
Quantum Simulation

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Abstract

Quantum systems pose a computationally difficult problem for simulation. This difficulty can be minimized by utilizing controllable quantum systems to simulate the systems desired. These more efficient simulations can be implemented using simple analog systems with a similar behavior as the system desired or through a universal digital quantum computer. This paper gives an overview of methods of quantum simulation, potential and current applications, and recent implementations of quantum simulators.

1 Introduction

Under the classical laws proposed by Newton, if one had a sufficiently large computer and a snapshot of the universe, one could predict the future. In the early twentieth century, quantum mechanical theories determined that dream impossible. At the smallest scale currently known to humans, we see probabilistic interactions and behaviors rather than deterministic. This results in a computational problem - to simulate all the possible configurations of a system requires an exponential increase of resources for a larger system. Though classical approximations such as Monte Carlo exist for tractable systems, they don't cover the full breadth of possible physical interactions (Georgescu et al., 2014).

In 1981, Richard Feynman proposed a quantum approach to physical simulation - "Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws" (Feynman, 1982). This revolutionary idea imagines a system with the capacity to simulate physical systems with only a polynomial overhead, making large-scale (and extremely small scale) simulations a reality.

Quantum simulation provides a direct and achievable utility for quantum computers - significant systems can be made with fewer coherent operations and qubits than are required for complex algorithms such as Shor's algorithm. Quantum systems which have a natural decoherence can be modeled with qubits that display a similar decoherence, allowing potentially large-scale simulations of some systems before more precise technology is developed. Quantum simulators are also predicted to be more efficient than classical simulators for local interactions. A local system with interactions can utilize the entanglement of the quantum simulator while also posing a larger computational problem for a classical computer (Lloyd, 1996).

2 Evolution of Quantum Systems

When a quantum state, $|\Psi\rangle$, evolves over time we express the evolution with an operator called the Hamiltonian. The Hamiltonian, \mathcal{H} can represent the total energy of a system, and contains important information about the system and its progression. To find the state of a system $|\Psi\rangle$ at some time t for a time-independent Hamiltonian, we solve the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\Psi\rangle = \mathcal{H} |\Psi\rangle \quad (1)$$

to achieve the result $|\Psi(t)\rangle = e^{-i\hbar\mathcal{H}t} |\Psi(0)\rangle$. In this system, \mathcal{H} is a $2^N \times 2^N$ matrix if no approximation methods can simplify the system. The job of a simulator of this quantum system is to compute or map this equation and feed the result of the desired state to the user. Our goal is to create a system which evolves via some \mathcal{H}_{sim} containing a state $|\phi(0)\rangle$ that is preparable. This system should obey the analogous solution to the Schrödinger equation $|\phi(t)\rangle = e^{-i\hbar\mathcal{H}_{sim}t} |\phi(0)\rangle$. It should contain a state $|\phi(0)\rangle$ which is mappable to $|\Psi(0)\rangle$, the target initial state, and an output state $|\phi(t)\rangle$ which maps to the target output state $|\Psi(t)\rangle$ in a known manner (Georgescu et al., 2014). There are two primary methods to simulate this system on a quantum device: to map the system to a controllable analog or to discretize the system into a digital format.

3 Analog Quantum Simulation

Analog Quantum Simulation, or AQS, is the process of mimicking the Hamiltonian of a target system to a similar system the user has control over. This is the method proposed by Feynman (1982), to create “an exact simulation” where “the computer will do exactly the same as nature.” To do an analog simulation, we need to find a controllable system with a Hamiltonian \mathcal{H}_{sim} that directly maps to that of the target system \mathcal{H}_{sys} , that is, $\mathcal{H}_{sys} \leftrightarrow \mathcal{H}_{sim}$. The next step is to find an efficiently computable, inevitable conversion operator g such that a preparable initial state $|\phi(0)\rangle$ maps to and from our target initial state $|\psi(0)\rangle$ via $|\psi\rangle = g|\phi\rangle$ and $|\phi\rangle = g^{-1}|\psi\rangle$. It is a design challenge to find an appropriate mapping where $\mathcal{H}_{sys} = g^{-1}\mathcal{H}_{sim}g$ to a tolerable approximation error. However, if the physical simulator has less noise than the system to be simulated, it is feasible for an imperfect analog system to provide a tolerable representation of the target system (Georgescu et al., 2014).

3.1 Analog Applications

Analog quantum simulators have a variety of applications including quantum chemistry, solid state physics, high-energy physics, cosmology, and atomic physics (Georgescu et al., 2014).

