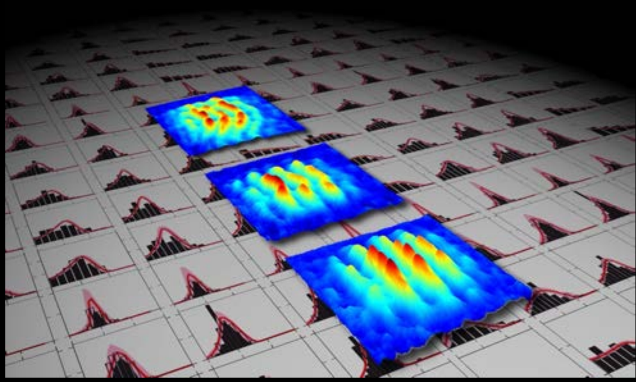
Quantum Simulation

an introduction



Jörg Schmiedmayer
Vienna Center for Quantum Science and Technology, TU-Wien

Outline

Lecture 1: Introduction

- Simulating physics with computers -> Quantum simulation
- Basic concepts

Lecture 2: Examples

- Analog quantum simulation
- Digital quantum simulation

Lecture 3: Simulating quantum fields in the lab

- Relativisitc quantum fields
- Emergent Sine-Gordon quantum simulator

Describing quantum systems
Many Body Quantum Systems (MBQuS)

On a fundamental level our nature is quantum.
Many Body Quantum Systems (= Quantum systems put together from many **interacting** constituents) are at the center of many of the most challenging problems

- Cosmology
- High energy / nuclear physics
- Material science
- Quantum chemistry
- Biology?

MBQuS are notoriously hard to describe, due to the exponential growth of the Hilbert space with system size.

This is especially true for systems out of equilibrium that are characterized by a rapid growth of entanglement

Describing Many Body Quantum Systems

There are powerful classical algorithms which are able to predict properties of MBQuS in many relevant regimes.

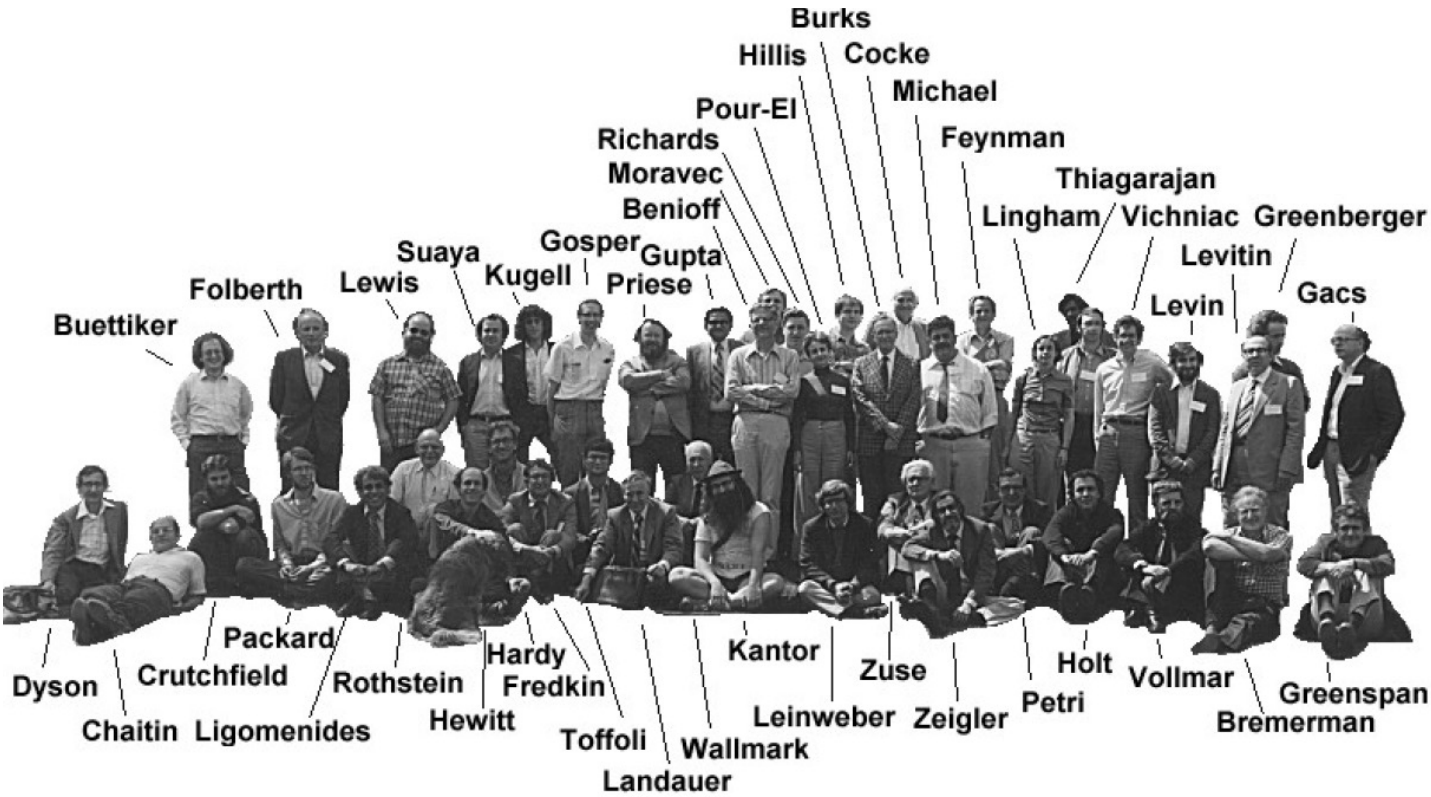
If strong correlations come into play they are seriously challenged even in predicting ground state properties, and even more for non equilibrium systems.

