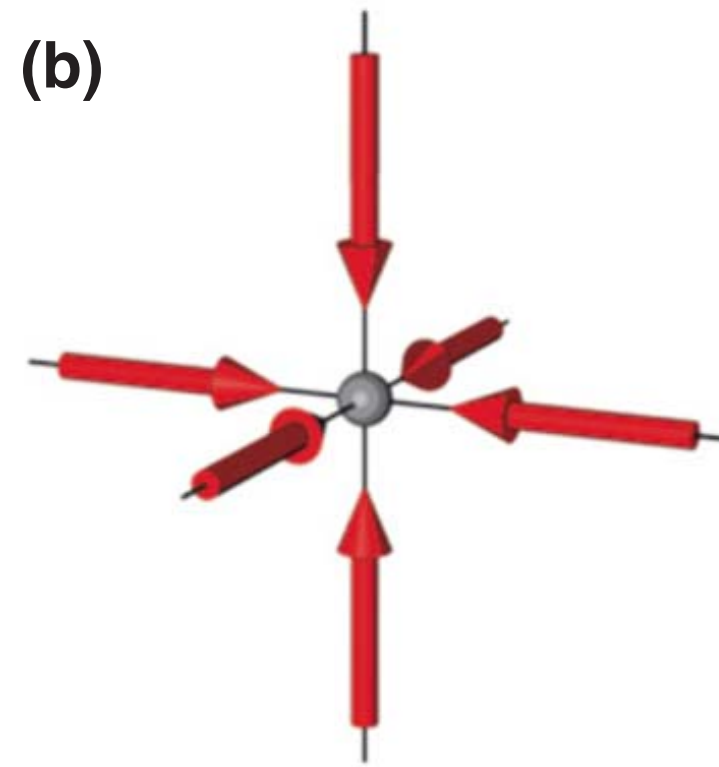
# Higher dimensional lattice



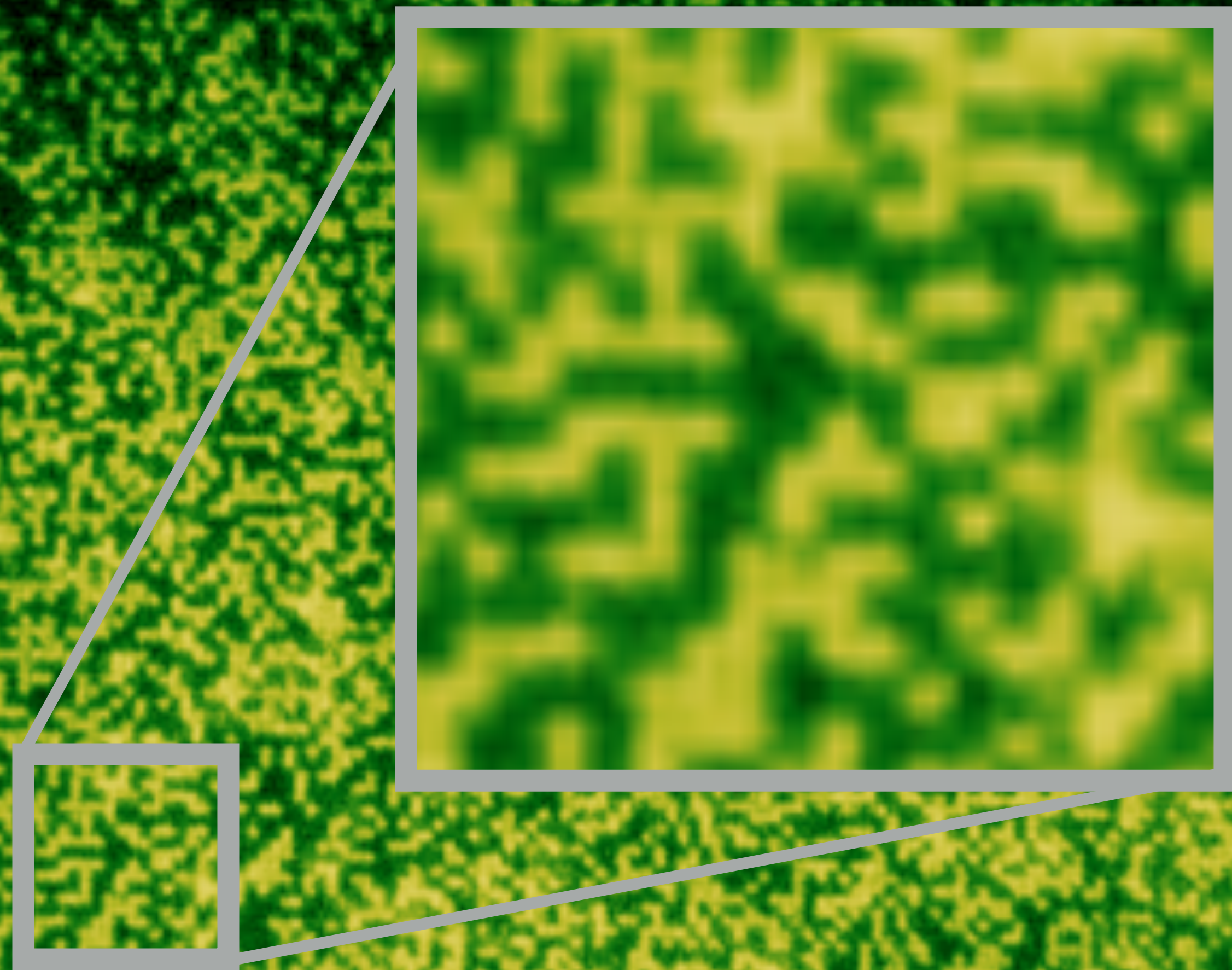
(a)



(b)

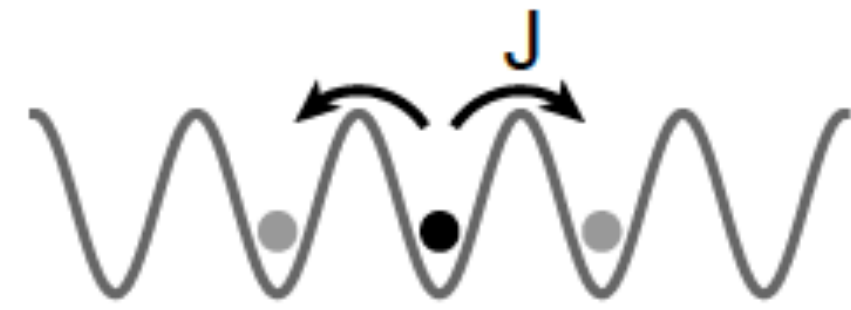


Zwenger et al. RMP



# Bose-Hubbard Model

$$H = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{h.c.}) + \frac{U}{2} \sum_i n_i(n_i - 1)$$



tunneling J

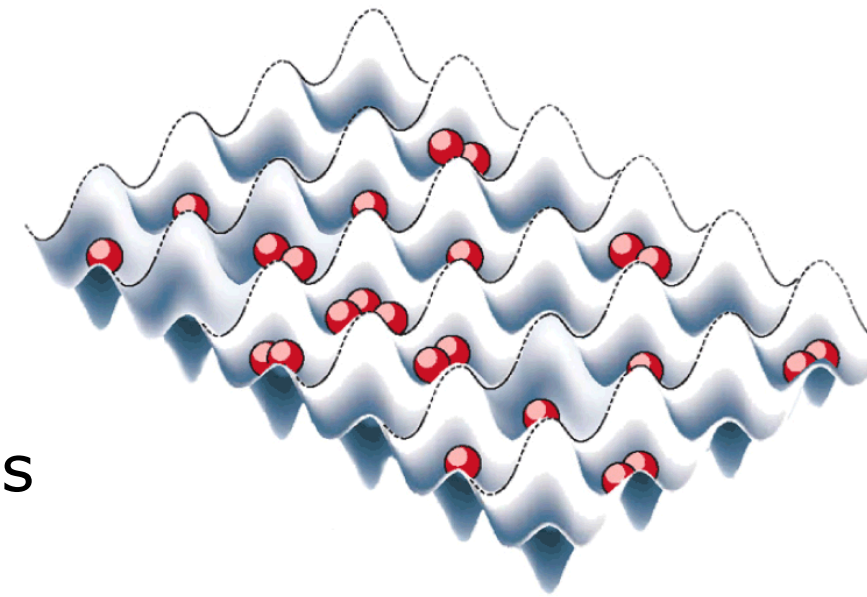


interaction U

$$U \ll J$$

## Superfluid

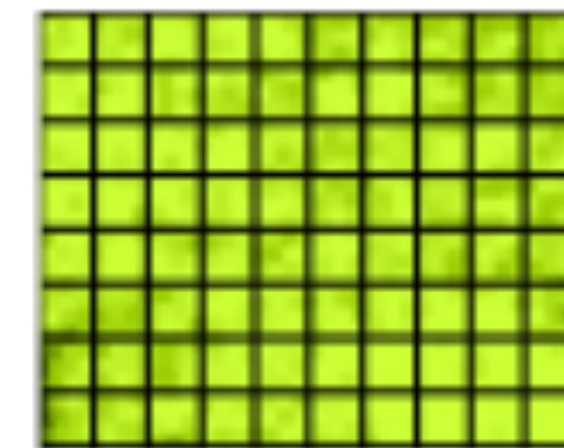
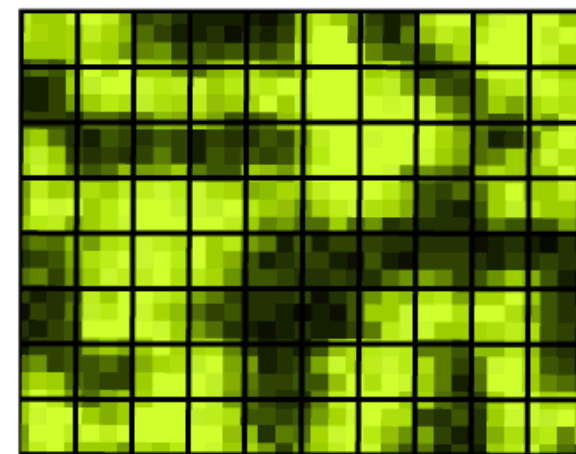
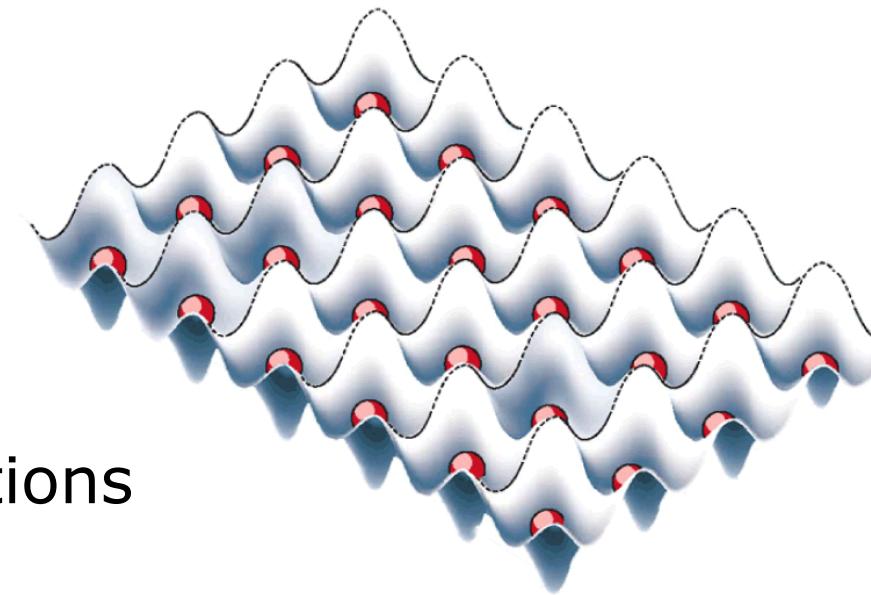
- Large number fluctuations
- Coherent state on-site



$$J \ll U$$

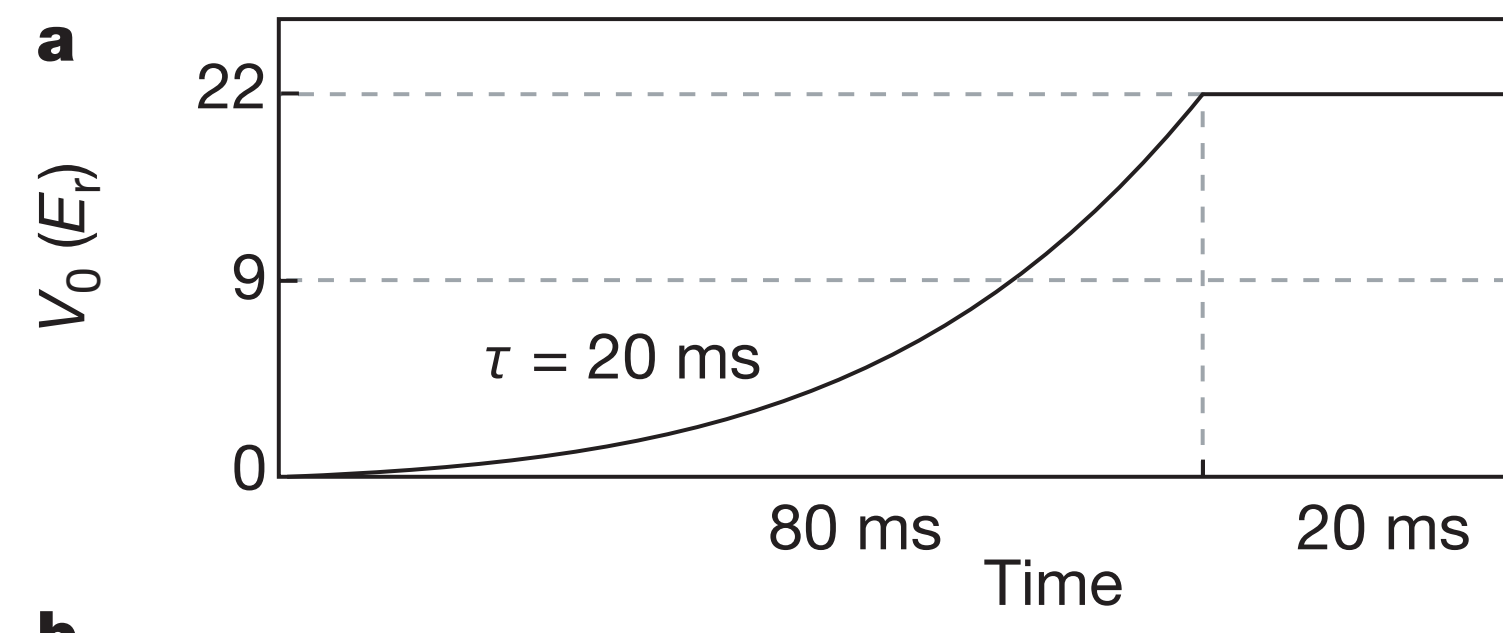
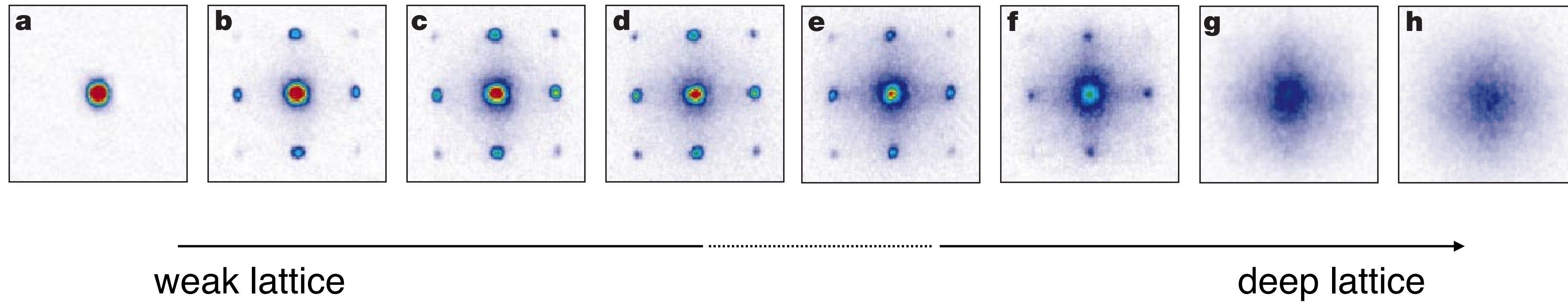
## Mott insulator

- No number fluctuations
- Fock state on-site



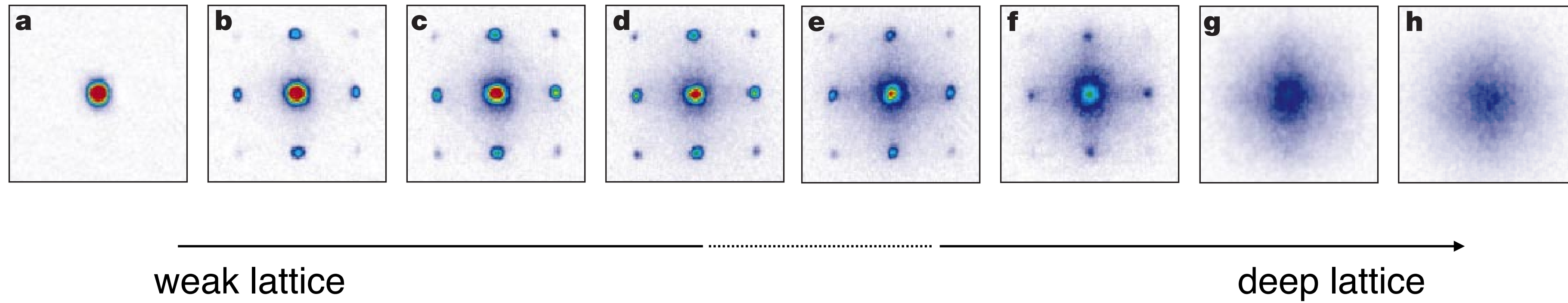


# Observation

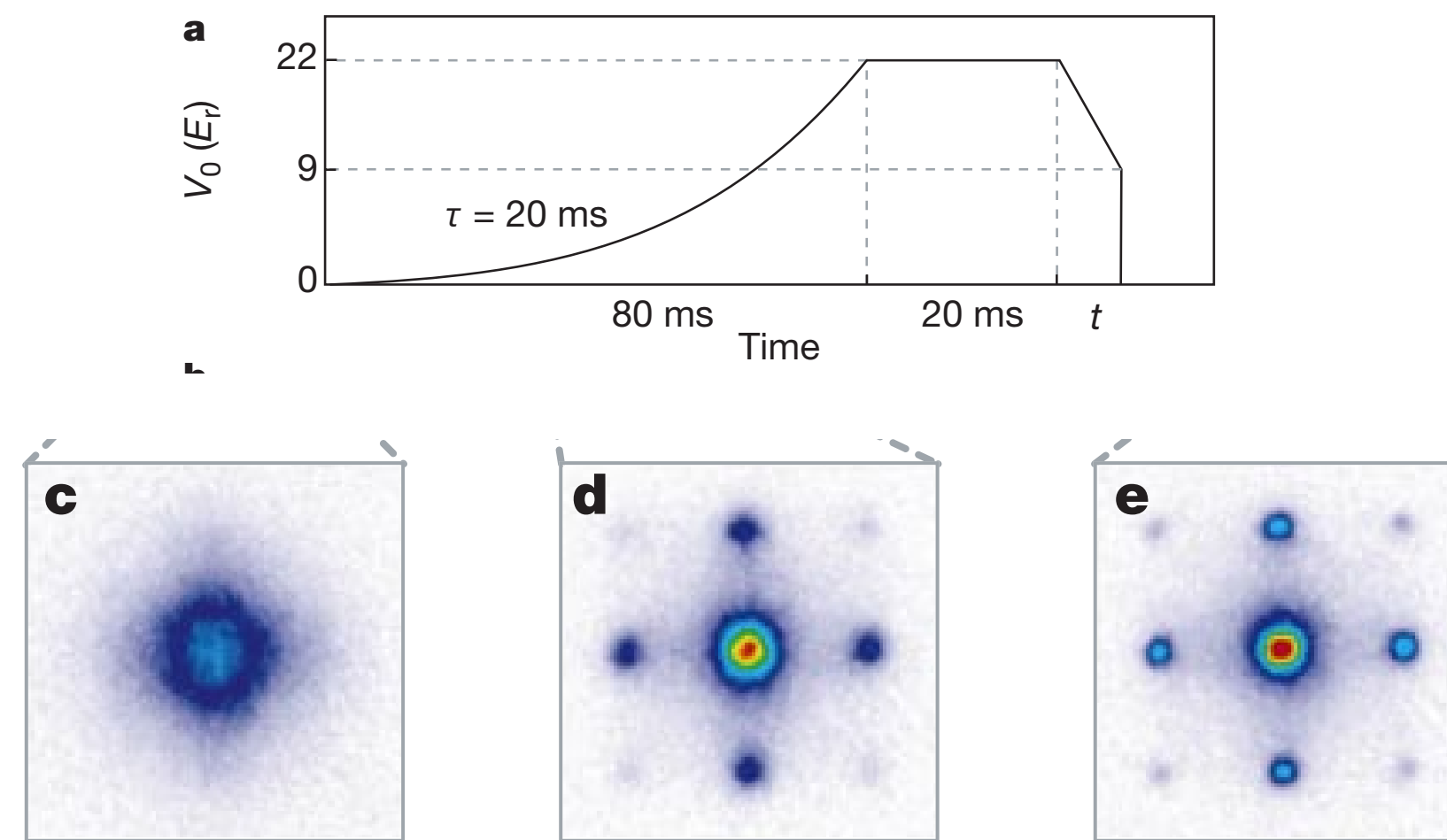


Greiner *et al.*, *Nature* **415** 39 (2002)

# Observation

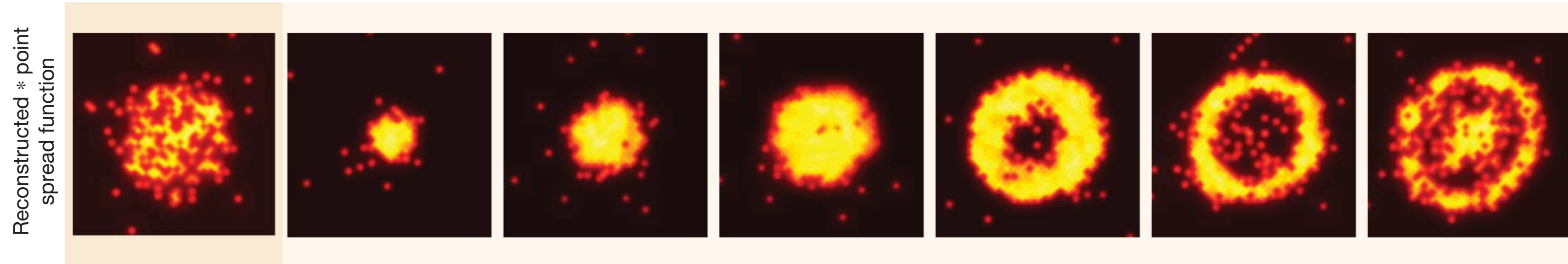


And it is reversible:

