







Quantum Simulation



Digital Quantum Simulators:

Trotter-Suzuki's decomposition of the many-body evolution operator into sequences of of elementary quantum gates.

Example: Real-time dynamics of lattice gauge theories with a few-qubit quantum computer E. A. Martinez et al. Nature 534, 516 (2016)

Analog Quantum Simulators:

Build the desired Hamiltonian directly in the Lab and prepare the ground state, observe time evolution. Quantum simulation with ultracold atomic gases, Example: Hubbard Model, ...

I. Bloch, et al. Nature Phys. 8, 267 (2012).

Emergent Quantum Simulators (lecture III)

The complexity of the many body wave function does not allow to 'observe' all the details. Every measurement we do is a 'coarse graining' which leads to an emerging effective description that is very different from the microscopic physics.

Example: Sine-Gordon model <-> two tunnel coupled superfluids



Scientific Opportunities for Quantum Simulators



Quantum simulators: Architectures and Opportunities, E. Altman et al., PRX-Quantum **2**, 017003 (2021).

1. Quantum materials

correlated electronic materials, high temperature superconductors, frustrated quantum magnets, spin ice, spin glass Bose-Hubbard, Fermi-Hubbard model QuSim: -> explore exotic phases

2. Quantum chemistry

calculation excitation rates, modelling catalysis ... , nitrogen fixation, light harvesting emulating models of reactions and molecules

3. Quantum devices and transport

calculation quantum properties of (nanoscale) electronic devices transport of spin, current, heat, information, ... quantum networks of devices

4. Gravity, particle physics and cosmology

lattice gauge theories, color superconductivity, defect formation, curved space time, horizons, Unruh radiation, many body quantum chaos and scrambling

5. Non equilibrium many body dynamics

spans all scales, really hard problems that can not be traced on classical computers from relaxation and thermalization -> emergence of classical world

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Platforms for Quantum Simulators: Architectures and Opportunities E. Altman et al., PRX-Ougntum 2, 01/003 (2021)



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- Cold and ultracold molecules
- Color centers
- Dopants in semi conductors
- Gate defined quantum dots
- Photons in nano structures
- Photons and atoms in cavities
- Rydberg atom arrays
- Superconducting quantum circuits
- Trapped atomic ions
- Ultra cold neutral atoms
- Van der Waals heterostructures, Moire materials, Exciton – Polariton, quantum fluids of light

rich internal structure, 'long range' dipole-dipole interactions for polar molecules

- Very many incarnations, NV-center in diamond, 'artificial' atoms, long coherence time, fixed in solid but inhomogeneous broadening
- Very many incarnations, 'artificial' atoms, fixed in solid but inhomogeneous broadening
- Flexible design, coherence time is an issue of material purity, recently big breakthroughs due t spin-0 hosts (²⁸Si)
- Mature technology, but problem with loss and detection that needs to be overcome, mostly probabilistic
- Light in cavity mediates long range interaction, exciting developments when combining with singles site detection/manipulation
- controllable strong interaction, fast loading and operation time, reusable samples, easily scalable, arbitrary arrangements
- Designed nodes (qubits) and designed connections. very fast (ns operation time), need exquisite fine tuning, ideal for disorder physics
- System with the best and most robust control, long coherence, difficult to scale up, digital quantum gate based quantum simulation
- Best isolation from environment, 100 thousand's identical nodes, wel Ideveloped techniques to cool, control, measure, bosons <-> fermions
- Many new possibilities. Excitons and quantum fluids of light allow to simulate driven dissipative systems



Challenges



Quantum simulators: Architectures and Opportunities, E. Altman et al., PRX-Quantum **2**, 017003 (2021).

 Scalability and complexity variability of the constituents <-> control connectivity <-> complexity operation speed <-> isolation and coherence

2. State preparation and control how to prepare the initial states: complexity <-> cooling error propagation <-> engineered baths optimal guantum control ...

3. Verification of simulators

how can I know if my simulator does what it is supposed to do?

4. Readout

how to read a simulator, how to read a complex wave function one can not do tomography (exponential difficult) correlation functions become very hard to analyse for non trivial (correlated) systems

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Verifying Quantum Simulation



Quantum simulators: Architectures and Opportunities, E. Altman et al., PRX-Quantum **2**, 017003 (2021).

