QUANTUM SIMULATION

Topics:
Present goals of quantum simulation
A set of criteria for a quantum simulator
Quantum simulations with ultracold quantum gases

Feynman legendarily noted that no classical computer can efficiently simulate a quantum system (although there are many clever approximations).

The computational power required to even describe a quantum system scales exponentially with the number of its constituents. For instance, to describe the most general (pure) quantum state for $N$ spin-½ particles, we have to store in our computer $2^N$ coefficients—a task that becomes practically impossible if $N$ is greater than ~50.
**Quantum Simulation**

**Problem:** How do you simulate the evolution of a quantum system, and extract useful predictions, efficiently?

Problem appears to be impossible classically for all but the simplest systems.

**Solution:** use the evolution of one quantum system to emulate the evolution of another.

\[
\begin{align*}
|s(0)\rangle & \xrightarrow{\text{Encode}} |\psi(0)\rangle \\
|s(t)\rangle & \xrightarrow{\text{Evolve}} |\psi(t)\rangle \\
|s(t)\rangle & \xleftarrow{\text{Measure}} |s(t)\rangle
\end{align*}
\]

Adapted from: Colin Williams

**Present goals of quantum simulation**

Feynman envisioned a quantum simulator to be “a quantum machine that could imitate any quantum system, including the physical world” (“digital quantum simulator” – just as hard to build as quantum computer).

**Present goal:** to build a simulator that can imitate certain physically interesting systems that cannot be simulated with classical computers. Such quantum simulator is expected to be more robust against imperfections than a quantum computer. Error correction, therefore, may not be needed.

A digital quantum simulator is an envisioned quantum device that can be programmed to efficiently simulate any other local system.

An “analog simulator” can also be considered, where the Hamiltonian $H(t)$ is built directly with a physical system that evolves continuously in time. A prominent example: which minimal Hamiltonian describes the phenomenon of high-temperature superconductivity? To answer this question, a quantum simulator could check the various candidate Hamiltonians for relevant phases.

Nature Physics 8, 264 (2012)
A set of criteria for a quantum simulator

The specific goal: to build a simulator that outperform classical devices and is capable of addressing questions in many-body quantum systems.

1. Quantum system. A quantum simulator should possess a system of bosons or/and fermions with or without internal degrees of freedom (pseudospin). The particles can be stored in a lattice or at least confined in some region of space. The system should contain a large number of degrees of freedom.

2. Initialization. A quantum simulator should be able to prepare (approximately) a known quantum state.

3. Hamiltonian engineering. It should be possible to engineer a set of interactions with external fields or between different particles, with adjustable values. These can be local (that is, acting among neighboring particles) or have a longer range. They may involve a reservoir if simulation of open-system dynamics is required. Among the accessible Hamiltonians there should be some that cannot be efficiently simulated (at present) with classical techniques.

\[ H_{\text{BH}} = -J \sum_{\langle i,j \rangle} \hat{b}^+_i \hat{b}_j + \frac{U}{2} \sum_j \hat{b}^+_j \hat{b}_j \hat{b}^+_j \hat{b}_j + \sum_j \epsilon_j \hat{b}^+_j \hat{b}_j \]

\( J \) – tunneling of atoms between neighboring wells
\( U \) – repulsion of atoms sitting in the same well

Adapted from: Nature Physics Insight 2012, Eugene Demler
A set of criteria for a quantum simulator

4. Detection. One should be able to perform measurements on the system. This could be individual (that is, addressing a few particular sites on the lattice) or collective (without the need of addressing any individual site). Ideally, one should be able to perform single-shot experiments that can be repeated several times. For instance, when measuring the collective magnetization in a set of spins along a given direction (corresponding to an observable $S$), one would be able to determine not only $S$, but also $f(S)$, where $f$ is an arbitrary function.

5. Verification. Although by definition there should be no way of verifying if the result of the simulation is correct, as long as a problem that cannot be classically simulated is being solved, there should be a way of increasing the confidence in the result.

For instance, the simulator could first be benchmarked with problems with known solutions. Or the evolution may be run forwards and backwards in time to check that it really ends up in the initial state. When an adiabatic algorithm is run, the technique may be used to adjust the time of the simulation by going back and forth with the parameters, each time getting closer to the target Hamiltonian. Alternatively, the results of simulations of different methods and systems could be compared.

