A Brief Exploration on Quantum Simulation

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Abstract: With the development of quantum simulations, recent investigations provide an alternative way to explore the quantum world and a more advanced computational tool. A quantum system of many particles could be simulated by a quantum computer using several quantum bits similar to the number of particles in the original system. This paper aims to give a short history of quantum simulators by presenting the difference between AQS and DQS and introducing the three most popular quantum simulators. Though there are many difficulties to perform and control these quantum systems, scientists have already successfully simulated many crucial and complicated physics models with these simulators.

1. Introduction

Quantum simulators are presented as modern technology and methodology to study the quantum systems that are difficult to study in the laboratory or on a supercomputer. These quantum systems in physics, like low-temperature physics and multi-body problems, are vastly complex so that the current computers, including the supercomputers, are impossible to simulate the systems with as few as 30 particles. Quantum simulators can solve the problem with the idea to exploit the real controllable particles through the properties of superposition and entanglement. A quantum system of many particles could be simulated by a quantum computer using several quantum bits similar to the number of particles in the original system. In 2016, Google announced that it had simulated the hydrogen molecule and estimated its ground-state energy using a quantum computer built around tiny superconducting circuits. IBM did the same for lithium hydride and beryllium hydride in 2017. And earlier this year, ionQ, a startup company in College Park, Maryland, simulated water, the largest molecule to date, using a computer in which trapped ions served as the qubits. Now, with the development of this field, quantum simulators have been applied on several experimental platforms, including-ultracold quantum gases, polar molecules, trapped ions, photonic systems, quantum dots, and superconducting circuits. This paper aims to introduce those different systems.

2. Definition of Quantum Simulator

Many important problems in physics, especially low-temperature physics and multi-body physics, remain poorly understood because the underlying quantum mechanics is vastly complex. Conventional computers, including supercomputers, are inadequate for simulating quantum systems with as few as 30 particles. Quantum simulators are born to solve those systems by directly exploiting the quantum properties of real particles. These simulators create straight and clear realizations of the interested specific systems which allow precise realizations of their properties. Precise manipulation and broad tunability of parameters of the system allow the influence of various parameters to be cleanly disentangled. In particular, they exploit a property of quantum mechanics called superposition, wherein a quantum particle is made to be in two distinct states at the same time, for example, aligned and anti-aligned with an external magnetic field. Crucially, simulators also take advantage of a second quantum property called entanglement, allowing the behavior of even physically well-separated particles to be correlated. To conclude the different types of all quantum simulators, quantum simulation can be loosely defined as a simulation of a quantum system by quantum mechanical means.

This very general definition allows us to include two types of simulation: 1) digital quantum simulation (DQS), 2) analog quantum simulation (AQS) [15].

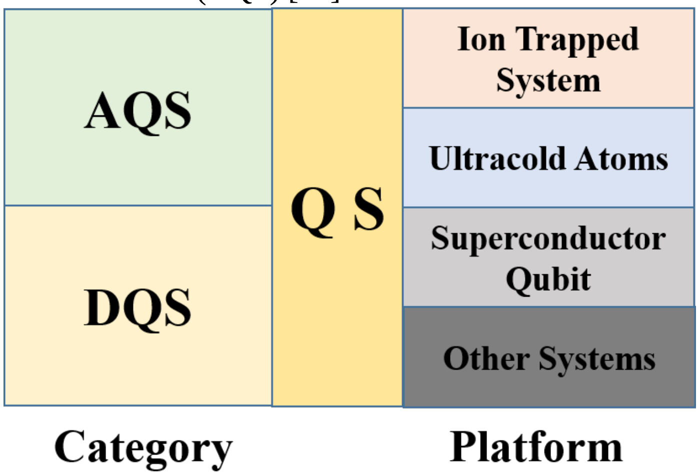

Figure 1 Categories and Platforms of quantum simulators.

The complicated many-qubit unitary transformation U is implemented through the application of a sequence of single-qubit and two-qubit gates. Such a circuit-based quantum simulation recreating the evolution through time is usually referred to as digital quantum simulation (DQS). In general, DQS consists of three steps: initial-state preparation, unitary evolution U, and the final measurement. Though DQS algorithms mainly depend on applying a time-ordered sequence of gates, thus implementing a unitary evolution of the simulator, DQS is not restricted to recreating the temporal evolution of the simulated system. Applications of DQS also include obtaining certain properties of a given quantum system e.g., phase estimation for computing eigenvalues of operators, particularly the Hamiltonian, or computing partition functions. In addition, it should also be possible to use quantum computers to simulate classical physics more efficiently.

