

Quantum Simulations: Report

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Currently, both small analog single-purpose simulators and few-qubit digital simulators represent important testbed applications enabling us to realize the industrial potential of certain many-body quantum systems and give understanding to the effects of environmental noise. The goal of this report is to give account of the complexity behind quantum simulations and provide insights about its feasibility.

I. INTRODUCTION

The aim of quantum simulations is to efficiently simulate quantum-mechanical behavior of a system in question using a hardware employing quantum effects of comparable qualities. The idea of using one quantum system to closely mimics the evolution of another quantum system was suggested in the early 80s by Yu. Manin and R. Feynman in a response to difficulties with simulating quantum physics on a classical computer.

At that time it was not clear whether a universal quantum simulator could be built so the main discussed simulators were of analog single-purpose nature. Few years later, D. Deutsch [1] worked out an abstract concept of a digital universal quantum computer which merely casted quantum simulations as a particular application for the computer - although a privileged one thanks to its practical use. Subsequently, Deutsch's computational model based on individually addressable quantum bits (qubits) and quantum logical operations (gates) on pairs of qubits was shown to represent a technically admissible implementation method.

The universality of a quantum computer implied that any quantum system can be simulated in principle, however, there were no implications regarding the efficiency of such process. This contrasted sharply with the original idea of analog single-purpose simulators founded on efficiency and natural mapping between the system being simulated and the simulator.

The problem of efficiency has been resolved in the 90s. S. Lloyd [2] presented a general framework for efficient simulations of quantum systems with local interactions and the algorithms of S. Wiesner [3] and C. Zalka [4] showed how to efficiently simulate the evolution of particles in a real space. The Wiesner-Zalka's algorithm is not limited to systems with local interactions although no quantum systems with non-local interactions are known. Both approaches work by approximate means allowing arbitrary precision.

The field of quantum simulations also subsumes algorithms for extracting relevant qualities of simulated systems. This adds additional complexity to the simulator, with an adequate initialization being far the biggest problem. For example, ground states, if needed, cannot be always prepared efficiently. In 2007, D. Aharonov, D. Gottesman, S. Irani and J. Kempe [5] proved that it is so even for one-dimensional systems. Therefore static

properties such as ground state energies can be harder to find than simulating the dynamics. A general scheme of a quantum simulator is depicted in Fig.1.

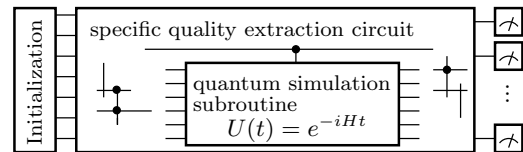


FIG. 1: A general scheme of quantum simulator.

Currently, both small analog single-purpose simulators and few-qubit digital simulators represent important testbed applications enabling us to realize the industrial potential of certain many-body quantum systems and give understanding to the effects of environmental noise.

The results will show whether a digital quantum simulator/computer is both a useful abstraction giving rise to genuine algorithms and viable implementation approach or the actual implementation must take an alternative path. Against purely analog simulators speak profound difficulties with suppressing errors in a systematic way. On the other hand, for Deutsch's-like models fault-tolerance is proven to be possible. Therefore digital simulators are currently at the frontier of interest.

II. THE ALGORITHMS

The key to quantum simulation algorithms is the convergence of the Trotter formula which allows us to deal with non-commuting hermitian operators. The Trotter formula states that for any real t and hermitian operators A, B ,

$$\lim_{q \rightarrow \infty} \left(e^{-iAt/q} e^{-iBt/q} \right)^q = e^{-i(A+B)t}. \quad (1)$$

Thus the evolution $U = \exp(-i(A+B)t)$ can be approximated by simulating the operators A and B over short discrete time slices. Let us write

$$e^{-i(A+B)t} = \left(e^{-i(A+B)t/q} \right)^q$$

and by taking $\Delta t = t/q < 1$ we get

$$e^{-i(A+B)\Delta t} = e^{-iA\Delta t} e^{-iB\Delta t} + O(\Delta t^2) \quad (2)$$

which results in

$$e^{-i(A+B)t} = (e^{-iAt/q} e^{-iBt/q})^q + O(t^2/q). \quad (3)$$

It is clear from (3) that the convergence of the Trotter formula is slow for practical purposes. The error decreases only linearly with q . Therefore it is advantageous to use the higher order Baker-Campbell-Hausdorff splitting formula

$$e^{-i(A+B)\Delta t} = e^{-iA\Delta t} e^{-iB\Delta t} e^{i\frac{1}{2}[A,B]\Delta t^2} + O(\Delta t^3), \quad (4)$$

which can be further splitted so that we get an error of order $O(\Delta t^\eta)$ using roughly 2η exponential factors. Hence with

$$\eta \geq \frac{\log(\varepsilon/q)}{\log(t/q)} \quad (5)$$

and $q > t$ chosen such that the product ηq is minimal, the evolution U can be approximated within error tolerance of $O(\varepsilon)$ at rather modest costs logarithmical in ε .