1. Validating analog quantum simulators

systems contain contributions to Hamiltonian that are not related to the model to be simulated universality of low energy physics may save the simulation quantification of the different perturbations and their effect on the simulation is mostly unknown

2. Validating digital quantum simulators

digitization errors, Trotter step errors, control errors on gates ... de-coherence tools exist for small scale systems (<10 qubits) ... need benchmarking tools that work for large systems

- 3. Comparison to classical calculation limited to cases where there are classical algorithms for some parameter space of the simulation
- **4. Verification of simulators** run simulation a different systems, self verification, new methods in the works
- 5. Error correction and mitigation identify and correct for unwanted interactions ... especially important for analog QuSim
- 6. Mesoscopic metric for quantum complexity models based on asymptotic limits ... but real systems are finite and mesoscopic



Analog Quantum Simulation



Build the desired Hamiltonian directly in the Lab and prepare the ground state, observe time evolution,

Example:

- Hubbard Model
- Lieb-Lininger Model
- Fermi-Hubbard antiferromagnet
- Disorder physics,
- MBL
- ...

Question:

- how good does one need to control the parameters?
- how to verify the results

...

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Main platforms:

Ultra cold atoms

- Bosons <-> Fermions
- Lattices <-> continuuse systems
- Atoms are identical 😊
- Slow (t_{op} ~ ms) $t_{coh} / t_{op} \sim 10^{5}$
- Experiment cycle time > seconds

Rydberg atoms in optical tweezers

- Atoms are identical 😊 Bosons <-> Fermions,
- Arbitrary designed configurations
- Not only next neighbor interactions
- Faster (t_{op} ~ μs) $t_{coh} / t_{op} \sim 10^{5}$
- Experiment cycle time > 10⁻³ seconds

Superconducting circuits

- Designed nodes and connectivity
- · Local control of node and connections
- Needs fine tuning
- $t_{coh} / t_{op} \sim 10^{5}$ • Fast $(t_{op} \sim ns)$
- Experiment cycle time $> 10^{-6}$ seconds



Analog Quantum Simulation



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Build the desired Hamiltonian directly in the Lab and Quantum simulation with ultracold atomic gases, prepare the ground state, observe time evolution,

I. Bloch, J. Dalibard, S. Nascimbène, Nature Phys. 8, 267 (2012).

Example:

- Hubbard Model
- Lieb-Lininger Model Fermi-Hubbard antiferromagnet
- Disorder physics, MBL
- ...

Question:

- how good does one need to control the parameters?
- how to verify the results







Crystalline solids



How to build a lattice



Superfluid to Mott insulator







Quantum gas microscope





energy scale:
$$E_{recoil} = \frac{\hbar^2 k^2}{2m}$$

confinement $\omega_T = \sqrt{4V_0 E_{rec}}$

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$$a_0 = \sqrt{1/\omega_T}$$

Optical Dipole Forces Optical lattice:

4 µm polystyrol particles on water surface

conservative light force for macroscopic particles \rightarrow optical tweezers





optical tweezers do amazing things in biology (measure the force of a ribosome)





lattice physics: bloch bands



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 $K = \frac{2\pi}{d}$







A typical lattice experiment



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...the "Greiner / Bloch machine"... now working on more than 10 labs

Atomic Species	⁸⁷ Rb
Wavelength	830-850 nm
Waist (1/e²)	125 μm
Polarization	Orthogonal between standing wave pairs
Intensity control	All beams intensity stabilized
Lattice geometry	Simple cubic
Lattice spacing	425 nm



BEC









varied by changing the depth of the 3D lattice potential

In 1998, D. Jaksch and P. Zoller proposed to observe the superfluid - Mott insulator transition using bosons in optical lattices (never observed in solid state system)

 $\frac{15}{V_0/E_R}$

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The Bose-Hubbard model superfluid limit



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Quantum Phase Transition Jaksch et al. PRL 81, 3108 (1998)







Quantum Phase Transition M. Greiner et al. Nature 415, p38 (2002)









the ultimate proof for the quantum phase transition: probing the excitation spectrum

there are many ways to loose and restore coherence:

Dalibard experiments questions Kesvich in 2004 by observing high contrast interference in 30 independent condensates

→ interference is not neccesarily a proof for coherent / Fock state

If one would apply a pertubation Δ to the system (e.g. shaking)



for atoms to hopping sites this costs interaction energy U No excitations below threshold energy ∆=U → gap in excitation spectrum

gradient:



If the gradient corresponds to the interaction energy, excitations are easily created

(actually, only applying the gradient is pertubation enough, tunneling is now allowed)



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Measuring the populatipon adiabatic switching off the lattice





-3hk -2hk -hk

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

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+hk +2hk +3hk

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



Populating higher energy bands stimulated Raman transitions





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Measuring the populatipon adiabatic switching off the lattice



so far, this has been "single particle physics with many particles", it doesn't need a BEC, not even bosons:

releasing ground state atoms from the same optical lattice:



difference in momentum is only due to different masses



Study Order by higher order Correlations Quantum Noise Interferometry









-100 -200 0 200

x (um)

200 400

x (µm)

_2 400

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Quantum Noise Interferometry Fermions in a Lattice