Another approach to simulating quantum systems by quantum mechanical methods is an analog quantum simulation (AQS), in which one quantum system mimics another. The simulator may only partially reproduce the dynamics of the system. The choice of the mapping depends on what needs to be simulated and on the capabilities of the simulator. In AQS, one is usually emulating an effective many-body model of the simulated system. A controllable “toy model” of the system is used to reproduce the property of interest, e.g., the dynamics or ground state.

The main advantage of the DQS is its universality. In general, the goal of digital quantum simulation is to obtain $|\psi(t)\rangle = \exp(-i\hbar H_{sys}t)|\psi(0)\rangle$, the solution of the Schrödinger equation for the time-independent Hamiltonian, H_{sys}, which can be written as a sum of many local interactions. Theoretically, any finite-dimensional quantum system can be simulated through this method. Compare to DQS, for AQS, the Hamiltonian of the system to be simulated, H_{sys}, is mapped onto the Hamiltonian of the simulator, H_{sim}, which can be controlled to some extent. An important advantage of AQS is that it could be useful even in the presence of errors, up to a certain tolerance level. For example, when scientists are interested in knowing whether a certain set of physical conditions leads to a given quantum phase transition, even without having the full quantitative details, a qualitative answer can be quite valuable in this context. If the quantum simulator suffers from uncertainties in the control parameters, the phase transition understudy could still be observed, hence providing the answer to the question of interest. Finding the mapping in an AQS might, at first glance, look simpler than obtaining the most efficient gate decomposition for a given Hamiltonian in DQS. Sometimes the mapping is indeed straightforward, but this is not always the case, and quite often clever mappings have to be devised, sometimes involving additional externally applied fields or ancillary systems to mediate various interactions.

Many platforms could be used as quantum simulators, such as ion-trapped systems, ultracold quantum gases, Superconducting circuits, etc.

2.1 Ion Trapped System

Currently, in all quantum simulator models, an ion-trapped system forms one of the most ideal environments for simulating interactions of quantum spin models. A qubit is coherently manipulated by lasers or microwaves resonantly coupling the qubit states as described by the Hamiltonian

$$H_I = \hbar \frac{\Omega}{2}(\sigma^+ e^{i\phi} + \text{h.c.}) \quad (1)$$

where the Rabi frequency Ω is controlled by the intensity $\mathrm{I} = |\Omega|^2$ of the exciting field, ϕ is the phase of the field and $\sigma^{\pm}$ denote the atomic raising and lowering operators. In trapped-ion physics, a landmark was produced by the proposal for simulating the Dirac equation and Zitterbewegung in a single ion, which was subsequently succeeded in the laboratory. The trapped-ion simulator was built by a tiny, single-plane crystal of hundreds of beryllium ions, less than 1 millimeter in diameter, hovering inside a device called a Penning trap. The outermost electron of each ion acts as a tiny quantum magnet and is used as a qubit, the quantum equivalent of a '1' or a '0' in a conventional computer. In the benchmarking experiment, physicists used laser beams to cool the ions to near absolute zero. Carefully timed microwave and laser pulses then caused the qubits to interact, mimicking the quantum behavior of materials that otherwise are very difficult to study in the laboratory. Although the two systems may outwardly appear dissimilar, their behavior is engineered to be mathematically identical. In this way, simulators allow researchers to vary parameters that couldn't be changed in natural solids, such as atomic lattice spacing and geometry, to perform quantum activities [17].

In the history of the development of ion-trapped quantum simulators, Friedenauer et al., adiabatically manipulated 2 spins, showing their separation into ferromagnetic and antiferromagnetic states. Kim et al., extended the trapped ion quantum simulator to 3 spins, with global antiferromagnetic Ising interactions featuring frustration and showing the link between frustration and entanglement, and Islam et al., used adiabatic quantum simulation to demonstrate the sharpening of a phase transition between paramagnetic and ferromagnetic ordering as the number of spins increased from 2 to 9. Barreiro et al. created a digital quantum simulator of interacting spins with up to 5 trapped ions by coupling to an open reservoir and Lanyon et al. demonstrated digital quantum simulation with up to 6 ions. Islam, et al., demonstrated an adiabatic quantum simulation of the transverse Ising model with variable range interactions with up to 18 trapped-ion spins, showing control of the level of spin frustration by adjusting the antiferromagnetic interaction range. Britton, et al. from NIST has experimentally benchmarked Ising interactions in a system of hundreds of qubits for studies of quantum magnetism. Pagano, et al., reported a new cryogenic ion trapping system designed for long-time storage of large ion chains demonstrating coherent one and two-qubit operations for chains of up to 44 ions. Currently, scientists found microwave is an alternative method to optical spin-dependent forces for entanglement creation. As the momentum transferred by absorption or emission of free-space microwave photons is too small to be useful, magnetic-field gradients provide a means of creating spin-dependent potentials for exhibiting a differential Zeeman shift or driving sideband transitions. Experiments have demonstrated coupling between two internal states of an ion and its motion using either static or oscillating field gradients. The latter has been recently used for entangling a pair of ions by inducing correlated spin flips. Quantum simulations of spin systems based on forces generated by magnetic-field gradients would have much less stringent low-temperature requirements than their laser-based counterparts. To achieve substantial ion-ion couplings, large field gradients of about 10–100 T m−1 are required, which can be achieved in microfabricated ion traps with current-carrying structures near the ions [17,18].