A. The Wiesner-Zalka's algorithm

The Zalka and Wiesner's algorithm [3, 4] describes an approach for quantum simulation of non-relativistic particles. The main idea is to discretize the wave function and perform a numerical simulation heavily founded in quantum parallelism.

The algorithm can be described as follows. For simplicity, let us have a time-independent Hamiltonian $H = T + V$ where $T = p/(2m)$ is the kinetic energy operator and $V = V(x)$ stands for the potential energy operator which depends only on position. Given the initial wave function $|\psi(0)\rangle$, the goal is to make the quantum simulator to prepare the wave function $|\psi(\Delta t)\rangle = e^{-iH\Delta t} |\psi(0)\rangle$.

First we discretize the wave function at multiples of Δx . For a single particle we have

$$\alpha_j = \psi(j\Delta x), \quad (6)$$

and we store these amplitudes in an n -qubit register

$$|\psi\rangle = \sum_{j=0}^{2^n-1} \alpha_j |j\rangle. \quad (7)$$

The number of qubits n determines the (exponentially good) spatial resolution. A system with d particles requires d n -qubits registers to be used. The overall state $|\psi\rangle_1 \otimes \dots \otimes |\psi\rangle_d$ can be think of as a grid of 2^{dn} points.

Next, we take an advantage of the operator V being diagonal in the position representation and thus the evolution $e^{-iV\Delta t}$ is nothing but a rephasing of position basis states

$$|j\rangle \rightarrow e^{-iV(j\Delta x)\Delta t} |j\rangle. \quad (8)$$

Since $f(j) = V(j\Delta x)\Delta t$ is an efficiently computable function, then, there exists a polynomial size quantum circuit U_f such that

$$U_f \sum_j |j, a\rangle = \sum_j |j, a \oplus f(j)\rangle, \quad (9)$$

and an initialization of ancillas to $|a\rangle = QFT^\dagger |0\dots 01\rangle$ gives us

$$U_f \sum_j |j, a\rangle = \sum_j e^{-if(j)} |j, a\rangle. \quad (10)$$

This handy implementation of diagonal rephasing is thanks to a generalized observation used in the Deutsch's problem. Now, an efficient implementation of quantum Fourier transform is well known and the implementation of U_f , in essence, follows replacing irreversible logical gates in a classical circuit for computing f with corresponding quantum reversible gates and dealing with ancilla qubits. The operator T is implemented in an analogous way since after being Fourier-transformed, $(QFT)T(QFT^\dagger)$, it is also diagonal in the position representation.

B. Lloyd's simulation of local interactions

S. Lloyd's approach [2] for simulation algorithms uniquely stems from Deutsch's gate model qualities. The key observation is that any efficient quantum circuit working with n qubits is in general described as

$$e^{-i(H_1+H_2+\dots+H_L)t} \quad (11)$$

where L is polynomial in n and each H_i acts non-trivially on at most two neighboring qubits. Now, following the universality of two-qubit gates, any evolution $e^{-iH_i t}$ where H_i' acts non-trivially on at most fixed number of neighboring particles, H_i' is a strict k -local Hamiltonian, can be simulated at a constant time proportional to k .

Additionally, since it takes at most n SWAP operations to work with any two qubits as with neighbors, we can simulate any k -local H_i' at time $O(kn)$ without assuming anything about the physical location of the particles. Thus for any quantum system \mathbb{S} with only local interactions and at most polynomially many H_i' s, this captures all known relevant quantum physics, there exists an efficient Trotter-approximate quantum circuit simulating \mathbb{S} with arbitrary precision.

The question of actually finding those efficient circuits in a systematic and again efficient way was addressed by G. Ortiz *et. al.* [6] and R. Somma *et. al.* [7]. The authors studied the relationship and mapping between different operator algebras and stressed the importance of the Jordan-Wigner transformation establishing an isomorphism between the fermion algebra and the spin algebra. Fermions are known to present the most intriguing system due to the dynamical sign problem and spin-1/2 algebra is the language of the quantum circuit model.