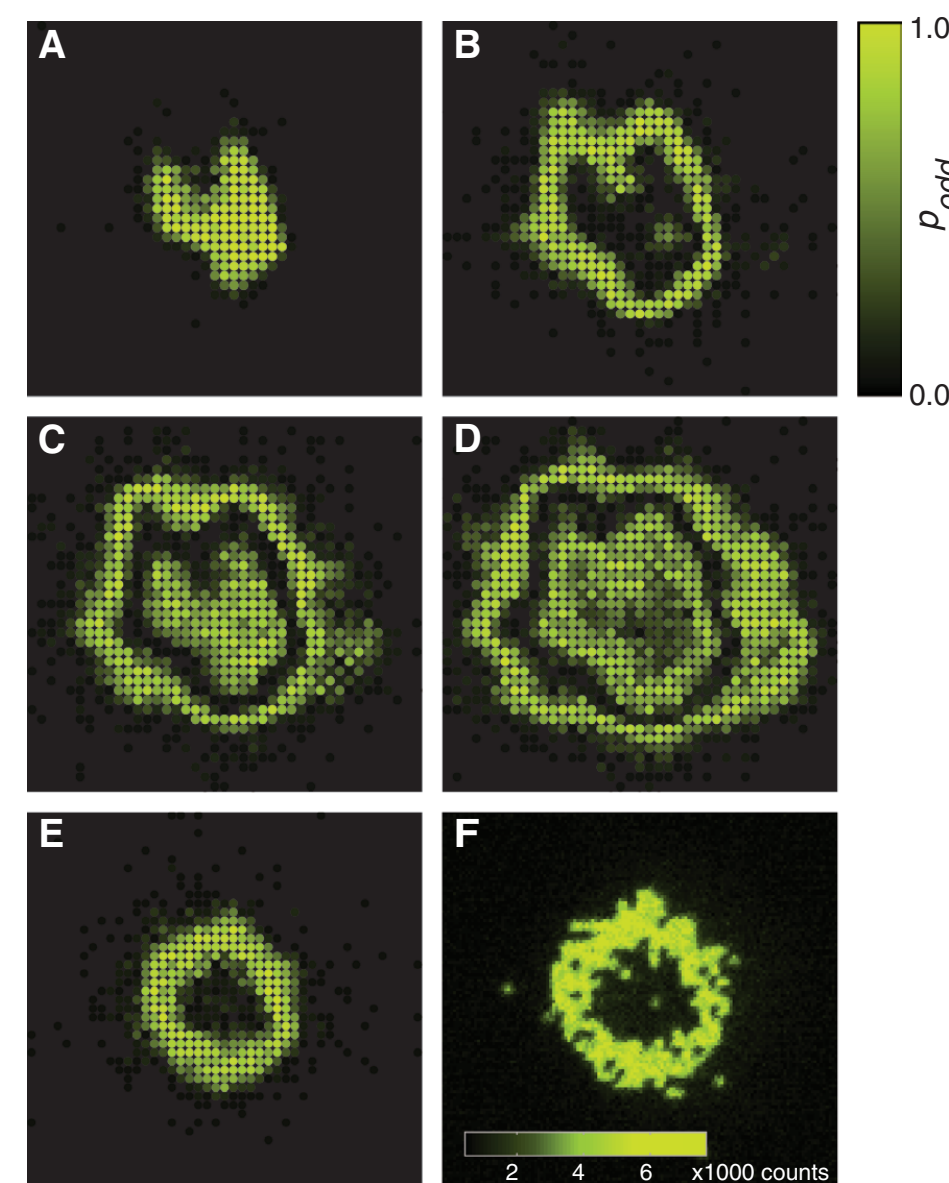


Greiner *et al.*, *Nature* **415** 39 (2002)

# In-situ observation



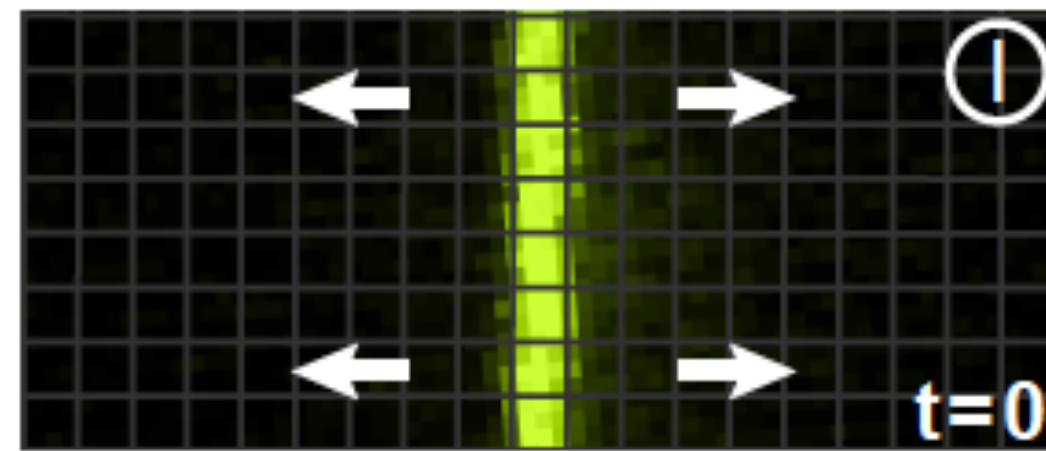
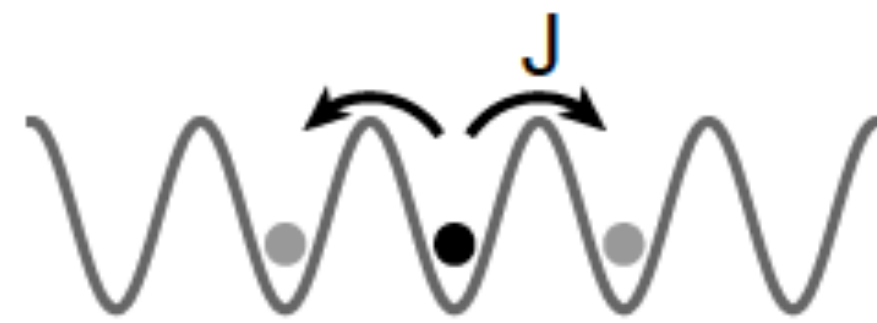
J. Sherson *et al.* *Nature* **467** 68 (2010)



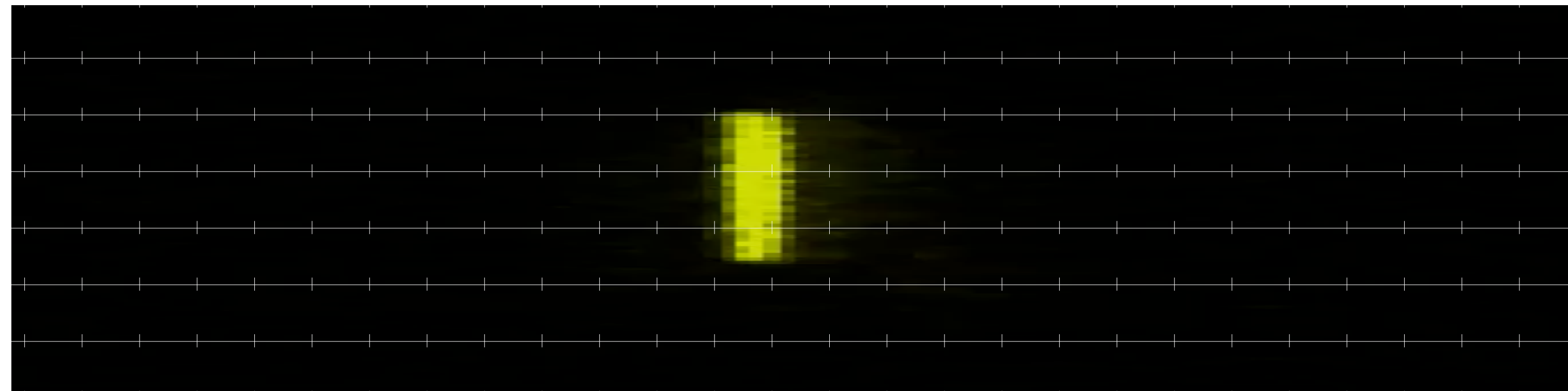
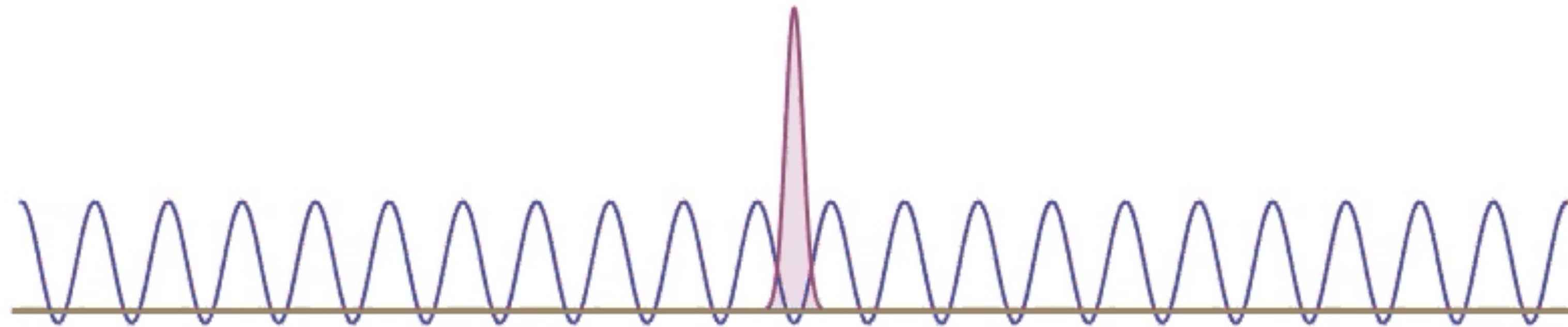
W. Bakr *et al.* *Science* **329** 547 (2010)

# Single-Particle Quantum Walk

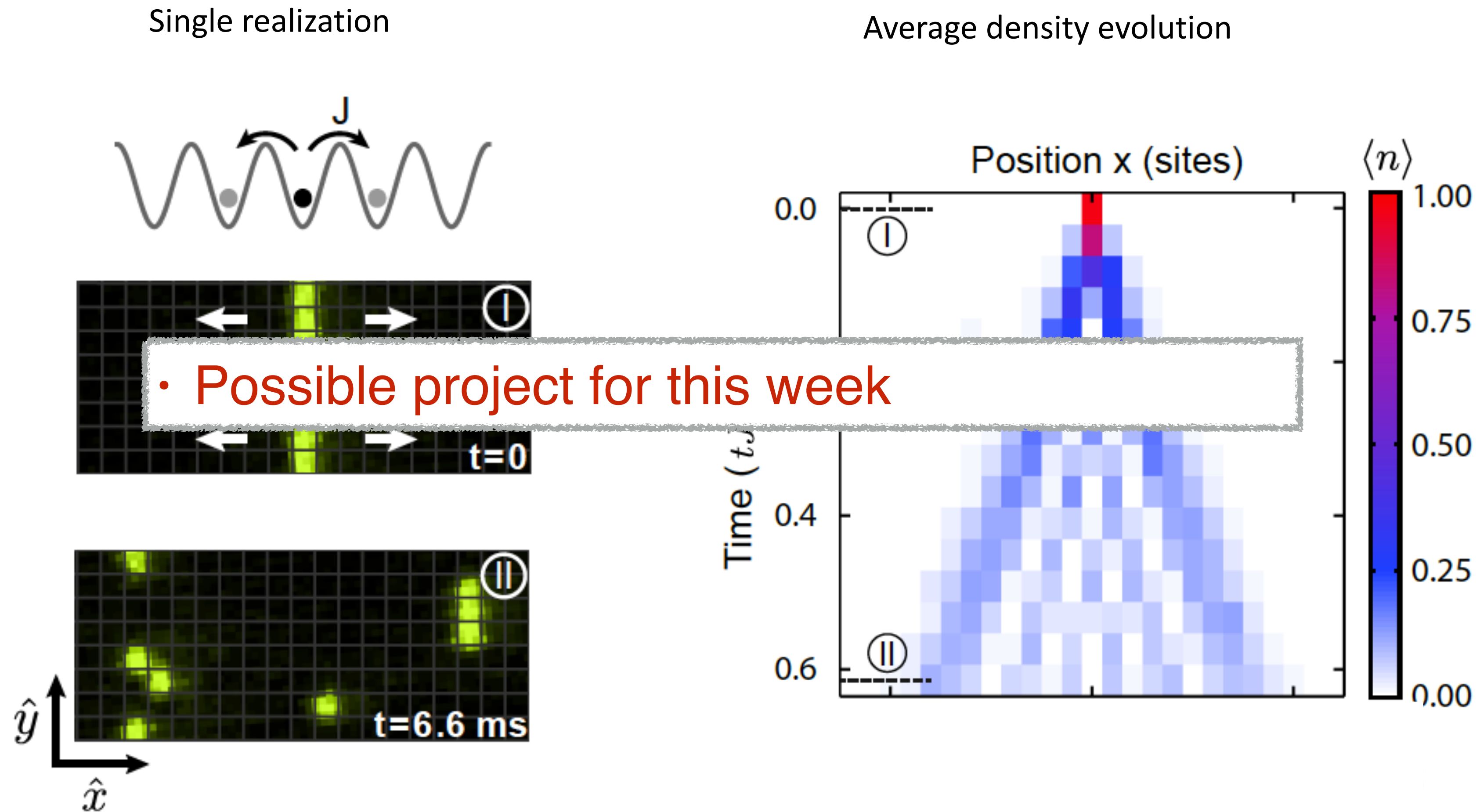
Single realization



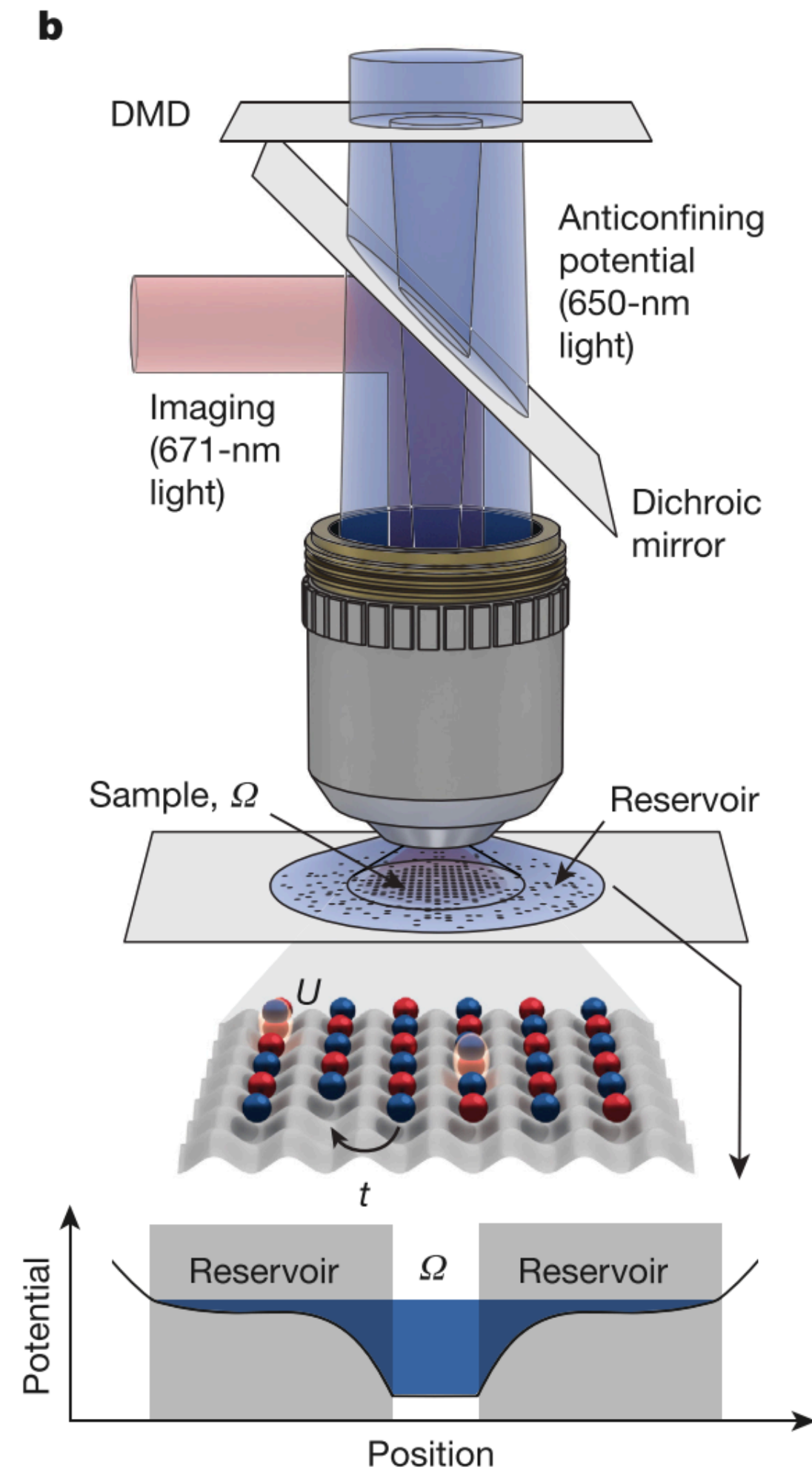
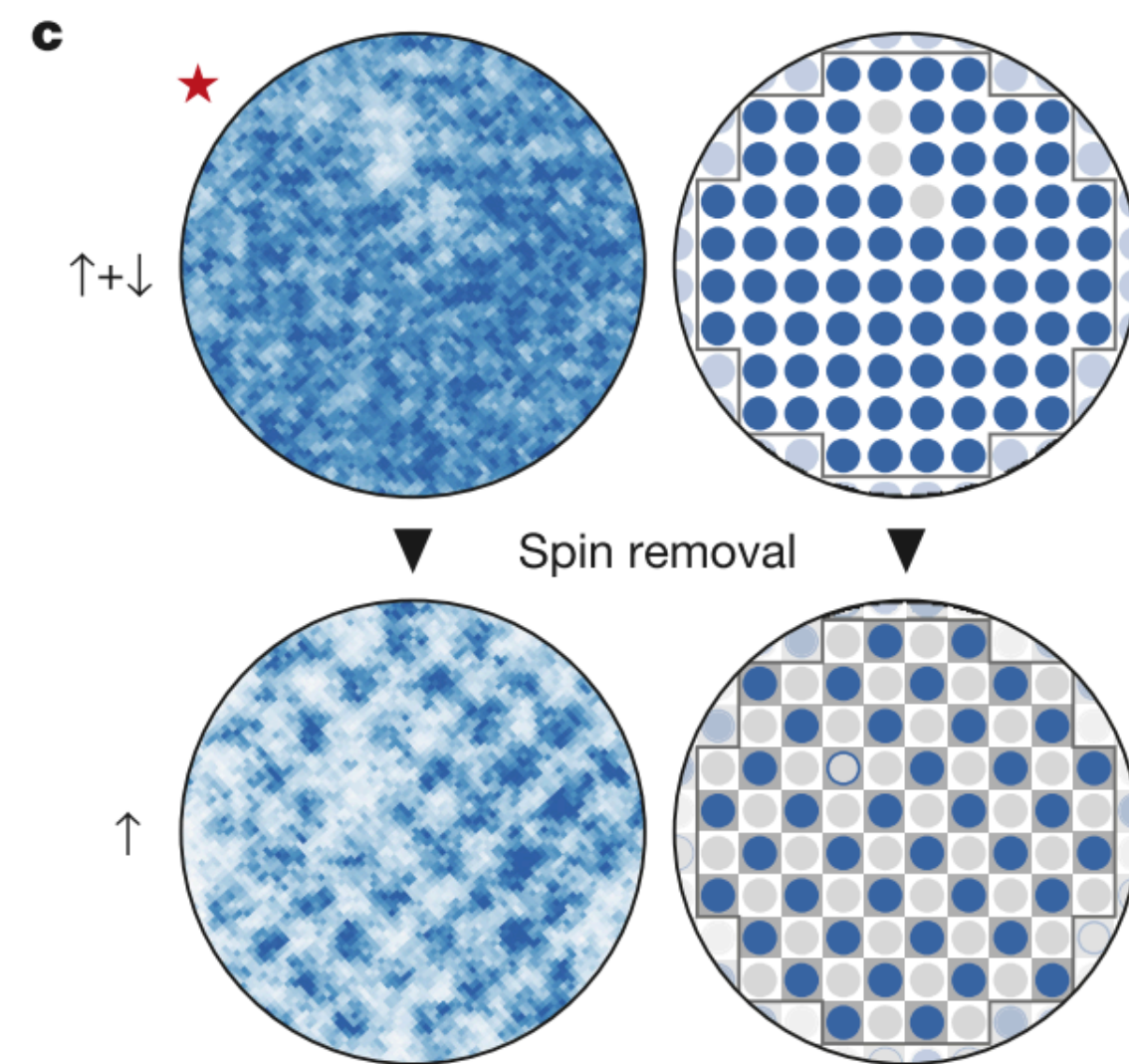
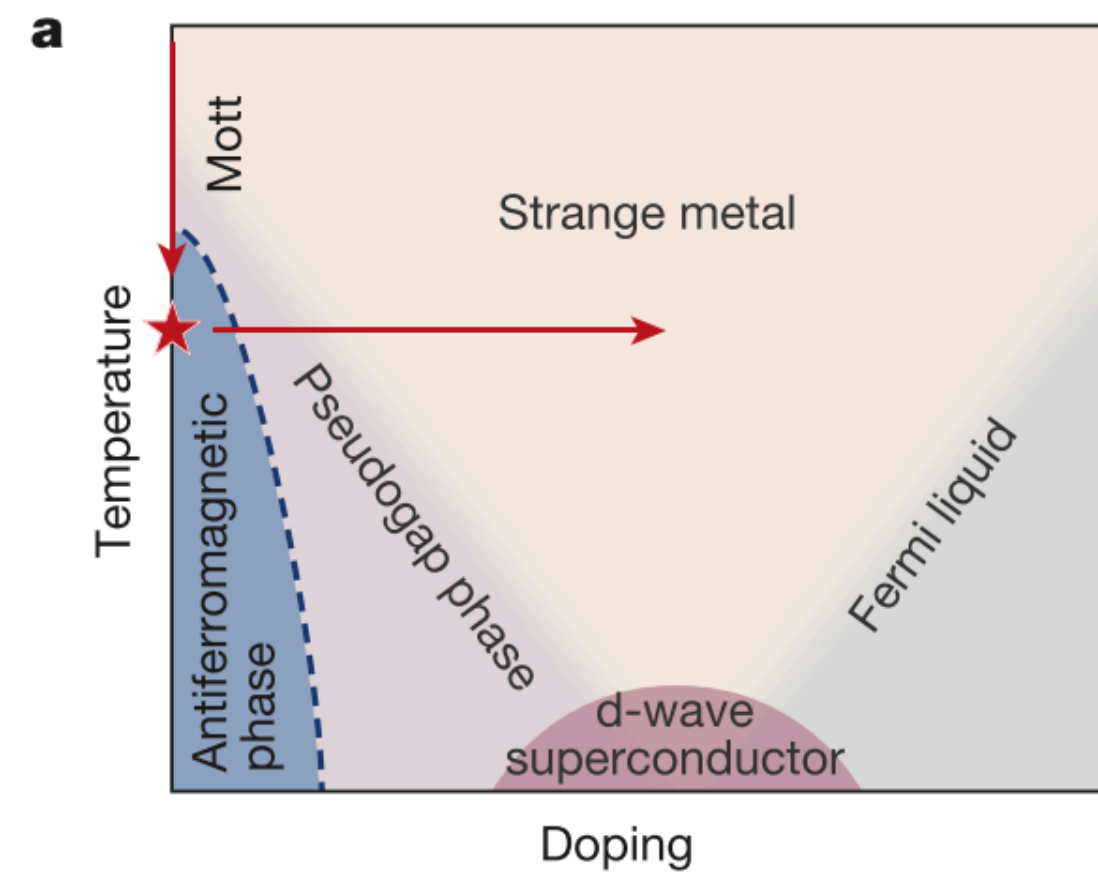
# Single-Particle Quantum Walk



