RESEARCH AND PRACTICAL APPLICATIONS

Quantum simulation: shaping the horizon of future technology

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Quantum wires and planet Earth. Conceptualization: Luisa Quiroga

Although the mass media often frames quantum computing as a revolution, in essence it is an extension of the enduring human endeavour to speed up information transfer and enhance its density. This journey began with pictographic data carved into cave walls by ancient civilizations, and then evolved to the use of paper, enabling written information to be transported by pigeons or horses. Information also transitioned from pictograms to alphabets, producing a higher density encoding of information. Similarly, the invention of fonts augmented the speed of information creation and replication beyond handwriting. The most substantial shift, however, emerged with the telegraph, which used electricity as a carrier of information.

Interestingly, this marked an approximate limit for the speed evolution of information distribution. With information in electrical cables travelling at roughly 70–80% of light speed, an increase achieved with optical fibres was only marginal when compared to the shift from horses to electricity. The revolutionary aspect of the telegraph also relied on the use of electrons to encode information. Put simply, the absence or presence of an electron represents 0 or 1, respectively, in a binary system that encodes all necessary information. This system, now known as a bit, is still used today in all our electronic devices.

So, what is quantum computing and why is it so appealing? Essentially, it is a progressive step beyond the contemporary binary method of encoding and processing information. Quantum computing delves deeper, controlling the carrier’s state and encoding information in its structure (the spin of an electron or the polarization of a photon, for example),

labelled as a qubit. This facilitates denser and thus more efficient information processing and transfer, the ultimate goal of all scientific explorations in quantum computing.

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Yet, this innovative approach to transmitting and processing information has substantial implications. It necessitates entirely new approaches to information processing, using quantum systems (qubits) as information carriers. The rules of quantum physics, such as entanglement and the superposition of states 0 and 1, should be harnessed for faster information processing, leading to quantum advantage. This occurs when a quantum computer outperforms a classical one in a computational task. To achieve this, however, entirely new logical gates must be designed and physically fabricated, full connectivity between qubits must be ensured, and innovative strategies to minimize potential errors must be established. Information encoded in quantum systems is extremely delicate and can be disrupted by environmental factors such as temperature. Moreover, the lack of quantum algorithms proven faster than classical computers is a notable hurdle, with limited progress since the introduction of Shor's (1994) and Grover's (1996) algorithms.

Some might wonder, therefore, whether quantum computing is simply hype. Yet we see it as less of a fleeting craze, and more of a significant and meaningful scientific journey. The public's scepticism may stem from exaggerated promises made by quantum companies that have failed to materialize. Moreover, there seems to be an excessive focus on achieving quantum supremacy. We suggest viewing quantum computing as a fresh, common scientific venture. It has already enabled us to manipulate atoms, photons, electrons and more, in ways we could never have imagined. Quantum computing has spurred enormous scientific and technological advancements in a host of areas including integrated photonics fabrication, superconducting circuits, cryogenics, light control, algorithm development, and entanglement generation. These achievements alone justify the ongoing support and development of quantum computing, even if "practical" quantum supremacy never materializes.

One undeniable advantage of developing a universal quantum computer would be the capacity to create a digital quantum simulator, capable of simulating any material or chemical reaction, an impossible feat for classical computers. Remarkably, no new algorithms are needed for this! The physics community has already developed the necessary formalism for such simulations, and is ready to implement them on a digital

quantum simulator when available. We believe this to be one of the most promising and impactful applications of quantum computing.

However, until problems of error corrected universal quantum computer are solved, achieving realistic and practical applications of quantum computing relevant to science and technology will remain in the domain of special purpose quantum computers, i.e., quantum simulators.

The idea behind quantum simulation can be briefly sketched as follows. We know that many interesting quantum phenomena such as superconductivity may have important technological applications. These phenomena are often difficult to describe with the help of classical computers. Instead, we can use a simpler and more easily controlled quantum system to simulate, understand and control these phenomena, as originally proposed by Y.I. Manin and R.P. Feynman. Such a system would thus work as a special-purpose quantum computer, and this is what we call a quantum simulator.

