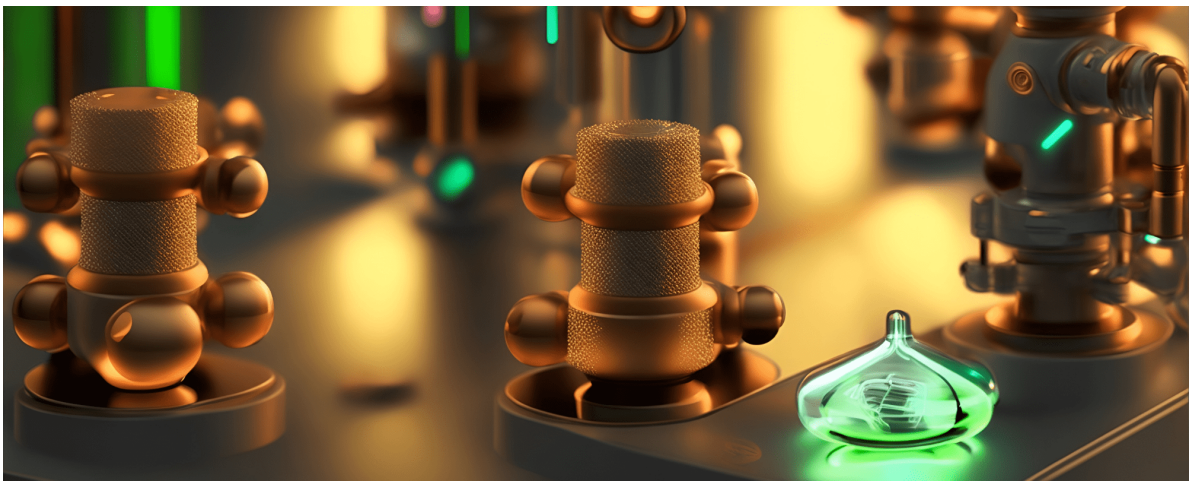
RESEARCH AND PRACTICAL APPLICATIONS

Solving difficult quantum problems with ultracold atoms

Leticia Tarruell



Artistic representation of ultracold atoms

What is quantum simulation?

Quantum computing has undergone dramatic developments in recent years. The new computing paradigm exploits the properties of quantum mechanics to perform calculations that are very complicated, if not impossible, to carry out using computers following the rules of classical physics. However, some formidable challenges will need to be overcome before we have at our disposal quantum computers that work in a similar way to the classical computers we are used to; that is, computers that are universal (can tackle any problem), digital, and can self-correct for errors arising in the calculations to ensure the quality of the final result. It is extremely difficult to make predictions in such a dynamic area, but the current consensus is that it will take years, if not decades, for such sophisticated quantum machines to become a reality.

To predict the outcome of difficult problems, however, full-blown quantum computers are not always required. Before classical computers, men used diverse tools to help them carry out complex calculations. An excellent example is the abacus, the origin of which remains unknown. Another is the armillary sphere, invented independently in both ancient China and ancient Greece, and used to predict the motion of the stars and planets. Similar devices can be exploited to assist us in solving difficult quantum mechanical problems and, because these problems are quantum in nature, the corresponding devices will naturally also be quantum. This idea was first proposed in 1981 by physicist Richard Feynman, who coined

the name “quantum simulators” to refer to them. [1] Quantum simulators are nothing other than special purpose quantum computers. Indeed, due to the limitations of the quantum hardware we currently have at our disposal, most quantum computing devices are currently run in quantum simulation mode when trying to obtain a quantum advantage with respect to classical machines.

> Quantum simulators allow us to solve complex quantum problems simple to formulate but hard to solve. Even the most powerful classical supercomputers may take an extremely long time –even beyond the age of the universe– to find the solution

Quantum simulators allow us to solve complex quantum problems because, in many cases, these are simple to formulate but hard to solve. In physics terms, the Hamiltonian – the quantum mechanical operator associated with the energy of a system – is very simple to write, but the size of the Hilbert space – the number of quantum mechanical configurations that need to be considered to describe the system – is tremendously large. Hence even the most powerful classical supercomputers may take an extremely long time – even beyond the age of the universe! – to find the solution. However, since the problem is simple to formulate, a quantum physical system can be used to engineer a model completely analogous to it, allow it to evolve until it reaches the state of interest, and then measure its properties to obtain the solution to the quantum problem. This is what is understood by “solving the problem using quantum simulation”.

