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PHYSICAL QUANTUM ALGORITHMS

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ABSTRACT

I review the differences between classical and quantum systems, emphasizing the connection between no-hidden variable theorems and superior computational power of quantum computers. Using quantum lattice gas automata as examples, I describe possibilities for efficient simulation of quantum and classical systems with a quantum computer. I conclude with a list of research directions.

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1. Introduction

There are two paths towards quantum computing: one is teleological and the other is practical. The *teleological* path—described 35 years ago in the prophecy known as Moore’s Law [1]—leads down through smaller and smaller device sizes where quantum effects become wilder and wilder. Eventually, rather than domesticating them for classical computation, experimental physicists and engineers believe they will be able to preserve them for quantum computation. The *practical* path, on the other hand, is paved with the desire to solve specific problems efficiently. In an amusing role-reversal, it is theoretical physicists, computer scientists, and mathematicians who follow this path. The first steps along it were taken 20 years ago by Feynman, who suggested that since quantum systems seem to be very hard to simulate on a classical computer, perhaps they could be simulated more efficiently on a quantum computer [2]. More recently, Deutsch [3], Jozsa [4], Simon [5], Shor [6], Grover [7] and others have noted that a quantum computer could solve *classical* problems as well. In this primarily pedagogical paper I describe some of the steps which have been taken along this practical path, and speculate about some steps further along it.

2. Simulating quantum systems classically

Let me begin by reviewing the reasons quantum systems are believed to be hard to simulate on classical computers. Traditionally these are known as ‘no hidden variable theorems’. Each is a statement that no classical model with specified constraints can reproduce quantum mechanical results. Consideration of two of them, the Gleason/Kochen-Specker theorem [8,9] and Bell’s theorem [10], reveals both their heuristic power and their weaknesses.

In 1957 Gleason proved that for Hilbert spaces of dimension at least 3, any non-negative measure on states which is quantum mechanical (*i.e.*, for any orthogonal basis $\{\hat{e}_i\}$ the measure sums to 1) must derive from a density matrix [8]. In 1967 Kochen and Specker made the contradiction with a classical hidden variable model more explicit [9]: They constructed a finite set of unit vectors in \mathbb{R}^3 with the property that every attempt to assign values 0 or 1 to each vector satisfying the condition that in each orthogonal triple two vectors get 1 and the third gets 0 must fail. That is, no classical ‘hidden variable’ can be assigned to pre-determine which outcome of each of some finite set of complete measurements of the spin-squared of a spin-1 particle will be observed (since the spin eigenvalues are $\{-1, 0, +1\}$, two of the spin-squareds are 1 and one is 0 for any complete measurement). Such a hidden variable would be *non-contextual*, in the sense that its value on each vector would specify the spin-squared observed for that measurement, independently of which complete measurement including it is performed. One can argue, however, that noncontextuality is too strict a condition to place on hidden variables—perhaps the results of measurement should depend on hidden variables inherent in the measuring device, which might differ for each complete measurement [11]. Furthermore, the the measurements must be exactly along the vectors Kochen and Specker constructed, but from a computational complexity perspective, infinite precision is suspect [12]—and in fact one can show that without additional assumptions one cannot prove a Kochen-Specker

theorem using only finite precision measurements [13].

Both of these weaknesses are absent from Bell's theorem [10]. He proved that the results of local measurements on specific states of pairs of spin- $\frac{1}{2}$ particles, *i.e.*, vectors in $\mathbb{C}^2 \otimes \mathbb{C}^2$, cannot be reproduced by any local, classical hidden variable model. Here 'local' means restricted to individual particles. This result is robust against measurement imprecision, and locality of the hidden variables seems justified on physical grounds—the finite speed of light and the locality of physical interactions. In fact, these are the same grounds upon which we base our models of computation: At each timestep a classical or quantum Turing machine changes only the state of the head and the symbol written on the tape cell where the head is located [14,3]; it does not make non-local changes of all the cells of the tape simultaneously, for example.

The states for which Bell's theorem rules out classical hidden variables are *entangled*, *i.e.*, ones for which the state of multiple particles cannot be described as the product of states for each particle individually. Since this is true for all but a set of measure 0 in the space of all pure states, Bell's theorem and its generalizations (see [15] for a recent survey) indicate that most quantum states cannot even be described by reasonable (in the sense of local) classical models. This is a more subtle problem than simply the large size of the state space, which we consider next.