Nowadays there are already several well-developed platforms where quantum simulation is being realized and “practical” quantum supremacy has been achieved. At this point, we should also stress that quantum simulation can be either analogue or digital. In the case of digital, any platform that offers tools for universal quantum computing can also be used for special purposes, i.e., for quantum simulation. Some examples from the long list of readily available platforms are provided in the paragraphs that follow.

Quantum simulation platforms

On the one hand, large companies such as Google and D-Wave use superconducting qubits, which in principle allow for noisy, but universal, quantum computing, and are very often used for digital quantum simulation. Other options for digital quantum simulation are circuit QED, systems of superconducting qubits located in micro-cavities, quantum dots, spin qubits in semiconductors, photonic systems – which, when combined with photon counting, may mimic universal quantum computers – or trapped ions, which allow for universal quantum computing but can also be used as analogue quantum simulators to describe spin-half systems, for instance, rather than Hubbard models.

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On the other hand, ultracold atoms make good candidates for analogue quantum

simulation, and can be realized in traps or, more frequently, in optical lattices. They are very flexible and allow the simulation of complex Hubbard models as well as spin systems. Other platforms for analogue quantum simulation include Rydberg atoms. These can be excited to high Rydberg states and trapped in optical tweezers, very useful for mimicking spin systems with long-range interactions, or twistronic systems, twisted bilayer graphene or other 2D materials systems. For small, “magic”-angle spinning, they lead to periodic moiré patterns at the length scale much larger than typical scale of condensed matter, such that they themselves can be considered as condensed matter quantum simulators of condensed matter.

All these platforms for quantum simulation are already being used for the tasks and goals listed at the end of this introduction. The most developed application is the study of the fundamental problems of physics, in which many of the results achieved are believed to have demonstrated the quantum advantage. Secondly, they can be used for quantum chemistry applications, although this field is rather new, and still a long way from achieving the precision and accuracy of contemporary theoretical quantum chemistry. Finally, quantum simulation can also be applied to classical or quantum optimization problems for technology. This application is also in an initial phase and cannot yet compete with classical supercomputer methods.

In the coming decades, as clearly reflected in future Quantum Flagship programmes, we expect the platforms being used to remain the same, though the challenges and focus are going to be vastly different. The quantum simulators of the future will need to be devices that are robust, scalable, programmable, externally accessible and standardized, as well as verifiable, demonstrable and certifiable. Moreover, prioritization of these tasks and goals will be inverted. We expect optimization problems with a technological application to rise to the top of the podium and quantum chemistry to remain in second place, while fundamental problems of physics will not become less important but will lose their unique status as the area where practical quantum advantage can be achieved. Summarizing, the future of quantum simulation will deal with the following list of priorities:

- Generation, manipulation and applications of massively entangled states, useful for quantum communication, quantum metrology, sensing and detection.
- Classical/quantum optimization problems for technology
- Quantum chemistry, including novel methods of simulating quantum chemistry, going beyond NISQ devices to analogue simulators
- Fundamental problems of physics, with a specific focus on simulations of systems for condensed matter, high energy physics (HEP) and quantum field theory (QFT).

Catalonia in the field of quantum simulations

In the following paragraphs, we present a number of quantum simulations of fundamental problems of physics currently being investigated in Catalonia, which feature some of the great achievements of quantum simulation over the last few years.

Fermi-Hubbard model: A “paradigmatic” and notoriously difficult to simulate classical system is, of course, the Fermi-Hubbard model, believed by many to lie at the heart of the high-temperature superconductivity phenomenon. The Markus Greiner group at Harvard is the World Master of Fermi-Hubbard quantum simulators. A good example of what quantum simulators can do in this context is, as the authors write: “Understanding strongly correlated quantum many-body states is one of the most difficult challenges in modern physics. For example, there remain fundamental open questions on the phase diagram of the Hubbard model, which describes strongly correlated electrons in solids. […] we realize the Hubbard Hamiltonian and search for specific patterns within the individual images of many realizations of strongly correlated ultracold fermions in an optical lattice.”