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Figure 1 | Origin of anticorrelations in a Fermi gas released from an optical lattice. Each occupied Bloch state, labelled by a crystal momentum ha, is represented by a dot in the reduced zone scheme (white region). The full occupation of the lowest energy band opposed to the empty second band describes the fermionic band insulating state. The periodically extended zone scheme (extension shown as green shaded region) shows that each Bloch state is a superposition of states with momenta equally spaced by 2 $\hbar k$. After the lattice is switched off abruptly, an atom with crystal momentum hap propagates freely during at time of flight r and can reach detectors equally spaced by a distance ℓ . If for example, detector number 3 detects a particle (yellow dot above detector), then owing to the single occupancy of each Bloch state lictated by the Pauli principle detectors 1, 2 and 4 will not detect a particle (white dots above detectors).



Figure 2 | Single shot absorption images and correlation analysis. a, Single absorption image of a fermionic ⁴⁰K atom cloud after 10 ms of free expansion. The inset shows a Brillouin zone mapping of the cloud, demonstrating that the Fermi gas is in a band insulating state. **b**, One-dimensional cut through a together with a gaussian fit (red). **c**, Spatial noise correlations obtained from an analysis of 158 independent images, showing an array of eight dark dots. **d**, A horizontal profile through the centre of the characteristic spacing ℓ . The profile has been high-pass filtered to suppress a broad gaussian background that we attribute to shot to shot fluctuations in the atom number. the atom number.



Quantum Gas Microscope detecting single atoms in lattice





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Quantum Gas Microscope Mott Insulator VC Ε W. S. Bakr et al., Science **329**, 547 (2010)

A 6E B 10E C 12E **D** 16*E*_r ⊷680nm x1000 counts

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increasing atom number averaged images



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Reconstructed -— 20 µm —> Increasing atom number BEC Mott insulators



What can they probe?





• Many-body localization (1D-2D)

15 U/J

• Debated in 2D

Schreiber, Hodgman, Bordia, Lüschen, Fischer, Vosk, Altman, Schneider, Bloch, Science 349, 842 (2015)

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• Ground state problems



Mazurenko, Chiu, Ji, Parsons, Kanász-Nagy, Schmidt, Grusdt, Demler, Greif, Greiner, Nature 545, 462 (2017) Esslinger, Ann Rev Cond Mat Phys 1, 129 2010





Digital Quantum Simulation



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Lloyd, S. Universal quantum simulators. Science 273, 1073 (1996)

In 1996 S. Lloyd, showed that quantum simulation can be performed with arbitrary precision in polynomial time, using a Trotter-Suzuki's decomposition of the many-body evolution operator into sequences of local Hamiltonian evolutions. This can be then implemented by sequence of elementary quantum gates.

Example:

- Universal digital quantum simulation with trapped ions,
 B. P. Lanyon, et al., Science 334, 57 (2011)
- Real-time dynamics of lattice gauge theories with a few-qubit quantum computer, E. A. Martinez et al. Nature **534**, 516 (2016)

What is the error accumulated by the 'Trotterisation'?

Quantum localization bounds Trotter errors in digital quantum simulation M. Heyl, P. Hauke, P. Zoller Science Advances **5**:eaau8342 (2019)







A cold-atom Fermi-Hubbard antiferromagnet



Nature 545, 462-466 (2017)

Exotic phenomena in systems with strongly correlated electrons emerge from the interplay between spin and motional degrees of freedom. For example, doping an antiferromagnet is expected to give rise to pseudogap states and high-temperature superconductors¹. Quantum simulation^{2,3,4,5,6,7,8} using ultracold fermions in optical lattices could help to answer open questions about the doped Hubbard Hamiltonian^{9,10,11,12,13,14}, and has recently been advanced by quantum gas microscopy^{15,16,17,18,19,20}. Here we report the realization of an antiferromagnet in a repulsively interacting Fermi gas on a twodimensional square lattice of about 80 sites at a temperature of 0.25 times the tunnelling energy. The antiferromagnetic long-range order manifests through the divergence of the correlation length, which reaches the size of the system, the development of a peak in the spin structure factor and a staggered magnetization that is close to the ground-state value. We hole-dope the system away from half-filling, towards a regime in which complex many-body states are expected, and find that strong magnetic correlations persist at the antiferromagnetic ordering vector up to dopings of about 15 per cent. In this regime, numerical simulations are challenging²¹ and so experiments provide a valuable benchmark. Our results demonstrate that microscopy of cold atoms in optical lattices can help us to understand the lowtemperature Fermi–Hubbard model.