2.2 Ultracold Quantum Gases System

Besides trapped ion systems, quantum simulation based on ultracold quantum gases is another hot topic in the field. Ultracold quantum gases offer a unique setting for quantum simulation of interacting many-body systems. The high degree of controllability, the novel detection possibilities, and the extreme physical parameter regimes that can be reached in these 'artificial solids' provide an exciting complementary set-up compared with natural condensed-matter systems, much in the spirit of Feynman's vision of a quantum simulator. A common thread for these experiments is the capability of realizing generic Hamiltonians. The main advantages of ultracold simulations include identifying low-temperature phases or tracking out-of-equilibrium dynamics for various models, problems that are theoretically or numerically intractable. Some experiments have realized condensed matter models in regimes that are difficult or impossible to realize with conventional materials, such as the Haldane model and the Harper-Hofstadter model.

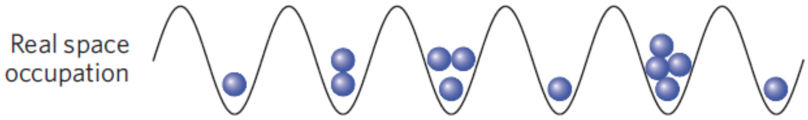

Figure 2 ultracold atoms in an optical lattice.

Recent years have seen tremendous scientific progress in the field of quantum simulations with ultracold atoms. Based on the idea of ultracold atoms, several models of quantum simulators were developed and can achieve several theoretical models, such as the Hubbard, Heisenberg, and Ising models, which are crucial in condensed matter physics. An optical lattice is one of the earliest systems utilized in the study of superfluid-to-insulator phase transition more than 20 years ago. An optical lattice — a periodic potential with the lattice spacing on the order of the laser wavelength — is a versatile tool to perform quantum simulations. Analogous to the lattice structure of solid-state systems, an optical lattice imprints a well-defined structure onto the atomic cloud and serves as the reference frame to define inter-atomic interactions; another convenient system is controlled interatomic interaction which mainly distinguishes between short-range and long-range interactions, such as the contact and the dipole-dipole interaction, and interactions intrinsic to the systems under study and dynamically controlled ones, such as magnetic moments and Feshbach resonances; since it is possible to change from a closed, equilibrated system to an open or nonequilibrium system in perturbing a quantum system, controlled perturbations can expand the range of accessible quantum simulation targets to go beyond the equilibrium properties in the ground states. Quantum gas microscopes have revolutionized our way of controlling and probing many-body systems, atom-by-atom, and with almost perfect control over the underlying potential. We believe that over the next years we will witness further improvements of cold atom-based quantum simulators; larger system sizes and longer coherent evolution times will enable even more complex quantum simulations [1, 19].

2.3 Superconducting Circuit System

The superconducting circuit is another successful platform of quantum simulations.

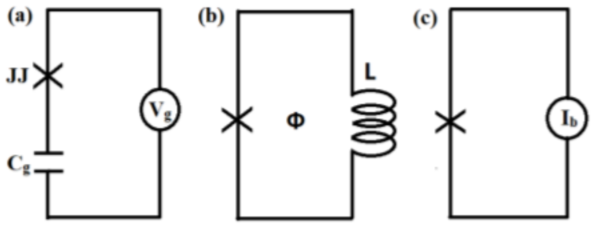

Figure 3 The structure of the superconducting qubit circuit. (a) The charge qubit is composed of a Josephson junction and a capacitor. Adjusting the voltage Vg can control the number of Cooper pairs. (b) Flux qubit. L is the loop inductance. Changing the bias flux ϕ can adjust the energy level structure of the qubit. (c) Phase qubit. Adjusting the bias current Ib can tilt the potential energy surface.