# Single-Particle Quantum Walk

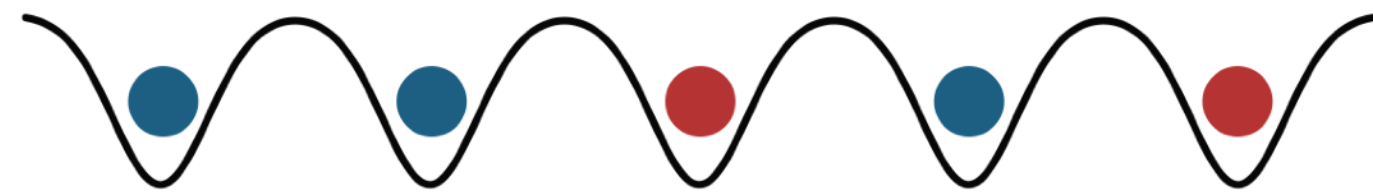
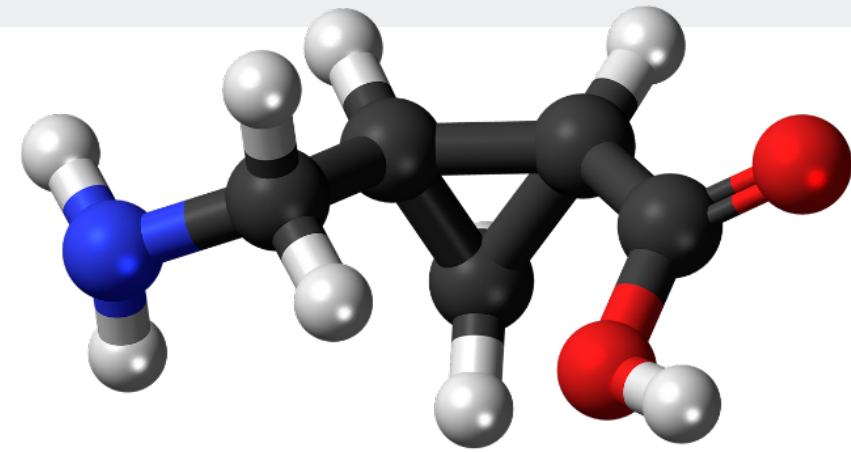


# The Fermi-Hubbard model

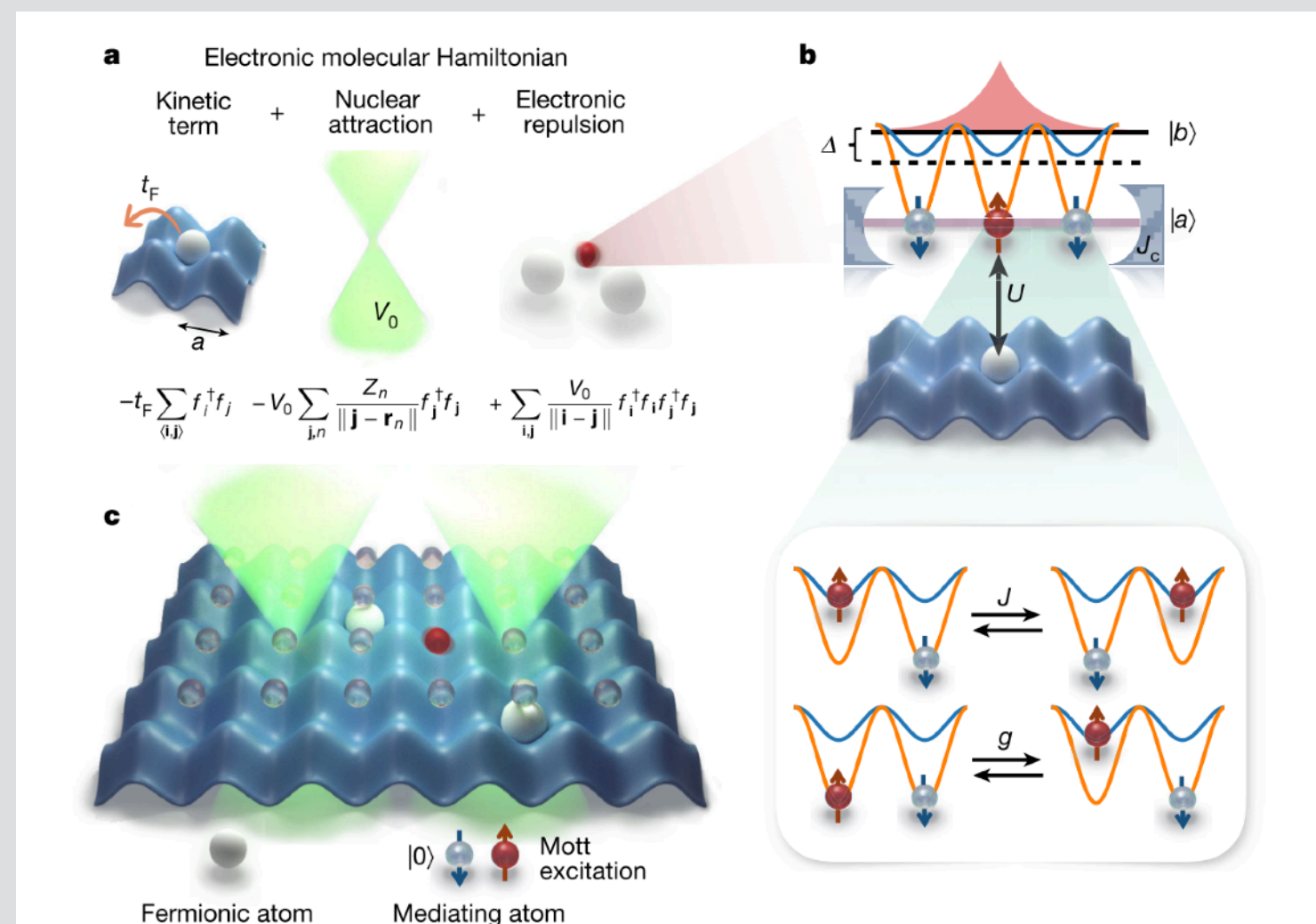


A. Mazurenko et al., Nature 545, 462 (2016).

# Putting chemistry into the machines - electronic structure



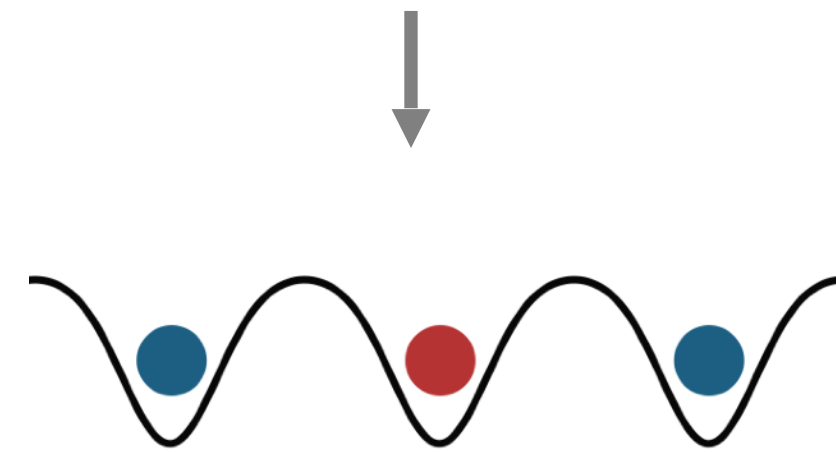
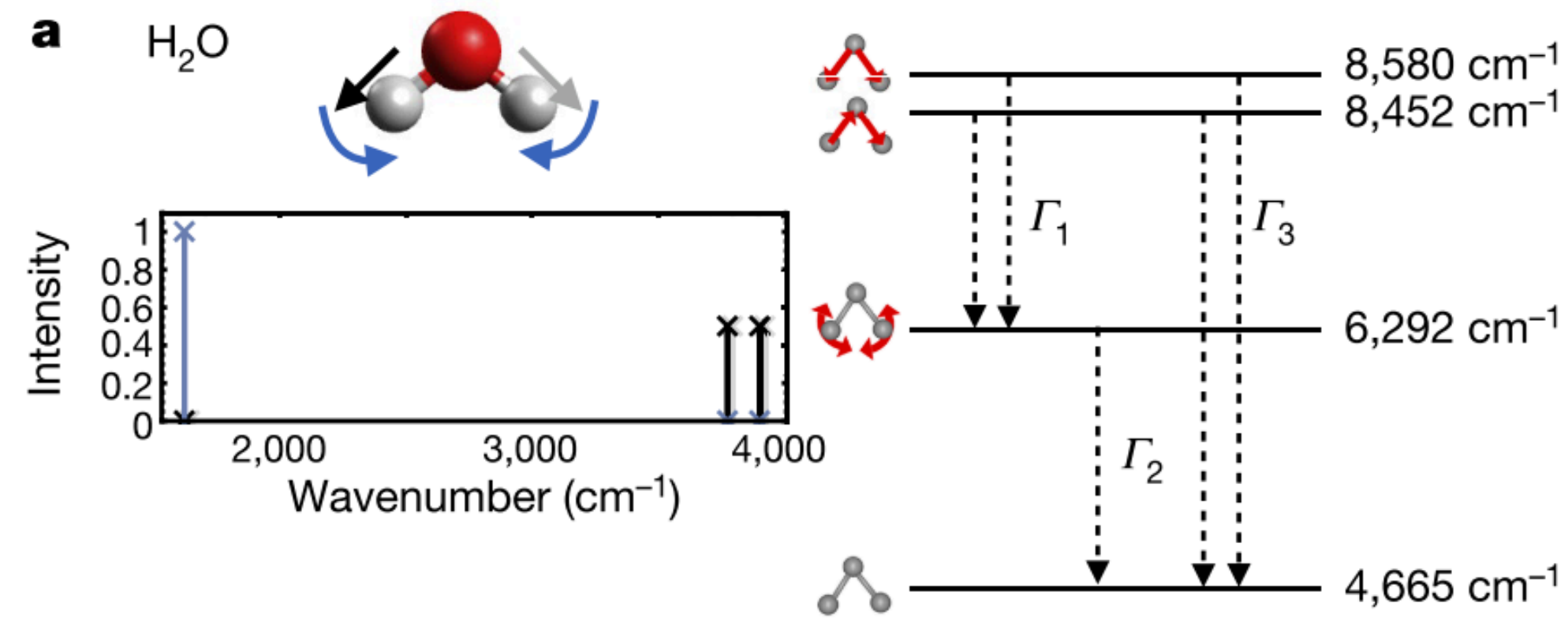
What are the electronic properties of molecules ?



J. Argüello-Luengo et al.  
Nature 574, 215 (2019).



# Putting chemistry into the machines - vibrational spectra

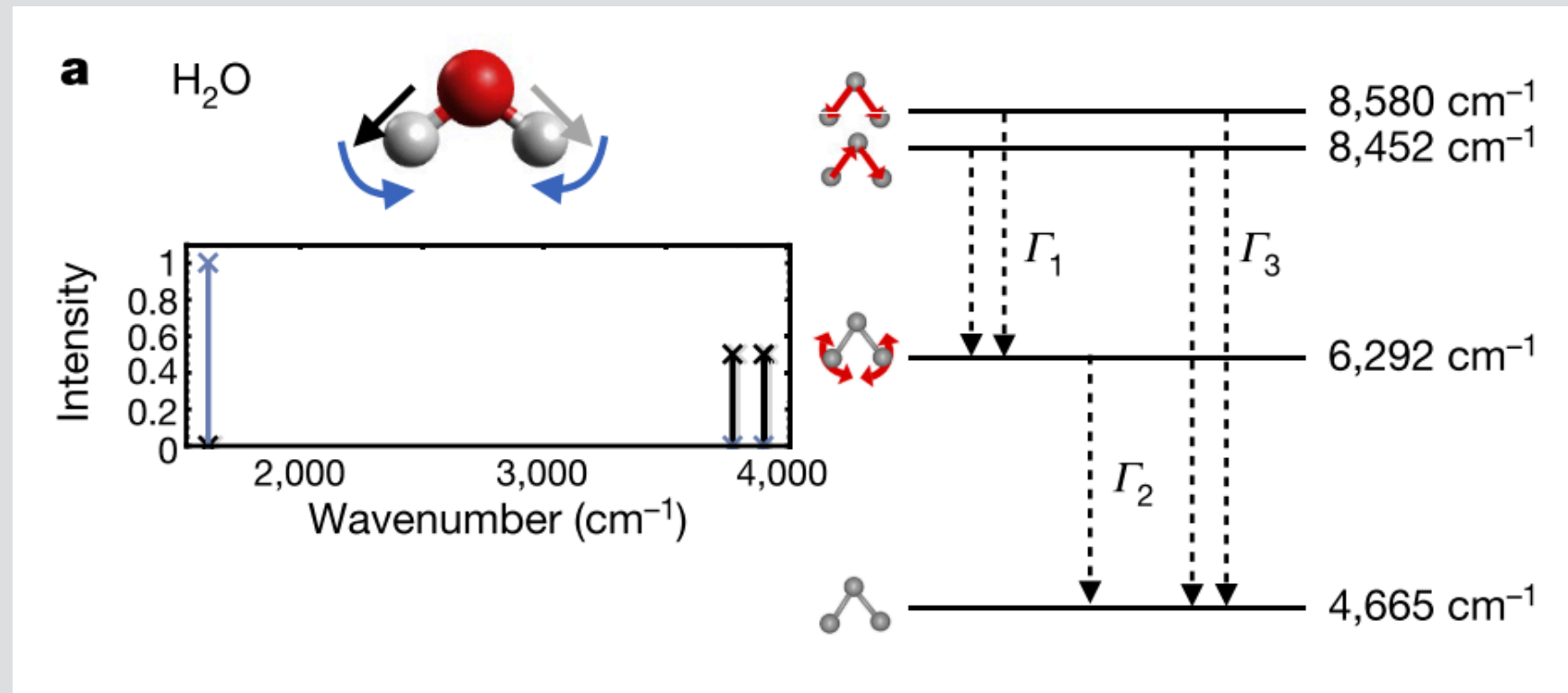


$$\hat{H}_a = \hat{H} + \hbar \sum_{i \leq j} \frac{x_{ij}}{2} \sqrt{\omega_i \omega_j} (a_i^\dagger a_i + a_j^\dagger a_j + 2a_i^\dagger a_j^\dagger a_i a_j)$$

$$\hat{H} = \sum_i \hbar \omega_i a_i^\dagger a_i$$

# Putting chemistry into the machines

## Vibrational spectra



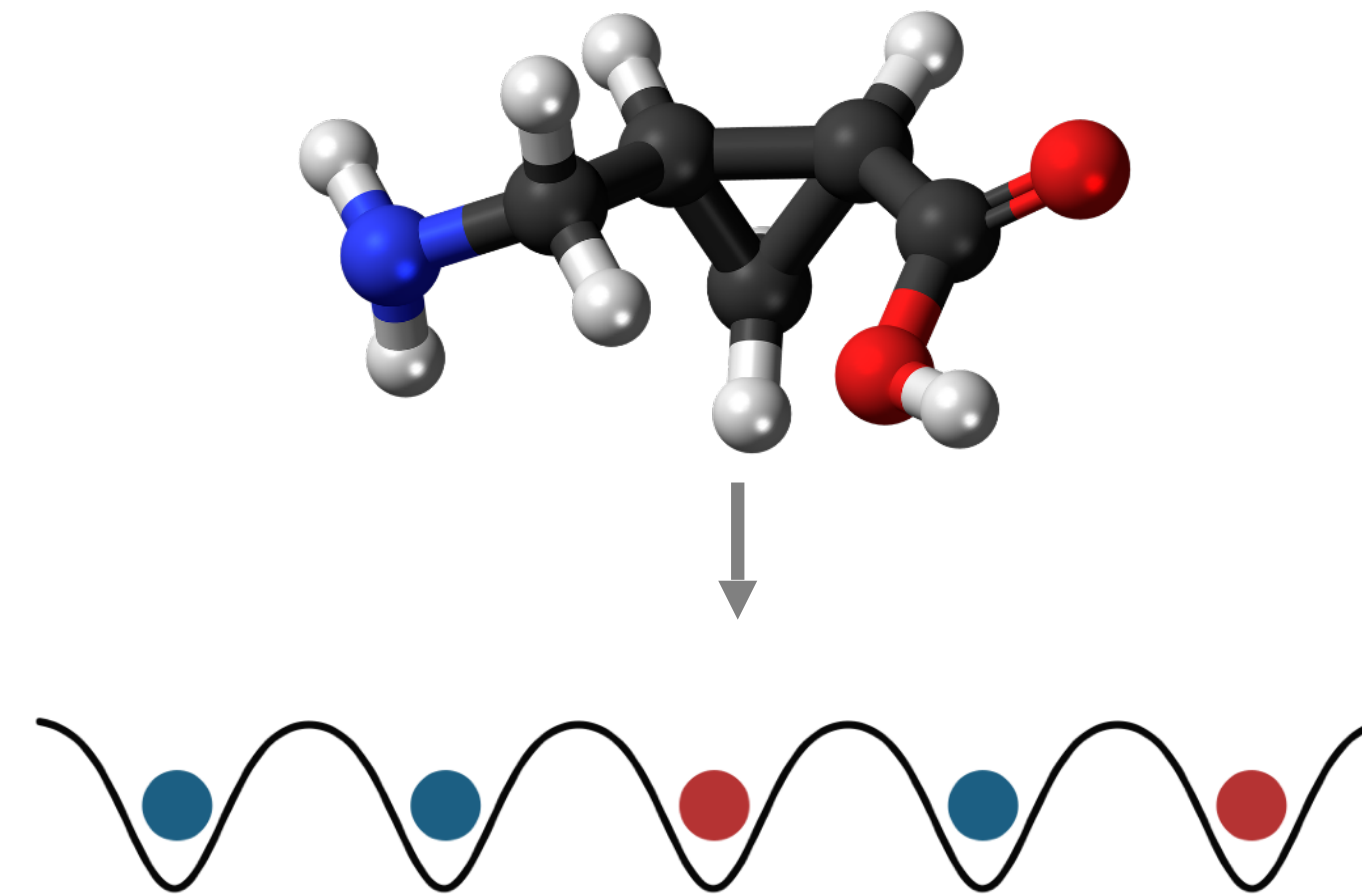
$$\hat{H} = \sum_i \hbar \omega_i a_i^\dagger a_i$$

$$\hat{H}_a = \hat{H} + \hbar \sum_{i \leq j} \frac{x_{ij}}{2} \sqrt{\omega_i \omega_j} (a_i^\dagger a_i + a_j^\dagger a_j + 2a_i^\dagger a_j^\dagger a_i a_j)$$

Looks an awful lot like **bosonic** Hubbard problem

C. Sparrow, Nature 557, 660 (2018).

## Electron structure

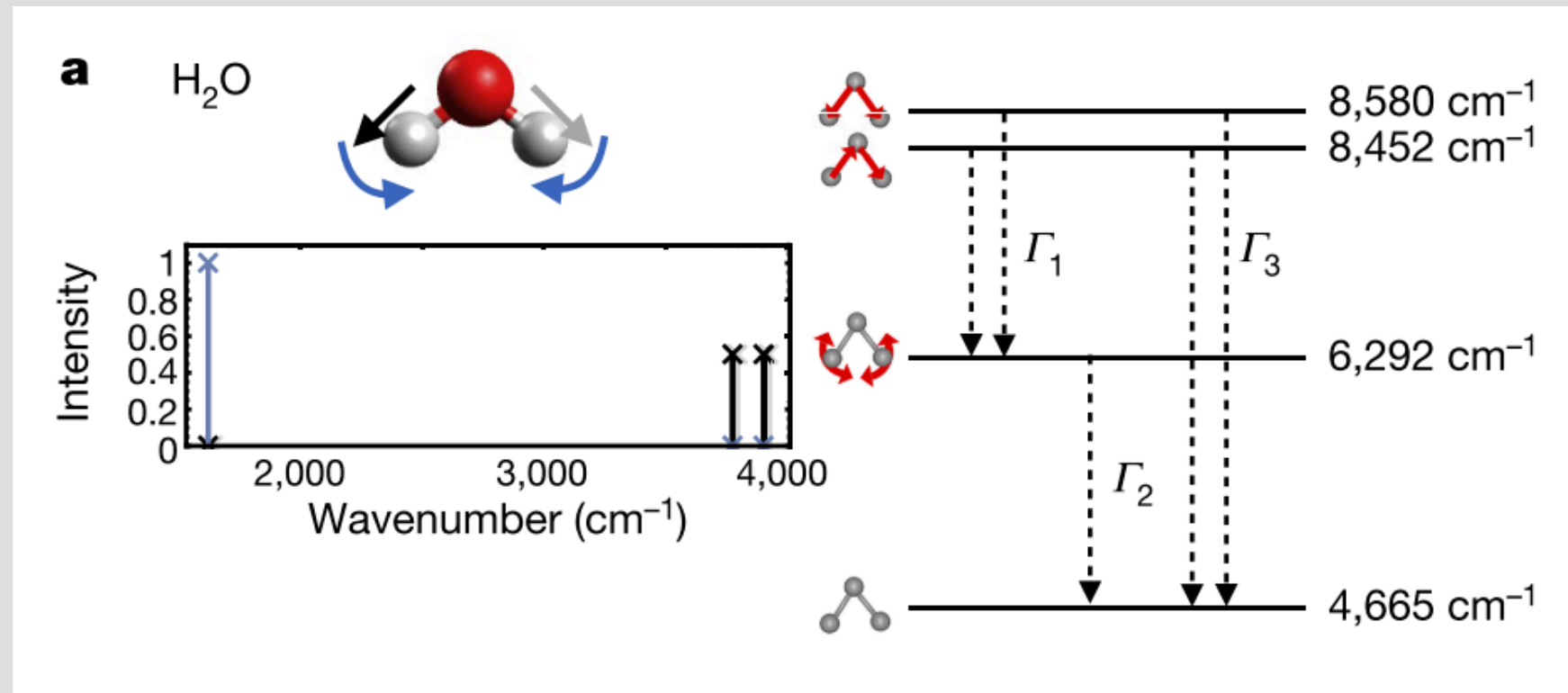


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# Putting chemistry into the machines

