

# Quantum Simulators

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This paper presents some of the main ideas of the theory, implementations and applications of quantum simulators. The paper is based on references [1] and [3], and reports their results. I start by a quick description of Feynman's ideas and speculations about simulating physics with computers and then move on to the concrete description of a universal quantum simulator, both in theory and in practice, based on [3]. Finally, I give a short example of the kind of simulations possible with the physical systems described.

## 1. INTRODUCTION

In a talk he gave at the California Institute of Technology in May 1981, Richard Feynman addressed the issue of simulating physical systems with computers ([1]). The realization that quantum physics can not be simulated efficiently (in a reasonable amount of time and memory) by classical, digital computers led him to the suggestion of a new kind of computer that would behave quantum mechanically by itself, and thus might be able to simulate quantum mechanical systems efficiently. He then suggested investigating which quantum systems are inter-simulatable (i.e. systems that behave identically, so one can simulate the other) and in particular, he conjectured that there might be a class of quantum systems that can serve as *universal quantum simulators*, which can simulate any (or almost any) other quantum system. He also “guessed” that a system of two-state microsystems could serve as such a universal quantum simulator, but left the problem to be worked out by others (he already had his Nobel prize).

In 1996, Lloyd showed that Feynman was right ([2]). He showed that quantum computers can simulate, to any given accuracy, any system governed by local interactions in a time that is proportional to the simulated time and using a number of qubits that is proportional to the number of variables of the system. In 2003, a paper by E. Jané, G. Vidal, W. Dür, P. Zoller and J. I. Cirac, [3], showed how such a universal quantum simulator can be achieved in practice. They described the use of two quantum optical systems to simulate quantum dynamics. Their first suggestion consists of neutral atoms in an optical lattice and the second consists of ions in an array of micro-traps.

In this paper, I will give a quick overview of Feynman's motivation for a quantum simulator and then move on to describe the arguments from the last paper I mentioned ([3]). I will summarize how a quantum simulator that is based on two level systems, qubits, can simulate any given system. Then, I will describe how this is done according to the first suggested scheme of atoms stored in an optical lattice. Finally, I will briefly describe how the Ising and Heisenberg models can be simulated by such a system.

## 2. MOTIVATION

As explained by Feynman ([1]), since we do not know everything about physics (if we did, we would not need to “pay any attention to computers”), exploring the possibilities of simulating physics on a computer can teach us about the characteristics of our physical theories and also about the possibilities of computers. The latter idea was proven to be right with the new field of quantum computing and quantum information. This field redefined the theoretical possibilities in computers (that is, of course, if a quantum computer can ever be built). So, the question of how to simulate physics on a computer, just by itself could lead to new interesting ideas. In addition, of course, by simulating certain systems and tracking their dynamics we can understand the different mechanisms that are in action to a greater extent, which in turn can lead to new discoveries.

Feynman explores what the requirements for a good simulation of a physical system are and what we would have to assume about physics in order to be able to simulate it exactly. For example, we would have to assume that time is discrete, which is not a problem for Feynman since “we don't have infinite accuracy in physical measurements so time might be discrete on a scale of less than  $10^{-27}$  sec” ([3]). However, the most important point for our purpose is to see how Feynman shows that classical computers cannot simulate quantum systems using resources (space and time) that do not grow exponentially with the space-time volume taken by the simulated system.

Since we want to simulate quantum mechanical systems, we only have the ability to predict probabilities. There are two ways to simulate probabilities according to Feynman. The first, is to calculate the probability of each outcome and interpret this number to represent nature. The second, is to use a computer which is itself probabilistic, that is, the probability that the computer will give each outcome is the same as the probability that the simulated system would give this outcome. There are two major problems with the first approach. The first problem is that if we calculate probabilities we would have to discretize them. If we have  $k$  digits to represent the probability, then if the probability of some event is less

