Stop thinking classically!

Thomas Busch

OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY
沖縄科学技術大学院大学

Quantum Simulators

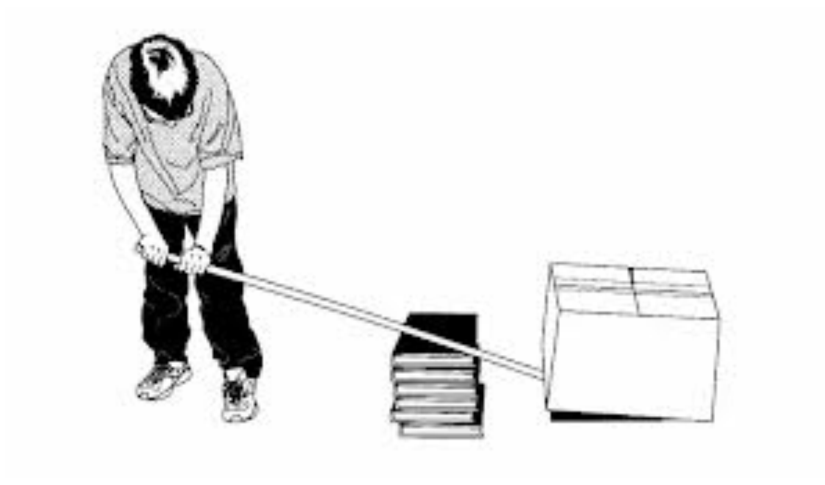
Thomas Busch

OIST OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY
沖縄科学技術大学院大学

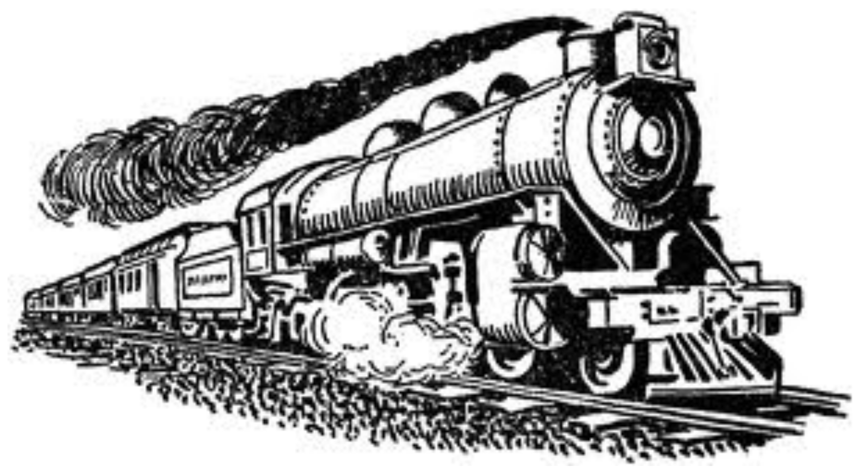
Motivation

New *physics* always lead to more insight and new technologies

Classical Mechanics
(Newton ~1700)



Thermodynamics
(Carnot ~1830)



Electrodynamics
(Maxwell ~1850)

Special/General Relativity
(Einstein ~1915)

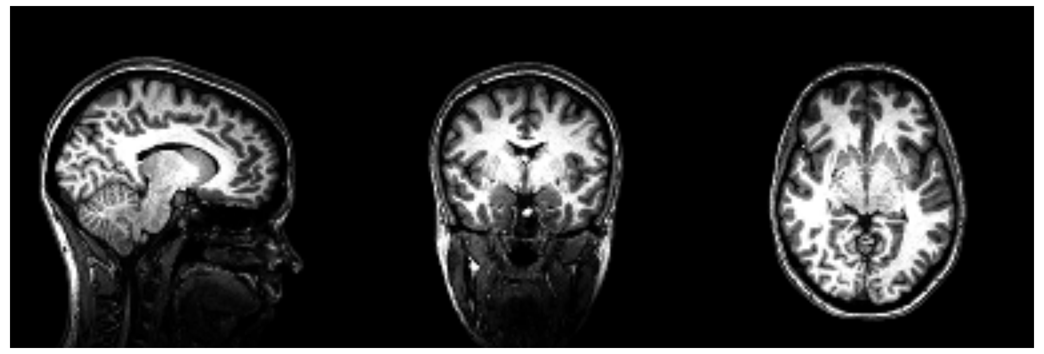
⟶ **what about the physics of the really small?**

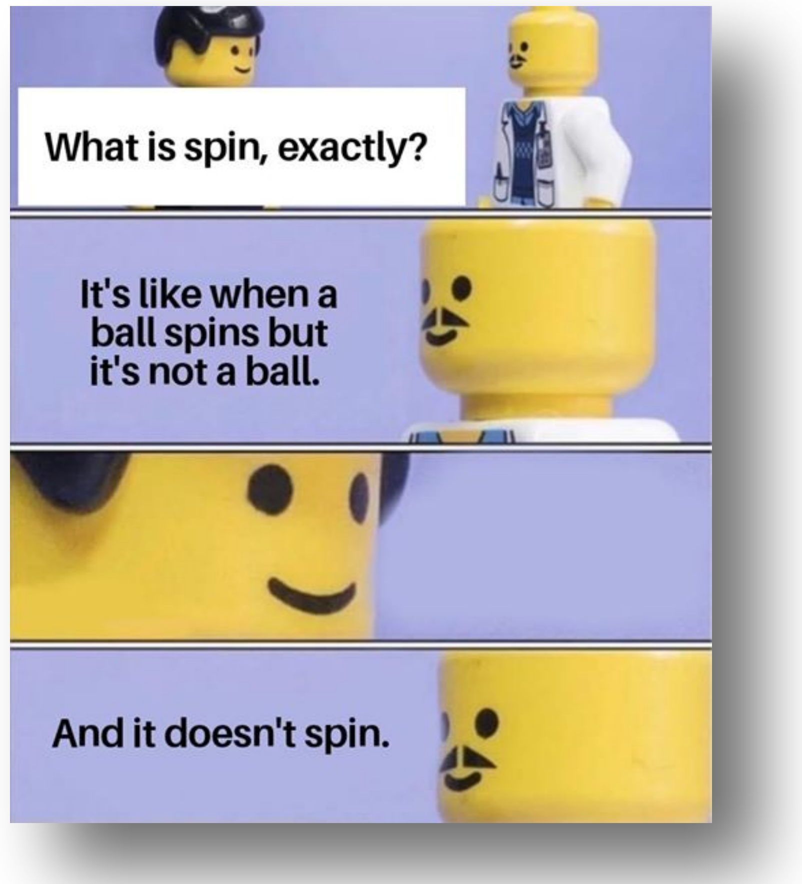
⟶ **Quantum Mechanics**

Motivation

Quantum Mechanics
(Bohr ~1920)

→ MRI scanners work on the spin of a particle (which are tiny magnets)

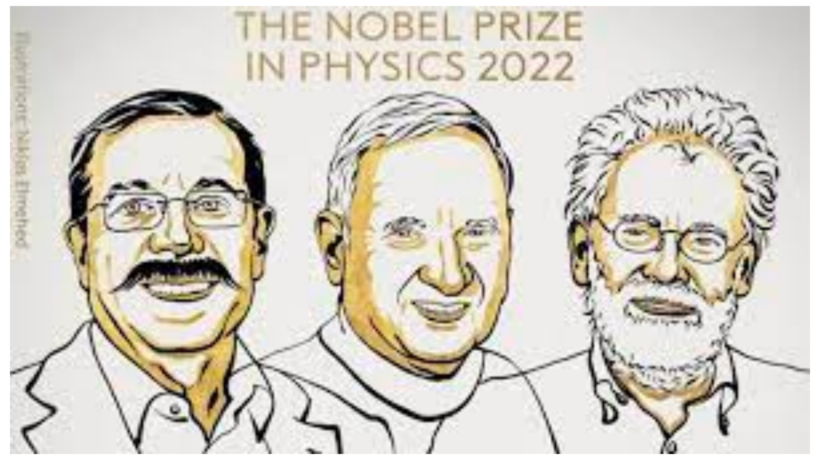




→ **But** these are many-particle quantum mechanical effects

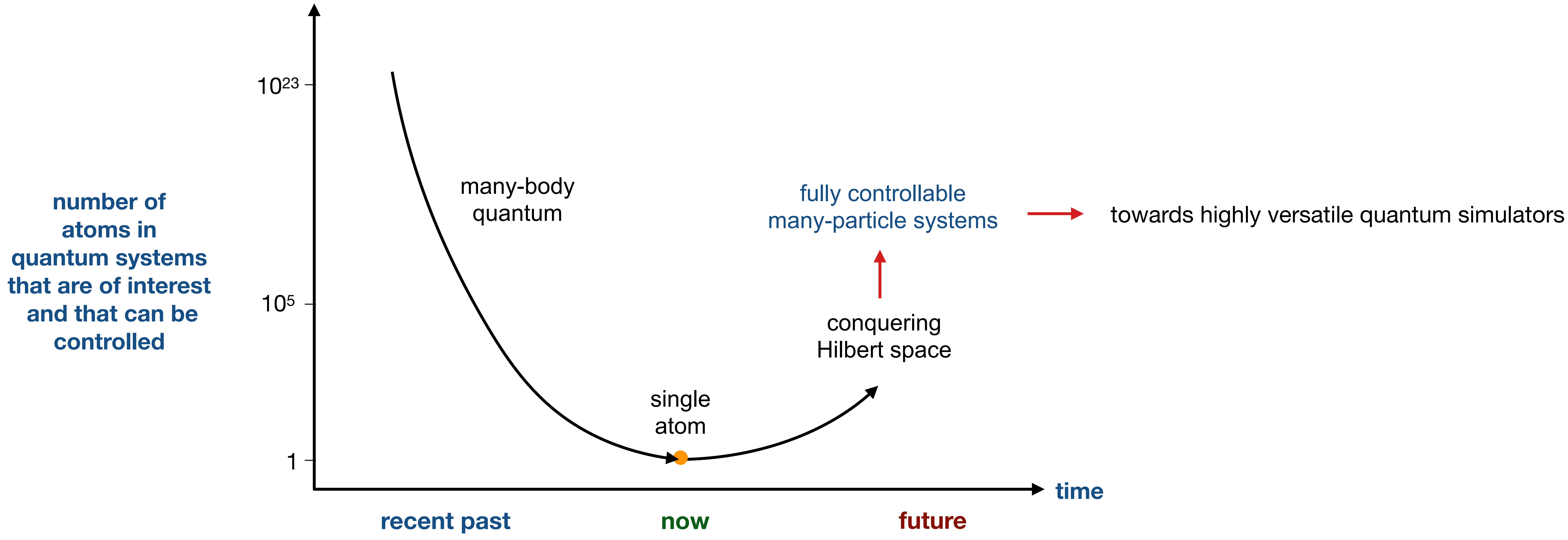
→ the world is too big and/or too hot and/or too slow to deal with single particle QM effects

→ until very recently...



→ The **second quantum revolution:** quantum computing, communication, metrology, simulations,….