3. Dynamics

The dimension of the Hilbert space describing the state of a system of multiple particles grows exponentially in the number of particles: 2^n for n spin- $\frac{1}{2}$ particles, for example. This exponential explosion, however, is not enough to preclude classical simulation. Consider a classical, probabilistic lattice gas. On a homogeneous one dimensional lattice of size n there are 4^n basis states s_i , since each lattice site can be occupied by no more than 1 particle with each of the two possible velocities. A general state s is a convex combination:

$$s = \sum_{i=0}^{4^n-1} p_i s_i \quad \text{with} \quad \sum_{i=0}^{4^n-1} p_i = 1, \quad p_i \geq 0.$$

Evolving the whole state, *i.e.*, the probability distribution, is therefore an exponentially difficult problem in the size of the lattice. Nevertheless, such lattice gas models are used regularly (see, *e.g.*, [16]). But one does not evolve the whole probability distribution. Rather, one samples it, by evolving a single s_i to a single s'_i at the next timestep, using some random number generator. Multiple runs sample the final distribution. A quantum lattice gas automaton (QLGA, which I will describe in more detail in §4) is also described at each timestep by a vector in a space with basis $\{|s_i\rangle\}$ —where $|\cdot\rangle$ is the standard Dirac notation for vectors in Hilbert space [17]:

$$|\psi\rangle = \sum_{i=0}^{4^n-1} a_i |s_i\rangle \quad \text{with} \quad \sum_{i=0}^{4^n-1} |a_i|^2 = 1, \quad a_i \in \mathbb{C}.$$

Evolving the QLGA state has classical computational complexity comparable to evolving the whole state of the probabilistic LGA. But in the quantum case, this cannot be reduced by sampling individual histories: each has a complex amplitude so the histories with each given final state interfere.

Thus interference seems to be the phenomenon which makes quantum dynamics hard to simulate classically. In fact, although the multi-particle structure of a system is important, entanglement *per se* seems to be less relevant: In liquid state NMR quantum computing experiments [18], for example, the state is not entangled at any timestep (more precisely, since the system is in a mixed state—a convex combination of pure states—the state is *separable*) [19]. Nevertheless, it seems to be difficult to construct a reasonable local hidden variable model for the dynamics [20], *i.e.*, the dynamics seems difficult to simulate classically. To make this more than heuristic, however, we would need a *dynamical* Gleason/Kochen-Specker/Bell-type theorem which applies even for evolution through a sequence of unentangled states. Perhaps some hint about a way to do this may be found in Laflamme’s response to the separability criticism of NMR quantum computation [21].

Of course, some demonstrations of the absence of classical models for quantum dynamics already exist. These are more commonly known as quantum algorithms for oracle problems; since each consists of a sequence of unitary operations, they are dynamical results. Grover’s quantum search algorithm, for example, solves the problem of identifying $a \in \{0, 1\}^n$ given an oracle which responds to a query $x \in \{0, 1\}^n$ by returning δ_{xa} , using only $O(\sqrt{2^n})$ queries [7]. Classically, any algorithm would require $O(2^n)$ queries. For $n > 2$, the state is entangled at every timestep after the first [22]. Possibly more to the point is Bernstein and Vazirani’s algorithm which solves the problem of identifying $a \in \{0, 1\}^n$ given an oracle which responds to a query $x \in \{0, 1\}^n$ by returning $x \cdot a \bmod 2$, using only 1 quantum query [23]. Classically, any algorithm would require $O(n)$ queries. And this quantum algorithm works without creating entanglement at any timestep [24]. These results suggest that while a theorem on the impossibility of efficient classical simulation of quantum dynamics may exist, it will have to count *all* the elementary operations, not just the queries, which will presumably make it more difficult to prove.

4. Quantum simulations

In §1–§3 I’ve tried to explain the heuristic that classical simulation of quantum systems is difficult, while noting what remains to be proved to make such a claim rigorous. Now let us consider Feynman’s proposed solution: simulation with quantum computers [2]. The standard model of quantum computation allows polynomially many local (*i.e.*, acting nontrivially on only 1 or 2 qubits) gate operations [25]. This is a reasonable model since in principle it can be realized by a quantum system with a local Hamiltonian. Feynman’s proposal has been verified in this model for quantum systems defined by local Hamiltonians [26,27,28,29,30,31]. More exotic quantum systems can also be simulated efficiently with a standard quantum computer: Fractional quantum Hall systems, for example, have Hamiltonians which vanish on the physical states; the only nontrivial unitary transformations have global (topological) origin. Nevertheless, Freedman, Kitaev and Wang have shown

that such topological quantum field theories can be simulated efficiently with a standard quantum computer [32].