Superconducting qubits are solid-state electrical circuits. Compared with the qubits based on other quantum systems, superconducting qubits have advantages, like high designability, scalability, ease to a couple and easy to control, etc. These advantages make superconducting qubits become the leading candidate for scalable quantum computing. According to different degrees of freedom, superconducting qubits are mainly divided into three typical categories: charge qubits [1], flux qubits [2], and phase qubits [3] as shown in Figure 1. Based on the three superconducting qubit archetypes, many new types of superconducting qubits are derived, such as transmon-type qubits [4], C-shunt flux qubits [5], Fluxonium [6], 0-π qubit [7], hybrid qubit [8], and so on. Taking a single Xmon qubit as an example showing introduce how superconducting qubits are manipulated to implement quantum gate, we usually couple microwave sources to Xmon by capacitance. The microwave drive can be expressed as $\Omega(\mathrm{t}) = \Omega_x \cos(\omega_d t - \phi)$ and the driving Hamiltonian can be simply expressed as

$$\mathrm{H} = -\frac{\hbar}{2}\omega\sigma_z + \Omega_x \cos(\omega_d t - \phi)\sigma_x \tag{2}$$

where the first term is Xmon's Hamiltonian and the second term is drive term. After transforming the Hamiltonian into the rotating frame, we get

$$\mathrm{H} = -\frac{\hbar}{2}\Delta\sigma_z + \frac{\hbar}{2}\Omega_x(\cos\phi\sigma_x + \sin\phi\,\sigma_y) \tag{3}$$

where$\Delta = \omega - \omega_d$ is the detuning between qubit frequency and microwave frequency. When the qubit resonates with the microwave which means$\Delta = 0$, the first term will be removed, and the angle of the rotation axis in the XY –plane is determined by the phase ϕ of the microwave drive. Besides the single-qubit gate, two-qubit gates and muti-qubit gates can also be realized.

Quantum simulators using superconducting qubits fall into two main categories: The first one is called quantum annealers which determine ground states of certain Hamiltonians after an adiabatic ramp. This approach is sometimes also called adiabatic quantum computing. Secondly, many systems mimic specific Hamiltonians and study their ground state properties, quantum phase transitions, or time dynamics. The superconducting qubits are potential platforms to simulate different quantum models, such as the Bose-Hubbard model [9], spin model [10], quantum Rabi model [11], and Lipkin-Meshkov-Glick model [12] were also investigated. Despite the great advances that have been achieved, several challenges and open questions we are facing in both theoretical and experimental work. There is still the need to develop and implement higher quality superconducting qubits, such as improving the qubit connectivity, the gate fidelity, and coherence time, which are the key challenge for the development of superconducting quantum computing [2-8, 16].

2.4 Other Systems

Besides the above quantum platforms, there are many other platforms, such as the Rydberg quantum simulator and Jaynes-Cumming lattice model. Rydberg quantum simulator is based on laser-trapped circular Rydberg atoms, which is a flexible and broad paradigm for quantum simulation of spin 1/2 arrays. The long intrinsic lifetimes of Rydberg atoms, combined with the inhibition of their microwave spontaneous emission and their low sensitivity to collisions and photoionization, make trapping lifetimes in the minute range realistic with state-of-the-art techniques. Ultracold defect-free circular atom chains can be prepared by a variant of the evaporative cooling method, which also leads to the detection of arbitrary spin observables with single-site resolution. The proposed simulator realizes an XXZ spin-1/2 Hamiltonian with nearest-neighbor couplings ranging from a few to tens of kilohertz. All the model parameters can be dynamically controlled at will, making a large range of simulations possible. The system evolution can be changed with times in the range of seconds, long enough to be relevant for ground-state adiabatic preparation and for the study of thermalization, disorder, or Floquet time crystals. This platform already presents unrivaled features for quantum simulation of regular spin chains [13].

The Jaynes–Cummings (JC) model is a platform to study light-matter interaction, where a quantum two-level system is coupled to a cavity mode. The light-matter coupling in a Jaynes-Cummings model induces intrinsic nonlinearity in the energy spectrum, which can be mapped to an onsite repulsive interaction between polariton excitations. The complex competition between this interaction and polariton jumping between neighboring sites results in many-body problems in Jaynes-Cummings lattices, such as quantum or dissipative phase transitions and photon blockade effects [14].

3. Conclusion

With the progress of modern physics, many fundamental problems are still barely understood because of the complexity of quantum mechanics. The development of quantum simulations provides an alternative way to explore the quantum world and a more advanced computational tool. This paper aims to give a short history of quantum simulators by presenting the difference between AQS and DQS and introducing the 3 most popular quantum simulators (trapped-ions, ultracold atoms, and superconducting circuits). Though there are many difficulties to perform and control these quantum systems, scientists have already successfully simulated many crucial and complicated physics models with these simulators. We believe the quantum simulators will be utilized more in future research and play a more significant role in theoretical physics studies.

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