Brief Review of Progress

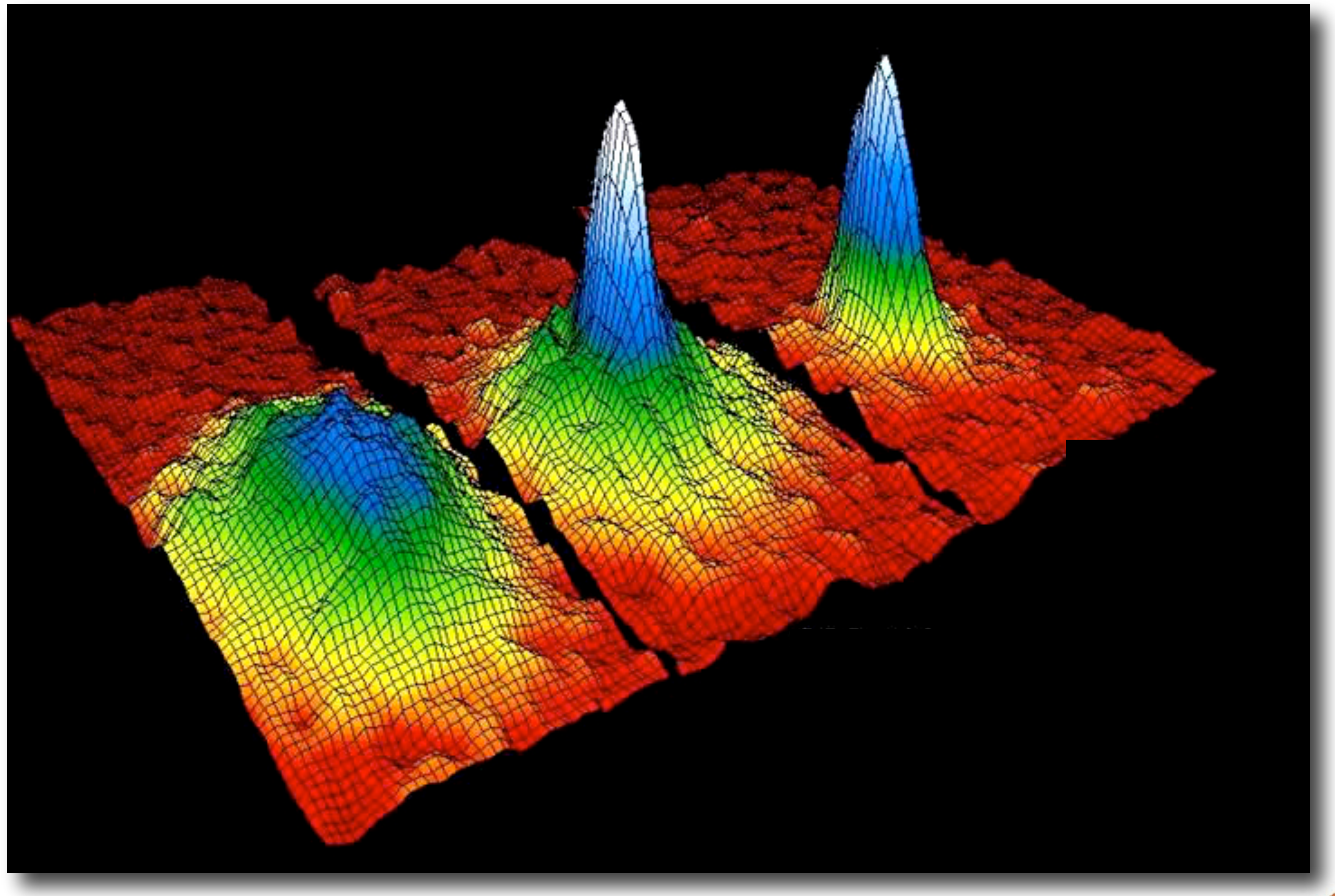


➔ the problem is that quantum systems are very fragile and the important coherences decay quickly

➔ need to find a good system

Ultracold Atoms

BEC 1995:

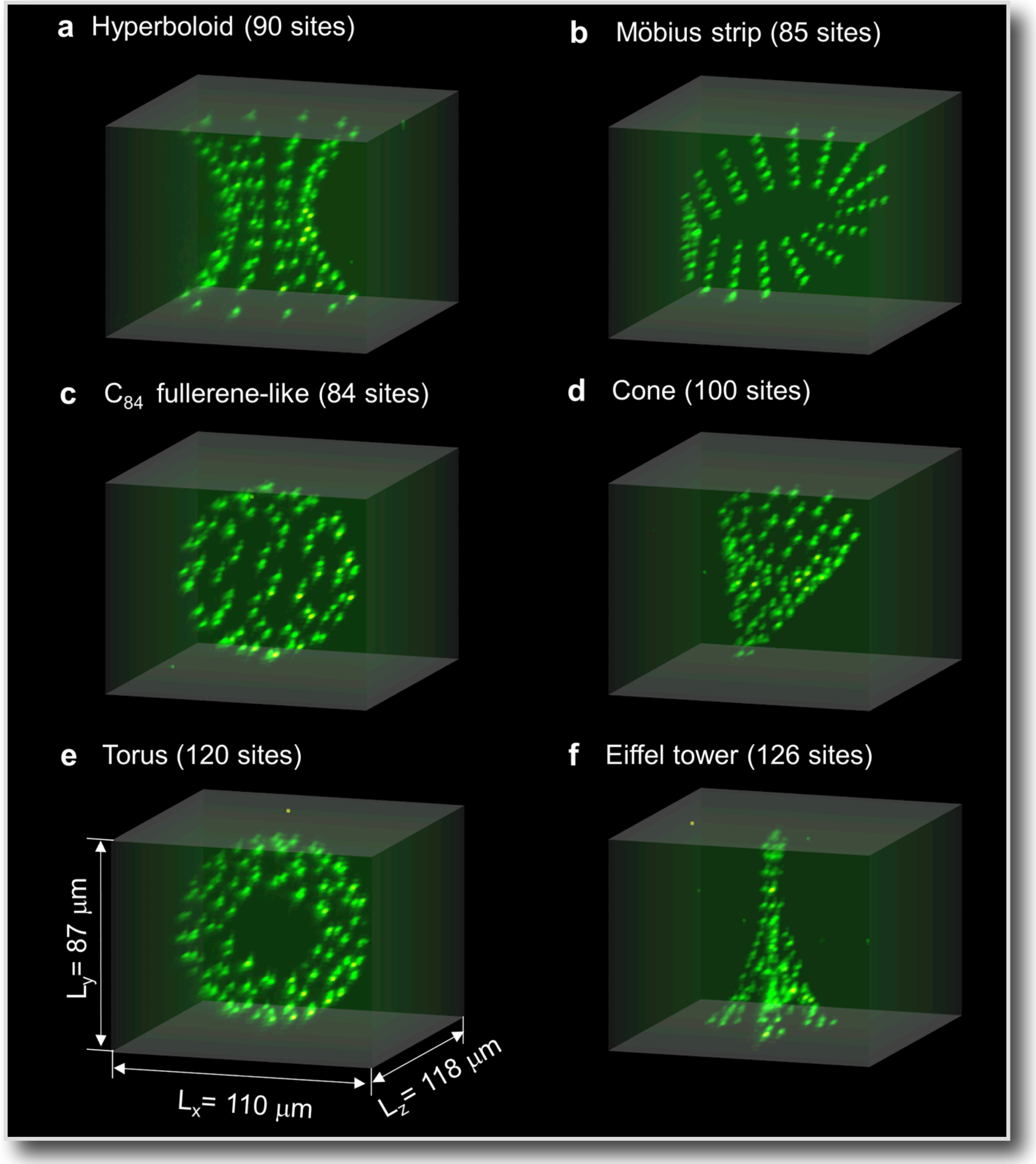


JILA 1995

2001

→ a <u>gas</u> of atoms at essentially zero temperature

Synthetic 3D atomic structures assembled atom by atom 2017:



CNRS 2017

→ full control over all degrees of freedom

Ultracold Atoms for Engineering

$$\mathcal{H} = \mathcal{H}_{\text{kinetic}} + \mathcal{H}_{\text{potential}} + \mathcal{H}_{\text{interactions}}$$

- $\mathcal{H}_{\text{kinetic}}$: artificial gauge fields, spin-orbit coupling, optical lattices
- $\mathcal{H}_{\text{potential}}$: dimensionality, painted potentials, optical lattices, optical tweezers, magnetic traps, atom chips
- $\mathcal{H}_{\text{interactions}}$: Feshbach resonances, Rydberg atoms, dipolar atoms, droplets

→ Floquet engineering

→ spinor wavefunction $|\Psi\rangle$
- → internal states
- → different species (bosons and fermions)
- → atoms and molecules

→ hybrid systems: interfacing atoms and photons

by no means complete!

cold atomic systems are highly controllable, versatile and can be measured in many ways

→ **foreordained for exploring new quantum few/many body physics with large control**

Ultracold Atoms for Quantum Simulations

real systems are often hard to access and can be noisy or impure

→ use a highly configurable quantum system to model the original system

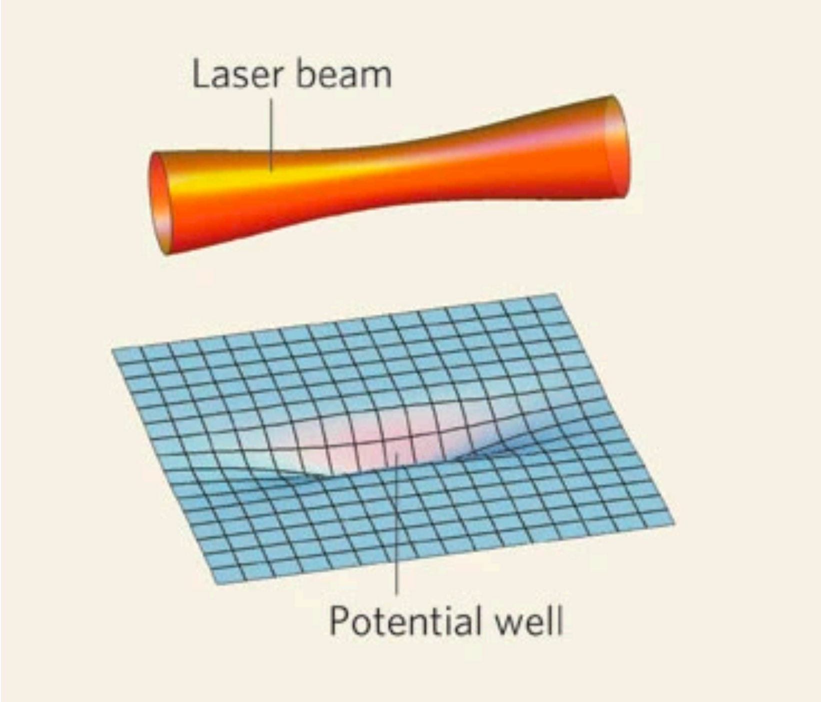
Example: **new materials that meet specific requirements**
classical computing is not powerful enough to predict relevant properties in systems with, for example, strong correlations

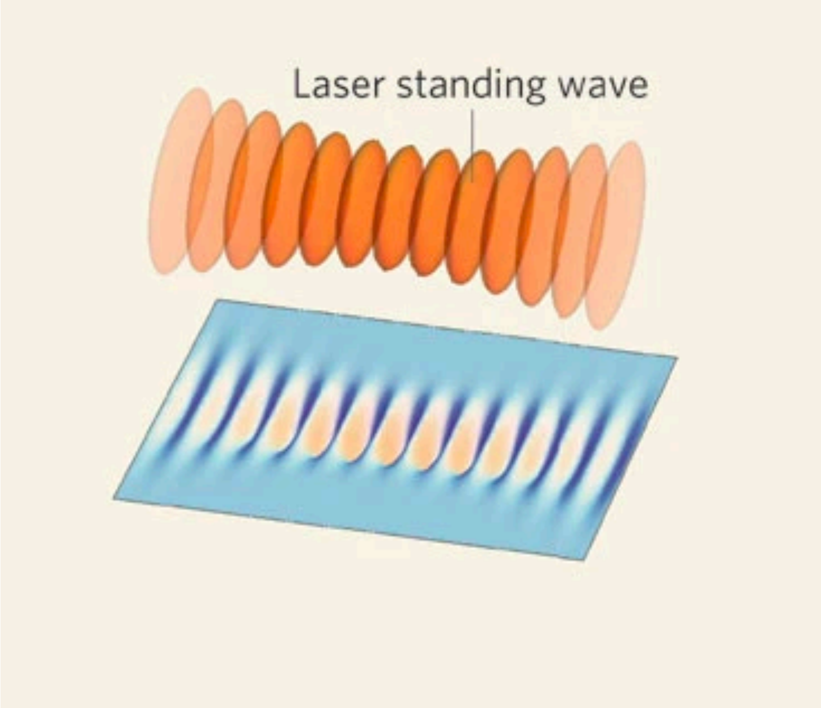
Example: **Alzheimers, Parkinsons and Huntingtons diseases are caused by misfolded protein molecules**
Quantum simulations can help understand protein folding and help cure these diseases.