In 1981 Richard Feynman, in a talk given at the *1st conference on Physics and Computation* reasoned that *other* quantum systems, assembled and manipulated under precisely controlled conditions following quantum laws, could come to rescue when simulating strongly correlated quantum systems.

=> Quantum Simulations

Simulating physics with computers,
R. Feynman, Int. J. Theor. Phys. 21, 467 (1982)

1st Conference on Physics and Computation
MIT, 1981



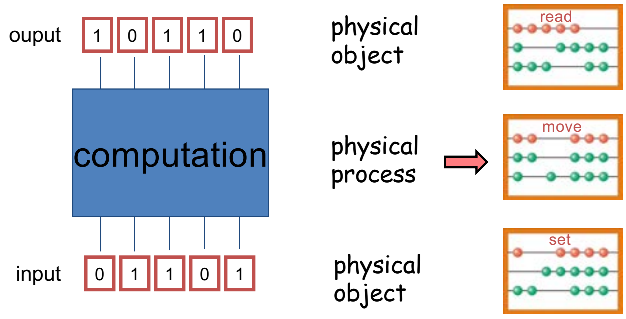
Outline

Lecture 1: Introduction

- Why is it hard to describe quantum systems
- Entanglement and the exponential growth of the resources neded.
- Where and why classical methods fail
- Basic concepts of quantum simulation
  - R. Feynman's proposal (1981)
  - S. Lloyd proofs it correct (1996)
- Analog quantum simulation
- Digital quantum simulation
- Emergent quantum simulation
- Quantum s9imulatiuon platforms

Information and Physics

computing as a *physical process*



Information is physical
Rolf Landauer

Our present computers process information according to the laws of classical physics: "classical computers".

Quantum Information Science

At at fundamental level nature obeys the laws of quantum physics.