## Vibrational spectra



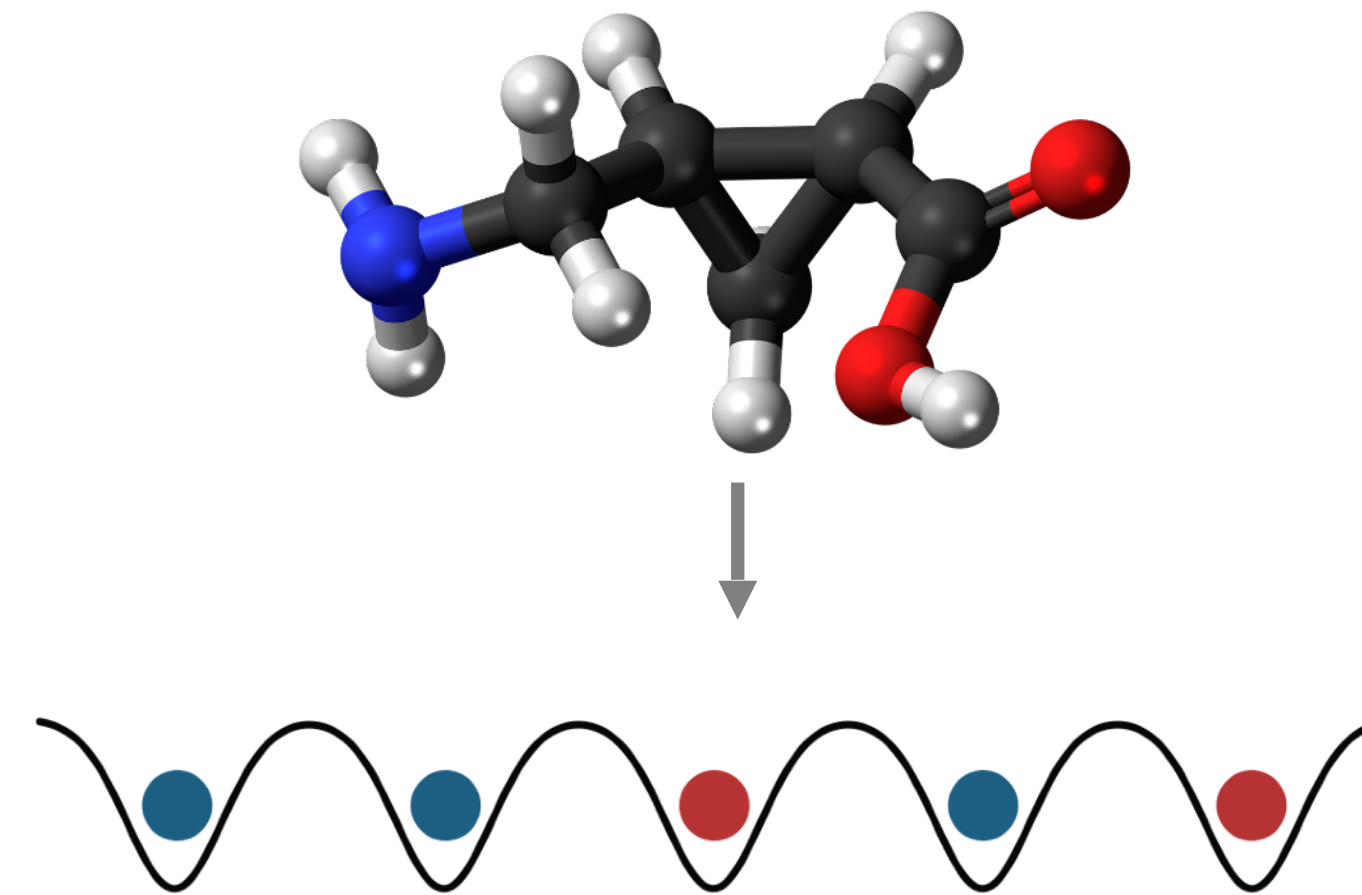
### • Possible projects for this week

$$\hat{H}_a = \hat{H} + \hbar \sum_{i \leq j} \frac{g_{ij}}{2} \sqrt{\omega_i \omega_j} (a_i^\dagger a_i + a_j^\dagger a_j + 2a_i^\dagger a_j^\dagger a_i a_j)$$

Looks an awful lot like **bosonic** Hubbard problem

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## Electron structure



Looks an awful lot like **fermionic** Hubbard problem

J. Argüello-Luengo et al.  
Nature 574, 215 (2019).

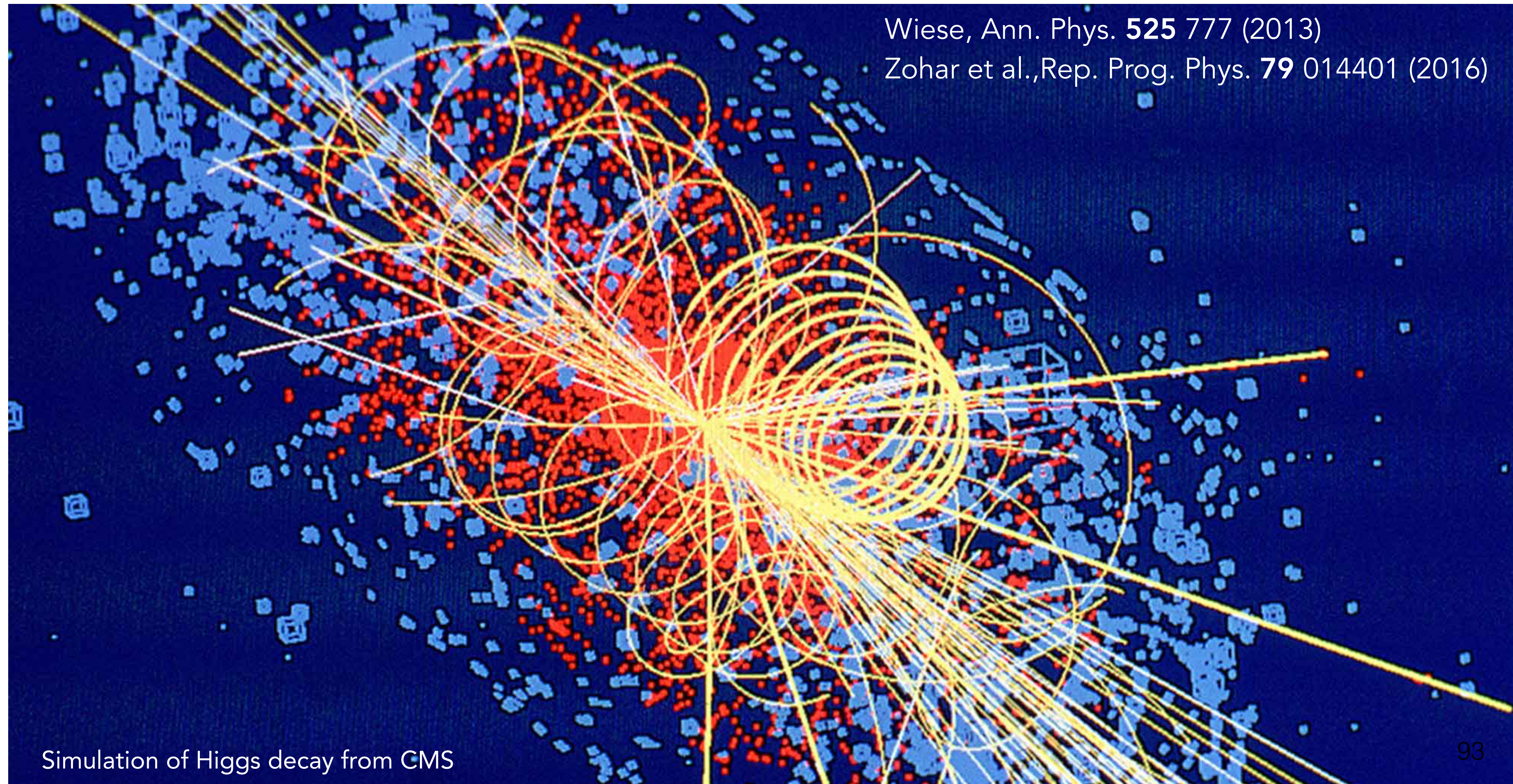
1. Atomic clocks — Qubits in cold atoms
2. Optical tweezers — Trapped qubits in atoms
3. Rydberg atoms — Large scale entanglement
4. Moving particles — Bosons vs Fermions and the link to chemistry
5. Lattice gauge theories — Working on a really hard physics problem

$$\mathcal{L}_{QED} = \bar{\psi} \left( i\gamma^\mu D_\mu - m \right) \psi - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}$$

$$\mathcal{L}_{QCD} = \sum_{fi} \bar{\psi}^{fi} \left( i\gamma^\mu D_{\mu ij} - m_f \right) \psi^{fi} - \frac{1}{2g^2} \text{Tr} \left( G^{\mu\nu} G_{\mu\nu} \right)$$

Particle

Gauge field



Simulation of Higgs decay from CMS

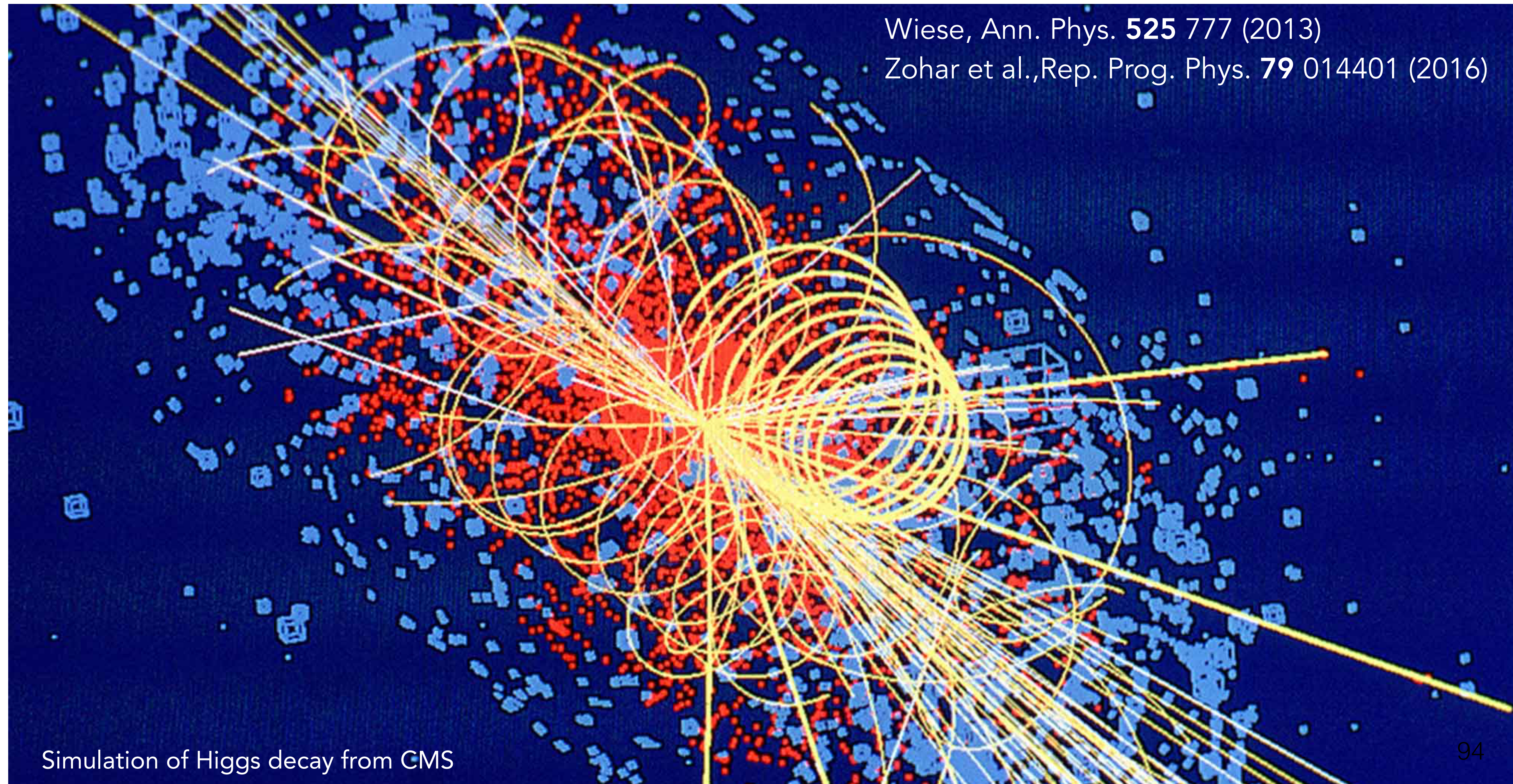
$$\mathcal{L}_{QED} = \bar{\psi} \left( i\gamma^\mu \mathbf{D}_\mu - m \right) \psi - \frac{1}{4} F^{\mu\nu} F_{\mu\nu}$$

$$\mathcal{L}_{QCD} = \sum_{fi} \bar{\psi}^{fi} \left( i\gamma^\mu \mathbf{D}_{\mu ij} - m_f \right) \psi^{fi} - \frac{1}{2g^2} \text{Tr} \left( G^{\mu\nu} G_{\mu\nu} \right)$$

Particle

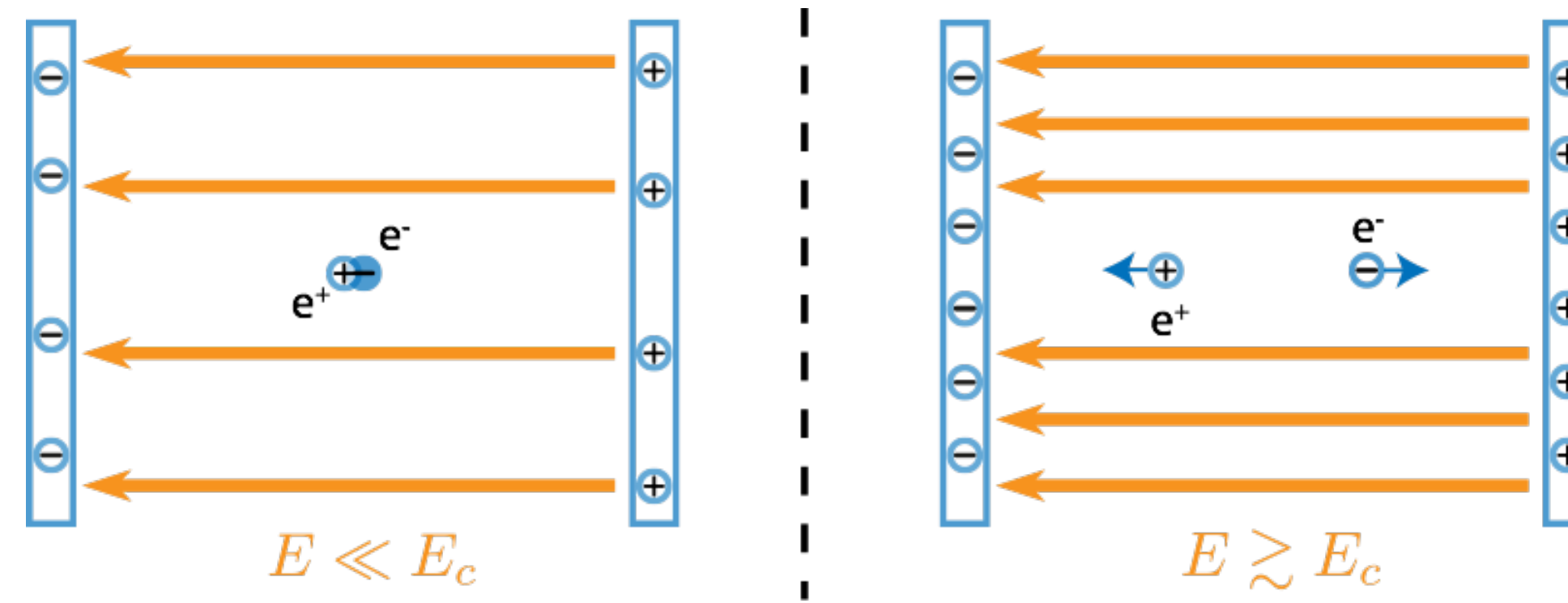
Gauge coupling

Gauge field

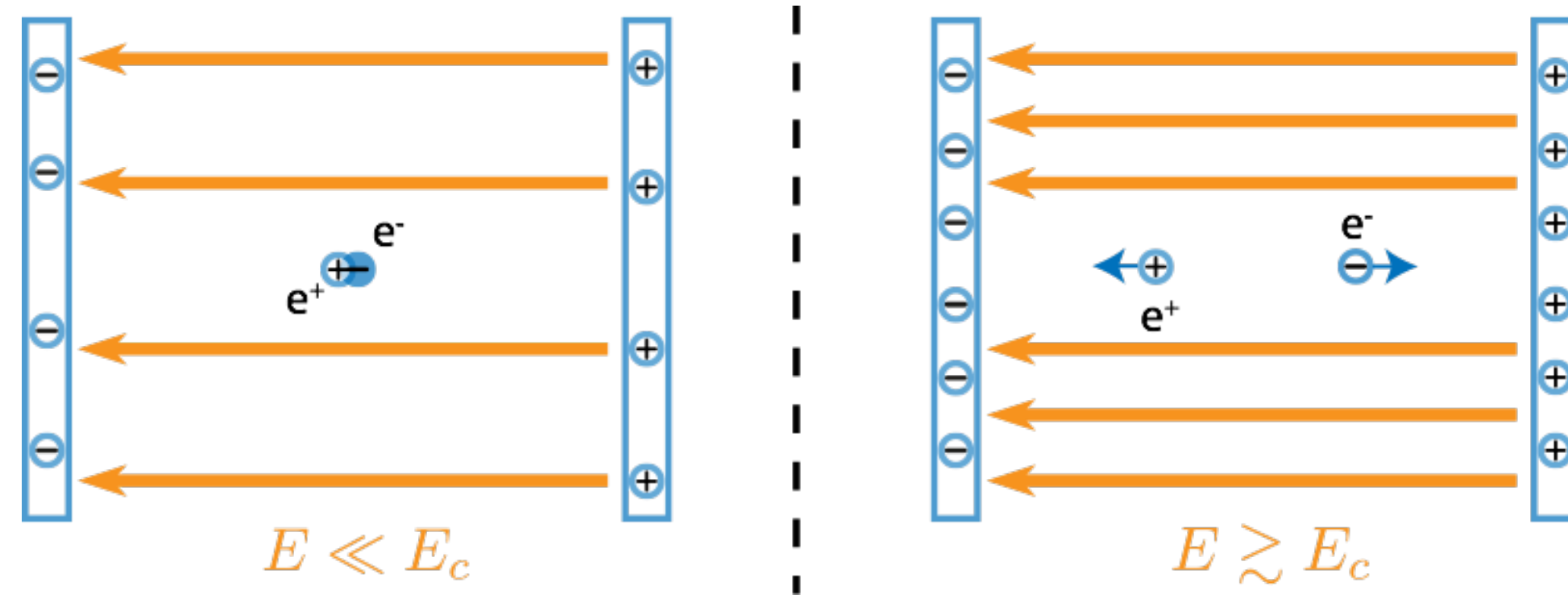


Simulation of Higgs decay from CMS

J. Schwinger, Phys. Rev. **714**, 16 (1951).



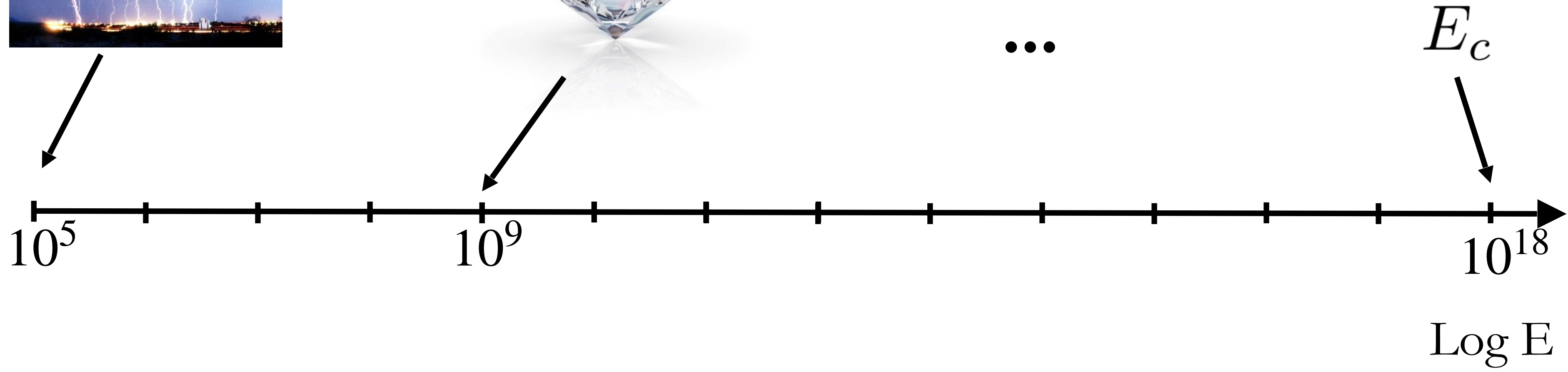
J. Schwinger, Phys. Rev. **714**, 16 (1951).



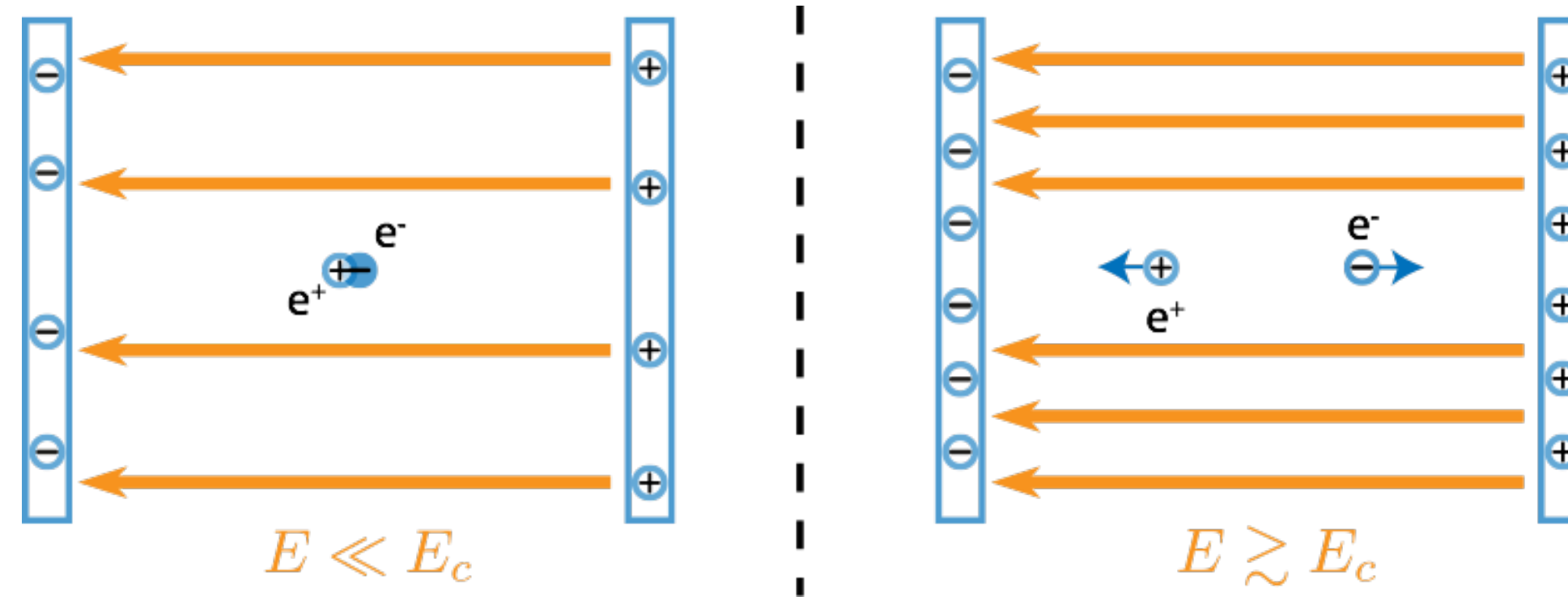
$$E_c = \frac{m_e^2 c^3}{\hbar q_e} \approx 10^{18} \text{ V/m}$$



...