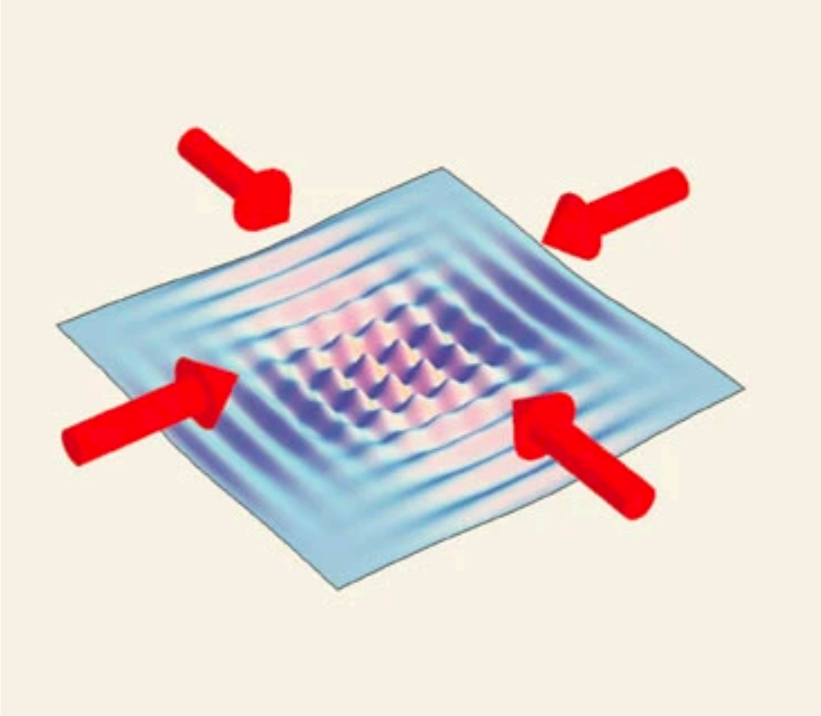
Example: **quantum for the environment**
understanding the precise quantum dynamics of chemical reactions can benefits our environment. Quantum simulators could find chemical catalysts to remove CO2 from the atmosphere, or reduce the massive amounts of energy needed to make fertilizers.

Example: Optical Lattices

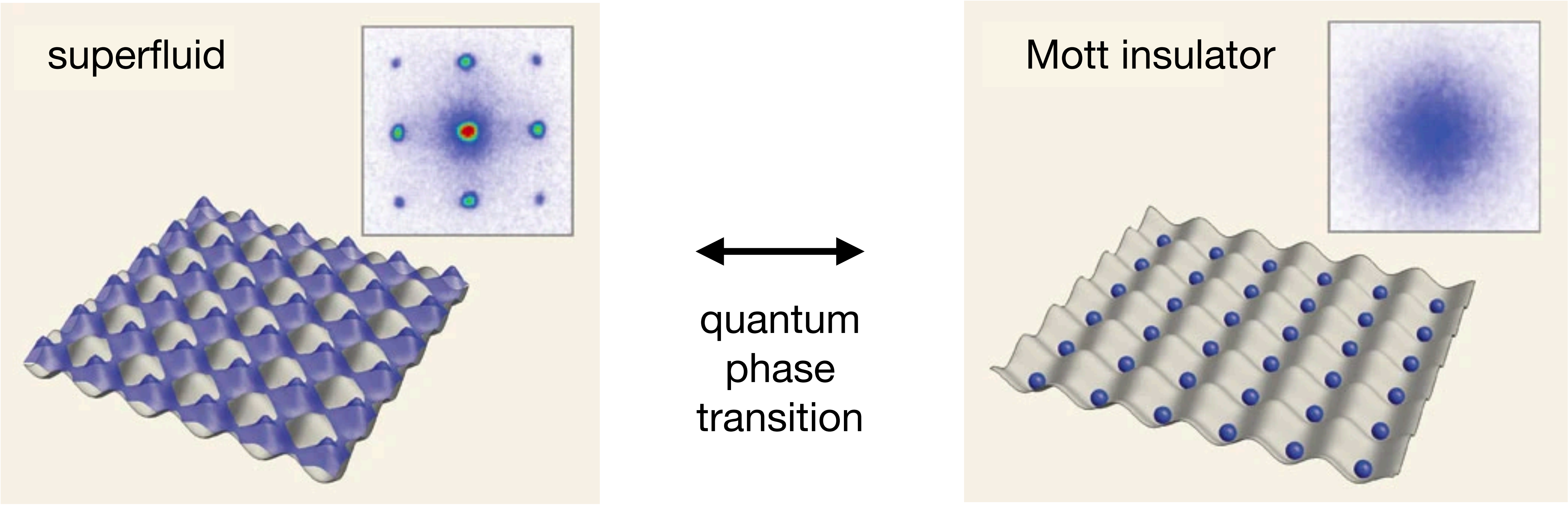
→ arrange single atoms in space; synthetic condensed matter systems







→ reduced complexity, reduced noisy, no imperfections etc.



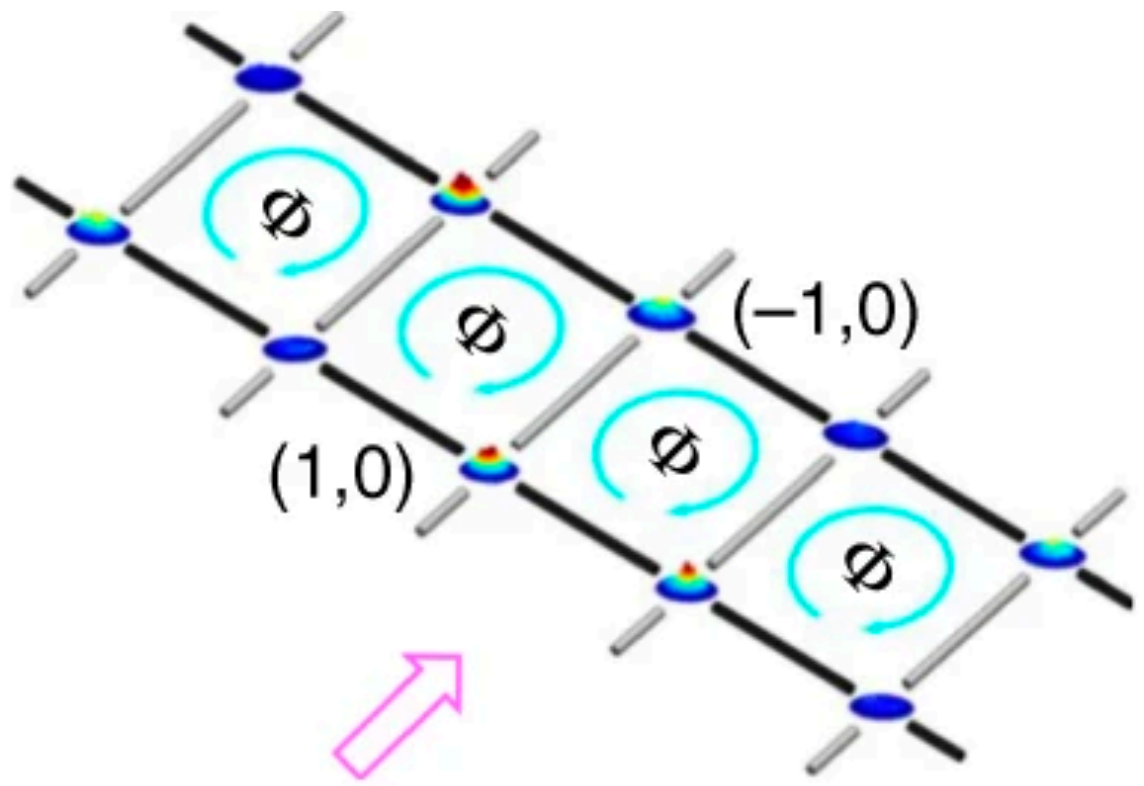
→ but quantum simulators can also help to get into new parameter regimes

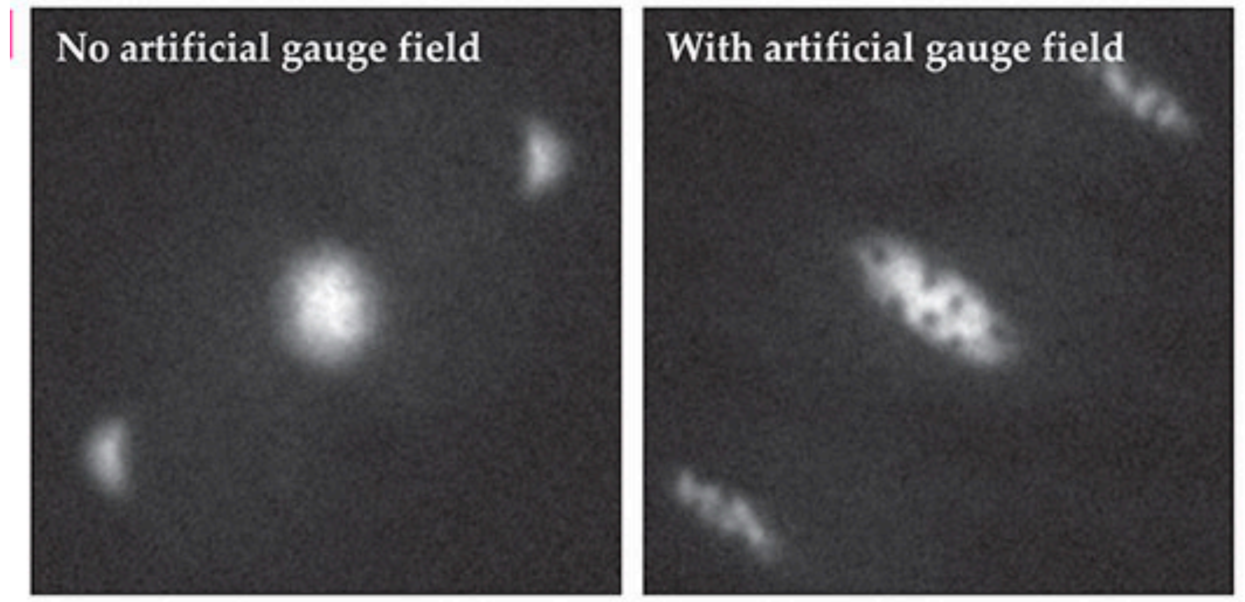
Example: Artificial Magnetic Fields

→ ultracold atoms are neutral, cannot be used to study the effects of magnetic fields

→ but, the effects of external magnetic fields is for a particle to pick up a phase when moving around a closed trajectory

→ we can do that in different ways: same physics, new regimes





Quantum Simulators: Example

→ these are all very helpful new experiments, but also very simple simulators

→ quantum engineering toolbox is growing quickly, but to solve all problems new ideas need to be developed

Develop and idea is four easy steps:

1. Remember the optical lattice? Distance between two atoms is given by the optical wavelength (100s nm)

2. But what if we want the atoms to be closer together? Cannot be done with optical waves…

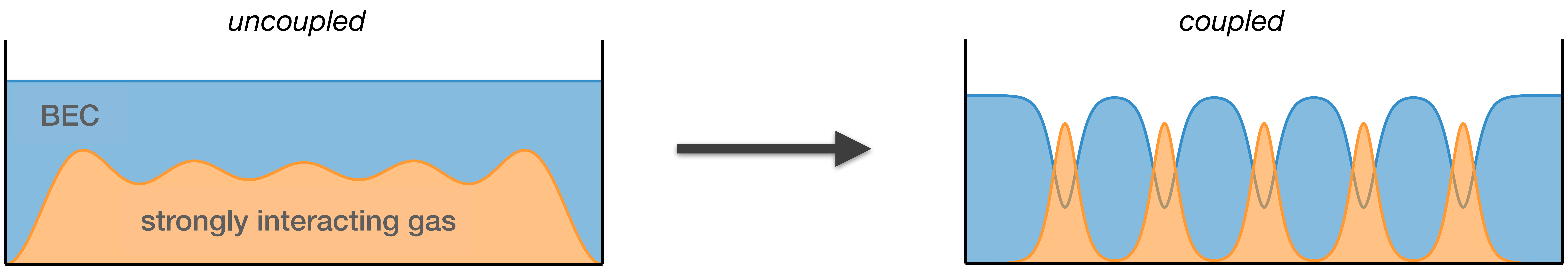
3. But, in quantum mechanics *particles are waves* (and *waves are particles*)

4. Can we use **matter waves?**

Quantum Phase Transition for interaction particles w/out a lattice?

Aim: Realise an insulator phase transition purely via atomic interactions and <u>without</u> an externally imposed lattice potential. **(effective 1D model)**

→ immerse a strongly interacting gas in a BEC (matter wave), imbalanced system



interacting gas is a superfluid

interacting gas is an insulator

→ can the BEC act like a matter-wave lattice?

→ what determines the distance between the trapped atoms?

→ extension of many-body quantum simulator?