than  $2^{-k}$ , this event will never happen according to the simulation! This might still be ok in practice if we make  $k$  very big. The other problem, however, is more severe. If there are  $N$  particles and  $M$  states that each particle can be in (could be position states for example), then there are  $M^N$  configurations for the system. At any time  $t$  we would need a  $k$  digit number for every configuration and that requires too much memory. For example, if we have 50 spin-1/2 particles, we would need  $2^{50}$   $k$ -digit numbers to record the state of the system. Moreover, to calculate the time evolution of such a system will require to exponentiate a  $2^{50} \times 2^{50}$  matrix. Thus, this strategy won't work. The other option is to use a probabilistic computer as described above. Feynman shows that quantum phenomena cannot be imitated by a classical probabilistic computer. By considering photon polarization, he essentially shows that quantum phenomena violates Bell's inequality. The argument is given in note [6].

After showing that a simulation of quantum systems can not be done by classical computers, we turn to the option of quantum simulators.

### 3. A UNIVERSAL QUANTUM SIMULATOR

A Universal Quantum Simulator, UQS, is a device that operates at the quantum level and that is able to simulate any quantum system that evolves under local interactions. Locality of the interactions implies that the total multi-particle Hamiltonian, can be written in the form

$$H_N = \sum_i H_i \quad (1)$$

Where each  $H_i$  is a Hamiltonian that involves only a few neighboring particles. This assumption is essential for an efficient simulation by a quantum computer as explained by Lloyd [2]. Some other systems that involve non-local interactions could also be described by this form of a Hamiltonian and could, therefore, be simulated efficiently as well. The requirement of local interactions, however, happens to be true in most cases (examples for such systems are van der Waals gases, Ising and Heisenberg spin systems and strong and weak interactions).

The idea in [3] is to use either neutral atoms in an optical lattice, or ions in an array of micro traps. In both cases the basic variables on which the manipulations are done are two level quantum systems, Qubits. Fast, single-qubit, unitary operations are done on single qubits using a laser beam. Also, by conditionally displacing the atoms (or ions) in space, some "raw" interaction between neighboring qubits is achieved. Then, by alternating this 2-qubit, raw interaction with the unitary, single-qubit operations in a way that will be described below, we can make the system evolve according to an effective Hamiltonian that we want to simulate. Although in theory a UQS can simulate any system that is described by local

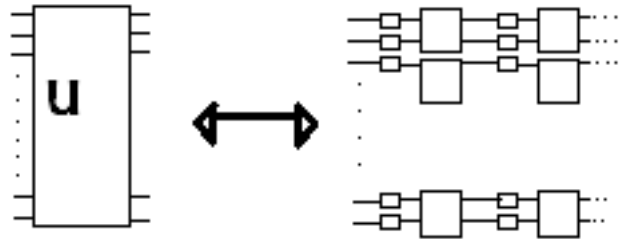


FIG. 1: We can simulate N-qubit evolution  $U = e^{-iH_N t}$  by alternating evolutions according to  $H_0^{(ab)}$  (represented by the bigger boxes) and single-qubit operations (represented by the small boxes)

interactions, in practice there are technological limitations. The above proposal, as explained in [3], can best be used to simulate systems of two level microsystems that have a Hamiltonian of the form

$$H_N = \sum_a H^{(a)} + \sum_{a \neq b} H^{(ab)} \quad (2)$$

(sum of single-qubit terms,  $H^{(a)}$ , and 2-qubit terms,  $H^{(ab)}$ ). Thus, we consider systems of this type and we want to see how we can produce the required Hamiltonian.