Georgescu et al. (2014) discusses proposals for AQS implementations in multiple fields. Atoms in optical lattices and quantum dots can model a Hubbard Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{hop} + \mathcal{H}_{interaction} + \mathcal{H}_{pot} + \mathcal{H}_{internal} \quad (2)$$

where \mathcal{H}_{hop} describes the tunneling of atoms from one site to another on the lattice, $\mathcal{H}_{interaction}$ describes interactions between atoms, \mathcal{H}_{pot} encompasses all non-uniform potentials affecting the atoms, and $\mathcal{H}_{internal}$ describes the internal energies of atoms. The application of the Hubbard model allows simulations of quantum phase transitions, ring-exchange models, and quantum magnets. Trapped ions also can provide an AQS for the Ising model and spin systems, and quantum dots can map the Hamiltonian of bulk

superconductors (Georgescu et al., 2014).

On a much larger scale, cosmological phenomena can be mapped to controllable analog quantum systems. Georgescu et al. (2014) cites proposals to investigate fields within the curved space-time structure of an expanding universe, cosmological particle creation, and quantum field effects. AQS also may allow testing of unobserved, theoretical phenomena such as an Unruh-like effect, the Schwinger effect, and Hawking radiation. Recently, Kim (2019) proposed another use of trapped ions for cosmology. He drew a parallel between the Wheeler-DeWitt equation for the Friedmann-Robertson-Walker quantum universe and properties of a trapped ion system. Kim (2019) showed the Hamiltonian of the action of the Wheeler-DeWitt equation as

$$\mathcal{H}_{WDW} = \int d\alpha d\phi_1 d\phi_2 [\Pi^2 + \Psi^* (-\frac{\partial^2}{\partial\phi_1} - \frac{\partial^2}{\partial\phi_2} + e^{6\alpha}\mu^2(\phi_1^2 + \phi_2^2))\Psi - \Psi^* V_G(\alpha)\Psi] \quad (3)$$

and the Hamiltonian of the transverse component of a charged scalar field in a magnetic field in scalar quantum electrodynamics as

$$\mathcal{H}_\perp(t) = \int d^2\mathbf{x}_\perp [\pi_\perp^* \pi_\perp + \Psi_\perp^* (\mathbf{p}_\perp^2 + \omega_\perp^2(t)\mathbf{x}_\perp^2 - 2\omega_L(t)L_z)\Phi_\perp]. \quad (4)$$

These equations map with the following relations:

$$\mathbf{p}_\perp^2 \Leftrightarrow \nabla_\perp^2 \Leftrightarrow \frac{\partial^2}{\partial\phi_1} + \frac{\partial^2}{\partial\phi_2}, \quad \omega_L(t) \Leftrightarrow e^{3\alpha}\mu, \quad m^2 + k_z^2 \Leftrightarrow -V_G(\alpha) \quad (5)$$

with a difference due to L_z reduced after further expansion of the functions. He concludes that appropriate manipulations of a trapped ion system can simulate current cosmological theories, opening a “new window for quantum simulation of the universe” (Kim, 2019).

Analog quantum simulators show promise in quantum chemistry. A proposition in 2007 shows a mapping between coupled semiconductor dots and molecules. According to Smirnov et al. (2007), the varying coupling strengths of the dots can emulate ionic and covalent bonds. This can allow accurate artificial atoms and their bonds, and simulate atomic and molecular interaction. The bonds between atoms can be manipulated via changes in the gates’ potentials, allowing the system to be controllable.

Electrons in the quantum dots' shells can emulate valence electrons, allowing dots to act as various atoms. The first two shell levels can hold 2 and 4 electrons, respectively, emulating s and p orbitals. As an example, one electron in the dot's shell can act as a hydrogen atom, and four electrons can emulate oxygen (the bottom shell is full and the outer shell has two vacancies). To create a water molecule, two one-electron dots and a four-electron dot can be coupled. Larger artificial chemical reactions are possible and controllable with tools such as magnetic fields, allowing difficult-to-create reactions. An additional benefit is the controllability of the speed of the reaction via the potentials and fields. Smirnov et al. (2007) shows the molecular Hamiltonian in the second-quantized form:

$$\mathcal{H} = \sum_{pq} \langle p | \mathcal{H}_0 | q \rangle a_p^\dagger a_q - \frac{1}{2} \sum_{pqrs} \langle pq | V_e | rs \rangle a_p^\dagger a_q^\dagger a_r a_s \quad (6)$$