A particularly simple architecture for a quantum computer is a QLGA [33]. Although I'm not aware of a demonstration that classical LGA are capable of universal computation, their similarity to the reversible billiard ball model of Margolus [34] suggests that they may be; since QLGA specialize to deterministic LGA, they would be also. Whether they can efficiently (*i.e.*, with polynomial overhead) simulate quantum gate arrays is, I believe, also an open question. In the other direction, QLGA can be simulated efficiently on a standard quantum computer, but have theoretical and possibly practical advantages: They directly simulate quantum systems and are possibly more easily realized experimentally than arbitrary quantum gate arrays.

The possible configurations for each particle on a one dimensional lattice L are labelled by pairs $(x, \alpha) \in L \times \{\pm 1\}$, where x is the position and α the velocity. A classical lattice gas evolution rule consists of an advection stage $(x, \alpha) \mapsto (x + \alpha, \alpha)$, followed by a scattering stage. Each particle in a QLGA [33] exists in states which are superpositions of the classical states: $|\psi\rangle = \sum \psi_{x,\alpha} |x, \alpha\rangle$, where $1 = \langle \psi | \psi \rangle = \sum \bar{\psi}_{x,\alpha} \psi_{x,\alpha}$. The evolution rule must be unitary; the most general with the same form as the classical rule is:

$$\begin{aligned} \sum \psi_{x,\alpha} |x, \alpha\rangle &\xrightarrow{\text{advect}} \sum \psi_{x,\alpha} |x + \alpha, \alpha\rangle \\ &\xrightarrow{\text{scatter}} \sum \psi_{x,\alpha} S_{\alpha\alpha'} |x + \alpha, \alpha'\rangle, \end{aligned}$$

where the scattering matrix is

$$S = \begin{pmatrix} \cos m & i \sin m \\ i \sin m & \cos m \end{pmatrix}.$$

Figure 1 illustrates this quantum evolution: at $m = 0$ it specializes to the classical deterministic lattice gas rule. The $\Delta x = \Delta t \rightarrow 0$ limit of this discrete time evolution is the Dirac equation [33]; the $\Delta x^2 = \Delta t \rightarrow 0$ limit is the Schrödinger equation [35].

This QLGA model can be extended to include multiple particles with a unitary two particle scattering rule

$$|x, \alpha, x, -\alpha\rangle \mapsto e^{is} |x, \alpha, x, -\alpha\rangle$$

shown in Figure 1. With these rules the 1 dimensional QLGA discretizes the quantum field theory described by the 1+1 dimensional massive Thirring model [36,33]. These rules also preserve the symmetry (*i.e.*, bosonic or fermionic) of the wave function under particle exchange [37]. The QLGA rules can be generalized to discretize the multi-particle Schrödinger equation in arbitrary

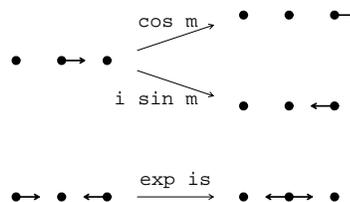


Figure 1. The general evolution rules for the one dimensional QLGA.

dimensions [35]; it seems more difficult, however, to create QLGA which discretize relativistic evolution in higher dimensions [38].

The fact that the QLGA rules are homogeneous, *i.e.*, the same at each lattice site and at each timestep, suggests that they might be easier to implement than general quantum gate arrays which are not. Possible physical systems in which they might be implemented include crystals—as originally proposed by Feynman [2] and more recently in the context of solid state NMR [39]—or optical lattices [40]. A detailed proposal for physical implementation in such systems could motivate experimental work towards realization of QLGA.

5. Simulating classical systems

In the previous sections we’ve seen that there are quantum algorithms to efficiently simulate multiparticle quantum systems which seem to be difficult to simulate classically. Since, as I noted in the Introduction, there are efficient quantum algorithms to solve classical problems, a natural question is whether quantum computers can simulate classical systems [41,42]. Assuming quantum mechanics is a correct description of the world, the existence of a classical description for macroscopic physics means that quantum computers can simulate classical physics with constant overhead—although the constant factor may be something like 10^{23} , *i.e.*, a number of quantum degrees of freedom sufficiently large that subsystems decohere and can be identified as the classical objects to be simulated.

Can we do better? That is, could there be quantum *speedups* for classical physics? Yezep has proposed that the answer is ‘yes’. Using a “Type II” quantum computer in which the state is measured, locally, after each timestep and then reset using a lattice Boltzmann rule [43]. A model like this can achieve at most a constant speedup, corresponding to reduced computational cost for local evolution. In practice, of course, a large constant improvement can be tremendously useful, but perhaps it is possible to do better. More precisely, using a standard quantum computer, can classical systems be simulated more efficiently than is possible classically? Lidar and Biham have shown that the answer to this question is also ‘yes’, for the non-dynamical problem of sampling the ground state distribution of a spin glass [41].