Pinned State

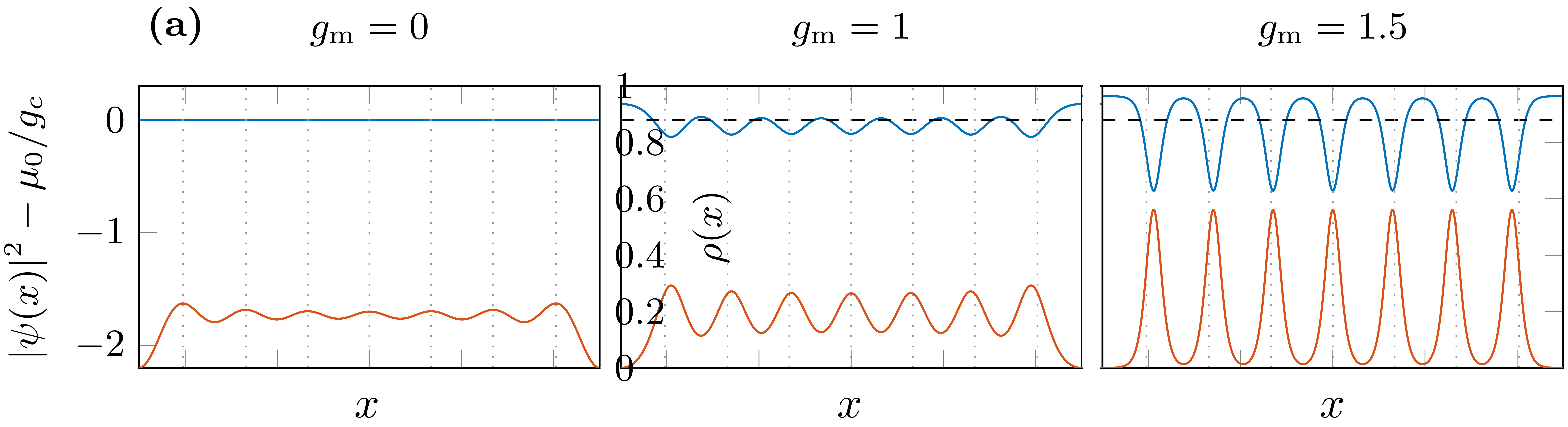
$T = 0$

BEC (GPE): $$i\dot{\psi}(x) = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} + g_c\,|\psi|^2 + g_m\,|\Phi|^2\right]\psi(x)$$

immersed gas (exact): $$i\dot{\Phi}(\mathbf{x}) = \left[\sum_l^N -\frac{1}{2}\frac{\partial^2}{\partial x_l^2} + V(x_l) + V_{int} + g_m\,|\psi|^2\right]\Phi(\mathbf{x})$$

→ numerically solve the coupled equations

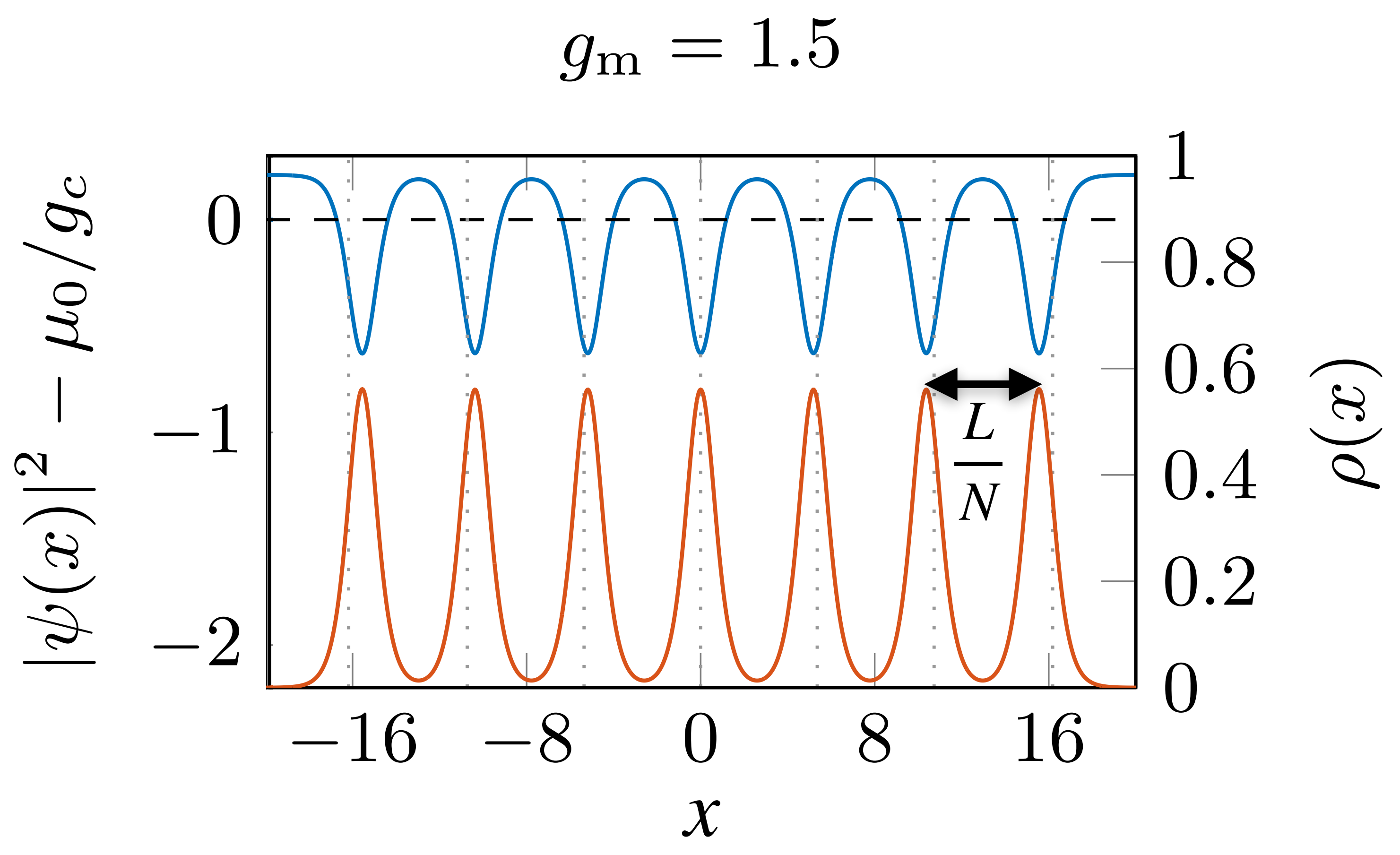
adiabatically ramp g_m



→ **periodic arrangement of localised impurities**

→ **period is given by inverse Fermi momentum**

Pinned State: effective model



pinned state density

$$\rho_{\text{pin}}(x) = \frac{a_{\text{pin}}}{2}\sum_{n=1}^{N}\frac{1}{\cosh^2[a_{\text{pin}}(x-x_n)]}$$

BEC in Thomas-Fermi regime for $g_{\text{m}} \ll \mu_0 L/N$

$$\psi(x,t) = \sqrt{\frac{1}{g_{\text{c}}}\left(\tilde{\mu} - g_{\text{m}}|\Phi(x)|^2\right)}e^{-i\tilde{\mu}t} \qquad \tilde{\mu} = \mu_0\left(1 + \frac{g_{\text{m}}N}{g_{\text{c}}N_{\text{c}}}\right)$$

effective model for single impurity

$$\hat{H}_1 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + g_m|\psi|^2 \rightarrow \hat{H}_1' = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{g_m^2}{g_c}|\phi_1|^2$$

→ $\phi_1(x) = \sqrt{\frac{a_0}{2}}\frac{1}{\cosh(a_0 x)}$ with $a_0 = \frac{g_{\text{m}}^2}{2g_{\text{c}}}$

Soliton-like state

→ take into account energy needed to prevent TG atoms from dispersing and required to displace BEC density

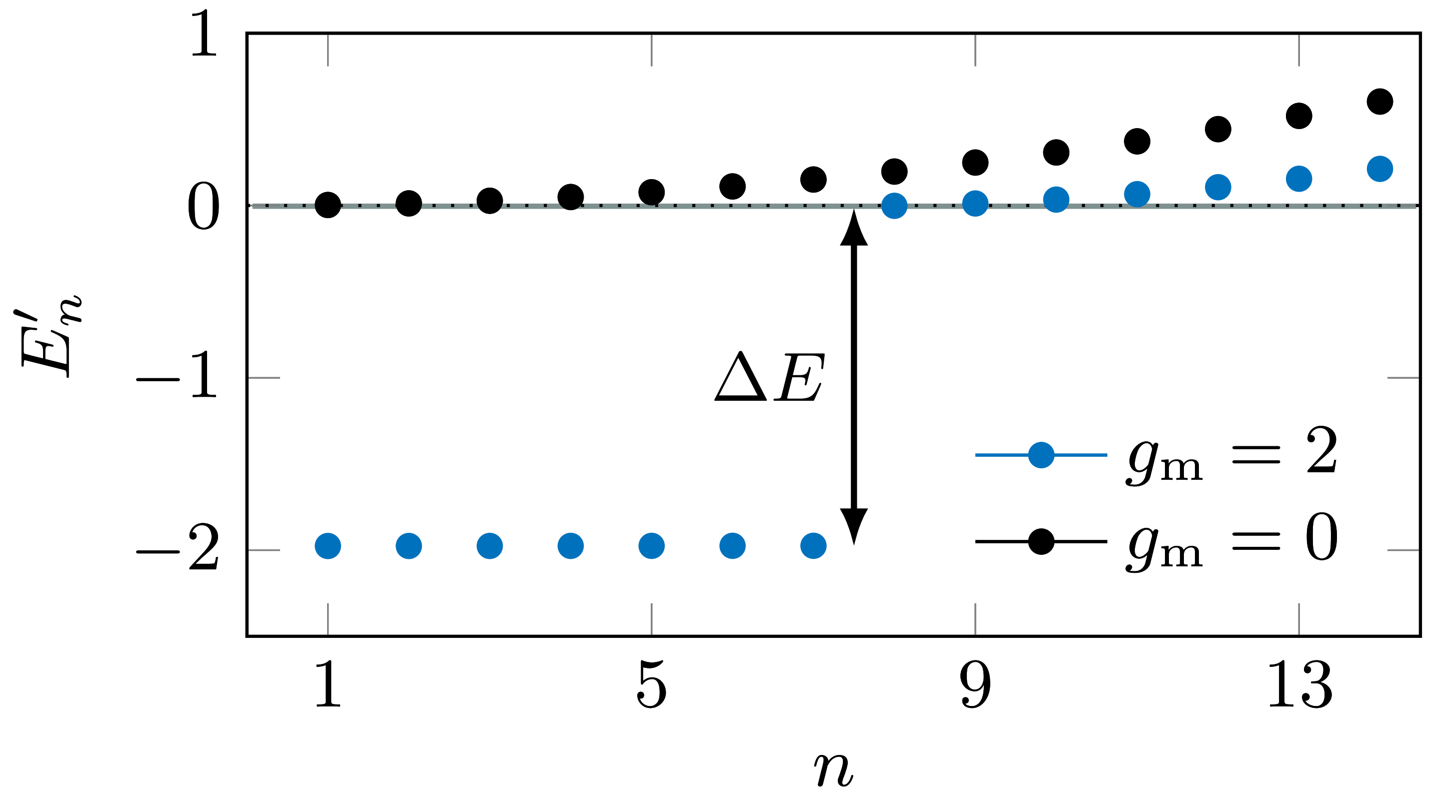
$$a_{\text{pin}} = a_0\frac{\sqrt{1+2\epsilon}-1}{\epsilon} < a_0 \quad \text{with} \quad \epsilon = \frac{6a_0^2}{5\tilde{\mu}}$$

Aside: state looks and smells somehow like a boson FFLO state…

Pinned State: phase transition

- energy gap separates the pinned states from the continuum
- when does the gap open?