When performing a quantum simulation, it is very important to be able to engineer the model required with great precision; in physics terms, to precisely realise the target Hamiltonian without any spurious terms that could modify the result. Excellent control over the initialisation of the system is also needed; another key aspect is to have a good method to probe the system once the simulation is performed, to read out the answer of the “calculation”. Ideally, the state of every single quantum component of the system would be available. Finally, it is crucial to be able to scan the different parameters of the Hamiltonian that has been realised, to determine how the solution depends on their value. This is exactly how numerical simulations are performed in classical computing, except that in quantum simulation the calculation is carried out by the quantum system.

These requirements – excellent model engineering, initialisation, probing, and the ability to independently scan the different system parameters – determine which quantum hardware is best suited to quantum simulation. Currently, the most developed experimental platforms are neutral atoms, trapped ions, superconducting circuits, and photonic circuits. Moreover, quantum simulators can be operated in digital or analogue mode. Digital simulators are, in principle, more flexible, that is, simpler to programme to address a broader class of

problems. But, in the absence of error correction protocols, the results are much more affected by the limitations of the hardware. Analogue simulators, in contrast, need to be reconfigured when addressing a different class of problem. However, they are much more robust against hardware imperfections and currently allow much larger system sizes to be simulated. In practice, the choice of a particular experimental platform and of an analogue or digital approach depends very much on the exact problem to be quantum simulated. In the section that follows, we will focus our discussion on ultracold neutral atoms, the system in which quantum simulation was first demonstrated and which currently allows the largest system sizes to be reached.

Cooling down, trapping and imaging neutral atoms

Ultradilute gases of neutral atoms constitute an excellent platform for quantum simulation. They naturally provide many identical particles – the atoms – which, however, need to be cooled to ultracold temperatures to enter the quantum regime. The first stages of cooling can be conveniently achieved using lasers, according to an invention by Steven Chu, Claude Cohen-Tannoudji and William D. Phillips, whose work was recognised with the 1997 Nobel Prize in Physics. [2][3][4] In practice, an ensemble of atoms are simply illuminated with laser beams whose wavelength (the colour of the laser) is near-resonant with an atomic transition. When an atom absorbs a photon – a particle of light – from a laser, its electron goes from the lowest energy (ground) state to an excited state. In this process, the atom receives a momentum kick that reduces its velocity along the laser direction. Because the excited state of the atom has a limited lifetime, the electron spontaneously falls back to the ground state, re-emitting a photon. However, in this case, the direction of emission is aleatory, and so is the momentum kick associated with it. If the process is repeated many times, the effect of the kicks due to the spontaneous emission events are cancelled out, but the effect of the laser kicks remains and reduces overall the velocity of the atoms along this direction. By shining lasers on the atoms along three perpendicular axes, the atoms are overall slowed down. Since the temperature of an ensemble of atoms is related to their velocity, their temperature is strongly reduced. With this method, temperatures of the order of 1 μK (or even lower, depending on the properties of the atomic transition used) can be attained, that is, just one millionth of a degree above the absolute zero of temperature.

Once such ultralow temperatures have been reached, additional lasers can be used to trap the atoms and subject them to precisely sculptured “landscapes”. This is achieved by exploiting the so-called optical dipole force.

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It relies on the fact that a laser of wavelength smaller than any atomic transition will polarise an atom, inducing a tiny electric dipole into it. This dipole will interact back with the electric field of the laser such that, in order to minimise its energy, the atom will want to move to the intensity maxima of the laser beam. Thus, the atoms will be attracted to the point where the laser beam is focused, getting effectively trapped there. As a result, a focused laser beam can act as an optical tweezer for the atom, not only trapping it but also allowing it to move around by displacing the point of maximum laser intensity. Moreover, one can generate essentially any landscape for the atoms can be generated by using, instead of a single laser beam, a spatial light modulator – the device inside the beamers used to project presentations or movies – which facilitates the creation of virtually any spatial light distribution. The atoms should be just sufficiently cold to stay in the trap.

This brings us to another key point. Even if laser-cooled atoms are very cold, they are not necessarily in the quantum regime yet. This will only occur once they start behaving simultaneously as particles and waves, which requires the wave packet intrinsically associated with each atom to have an extent larger than the distance between neighbouring atoms, so that quantum interference effects between different atoms can arise. This situation only takes place at even lower temperatures, on the nK scale (a billionth of a degree above absolute zero) or even lower. These are really the lowest temperatures in the universe, as certified in 2008 by a Guinness World Record.

Eric A. Cornell, Carl E. Wieman and Wolfgang Ketterle were awarded the Nobel Prize in Physics in 2001 for attaining this quantum regime for the first time. [5][6] Such temperatures can be achieved using an additional cooling technique that is conceptually analogous to the way one cools a hot cup of coffee by blowing on its surface, and which because of this similarity is known as evaporative cooling. For it to work, the atoms must interact with each other. They do so by colliding with each other, which is also the basic resource that we use to engineer interacting models with ultracold atoms (although other types of more complex interactions are also possible).