Quantum simulations with ultracold quantum gases

Ultracold quantum gases offer a unique setting for quantum simulation of interacting many-body systems. By carefully manipulating the laser light and magnetic fields trapping an ensemble of ultracold atoms, researchers can control the interactions between atoms – and therefore simulate interactions that occur between electrons in solids. But unlike electrons in solids, the strength of these interactions can be easily adjusted, allowing to test theories of condensed-matter physics.

Atoms in optical lattices (A) or in 1D (B) or 2D (C) arrays of cavities.

Density profile of a trapped ultra-cold Fermi gas. Although density is 24 times smaller than in the upper crust of a neutron star, these two systems obey the same equations.
Quantum gases: bosons and fermions

Ideal gas at zero temperature

Bose-Einstein: integer spin
Fermi-Dirac: half-integer spin

In neutral atoms $N_{\text{electrons}} = N_{\text{protons}}$

Statistical properties are governed by the number of neutrons in an atom $N_{\text{neutrons}}$.

Boson if $N_{\text{neutrons}}$ is even
Fermion if $N_{\text{neutrons}}$ is odd

Quantum simulations with ultracold quantum gases

The examples of implementing analog quantum simulation with cold atoms.

1. Ultracold quantum gases as a quantum simulator for strongly interacting fluids. It is possible to achieve strongly interacting regime where the fluid becomes scale-invariant and its behaviour is characterized by a few dimensionless coefficients. Example of system to simulate: neutron stars. The control of interactions provided by Feshbach resonances.

2. Atoms in optical lattices or arrays of traps as a quantum simulator for condensed matter systems. Study of quantum phase transitions, quantum magnetism, high-temperature superconductors, etc. The control of the system: control of optical lattice parameters, loading, external fields, etc.

3. Atomic gases as a quantum simulator for charged quantum many-body systems, such as an electron fluid in an external magnetic field.

Applications: study of quantum Hall effect, addressing problems if quantum field theory. The control of the system: the control of the topology in which the quantum fluid evolves.

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**Neutron stars**

X-ray image of RCW 103

1 to 2 solar masses
R=12 km !!!
T= 10^6 Kelvins

A neutron star is a type of stellar remnant that can result from the gravitational collapse of a massive star during a supernova event. Such stars are composed almost entirely of neutrons (which are fermions). Neutron stars are very hot and are supported against further collapse by quantum degeneracy pressure due to the Pauli exclusion principle.

http://www.astro.umd.edu/~miller/nstar.html#internal
Fermionic superfluidity

**Superfluid** is a state of matter in which the matter behaves like a fluid with zero viscosity and zero entropy.

The substance, which looks like a normal liquid, will flow without friction past any surface, which allows it to continue to circulate over obstructions and through pores in containers which hold it, subject only to its own inertia.

Fermionic superfluidity, whether it occurs in superconductors, helium-3, or inside a neutron star, requires pairing of fermions, particles with half-integer spin.

In an equal mixture of two states of fermions ("spin up" and "spin down"), pairing can be complete and the entire system will become superfluid.

The superfluid behaviour of the gas can be understood using the Bardeen–Cooper–Schrieffer (BCS) theory of pairing.
Our simulator “toolbox”: BEC–BCS crossover

The superfluid behaviour of the gas can be understood using the Bardeen–Cooper–Schrieffer (BCS) theory of pairing. This theory has proven extremely successful for the understanding of conventional superconductors, and constitutes a starting point for modelling more complex systems. For weak attractive interactions, atoms of opposite spin and momentum form Cooper pairs whose spatial extent greatly exceeds the mean interparticle distance.

In the opposite limit of strongly attractive interactions, the gas is made of molecules forming a Bose-Einstein condensate (BEC). Weakly bound dimers are produced via magnetically tuned Feshbach resonances. Such a scattering resonance occurs when a free colliding atom pair energetically coincides with a bound molecular state. On the side of the resonance where the energy of the molecular level is below the dissociation limit, a weakly bound dimer state exists.


What parameter can we change in our quantum simulation with ultracold gases?

We can change the scattering properties of the atoms, i.e. the scattering length \( a \).

Scattering length is a parameter used in analyzing scattering at low energies. At low energies, only s-wave makes non-zero contribution to the cross section and the scattering cross section approaches that of an impenetrable sphere whose radius equals this length \( a=a_0 \).

\[
\sigma_{\text{tot}} = \frac{4\pi}{p^2} \sin^2 \delta_0 \xrightarrow{p \to 0} 4\pi a_0^2
\]

Changing scattering length allows us to control pairing of fermions! We can make loosely bound Cooper pairs or make molecules.
Feshbach resonances

The scattering of ultracold atoms can be altered significantly through a so-called ‘Feshbach resonance’.