$E'_n = E_n - g_m\tilde{\mu}/g_c$



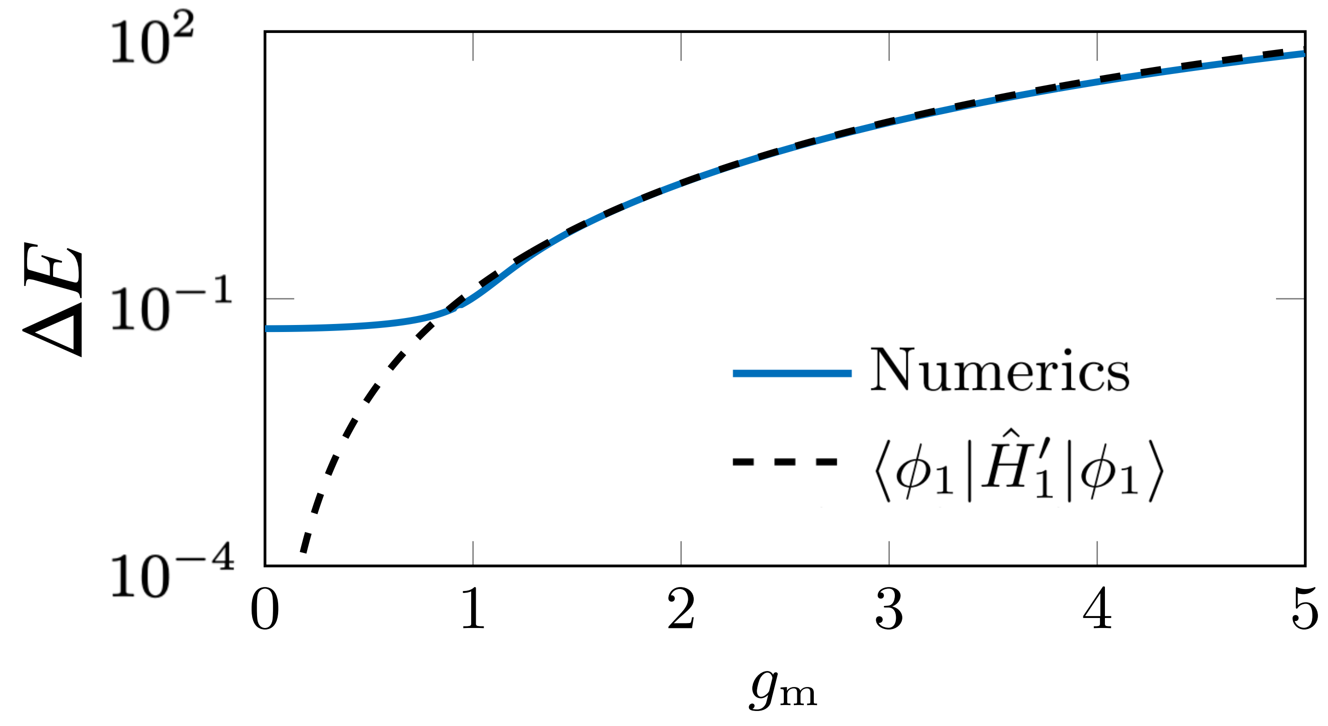
In the shifted reference frame:

$$\Delta E = E'_{N+1} - E'_N \approx |E'_1|$$

Can we use the effective model to estimate the size of the energy gap?

$$\hat{H}_1{}' = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{g_m^2}{g_c}|\phi_1(x)|^2$$

- $\Delta E \approx \langle\phi_1|\hat{H}'_1|\phi_1\rangle = |a_{\rm pin}^2/6 - 2a_0 a_{\rm pin}/3|$



- these are all results for zero temperature.

Pinned State: finite temperature

- does the self-pinning state survive at finite temperature?

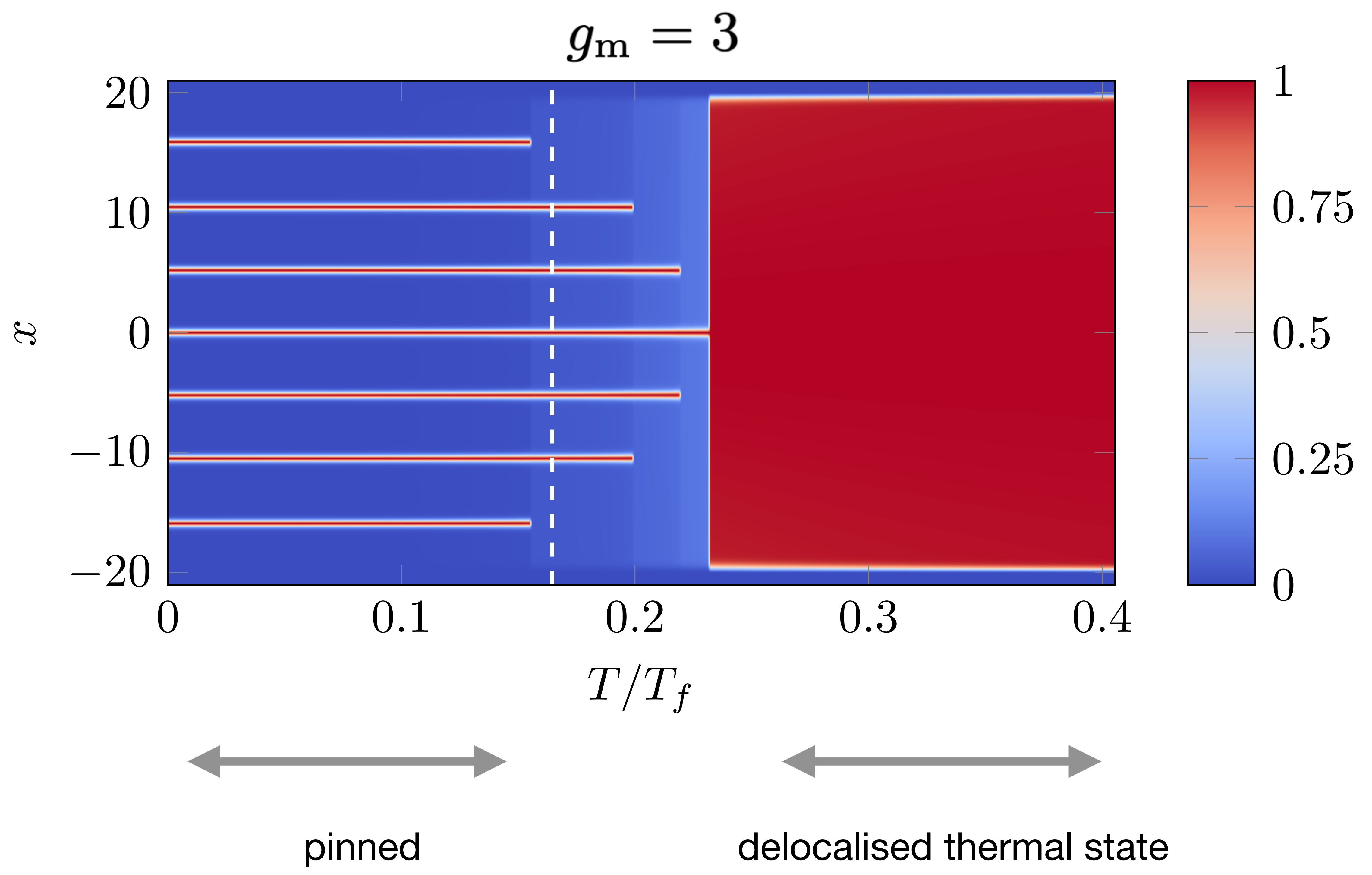
density of the Tonks-Girardeau gas at finite temperature:

$$|\Phi(x)|^2 = \sum_{n=1}^{\infty} f_n \, |\phi_n(x)|^2$$

with Fermi-Dirac distribution

$$f_n = \frac{1}{\exp\left[\beta\left(E_n - \mu\right)\right] + 1}$$

and assuming that the temperature of the BEC does not change



- initially a large energy gap protects the pinned state
- particles start to be ejected from the pinned state in a crossover region
- at high temperature all particles are delocalised

Pinned State: finite temperature

- modify the effective Hamiltonian to include thermal effects $\phi_1 \to \sqrt{f_1}\phi_1$

- $$\hat{H}_{\mathrm{eff}} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{g_{\mathrm{m}}^2}{g_{\mathrm{c}}}|\phi_1(x)|^2$$

- temperature effectively reduces the interaction!

- reduced interaction changes the energy E_1' and therefore f_1, etc...

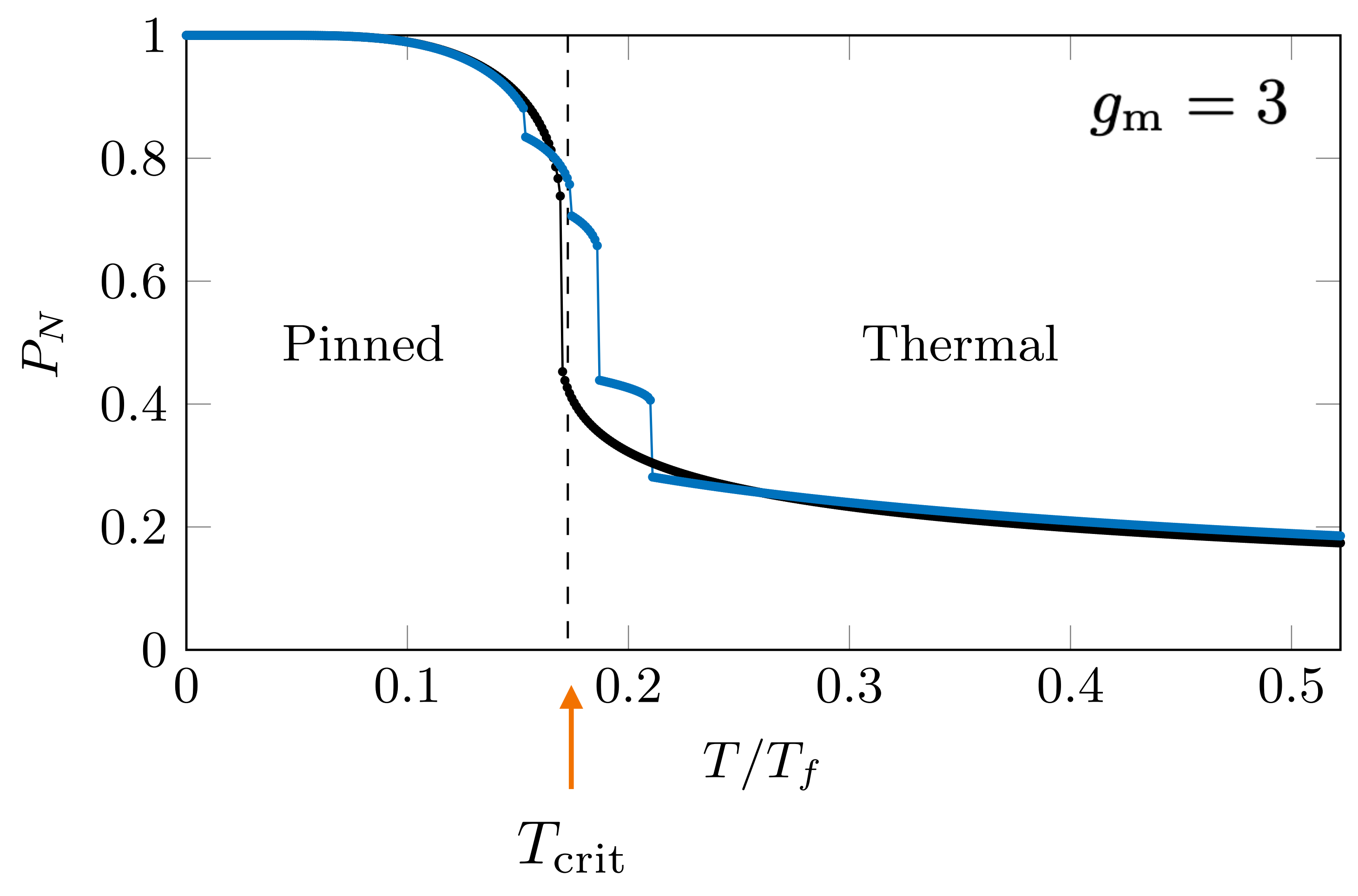
- needs a self-consistency criterion for finding the energies and occupations