For any Hamiltonian of the form  $H = \sum_{i=1}^s H_i$  we can write

$$e^{-iHt} = \lim_{n \rightarrow \infty} (e^{-iH_1/n} e^{-iH_2/n} \dots e^{-iH_s/n})^n \quad (3)$$

Therefore, if we have a system that is composed of  $N$  two level microsystems that evolves according to the Hamiltonian (2), we can simulate it by applying short 2-qubit and single-qubit evolutions (that are produced by the 2-qubit and single-qubit Hamiltonians  $H^{(ab)}$  and  $H^{(a)}$ ) successively and in the right order to our qubits. Now, all the single-qubit evolutions can be achieved directly, by shining a laser on the atoms (or ions). The 2-qubit evolutions are a bit more tricky so let's see how to produce them. The idea is that we have some available 2-qubit interaction,  $H_0^{(ab)}$ , and we can produce the required interaction,  $H^{(ab)}$ , by alternating  $H_0^{(ab)}$  with single-qubit, unitary transformations (that we assume we can perform much faster compared with the interaction times of  $H_0^{(ab)}$ ). The evolution we get is

$$U(t) = \prod_{i=1}^n V_i \exp(-iH_0^{(ab)} t_i) V_i^\dagger = \prod_{i=1}^n \exp(-iV_i H_0^{(ab)} V_i^\dagger t_i) \quad (4)$$

Here  $t = \sum t_i$  is the total time and  $V_i = v_i^{(a)} \otimes u_i^{(b)}$ , where  $u_i$  and  $v_i$  are single-qubit, unitary transformations.

Then, we assume  $-I \ll tH_0^{(ab)} \ll I$  so we can approximate the exponentials to get

$$U(t) \simeq I - it \sum_{i=1}^n p_i V_i H_0^{(ab)} V_i^\dagger + O(t^2) \quad (5)$$

with  $p_i = t_i/t$ . This means that our two qubits will evolve according to the effective Hamiltonian

$$H_{eff}^{(ab)} = \sum_{i=1}^n p_i V_i H_0^{(ab)} V_i^\dagger + O(t) \quad (6)$$

for a time  $t$ . To simulate  $H_{eff}^{(ab)}$  for longer times, we can apply several gates of the form  $U(t)$ .

After describing this procedure, the authors of [3] discuss the *time cost* and the *control complexity* (the number of required control operations per unit time of simulation) of such a simulation. They conclude that the simulation time,  $T$ , is proportional to the simulated time,  $T'$ , and that the control complexity grows linearly with  $T'$ . They also consider how these parameters depend on the size of the system,  $N$ . It turns out that if a parallel manipulation of all  $N$  qubits is available, the time cost does not depend on  $N$  and the control complexity grows linearly in  $N$ .

Next, the authors of [3] move on to describe what kinds of 2-qubits Hamiltonians can be simulated by

$$H_0^{(ab)} = \gamma \sigma_z \otimes \sigma_z \quad (7)$$

with real  $\gamma$ , and by fast, unitary, single-qubit operations. The classes of Hamiltonians that could be simulated depend on the degree of independence of  $u_i$  and  $v_i$  in the operation  $V_i = v_i^{(a)} \otimes u_i^{(b)}$  above. This independence, in turn, depends on how well we can address each qubit separately (with the laser). Using references [4] and [5], they state the results for two extreme cases. The first case, is the perfectly homogeneous manipulation in which the laser affects all the qubits and in the same way so  $u = v$ . The second case, is the perfectly inhomogeneous manipulation in which the laser can be focused only on one qubit, and  $u$  and  $v$  are arbitrary.

For the homogeneous case it turns out ([3],[4]) that by using the above strategy, it is possible to simulate any 2-qubit Hamiltonian that is symmetric under the exchange of qubits,

$$H = \sum_{i,j=x,y,z} M_{ij} \sigma_i \otimes \sigma_j, M_{ij} = M_{ji} \quad (8)$$

and with the additional condition that the sign of  $\gamma$  coincides with the signs of all non-vanishing eigenvalues of  $M$ . For the inhomogeneous case, it turns out that any 2-qubit Hamiltonian

$$H = \sum_{i,j=x,y,z} M_{ij} \sigma_i \otimes \sigma_j \quad (9)$$

can be simulated by the above scheme.