Quantum droplets: Another classically difficult to simulate system is the type that exhibit intrinsic instability compensated by strong interactions, quantum fluctuations or other mechanics, leading to the creation of self-bounded solitons, liquid droplets (see Fig. 2) and similar textures. Liquids and gases are two distinct phases of matter that are part of our everyday life. While gases are dilute, compressible and take the size of their container, liquids are dense, with fixed volume and form droplets in small quantities. These are ensembles of particles that remain bound by themselves and have a free surface that separates them from their environment. By increasing the temperature, a transition phase between liquid and gas can be induced. This is exactly what happens when we boil water in a pan. But are gases always dilute and liquids always dense? Normally yes, but things can become very different at ultralow temperatures. Recently, the Leticia Tarruell group at ICFO created a liquid one hundred million times more dilute than water and a million times thinner than air.



Figure 1. Artistic view of a drop of quantum liquid formed by mixing two gases of ultracold potassium atoms. Graphic adaptation. Original image: ©ICFO/PovarchikStudiosBarcelona

Fundamental systems of condensed matter, HEP and QFT: In recent years, there has been a

strong focus on quantum simulation of HEP (High Energy Physics) models, lattice gauge theories and related systems. The challenge here is to control many-body interactions: “magnetic” interactions on the lattice plaquettes, and “electric” interactions governed by the Gauss law, i.e., local gauge invariance.

Schwinger model: The versatility of trapped ions makes them particularly suited to either digital or analogue simulation of LGTs. These systems may serve as universal quantum computers and, in principle, realize any few-body interactions and constraints. Here we quote an achievement of the Rainer Blatt group, who reported “the first experimental demonstration of a digital quantum simulation of a lattice gauge theory, by realizing (1 + 1)-dimensional quantum electrodynamics (Schwinger model) on a few-qubit trapped-ion quantum computer”. They were interested in the real-time evolution of the Schwinger mechanism, describing the instability of the bare vacuum due to quantum fluctuations, which manifests itself in the spontaneous creation of electron-positron pairs.

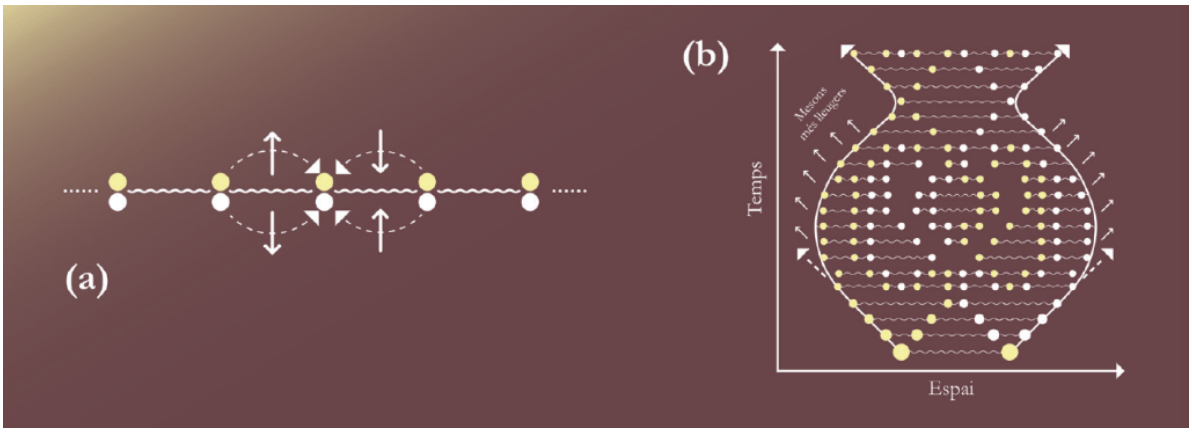


Figure 2. A particle-antiparticle pair (a meson) begins to expand and thermalize, but soon begins to experience confinement effects and oscillates ad infinitum with no apparent thermalization. Image credit: Titas Chanda