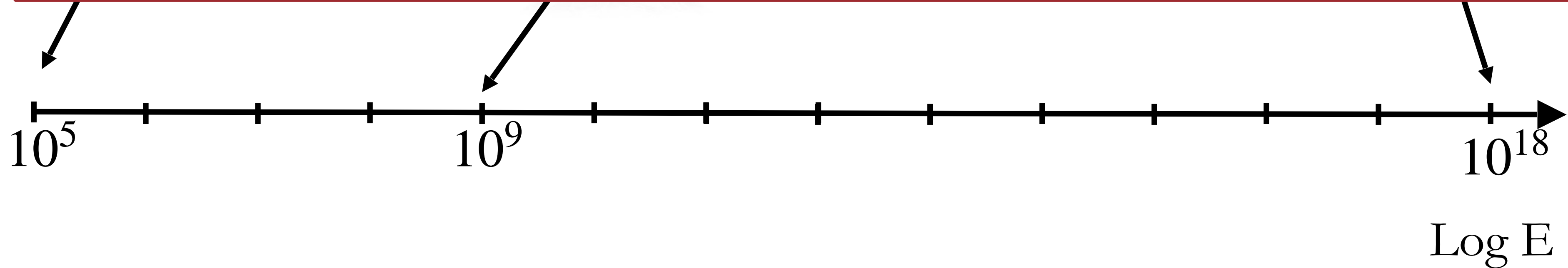


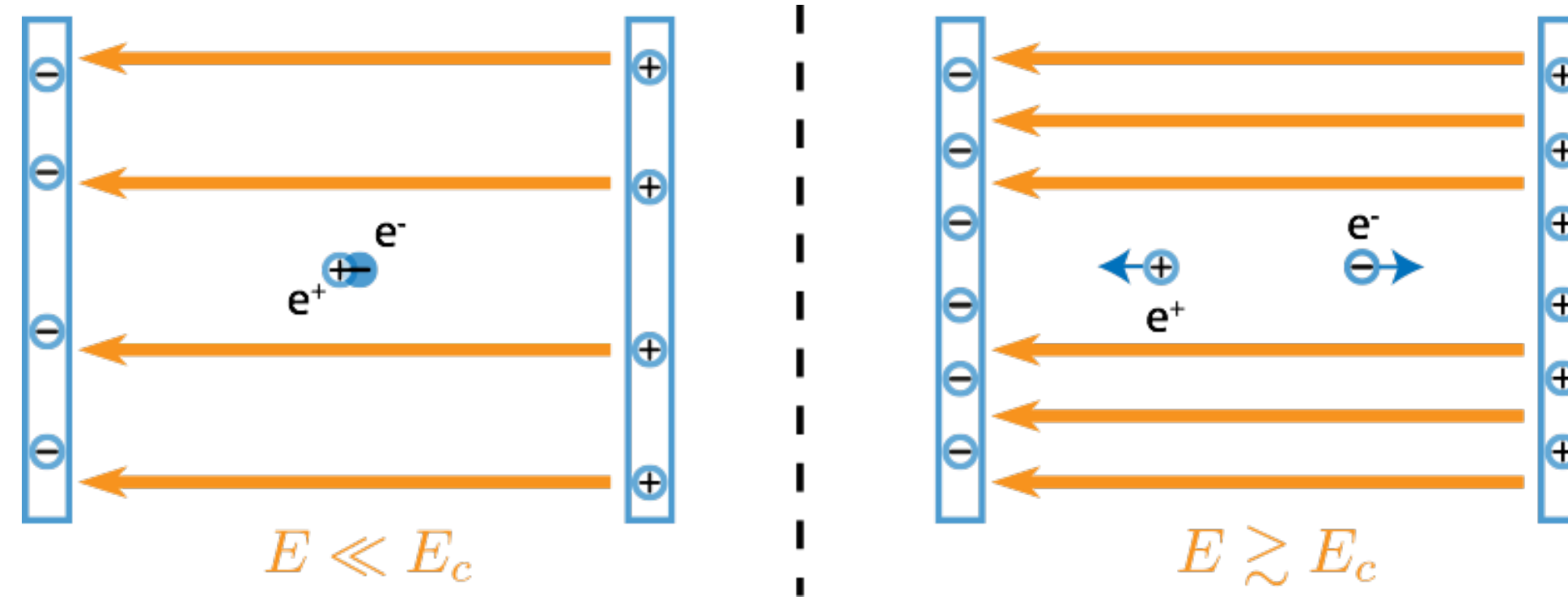


$$E_c = \frac{m_e^2 c^3}{\hbar q_e} \approx 10^{18} \text{ V/m}$$

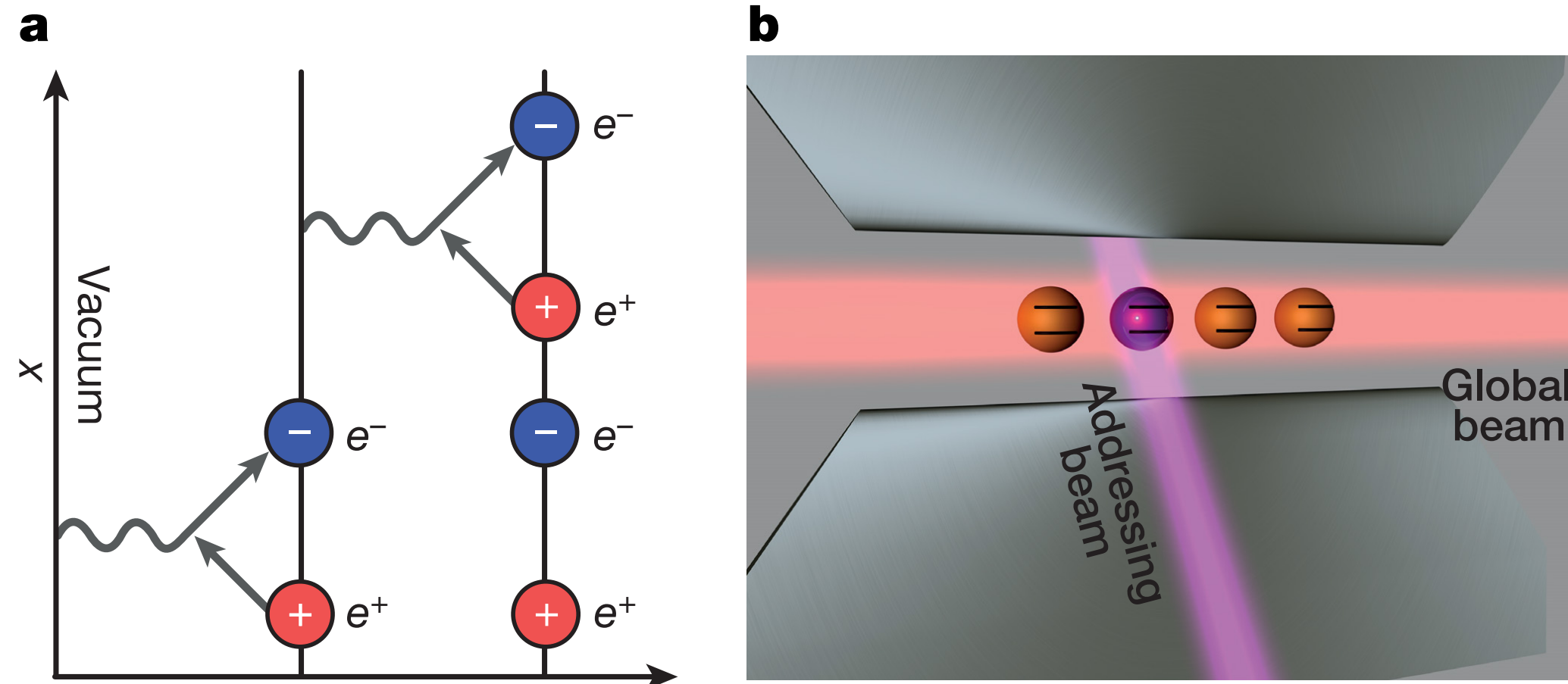


Can we construct a quantum simulator ?



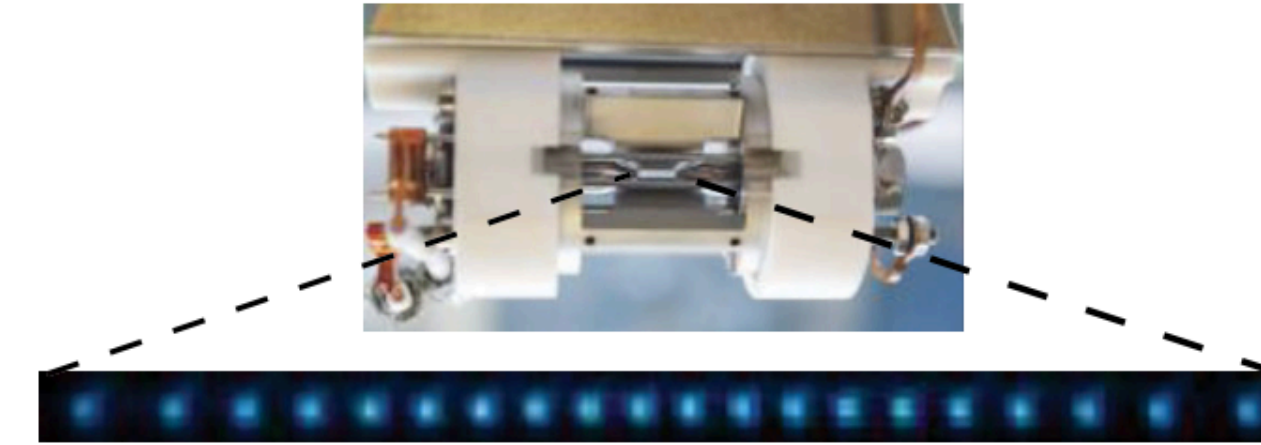


First digital implementation with ions

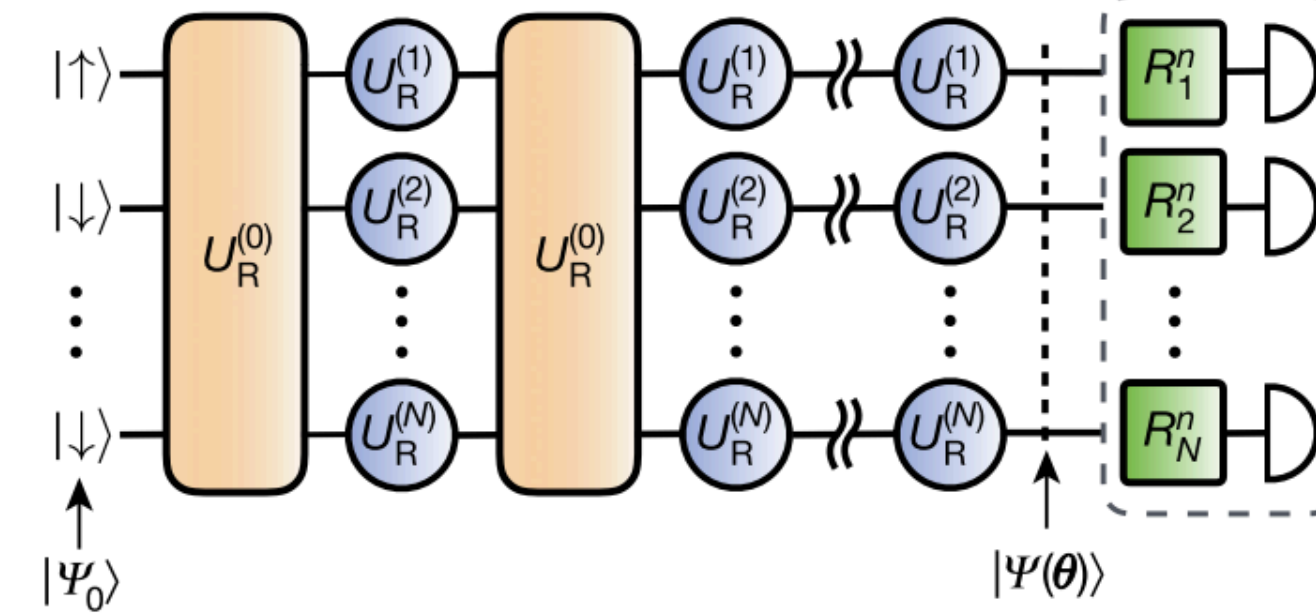


E. Martinez et al., Nature **534** 516 (2016).

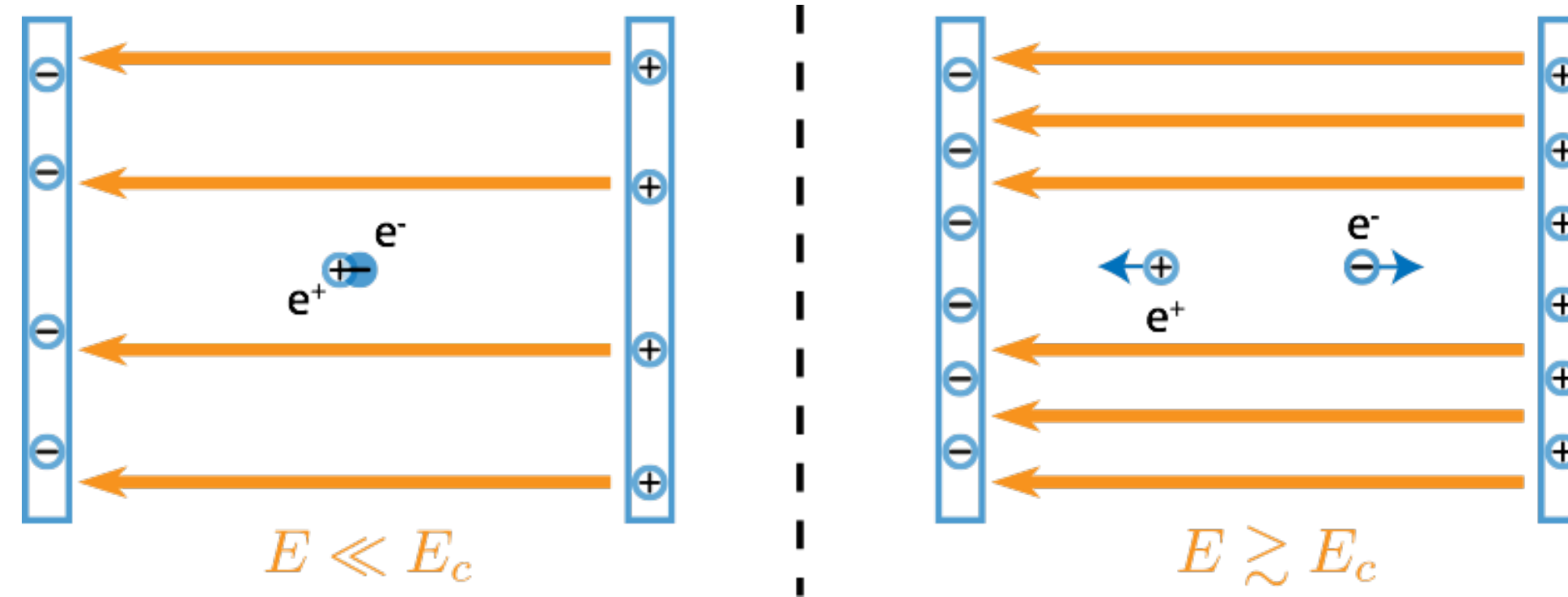
Analogue quantum simulator



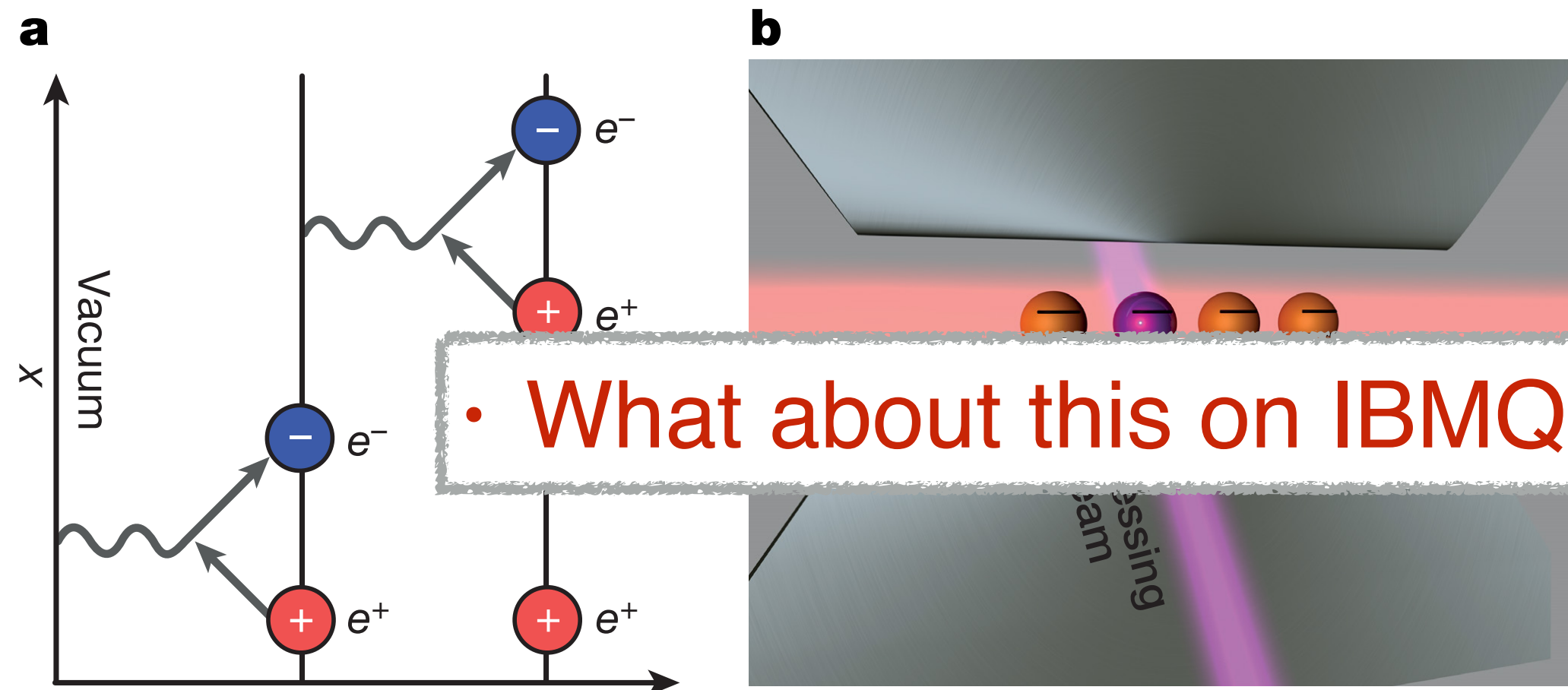
Symmetry-protecting quantum circuit



C. Kokail et al., Nature **569**, 355 (2019).



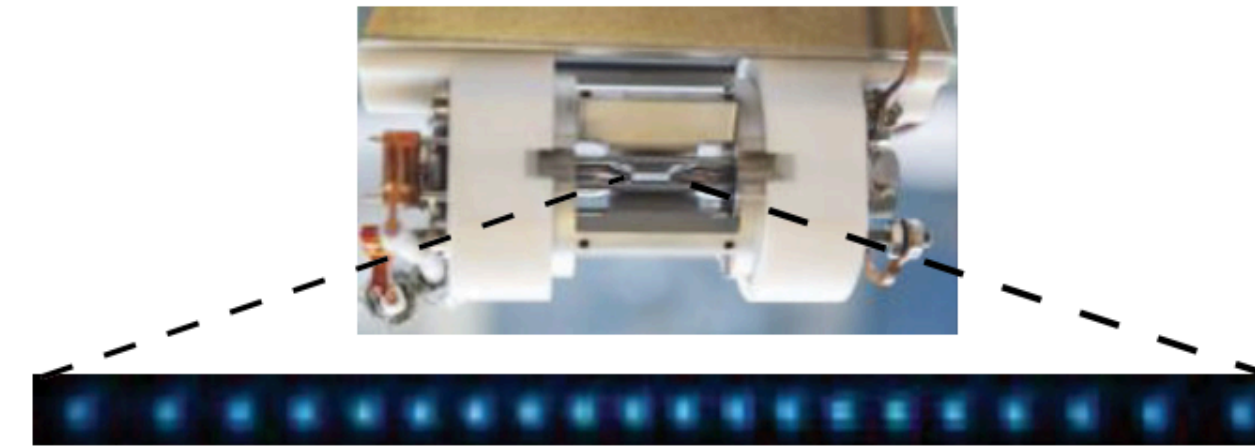
First digital implementation with ions



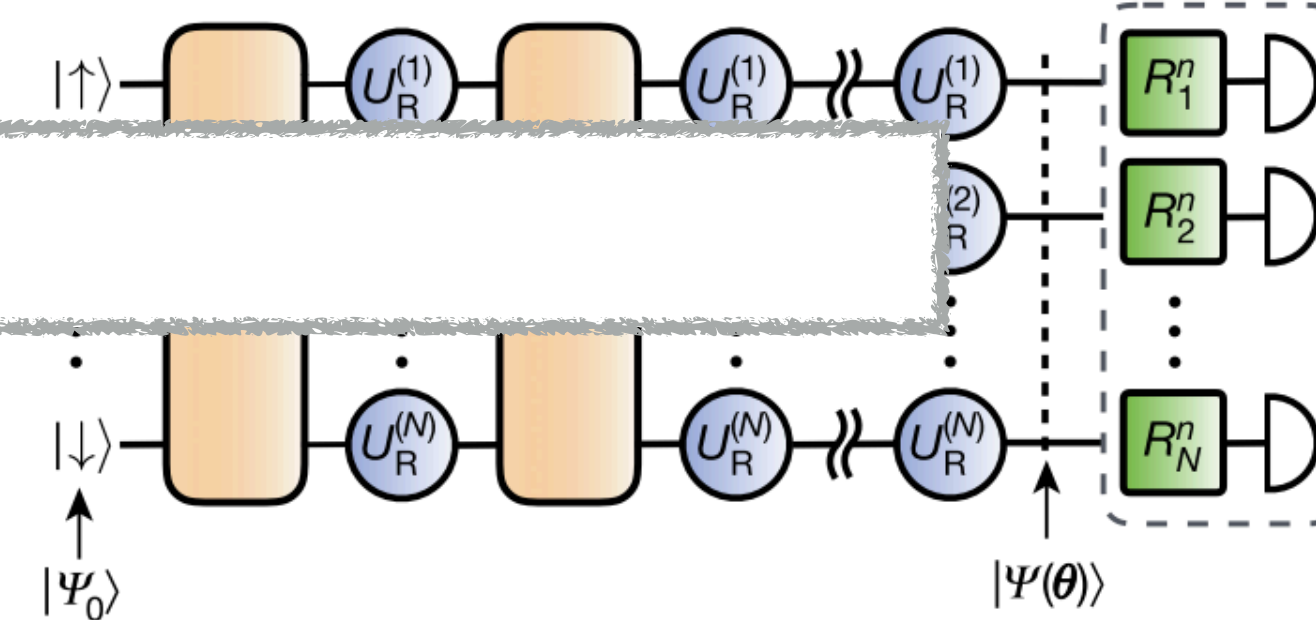
E. Martinez et al., Nature **534** 516 (2016).

• What about this on IBMQ ?