## 4. IMPLEMENTATION

As mentioned above, [3] describes two different schemes to implement the UQS. The first, consists of neutral atoms in an optical lattice and the second, of ions in an array of micro-traps. Both schemes are based on qubits and are described by spin-1/2 algebra, which make them suitable for the above simulation technique. In both schemes the single-qubit, unitary operations are achieved by directly shining a laser on the qubits. Finally, in both schemes the 2-qubit interactions are achieved by conditionally displacing the qubits. The difference between the schemes, however, is that in the first scheme, according to present experiments, only *homogeneous*, single-qubit operation can be performed, while in the second scheme we can perform *inhomogeneous*, single-qubit operations that act on individual ions. This limits the first scheme. However, the high level of parallelism in the qubits manipulation in this scheme makes it very suitable in some cases, such as for simulating some spin models. Also, as mentioned in [3], the first scheme seems very feasible with current technology. Here I describe how the first scheme is implemented according to [3].

We have 2 identical, one-dimensional, optical lattices with period  $d$  that are homogeneously filled with  $N$  atoms (one per lattice site). The atoms have internal states  $|0\rangle$  and  $|1\rangle$ . The lattices are designed such that one lattice traps the atoms when their internal state is  $|0\rangle$ , and the other lattice traps the atoms when their internal state is  $|1\rangle$ . The atoms are all in their vibrational ground state (Bose Einstein Condensate) and can be brought into internal state  $|0\rangle$  by optical pumping. To measure (or read out) the qubits we measure the phosphorescence of the atoms as a result of a laser. As mentioned above, the single-qubit, unitary operations are done by shining a laser on the atoms. Thus, we are left with figuring out how to create some raw, 2-qubit interaction,  $H_0^{(ab)}$ .

To create the optical lattice, two interfering laser beams are superimposed, which creates a standing wave. The two lattices can be displaced relative to each other by tuning the phases of the laser beams. This causes the atoms to displace conditionally to their internal state (We do this process adiabatically so the atoms will stay in their vibrational ground state). If we choose the displacement to be one lattice period,  $d$ , we cause the  $|1\rangle$  component of atom  $a$  to interact (collide) with the  $|0\rangle$  component of atom  $a + 1$ . Finally, the lattices are displaced back to their previous position. Figure 2, which is taken from [3], illustrates the process. This interaction between the  $|1\rangle$  component of atom  $a$  and the  $|0\rangle$  component of atom  $a + 1$  causes a phase shift in the  $|1\rangle_a |0\rangle_{a+1}$  component of the total wave function of the two qubits at positions  $a$  and  $a + 1$ . The phase shift gives a non-local

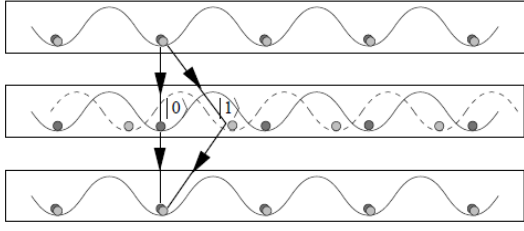


FIG. 2: In the first step, the two lattices overlap. The  $|0\rangle$  components are represented by dark balls and the  $|1\rangle$  components by light balls. In the second step the lattice that traps the  $|1\rangle$  components is displaced so the  $|1\rangle$  component of atom  $a$  move toward the  $|0\rangle$  component of the  $a + 1$  atom. After the interaction, in the third step, the lattices move back to the initial position

evolution according to the interaction Hamiltonian

$$H_1 = \sum_a \sigma_z^{(a)} \otimes \sigma_z^{(a+1)} \quad (10)$$

There are actually some other phases that are introduced by this process, but these are described by local Hamiltonians of the form  $\sum_a \sigma_z^{(a)}$  and can be removed by our local unitary operations to get the evolution

$$U_1 = e^{-i\theta_1 H_1} = \prod \exp(-i\theta_1 \sigma_z^{(a)} \otimes \sigma_z^{(a+1)}) \quad (11)$$

where  $\theta_1$  can be adjusted by adjusting the interaction (collision) time. By using this evolution and the unitary single-qubit operations in the way described above, we can simulate first neighbor interactions. If we displace the lattices  $k$  periods instead of one, the same argument shows that we can simulate  $k^{th}$  neighbor interactions. Also, this procedure works in 2D and 3D in the same way, by displacing the lattices in different directions.