There are also QLGA results which suggest that certain aspects of classical dynamics can be simulated more efficiently quantum mechanically. Consider classical diffusion of a particle in a linear potential, as shown in Figure 2. A discrete model for the evolution is a biased random walk, with $\text{prob}(\Delta x) \propto e^{-\nabla V \Delta x}$. The results of

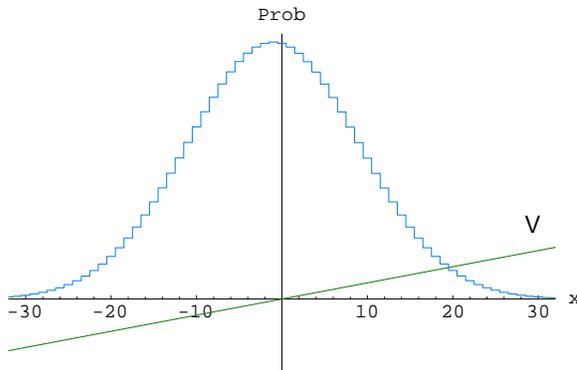


Figure 2. The probability distribution for the position of a classical particle after diffusing in a linear potential. The particle was initially at the origin.

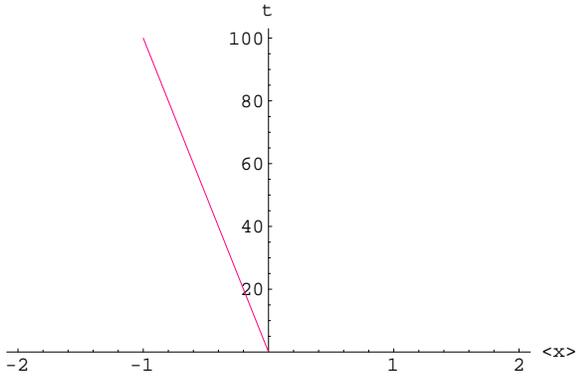


Figure 3. The evolution of expected position for the random walk model of a classical particle diffusing in a linear potential.

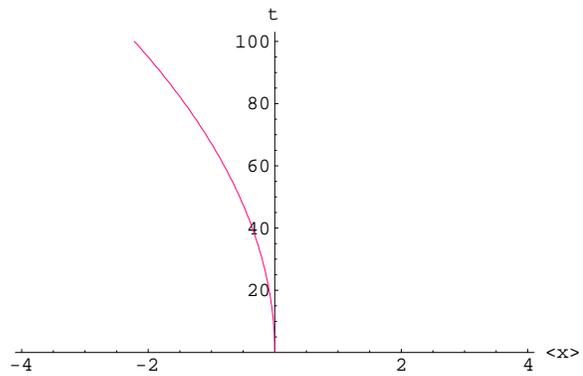


Figure 4. The evolution of expected position for the QLGA model of a quantum particle subject to a linear potential.

simulating the evolution with a classical (probabilistic) LGA are shown in Figure 3. The average position of the particle satisfies

$$\langle x(t) \rangle - \langle x(0) \rangle \propto -\nabla V t.$$

In QLGA the evolution rules can be modified to include a potential by incorporating an x dependent phase multiplication, *i.e.*, $e^{-iV(x)}$ at each timestep [44], which one might imagine implementing in a physical system with an applied, spatially varying magnetic field, for example. Figure 4 shows the result of a QLGA simulation with a linear potential. Now the average position of the particle approximately satisfies

$$\langle x(t) \rangle - \langle x(0) \rangle \propto -\nabla V t^2.$$

That is, this quantum system simulates the evolution of the average position of a classical particle diffusing in a linear potential *quadratically faster* than does the classical simulation shown in Figure 3. I must emphasize that it is only the average position which is being simulated accurately, not the whole probability distribution. Furthermore, the quadratic speedup only holds on timescales $t \ll 2\pi/\nabla V$. On longer timescales the evolution is periodic [45]. Nevertheless, this very simple example suggests that efficient simulation of more complicated classical dynamics may be possible.

6. Conclusion

In conclusion, let me reiterate the open questions discussed in this paper:

Is there a proof that (some) quantum dynamics is difficult to simulate classically? Can it be difficult even when the state is unentangled (separable) at each timestep?

In case QLGA become a practical architecture for quantum computers, can they simulate the standard model of quantum computation with no more than polynomial overhead?

What are possible physical implementations of QLGA?

What are the correct QLGA models for relativistic quantum systems in more than 1 spatial dimension?

and most importantly,

Are there quantum algorithms which speed up the simulation of classical physics?

Positive answers to this last question will broaden the possible uses for a quantum computer and help justify the immense commitment of resources which seems likely to be necessary to develop a scalable one.

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