Probing antiferromagnetism in the Hubbard model with a quantum gas microscope





A Mazurenko *et al. Nature* **545**, 462-466 (2017) doi:10.1038/nature22362

Figure 1 | Probing antiferromagnetism in the Hubbard model with a quantum gas microscope. a, Schematic of the two-dimensional Hubbard phase diagram, including predicted phases. We explore the trajectories traced by the red arrows for a Hubbard model with U/t = 7.2(2). The strongest antiferromagnetic order is observed at the starred point. b, Experimental set-up. We trap ⁶Li atoms in a two-dimensional square optical lattice. We use the combined potential of the optical lattice and the anticonfinement that is generated by the digital micromirror device (DMD) to trap the atoms in a central sample Ω of homogeneous density, surrounded by a dilute reservoir, as shown in the plot. The system is imaged with 671-nm light along the same beam path as the projected 650-nm potential, and separated from it by a dichroic mirror. c, Exemplary raw (left) and processed (right) images of the atomic distribution of single experimental realizations, with both spin components present (upper; corresponding to the starred point in a) and with one spin component removed (lower). The observed chequerboard pattern in the spin-removed images indicates the presence of an antiferromagnet.

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Observing antiferromagnetic long-range order



A Mazurenko *et al. Nature* **545**, 462–466 (2017) doi:10.1038/nature22362

Figure 2 | Observing antiferromagnetic long-range order. a, The spin correlator C_d is plotted for different displacements $d = (d_x, d_y)$ ranging across the entire sample for five temperatures T/t. We record more than 200 images for each temperature (Methods). Correlations extend across the entire sample for the coldest temperatures, whereas for the hottest temperature only nearest-neighbour correlations remain. b, The sign corrected correlation function $(-1)^i C_d$ is obtained through an azimuthal average. The exponential fits to the data (|d| = d > 2 sites) are shown in blue, from which we determine the correlation length ξ ; the fit of the coldest sample is plotted in grey in the other panels for comparison. c, The measured spin structure factor $S^{z}(q) - S^{z}(0)$ obtained from Fourier transformations of single images. A peak at momentum $q_{\text{AFM}} = (\pi/a, \pi/a)$ signals the presence of an antiferromagnet. **d**, The measured correlation length ξ (data), fitted to equation (2) (curve), diverges exponentially as a function of temperature T/t and is comparable to the system size for the lowest temperature. The temperature is varied by holding the atoms in the trap for a variable time. The inset is a semi-logarithmic plot of the same quantity versus inverse temperature. e, The measured corrected staggered magnetization m_c^z (large blue circles) increases markedly below temperatures $T/t \approx 0.4$. We find good agreement with quantum Monte Carlo calculations of the Hubbard model (small grey circles). The trajectory followed in this figure is shown schematically in the phase diagram in the inset. Error bars in d and e are standard deviations of the sampled mean; error bars in b (smaller than the markers) are computed as in Methods. The figure is based on 2,282 experimental realizations





Full counting statistics of the staggered magnetization operator



A Mazurenko *et al. Nature* **545**, 462-466 (2017) doi:10.1038/nature22362



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Figure 3 | Full counting statistics of the staggered magnetization operator. a, Selected images with one spin component removed (chequerboard overlaid to guide the eye) show a large variation in ordering strength at the coldest temperature. This variation is a consequence of the SU(2) symmetry of the underlying Hamiltonian, which leads to different orientations of the staggered spin-ordering vector \hat{m} relative to the measurement axis z, as shown schematically by the spin vectors (red and blue arrows) relative to the axis defined by δ^{2} (black arrows). **b**, Measured distributions of the staggered magnetization operator, $p(\hat{m}_{z})$, are plotted at different temperatures T/t (histograms). We find excellent agreement with quantum Monte Carlo simulations of the Heisenberg model with no free fitting parameters (black lines). The figure is based on 2,282 experimental realizations.



Doping the antiferromagnet



A Mazurenko *et al. Nature* **545**, 462–466 (2017) doi:10.1038/nature22362



Figure 4 | Doping the antiferromagnet. a, We dope the system with holes and reduce the density from half-filling, with $0.0 \le \delta \le 0.25$ (corresponding to $0.95 \ge n_8 \ge 0.73$). The corrected staggered magnetization me settles at the critical hole doping $\delta_c \approx 0.15$. The trajectory followed in this figure is shown schematically in the phase diagram in the inset. b, The relative strength of the sign-corrected spin correlations $(-1)^{i}C_{d}$ decreases less rapidly with hole doping at smaller distances (d = 1.0) than at larger distances (d = 3.6). For large doping, only the nearest-neighbour correlator is appreciable, so this correlation is predominantly responsible for the non-zero staggered magnetization away from the antiferromagnetic phase. c, We show the spin structure factor $S^{c}(\mathbf{q}) - S^{c}(\mathbf{0})$, as in Fig. 2c, for each doping value. Error bars in **a** are standard deviations of the sampled mean; those in **b** are computed as in Methods. The figure is based on 1,470 experimental realizations.