The spin-1/2 chain Jordan-Wigner transformation

Creation and annihilation operators are operators that allow us to deal in a very compact way with the concept of increasing and lowering the number of particles in a given state by one. The creation operator is denoted a^\dagger and the adjoint annihilation operator is written simply as a . For fermions, the operators a_k^\dagger and a_k acting on the fermionic occupation state (site) k satisfy the following anticommutator relations

$$\{a_k, a_l\} = \{a_k^\dagger, a_l^\dagger\} = 0, \quad \{a_k^\dagger, a_l\} = \delta_{kl}. \quad (12)$$

The basis for the operators on spin-1/2 particles (qubits) is generated by the Pauli matrices σ_x, σ_y and σ_z . Now, identifying an unoccupied fermionic site with the std. basis state $|1\rangle$ and an occupied site with the state $|0\rangle$, we can define raising and lowering matrices

$$\sigma_+ = \frac{1}{2}(\sigma_x + i\sigma_y), \quad \sigma_- = \frac{1}{2}(\sigma_x - i\sigma_y), \quad (13)$$

which acts as a^\dagger and a , respectively. Then, the Jordan-Wigner transformation for a chain of spin-1/2 particles is defined as

$$a_k^\dagger = \left(\prod_{j=1}^{k-1} -\sigma_z^j \right) \sigma_+^k, \quad a_k = \left(\prod_{j=1}^{k-1} -\sigma_z^j \right) \sigma_-^k. \quad (14)$$

The product of $-\sigma_z$ matrices reflects on the anticommutator relations. For example,

$$a_1^\dagger a_2^\dagger = \sigma_+^1 (-\sigma_z^1) \sigma_+^2 = \sigma_+^1 \sigma_+^2 = -\sigma_+^2 \sigma_+^1 = -a_2^\dagger a_1^\dagger.$$

The generalized Jordan-Wigner transformations were discussed by C. D. Batista and G. Ortiz in [8].

Let us summarize what can be achieved using the Jordan-Wigner transformation as follow. A local Hamiltonian acting on n fermionic occupation states, for example with at most two-body interactions,

$$H = \sum_{i,j=1}^n E_{ij} a_i^\dagger a_j + \sum_{i,j,k,l=1}^n E_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \quad (15)$$

is transformed into a sum of polynomially many n -qubit operations

$$H' = \sum_{l=1}^{\text{poly}(n)} \left(E_l \prod_{j=1}^n \sigma_\mu^j \right), \quad (16)$$

where $\sigma_\mu \in \{\sigma_x, \sigma_y, \sigma_z, \mathbf{1}\}$ and $\text{poly}(n) = O(n^4)$ since (15) is described roughly by $n^2 + n^4$ parameters.

Factorization of multi-qubit operations

The next step is to factorize multi-qubit operations into single and two-qubit operations. The most difficult

part is solved by the Trotter approximation

$$e^{-iH'\Delta t} \approx \prod_{l=1}^{\text{poly}(n)} e^{-iE_l(\prod_{j=1}^n \sigma_\mu^j)\Delta t}.$$

Now, since each evolution of the form

$$e^{-iE_l(\prod_{j=1}^n \sigma_\mu^j)\Delta t} \quad (17)$$

has a very simple product structure, almost any brute force decomposition would led to an efficient implementation with only single and two-qubit gates. However, the process of brute force decomposition is in this situation unnecessarily complex and, more importantly, we loose track of the information flow and control over possibly exploitable symmetries.

A better way is to use the algebraic properties of the Pauli matrices. The key is the relation

$$e^{i\theta\sigma_\mu} = \cos(\theta)\mathbf{1} + i\sin(\theta)\sigma_\mu, \quad (18)$$

for any real θ , from which we derive the following. First,

$$(e^{-i\frac{\pi}{4}\sigma_\mu^j})\sigma_{\mu'}^j (e^{i\frac{\pi}{4}\sigma_\mu^j}) = \epsilon\sigma_{\mu''}^j, \quad (19a)$$

where $\sigma_\mu \neq \sigma_{\mu'} \neq \sigma_{\mu''} \neq \mathbf{1}$ and ϵ is the Levi-Civita symbol, and a generalization of (19a) for a tensor product of two σ -matrices including the identity matrix $\mathbf{1}$, e.g.

$$(e^{-i\frac{\pi}{4}\sigma_z^j\sigma_z^{j+1}})\sigma_x^j \mathbf{1}^{j+1} (e^{i\frac{\pi}{4}\sigma_z^j\sigma_z^{j+1}}) = \sigma_y^j \sigma_z^{j+1}. \quad (19b)$$

Second,

$$e^{-i\theta(U\sigma_\mu^j U^\dagger)} = U e^{-i\theta\sigma_\mu^j} U^\dagger \quad (20)$$

and its variant for two-qubit operations.