Bosonic Schwinger model: Relativistic quantum gauge theories are fundamental theories of matter describing nature. Paradigmatic examples are quantum electrodynamics (describing electro-magnetic interactions of charged particles and photons), chromodynamics (describing strong interactions of quarks and gluons), and the Standard Model, whereby the latter two are unified with the weak interactions. Despite enormous progress in our understanding of quantum gauge theories, questions concerning the behaviour of the systems described by these theories in the presence of strong correlations remain widely open: from the very nature of quark confinement to the behaviour of quark-gluon-plasma at high densities and temperatures. Moreover, out-of-equilibrium quantum dynamics of quantum gauge theories is beyond the reach of present computers. For these reasons, a great deal of effort is going into designing and investigating quantum simulators of such systems.

In the Schwinger model, the paradigmatic model of quantum gauge theory in one spatial dimension and time, “charged” electrons (fermions) interact with photons (bosons) in one dimension. Since quantum simulations with fermions are notoriously difficult, the quantum

optics group at ICFO, working in collaboration with the Cracow group of Jakub Zakrzewski, proposed a bosonic version of the Schwinger model. Using state-of-the-art theoretical physics methods, we investigated how the bosonic matter behaves when it is driven out of equilibrium by the creation of a particle-antiparticle pair on top of the vacuum of the system. The three main results are important for the understanding of quantum gauge theories in general (see Fig. 3). This work opens up a path towards quantum simulations of quantum gauge theories in novel, unexplored regimes.

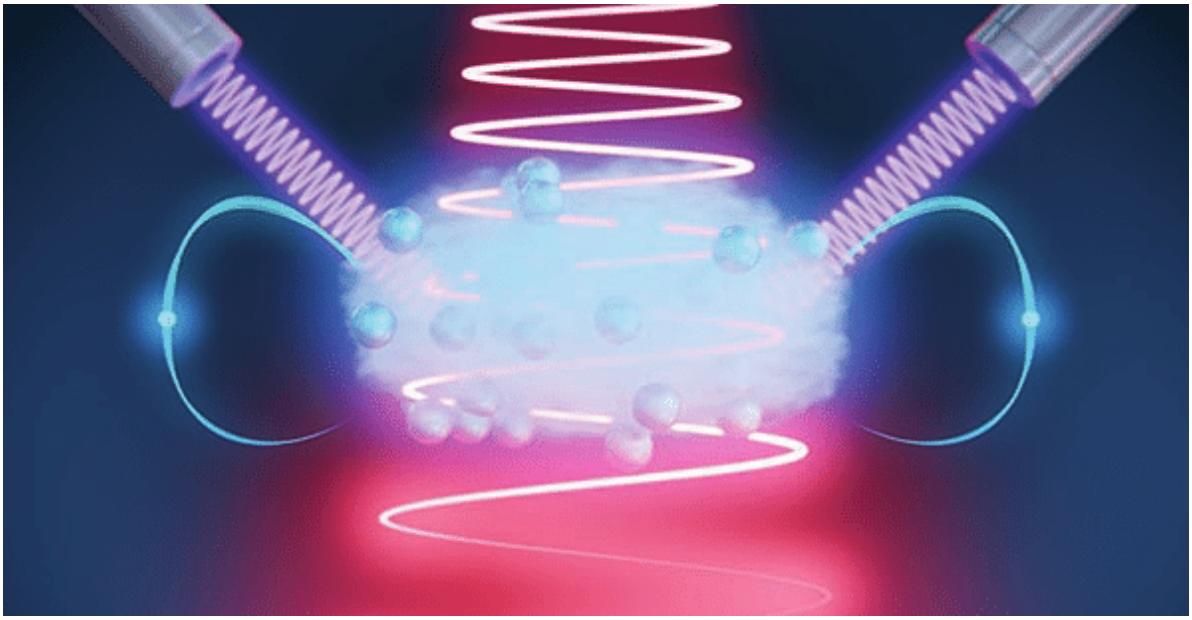


Figure 3. Optical states of Schrödinger's cat in intense laser-matter interaction. ©ICFO / Scixel – E. Sahagun