At a fundamental level information science must be based on quantum theory.

quantum information science

Question:
„Can the computers of the future exploit quantum properties of information, to perform tasks that are beyond what can conceivably be achieved with conventional (classical) information technolgoy?“

David Deutsch

Quantum Physics

what is different I

- **Quanta**
  one Photon, Atom, Neutron
  smallest unit = 1 Bit

$$|H\rangle,\ |V\rangle \quad |\sigma^+\rangle,\ |\sigma^-\rangle$$
$$|\uparrow\rangle,\ |\downarrow\rangle \quad |L\rangle,\ |R\rangle$$
$$|p\rangle,\ |x\rangle,\ |\ell\rangle$$

- Superposition
  Polarisation
  Double slit
- Measurement
  Which state?
  Through which slit?
- Entanglement
  composite systems built from sub systems

Quantum Physics
what is different II

- **Quanta**
  one Photon, Atom, Neutron
  smallest unit = 1 Bit

$|H\rangle,\ |V\rangle \quad |\sigma^+\rangle,\ |\sigma^-\rangle$
$|\uparrow\rangle,\ |\downarrow\rangle \quad |L\rangle,\ |R\rangle$
$|p\rangle,\ |x\rangle,\ |\ell\rangle$

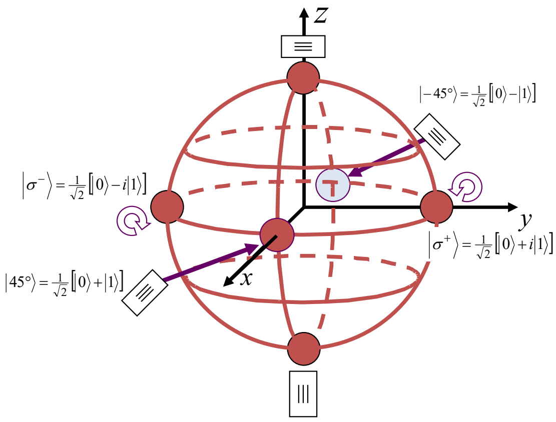
- **Superposition**
  Polarisation
  Double slit

$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle \quad \text{with} \quad \sum_i |\alpha_i|^2 = 1$
$|+45^\circ\rangle = \frac{1}{\sqrt{2}}[|H\rangle + |V\rangle]$
$|-45^\circ\rangle = \frac{1}{\sqrt{2}}[|H\rangle - |V\rangle]$

- Measurement
  Which state?
  Through which slit?

- Entanglement
  composite systems built from sub systems

Two state system
example: polarisation



Quantum mechanics allows all states on the sphere in the form of superposition states.

Which resources do i need to write down a quantum state

N - two state systems

classical Bit

1

0 or 1

0

classical register for 3 bits

101

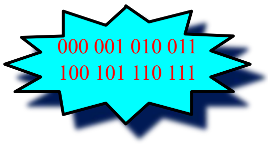
Quantum mechanics allows superpositions

A superpositiopn can acess all states

300 two state systems : 2^{300} states
> # atoms in the universe

quantum Bit: qubit

quantum register for 3 qubits



exponential growth of the state space quantum systems live in

Quantum Physics
what is different III

- **Quanta**
  one Photon, Atom, Neutron
  smallest unit = 1 Bit

$|H\rangle,\ |V\rangle \quad |\sigma^+\rangle,\ |\sigma^-\rangle$
$|\uparrow\rangle,\ |\downarrow\rangle \quad |L\rangle,\ |R\rangle$
$|p\rangle,\ |x\rangle,\ |\ell\rangle$

- **Superposition**
  Polarisation
  Double slit

$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle \quad \text{with} \quad \sum_i |\alpha_i|^2 = 1$
$|+45°\rangle = \frac{1}{\sqrt{2}}[|H\rangle + |V\rangle]$
$|-45°\rangle = \frac{1}{\sqrt{2}}[|H\rangle - |V\rangle]$

- **Measurement**
  Which state?
  Through which slit?

$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle \xrightarrow{\text{Messung}} |\varphi_i\rangle$
$\text{with} \quad P_{|\varphi_i\rangle} = |\alpha_i|^2$

Non-deterministic!