Analogue quantum simulator



Symmetry-protecting quantum circuit



C. Kokail et al., Nature **569**, 355 (2019).

Sodium



$$N_{at} \sim 300 \times 10^3$$

$$\bar{\omega}/2\pi \sim 250\text{Hz}$$

$$B_0 \sim 2\text{G}$$

Gauge field



Sodium

Bosonic  ${}^7\text{Li}$



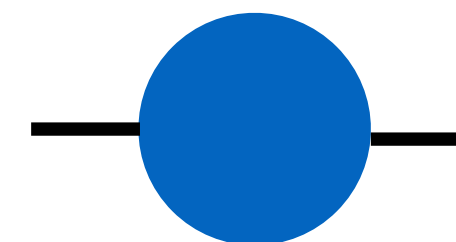
$$N_{at} \sim 60 \times 10^3$$

$$\bar{\omega}/2\pi \sim 500\text{Hz}$$

$$B_0 \sim 2\text{G}$$

Sodium

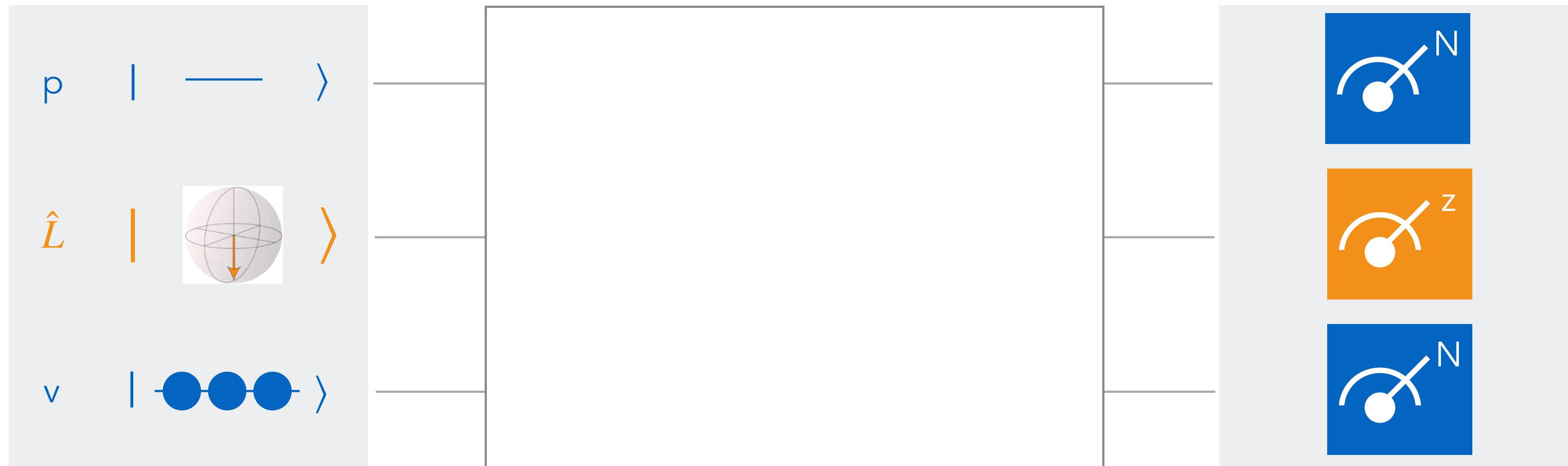
Matter field



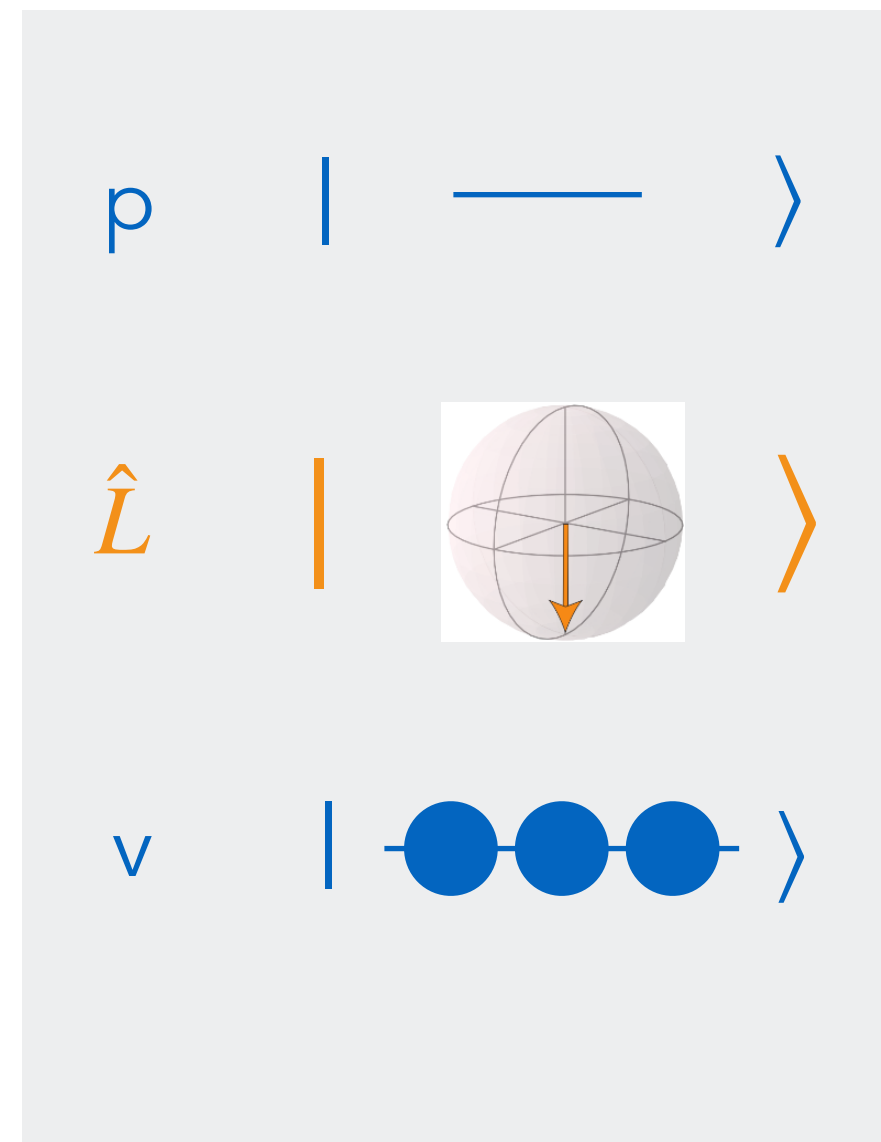
1.) Initialization

2.) Manipulation and evolution

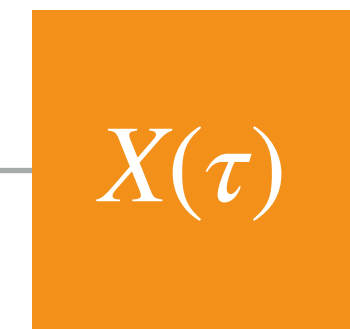
3.) Read-out



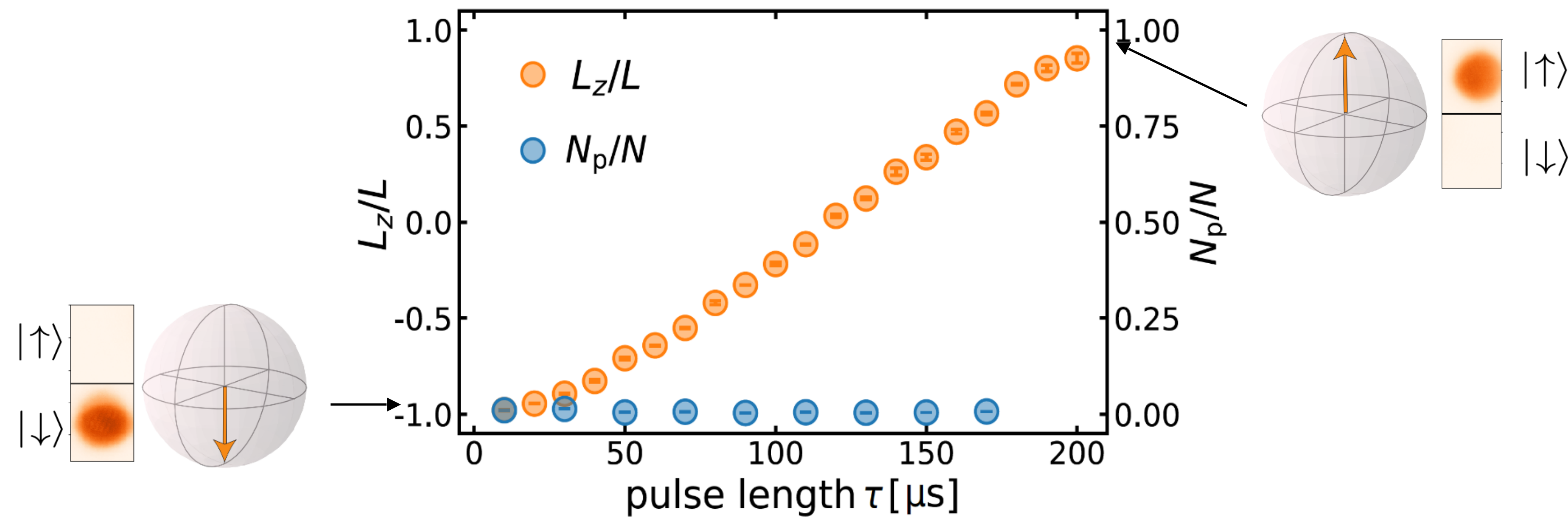
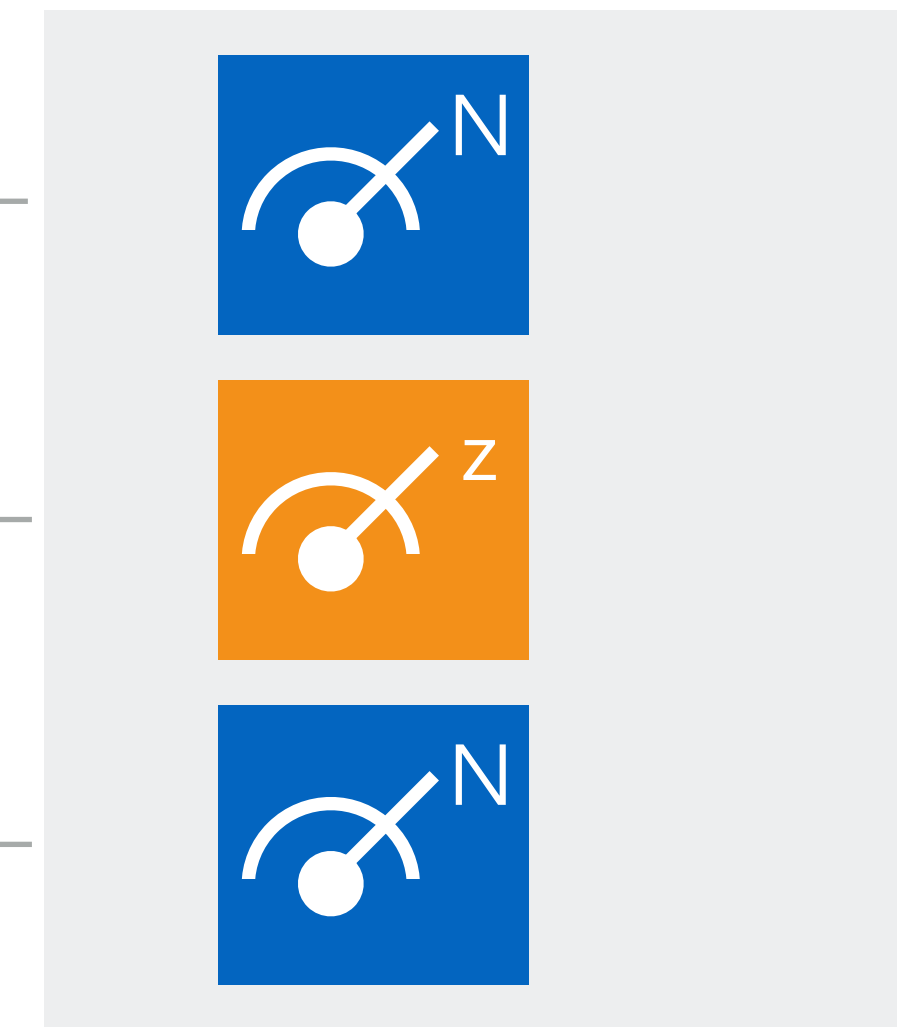
1.) Initialization



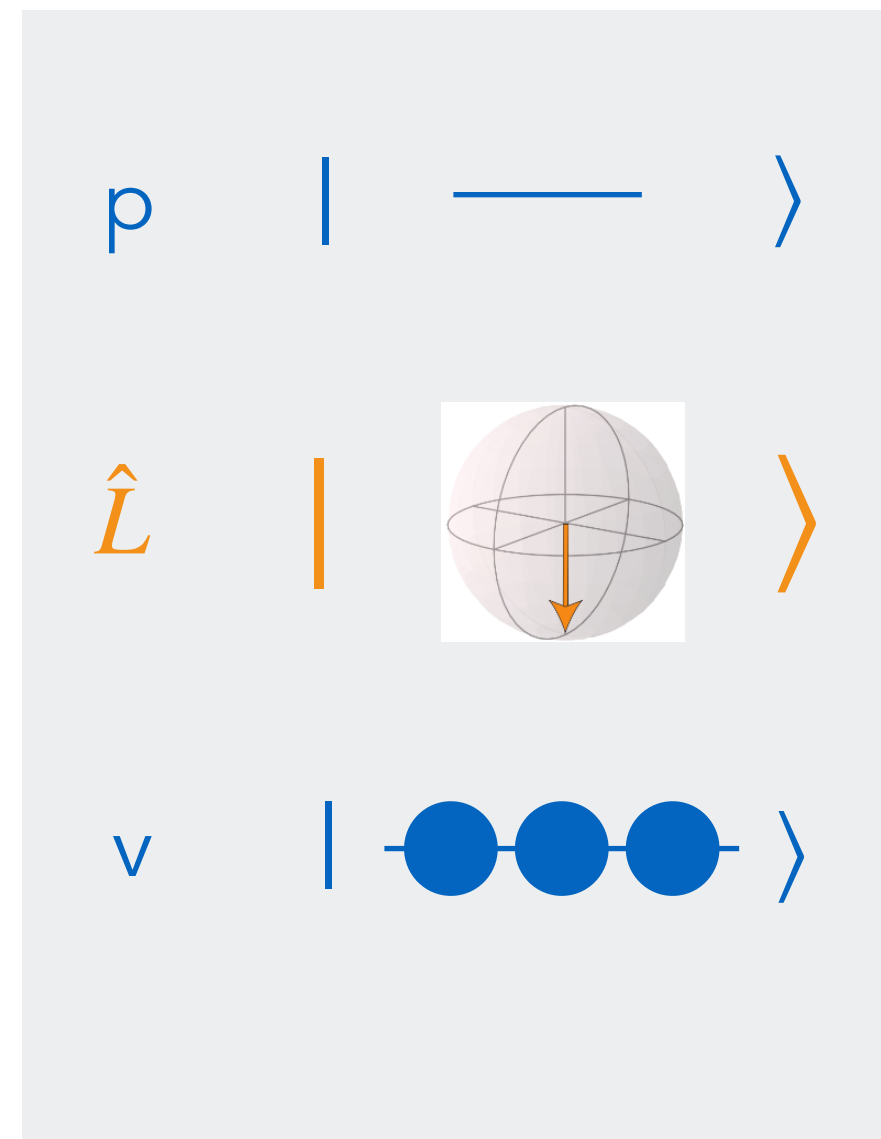
2.) Manipulation and evolution



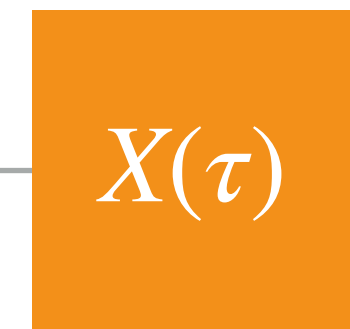
3.) Read-out



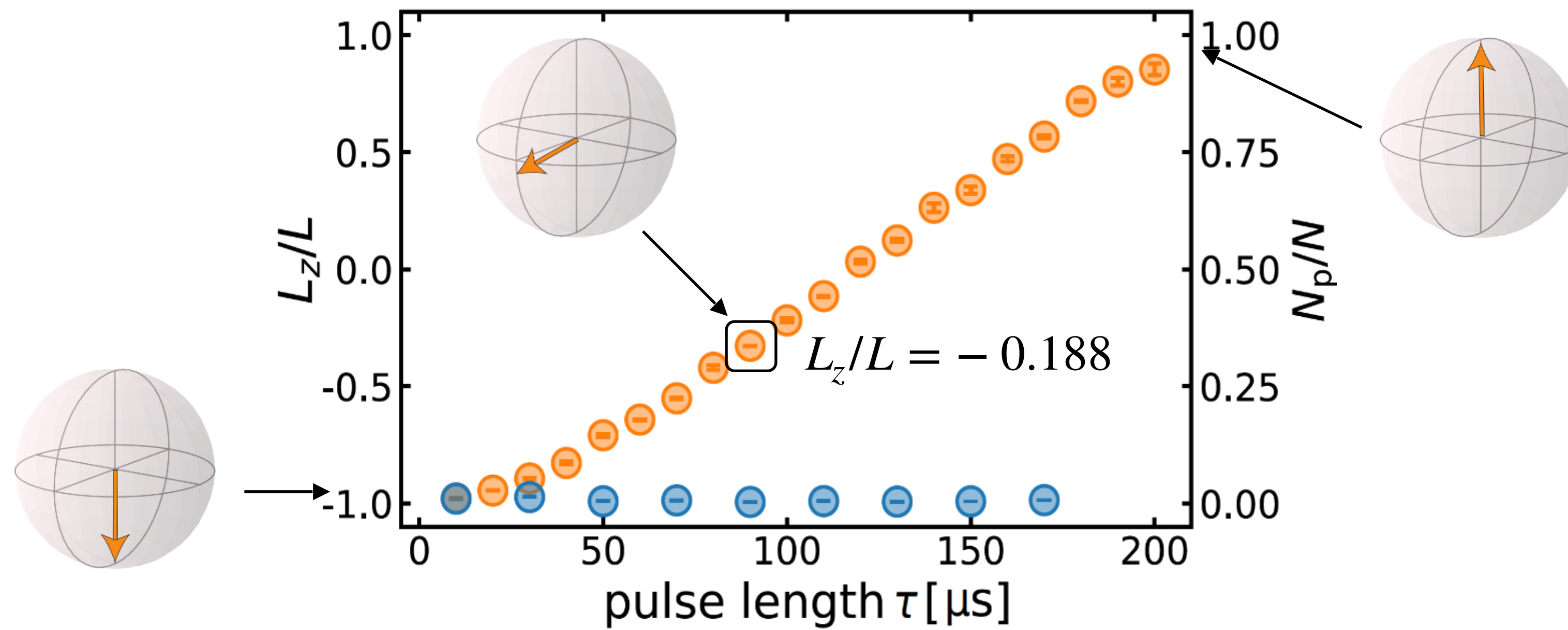
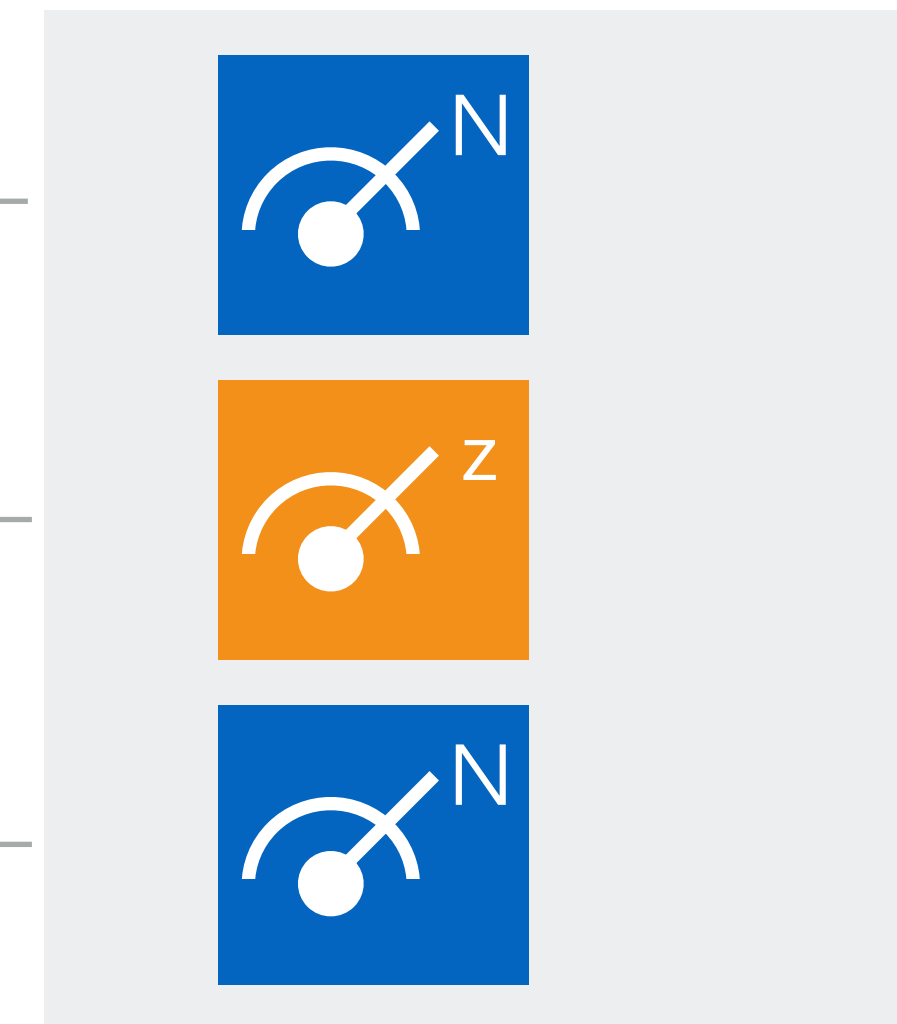
1.) Initialization