Novel quantum simulators (NOQIA) – ICFO recently proposed a completely new platform for quantum simulation of attoscience and ultrafast processes. Over the past four decades, astounding advances have been made in the field of laser technologies and the understanding of light-matter interactions in the non-linear regime. Thanks to this, scientists have been able to carry out extremely complex experiments related to, for example, ultrafast light pulses in the visible and infrared range, and reach crucial milestones such as using a molecule's own electrons to image its structure, to see how it rearranges, vibrates or breaks apart during a chemical reaction.

The development of high-power lasers has allowed scientists to study the physics of ultra-intense laser-matter interactions. The standard version of the study model, however, treats ultra-strong, ultra-short driving laser pulses from only a classical point of view. The famous theory known as the "simple man's model" or the "three-step model" – which had its 25th anniversary in 2019 – elegantly described the interaction of an electron with its parent nucleus sitting in a strong laser field environment according to classical and quantum processes. However, since these laser pulses are highly coherent and contain huge numbers of photons, the description of the interaction in the strong laser field remains incomplete, because the atomic system is given a quantum treatment, while the electromagnetic field is given a classical treatment.

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Nowadays, in the description of the most relevant processes of ultra-intense, laser-matter physics (such as high-harmonic generation, above threshold ionization, laser-induced electron diffraction, sequential and non-sequential multi-electron ionization, etc.), the quantum-fluctuation effects of the laser electric field, not to mention the magnetic fields, are negligible.

However, the quantum nature of the entire electro-magnetic field is always present in these processes, giving rise to the question, does this quantum nature exhibit itself? And in which situations does it appear? In a recent study in collaboration with the FORTH Paraskevas Tzallas group, we reported on the theoretical and experimental demonstration that intense laser-atom interactions may lead to the massive generation of highly non-classical states of light, one of the holy grails of contemporary quantum simulation (see Fig. 4). These results were obtained using the process of high-harmonic generation in atoms, in which large numbers of photons from a driving laser pulse of infrared frequency are up-converted into photons of higher frequencies in the extreme ultraviolet spectral range. The quantum electrodynamical theory formulated in this study predicts that, if the initial state of the driving laser is coherent, it remains coherent, but shifts in amplitude after interactions with the atomic medium. Similarly, the quantum states of the harmonic modes become coherent with small coherent amplitudes. However, the quantum state of the laser pulse that drives the high-harmonic generation can be conditioned to account for this interaction, which transforms it into an optical Schrödinger’s cat state. This state corresponds to a quantum superposition of two distinct coherent states of light: the initial state of the laser, and the coherent state reduced in amplitude that results from the interaction with the atoms.

Enjoy physics & beyond

The field of quantum simulators is one of the most beautiful areas of contemporary physics, melting together in a common pot all the branches and genres of physics, and not only physics. The conclusion we always reiterate is to enjoy physics and beyond. At ICFO we delight in going beyond physics to try to interpret quantum mechanical processes and, more specifically, quantum randomness in contemporary avantgarde music. We call this project the sonification of quantum physics. We also try to incorporate quantum random processes, using the genuine quantum random number generators provided to us by ICFO’s spinoff company, QUSIDE. A recent highlight of this endeavour was the nearly one-hour long concert “Interpreting Quantum Randomness” at the famous SONAR Festival 2021, and the vinyl and digital album available on Bandcamp.

CRÈDITS

This article is a shortened and simplified version of the chapter “The Coming Decades of Quantum Simulation” by the same authors, Joana Fraxanet, Tymoteusz Salamon and Maciej Lewenstein, in «Sketches of Physics», *Lecture Notes in Physics*, vol. 1.000, eds.: Roberta Citro, Maciej Lewenstein, Angel Rubio, Wolfgang P. Schleich, James D. Wells i Gary P. Zank.



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