- Entanglement
  composite systems built
  from sub systems

Quantum Physics
what is different IV

- **Quanta**
  one Photon, Atom, Neutron
  smallest unit = 1 Bit

$|H\rangle,\ |V\rangle \quad |\sigma^+\rangle,\ |\sigma^-\rangle$
$|\uparrow\rangle,\ |\downarrow\rangle \quad |L\rangle,\ |R\rangle$
$|p\rangle,\ |x\rangle,\ |\ell\rangle$

- **Superposition**
  Polarisation
  Double slit

$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle \quad \text{with} \quad \sum_i |\alpha_i|^2 = 1$
$|+45°\rangle = \frac{1}{\sqrt{2}}[|H\rangle + |V\rangle]$
$|-45°\rangle = \frac{1}{\sqrt{2}}[|H\rangle - |V\rangle]$

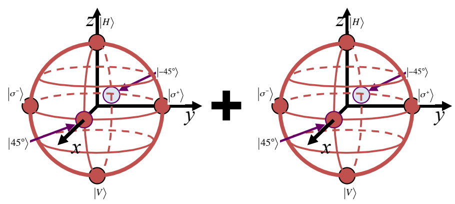
- **Measurement**
  Which state?
  Through which slit?

$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle \xrightarrow{\text{Messung}} |\varphi_i\rangle$
$\text{with} \quad P_{|\varphi_i\rangle} = |\alpha_i|^2$

- **Entanglement**
  composite systems built
  from sub systems

$|00\rangle,\quad |10\rangle,\quad |01\rangle,\quad |11\rangle$
$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle_1|0\rangle_2 \pm |1\rangle_1|1\rangle_2)$
$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|1\rangle_1|0\rangle_2 \pm |0\rangle_1|1\rangle_2)$

2 two-state systems
(2 photons)



4 basis vectors

$\Psi_1 = |H\rangle_1|H\rangle_2$
$\Psi_2 = |H\rangle_1|V\rangle_2$
$\Psi_3 = |V\rangle_1|H\rangle_2$
$\Psi_4 = |V\rangle_1|V\rangle_2$

Add superposition

$$\psi_1 = \frac{1}{\sqrt{2}}[|H\rangle_1|H\rangle_2 + |V\rangle_1|V\rangle_2]$$
$$\psi_2 = \frac{1}{\sqrt{2}}[|H\rangle_1|H\rangle_2 - |V\rangle_1|V\rangle_2]$$
$$\psi_3 = \frac{1}{\sqrt{2}}[|H\rangle_1|V\rangle_2 + |V\rangle_1|H\rangle_2]$$
$$\psi_4 = \frac{1}{\sqrt{2}}[|H\rangle_1|V\rangle_2 - |V\rangle_1|H\rangle_2]$$

In the space created by the 4 basis vectors there are **non-separable states**

entanglement

Entanglement

Entanglement is a pure (the essential) quantum phenomenon.

Independent of basis
Independent of distance
Leads to Strong correlations (stronger then possible in classical physics)
=> EPR paradoxon: Bell inequalities

In nature entanglement is created by conservation laws:

momentum conservation in scattering or decay
angular momentum conservation
....

Or in conditional dynamics (interaction mediated)

(see quantum information: no cloning, quantum gates)

=> Dynamics in an interacting quantum many body system leads to rapid growth of entanglement (system can not be separated into subsystems
=> exponential growth of resources needed to describe the system

Quantum Simulations
Describing Many Body Quantum Systems

Spreading of entnaglement and the connected strong correlations limits even the most powerful classical algorithms to predict properties of MBQuS in many relevant regimes, especially out of equilibrium.

1981 **Richard Feynman**: *other* quantum systems, assembled and manipulated under controlled conditions following quantum laws, could simulate strongly correlated quantum systems.