Finally, recursively applying the above written rules $O(n)$ times, we get

$$e^{-iE_l(\prod_{j=1}^n \sigma_\mu^j)\Delta t} = \left(\prod_{k=1}^{O(n)} U_k \right) e^{-iE_l\sigma_{\mu'}^1\Delta t} \left(\prod_{k=1}^{O(n)} U_k^\dagger \right), \quad (21)$$

up to the global phase, where $\sigma_{\mu'} \neq \mathbf{1}$ and U acts non-trivially on at most two neighboring qubits.

Compact mapping

The Jordan-Wigner transformation as defined by (14) establishes a direct mapping between fermionic occupation states and qubits so that n occupation states are mapped to n qubits. One consequence of such mapping is a block diagonal structure of a matrix representation of (16) in the standard basis, see Fig.2. Each block corresponds to a fixed number of particles subspace and it is the input wave function that determines the number of particles in the system, $0 \leq \ell \leq n$, and selects the effective block (Hamiltonian). The effective Hamiltonian matrix is of size $\binom{n}{\ell} \times \binom{n}{\ell}$ and therefore $\lceil \log_2 \binom{n}{\ell} \rceil$ qubits

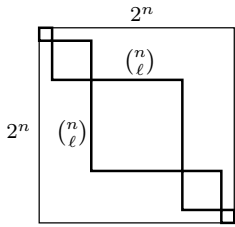


FIG. 2: Block diagonal structure of Hamiltonian (16).

would suffice for the simulation. We talk about a compact mapping.

The compact mapping becomes very useful if $|n/2 - \ell| \gg 0$ or a reduction from 7 to 3 qubits bridges the gap between a theory and an experiment. Unfortunately, rewriting a Hamiltonian of the form (15) into a Hamiltonian with a fixed number of particles is not an easy task but for special cases. No general rewriting algorithm is known up to date.

For small systems, one can directly arrive at the effective Hamiltonian matrix simply by enumerating and equating all allowed transitions in the simulated system. Subsequent isolation of the structure of (16) can be a tedious job. An advantage is the possibility to come up with an arbitrary dense compact mapping. One can choose the most relevant subspaces of fixed number of particles subspace.

III. QUANTITIES OF INTEREST READOUT

Algorithms for extracting relevant properties of simulated systems usually involve controlled version of the quantum simulation subroutine, as shown in Fig. 1, in one or another way. Main ideas follow the eigenvalue equation

$$U |\psi\rangle_U = e^{i2\pi\phi} |\psi\rangle_U \quad (22)$$

which is the key behind Kitaev's phase estimation algorithm [9] and, later, D. S. Abrams and S. Lloyd [10] put this very procedure into use in the field of quantum simulations. Given that $|\psi\rangle_U$ is the (approximate) ground state of the simulated system, the ground state energy can be easily reconstructed from an accurate estimate of the eigenphase ϕ .

Fig.3 shows how to transfer the eigenphase ϕ into the relative phase of an ancilla qubit which is to be measured. In order to estimate the resulting expectation value, with respect to the σ_x -observable in this case, various classical/quantum strategies operating at the standard quantum limit or the Heisenberg limit are known. For quantum metrology overview see V. Giovannetti *et. al.* [11], and S. M. Roy and S. L. Braunstein [12]. In general, strategies operating close to the Heisenberg limit require an implementation of powers $U^{2^k}(t) = U(t2^k)$ and therefore have a limited use under strong dephasing due to a

rapid growth of simulation time, see M. Dobšiček *et. al.* [13, 14].

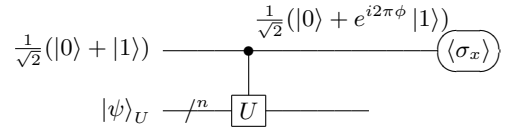


FIG. 3: Estimation of an eigenphase.

In 1998, E. Knill and R. Laflamme [15] studied the power of an idealized NMR quantum computer with one coherent qubit and many qubits in a completely mixed state, so called DQC1 model. Despite the limitations of such system (not as powerful as a circuit model with many coherent qubits), the authors showed how to estimate a normalized trace of U within the DQC1 framework. See Fig.4 for the circuit.