At low temperatures, the interaction energy in a cloud of atoms is proportional to the density and a single atomic parameter, the scattering length $a$ which depends on the quantum-mechanical phase shift in an elastic collision.

Feshbach resonance works as follows. When two fermion atoms interact in a vacuum, they can jump between a “closed channel” and an “open channel.” In the closed channel, they form a small (atomic-scale) molecule, whereas they are unbound in the open channel. The energy difference between the two states can be tuned with a magnetic field. Feshbach resonance occurs when the energy difference is tuned to zero, at which point a bound pair is about to emerge.

Ultracold Fermi gases

The phenomenon of Feshbach resonance provides a means to tune the strength of interactions between atoms over several orders of magnitude by means of an external magnetic field. This leads to the possibility of investigating different regimes of superfluidity with a single physical system.

For negative scattering length $a$, no weakly bound dimer state exists. Then, the $^6$Li gas exhibits a remarkable stability against collisional decay, and deeply degenerate Fermi gases have been created.
In the middle of the crossover between the BCS and BEC regimes, the scattering length diverges at the unitary limit, leading to a strongly correlated state of matter. In this regime the gas is strongly interacting and its theoretical understanding defies standard many-body techniques. Analytical results for these systems are relatively rare, limited either to a few particles or to short-range correlations for the many-body problem. As the interaction energy is comparable to the Fermi energy, there is no small parameter in the system and standard many-body techniques based on perturbation expansions cannot be used.

In this regime, fermionic atoms instead of neutrons or quarks. At low temperature one is left with just two energy scales, the chemical potential $\mu$ and the Fermi energy $E_F$. These quantities are then necessarily proportional, resulting in a simple expression for the equation of state $\mu = \xi E_F$. The quantity $\xi$ is a dimensionless number that describes the full thermodynamic properties of a unitary Fermi gas.

- It is expected to be independent of the elementary constituents of the gas, as long as they interact with short-range interactions described by an infinite scattering length.
- This universal character of $\xi$ makes it relevant for modelling low-density neutron matter in the neutron stars, despite densities twenty-five orders of magnitude larger than cold-atom systems.
- The measurement of the parameter $\xi$ constitutes a simple prototype of a quantum simulation with ultracold atoms.
Quantum simulation

The theoretical understanding of finite-temperature effects is even more difficult and until recently no consensus was established for the equation of state. Measurements of the equation of state in the unitary limit, thus proved useful in discriminating between various theoretical approaches.

One of the defining characteristics of a quantum simulator is the ability to perform high-precision measurements of key observables. The combined measurement of several intensive quantities, such as the gas density $n$, chemical potential $\mu$ and temperature $T$, allows one to reconstruct the equation of state $n(\mu, T)$ of the investigated system.

Measuring the local pressure inside a trapped gas.

The CCD (charge-coupled device) camera signal corresponds to the atom density integrated along the line of sight $x$. An further integration along $y$ provides a one-dimensional profile, which is proportional to the local gas pressure $P(z)$ inside the gas along the $z$ axis.

Superfluid or not with spin imbalance?

Fermionic superfluidity, whether it occurs in superconductors, helium-3, or inside a neutron star, requires pairing of fermions, particles with half-integer spin.

In an equal mixture of two states of fermions ("spin up" and "spin down"), pairing can be complete and the entire system will become superfluid.

When the two populations of fermions are unequal, however, not every particle can find a partner, raising the question of whether superfluidity can persist in response to such a population imbalance.

This problem arises in many different fields of physics—for example, in the study of superfluidity of quarks in the neutron stars or dense matter of the early universe, where charge neutrality and differing masses impose unequal quark densities.

Science 311, 492 (2006)
Quantum simulation: superfluidity with spin imbalance

Quantum simulations with ultracold atoms: the superfluidity with imbalanced spin populations was observed.

Contrary to expectations for the weakly interacting case, superfluidity in the resonant region is extremely stable against population imbalance.

As the asymmetry is increased, we observe the quantum phase transition to the normal state, known as the Pauli limit of superfluidity.

Carry out experiments with different imbalanced spin state mixture of $^6$Li atoms.