where a_p^\dagger, a_p are Fermi operators responsible for the creation and annihilation respectively of an electron in a single-particle orbital, $|pq\rangle$ is a two-electron state, \mathcal{H}_0 is the single-particle Hamiltonian with kinetic and nuclear attraction operators, and V_e is a repulsion term. They go on to simplify the Hamiltonian into an invariant component, \mathcal{H}_0 , and a reaction component, $\lambda(t)V$:

$$\mathcal{H} = \mathcal{H}_0 + \lambda(t)V \quad (7)$$

They map the molecular Hamiltonian of a three-hydrogen system ($H + H_2 \rightarrow H_2 + H$) to quantum dots, with a component containing on Zeeman energies, \mathcal{H}_{3D} , a component containing inter-dot and intra-dot energies, \mathcal{H}_C , and a tunneling component \mathcal{H}_{tun} :

$$\mathcal{H} = \mathcal{H}_{3D} + \mathcal{H}_C + \mathcal{H}_{tun} \quad (8)$$

$$\mathcal{H}_{3D} = \sum_{S=1,2} (E_{AS}N_{AS} + E_{BS}N_{BS} + E_{CS}N_{CS})$$

$$\mathcal{H}_C = U_A N_{A1} N_{A2} + U_B N_{B1} N_{B2} + U_C N_{C1} N_{C2} + U_{AB} N_A N_B + U_{BC} N_B N_C + U_{AC} N_A N_C$$

$$\mathcal{H}_{tun} = - \sum_{S=1,2} (\Delta_{AB} a_{AS}^\dagger a_{BS} + \Delta_{BC} a_{BS}^\dagger a_{CS} + \Delta_{AC} a_{AS}^\dagger a_{CS} + h.c.)$$

In these equations, S represents the spin - 1 for up, 2 for down - of electrons. $A, B,$ and C are the dot indices, and $N_{A,B,C}$ is the population of the dot or component of the dot with the appropriate spin. $E_{A,B,C}$ are the Zeeman energies of the dots, and U_A, U_{AB} are intra-dot and inter-dot energies, respectively. The researchers found that varying the speed and initial state of the simulation allowed for outputs in different energy states. The ground state of the system is all three atoms holding one electron, and an excited state contains a bond between two atoms (or dots). A slow, adiabatic progression of the system resulted in output states at or close to the ground state, and very fast sweeps resulted in a high probability ($\sim 90\%$) of covalent bond between dots A and B. Smirnov et al. (2007) was also able to restore the system to continue using the Hamiltonian and achieve bonds between different atoms by sweeping the system at a varying, selective speed.

4 Digital Quantum Simulation

Digital quantum simulation (DQS) uses a series of discrete gates to transform a set of qubits to achieve the same result as the target Hamiltonian. Each gate can be represented as a unitary transformation, and the final Hamiltonian is created via performing the unitary transformations on the target state in series.

To perform a digital quantum simulation, one first maps the target initial state to a superposition of binary bit strings. Next, the target Hamiltonian is decomposed into a series of fundamental gates including rotations of the qubit about the Bloch sphere, Pauli gates, controlled-not gates, and even Toffoli 3-qubit gates. This process uses the Suzuki-Trotter expansion. To obtain an approximation, the Hamiltonian is broken down into components, cast into its unitary form, and decomposed into simpler unitaries.

$$\mathcal{H} = \sum_i a_i O_i \Rightarrow U(t) = \exp\left(-i \sum_j a_j O_j t\right) \quad (9)$$

leads to the decomposition of the unitary:

$$U(t) = \exp\left(-i \sum_j a_j O_j t\right) = \lim_{n \rightarrow \infty} \left(\prod_j \left(1 - \frac{i \mathcal{H}_j t}{n}\right)^n\right) \quad (10)$$

$$\approx \prod_j \exp\left(\frac{-i \mathcal{H}_j t}{n}\right) \quad (11)$$

The final product of exponentials is simply the progression of a quantum system via gates and can approximate the desired quantum system. After this decomposition is complete, the initial state and gates can be fed into a universal quantum computer to obtain the desired result (Georgescu et al., 2014).

With a digital simulation, accuracy comes at the cost of speed. According to the Solovay-Kitaev theorem, the decomposition of the unitary formed by the Hamiltonian can be performed to a desired precision, though higher accuracy requires a greater number of gates. An approximation of the desired Hamiltonian with error 2^{-d} is obtainable with some polynomial function $p(d)$, demonstrating a greater efficiency for quantum simulations over classical simulations. However, like their analog counterpart, digital quantum simulators may have their limits. Some theoretical Hamiltonians which have no physical realizations are likely not efficiently implementable. However, it is predicted that all physically possible quantum systems can be efficiently decomposed (Rieffel and Polak, 2011).