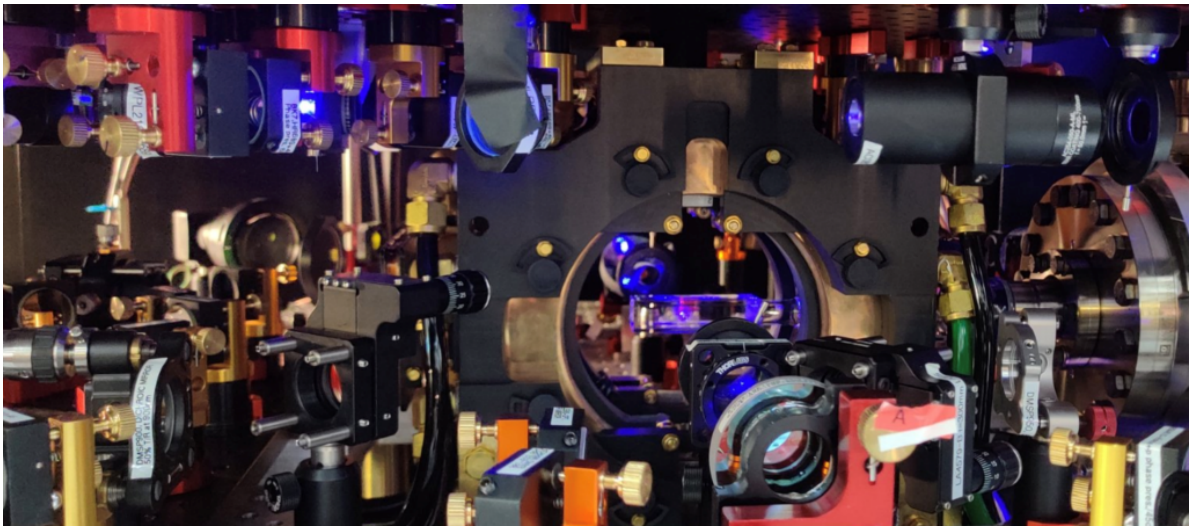


Figure 1.1. One of ICFO’s quantum simulators with ultracold neutral atoms, where strontium atoms are laser-cooled down to μK temperatures

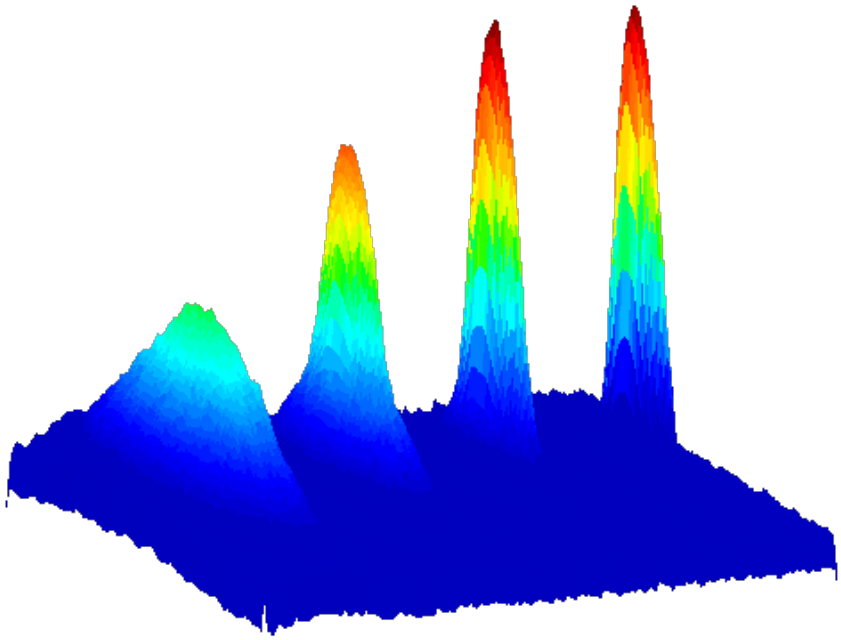


Figure 1.2. First Bose-Einstein condensate (a set of bosonic atoms in the quantum regime) made in Catalonia in 2015 by our ICFO group. The image shows how the velocity distribution of a gas of potassium atoms changes when it goes from the classical to the quantum regime

Once the quantum regime is reached, the atoms will behave very differently if they have an even or an odd number of components; in physics terms, if their intrinsic angular momentum (their spin) takes integer or half-integer values. In the first case, the atoms are called bosons and all tend to occupy the same state. In the second case, we refer to them as fermions, two identical atoms that can never be in the same state at the same time. Having these two classes of atom allows us to mimic the behaviour of the different types of particles existing in nature because matter particles – like electrons, protons, quarks, etc. – are fermions, while the interactions between them arise from the exchange of bosonic particles: photons for electromagnetic forces, for instance.