2.) Manipulation and evolution



3.) Read-out

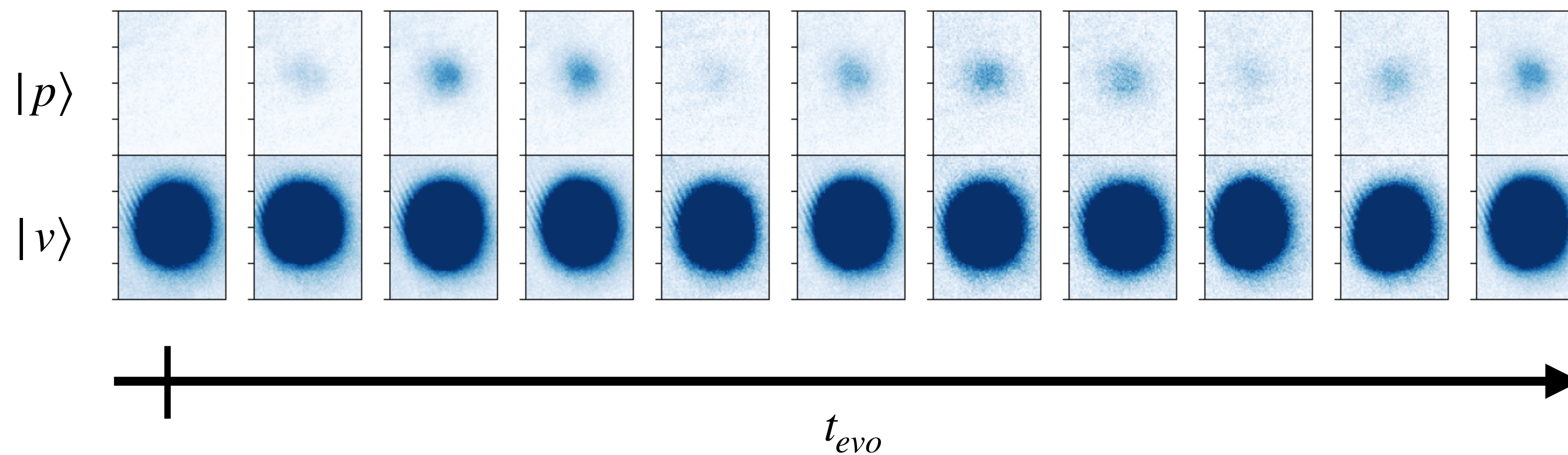
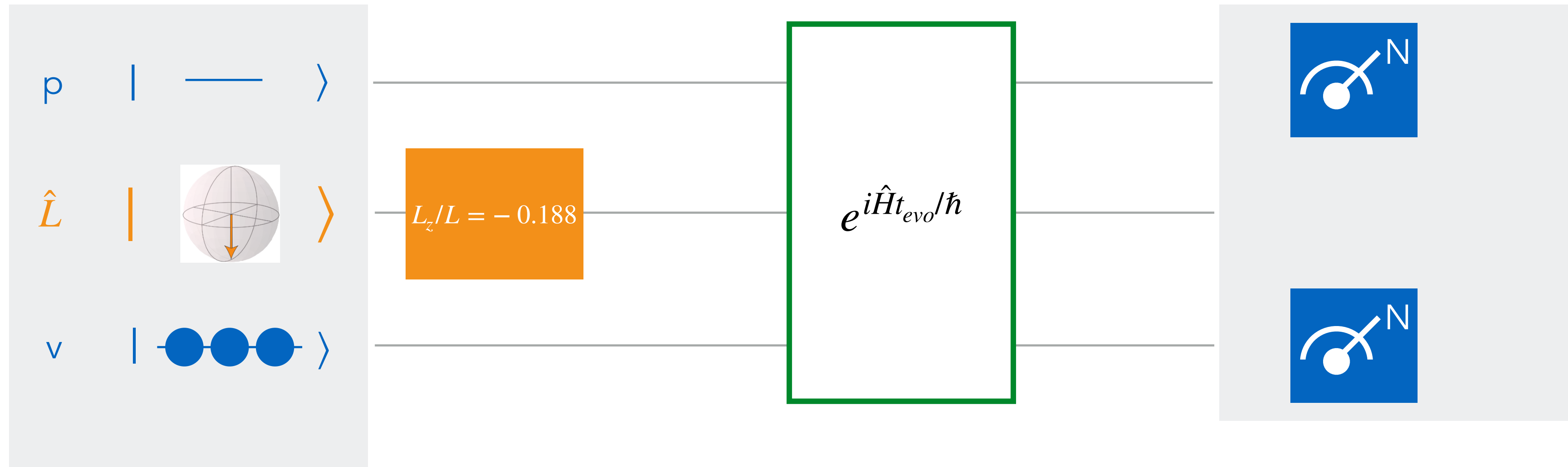


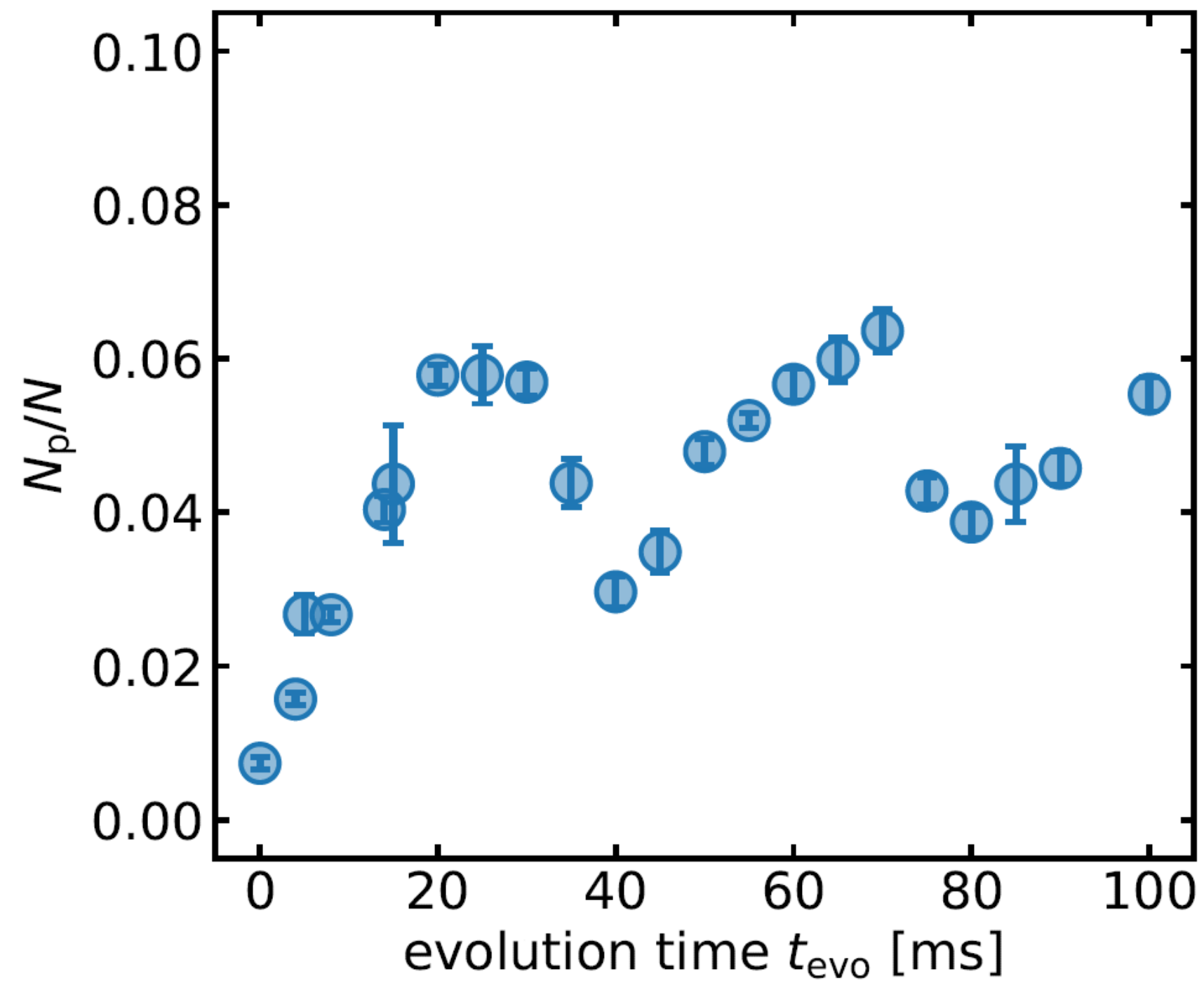
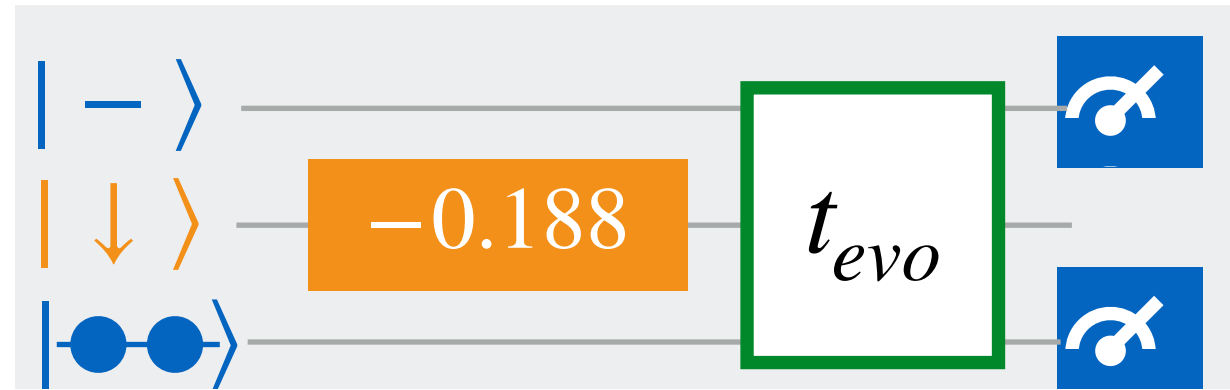


1.) Initialization

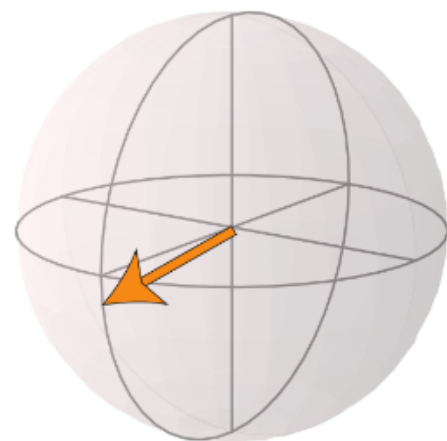
2.) Manipulation and evolution

3.) Read-out

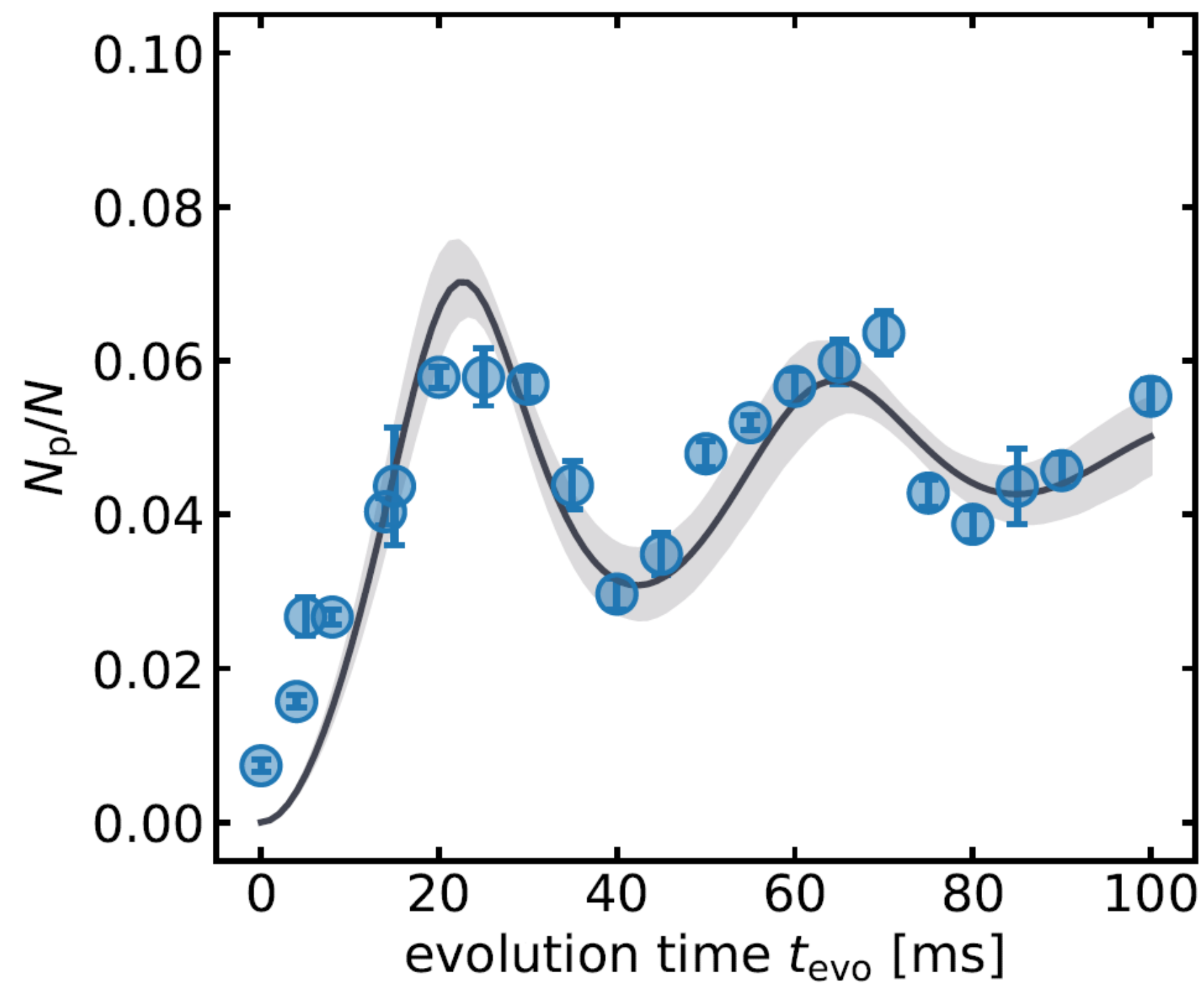
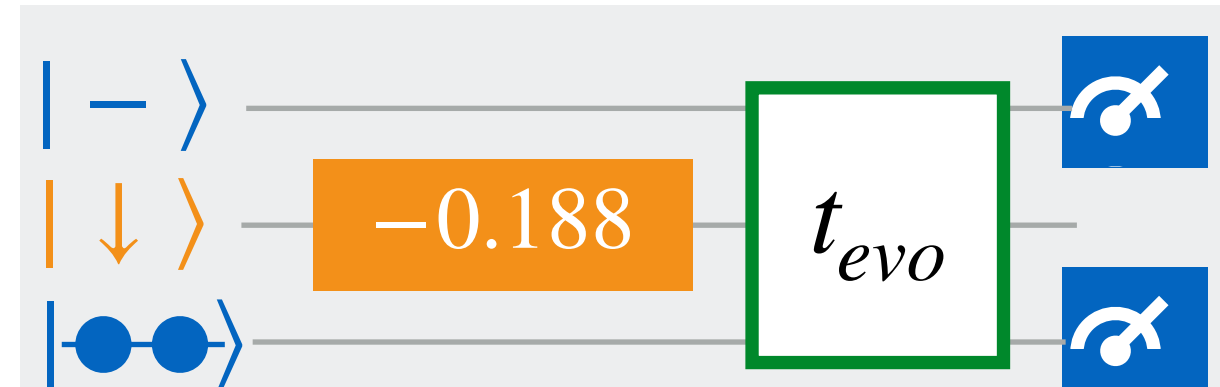




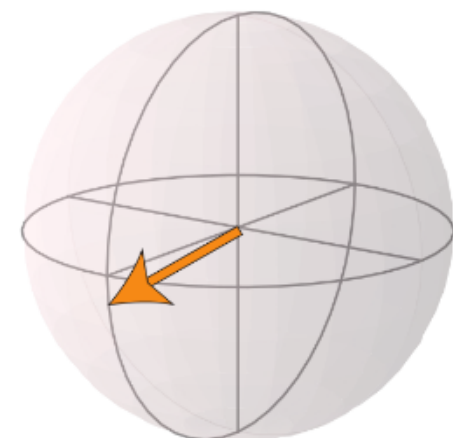
$L_z/L = -0.188$



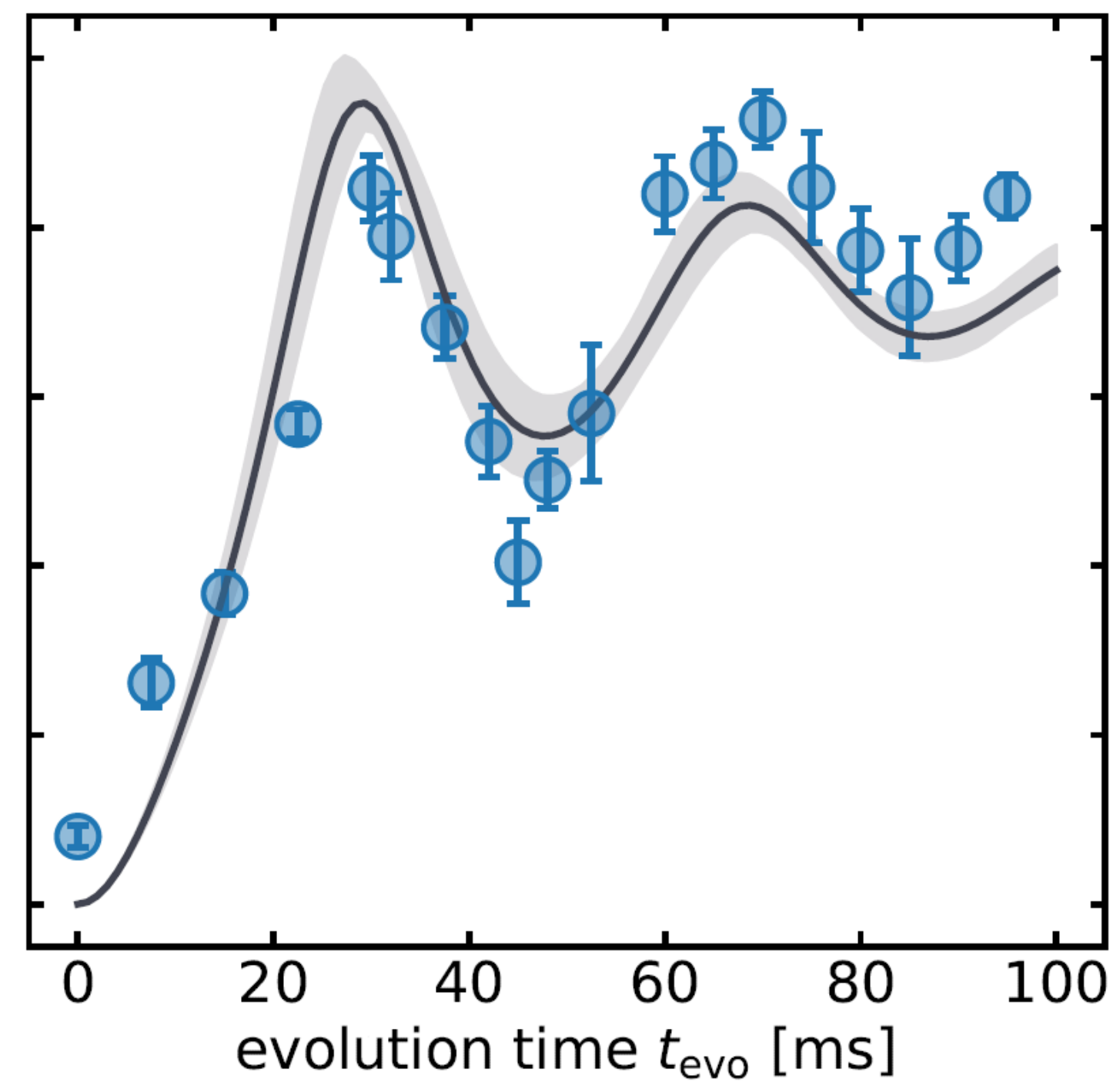
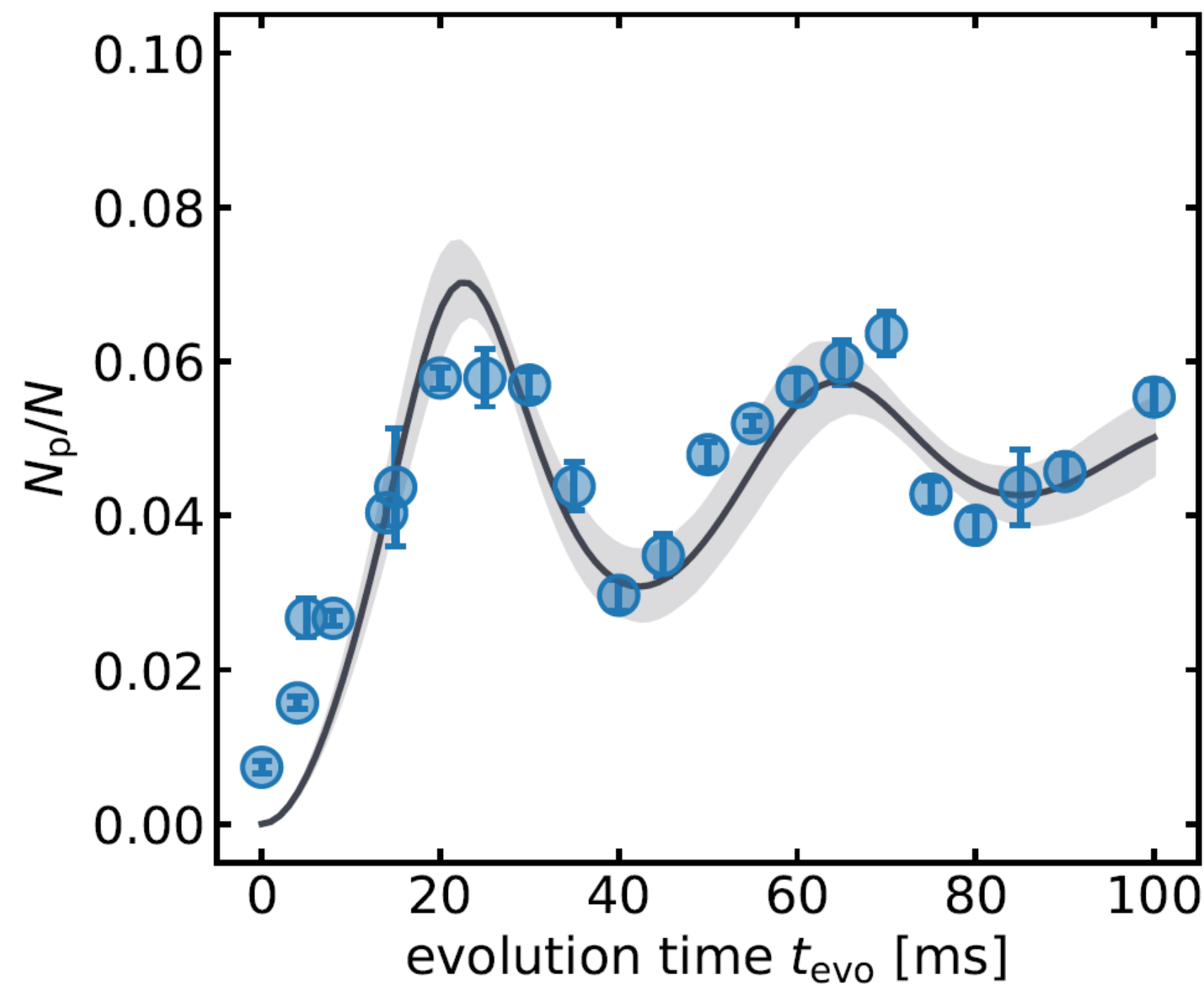
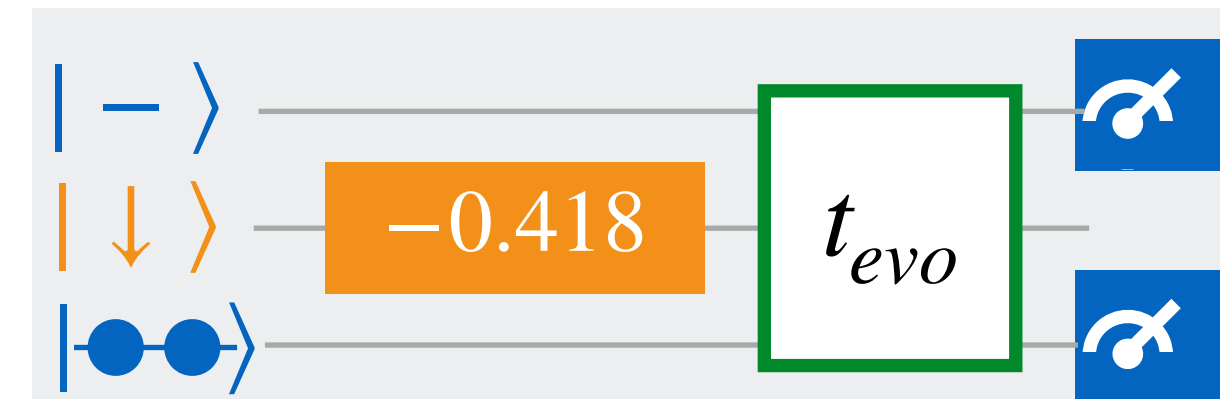
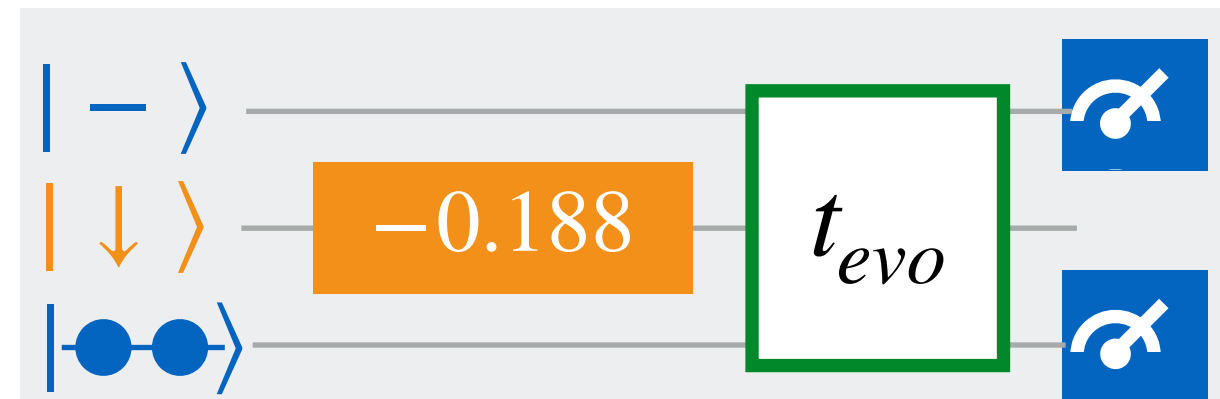
$$\hat{H}/\hbar = \chi \hat{L}_z^2 + \frac{\Delta}{2} \left( \hat{b}_p^\dagger \hat{b}_p - \hat{b}_v^\dagger \hat{b}_v \right) + \lambda \left( b_v^\dagger \hat{L}_- \hat{b}_v + b_v^\dagger \hat{L}_+ \hat{b}_p \right)$$