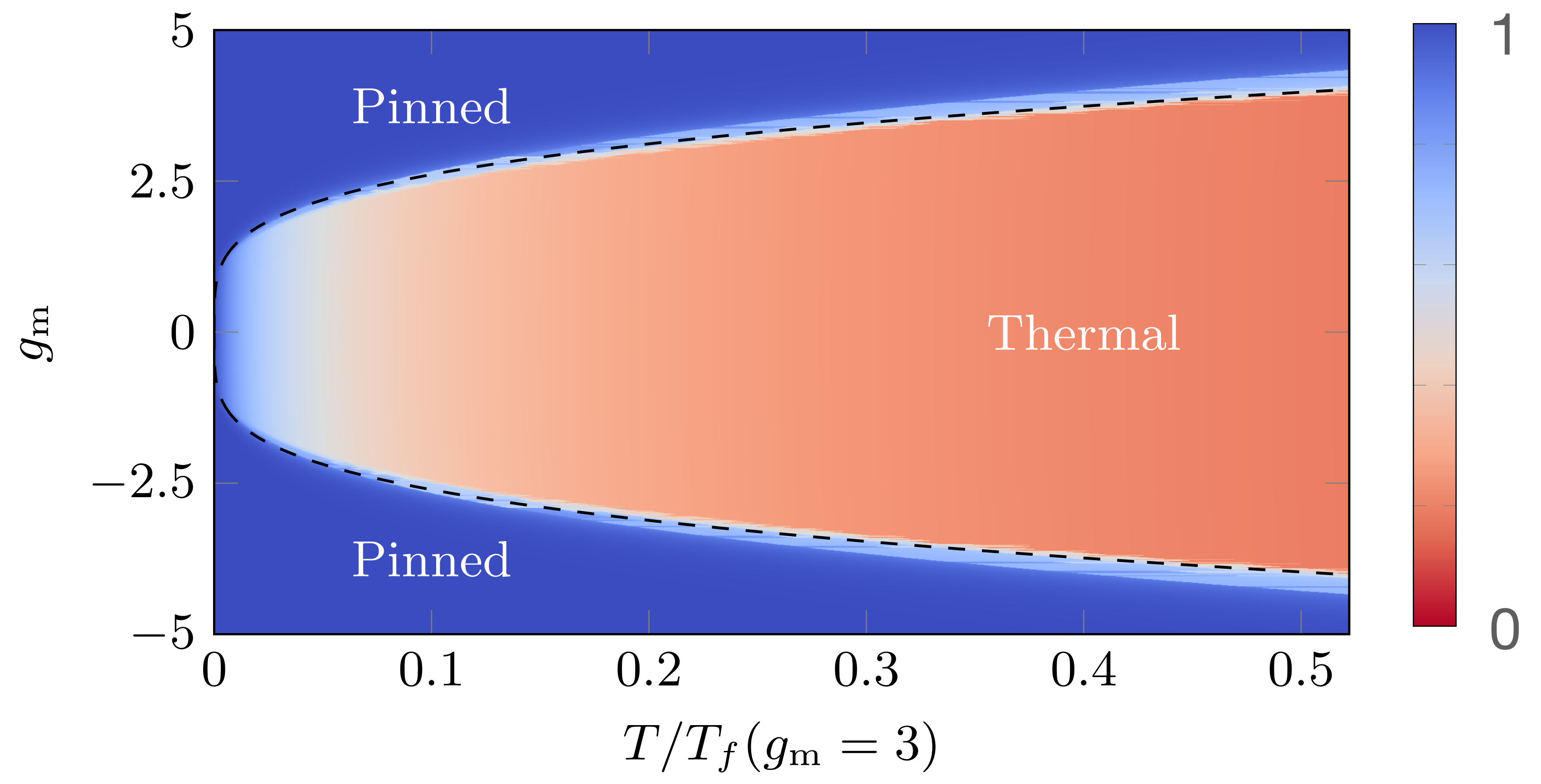
$$f_{\mathrm{pin}} = \frac{1}{\exp\left[\beta\left(E(f_{\mathrm{pin}}) - \mu(f_{\mathrm{pin}})\right)\right] + 1}$$

- one can estimate a **critical temperature** for the pinned state phase transition from the point where the change in the ground state occupancy is maximal

$$\frac{T_{\mathrm{crit}}}{T_f} = C(f^*)\frac{\sqrt{1 + 2\left(f^*\right)^2\epsilon} - 1}{\sqrt{1 + 2\epsilon} - 1}$$

Ground state occupancy $P_N = \sum_{n=1}^{N} \frac{f_n}{N}$





But there is more. Quantum can also do stuff differently…

Quantum Tech: Work & Heat & Engines

→ two fundamental forms of energy transfer

	macroscopic	**microscopic**	
Work:	energy change induced by the variation of a mechanical parameter	displacement of energy levels in quantum systems	$W = \sum_n f_n \Delta E_N$
Heat:	energy exchanged with a thermal bath	modification of a systems population probability distribution	$Q = \sum_n \Delta f_n E_N$

Heat Engine: *convert thermal energy into mechanical work* by cyclically operating between effective thermal reservoirs at different temperatures

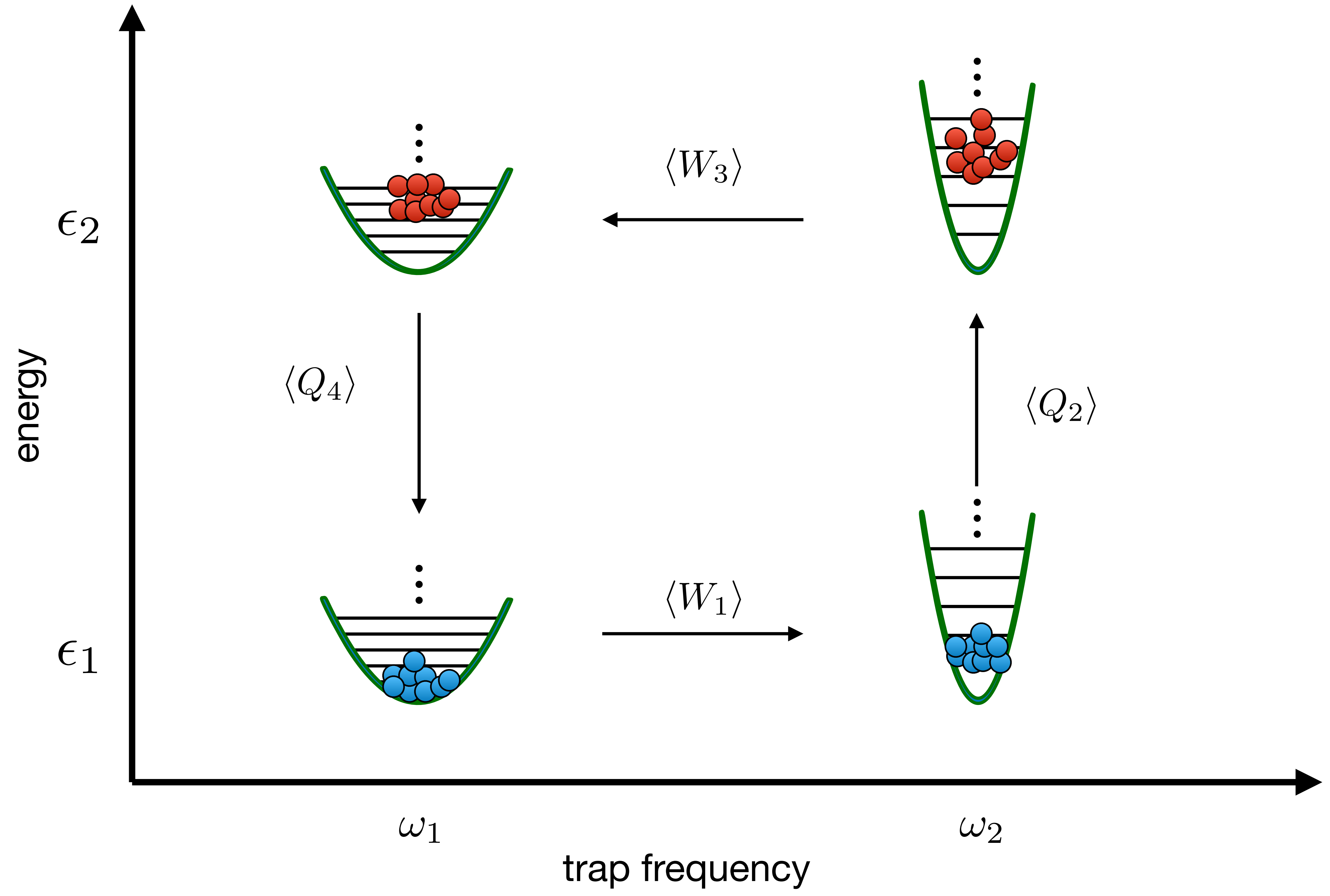
→ heating/cooling strokes redistribute the quantum state populations

Quantum Heat Engine: uses *quantum effects* in the heat engine process (squeezed baths, quantum STAs, etc)

Quantum Engine: uses genuinely non-classical forms of energies in a heat-engine-like cycle

Otto Cycle

- consider a gas of particles in a harmonic trap



- heat stroke changes temperature
- changes the distribution function

$$f_n = \frac{1}{\exp\left(\frac{E_n - \mu}{k_B T}\right) \pm 1}$$

- energy is added to the engine

- but there are other ways one can change the distribution function: change the chemical potential
- or change the *quantum part* by turning the ‘plus one’ into a ‘minus one’ or v.v.

Statistical Quantum Engine Considerations

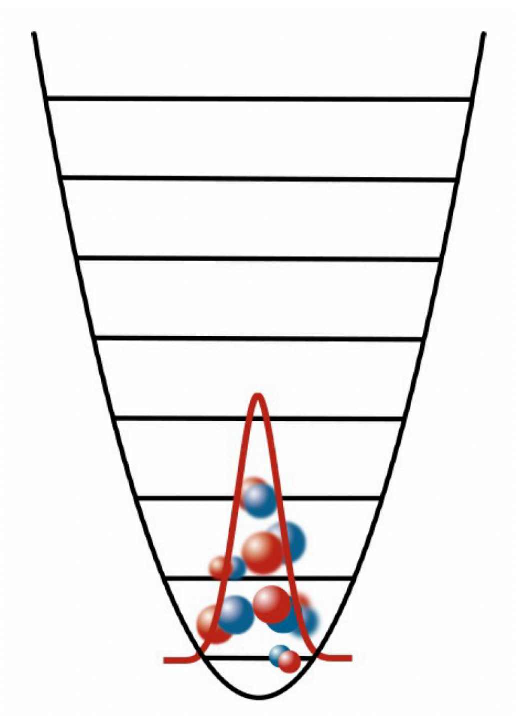
$$f_n = \frac{1}{\exp\left(\frac{E_n - \mu}{k_B T}\right) \pm 1}$$

→ switch the working medium cyclically from a Bose-Einstein statistics to a Fermi-Dirac statistics

→ at fixed temperature

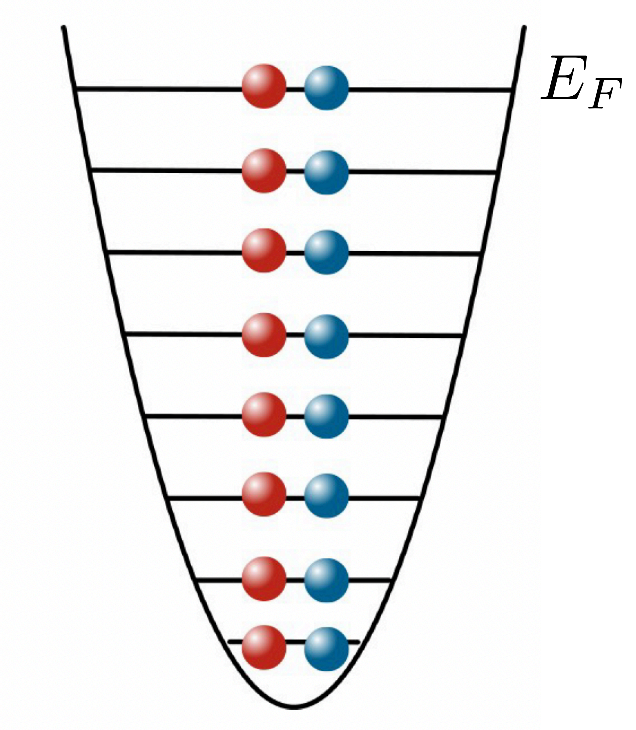
$$T = 0$$

bosons



Bose-Einstein condensate

fermions



Fermi sea

Remember:

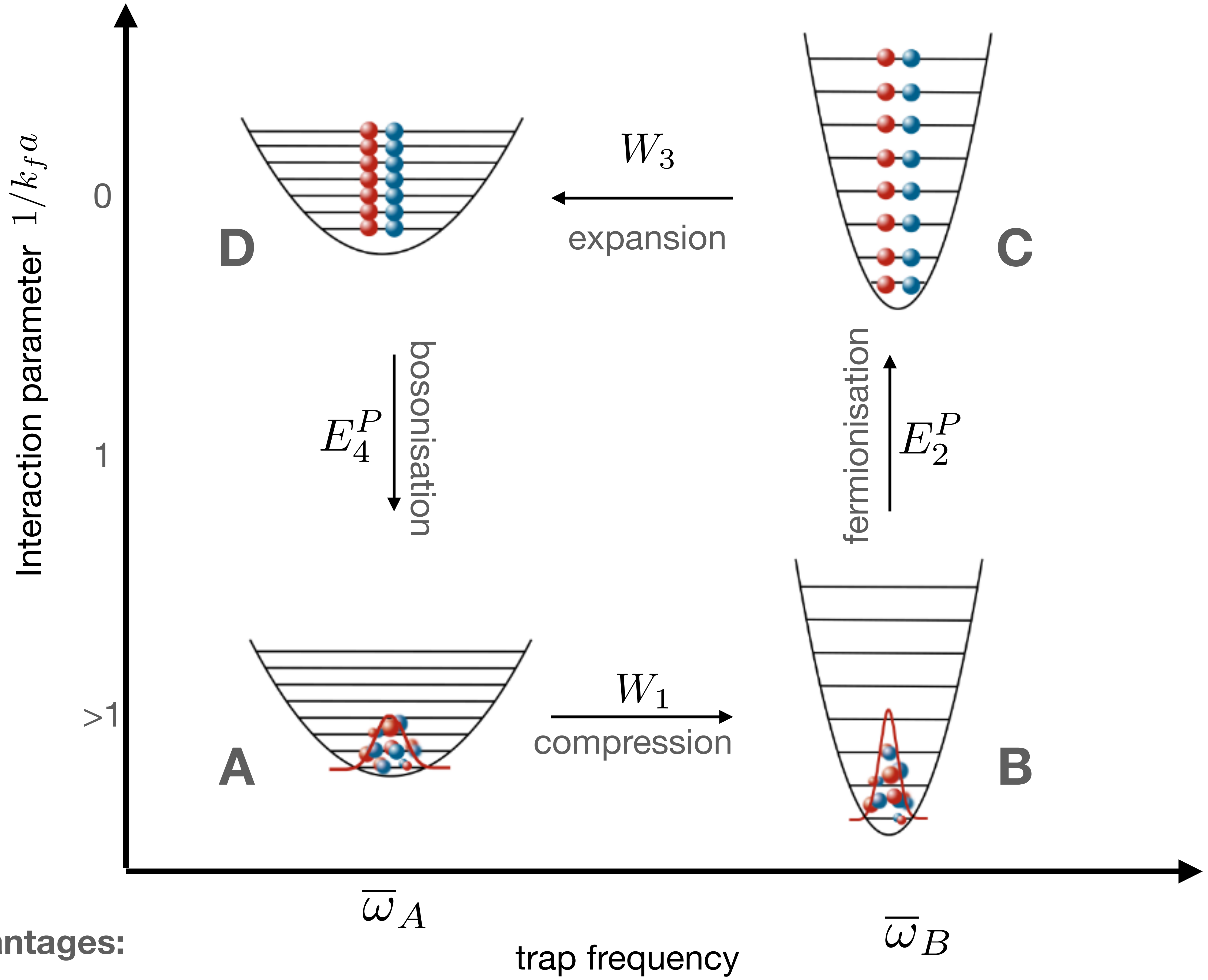
$$Q = \sum_n \Delta f_n E_N$$

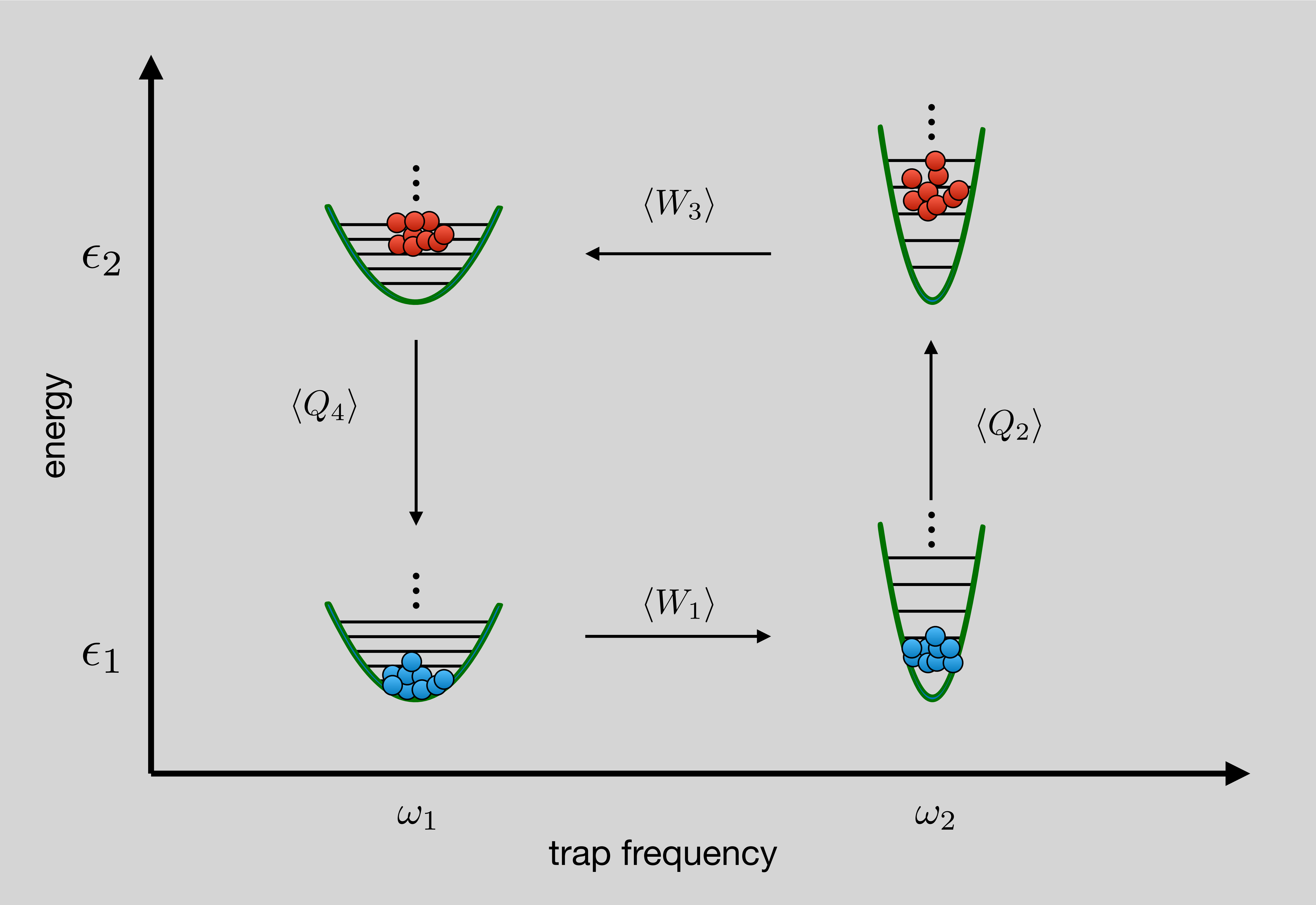
→ first idea: use nuclear processes! Hard to do cyclically, known nuclear decay processes do not change statistics,….

→ use BEC-BCS transition region, where fermionic atoms can be turned into bosonic molecules via a Feshbach resonance

Pauli Engine

→ cyclically converts energy stemming from the Pauli exclusion principle (”Pauli energy”) into mechanical work





advantages:

→ fully reversible process

→ no coupling to a bath required

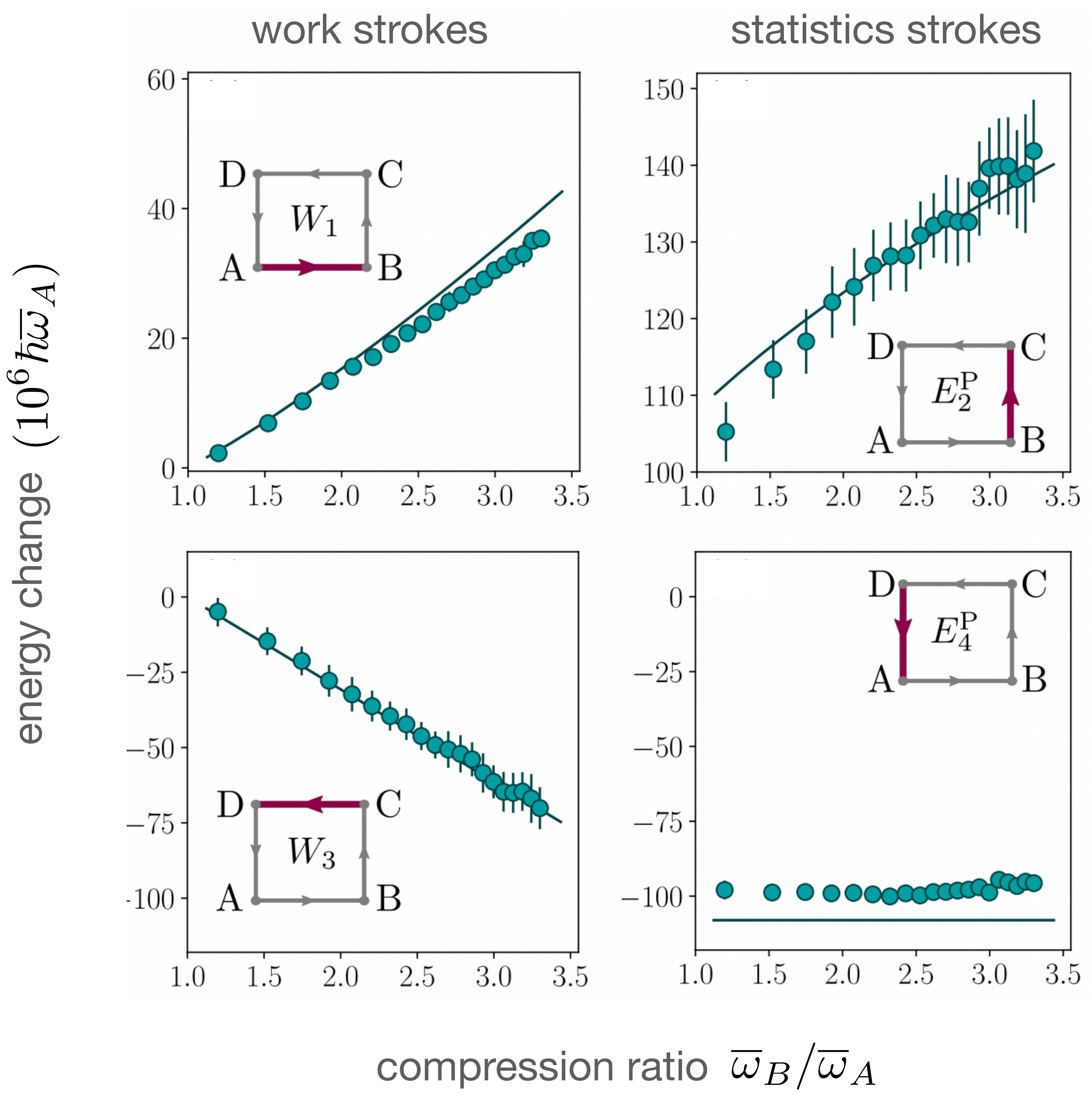
→ minimal dissipation, entropy constant

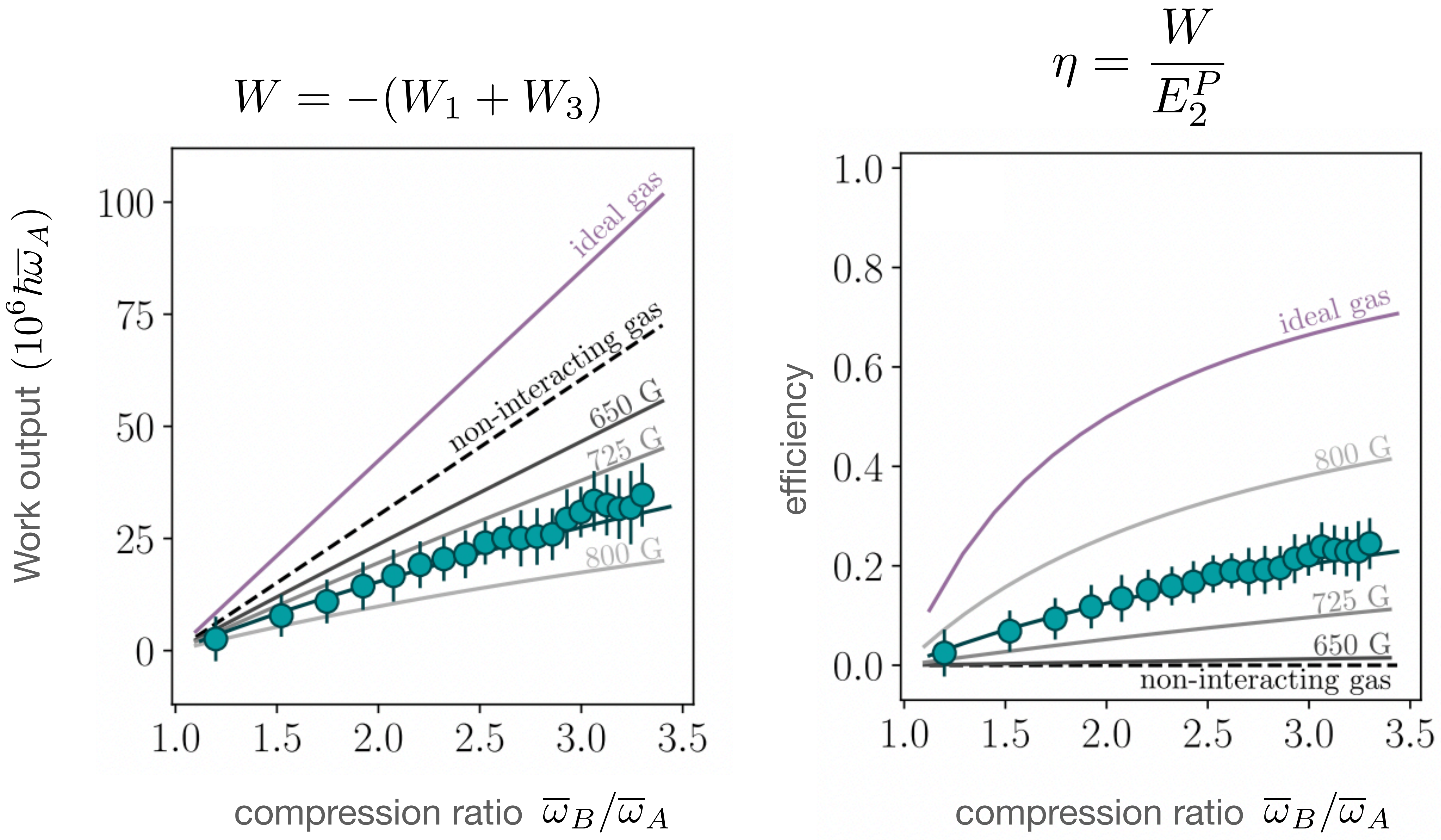
Performance of the Pauli Engine

$B_{\mathrm{FB}} = B_C = B_D = 832.2G$

$N_A^i \approx 2.5 \times 10^5$

→ extract energy from every stroke using absorption pictures





→ work output and efficiency increase with (experimentally accessible) compressions ratios

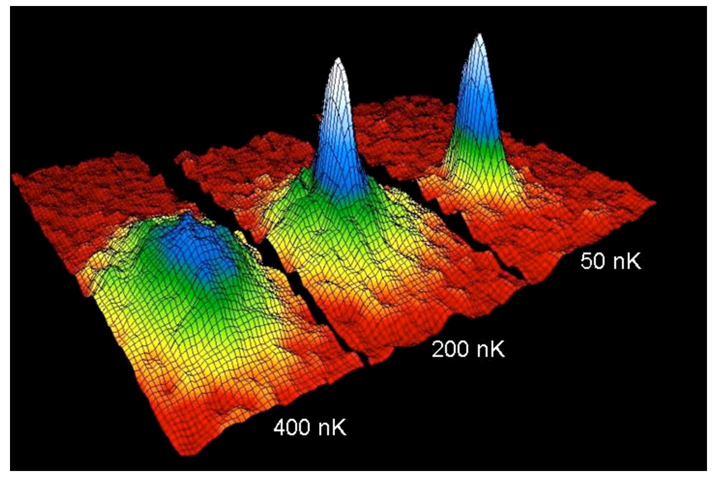
→ efficiencies are significant (>10%) for modest aspect ratios already

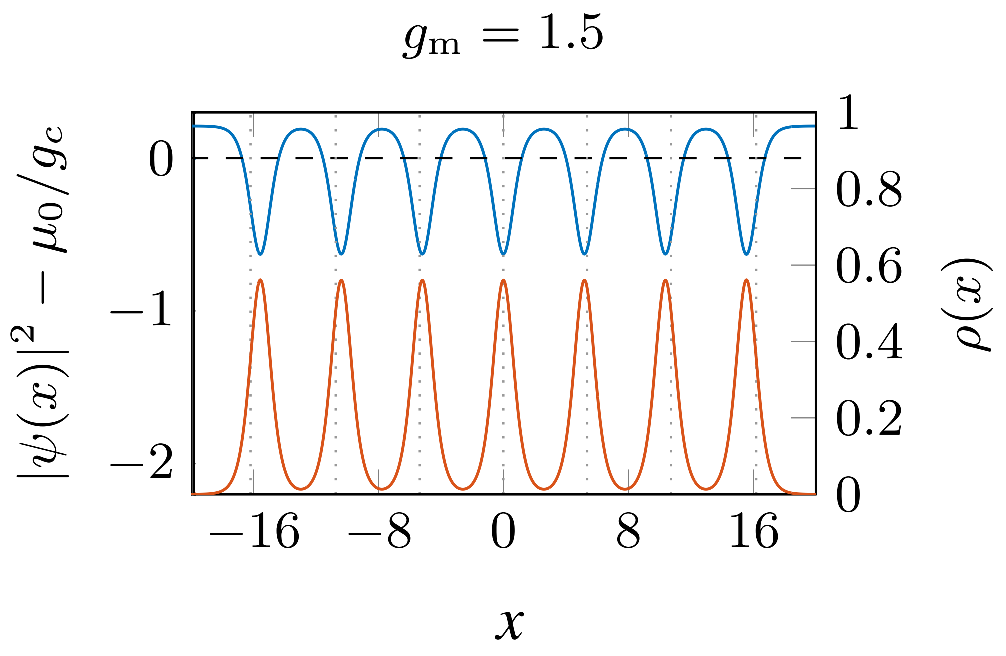
→ for compression ratios larger than 10, theoretically efficiencies > 50% possible

J. Koch, K. Menon, E. Cuestas, S. Barbosa, E. Lutz, T. Fogarty, TB, A. Widera, arXiv:2209.14202 (2022)

Summary and outlook

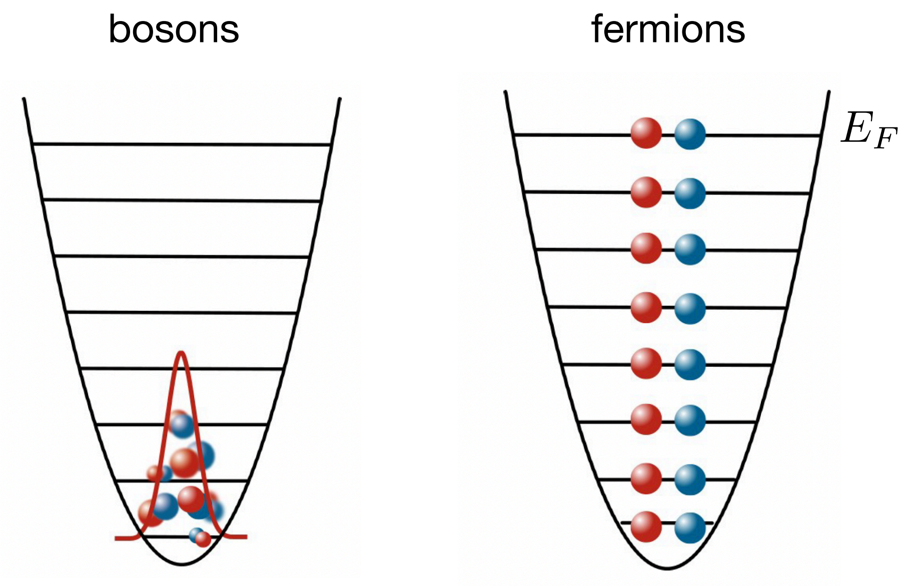
ultracold atoms are highly suitable systems to build quantum simulators, which can have applications in many different areas





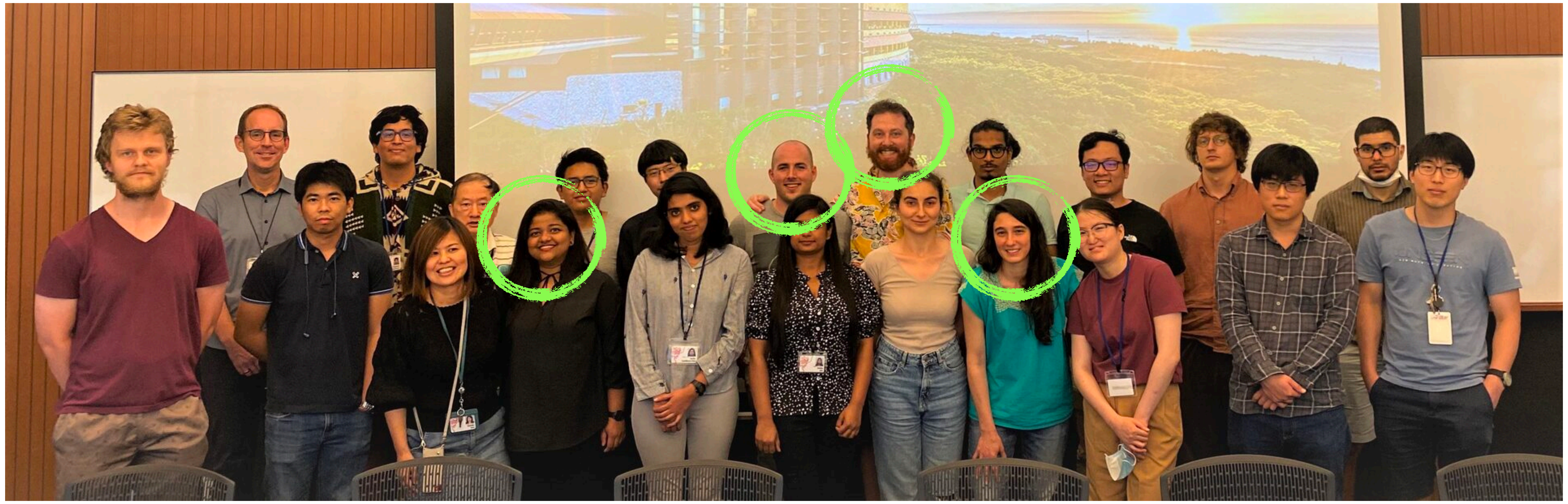
a gas immersed into a BEC undergoes a self-pinning transition even in the absence of a lattice; matter waves are part of the quantum engineering toolbox

quantum systems have new properties that can lead to new ways of carrying out fundamental technical tasks



Tim Keller, T. Fogarty, TB, Phys. Rev. Lett. **128**, 053401 (2022)

Das Team



Jennifer Koch (KL)

Sian Babosa (KL)

Artur Widera (KL)

Eric Lutz (Stuttgart)

Pham Le Kien
Thomás Fogarty
Karol Gietka
Eloisa Cuestas
Hao Lyu
Seyyare Aksu
Kritika Jain
Christopher Campbell
Tim Keller
Friederike Metz
Lewis Ruks
Muhammad Sirajul
Mohamed Boubakour
Jose Carlos Pelayo
Keerthy Menon
Tai Tran
Hoshu Hiyane
Sarika Sasidharan Nair
Sawako Koki

OIST
Japan Society for the Promotion of Science 日本学術振興会
科研費 KAKENHI
Technische Universität Kaiserslautern
Universität Stuttgart