Finally, to read out the result of a quantum simulation, it is crucial to be able to detect the state of the system extremely accurately. Ideally, this should be done at the single atom level, which can be achieved by shining resonant light on an atomic transition. After absorbing the corresponding photons, the atoms will re-emit fluorescence light. By collecting the fluorescence photons with a microscope objective and forming the image on a

CCD camera, the spatial distribution of the system, with a resolution that goes down to each single atom, can be obtained. [7]

We have seen, then, that ultracold neutral atoms provide all the ingredients required for successful quantum simulations. They provide many identical particles, the nature of which (boson or fermion) can be easily selected, and which can be brought to the quantum regime. They can be made to interact with each other and can be subjected to various energy landscapes, enabling the realisation of a broad variety of models. The parameters of these models can be scanned in a flexible manner, allowing them to be “solved”. And this solution can be read out by detecting the state of each atom in a very precise way. In conclusion, ultracold neutral atoms provide an extremely malleable form of quantum matter to perform quantum simulations.

From engineering artificial materials to exploring exotic states of matter

We conclude this article by giving some examples of difficult quantum problems that can be tackled with these systems. Our first example is the electrical conductance properties of solids, a problem that naturally lends itself to quantum simulation. This is a situation that involves many quantum particles – the electrons – which, when interactions between them are very strong, can be extremely hard to tackle using classical methods. At the same time, it is also a problem with important practical applications. One key example is high-temperature superconductivity – the fact that certain materials conduct electricity without any losses at temperatures much higher than usually observed. The phenomenon was discovered in the 1980s but, despite its potential technological importance – for instance, in the fabrication of high-field magnets for applications as crucial as fusion reactors – it remains only partially understood. Quantum simulation is a very serious candidate to shed light on the mechanisms behind high-temperature superconductivity.

To investigate such phenomena, a quantum simulator must engineer an artificial material. When considering its electronic transport properties, the two key ingredients of a material are the electrons and the crystalline structure under which they evolve. In an ultracold atom quantum simulator, fermionic atoms can be used to mimic the electrons. The crystalline structure is realised using interfering laser beams, which will create a periodic potential – very similar to an “egg carton” – for the atoms. Indeed, the interference of two counter-propagating laser beams gives rise to a standing wave with a succession of bright and dark fringes, and by choosing the wavelength of the lasers appropriately, the atoms can be trapped in the bright fringes. Moreover, by interfering not just two but several laser beams, and properly adjusting their angles, wavelengths and intensities, it is possible to realise two- and three-dimensional artificial materials with basically any crystalline structure. [8]

These systems are certainly the purest and cleanest “solids” existing in nature, and their tunability can be exploited to investigate a broad range of materials including insulators, conductors, superconductors and magnets, as well as to identify the key ingredients that

give rise to a behaviour of interest. The long-term goal is to exploit quantum simulators as a practical tool to guide the design of new materials, by testing new ideas and concepts prior to synthesising the corresponding compounds in a laboratory; in other words, to make quantum simulators play a role similar to wind tunnels in the design and testing of automobiles and planes. In Catalonia, at the Institute of Photonic Services (ICFO), we have developed a quantum simulator ideally suited to this type of “quantum calculation”, which will allow us to engineer artificial materials where every single atom will be controlled, and where the solution to the problems will also be read out at the single-atom and single-site level.