Digital quantum simulators show their difference from analog quantum simulators in the area of error correction. Digital systems can utilize a variety of error correction codes including rudimentary bit flip codes, Shor's qubit codes, and the Steane code. If/once a fault-tolerant universal quantum computer is created, many simulations can simply be run without needing to create a device specific to the simulation.

4.1 Digital Applications

Much like analog quantum simulators, digital quantum simulators have applications in a variety of physical sciences. DQS is predicted to be able to simulate bulk semiconductors, molecular systems, and quantum statistical models such as the Ising model. DQS also has

the potential to predict properties of superconductors along with many cross-discipline models (Georgescu et al., 2014).

Many applications of quantum simulation that work with analog systems can be decomposed into gates and simulated on a DQS. The Fermi-Hubbard Hamiltonian,

$$\begin{aligned} \mathcal{H}_H = & - \sum_{(i,j);\sigma} [t_x(a_{(i,j);\sigma}^\dagger a_{(i+1,j);\sigma} + a_{(i+1,j);\sigma}^\dagger a_{(i,j);\sigma}) \\ & + t_y(a_{(i,j);\sigma}^\dagger a_{(i,j+1);\sigma} + a_{(i,j+1);\sigma}^\dagger a_{(i,j);\sigma})] \\ & + \tilde{U} \sum_{(i,j)} n_{(i,j);\uparrow} n_{(i,j);\downarrow} \end{aligned} \quad (12)$$

has been decomposed into quantum gates. In this equation, \tilde{U} represents the on-site repulsion potential energy and t_x and t_y are the hopping matrix elements which allow fermions to move about the lattice. DQS implementations have also been analyzed for the Holstein model, spin lattice Hamiltonians, the Fano-Anderson Hamiltonian to represent disordered systems, spin glass models, and BCS pairing in superconductors. In 2006, the BCS pairing Hamiltonian was implemented,

$$\mathcal{H}_{BCS} = \sum_{m=1}^N \frac{\epsilon_m}{2} (n_m^F + n_0^F m) + \sum_{m,l=1}^N V_{ml}^+ c_m^\dagger c_{-m}^\dagger c_{-l} c_l \quad (13)$$

where c_m^\dagger, c_m are fermionic creation and annihilation operators, m represents quantum numbers, $n_m^F = c_m^\dagger c_m$ is the number operator, and V_{ml}^+ is the matrix element $\langle m, -m | V | l, -l \rangle$.

A two-qubit demonstration of the DQS algorithm for this Hamiltonian was constructed on a nuclear magnetic resonance quantum computer (Georgescu et al., 2014).

A recent study, Hempel et al. (2018), utilized a digital quantum simulator based on trapped ions to calculate the ground-state energies of molecules. The researchers used the variational quantum eigensolver algorithm for molecular hydrogen and lithium hydride. They took the Hamiltonian of a collection of nuclear charges Z_i where the positions of nuclei are R_i , the positions of electrons are r_i , and the masses are denoted M_i :

$$\mathcal{H}_1 = - \sum_i \frac{\nabla_{R_i}^2}{2M_i} - \sum_i \frac{\nabla_{r_i}^2}{2} - \sum_{i,j} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \left(\frac{Z_i Z_j}{|R_i - R_j|} + \frac{1}{|r_i - r_j|} \right) \quad (14)$$

which is the first-quantized formulation of quantum chemistry in atomic units ($\hbar = 1$). Hempel et al. (2018) then used the second-quantized formulation (equation 2), but decomposed the formulation differently:

$$\mathcal{H}_2 = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \quad (15)$$

They then decomposed h_{pq} and h_{pqrs} to encode the electron's spatial and spin coordinates as $\sigma_i = (r_i, s_i)$:

$$h_{pq} = \int d\sigma \phi_p^*(\sigma) \left(\frac{\nabla_r^2}{2} - \sum_i \frac{Z_i}{|R_i - r|} \right) \phi_q(\sigma) \quad (16)$$

$$h_{pqrs} = \int d\sigma_1 d\sigma_2 \frac{\phi_p^*(\sigma_1) \phi_q^*(\sigma_2) \phi_s(\sigma_1) \phi_r(\sigma_2)}{|r_1 - r_2|} \quad (17)$$