Our “quantum simulator” toolbox allows preparation of various spin mixtures.

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2. Atoms is optical lattices or arrays of traps as a quantum simulator for condensed matter systems. Study of quantum phase transitions, quantum magnetism, high-temperature superconductors, etc. The control of the system: control of optical lattice parameters, loading, external fields, etc.
Rotating Superfluid

In a classical solid, each individual particle resides on one particular site — a lattice site if the solid is a crystal — and is localized such that the crystal is rigid and responds elastically to shear stress.

A classical solid inside a box is forced to rotate with the box walls when the box rotates.

However, in a quantum solid, particles fluctuate a lot around their average positions, with the result that atoms may exchange places with their neighbours. If this exchange is easy enough, some of the atoms may flow through the otherwise rigid network and some of the mass may stay at rest while the rest rotates. Eventually, if this flow becomes superfluid, the solid is said to be supersolid. Some of the mass is delocalized and the remainder is localized.

Supersolid

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*Nature*  
*464*, 176-182 (11 March 2010)
Quantum simulations with atoms in optical lattices

In a typical condensed-matter system, electrons can be modelled as moving on a lattice generated by the periodic array of atom cores. Such a general setting can be simulated with ultracold atoms using the concept of an 'optical lattice'.

An optical lattice works as follows. When atoms are exposed to a laser field that is not resonant with an atomic optical transition (and thus does not excite the atomic electrons), they experience a conservative potential that is proportional to the laser intensity. With two counterpropagating laser fields, a standing wave is created and the atoms feel a periodic potential. With three such standing waves along three orthogonal spatial directions, one obtains a three-dimensional optical lattice. The atoms are trapped at the minima of the corresponding potential wells.

Optical lattices vs. real crystals

Figure 1: Crystal simulation. Ultracold atoms in an optical lattice can simulate condensed-matter phenomena that usually occur only in the 'electron gas' of a solid-state crystal. In an optical lattice (a), atoms are trapped in a sinusoidal potential well (grey) created by a standing-wave laser beam. The atoms' wavefunctions (blue) correspond to those of valence electrons in a real crystal (b). Here, the periodic potential is caused by the attractive electrostatic force between the electrons (-) and the ions (+) forming the crystal. The motion and interaction of the particles, whether ultracold atoms or electrons, determine the physics of the material. Thus, for example, superfluidity in a gas of ultracold atoms corresponds to superconductivity in an electron gas.

Why optical lattices for quantum simulation?

An optical lattice is essentially an artificial crystal of light - a periodic intensity pattern that is formed by the interference of two or more laser beams.

Imagine having an artificial substance in which you can control almost all aspects of the underlying periodic structure and the interactions between the atoms that make up this dream material.

Such a substance would allow us to explore a whole range of fundamental phenomena that are extremely difficult - or impossible - to study in real materials.

Bose Hubbard model

The statistical nature of the atoms—whether they are fermions or bosons—plays a key role in such a lattice.

Fermions obey the Pauli exclusion principle, such that two fermions cannot occupy the same quantum state, whereas for bosons, multiple occupation of a single quantum state is allowed.

Bosons in an optical lattice can be described by the Bose Hubbard model.

\[ J \] – tunneling of atoms between neighboring wells

\[ U \] – repulsion of atoms sitting in the same well
What parameters can we change?

Practically anything!
- 1D, 2D, 3D
- Lattice wavelength
- Lattice geometry
- J/U (depth of the potential)
- Lattice loading
- Bosons or fermions or both
- Spin arrangements
- Introduce disorder, etc.

What can we do with optical lattice quantum simulator?

- Study of quantum phase transitions
- Quantum magnetism
- High-temperature superconductors
- Quantum Hall effect
- Address problems in quantum filed theory
- ???
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• Study of quantum phase transitions
• Quantum magnetism
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• Quantum Hall effect
• Address problems in quantum field theory
• ????

Superconductivity

Superconductivity is a phenomenon occurring in certain materials at extremely low temperatures, characterized by exactly zero electrical resistance and the exclusion of the interior magnetic field (the Meissner effect).

A magnet levitating above a high-temperature superconductor, cooled with liquid nitrogen. Persistent electric current flows on the surface of the superconductor, acting to exclude the magnetic field of the magnet (the Meissner effect). This current effectively forms an electromagnet that repels the magnet.