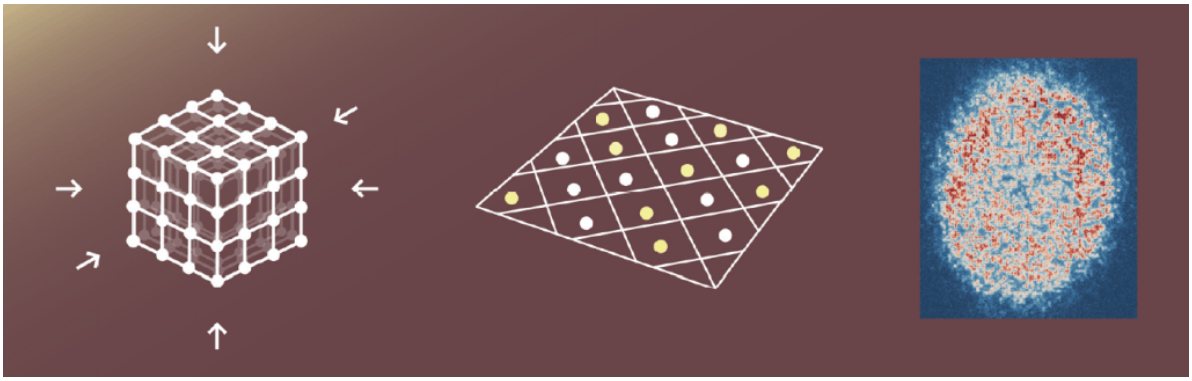


Figure 2. Engineering of artificial materials with ultracold atoms in light crystals. Left: arrangement of interfering laser beams leading to a three-dimensional crystal, known as an optical lattice. Center: Schematics of an optical lattice, where atoms are trapped in a series of potential wells and experience an “egg” landscape. Right: One of the first images of strontium atoms in an optical lattice taken in the ICFO quantum simulator in 2023. The fluorescence images allow each individual atom to be seen, which in the image appears as a dot bright

Another type of problem where quantum simulators offer an important advantage is the exploration of exotic phases of matter. Ultracold atoms enable the realisation of forms of quantum matter that have existed in the minds of physicists for decades as abstract constructions, but which up to now could not be observed in natural systems. This may be because they correspond to extreme parameter regimes not accessible in nature, such as extremely strong magnetic fields, materials subjected to enormous stress, or unrealistically high temperatures; or because they are expected to occur in systems where performing measurements is extremely difficult, if not impossible, such as the core of a neutron star or the inside of a nucleus. While interest in these problems is more fundamentally scientific than applied, the existence of laboratory experiments where they can be addressed is not only very exciting for scientists, it also leads to advances in our understanding of nature that will certainly spread to other areas of knowledge.

At ICFO, we have a quantum simulator that specialises in this type of exotic problem. Over the last few years, for instance, we have realised liquids 100 million times more dilute than water and 1 million times thinner than air, and which exist due to tiny quantum effects – so-called quantum fluctuations – that are normally very difficult to observe. [9] We have also

engineered chiral quantum matter, in which the interactions between the atoms are different according to whether they move to the right or to the left. This has allowed us to observe phenomena that were predicted theoretically almost twenty years ago, but had never been "seen" in a laboratory. [10] Very recently, we have realised a very intriguing phase of matter, a supersolid, which at the same time flows without any friction and crystallises spontaneously. These are just some examples of the very strange forms of matter that exist once we get very close to absolute zero.

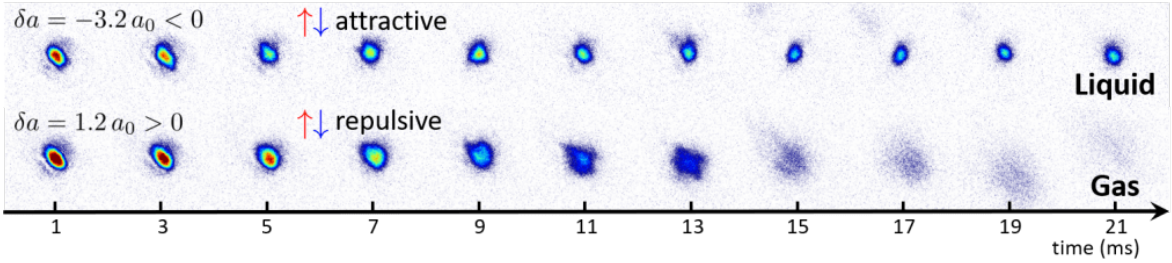


Figure 3. Observation of exotic quantum phases of matter with quantum simulators; here, quantum liquid droplets in a mixture of two gases of potassium bosonic atoms with competing interactions. When opening a "laser box" at time t = 0 ms, a gas expands while a liquid maintains its shape because it has formed a drop

Conclusion

In this article, we have offered a short introduction to quantum simulation: the "art" of solving difficult quantum problems that traditional (classical) computers cannot tackle and realising novel forms of quantum matter beyond what is accessible in nature. We have discussed how quantum simulators can be understood as special purpose (and in many cases analogue) quantum computers. We have gone on to present ultracold neutral atoms as a highly advanced quantum hardware that is already available for performing such quantum simulations. Finally, we have discussed some of the problems currently being explored using quantum simulators, giving as examples some of the capabilities that we have developed in Catalonia in recent years. Quantum simulation is a very rapidly evolving field, and in the near future we expect to see a steady increase in both the quality and power of quantum simulation hardware and the range of problems it can help to solve.

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