To translate the Hamiltonian into its implementation on trapped ions, the researchers used the Bravyi-Kitaev transformation to map the fermionic Hamiltonians of the electrons onto the spin Hamiltonians of the ions. For molecular hydrogen (H_2), after the Bravyi-Kitaev transformation, the team obtained the effective Hamiltonian:

$$\mathcal{H}^{BK} = c_0(I) + c_1 \sigma_0^z + c_2 \sigma_1^z + c_3 \sigma_0^z \sigma_1^z + c_4 \sigma_0^x \sigma_1^x + c_5 \sigma_0^y \sigma_1^y \quad (18)$$

for two qubits. The team then ran the variational quantum eigensolver algorithm at various internuclear separations with randomly generated initial ansätze. They measured the expectation values corresponding to the terms in the Hamiltonian and simplified the results on a classical computer using the Nelder-Mead simplex algorithm. They then passed the intermediate unitary coupled-cluster ansätze back into the VQE algorithm and checked that the convergences of the quantum simulations matched those of simultaneously performed classical simulations. The gates showed a 99(3)% fidelity and the team found a convergence within their 1σ confidence band.

The next step of the experiment was to up the complexity. Hempel et al. (2018) moved to simulate the ground-state energy of lithium hydride (LiH). Unlike previous experiments which used four qubits, the team worked to implement the simulation using

three ion qubits. The researchers approximated the system by finding an active space of two electrons in three spacial orbits to average out the electrons thought to be involved only weakly in the bond. After a further simplification using classical configuration interaction singles and doubles (CISD), only dominant singlet excitations were simulated. After the classical simplifications, they used the Bravyi-Kitaev transformation to obtain the final operator:

$$U_{UCCSD}^{BK}(\alpha, \beta) = e^{-i\alpha\sigma_2^x\sigma_4^y} \cdot e^{-i\beta\sigma_2^x\sigma_6^y} \quad (19)$$

The team then ran a projective measurement over values of α and β and implemented the VQE algorithm on a set of internuclear separations. Their run of the VQE algorithm utilized a hybrid classical algorithm between quantum steps which incorporated simulated annealing. Their final results predicted that the simulation should be run and measured over 14,000 times to achieve a result within chemical accuracy. As expected, the more complex simulation had a greater runtime. Their study shows some of the current applications and technological bounds of digital quantum simulation, and suggests future use in more complex simulations that classical computers cannot efficiently compute.

Even more recently another team of researchers (Nam et al., 2019) used a generic VQE approach to compute the ground-state energy of the water molecule. This paper boasts computational errors approaching chemical accuracy, projecting future computations “reaching beyond the capability of classical methods.” Similar to the previous experiment, the group used the second-quantized Hamiltonian representation of the molecule. The group also used classical methods to generate an initial unitary coupled-cluster ansatz state and the expectation value of the Hamiltonian. The VQE algorithm was run repeatedly to improve the ansatz, reaching the full configuration-interaction result within chemical accuracy after 17 terms were included in the ansatz. The simulation used 11 qubits using 143 entangling gates. The team utilized properties of their quantum computer (the IonQ trapped-ion quantum computer) to optimize gates and used classical techniques to estimate uncertainties (Nam et al., 2019).

The recent studies of DQS using trapped ion universal quantum computers show the promise of quantum simulation. Even in the noisy intermediate-scale quantum (NISQ)

device era, computations approaching useful accuracy are possible for simple molecules. As scaling and precision improve on quantum devices, currently unfeasible simulations may be possible and accessible.

5 Conclusion

The theoretical potential of quantum simulation forecasts a greater ability to model and understand the world. Recent experimental results in the NISQ era show quantum simulations approaching the accuracy of current classical methods, giving an indication of future potential. Current quantum machines suffer from large amounts of noise and low scale, but engineering improvements are rapidly progressing the size and precision of quantum computers and simulators.

Recently, many quantum algorithms are seeing quantum-inspired classical algorithms that approach and even match the quantum algorithms' efficiency, challenging the perceived quantum supremacy (Tang, 2018). Many classical quantum approximations have been made for quantum simulations, though it is predicted that some quantum systems will remain exponentially complex to fully characterize and compute (Georgescu et al., 2014), and Feynman (1982) conjectured that the simulation of the full time evolution of an arbitrary quantum system is intractable for classical computers. Even if the notion of quantum supremacy is disproven, many algorithms approaching the efficiency of those of quantum computers are inspired by quantum algorithms and quantum effects.

The improvement of quantum simulation will likely lead to breakthroughs in the physical sciences, enabling researchers to simulate systems that are impractical or impossible to measure in the real world. In the near future, simulations with only tens of qubits have the potential to surpass the current limits of classical simulations, providing a new tool for testing physical theories and predicting physical systems to push the limits of scientific knowledge.

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