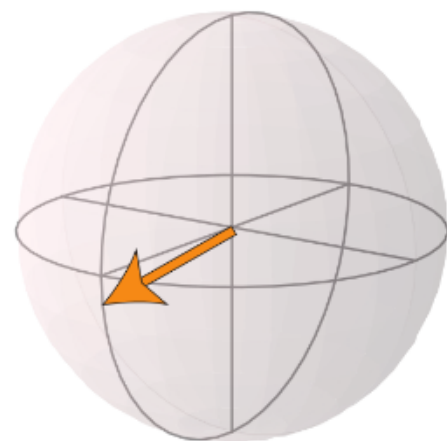
$$L_z/L = -0.188$$



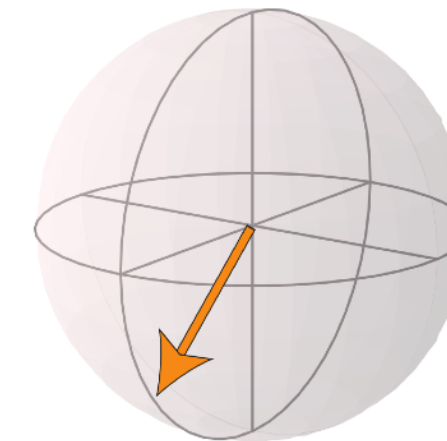
$$\hat{H}/\hbar = \chi \hat{L}_z^2 + \frac{\Delta}{2} (\hat{b}_p^\dagger \hat{b}_p - \hat{b}_v^\dagger \hat{b}_v) + \lambda (b_v^\dagger \hat{L}_- \hat{b}_v + b_v^\dagger \hat{L}_+ \hat{b}_p)$$

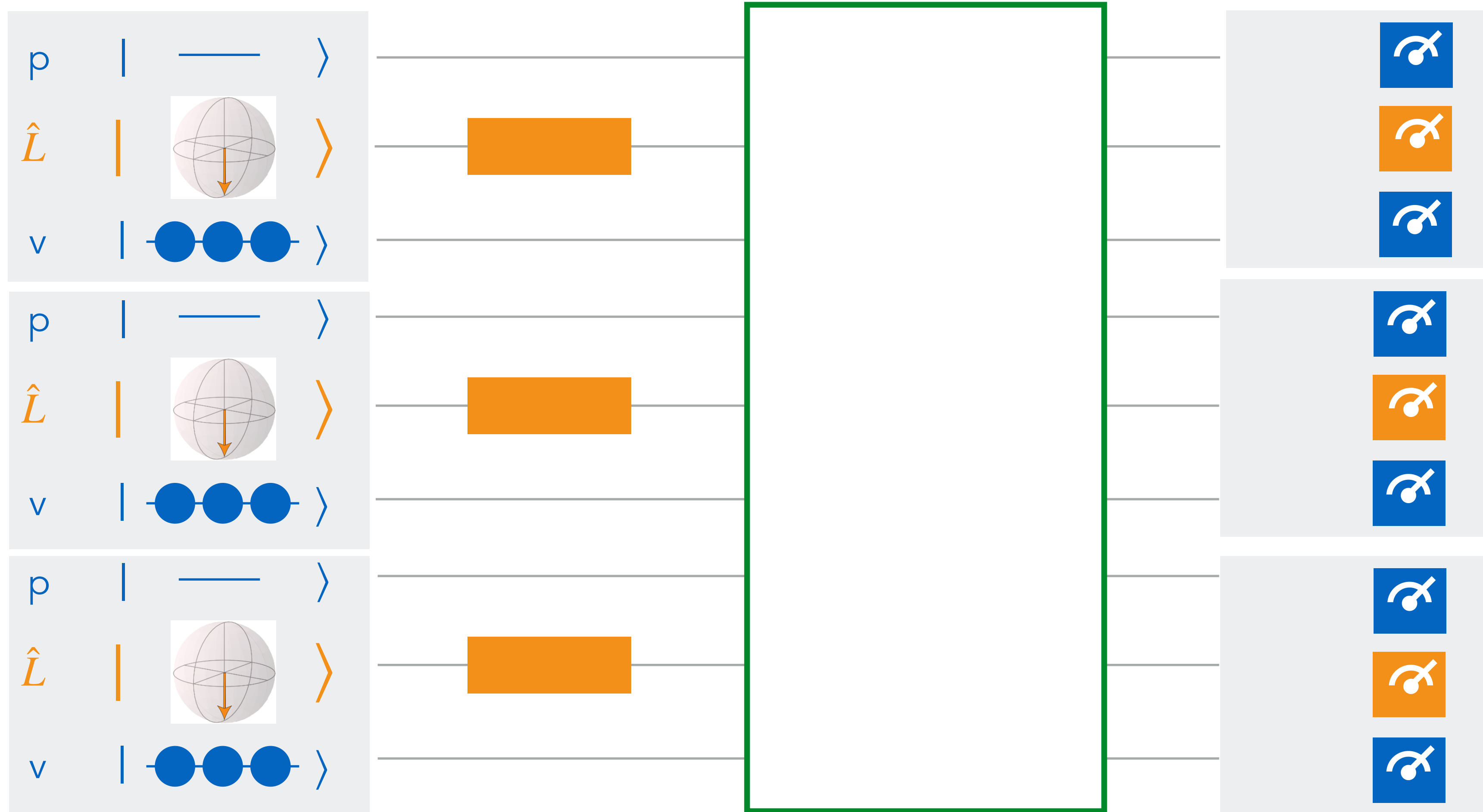
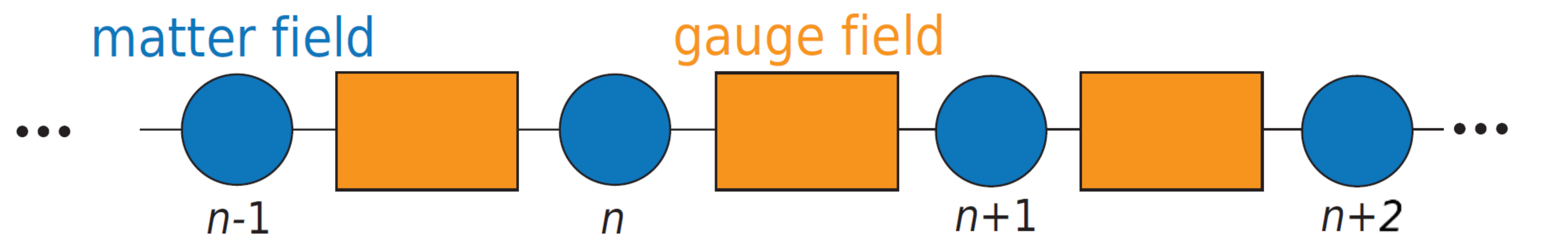


$L_z/L = -0.188$



$L_z/L = -0.418$



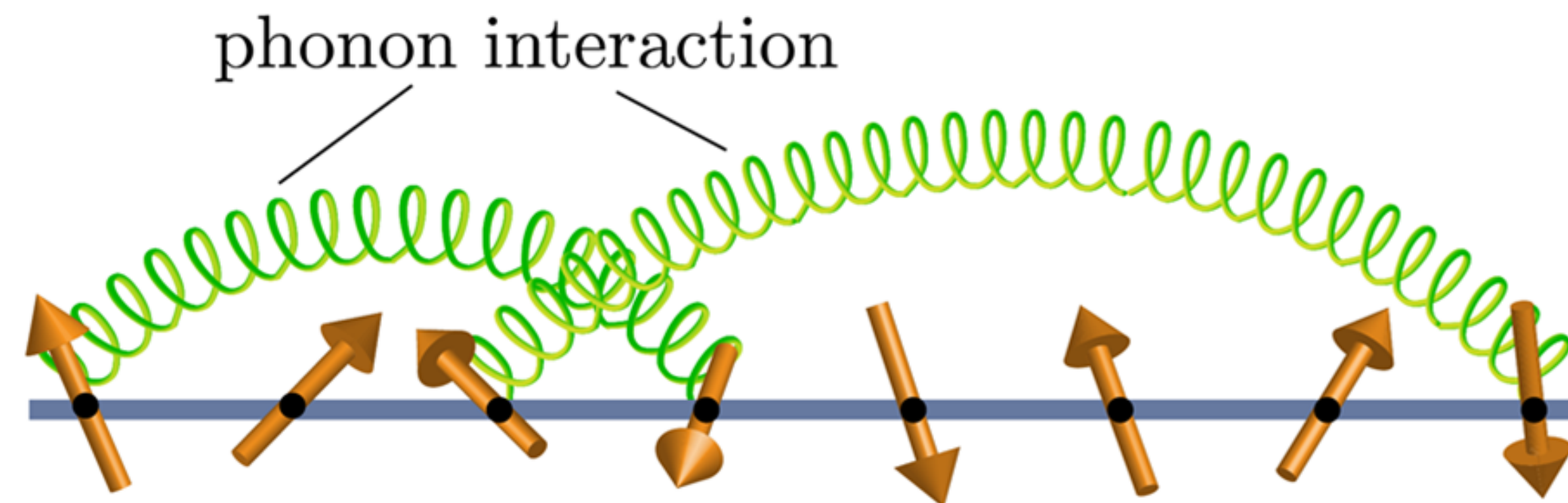
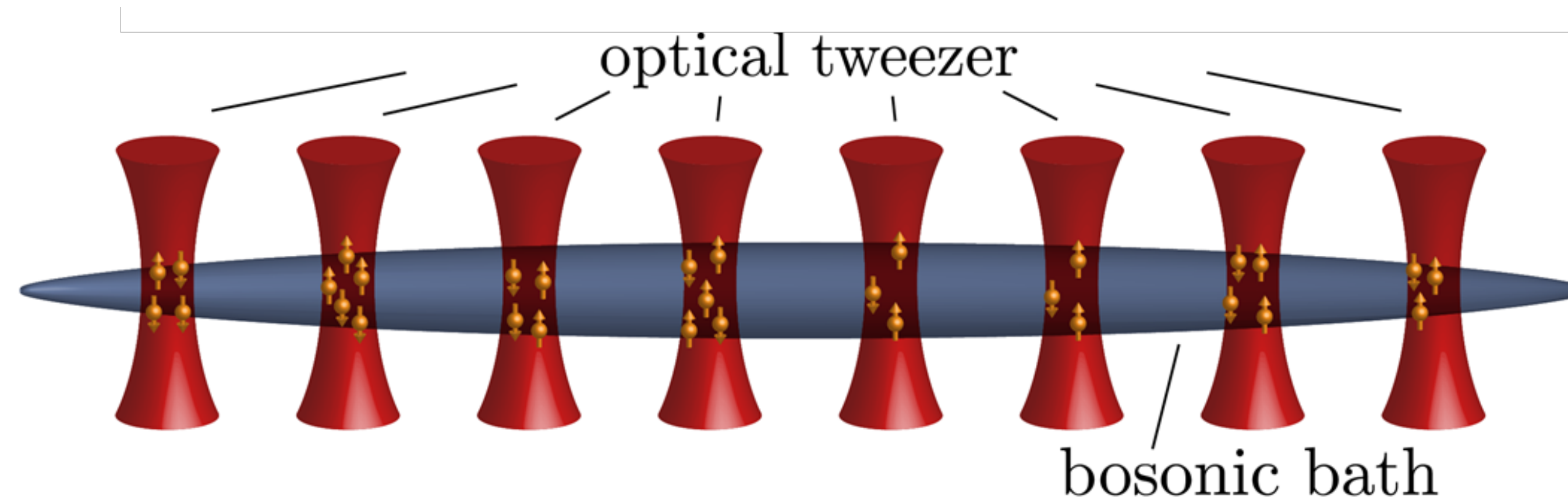


1.) Initialization

2.) Manipulation and evolution

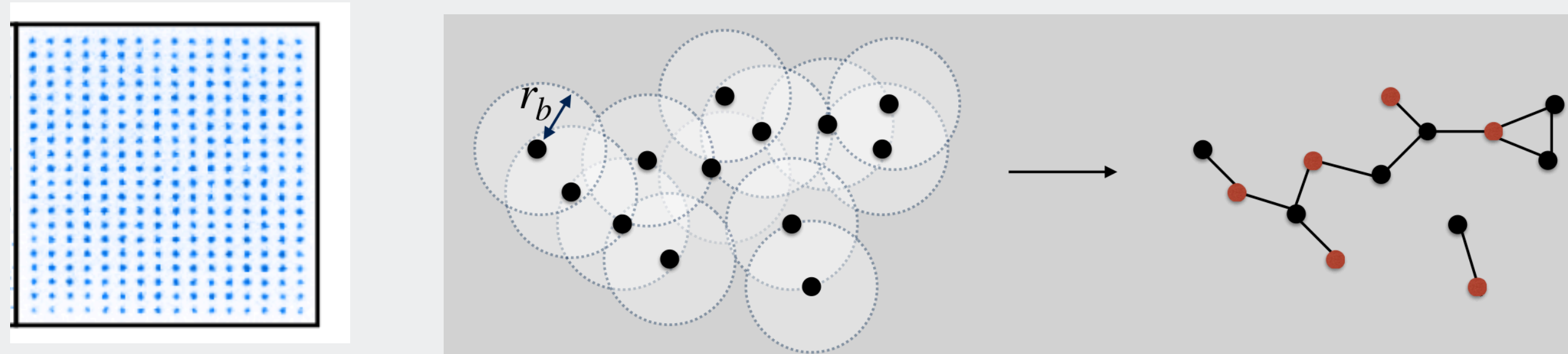
3.) Read-out

# Universal QC with atomic mixtures

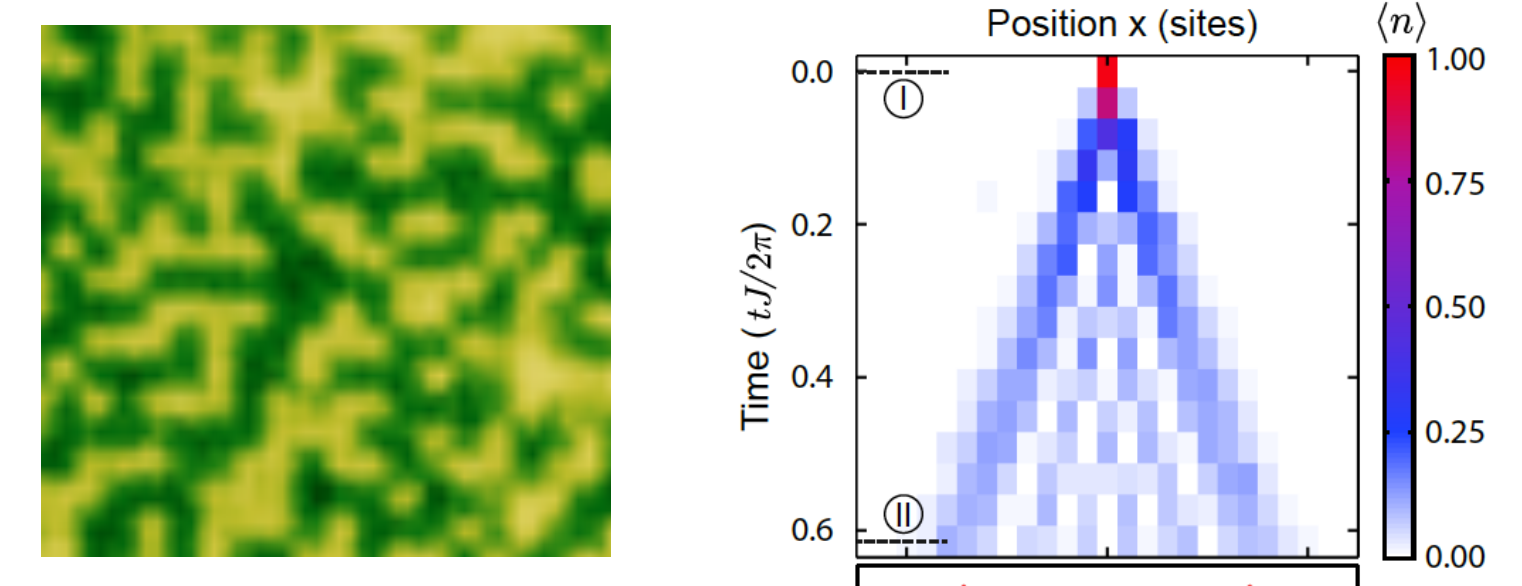


# Possible projects (in qiskit-cold-atoms)

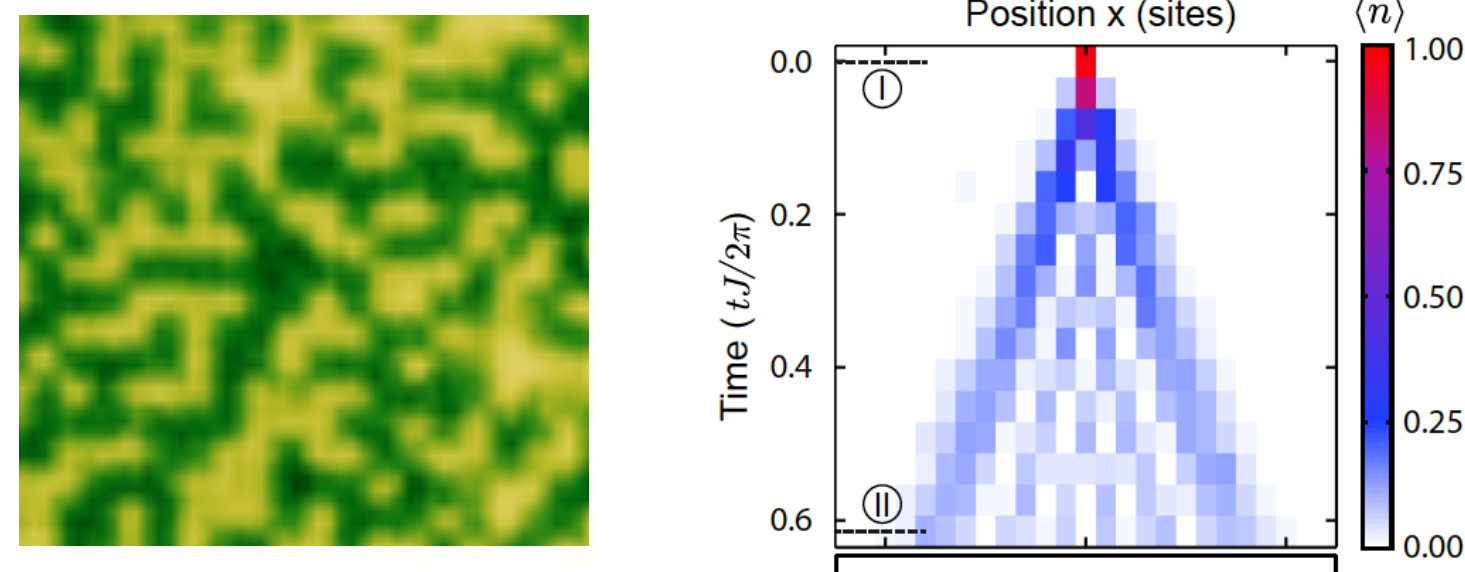
## Rydberg atoms for optimization problems



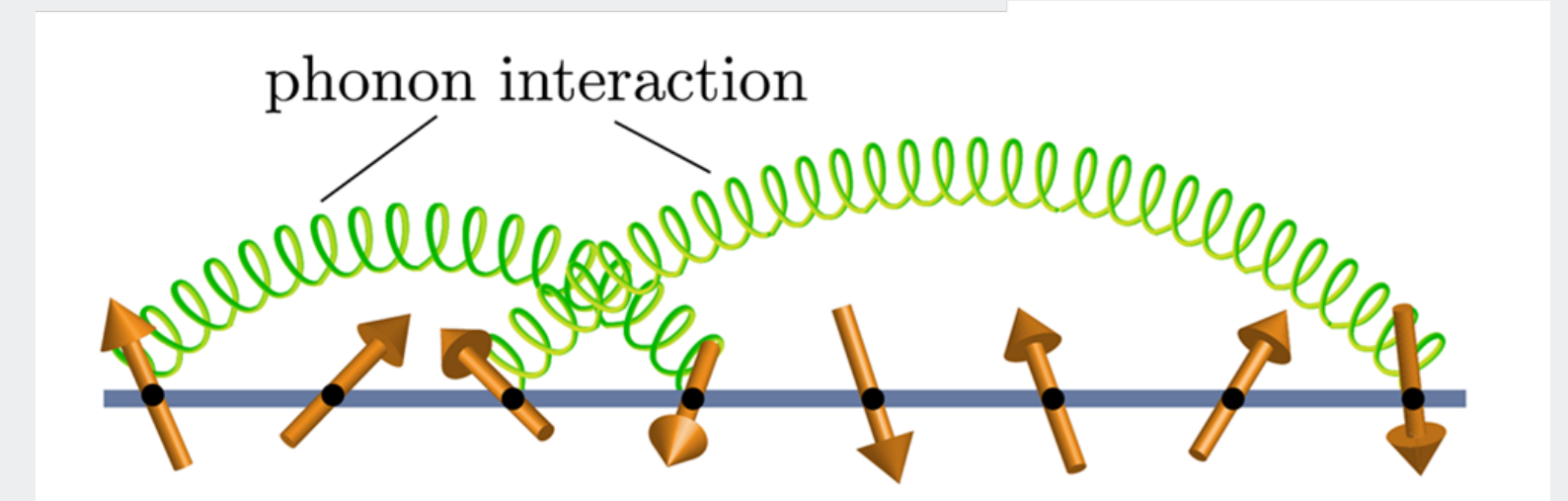
## Squeezing on superconducting circuits



## Lattice systems for itinerant particles



## Universal QC with atomic mixtures



## Digital and analog quantum simulators for lattice gauge theories