Simulating physics with computers,
R. Feynman, Int. J. Theor. Phys. 21, 467 (1982)

Behind the Iron Curtain:

1975: **R. P. Poplavskii**: Computational infeasibility of simulating quantum systems on classical computers, due to superposition principle:

Thermodynamical models of information processing,
R. P. Poplavskii Uspekhi Fizicheskikh Nauk, 115:3, 465-501, (1975)

1980: **Yuri I. Manin**, Computable and un-computable (in Russian), Moscow, Sovetskoye Radio

- Exploit the exponential number of basis states of quantum systems.
- Need a theory of quantum computation that captures the fundamental principles without committing to a physical realization.

Universal Quantum Simulators

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

1996 S. Lloyd:
Quantum simulation of quantum systems that evolve according to local interactions can be performed with arbitrary precision in polynomial time.

'Programming' a simulator: inducing interactions between the variables of the simulator that imitate the interactions between the variables of the system to be simulated
=> dynamics of the simulator and the system are the same within a desired accuracy

Classical: 40 spin ½ particles require $2^{40} \approx 10^{12}$ numbers to describe the state and $2^{40} \times 2^{40} \approx 10^{24}$ for dynamics
Quantum: 40 spin ½ particles require 40 quantum bits evolving over time

Analysis of simulation efficiency:
arbitrary unitary evolution would require too many steeps
systems that evolve with local intertactions are simpler and can be efficiently simulated using a Trotter-Suzuki's decomposition of elementary quantum gates.

Quantum Simulation

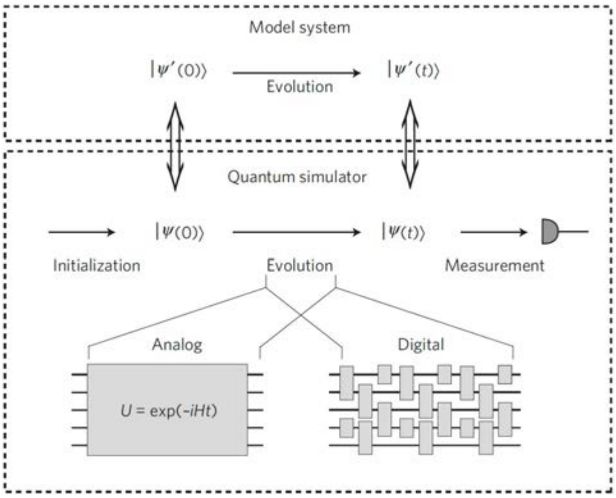
Digital Quantum Simulators:
Trotter-Suzuki's decomposition of the many-body evolution operator into sequences of of elementary quantum gates.
Example: *Real-time dynamics of lattice gauge theories with a few-qubit quantum computer*
E. A. Martinez et al. Nature **534**, 516 (2016)

Analog Quantum Simulators:
Build the desired Hamiltonian directly in the Lab and prepare the ground state, observe time evolution.
Example: Hubbard Model, ... *Quantum simulation with ultracold atomic gases,*
I. Bloch, et al. Nature Phys. 8, 267 (2012).

Emergent Quantum Simulators
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

Schweigler , et al. Nature **545**, 323 (2017)
Zache et al. arXiv:1909.12815.

Quantum Simulation



Digital Quantum Simulation

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)

Analog Quantum Simulation

Quantum simulation with ultracold atomic gases,
I. Bloch, J. Dalibard, S. Nascimbène,
Nature Phys. 8, 267 (2012).

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
- …

Question:

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

Emergent Quantum Simulation

The complexity of the many body wave function does not allow to 'observe' all the details. We can only measure few body observables.

Every measurement we do of many body system is therefor a 'coarse graining'. This leads to an effective description of the system that can be very different from the microscopic physics.

The question I will ask in my third lecture:

Can we use these 'emerging' properties to build interesting quantum systems (simulators)

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

Platforms for Quantum Simulation

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

- 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 and excitons

Challenges

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

1. **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 quantum 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

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