## 5. EXAMPLE: ISING AND HEISENBERG SPIN MODELS

The Ising spin model consists of an array of spins that interact with their first neighbors only. If two neighboring spins are aligned in the same direction, they have energy  $J/2$ . If they are anti-aligned, meaning point in opposite directions, they have energy  $-J/2$ .  $J$  can be positive, negative or zero corresponding to ferromagnetism, antiferromagnetism and noninteracting spins, respectively. Thus, the energy of the system can be written as

$$E = \sum_{\langle a,b \rangle} \frac{J}{2} S_a S_b \quad (12)$$

where  $S_a$  and  $S_b$  are 1 for spin up and  $-1$  for spin down,  $a$  and  $b$  label the different spins, and the  $\langle, \rangle$  symbol indicates that the sum includes only neighboring spins  $a$  and

$b$ . Therefore we can write the Hamiltonian as

$$H_I = -\frac{J}{2} \sum_{\langle a,b \rangle} \sigma_z^{(a)} \otimes \sigma_z^{(b)} \quad (13)$$

Simulating this Hamiltonian is a trivial task for the scheme of the neutral atoms in an optical lattice. Since  $H_I$  includes only first neighbor interactions, to achieve it we simply use  $H_1$  from above together with single-qubit unitary operations in the way described in section 3. For the trapped ions scheme, achieving this simulation is also not particularly hard, as described in [3].

The Heisenberg model replaces the simple Hamiltonian (13) with the more complicated one

$$H_H = -\frac{J}{2} \sum_{\langle a,b \rangle} (\sigma_x^{(a)} \otimes \sigma_x^{(b)} + \sigma_y^{(a)} \otimes \sigma_y^{(b)} + \sigma_z^{(a)} \otimes \sigma_z^{(b)}) \quad (14)$$

It turns out ([3]) that this Hamiltonian can be simulated by the technique described in section 3 and in Eq. (6), using the Ising Hamiltonian that we just discussed,  $H_I$ , as the raw Hamiltonian,  $H_0^{(ab)}$ , and using the homogeneous operations

$$\begin{aligned} p_1 &= 1/3, V_1 = I^{\otimes N} \\ p_2 &= 1/3, V_2 = \left( \frac{I - i\sigma_x}{\sqrt{2}} \right) \otimes N \\ p_3 &= 1/3, V_3 = \left( \frac{I - i\sigma_y}{\sqrt{2}} \right) \otimes N \end{aligned}$$

## 6. CONCLUSION

As far away as we are from actually being able to perform real calculation on a quantum computer, the enormous efforts in this field are already beginning to yield fruits. The ability to simulate quantum mechanical systems seems feasible with current technology and might begin to serve as a research tool for studying these systems in the near future (for example, as mentioned in [3], the Quantum Hall Effect can be studied using the Heisenberg model). Furthermore, designing a quantum simulator of the type described above can lead to developments in the design of a quantum computer in the future. In his original talk in 1982 Feynman says about quantum mechanics,

“Might I say immediatly, so that you know where I really intend to go that we always have had - secret, secret, close the doors! - a great deal of difficulty in understanding the world view that quantum mechanics represents. At least I do, because I’m old enough man that I haven’t got to the point that this stuff is obvious to me. Okay, I still get nervous with it... I cannot define the real problem and therefore I suspect there’s no real

problem, but I'm not sure there's no real problem. "[1]

Quantum mechanical systems are hard to understand. Perhaps, by being able to simulate them in a controlled way and track their dynamics we can better understand them.

