Quantum simulators developed to study inaccessible physical systems

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Quantum simulators recreate the behaviour on a microscopic scale of biological and quantum systems and even of particles moving at the speed of light. The exact knowledge of these systems will lead to applications ranging from more efficient photovoltaic cells to more specific drugs. Researchers in the UPV/EHU's department of Physical Chemistry are working on the design of several of these quantum simulators so they can study the dynamics of complex physical systems.

Quantum mechanics is the mathematical tool that enables us to describe the physical processes that take place on a microscopic level; it is capable of satisfactorily predicting the stability of atoms and molecules, the reactivity of different chemical compounds, or the result of the interaction between radiation and matter. They are all situations that constitute the basis of our physical world and for which there is no explanation within the framework of classical physics. "The physical processes that take place on a quantum level obey such sophisticated mathematical models that they cannot be analysed by means of today's computers because of the computational limitations of these devices," explained Dr Jorge Casanova, researcher in the UPV/EHU's department of Physical Chemistry. One possible way of solving the problem of computational complexity of physical systems is to use a quantum platform or technology as a simulator.

Quantum simulators are systems capable of reproducing the dynamics of a specific physical system, and overcoming the limitation of conventional computers. Among the various technologies that are studied

with a view to developing efficient quantum simulators, this UPV/EHU research group has been focussing on the technology of trapped ions. "Basically, these systems work by isolating individual atoms in a controlled environment so that there is no interference with the environment. They then undergo laser treatment, and after that, it is possible to conduct operations like exciting or de-exciting the electrons of these atoms. That way they are made to behave like the system we want to study," explained Casanova, the lead author of the work.

Basing themselves on the technology of trapped ions, Casanova and his collaborators have designed various protocols for developing controlled quantum simulations. "We are theoretical physicists; we work by designing the processes that will subsequently take place in a specific experiment. We base ourselves on the laws of quantum mechanics, the ones that govern these systems, and we put forward ideas that are then verified in the laboratories we are working in collaboration with," explained the researcher.

Simulators for a range of physical situations

In the course of this research the UPV/EHU group designed quantum simulation protocols for various physical situations. The first was a simulator of relativist systems, in other words, of particles that move at speeds close to that of light. "This experiment is no trivial matter, because the ions used remain still, and yet we manage to get them to behave as if they were moving at the speed of light". The experiment proposed by this group in the department of Physical Chemistry was carried out in Austria, "and had quite an impact internationally, because until now this has been the experiment in which the highest level of quantum control has been achieved worldwide on ion movement states," remarked Casanova.

Following the success achieved, they went on proposing quantum

simulators for other types of systems, like those of interacting fermions and bosons. "This is very important," pointed out Casanova, because in nature both types of particles basically exist: some are fermions (in atoms, for example, the electrons) and the others are bosons (photons or light particles or the Higgs boson)."Our idea was to design the system under study artificially, so that we could gain access and extract information from it. The problem with these systems is that their dynamics are so complex that it is not possible to gain access to them by means of computations produced in classical computers, in other words, we are fully familiar with the equations that describe their dynamics, but we cannot resolve them," he remarked.

They then went on to consider another two types of simulators. Firstly, they designed simulators for quantum field theory models. These theories "are the ones that describe the most basic processes, like collisions between beams of particles that take place in accelerators, which are also very complex," explained Casanova. After that they focussed on the simulation of quantum chemistry models; "this is a proposal that we have in collaboration with research personnel at Harvard University (USA), where we designed a specific protocol for quantum chemistry molecular models. "They also proposed fusing a quantum simulator with a quantum computer, "a new concept to increase the versatility of quantum simulations; what we did was to create a mathematical framework that provides the simulators with access to a larger number of tasks."

Casanova explained the interest from the technological perspective of all these quantum simulators: "The whole pharmaceutical industry, the chemical and materials industry, and even the energy industry are seeking to design molecules that are more efficient for a specific function. Photovoltaic cells, for example, which we use to capture solar energy, only trap 20% of the energy that reaches them. So a molecule model that is more efficient in capturing solar energy would increase the

energy capture of these photovoltaic cells. To do this you need to be capable of designing molecules and knowing how they are going to behave.

"I reckon that within about 5 to 10 years we'll be able to design specific molecules for certain processes, like the capture of solar energy or even to design materials and drugs. Once we can understand complex systems, we will be able to predict their behaviour and design new technology based on that knowledge."

More information: M.-H. Yung, J. Casanova, A. Mezzacapo, J. McClean, L. Lamata, A. Aspuru-Guzik eta E. Solano. 2014. "From transistor to trapped-ion computers for quantum chemistry". *Scientific Reports* 4: 3589. DOI: 10.1038/srep03589.

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