Superconductors are also able to maintain a current with no applied voltage whatsoever. Experimental evidence points to a current lifetime of at least 100,000 years, and theoretical estimates for the lifetime of persistent current exceed the lifetime of the universe.
Superconductivity: Cooper pairs

- Singe electrons: only one electron can occupy a particular state
- Cooper pairs: the above restriction no longer applies as electron pairs are bosons and very large number of pairs can occupy the same state (BCS theory)

1. Therefore, the electron pairs do not have to move from an occupied state to unoccupied one to carry current.

2. The normal state is an excited state which is separated from the ground state (in which electrons form Cooper pairs) by an energy gap. Therefore, electrons do not suffer scattering which a source of resistance as there is an energy gap between their energy and the energies of the states to which they can scatter.

Superconductivity: How are Cooper pairs formed?

Low-temperature superconductivity – below 30K

Normally electrons do not form pairs as they repel each other. However, inside the material the electrons interact with ions of the crystal lattice. **Very simplify, the electron can interact with the positively charged background ions and create a local potential disturbance which can attract another electron.**

The pairing alters the spacing of the rungs on the energy ladder, creating a gap near the top of the stack. To break from its partner, an electron must jump the gap to an empty state. There isn't enough energy around to allow that, so the pairs glide along unperturbed.

From BCS theory we learn that the lowest state of the system is the one in which Cooper pairs are formed.

### Transition temperatures of well-known superconductors

<table>
<thead>
<tr>
<th>Transition temperature (in kelvin)</th>
<th>Material</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>195</td>
<td>HgBa₂Ca₂Cu₃O₧</td>
<td>Copper-oxide superconductors</td>
</tr>
<tr>
<td>133</td>
<td>Bi₂Sr₂Ca₃Cu₄O₁₀ (BSCCO)</td>
<td>Copper-oxide superconductors</td>
</tr>
<tr>
<td>110</td>
<td>YBa₂Cu₃O₇ (YBCO)</td>
<td>Copper-oxide superconductors</td>
</tr>
<tr>
<td>90</td>
<td>SmFeAs(O,F)</td>
<td>Iron-based superconductors</td>
</tr>
<tr>
<td>55</td>
<td>CeFeAs(O,F)</td>
<td>Iron-based superconductors</td>
</tr>
<tr>
<td>41</td>
<td>LaFeAs(O,F)</td>
<td>Iron-based superconductors</td>
</tr>
<tr>
<td>77</td>
<td>Boiling point of liquid nitrogen</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>Boiling point of liquid hydrogen</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>NbSn</td>
<td>Metallic low-temperature superconductors</td>
</tr>
<tr>
<td>10</td>
<td>NbTi</td>
<td>Metallic low-temperature superconductors</td>
</tr>
<tr>
<td>9.2</td>
<td>Nb</td>
<td>Metallic low-temperature superconductors</td>
</tr>
<tr>
<td>4.2</td>
<td>Hg (mercury)</td>
<td>Metallic low-temperature superconductors</td>
</tr>
</tbody>
</table>

### Applications of superconductivity

Superconducting magnets are some of the most powerful electromagnets known. They are used in MRI/NMR machines, mass spectrometers, and the beam-steering magnets used in particle accelerators. They can also be used for magnetic separation, where weakly magnetic particles are extracted from a background of less or non-magnetic particles, as in the pigment industries.

Superconductors are used to build Josephson junctions which are the building blocks of SQUIDs (superconducting quantum interference devices), the most sensitive magnetometers known.

Promising future applications include, electric power transmission, transformers, power storage devices, electric motors (e.g. for vehicle propulsion, as in vactrains or maglev trains), magnetic levitation devices, fault current limiters, nanoscopic materials and superconducting magnetic refrigeration.
High-temperature superconductivity

High-temperature superconductive compounds contain planes of copper and oxygen ions that resemble chess boards, with a copper ion at every corner of a square and an oxygen ion along each side.

Electrons hop from copper ion to copper ion.

Between the planes lie elements such as lanthanum, strontium, yttrium, bismuth, and thalium. But it is along the copper-and-oxygen planes that the electrons pair and glide.

Just how that happens is anything but clear.

Example: $T_c=93K$

$YBa_2Cu_3O_7$

Possible explanations for high-$T_c$ superconductivity

Interaction of the electrons only (waves of magnetism associated with antiferromagnetic ordering of electron spins)

The resonating valence bond theory (involves interactions of electrons on neighboring copper ions).

There is experimental evidence for d-wave pairing