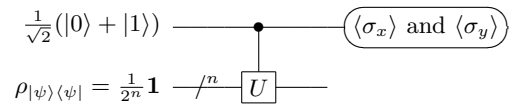


FIG. 4: Estimation of the normalized trace of U .

Expectation values $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ are estimated independently and the sum $\langle\sigma_x\rangle + i\langle\sigma_y\rangle$ equals to the normalized trace of U .

$$\begin{aligned} \langle\sigma_x\rangle + i\langle\sigma_y\rangle &= \langle 2\sigma_+ \rangle \\ &= \frac{1}{2} \left(\langle 0, \psi | + \langle 1, \psi U^\dagger | \right) 2\sigma_+ \left(|0, \psi\rangle + |1, U\psi\rangle \right) \\ &= \langle \psi | U | \psi \rangle = \text{Tr}(U | \psi \rangle \langle \psi |) = \frac{1}{2^n} \text{Tr}(U). \end{aligned} \quad (23)$$

It is interesting to note that in special cases, diagonal U being the most obvious case, both the input state and the output state before measurement are a mixture of separable states. Thus there is no entanglement and, yet, we get an exponential speed-up compared to classical algorithms. The non-classical correlations behind the efficient estimation are quantified by quantum discord. For theory and experimental verification see A. Datta *et. al.* [16] and B. P. Lanyon *et. al.* [17], respectively.

With many coherent qubits, the circuit in the Fig.4 can be also used to estimate the expectation value $\langle U \rangle$ with respect to input state $|\psi\rangle$. We get straightforwardly $\langle \psi | U | \psi \rangle = \langle U \rangle$. This observation was used by R. Somma [7] giving a circuit for an estimation of expectation values of the form

$$C_{AB}(t) = \langle U^\dagger(t) A U(t) B \rangle. \quad (24)$$

This class subsumes variety of spatial and time correlation functions and the corresponding circuit is shown in the Fig.5.

Recently, focusing on chemical dynamics, I. Kassal *et. al.* [18] discussed how to readout observables such as

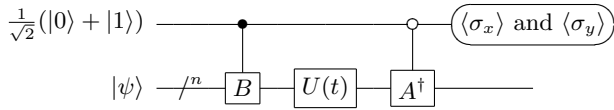


FIG. 5: Estimation of the expectation values of the form $\langle U^\dagger(t)AU(t)B \rangle$.

thermal reaction rates and state-to-state transition probabilities.

The question of preparing appropriate input states is addressed by many authors. A. Aspuru-Guzik *et. al.* [19] used an adiabatic state preparation approach in order to approximate the electronic ground state. L. Grover and T. Rudolph [20] showed how to create superpositions corresponding to efficiently integrable probability density functions. A. Kitaev and W. A. Webb [21] presented an algorithm for preparing wavefunctions corresponding to a multi-dimensional Gaussian. D. S. Abrams and S. Lloyd [22] proposed an efficient algorithm for antisymmetrization. The paper of R. Somma *et. al.* [7] also discusses initial state preparation in some details. Although not all initial states can be prepared efficiently, the general consensus is that the set of efficiently preparable states is large and captures many relevant problems.

IV. CONCLUSIONS

Reading through European and American quantum information processing and communication strategic report/roadmap [23, 24], one can find paragraphs referring to the question of what can be done with few qubits with-

out using, so far unfeasible, quantum error correction. Going beyond testing fundamentals, this question targets somewhere between exponential speed-up in Shor's algorithm and things that cannot be achieved classically such as certain primitives in quantum cryptography.

In order to answer this question, we find two limit-case approaches. The first one is to well characterize a given quantum hardware, including easy-to-do and do-not-try operations, sensitivity to different types of noise, timing, and so on, so that in effect an algorithmic toolkit is created. The goal is to create analogues to the success of the DQC1 model of an NMR quantum computer and within it derived fast algorithm for an estimation of a normalized trace. The second approach is to employ quantum-enhanced subroutines in rather any classical computation. Almost generally achievable Grover-like square root speed-up is by no means less striking than a specially tailored routine, L. M. K. Vandersypen *et. al.* [25], factoring 15 into 5 and 3.

We believe that both these approaches will give rise to testbed applications sufficient enough to help us to realize the industrial potential of certain many-body quantum systems, and, moreover, we find quantum simulations to be a natural convergent of a research done along this path. The goal of this report was to give account of the complexity behind quantum simulations and provide insights about its feasibility.

V. ACKNOWLEDGEMENTS

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