We consider the case of angles that are multiples of  $30^\circ$  only. A photon goes to Alice in a particular state. After it leaves the atom it is already determined what it will be for every given angle. Let's say that it will give the results shown in figure 4a, which is taken from [1], where a white dot represents O and a black dot represents E. As explained above, Bob's pattern must be the

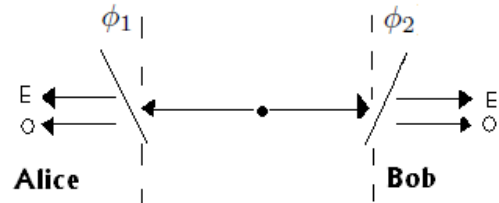


FIG. 3: Figure 3

1. R. P. Feynman, Simulating Physics with Computers, Int. J. Theo. Phys, 21, 467 (1982)
2. S. Lloyd, Universal Quantum Simulators, Science, 273, 1073-1078 (1996)
3. Jane, E., Vidal, G., Dur, W., Zoller, P. Cirac, J. I., Simulation of Quantum Dynamics with Quantum Optical Systems, Quant. Inform. Comput. 3, 15-37 (2003)
4. Ll. Masanes, G. Vidal, J. I. Latorre, Quant. Inform. Comput., 2, 275-285 (2002)
5. C. H. Bennet, J. I. Cirac, M. S. Leifer, D. W. Leung, S. Popescu and G. Vidal, quant-ph/0107035
6. When a photon goes through a calcite it either comes out in the Ordinary ray (O) or in the Extraordinary ray (E) and we can place detectors on the other side so after it goes through we know if it is O or E. Now consider the situation in figure 3. An atom emits two photons at the same time, one to Alice and one to Bob. Alice has her calcite at an angle  $\phi_1$  and Bob has his at an angle  $\phi_2$ . According to quantum mechanics the probabilities for the four different possible results are

$$\begin{aligned} P_{OO} &= P_{EE} = \frac{1}{2} \cos^2(\phi_1 - \phi_2) \\ P_{OE} &= P_{EO} = \frac{1}{2} \sin^2(\phi_1 - \phi_2) \end{aligned} \quad (15)$$

So, if Alice and Bob set their angles to be the same ( $\phi_1 = \phi_2$ ), then  $P_{OO} = P_{EE} = \frac{1}{2}$  and  $P_{OE} = P_{EO} = 0$ , so Bob can predict Alice's result exactly, by measuring his result. If they decide to set the angles such that  $\phi_2 - \phi_1 = 30^\circ$ , the probability that they will get the same result is  $\frac{3}{4}$ .

Now, we want to see what will happen on a classical probabilistic computer. Feynman explains that once a photon 'leaves the atom' in the simulation, whether it is O or E must be already determined. Otherwise it would not have been possible to predict it on the other side.

same, shown in figure 4a. Now, suppose after the photons leave the atom, Alice and Bob set the calcites such that  $\phi_2 - \phi_1 = 30^\circ$ . Then they will get the same result only if the two neighboring dots are the same color. As can be seen from the picture, the probability for that is  $\frac{2}{3}$ . Moreover, no other pattern would yield a probability greater than  $\frac{2}{3}$ ! (For example for the case in figure 4b the probability to get the same result is 0). Thus, we see that a classical probabilistic computer can not imitate quantum phenomena.

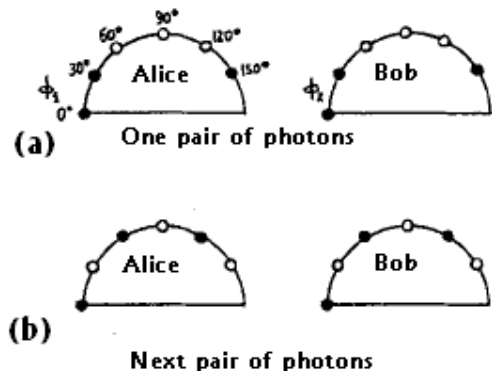


FIG. 4: In (a) and (b) we see the case that give the greatest probability to get the same answer. (c) and (d) show the case of the worst probability (0).